Gaussian 09 使用手册目录

Last update: *1 September* 2009

Gaussian 09 计算输入档案

Gaussian 09 计算输入档是一个包含一系列的行所构成的 ASCII 文字文件。Gaussian 计算输入党的基本结构包含几个段落：

- *Link 0 指令：*确定站存盘的位置和名称（段落结束时不需要空行）。
- *计算路径段落 (# 行)*：指定所要进行的计算工作类型，模型化学和其它选项（用空行结束这个段落）。
- *标题段落：*计算工作的简短描述（用空行结束这个段落）。输入档内要有这个段落，但 Gaussian 09 程序不会加以处理。这行数据汇出现在计算输出档作为识别之用。通常，这一段落会包含化合物名称，对称性，电子状态，以及其它任何相关的信息。标题段落不能超过五行，必须以空行终止。在这段落中应避免使用这些符号：
  @ # ! - _ \ *control 字母 (尤其是 Ctrl-G)*。
- *分子系统设定段落：* 设定要研究的分子系统（以空行终止这个段落）。
- *额外的段落选项：* 某些计算工作类型需要无外的输入数据（通常以空行终止段落）。

许多 Gaussian 09 计算工作输入档只有第二，第三和第四个段落。以下是一个输入文件的范例，要求对水分子做单一结构能量计算：

```
# HF/6-31G(d)                                    计算路径段落

water energy                                     标题段落

0 1                                                  分子系统设定
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
```

这计算中，计算路径和标题段落各占一行。分子系统设定段落第零行是分子电荷和自旋多重态。电荷为零（中性分子），自旋多重态为 1（单一态）。电荷和自旋多重态行之后是描述分子中各原子位置的行，一个原子一行。这个粒子中使用直角坐标。分子系统设定在后面会有详细的讨论。

以下这个计算输入文件范例使用 Link 0 指令和一个额外的输入段落：

```
%Chk=heavy                                                    Link 0 段落
# HF/6-31G(d) Opt=ModRedundant      计算路径段落
```

Opt job *标题段落*

0 1 *分子系统设定*
段落
原子坐标 ...

3 8 *在用来*
做几何优选的内坐标系统内增加一个键长和一个键角
2 1 3

这计算工作指定进行几何优选计算。分子系统设定段落后面的输入段或是关键词 Opt=ModRedundant 需要的输入数据，指定在几何优选计算中使用的内坐标里增加一个键长和键角。这计算工作同时指定检查档的档名。

为方便查询，以閒表中列出 Gaussian 09 程序计算输入文件中可能会出现的段落，依照各段落出现的次序排列。每个段落对应的关键词也列在表中。

Gaussian 09 计算输入档各段落的次序

段落	需要这输入段落的关键词	是否需要空行做结束？
Link 0 指令	% 指令	否
计算路径段落 (# 行)	所有关键词	是
额外层组 Extra Overlays	ExtraOverlays	是
标题段落	所有关键词， Geom=AllCheck 除外	是
分子系统设定	所有关键词， Geom=AllCheck 除外	是
原子连接关系	Geom=Connect 或 ModConnect	是
冻结原子位置	Geom=ReadFreeze	是
坐标修改	Opt=ModRedundant	是
第二个标题和分子系统设定	Opt=QST2 或 QST3	两者皆是
第二组坐标的原子连接关系	Geom=Connect 或 ModConnect 和 Opt=QST2 或 QST3	是
第二组冻结原子	Geom=ReadFreeze	是
第二组坐标修改	Opt=QST2 或 QST3	是

第三组标题和分子系统设定，过渡状态的最初猜测结构	Opt=QST3	两者皆是
第三组坐标的原子连接关系	Geom=Connect 或 ModConnect Opt=(ModRedun, QST3)	是
第三组冻结原子	Geom=ReadFreeze	是
第三组坐标修改	Opt=(ModRedun, QST3)	是
PDB 二级结构数据	若分子设定段落中有胺基酸分子团的信息	是
原子质量	ReadIsotopes 选项	是
分子力学参数	HardFirst, SoftFirst, SoftOnly, Modify	是
感兴趣的振动频率	CPHF=RdFreq	是
背景电荷分布	Charge	是
BOMD/ADMP 输入 (1 或多个段落)	ADMP 和 BOMD 需要的输入数据， ReadVelocity, ReadMWVelocity 选项	是
PCM 输入数据	SCRF=(ExternalIteration,Read)	是
IRC 表的坐标	IRC=Report	是
简协限制 Harmonic constraints	Geom=ReadHarmonic	是
半经验方法参数 (Gaussian 格式)	Input 选项, AM1=Both	是
半经验方参数 (MOPAC 格式)	MOPAC, Both 选项	是
基底函数设定	Gen, GenECP, ExtraBasis	是
基底函数更改	Massage	是
有现场系数 Finite field coefficients	Field=Read	是
ECP 设定	Pseudo=Cards, GenECP	是
密度释配基底组设定	ExtraDensityBasis	是
PCM 溶解模型输入	SCRF=Read	是
DFTB 参数	DFTB	是
最初猜测的来源	Guess=Input	是
要结合的对称类型	Guess=LowSymm	否
轨域设定(分离 α 和 β)	Guess=Cards	是
轨域更改(分离 α 和 β)	Guess=Alter	是

轨域排序(分离 α 和 β)	Guess=Permute	是
# 轨域/GVB 电子对	GVB	否
CAS 状态平均的权重	CASSCF=StateAverage	否
要计算自旋轨道耦合效应的状态	CASSCF=SpinOrbit	否
轨域冻结信息	ReadWindow 选项	是
要精制的 EPT 轨域	EPT=ReadOrbitals	是
要计算自旋-自旋耦合常数的原子清单	NMR=ReadAtoms	是
另一种原子半径	Pop=ReadRadii 或 ReadAtRadii	是
静电性质的数据	Prop=Read 或 Opt	是
NBO 输入数据	Pop=NBORead	否
简协正振动模式选择	Freq=SelectNormalModes	是
障碍旋转体 Hindered Rotor 输入数据	Freq=ReadHindered	是
非简协正则振动模式选择	Freq=SelectAnharmonicNormalModes	是
FCHT 的正则振动模式	Freq=SelectFCHTNormalModes	是
非简协性的输入数据	Freq=ReadAnharmonic	是
FCHT 输入数据	Freq=ReadFCHT	是
Pickett 输出档名	Output=Pickett	否
PROAIMS 输出档名	Output=WFN	否

输入数据的语法

通常 Gaussian 计算输入数据遵循以下语法规则：

- 输入的数据没有固定的格式，和字母大小写无关。
- 空格，跳格（tabs），逗点，或前斜线可以任何组合方式分隔在一行中的各项。连续多个空格当做一个区隔。
- 关键词的选项可用以下方式设定：
  - *keyword* = *option*
  - *keyword*(*option*)
  - *keyword*=(*option*1, *option*2, …)
  - *keyword*(*option*1, *option*2, …)

- 多重选项要用括号聚集，各选项之间可用有效的符号加以区隔（通常使用逗点符号）。括号前的等号可以省略，括号之前和之后也可以有空格。注意，有些选项要设定数值，这时选项的名称后面接着等号，例如 CBSExtrap(NMin=6).
- Gaussian 09 所有关键词和选项可以用缩写到最短且唯一缩写字符串代替。因此 Conventional option to the SCF 关键词选项 Conventional 可以缩写成 Conven，但不能缩写成 Conv（因为有另一个 Convergence 选项存在)。不论是否刚好 Conventional 和 Convergence 都是某一个关键词有效的选项，这个规定都成立。
- Gaussian 09 计算输入资料可以包含外部档案的内容，利用这个语法 @*文件名*。将整个档案的内容放到计算输入文件中这个字符串出现的位置。在这指令后附加 /N ，计算输出档的开头将不会印出这外部档案的内容。
- 行中惊叹号 (!)右边的信息是当作批注，惊叹号可出现在一行中的任何位置。 独立的批注行可出现在输入文件中任何位置。

Last updated on: 2 September 2009

Gaussian 09 计算工作类型

Gaussian 09 计算输入文件的计算路径段落指定计算工作的类型。这设定的内容有三个主要部份：

- 计算工作类型
- 计算方法
- 基底函数组

以下是 Gaussian 09 程序可用的计算类型清单：

- SP: 分子单一结构能量。
- Opt: 分子几何结构优选。
- Freq: 振动频率和热化学分析。
- IRC: 化学反应路径探索。
- IRCMax: 在指定的话学反应路径上找到能量最大值的分子结构。
- Scan: 位能曲面扫描。
- Polar: 极化张量和超极化张量。
- ADMP 和 BOMD: 直接运动轨迹计算。
- Force: 计算原子和尚的作用力。
- Stable: 测试波函数的稳定性。
- Volume: 计算分子体积。
- Density=Checkpoint Guess=Only: 纸重新计算电子分布分析。

- Guess=Only: 纸印出最初猜测波函数，产生片段结构的最初猜测波函数。

一般而言，一个计算只能指定一个计算工作类型。但有几个例外：

- Polar 和 Opt 可和 Freq. 结合在一个计算工作内。在后者的情况，几何优选计算结束后自动接着对优选过得分子结构进行振动频率计算。
- Opt 可和复合方法关键词合用，以便指定优选计算部份的选项：例如，Opt=(TS,ReadFC) CBS-QB3.

若在计算路经段落中没有指定计算工作类型，预设的选项是单一结构能量计算（SP）。但是，具有这种格式 *method*2/*basis*2 // *method*1/*basis*1 的计算路径可用来指定一个几何优选计算（ *采用 method*1/*basis*1）接着对优选过得几何结构做一次单结构能量计算（采用 *method*2/*basis*2）。例如，以下的计算路径范例指示进行一个 B3LYP/6-31G(d) 几何优选计算，接着用 CCSD/6-31G(d) 模型化学进行一个单一结构能量计算：

```
# CCSD/6-31G(d)//B3LYP/6-31G(d) Test
```

在这种情况， Opt 关键词视域设的选项，不需标示。注意 Opt Freq 计算不能采用这种语法。

分子性质预测

以下窗体列出各种可预测的分子性质，和产生这些分子性质的 Gaussian 09 程序的关键词：

- 反铁磁性耦合常数 Antiferromagnetic coupling: Guess=Fragment, Stability
- 原子电荷 Atomic charges: Pop
- 溶解自由能 ΔG of solvation: SCRF=SMD
- 双极矩 Dipole moment: Pop
- 电子亲和能 Electron affinities: CBS-QB3, CCSD, EPT
- 电子密度 Electron density: cubegen
- 电子圆二色性 Electronic circular dichroism: CIS, TD, EOM, SAC-CI
- 就电位能 Electrostatic potential: cubegen, Prop
- 静电位能感应电荷 Electrostatic potential-derived charges: Pop=Chelp, ChelpG or MK
- 电子跃迁能带形状 Electronic transition band shape: Freq=FC, Freq=HT
- 极化张料和超极化张量 Polarizabilities/hyperpolarizabilities: Freq, Polar [CPHF=RdFreq], Polar=DCSHG
- 高准确能量 High accuracy energies: CBS-QB3, G2, G3, G4, W1U, W1BD
- 超细微耦合常数 Hyperfine coupling constants (anisotropic): Prop
- 超细微光谱张量 Hyperfine spectra tensors (包含 *g* 张量): Freq=(VCD, VibRot [, Anharmonic])

- 游离能 Ionization potentials: CBS-QB3, CCSD, EPT
- 红外线和拉曼光谱 IR and Raman spectra: Freq[=Anharmonic]
- 共振前拉曼光谱 Pre-resonance Raman spectra: Freq CPHF=RdFreq
- 分子轨域 Molecular orbitals: Pop=Regular
- 电多极矩 Multipole moments: Pop
- 核磁共振遮蔽和化学位移 NMR shielding and chemical shifts: NMR
- 核磁共振自旋-自旋耦合常数 NMR spin-spin coupling constants: NMR=Mixed
- 光学旋转系数 Optical rotations: Polar=OptRot
- 拉曼光学活性 Raman optical activity: Freq=ROA, CPHF=RdFreq
- 热化学分析 Thermochemical analysis: Freq
- 紫外线和可见光光谱 UV/Visible spectra: CIS, ZIndo, TD, EOM, SAC-CI
- 振动旋转耦合 Vibration-rotation coupling: Freq=VibRot
- 振动圆二色性 Vibrational circular dichroism: Freq=VCD

Last updated on: 2 September 2009

模型化学

计算方法结合基底函数组设定一个 Gaussian 程序的模型化学，指定理论的层级。每一个 Gaussian 计算工作必须指定一个计算方法和一组基底函数。在计算输入文件中的计算路径内用两个独立的关键词做设定，有些计算方法本身及隐含使用特定的基底函数组。有些计算工作使用密度泛函理论也包括密度适配基底组（见 基底函数组章节 更多的说明）。

以下表中列出 Gaussian 程序可用的计算方法，以及其对应的计算工作类型。星号标示解析方法计算，只有数值方法的计算用 *n* 标示（见各关键词章节更多的说明）。

Method Availabilities in Gaussian 09

	SP, Scan	Opt, Force, BOMD	Freq	IRC	ADMP	Polar	Stable	ONIOM	SCRF	PBC
Molecular Mechanics methods	*	*	*					*	*	
AM1, PM3, PM3MM, PM6, PDDG	*	*	*	*		*	*	*	*	
HF	*	*	*	*	*	*	*	*	*	*
DFT methods	*	*	*	*	*	*	*	*	*	*
CASSCF	*	*	*	*		*		*	*	
MP2	*	*	*	*		*		*	*	
MP3, MP4(SDQ)	*	*	*num*	*		*num*		*	*	
MP4(SDTQ), MP5	*	*num*						*		
QCISD, CCD, CCSD	*	*	*num*	*		*num*		*	*	
QCISD(T) or (TQ)	*	*num*						*		
BD	*	*						*	*	
EPT	*							*		
CBS, G*n*, W1 methods	*									
CIS	*	*	*	*		*		*	*	
TD	*	*	*num*	*		*num*		*	*	
EOM	*	*num*						*	*	
ZINDO	*							*	*	
DFTB	*	*	*	*		*		*		
CI	*	*		*				*		
GVB	*	*		*				*		

*=Analytic algorithm available *num*=Available via numerical differentiation

计算方法和可用的计算工作类型清单

若没有指定计算方关键词，预设的方法是 HF 。以 R 开头的方法关键词用于填满壳层自旋限制波函数，以 U 开头的方法关键词用于不限制自旋未填满壳层波函数，或以 RO 开头的方法关键自用于自旋限制未填满壳层波函数：例如，ROHF，UMP2，或 RQCISD。RO 只适用于 Hartree-Fock 和密度泛函方法，AM1，PM3，PM3MM，PM6 和 PDDG 能量和梯度，和 MP2，MP3，MP4，和 CCSD 能量。

通常，只能设定一个计算方法关键词，若指定的计算方法关键词超过一种，或产生怪异的结果。但是有利外情况：

- CASSCF 可和 MP2 共享，要求在做 CASSCF 计算时纳入动态电子相干计算。
- ONIOM 和 IRCMax 计算工作需要设定多种计算方法，但是当作对应关键词的选项做设定。
- 前面提到的 *model*2 // *model*1 形式，要求几何优选计算（model2）后，对优选过得结构自动进行一次单结构能量计算（model 1）。

Last updated on: 9 Jun 2009

基底函数

大部分的计算方法都需要指定基底函数；若计算路径段落中没有指定基底函数，程序将使用 STO-3G 基底函数。某些计算方法本身内含指定的基底函数，则不需要指定基底函数，这些方法包括：

- 所有半经验方法，包括激发态所用的 ZIndo 。
- 所有分子力学方法。
- 复合式模型化学：所有 G*n*，CBS 和 W1 方法。

以下是 Gaussian 09 程序提供的基底函数清单，各基底函数的详细描述请参考相关文献。清单中基底函数的名称对应 Gaussian 09 程序的关键词（只有两个例外）：

- STO-3G [Hehre69, Collins76]
- 3-21G [Binkley80a, Gordon82, Pietro82, Dobbs86, Dobbs87, Dobbs87a]
- 6-21G [Binkley80a, Gordon82]
- 4-31G [Ditchfield71, Hehre72, Hariharan74, Gordon80]
- 6-31G [Ditchfield71, Hehre72, Hariharan73, Hariharan74, Gordon80, Francl82, Binning90, Blaudeau97, Rassolov98, Rassolov01]
- 6-31G†: Gaussian 09 还提供 George Petersson 和同僚的 6-31G† 和 6-31G‡ 基底函数，作为完全基底函数方法的一部分 [Petersson88, Petersson91]。对应的关键词是 6-31G(d') 和 6-31G(d',p') ，在这基底函数上还可以加上一个或两个扩散函数，也可以加上 f 函数，例如，6-31G(d'f)。
- 6-311G: 指定周期表第一列元素使用 6-311G 基底函数，第二列元素使用 McLean-Chandler (12s,9p) → (621111,52111) 基底函数 [McLean80, Raghavachari80b] （注意 P，S，和 Cl 的基底函数被 McLean 和 Chandler 称为负离子基底函数 negative ion basis sets，但对中性分子也可产生较佳的结果）。Ca 和 K 原子使用 Blaudeau 和同僚的基底函数 [Blaudeau97]，第一列过渡元素使用 Wachters-Hay [Wachters70, Hay77] 的全电子基底函数，并使用 Raghavachari 和 Trucks 的调幅因子（scaling factor）[Raghavachari89]，第三列其它元素使用 nd the 6-311G basis set of McGrath, Curtiss 和同僚的 6-311G 基底函数 [Binning90, McGrath91, Curtiss95]。注意 Raghavachari 和 Trucks 建议对前两列过渡元素使用 Wachters-Hay 基底函数时要使用调幅因子，并加上扩散函数。包含扩散函数时需指定使用 6-311+G 关键词。MC-311G 和 6-311G 同义。
- D95V: Dunning/Huzinaga valence double-zeta [Dunning76].
- D95: Dunning/Huzinaga full double zeta [Dunning76].
- SHC: 第一列元素用 D95V，第二列元素用 Goddard/Smedley ECP [Dunning76, Rappe81].，和 SEC 同义。
- CEP-4G: Stevens/Basch/Krauss ECP minimal basis [Stevens84, Stevens92, Cundari93].
- CEP-31G: Stevens/Basch/Krauss ECP split valance [Stevens84, Stevens92, Cundari93].

- CEP-121G: Stevens/Basch/Krauss ECP triple-split basis [Stevens84, Stevens92, Cundari93].

  第二列之后的元素只有一种 CEP 基底函数，对这些原子来说，这三种关键词没有差别。

- LanL2MB: 第一列元素使用 STO-3G [Hehre69, Collins76] ，Na-La，Hf-Bi 使用 Los Alamos ECP plus MBS 基底函数 [Hay85, Wadt85, Hay85a]。
- LanL2DZ: 第一列元素使用 D95V [Dunning76]，Na-La，Hf-Bi 使用 Los Alamos ECP plus DZ [Hay85, Wadt85, Hay85a]。
- SDD: 周期表中 Ar 以前的元素都使用 D95 [Dunning76] ，其余的元素使用 Stuttgart/Dresden ECPs [Fuentealba82, Szentpaly82, Fuentealba83, Stoll84, Fuentealba85, Wedig86, Dolg87, Igel-Mann88, Dolg89, Schwerdtfeger89, Dolg89a, Andrae90, Dolg91, Kaupp91, Kuechle91, Dolg92, Bergner93, Dolg93, Haeussermann93, Dolg93a, Kuechle94, Nicklass95, Leininger96, Cao01, Cao02]。在 Gen 基底函数关键词输入段落中可用关键词 SDD，SHF，SDF，MHF，MDF，MWB 指定使用这些基底函数/位能。注意这字符串后面必须接着指定内层电子的数目 （例如，MDF28 表示 MDF 位能代替 28 个内层电子）。
- SDDA11: 原子序 Z > 2 的原子采用 Stuttgart 位能。.
- cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z, cc-pV6Z: Dunning’s 相干作用医治性基底函数 （correlation consistent basis sets） [Dunning89, Kendall92, Woon93, Peterson94, Wilson96]（分别代表双重，三重，四重，五重，和六重-zeta 函数）。为了增加计算效能，重复的函数已经移除，并且已经旋转到适当的方位 [Davidson96] i。

  这些基底函数已内含极化函数。以下这表格列出这些基底函数对各种原子所包含的价电子极化函数：

Atoms	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV5Z
H	2s, 1p	3s, 2p, 1d	4s, 3p, 2d, 1f	5s, 4p, 3d, 2f, 1g
He	2s, 1p	3s, 2p, 1d	4s, 3p, 2d, 1f	5s, 4p, 3d, 2f, 1g
Li-Be	3s, 2p, 1d	4s, 3p, 2d, 1f	5s, 4p, 3d, 2f, 1g	6s, 5p, 4d, 3f, 2g, 1h
B-Ne	3s, 2p, 1d	4s, 3p, 2d, 1f	5s, 4p, 3d, 2f, 1g	6s, 5p, 4d, 3f, 2g, 1h
Na-Ar	4s, 3p, 1d	5s, 4p, 2d, 1f	6s, 5p, 3d, 2f, 1g	7s, 6p, 4d, 3f, 2g, 1h
Ca	5s, 4p, 2d	6s, 5p, 3d, 1f	7s, 6p, 4d, 2f, 1g	8s, 7p, 5d, 3f, 2g, 1h
Sc-Zn	6s, 5p, 3d, 1f	7s, 6p, 4d, 2f, 1g	8s, 7p, 5d, 3f, 2g, 1h	9s, 8p, 6d, 4f, 3g, 2h, 1
Ga-Kr	5s, 4p, 2d	6s, 5p, 3d, 1f	7s, 6p, 4d, 2f, 1g	8s, 7p, 5d, 3f, 2g, 1h

分子系统设定

这输入段落设定分子中所有原子核的位置和 α- 及 β-自旋的电子数。有几种方式可以设定原子核的组态：一个 Z-矩阵，一个直角坐标，或两者混合的形式（注意直角坐标只是 Z-矩阵的一个特例）。

分子系统设定段落第一行设定分子净电荷（一个整数）和自旋多重态（通常是一个正整数）。因此一个中性分子的自旋单一态，这一行的内容是 0 1。阳离子自由基，这一行的内容是 -1 2 。在某些计算类型中，这一行可能包含多组电荷/自旋多重态 的数据。

若在计算路径段落中使用关键词 Geom=CheckPoint ，分子系统设定段落只需要电荷自旋多重态这一行数据。若在计算路径段落中使用关键词 Geom=AllCheck ，整个分子系统设定段落（以及标题段落）都可以省略。

分子系统设定段落剩下的部份对分子中每一个原子设定元素类型和原子位置。这一行数据最常见的形式是：

Element-label[-*Atom-type*[-*Charge*]][(*param*=*value*[, …])]
Atom-position-parameters

每一行包含一个元素类型，和可能的分子力学原子类型和部份电荷选项。这原子的原子核参数在括号内的清单中设定。这一行剩下的部份是原子的位置，可用直角坐标，也可以用 Z 矩阵内坐标来定义。我们先考虑最初和最后的项目，然后在讨论剩下的项目。

这是分子系统设定段落内原子设定的基本形式（省略其它所有选项）：

Element-label [*freeze-code*] *x y z*

这些范例中使用空格作为各项的区隔符号，其它有效的区隔符号也可以使用（例如，逗点）。原子的位置用直角坐标设定。 *freeze-code* 是一选项参数，用来在 ONIOM 计算中标示几何优选计算中位置要固定的原子（见 ONIOM 的说明）。

元素卷标 *Element-label* 是一个字符串，由原子的化学符号或原子序构成。若使用元素符号，可以选择在元素符号后加上一个数字，产生这原子的识别标签。通常是在元素名称后加上一个识别整数： C1，C2，C3，等等；这技术在遵循传统的化学编号上很有用。元素卷标最多只能有四个字母。

第一种形式中，每一行剩下的部份是指定该原子核位置的直角坐标。第二种形式，*atom*1，*atom*2，*atom*3 是前面已设定的原子，用来定义这一行原子的位置（另一种方式，可用分子结构设定段落中，各原子出现所在的行数代入上述的原子变量，电荷和自旋多重态所在的行当作第零行）。

目前这个原子的位置，可用和原子 1 间的键长，连接这原子与原子 1 的键和连接原子 1 与原子 2 键的键角，以及这原子原子 1，原子 2 构成的平面，与原子

1，原子 2 ，原子 3 构成的平面，两平面间的双面角（扭角）所定义。这是 Z 矩阵的定义。

以下是一个乙烷分子简单的分子系统设定段落，使用元素卷标（元素类型+原子编号）指定碳原子，使用元素类型指定氢原子：

```
0,1
C1  0.00    0.00    0.00
C2  0.00    0.00    1.52
H    1.02    0.00 -0.39
H -0.51  -0.88  -0.39
H -0.51    0.88  -0.39
H -1.02    0.00    1.92
H    0.51  -0.88    1.92
H    0.51    0.88    1.92
```

Z-matrix molecule specifications are also accepted. See Appendix C for details.

设定同位素和其它原子核参数

在原子类型字段中，用括号内的关键词和数值，可指定同位素和其它原子核参数，例如：

```
C(Iso=13,Spin=3) 0.0 0.0 0.0
```

这一行指定一个 ^{13}C 原子，原子核自旋为 3/2 (3 * 1/2)，位于原点。以下是可以被包含在括号里的项目：

- Iso=*n*: 选择同位素，若用整数当作原子质量，程序会自动使用最接近的真正同位素质量（例如， 18 指定 ^{18}O，而 Gaussian 程序使用的数值是 17.99916）。
- Spin=*n*: 原子核自旋，单位是 1/2。
- ZEff=*n*: 有效电荷。照参数用在自旋轨域耦合（见 CASSCF=SpinOrbit），和 ESR g 张量与电子自旋--分子旋转超细微张量（NMR Output=Pickett）的计算。
- QMom=*n*: 核四极举。
- GFac=*n*: 核磁矩，单位是 nuclear magnetons。

分子片段设定

分子系统内的分子片段可用参数 Fragment 定义，出现在原子符号后的括号内，括号内也可设定同位素和原子核参数值。Fragment 设定的数值是一个整数。具

有相同片段编号的原子同属一个分子片段。分子片段用于分子片段猜测计算，补偿（ counterpoise）计算，等等。

例如，以下的 biphenyl 结构分成两个苯环分子片段：

0,1 0,1 0,1　　*总电荷和总自旋多重态，后便是每个分子片段的总电荷和总自旋多重态*

```
C(Fragment=1) -3.05015529 -0.24077322    0.00000698
C(Fragment=1) -1.64875545 -0.24070572    0.00067327
C(Fragment=1) -0.94811361    0.97297577    0.00020266
C(Fragment=1) -1.64887160    2.18658975 -0.00093259
C(Fragment=1) -3.05027145    2.18652225 -0.00159819
C(Fragment=1) -3.75091329    0.97284076 -0.00112735
H(Fragment=1) -3.58511088 -1.16744597    0.00036555
H(Fragment=1) -1.11371117 -1.16732692    0.00154256
H(Fragment=1) -1.11391601    3.11326250 -0.00129286
H(Fragment=1) -3.58531573    3.11314346 -0.00246648
H(Fragment=1) -4.82091317    0.97278922 -0.00163655
C(Fragment=2)    0.59188622    0.97304995    0.00093742
C(Fragment=2)    1.29252806    2.18673144    0.00046795
C(Fragment=2)    1.29264421 -0.24056403    0.00207466
C(Fragment=2)    2.69392790    2.18679894    0.00113535
C(Fragment=2)    2.69404405 -0.24049653    0.00274263
C(Fragment=2)    3.39468590    0.97318496    0.00227326
H(Fragment=2)    0.75768862 -1.16723678    0.00243403
H(Fragment=2)    0.75748378    3.11335264 -0.00040118
H(Fragment=2)    3.22888349    3.11347169    0.00077519
H(Fragment=2)    3.22908834 -1.16711773    0.00360969
H(Fragment=2)    4.46468577    0.97323650    0.00278063
```

这个范例说明分子片段的电荷和自旋多重态设定方式。计算输入档中对应这设定行的格式如下：

总电荷，总自旋多重态，片段 1 的电荷，片段 1 的自旋多重态，片段 2 的电荷，片段 2 的自旋多重态

Guess=Fragment 计算中负值的自旋多重态有特殊的含意，指示对应的分子片段未成对轨域的自旋状态为 β 自旋轨域。其它计算工作类型中设定负直得自旋多重态都会产生错误。

Guess=Fragment 和 Counterpoise 计算中，分子片段编号要从 1 开始，依序指定。其它计算工作类型则无此严格要求，但违反这个规则可能会在输出文件中造成一些冗长得空白数据段落（例如，所有片段分布分析的数据都是零）。

GaussView 图形程序提供定义分子片段的图形工具。

分子力学原子类型

分子力学计算所用的分子系统设定也可包含原子类型和部份电荷等信息。这是一个范例：

C-CT　　*指定一个 SP3 脂肪族 （aliphatic） 碳原子*
C-CT-0.32　　*指定一个 SP3 脂肪族（aliphatic） 碳原子，部份电荷为 0.32.*
O-O--0.5　　*指定一个 羰基 氧原子，部份电荷为 -0.5.*

原子类型和选项部份电荷可对每一个原子做设定。也可定义原子核参数，例如：

C-CT(Iso=13)
C-CT--0.1(Spin=3)

PDB 档案参数

原子核参数和分子团的定义之后可附加几项定义，这些项目是要和 PDB 格式档案搭配，以保留档案中包的分子团和其它结构信息，这些信息使用者不会做定义。若 Gaussian 09 计算输入档案来自 GaussView 程序，而分子结构数据源自一个 PDB 格式档案，这计算输入档中可能会有这些标示。

- RESNum 指定这原子所属的分子团（胺基酸）编号。这数值的格式是 *n*[*X*[*Y*]]， *n* 是一个整数（不一定是正数），*X* 是选项单字母插入码，*Y* 是选项分子炼字母。若指定分子炼，但是没有插入码，则 *X* 可用底现代替：ResNum=-17_C 代表在分子炼 C 上的编号 -17 的胺基酸分子团。
- RESName 指定三个字母的胺基酸名称。
- PDBName 若不只是元素名称，指定这名称给这原子。

设定虚拟原子（ Ghost Atoms）

分子力学原子类型标示为 Bq （即，O-Bq）的原子是对应原子的虚拟原子 ghost [Macbeth]，虚拟原子举有和对应原子相同的正常基底函数和数值积分格点，但不具核电荷或电子。进行补偿（counterpoise）计算时需要虚拟原子的设定。这样的计算和旧版 Gaussian 程序使用关键词 Massage 所做的计算有一些不同，差异在于包含 DFT XC 积分计算中虚拟原子使用的格点。新版的计算方法提供较一致性的重迭校正，比较容易使用。注意补偿计算也可用关键词 Counterpoise 启动。

设定具周期边界条件的分子系统

周期性系统用一个单位晶格内的分子系统设定做设定，只需要在正常的分子设定段落后紧跟上一个，两个或三个平移向量（之间不要有空行），指定结构重复的

方向。例如以下段落设定 neoprene 分子一维周期边界条件系统的单结构能量计算：

```
# PBEPBE/6-31g(d,p)/Auto SCF=Tight

neoprene, -CH2-CH=C(Cl)-CH2- optimized geometry

0 1
C,-1.9267226529, 0.4060180273, 0.0316702826
H,-2.3523143977, 0.9206168644, 0.9131400756
H,-1.8372739404, 1.1548899113,-0.770750797
C,-0.5737182157,-0.1434584477, 0.3762843235
H,-0.5015912465,-0.7653394047, 1.2791284293
C, 0.5790889876, 0.0220081655,-0.3005160849
C, 1.9237098673,-0.5258773194, 0.0966261209
H, 1.772234452, -1.2511397907, 0.915962512
H, 2.3627869487,-1.0792380182,-0.752511583
Cl,0.6209825739, 0.9860944599,-1.7876398696
TV,4.8477468928, 0.1714181332, 0.5112729831
```

最后一行设定平移向量。注意 TV 当作一个原子符号处理。

以下这分子系统设定可用来做一片石墨的二维周期边界条件计算：

```
0 1
C     0.000000 0.000000 0.000000
C     0.000000 1.429118 0.000000
TV    2.475315 0.000000 0.000000
TV -1.219952 2.133447 0.000000
```

以下这分子系统设定可用来做砷化镓三维周期边界条件（晶体）计算：

```
0 1
 Ga 0.000000 0.000000 0.000000
 Ga 0.000000 2.825000 2.825000
 Ga 2.825000 0.000000 2.825000
 Ga 2.825000 2.825000 0.000000
 As 1.412500 1.412500 1.412500
 As 1.412500 4.237500 4.237500
 As 4.237500 1.412500 4.237500
 As 4.237500 4.237500 1.412500
 TV 5.650000 0.000000 0.000000
 TV 0.000000 5.650000 0.000000
 TV 0.000000 0.000000 5.650000
```

Last updated on: 9 Jun 2009

多步骤计算工作

多重 Gaussian 计算工作可结合在一个计算输入档内。各计算工作的计算输入数据之以这一行做区隔：

--Link1--

例如这个计算输入档内有两个计算步骤：

```
%Chk=freq
# HF/6-31G(d) Freq

Frequencies at STP

分子结构设定段落

--Link1--
%Chk=freq
%NoSave
# HF/6-31G(d) Geom=Check Guess=Read Freq=(ReadFC,ReadIsotopes)

Frequencies at 300 K

电荷和自旋多重态

300.0 2.0
同位素设定段落
```

这计算输入文件计算振动频率并在两组不同的温度和压力下做热化学分析：首先是 298.15 K 和 1 大气压，然后是 300 K 和 2 大气压。--Link1-- 行之前必须要有一行空行。第二个计算工作从检查档读入分子结构（Geom=Check），因此在分子结构设定段落中只需设定电荷和自旋多重态。

Last updated on: 9 Jun 2009

Gaussian 09 关键词

关键词依照字母顺序排列，但有以下例外：

- 基底函数组关键词不在这里；可用的基底函数组和对应的关键自相系说明请参考 基底函数组章节 。注意，ChkBasis，ExtraBasis，Gen，和 Pseudo 关键自有自己的说明章节。
- 所有 DFT-有关的关键词集中在 DFT Methods 章节内讨论。
- Link 0 指令章节放在所又字母排列关键词之后（即在 ZIndo 关键词章节之后），倒数第二个章节。
- 和指定更动计算路径有关的关键词—ExtraLinks， ExtraOverlays，NonStd， Skip，和 Use—在章节 Specifying Nonstandard Routes 中讨论。有关的信息也出现在 testrt 工具程序的讨论中。

每一关键词的讨论中，选项依照重要性和使用的频繁程度排序，而非严格遵照字母排序。庞大的选项清单还将功能类似的选项集中成小的章节。

Last updated on: 3 September 2009

Gaussian 09 关键词

关键词清单	关键词主题和分类
ADMP	CBS 方法
AM1	密度泛函数方 (DFT)
Amber	G1-G4 方法
B3LYP	内层冻结选项
BD	分子力学方法
BOMD	MP 和双重混合 DFT 方法
CacheSize	半经验方法
CASSCF	W1 方法
CBSExtrapolate	
CCD, CCSD	Link 0 指令总结
Charge	Gaussian 09 工具程序
ChkBasis	FormChk 工具程序
CID, CISD	程序发展关键词
CIS, CIS(D)	废弃的关键词和不建议使用

CNDO 的功能
Complex
Constants
Counterpoise
CPHF
Density
DensityFit
DFTB
Dreiding
EOMCCSD
EPT
ExtendedHuckel
External
ExtraBasis
ExtraDensityBasis
Field
FMM
Force
Freq
Gen, GenECP
GenChk
Geom
GFInput
GFPrint
Guess
GVB
HF
Huckel
INDO
Integral
IOp
IRC
IRCMax
LSDA
MaxDisk
MINDO3
MNDO
Name
NMR
NoDensityFit
ONIOM
Opt
Output
OVGF

工具程序 Utility Programs

这章节讨论 Gaussian 09 程序所附的各种工具程序，依照程序名称的字母顺序依次讨论。

大部分的工具程序同时有 UNIX 和 Windows 版本， 使用前请务必参考 Gaussian 09 程序发行说明，以取得这些工具程序与操作系统相关的信息。工具程序用来处理计算的输入档或计算所产生的检查档，以产生有用的数据和数据。

以下是工具程序清单以及各工具程序的功能 （ 有星号的项目放在程序 Gaussian 09W Utilities 选单）：

c8609
将旧版的检查档转换成 Gaussian 09 检查档的格式。

chkchk*
显示检查文件中的计算路径和标题段落。

cubegen*
独立的方块数据产生工具，可产生分子轨域，电子密度，和静电位场在指定空间内的数值资料，以便后续的图形显示。

cubman*
可对 Gaussian 程序计算所得的电子密度和静电位能存在的空间分布数据做操作，例如可以做相加或相减等等）。

formchk*
将二元检查文件转换成 ASCII 文字文件，以便搭配绘图软件，或在不同类型的计算器之间做迁移。二元档和计算器的架构有关，不同架构计算机产生的二元党部能互通，必须先转换成 ASCII 文字文件后，才能被其它计算机识别。

freqchk*
从一个检查档中读取并印出振动频率和热化学性质数据。可指定与原计算不同的同位素，温度，压力和幅度调整常数，进行热化学分析计算。

freqmem
决定频率计算所需的内存大小。

gauopt
对分子坐标之外的变量进行优选计算。

ghelp
Gaussian 程序的在线说明。

mm
独立的分子力学程序。

newzmat*
将分子几何结构在各种格式之间做转换。

testrt*
检查计算输入文件中计算路径的语法，也可用来产生非标准计算路径。

unfchk*
将格式化的检查档转换为二元档格式(将来自其它计算机的格式化检查文件转换成本机计算机可用的二元档）。

GAUSS_MEMDEF 环境变量

使用这些工具程序的时候，若工具程序本身没提供内存大小选项，环境变量 GAUSS_MEMDEF 可用来增加可用的内存大小。单位是计算器字（word，64bits）。

G09 IOps 参考手册

- Overlay 1
- Overlay 2
- Overlay 3
- Overlay 4
- Overlay 5
- Overlay 6
- Overlay 7
- Overlay 8
- Overlay 9
- Overlay 10
- Overlay 11
- Overlay 9999

Last update: 11 June 2009

执行 Gaussian 计算

这章节描述在 UNIX/Linux 计算机系统上执行 Gaussian 程序所需的计算机系统指令。在其它操作系统计算机上执行 Gaussian 程序应参考对应该操作系统的章节。以下的讨论假设 Gaussian 程序已经安装完成。

执行 Gaussian 程序涉及以下动作：

- 产生描述所要计算的 Gaussian 计算输入档。
- 指定各种站存盘的位置和文件名。
- 指定所需的计算资源。
- 用互动或批次模式启动程序执行。

在这章节假设基本的 Gaussian 计算输入档已经产生，以下将讨论盛下的三个动作。

指定暂存盘的处理方式和存放位置

Gaussian 成是在计算＼的过程中使用几个站存盘。包括：

- 检查档 Checkpoint file: *name*.chk
- 读写档 Read-Write file: *name*.rwf
- 双电子积分文件 Two-Electron Integral file: *name*.int (预设的选项是空档案)
- 双电子积分的微分文件 Two-Electron Integral Derivative file: *name*.d2e (预设的选项是空档案)

根据预设的设定，以上档案的档名来 *name* 自 Gaussian 程序执行程序的程序编号，存放在 GAUSS_SCRDIR 环境变量（UNIX）指定的暂存目录区。在这目录区内还可以看到档案 *name*. inp。这些是程序使用的内部输入文件。若这环境变量没有定义，预设的暂存盘目录区位置就是启动 Gaussian 计算程序时所在的工作目录区。

根据预设的设定，计算工作成功完成后，这些临时文件都会被删除。但是，也可选择保留检查档或其它暂存盘，留给后续的 Gaussian 计算工作中使用，或给图形程序使用，或重启失败的计算工作，等等。要保留检查档，可在 Gaussian 计算输入文件中用指令 %Chk 指定检查档的文件名和储存位置，计算结束时这检查档不会被删除。例如：

```
%Chk=water
```

这指令方在计算输入文件的开头（计算路径段落之前），指定检查档的档名为 water.chk，取代预设的档名，并要求计算结束时保留这检查档。在这个范例中，检查文件会放在目前的工作目录区。但是这样的指令也可以同时指定另一个存放位置：

```
%Chk=/chem/scratch2/water
```

若某一磁盘空间有限，但在计算机系统其它目录区还有空间，可将站存档分割成几部份，分别放到几个磁盘位置。以下指令可用来指定其它暂存档的文件名和存放位置：

%RWF=*路径*　　*读写档名*
%Int=*路径*　　*积分档名*
%D2E=*路径*　　*机分的微分档名*

通常，读写档是最大的档案，因此常被指定分割存放。

将暂存盘分割存放的几个磁盘位置

在 Windows 和 IA32 Linux 等 32 位计算机系统上，Gaussian 09 程序单一暂存盘可以寻址到 16 GB，因此不再需要将暂存盘切割成 2 GB 大小的档案。32 位

整数限制单一暂存档大小的上限为 16 GB，即使分割成多的档案，合并的档案大小还是不能超过 16GB。

另一种指令语法可用来设定分割读写档，积分档和积分的微分挡到两个或多个档案系统上。这是 %RWF 指令的语法：

%RWF=*loc*1,*size*1,*loc*2,*size*2, …

这里 *loc* 是目录区位置或档案路径，每一个 *size* 是在该位置存放部份档案的最大空间。若 *loc* 只设定目录区，Gaussian 程序会自动产生独一无二的档名。UNIX 操作系统中，目录区的指定（不包含档名）必须用前斜线（ / ）最为终端符号。

磁盘空间大小的预设单位是计算器字，这数值后可接上 KB，MB 或 GB （中间不能有空格）分别标示 KB，MB 或 GB，或接上 KW，MW 或 GW 分别标示单位是千字，百万字，或兆字（ gigawords）。注意 1 MB = 1024^2 bytes = 1,048,576 bytes （不是 1,000,000 bytes）。

磁盘空间大小参数的数值为 -1 表示任何和所有可用的空间都可使用，数值为 0 表示使用已存在目录区目前的大小。 -1 只用在最后一个档案指定，这也是预设的选择。

例如，以下指令将读写文件分割到三个磁盘位置：

%RWF=/dalton/s0/,4GB,/scratch/,3GB,/temp/s0/my_job,-1

指定档案片段的最大空间，分别是 4 GB，3 GB，和无限。Gaussian 程序会给前两个档案片段档名，第三个档案片段已经取名为 my_job。 注意前两个定的目录区设定都有终端的前斜线。

由于目前 UNIX 版本时做的限制，使用 -1 需要小心，因为程序会尝试将这档案片段扩展，超过这档案系统的剩余空间，另一个副作用是一些不会再用到的其它档案片段部份也会写到这个空间里。

临时文件的保存和删除

Gaussian 计算成功结束时，没有特定取档名的临时文件会被删除，有取档名的暂存档会保留。指令 %NoSave 可用来改变这预设的作法。计算输入文件出现这个指令的时候，出现在这 %NoSave 指令之前的已命名暂存档，和所有未命名的暂存档，在计算结束时都会被删除。但是，出现在 %NoSave 之后，用 % 指令明的暂存盘会被保留。例如，住些指令设定检查文件的文件名，设定读写文件到另一个位置，并且命名，Gaussian 计算结束时只有检查档被保留：

%RWF=/chem/scratch2/water　　*会被删除的档案放在这里*
%NoSave
%Chk=water　　*会被保留的档案放在这里*

当计算工作不正常结束时，所有暂存盘都会不会被删除。

启动档案

Gaussian 程序系统提供启动档案，用来建立使用者执行程序的系统环境，这些档案是：

$g09root/g09/bsd/g09.login　　*C shell*
$g09root/g09/bsd/g09.profile *Bourne shell*

注意，g09root 环境变量必须由使用者设定。习惯上会在 Gaussian 程序使用者计算机账号内的 .login 或 .profile 档案中加入这几行指令：

.login files:
setenv g09root *location*
source $g09root/g09/bsd/g09.login

.profile files:
g09root=*location*
export g09root
. $g09root/g09/bsd/g09.profile

这里 location 是计算机系统的目录区路径，g09 目录区在这目录区下。若设定正常，就可以用 g09 指令执行 Gaussian 09 程序的计算工作。(见以下的说明)。

内存使用的控制

指令 %Mem 控制 Gaussian 计算所用的动态内存大小。预设的大小是 256 MB (32MW) 。可用以下指令指定使用 *n*
个双精度计算器字：

%Mem=*n*

例如，以下指令要求使用 320 million bytes：

%Mem=40000000

%Mem 设定的数值后面可接上 KB, KW, MB, MW, GB 或 GW (中间不能有空格) 标示单位。例如，这指令设定 1 GB 的动态内存空间：

%Mem=1GB

非常大的直接 SCF 计算也需要指定更大的内存空间，至少 $3N^2$ 个计算器字， N 是基底函数的数目。

警告：指定的内存空间超过计算机系统可用的内存容量会造成极差的计算效能。

若执行 Gaussian 程序的计算机内存空间有限，无法提供预设的 256 MB，预设的计算方法和预设的内存大小应在安装程序的时候做适当地设定。见 Efficiency Consideration 章节有关有效率的使用 Gaussian 程序的说明。

在 UNIX 计算机系统上执行 Gaussian

一旦所有输入档案和使用资源设定都已被妥，就可以执行程序了。可用以下两种指令形式以互动模式执行 Gaussian 09 计算：

g09 *job-name*
g09 < *input-file* >*output-file*

第一种形式，程序读取输入文件 *job-name*.com 并将程序输出数据写到输出文件 *job-name*.log。若 *job-name* 没有指定，程序将从标准输入（键盘）读取输入数据，并将程序出出数据写到标准输出（屏幕），这些数据可用 UNIX 常用的数据引导指令，存放到档案中。这两种形式的指令启动计算后都可用 & 符号强制在计算机系统背景触执行，不影响计算机交互式的操作。

指令文件和 Gaussian 程序

执行 Gaussian 09 程序用的指令文件 (scripts)可用几种方式产生（这里用 C shell 做例子）。 首先 g09 指令可包含在一个指令文件内，其次，真正的 Gaussian 计算输入数据可包含在指令文件中，使用 << 语法结构:

```
#!/bin/csh
g09 <<END >water.log
%Chk=water
#RHF/6-31G(d)

water energy

0 1
O
H 1 1.0
H 1 1.0 2 120.0
```

```
END
echo "Job done. "
```

<< 符号之后到 END 之前的这些行，当作 g09 指令的输入数据。

最后，在指令文件内可用循环安排依序执行一系列的 Gaussian 计算工作。以下范例指定所有 Gaussian 计算输入文件当作指令行的参数，并将所有动作记录到档案 Status 里：

```
#!/bin/csh
echo "Current Job Status:"  > Status
foreach file ($argv)
 echo "Starting file $file at `date`"  >> Status
 g09 < $file > $file:r.log
 echo "$file Done with status $status"  >> Status
end
echo "All Done."  >> Status
```

$argv 变量代表一个输入文件名清单，是这指令文件的指令行参数。在工作目录区内必须要有这些档案存在。

以下是一个比较复杂的指令文件，对每一个部份输入档实时产生 Gaussian 计算输入档，这部份输入文件清单由指令文件的指令行参数输入的。部份输入文件区没有完整的计算路径段落，其计算路径段落只有一个 # 符号，或一个 # 行，包含只用在这分子系统的特殊关键词，但不包含计算方法，基底函数组或计算工作类型。

这指令文件对每一个部份输入档产生一个两步骤计算工作的计算输入档—一个 Hartree-Fock 优选计算，接着一个 MP2 单结构能量计算—这计算输入文件包括指令文件内的文字指令，以及指令文件执行时引进的每一个外部档案的内容。这里利用了 Gaussian 09 @ 纳入外部档案机制：

```
#!/bin/csh
echo "Current Job Status:"  > Status
foreach file ($argv)
echo "Starting file $file at `date`"  >> Status
g09 <<END> $file:r.log
%Chk=$file:r
# HF/6-31G(d) FOpt
@$file/N

--Link1--
%Chk=$file:r
%NoSave
# MP2/6-31+G(d,p) SP Guess=Read Geom=AllCheck
```

```
END
echo "$file Done with status $status"  >> Status
end # end of foreach
echo "All Done."  >> Status
```

以 NQS 进行批次计算

在提供 NQS 批次计算功能的 UNIX 计算机上，可用批次模式进行 Gaussian 计算。在 Gaussian 启动档案内定义的指令 subg09 可用来将计算工作送到批次计算环境中排序执行。以下是指令语法：

subg09 *queue-name job-name* [-scrdir *dir1*] [-exedir *dir2*] [-p *n*]

只领需要两个参数，排序名称和计算工作名称。计算输入档来自档案 *job-name*.com 计算输出档是 *job-name*.log， 和互动模式一样。NQS 记录文件名是 *job-name*.batch-log。选想参数 -scrdir 和 -exedir 分别用来取代预设的暂存目录区和执行文件目录区。其它的参数都当作是 NQS 的选项。尤其是 -p *n* 可用来指定在排序中的优先级为 *n*。 这是程序启动的优先级（1 是最低），但不影响后续程序的优先级。

从一互动环境中送出一个 NQS 计算工作，需先产生一个这样的档案（档名为 *name*.job）：

```
# QSUB -r name -o name.out -eo
# QSUB -lt 2000 -lT 2100
# QSUB -lm 34mw -lM 34mw
g09 <name.com
```

这里 *name* 应换成适合该计算工作的名称。第一行指定计算工作的名称，输出档案档名，并要求错误讯息包含在输出党内。两个时间参数设定略有差异，容许额外的计算工作控制指令做清理的动作(例如超过时间限制的时候将检验档做归档整理）。内存参数设定的数值用在执行计算工作时最初的程序安排，也用在程序执行时使用的动态内存。

这计算工作用以下指令送出排序执行：

$ qsub *name*.job

计算输出档案会放在目前的工作目录区内。

Last updated on: 9 Jun 2009

计算效能的考虑

Gaussian 程序的设计是要在各种计算机组态上能够很又效率的执行。通常，这程序尝试在已给的内存和磁盘空间限制下选择最有效率的计算方法。因为 Gaussian 提供许多种计算方法的选择，了解各种方法的可能性和折衷，有助于达到最佳的计算效能。

进行之前，先强调两点：

- 程序选择的预设方法，除了非常大的计算工作外，都能提供很好的计算效能。注意，为了反映目前典型的问题大小，Gaussian 09 程序预设的计算方法已经做了调整。旧版预设的计算方法适用于最多 100 个基底函数的小型计算工作。通常 Gaussian 程序预选的计算方法是针对较长时间计算所做的设计。
- 若经常性的需要执行非常大的计算工作，为了较加的计算效能，建议在档案 Default.Route f 内设定适当的选项默认值，像是可用的内存容量和磁盘空间，例如：
- -M- *可用内存大小*
  -#- MaxDisk=*可用磁盘空间大小*

  可用内存容量看磁盘空间大小的设定单位是 8 bytes （默认值）的计算器字；整数后可紧跟着 KB，MB，GB，KW，MW 或 GW （中间不能有空格），分指定单位是 kilo-，mega- 或 giga- bytes 或计算器字。预设的内存大小是 256 MB，预设的暂存磁盘空间是无限 (-1)，也就是假设有足够的磁盘空间完成所指定的计算工作。大部分的计算机上要求整体的程序执行效能，一旦档案 Default.Route 建立之后，就不需要再采取其它特别的动作。

内存需求的估算

在现代的计算机上使用 Gaussian 09 程序， 对大部分计算工作类型和方法，以及使用到包含 g 函数的基底函数，预设的内存大小 256 MB 是足够的。若基底函数包含 h 或更高阶角动量函数（例如 cc-pVQZ），则需要增加内存空间。以下公式可用来预估各种类型 Gaussian 计算工作所需的内存大小（单位是 8-byte 计算器字）：

$$M + 2(N_B)^2$$

这里 N_B 是计算中所用基底函数的数目， M 所需内存的最小值，通常用预设的内存大小足够代表这个值。注意 1 MW = 1,048,576 计算器字 (= 8,388,608 bytes)。合并的高阶角动量函数（ f 和更高阶的函数）的微分需要更多的内存。

这一章其余的部份说明各种选择隐含的取舍，了解这些知识才能设法在各别的计算工作获得最佳的效能，而不只是整体的最佳效能。所用的技巧涵盖非常大和非常小的计算工作。更多的相关资料可在参考文献中找到 [Schlegel91]。

并行计算的内存需求

使用共享内存的多个计算何新的时候，所需内存和使用单一计算核心所需的内存容量相近。在分散内存环境下使用多个计算核心（即经由 Linda），the amount of memory specified in %Mem 所设定的内存空间应该等于或大于使用单计算核心所需的内存大小。

Gaussian 09 程序中，两种并行计算的方式可以合并。例如，可用以下指令在四个计算机上使用八个计算核心，每个计算机上有两个计算核心共享该计算机的内存：

```
%Mem=128MW                                          每一个
计算核心需要的内存大小
%LindaWorkers=sysa,sysb,sysc,sysd          指定四个 Linda 计算机，每个计算
机有多个计算核心.
%NProcShared=2                                      在每个计算
机上使用两个共享内存的计算核心.
```

SCF 程序

为了要加速直接 HF 和 DFT 计算，迭代工作分两个阶段进行：

- 使用积分准确渡到小数点下六位，DFT 计算使用中等程度的积分网格，使电子密度收敛到 10^{-5} 。进行 21 不迭代计算后结束，不论是否以完全收敛。若分子系统中有任何过渡金属，这步骤自动省略。
- 继续 SCF 迭代计算，使用积分准确渡到小数点下十位数，密度收敛到 10^{-8} 。者两阶段的迭代次数最高到 128 步。

和整个计算过程中采用完全积分准确度相比，这方法要快上许多，在目前为止所做过的测试中，绝大部分的情况也没有降低收敛的速度。遇到困难的情况的时候，可用 SCF=NoVarAcc 选项要求采用完全积分准确度，进行计算。见 SCF 关键词章节。

收敛问题情况

预设的 SCF 计算方法使用在迭代子空间（DIIS）外插方法中两种直接反转（Direct Inversion）的结合：EDIIS 和 CDIIS。EDIIS [Kudin02] 使用能量外插，主宰 SCF 收敛程序的早期迭代步骤。CDIIS，根据 Fock 和密度矩阵的对易式

（commutator）做外插，处理 SCF 收敛后期迭代。这计算方法很可靠，旧版程序遇到的 SCF 收敛困难问题，现在用这预设的计算方法几乎都可以解决。少数有收敛困难的情况，Gaussian 09 提供 Fermi 增宽（broadening）和阻尼（damping）方法，搭配 CDIIS （帮含自动能阶移动 level shifting）。

若预设的方法无法收敛，可用以下替代选项（用对应的关键自作标签）：

SCF=Fermi
要求在早期迭代试作温度增宽（temperature broadening） [Rabuck99]，在开始的几次 SCF 迭代计算中，结合 CDIIS 和动态阻尼（dynamic damping）。遇到 SCF 收敛问题的时候，这是第一种选择。

SCF=QC
这是二次收敛的 SCF 方法，根据 Bacskay [Bacskay81] 方法。这方法结合线性极小化，加上 Bacskay 提出的 Newton-Raphson 计算方法，保证最后会到达一个稳定点。通常，SCF=QC 比传统的 SCF 方法贵两倍。因为 SCF=QC 是可靠的，可用在直接 SCF 方法，当遇到收敛困难的问题是，这方法常是第二种选择。可用在 RHF 和 UHF，但不能用在复数或 ROHF 计算。

Guess=Alter
有时收敛困难是警告最初猜测中的电子填入错误的轨域。最出的猜测必须先检查，特别是填入轨域的对称性。Guess=Alter 可用来更改要填入的分子轨域选择。

SCF(MaxCyc=*N*)
将 SCF 迭代总数增加到 *N*。 注意，只增加预设方法的 SCF 迭代总数几乎没用。

这些方法都趋向于强制收敛到轨域空间内最接近的稳定点，相对于轨域旋转来说，不一定是能量最小的点。稳定性计算可用来检查是否适当的 SCF 解已经获得（见 Stable 关键词）。另外，还需要确认最后的波函数对应所要的电子状态，特别是使用关键词 Guess=Alter 的时候。

工具程序 freqmem 可用来估算不同参数的频率计算所需最佳的内存大小（亦即，一次完成主要步骤所需内存的容量）。

MP2 能量，梯度和振动频率

MP2 有四种计算方法，但大部分的情况由程序自动决定选用哪一种方法。方法选择的重要关键是 MaxDisk 的数值，这变量的数值依据计算机系统的组态环境做设定（见第三章），设定可用磁盘空间的最大值。若在计算路径或档案 Default.Route 内没有设定 MaxDisk，Gaussian 程序会假设计算机系统会提供足够的磁盘空间进行计算，但遇到大型的计算工作时，可能不是这种情况。因此，*设定可用的内存和磁盘空间的大小，是目前改善 MP2 计算效能最重要的方式*。设定后，可让程序在种可用的计算方法中，选出一种最适合计算机组态的计算方

法。在档案 Default.Route 内用 -M- 指令和 MaxDisk i 关键自作设定（计算输入档内也可用 MaxDisk 和 %Mem 指令做设定）。

高阶相干方法

MP2 以上的相干作用方法 （MP3，MP4，CCSD，CISD，QCISD，等等...都需要将某些转换过的分子轨域积分储存到磁盘上，因此（和 MP2 能量和梯度的计算不同）对磁盘空间的需求会随分子的大小成长而有巨大的成长。但是，有几种另类的方式，像是转换过的机分的产生方式，有多少积分要被储存，以及剩下的项要如何计算等等，以改善对计算机系统资源的需求。

Gaussian 程序预设的选项是半直接计算方法。在计算工作的 SCF 计算阶段，原子轨域可被写出和使用，或用直接计算或 in-core 方式进行 SCF。要用到的时候重新计算原子轨域积分，在磁盘上只储存最少数量的分子轨域（见以下说明）。剩余的项用重新计算的原子轨域积分计算。

以下几点书名 MaxDisk 对后-SCF 方法的影响：

- CID，CISD，CCD，BD，和 QCISD 能量计算有固定的储存空间需求，和 O^2N^2 成比例，比例因子很大，但遵循 MaxDisk 的限制，以避免更大的储存空间需求。
- CCSD，CCSD(T)，QCISD(T)，和 BD(T) 能量计算有固定的磁盘空间需求，和 ON^3 成比例，这无法用 MaxDisk 做限制。
- CID,CISD,CCD,QCISD 密度和 CCSD 梯度有固定的磁盘空间需求，和 $N^4/2$ 成比例（填满壳层系统），或和 $3N^4/4$ 成比例（未填满壳层系统）。

CIS 和 TD 能量和梯度

除了积分储存方式的选择，明智使用重新启动计算的功能能够改善 CIS 和 TD 计算的成本。

积分储存方式

用单激发 CI 计算分子激发态有五种方法（用 CIS 关键词中对应的选项做设定）。注意， TD 计算只能使用前两种：

Direct
利用迭代对角化方法，计算指定数目的电子态，从双电子积分建构乘积向量，需要用的时候才计算双电子积分。这计算方法降低了内存和词空间的需求到 $O(N^2)$。这是 TD 计算的预设选项。

InCore
要求原子轨域 Raffenetti 组合要存放在内存内。In-core 计算效能很高，但只适用于小型分子系统或使用具有大内存的计算机，因为这计算方法需要 $N^4/4$ 计算器字的内存。若计算机系统有足够的内存，这计算方法会自动采用。

MO
利用迭代（Davidson）对角化方法解出指定数目的电子态，利用分子轨域积分构成乘积向量。这是最快的计算方法，并且是预设选项。基底函数数目不超过 150 的分子系统，这计算方法效能做好，并且和填满电子的分子轨域数目有关。填满电子个分子轨域数目越多，应越早采用直接计算方法。因为只有两个虚拟（未填电子）轨域的积分（甚至还有梯度的计算）才会用到，程序并且尝试遵循 MaxDisk 的限制。所需最小磁盘空间 40^2N^2（未填满壳层系统的需求是 60^2N^2 ）。这是 CIS. 方法的预设选项。

重新启动计算工作和波函数的再利用

CIS 和 TD 计算工作可从 Gaussian 检查档重新启动，继续未完成的计算工作。在小型计算工作这这功能用处不大，因为小型计算可用分子轨域进行，因为必须完成新的积分计算和今分转换，但这功能在直接 CIS 计算中很有用。若直接 CIS 计算工作在 CIS 计算阶段因故中断，应在 CIS=Restart 或 TD=Restart 关键词的设定中加上 SCF=Restart ，因为整个计算步骤（或优选计算步骤）完成后，最后的 SCF 波函数才会搬到检查文件中永久的位置（可用 Guess=Read 读取）。

CIS 和 TD 激发态电子密度

若只要做电子密度分析，并且已经找到激发态，CIS 电子密度可从检查文件中复原，利用 Density=(Check,Current) Guess=Only, 指示对应目前的计算方法（假设为 CIS）取回任何储存在档案内的的广义密度，然后重复电子分布分析。注意可以检查单粒子（unrelaxed）密度和广义（relaxed）密度，但在 CIS 理论的店双极矩和其它性质已知是不太准确，若使用单粒子电子密度（亦即，若轨域放松(orbital relaxation)项被忽略） [Foresman92, Wiberg92]。因此，强烈不建议使用 CIS 单粒子电子密度，除非是为了要和采用正确的电子密度的计算做比较，或和无法计算广义电子密度的方法的计算结果做比较。

要产生多个状态的广义电子密度需要做另外的计算，因为每一个状态都要执行一次 CPHF 计算。要进行这类计算，先解出第一个激发态所有的状态和电子密度：

```
# CIS=(Root=1,NStates=N) Density=Current
```

若要计算 *N* 个状态。然后进行 *N*-1 次计算，使用以下的计算路径：

```
CIS=(Read,Root=M,NStates=N) Density=Current
```

从状态 M=2 到 N。

未填满壳层激发态的陷阱

因为 UHF 参考状态不是 S^2 的本征函态，因此也不是 CIS 或 TD 方法产生的激发态 [Foresman93]。

稳定性计算

使用关键词 Stable 可用来检查 RHF 和 UHF 以及受限与非受限 DFT 方法的自旋三重态与单一态的稳定性。稳定性计算可以在中断后重新启动接续进行，和前述的 CIS. 计算一样。

CASSCF 计算效能

使用 CASSCF 方法的首要挑战是选择适当地主动空间轨域（active space orbitals）。有几种可能的策略：

- 使用选项 Pop=SaveMixed 将填满轨域的 NBO 和未填满轨域的 NLMO 写到检查档内。然后用 GaussView 将所需要的轨域填入电子并重新排序，建构主动空间。这是目前最容易也最有效的方法。
- 使用标准非局部化最初猜测轨域。若主动空间包含所有的 p 电子，这种选择就足够了。使用 Guess=Only 检查这些轨域，在执行真正计算之前决定是否需要做任何调整。
- 使用局部化的最初猜测轨域。若包含指定的键结电子对，这个策略有效，因为局部化轨域会分离电子。
- 使用来自 UHF 计算 (CAS-UNO)的总电子密度的自然轨域 [Hamilton88, Bofill89]。对于自旋单一态系统，要求设法让 UHF 计算收敛到一个对称破坏的波函数（通常指定 Guess=Mix）。对于不清楚哪些原子最不适宜用双重填入轨域描述的复杂系统，这个策略最有用。

在所有情况下，任何优选计算之前应该先做一次单点能量计算，以便检查收敛的主动空间，确定所要的电子在进行优选计算之前已经产生相干。激发态 CASSCF 波函数的计算还有额外的考虑（参考 CASSCF 关键词的说明）。

CASSCF 频率计算

CASSCF 频率计算需要庞大的内存。增加内存容量总是能够改善 CASSCF 频率计算工作的效能 （用其它方法频率计算的效能不一定会阴内存容量增加而改善）。这计算还需要 O^2N^2 的磁盘空间。

Last updated on: 2 September 2009

Gaussian 09 程序限制

这章节列举程序 Gaussian 09 各种数量大小的限制

- 积分程序有以下限制：
  - 原子数最大值为 250,000.
  - 原始电子壳层函数（primitive shells）总数最大值 750,000.
  - 原始 d-壳层及更高阶壳层函数总数最大值 250,000.
  - 合并壳层函数（contracted shells）总数最大值 250,000.
  - 合并壳层函数的合并程度(被合并的壳层函数的数目)最大值 100.
- Opt=(EF,EnOnly) 几何优选—只对不具解析梯度的计算方法有用—最多只能有 50 个变数.
- GVB 程序最多只能有 100 个成对轨域（ 实务上这不构成一个限制).
- NBO 程序的数组空间能容纳 250,000 个原子和 10,000 个基底函数.

建构 Z-矩阵

这章节简短说明描述分子系统的传统 Z-矩阵。Z-matrix 的大小有限制：在一计算内原子总数和变量的总数不能超过一个最大值。真实原子的数目不能超过 250,000（包含虚拟原子，但不包含哑原子），and a maximum of 250,000 Z-矩阵的中心点数目不能超过 250,000 个 （中心点包括原子，虚拟原子和哑原子）。

使用内坐标

Z-矩阵的的一行指定分子内一个原子的内坐标。最常用的 Z-矩阵格式的语法如下：

元素卷标，原子 1，键长，原子 2，键角，原子 3，双面角 [，标示码]

这里用逗点作各字段间的区隔符号，其它有效的符号也可以。元素卷标是一字符串，由原子的化学符号和原子序构成。若使用元素的化学符号，通常在其后可紧接一个数字用来当作这原子的识别标签。通常的作法是在元素化学符号后接上一个识别用的整数： C1，C2，等等。

原子 1，原子 2，原子 3 是在这行之前已经指定过的原子识别标签，利用和这些原子间的关系决定目前这个原子的位置。另一种方式，也可用这几个原子在分

子结构设定段落内的行数当作识别标签，分子电荷和电子自旋多重态这一行当作第零行。

目前这个原子的位置指定的方式，是指定和原子 1 距离为*键长*，这原子与*原子 1*，及*原子 2* 与*原子 1* 两个键结间的夹角指定为为*键角*，这原子，*原子 1* 和*原子 2* 定义的平面，与*原子 1*，*原子 2*，和*原子 3* 定义的平面，这两个平面间的夹角指定为*双面角*。*键角*的范围必须是 0° 和 180° 之间（不能为负值），*双面角*可以是任何数值。

标示码是选项，指定 Z 矩阵输入的格式。这里描述的文意下，这标示码总是 0。只有当正常 Z 矩阵指定数据之后还有额外的参数的时候，例如 ONIOM 计算，这标示码才有其它的值。

例如，这个过氧化氢的例子。这结构的 Z-矩阵是：

```
H
O 1 0.9
O 2 1.4 1 105.0
H 3 0.9 2 105.0 1 120.0
```

Z-矩阵的第一行指定一个氢原子。第二行指定一个氧原子，并指定和氢原子间的距离是 0.9 埃。第三行定义第二个氧原子，指定 O-O 距离是 1.4 埃（ 即，和原子 2，第一个氧原子，的距离），指定 O-O-H 夹角 （和原子 2 及原子 1 构成的夹角）是 105 度。第四也是最后一行，是唯一需要指定三个内坐标的原子，这是第二个氢原子的定义，和第二个氧原子距离是 0.9 埃，H-O-O 夹角是 105 度，H-O-O-H 双面角是 120 度。

Z-矩阵内所有或部份的数值可用变量指定，过氧化氢分子的 Z 矩阵也可写成这种形式：

```
H
O 1 R1
O 2 R2 1 A
H 3 R1 2 A 1 D
Variables:
R1 0.9
R2 1.4
A 105.0
D 120.0
```

分子的对称性限制可反映在内坐标的定义上。两个 H-O 距离用相同的变数指定，两个 H-O-O 夹角也是。使用这样的 Z-矩阵做内坐标几何结构优选计算时（Opt=Z-matrix），这些变量的数值会被优选，以决定能量最低的结构。做全优选计算（FOpt）的时候，这些变量必须彼此线性独立，并且包含分子所有的自由

度。做部份优选计算（POpt）时，在第二段落的变量（ 通常标示为 Constants:）会维持固定不变，而在第一段落的变量会变优选：

```
 Variables:
R1 0.9
R2 1.4
A 105.0
 Constants:
D 120.0
```

参考关键词 Opt 章节有关使用内坐标做优选计算的说明和范例。

混合内坐标和直角坐标

直角坐标其实是　Z-矩阵的一个特殊情况，例如：

```
C    0.00    0.00    0.00
C    0.00    0.00    1.52
H    1.02    0.00 -0.39
H -0.51 -0.88 -0.39
H -0.51    0.88 -0.39
H -1.02    0.00    1.92
H    0.51 -0.88    1.92
H    0.51    0.88    1.92
```

在一个 Z 矩阵内可以使用同时内坐标和直角坐标，例如：

```
O 0 xo       0.    zo
C 0    0.     yc     0.
C 0    0.    -yc     0.
N 0 xn       0.     0.
H 2 r1 3 a1 1    b1
H 2 r2 3 a2 1    b2
H 3 r1 2 a1 1 -b1
H 3 r2 2 a2 1 -b2
H 4 r3 2 a3 3    d3
 Variables:
xo -1.
zo    0.
yc    1.
xn    1.
r1    1.08
r2    1.08
r3    1.02
```

```
a1    125.
a2    125.
d3    160.
b1    90.
b2  -90.
```

这 Z-矩阵有几点值得注意：

- 直角坐标使用的变量名称和内坐标的变量名称用相同的方式指定。
- 原子的元素符号后面的整数 0 （第二字段）表示这一行后面接着的字段是直角坐标。
- 直角坐标的变量前可直接使用负号，表示负值，和双面角变量一样。

另一种 Z-矩阵格式

这 Z-矩阵格式容许原子核的位置用两个键角指定，而非用一个键角和一个双面角。在第二个键角后新增一个字段内，用 1 做标示。（这字段预设的数值是 0，表示前面这个字段是双面角）：

```
C4 O1 0.9 C2 120.3 O2 180.0 0
C5 O1 1.0 C2 110.4 C4 105.4 1
C6 O1 R C2 A1 C3 A2 1
```

第一行使用双面角，第二和第三行使用第二个键角。

使用哑原子

这章节说明 Z-矩阵内如何使用哑原子，哑原子的原子符号是 X。 以下这个范例说明如何使用一个哑原子固定 C_{3v} 氨分子的三重对称轴：

```
N
X 1 1.
H 1 nh 2 hnx
H 1 nh 2 hnx 3 120.0
H 1 nh 2 hnx 3 -120.0

nh 1.0
hnx 70.0
```

哑原子在对称轴上的位置无关紧要，这里设定的距离 1.0 可用其它数值取代。hnx 是三重对称轴和 N-H 键结间的夹角。

这是 oxirane 分子的 Z 矩阵：

```
X
C1    X halfcc
O     X ox C1 90.
C2    X halfcc O 90. C1 180.0
H1 C1 ch X hcc O    hcco
H2 C1 ch X hcc O -hcco
H3 C2 ch X hcc O    hcco
H4 C2 ch X hcc O -hcco

halfcc 0.75
ox        1.0
ch        1.08
hcc       130.0
hcco     130.0
```

这个范例说明两点。首先，哑原子放在 C-C 渐得中间，协助固定 cco 三角形成为等腰三角形。 ox 是从 O 到 C-C 键的垂直距离，键角 oxc 设定为 90 度。第二， Z-矩阵内某些项用双面角变数 hcco. 加一负号表示。

以下这个范例说明使用哑原子设定线性键结。用内坐标做几何优选计算无法处理接近 180 度的键角，像乙炔或丁三烯的 C_4 炼等分子的线性片段结构，就有这种情况。含有线性的分子团（如乙烯基）的无对称性分子也会遇到几何优选计算的困难。遇到这种情况，可在分角在线放置哑原子，并使用半角作为变量或常数，即可排除优选计算的困难：

```
N
C 1 cn
X 2 1. 1 90.
H 2 ch 3 90. 1 180.

cn 1.20
ch 1.06
```

同样的，这用来做几何优选计算的 Z-矩阵，half 代表 N-C-O 角度（接近 180 度）的一半。注意 half 的数值小于 90 度，对应一个顺式排列：

```
N
C 1 cn
X 2 1. 1 half
O 2 co 3 half 1 180.0
H 4 oh 2 coh 3 0.0

cn 1.20
co 1.3
oh 1.0
```

half 80.0
coh 105.

模型建构（Model Builder）几何设定

模型建构是 Gaussian 程序提供的工具，用来快速设定某类型的分子系统[Pople67a]。可用关键词 Geom 的 ModelA 或 ModelB 选项做指定，在计算输入档内需有有一个独立的段落提供适当地设定。

模型建构的基本输入数据称为简短公式矩阵（ *short formula matrix*），由好几行构成，每一行定义一个原子（用原子符号表示）和这原子与其它原子间的连接关系，最多可以有六个字段（表示最多可和六个原子键结）。每一个字段上可以是一个整数，代表键结原子在分子结构设定段落里的行的位置，或是一个原子符号（例如 H，F）表示和这原子以末端键结连接，或是一个和这原子连接的末端分子团。可用的末端分子团有 OH，NH2，Me，Et，NPr，IPr，NBu，IBu，和 TBu。

简短公式矩阵隐含绕着每一个键结旋转几何的定义。假设原子 X 和 Y 已明确定义。X 出现在 Y 列，且 Y 出现在 X 列。令原子 *I* 在 Y 列中出现在 X 的右边，原子 *J* 在 X 列中出现在 Y 的右边。则原子 *I* 和 *J* 和 X-Y 键结是处在反式 （trans）的取向。简短公式矩阵后可加入几行的设定，修改所产生的结构。有需要时才加入这几行，并且要用以下的次序，同一类型的设定要放在一起：

AtomGeom, *I*, *Geom*
通常一个原子附近的局部几何关系用和这原子键结的数量和类型定义（例如，甲烷的碳是四面体，乙烯的碳是三角形，等等）。在中心原子触的所有键角都相等。AtomGeom 这行可来改变在中心原子 *I* 的键角数值。*Geom* 是一个键角，可以是一个浮点数，或是以下字符串之一 Tetr，Pyra，Trig，Bent，或 Line。

BondRot, *I, J, K, L, Geom*
这行改变 *I-J* 和 *K-L* 键箱对于 *J-K* 渐得方位取向。*Geom* 是双面角的数值，或是以下字符串之一 Cis（≥0），Trans（≥180），Gaup（≥+60），或 Gaum（≥－60）。

BondLen, *I, J, NewLen*
这行设定 *I-J* 键长为 *NewLen* （一个浮点数）。

模型建构只能建构正常价键（valance）原子组成的分子结构。若要建构自由基分子，多出来的价键方位可用哑原子锁定，可在原子符号前加上一个负号做指定（例如， －H）。只有在末端的原子才可以这样设定。

这两个模型建构（A 和 B）的差别是，模型 A 在指定键长时考虑到键结的类型（单键，双键，三键，等等），而模型 B 的键长只考虑和相关原子的类型。模型 B 适用于从 H 到 Cl 的所有原子，除了 He 和 Ne。若采用模型 A，但某个原子在模型 A 内没有定义键长，将会使用适当地模型 B 键长。

Last updated on: 1 Jul 2009

Gaussian 09 模块 Links

以下是 Gaussian 09 程序的模块清单，以及各模块的主要功能：

L0	启动程序并控制层组 overlaying
L1	处理计算路径段落，建立要执行的模块清单，并打开或建立暂存档
L101	读进标题段落和分子系统设定段落
L102	Fletcher-Powell 优选计算
L103	Berny 优选计算，用于能量最小化，过渡状态，STQN 过渡状态搜寻
L105	Murtaugh-Sargent 优选计算
L106	of 作用力/双极矩的数值差分，计算极化张量和超极化张量。
L107	线性同步跃迁 Linear-synchronous-transit (LST) 过渡状态搜寻
L108	未松弛（Unrelaxed）位能曲面扫描
L109	Newton-Raphson 优选计算
L110	能量的双重数值差分，产生振动频率
L111	能量的双重数值差分，计算极化张量和超极化张量
L113	使用解析梯度做 EF 优选计算
L114	数值 EF 优选计算（只用到能量）
L115	使用 GS3 方法探索化学反应路径
L116	数值自洽反应场 (SCRF)计算
L117	IPCM 溶液模型计算
L118	BOMD 计算
L120	控制 ONIOM 计算
L121	ADMP 计算
L122	补偿（Counterpoise） 计算
L123	以 HPC 计算方法（和其它方法）探索化学反应路径
L124	利用 PCM 和外迭代（external-iteration） PCM 进行 ONIOM 计算
L202	重新调整分子方位，计算分子对称性，检查变数
L301	产生基底函数组信息
L302	计算重迭，运动项和位能积分

L303 计算多极积分
L308 计算电双极速度和 Rx∇积分
L310 以原始型计算 spdf 双原子积分
L311 计算 sp 双电子积分
L314 计算 spdf 双电子积分
L316 印出双电子积分
L319 计算近似自旋轨域偶合作用所需的单电子积分
L401 建立分子轨域最初猜测
L402 半经验和分子力学计算
L405 启动 MCSCF 计算
L502 迭代解 SCF 方程式(传统方法,UHF 和 ROHF,所有直接方法, SCRF)
L503 使用直接能量最小迭代解 SCF 方程式
L506 进行 ROHF 或 GVB-PP 计算
L508 二阶收敛 SCF 程序
L510 MC-SCF
L601 电子分布和相关的分析 (包括多极矩)
L602 单电子性质(静电位能,静电位场和静电位场梯度)
L604 在一格网上计算分子轨域或电子密度
L607 进行自然键节轨域 NBO 分析
L608 非迭代 DFT 能量
L609 Atoms in Molecules 性质
L610 数值积分 (测试积分程序)
L701 单电子积分一次和二次微分
L702 双电子积分一次和二次微分 (sp)
L703 双电子积分一次和二次微分 (spdf)
L716 整理优选计算和频率计算所需数据
L801 启动双电子积分转换
L802 积分转 (N^3 内存 in-core)
L804 积分转换
L811 转换积分的微分,并计算对这些积分的微分对 MP2 2^{nd} 为分的贡献
L901 双电子积分的反对称化
L902 决定 Hartree-Fock 波函数的稳定性
L903 旧版内存 MP2
L904 完全基底函数组 (CBS) 外插方法(Petersson, et. al.)

L905	复数 MP2
L906	半直接 MP2
L908	电子传布程序 Electron Propagator Program
L913	后-SCF 能量和梯度项
L914	CI-Singles， RPA 和 ZIndo 激发态；SCF 稳定性
L915	计算第五阶量（计算 MP5，QCISD(TQ) 和 BD(TQ)）
L916	旧版 MP4 和 CCSD
L918	波函数重新优选计算
L923	SAC-CI 程序
L1002	CPHF 方程是的迭代解；计算各种分子性质（包括 NMR）
L1003	CP-MCSCF 方程是的迭代解
L1014	解析 CI-Singles 二次微分
L1101	单电子积分的微分
L1102	电双极为分的积分
L1110	$F^{(x)}$ 的双电子积分的微分
L1111	双粒子密度矩阵和后-SCF 微分
L1112	MP2 二次微分
L9999	结束计算和关闭输出档案

Last updated on: 1 Jul 2009

和 Gaussian 03 的差异

这一节总结 Gaussian 09 和 Gaussian 03 的主要差异。相关功能的细节请参考这手册前面的章节（包括参考文献）。Gaussian 个本版功能回顾式总结档案放在网页 www.gaussian.com/g_tech/gdiffs.pdf.

新方法和新功能

能量和能量微分

- 最近发展的半经验模型已重新纳入，包括 AM1，PM3，PM3MM，PDDG 和 PM6，包括能量的解析一阶和二阶微分，使用者自定参数，以及 PCM 溶液模型方法。

- TD-DFT 梯度和数值频率。
- EOM-CCSD 方法计算电子激发能。
- 许多新的 DFT 泛函数， 包括 HSE， wB97， m05/m06， LC 系列和双重混合 B2PLYP。
- 各泛函数包含所对应的经验散频模型 （Empirical dispersion models）。
- ROMP3，ROMP4，ROCCSD，和 ROCCSD(T) 能量。
- W1RO，W1BD，和 G4 复合式能量计算方法。
- DFTB 半经验模型和使用解析矩阵元素方法的 DFTBA 版本。

ONIOM

- ONIOM 和 PCM 能够合并使用。有几种 ONIOM+PCM 模型。
- IRCs 现在可以在 ONIOM 模型下进行，甚至含有数千个原子的分子系统上也有很好的计算效能。

溶液模型

- 新的 PCM 溶液模型计算方法，使能量成为原子核坐标适当的的连续函数，对所有 SCF 性质的溶剂效应计算提供效能很高的计算方法。PCM 溶液模型和气态态环境下的分子的几何优选计算收敛程度相近。
- 可进行溶液环境内指定电子状态的自洽计算，模拟荧光和其它放射（emission）现像。
- SMD 溶液模型。这模型的参数得自对一百多种溶剂的总溶解自由能所做的最佳调适。

几何优选和 IRCs

- GEDIIS 分子几何优选计算方法式能量最小化计算的预设方法。对于大型扁平柔软的分子结构特别有效。
- ONIOM(MO:MM) 二阶收敛几何优选计算，不论是纯力学的或是内含电子效应的情况，对能量最低和对过渡状态的分子结构，都能使用。
- 输入档中有一个段落指示在优选计算中哪些原子的坐标要被冻结，哪些原子要被解冻。可根据原子，元素，分子团，或 ONIOM 层的类型做标示。

分子性质

- 和频率有关的解析 ROA 强度。
- 解析 DFT 超极化张量 hyperpolarizabilities。
- 电子激发，放射 emission，和光游离光谱形状（photoionization band shapes），根据 Franck-Condon 理论和双态（two states）简谐正则振动方法。

- 电子激发光谱形状 （Electronic excitation band shapes），根据 Herzberg-Teller 或 Franck-Condon-Herzberg-Teller 理论。
- 可选取正则振动做显示，或做非简谐校正，或做 FC/HT/FCHT 分析。可根据原子，元素，分子团，或 ONIOM 层的类型做选取。

分析和输出

- 在计算输入档和格式化的检查档 .fchk 中的分子结构设定段落中可包含蛋白质分子的二级结构信息。
- 可进行每个分子轨域的电子分布分析（ population analysis），可显示个别原子轨道和个别角动量波函数对分子轨域的贡献。
- 正则（Canonical） UHF/UDFT 轨域可以做双重正交处理（ biorthogonalized），可用来作图形显示，或当做 ROHF 计算的最初猜测轨域。
- 可做 CIS 和 TD 激发态的自然过渡轨域分析（Natural Transition Orbital analysis）。
- 被占轨域被投射在一组最小基底函数后，可做 Mulliken 电子分布分析。使用延展的基底函数组时，可以得到稳定的电子分布分析。

其它新功能

- SCF 计算的最初猜测，可从各分子片段的计算组合而成，每个分子片段的计算需指定电荷和自旋多重态。
- 数值频率可用四点差分方法计算，比预设的两点差分发法更准确，数值上也更稳定。

计算效能的改善

- 大型分子的 HF 和 DFT 频率计算效能改善很大，特别是做并行计算时更显著。
- 做跨节点并行计算时，FMM 和静电（Coulomb）与交换（Exchange）能量的计算可符合线性增幅（ linear scaling）。
- 大型分子系统的 ONIOM(MO:MM) 频率计算计算效能有很大的提升，特别是内涵电子效应的计算。对包含 100-200 个 QM 原子和 6000 个 MM 原子的分子系统做频率计算现在是可行的。
- 大型频率计算个过程中可以储存基本震动模式 （normal modes），并且可用来作展示或打印，启动一个 IRC=RCFC 计算工作。
- CC，BD 和 EOM-CCSD 振幅可以储存到检查档内，在后续的计算中读取，后续计算使用不同基底函数也行。 BD 轨域也可以储存然后再读取。
- 半经验，HF，和 DFT 方法的频率计算可从前一计算半途中重新启动。
- CC 和 EOM-CC 计算可从前一计算半途中重新启动。

- 在单一 ONIOM 计算中个别步骤的最初猜测可从其它检查档案中读取。ONIOM=OnlyInputFiles 选项会印出输入文件中对应 ONIOM 计算中各区块的数据，便利产生各区块的波函数。
- 提供对应 SVP，TZVP，和 QZV 基底函数的密度适配组。 /Fit 关键词指示适配组要对指定的原子轨域基底做适配（matching），若没有指定的适配组，则用关键词 /Auto。因此 BVP86/SVP/Fit 表示使用伴随 SVP 基底函数定义的适配组所做的密度适配（ density fitting），而 BVP86/6-31G*/Fit 和 BVP86/6-31G*/Auto 同义。
- 关键词 DensityFit 可包含在档案 Default.Route 内，指示当要求使用群密度泛函数的时候使用适配预设的泛函数。
- 密度基底函数可读入使用未归一化的原始函数的系数，密度归一化的原始函数的系数，或是当做原子轨道归一化的原始函数的系数。每一种方式都有一些程序采用，若在 Gaussian 09 程序中要使用这些基底函数，需要使用对应的关键词选项。

Gaussian 09 和 Gaussian 03 功能上的差异

- 单点 SCF 计算是完全精确选项的预设选项 (SCF=Tight)。
- Freq=ROA 的预设选项是 CPHF=RdFreq，因为频率相关的 ROA 强度有解析方法做计算，但在静态极限内的只有数值方法可做计算，比较不准。
- 后-SCF 方法，像 MP，BD 和 CC 的预设选项是 Tran=IABC，在大部分的计算机上，这方法比完全转换（full transformation ）要更有效率。
- IRCs 预设的计算采用新的模块，L123。除非明确指定，IRCMax 的计算工作或采用旧的 IRC 模块 (L115)。 L123 预设的计算方法是 IRC=HPC，除了 ONIOM(MO:MM) 计算，这计算采用 IRC=EulerPC。L123 可用 IRC=GS2 计算方法（ L115 使用的方法）），但通常这方法比预设的方法昂贵（花更常的计算时间）。
- 预设的设定，IRCs 只输出反应路径上每一点的能量和原子坐标，用 IRC=Report 可指定哪些内坐标的数值也要列表输出。
- 普通的 QM 频率计算和 ONIOM(MO:MM) 频率计算是 CPHF=Simultaneous 的预设选项，和 Gaussian 03 一样。但使用 CPHF=Separate 时，半经验频率计算会较有效率，因此是这种情况下的预设选
- Counterpoise 和 Guess=Fragment 计算或做根据分子片段做的电子分布分析时，时要对原子指定所属的分子片段，这是在原子设定段落的原子核性质设定完成，而非在该行的最后做设定，这和 ONIOM 的输入数据乡冲突，例如：

  C(Fragment=3) 0.0 1.0 2.0

  而非旧的格式：

  C 0.0 1.0 2.0 3
- 同位素通常是在原子核性质字段中指定，是原子定义行的一部分。若这些数据要另外读取，在读入分子结构段落之后，一次读取，而不是由个个子程序（例如 IRC，Freq 等等）个别读取。

附属工具程序的强化

- 工具程序 formchk 可将额外的信息加入 .fchk 档案，包括使用者指定的 MM 类型和其它字符串。 执行 formchk 时加上 -3 选项，可加入这些讯息。
- 工具程序 freqchk 可从 .chk 或 .fchk 档案取出分子基本震动模式（normal mode），并可将所惨生的基本震动模式储存到所产生的 .chk 档案内（但不能储存到 .fchk 档案内）。.

Last updated on: 1 September 2009

计算输入档	计算执行路径
test000.com	# SP, RHF/STO-3G punch=archive trakio scf=conventional
test001.com	#P TEST STO-3G COMPLEX pop=full scf=tight
test002.com	#p rohf/4-31g pop=(reg,npa) test force scf=conventional #p rohf/4-31g test force #p rohf/4-31g test force scf=noincore #p rohf/4-31g test force scf=noincore raff #p rohf/4-31g test force scf=noincore noraff #p rohf/4-31g test force scf=noincore iop(5/29=3) #p gvb(0)/4-31g pop=(reg,npa) test force scf=conventional #p gvb(0)/4-31g test force #p gvb(0)/4-31g test force scf=noincore noraff #p gvb(0)/4-31g test force scf=noincore raff #p gvb(0)/4-31g test force scf=noincore iop(5/29=3)
test003.com	#P TEST 3-21G SCFDM
test004.com	#P TEST UHF/6-31G* scf=conventional
test005.com	#P TEST 6-311G** scf=conventional
test006.com	#p rhf/gen 6d iop(5/8=2) test pop=reg scfdm
test007.com	#P NONSTD OLDCONSTANTS 1//1; 2//2; 3/5=1,6=6,7=1,11=0,25=14/1,2,3,11,14; 4//1; 5/6=7/2; 6//1;
test008.com	#P rhf/6-31g* use=l310 test scf=conventional

test009.com	#P TEST OPT STO-3G scf=conventional
test010.com	#P TEST OPT=FP STO-3G OPTCYC=2 scf=conventional #P TEST OPT=(FP,RESTART) STO-3G OPTCYC=20 scf=conventional
test011.com	#P TEST opt RHF/LP-31G scf=conventional
test012.com	#P TEST MP4SDTQ/6-31G* scf=conventional
test013.com	#P TEST CID/4-31G scf=conventional
test014.com	#P TEST RCISD/4-31G density=all pop=full scf=conventional
test015.com	#P TEST CCD/4-31G scf=conventional
test016.com	#P TEST RMP2/4-31G force scf=conventional #P TEST RMP2/4-31G force iop(9/8=20) #P TEST RMP2/4-31G force iop(9/8=30)
test017.com	#P TEST 3-21G FREQ scf=conventional #P TEST 3-21G FREQ=noraman scf=conventional
test018.com	#P TEST RHF/4-31G STABLE(OPT,RUHF,REXT,INT) #P TEST RHF/4-31G STABLE(1OPT,RUHF,REXT,INT) use=l902 scf=conventional
test019.com	#P TEST RHF/4-31G STABLE(1OPT,CRHF,CEXT,INT)
test020.com	#P TEST UHF/4-31G ALTER STABLE #P TEST UHF/4-31G ALTER STABLE use=l902 scf=conventional
test021.com	#P TEST CISD=FULL pop=none GEN
test022.com	#P TEST CCD=FULL GEN
test023.com	#P TEST HF/STO-3G OPT=(CALCFC,TS)
test024.com	#P TEST FREQ RHF/STO-3G
test025.com	#P TEST OPT=MS STO-3G #P TEST OPT=(MS,RESTART) STO-3G OPTCYC=32
test026.com	#p rmp2/3-21g freq=numer test polar #p rmp2/3-21g freq=(numer,restart) test polar
test027.com	#p rhf/3-21g freq=numer test polar
test028.com	#p rhf/3-21g freq=anal
test029.com	#P TEST RHF/6-31G* FORCE #P TEST GVB(0)/6-31G* FORCE
test030.com	#P TEST UHF/6-31G* FORCE
test031.com	#P TEST MP4/3-21G
test032.com	#P TEST MP4/3-21G

test033.com	#P TEST CISD/3-21G
test034.com	#P TEST CISD/3-21G
test035.com	#P TEST RMP2=full/3-21G force
test036.com	#P TEST FREQ UHF/3-21G
test037.com	#p UMP2(full)/3-21G force test density=all popu=full
test038.com	#P CID RHF/3-21G force test
test039.com	#P CISD RHF/3-21G force test
test040.com	#P TEST MP4(SDTQ)/3-21G
test041.com	#P TEST MP4(SDTQ)/3-21G #P TEST MP4(SDTQ)/3-21G use=l802
test042.com	#P TEST FREQ RHF/STO-3G #P RHF/STO-3G pop=none geom=check guess=read test opt=readfc

test043.com	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq scf=conventional scfcon=12
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq scf=conventional int=writed2e
	iop(10/32=1,10/50=1) scfcon=12 geom=check guess=read
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq scf=conventional
	iop(5/17=1000400,10/17=400) scfcon=12 geom=check guess=read
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq scfcon=12 geom=check guess=read
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq scfcon=12 scf=noincore geom=che
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq iop(10/50=1) scfcon=12 scf=noin
	guess=read
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq iop(10/50=3) scfcon=12 scf=noin
	guess=read
	#p cas(6,6)/6-31g(df,pd) 5d 7f test freq iop(10/32=2) scfcon=12 scf=noin
	guess=read

test044.com	#P RHF/6-31G* Pop=NBORead test
test046.com	#P TEST OPT RHF/6-31G* 5D #P TEST FREQ=NUMER RHF/6-31G* 5D GEOM=CHECK GUESS=READ
test047.com	#P TEST OPT RHF/6-31G* 5D #P TEST FREQ RHF/6-31G* 5D GEOM=CHECK GUESS=READ
test048.com	#P TEST FORCE RHF/6-31G*
test049.com	#P TEST MP4(SDTQ)/6-31G* #P TEST RMP4=noincore/6-31G* scf=noincore tran=semidirect #P TEST RMP4/6-31G* scf=noincore tran=(full,incore) #P TEST RMP4/6-31G* scf=direct tran=(full,fulldirect,sort) #P TEST RMP4/6-31G* scf=direct tran=(semidirect,full) #P TEST RMP4/6-31G* tran=conventional

test050.com	#P TEST FREQ RHF/6-31G* #P TEST FREQ RHF/6-31G* scf=direct geom=check guess=read #P TEST FREQ RHF/6-31G* scf=noincore geom=check guess=read raff #P TEST FREQ RHF/6-31G* scf=direct geom=check guess=read iop(11/11=8,11/ #P TEST FREQ RHF/6-31G* scf=noincore geom=check iop(3/47=32) noraff #P TEST FREQ RHF/6-31G* scf=noincore geom=check iop(3/47=32) raff
test051.com	#P TEST UHF/6-311G* FORCE prop=epr
test052.com	#P TEST FREQ UHF/6-31G* #P TEST FREQ UHF/6-31G* scf=direct guess=read geom=check #P TEST FREQ UHF/6-31G* scf=direct guess=read geom=check raff #P TEST FREQ UHF/6-31G* scf=direct iop(11/11=8,11/31=1) guess=read geom= #P TEST FREQ UHF/6-31G* scf=noincore geom=check noraff int=revdagsam #P TEST FREQ UHF/6-31G* scf=noincore geom=check int=revdagsam raff
test053.com	#p test mp4(sdtq)/6-31g* popu=min #p test mp4/6-31g* popu=min tran=semidirect iop(8/2=2000000) #p test mp4/6-31g* popu=min scf=noincore tran=(full,incore) #p test mp4/6-31g* popu=min scf=direct tran=(full,fulldirect,sort) iop(8, #p test mp4/6-31g* popu=min scf=direct tran=(semidirect,full) iop(8/2=20 #p test mp4/6-31g* tran=conventional #p test mp4=noincore/6-31g* popu=min scf=direct tran=incore
test054.com	#P test MP2/6-31G* force #P test MP2/6-31G* force iop(9/8=20,9/16=-2) #P test MP2/6-31G* force iop(9/8=30,9/16=-2)
test055.com	#P rhf/gen prop=(read,opt) test scf=conventional #P rhf/chkbas prop=(read,potential) test geom=check guess=read scf=tight #P rhf/chkbas prop=(read,field) test geom=check guess=read scf=tight
test056.com	#p rhf/lp-31g test pop=reg
test057.com	#P TEST opt RHF/LP-31G*
test058.com	#P TEST FORCE rqcisd/6-31G* 5d density=curr
test059.com	#P TEST MP4SDTQ/6-311G(df,p)
test060.com	#P TEST uqcisd/6-311G* FORCE density=curr
test061.com	#p rhf/3-21g complex geom=(modela,print) force test #p rhf/3-21g complex geom=(modela,print) force test int=dsrys #p rhf/3-21g complex geom=(modela,print) force test int=(berny,dsrys)
test062.com	#p rmp2/3-21g complex geom=(modela,print) test
test063.com	#p rmp2/3-21g use=l903 geom=(modela,print) test
test064.com	#p rhf-cid=full/3-21g freq=numer geom=(modela,print) test
test065.com	#P ump2/3-21g test density=curr

	#P ump2=noincore/3-21g test density=curr iop(9/16=-1) #P ump2=noincore/3-21g test density=curr iop(9/8=20,9/16=-4) #P ump2=noincore/3-21g test density=curr iop(9/8=30,9/16=-4) #P ump2/3-21g tran=conv density=curr test #P ump2/3-21g use=l903 test
test066.com	#p ump2/sec** geom=(modela,print) pop=nboread test
test067.com	#p uhf/6-311g(df,pd) test
test068.com	#p ump2/6-311g(df,pd) nosymm test #p ump2/6-311g(df,pd) nosymm test iop(9/8=10)
test069.com	#p rmp2/d95** geom=(modela,print) test pop=full density=curr #p rmp2/d95** geom=(modela,print) test pop=full density=curr iop(9/16=-2 #p rmp2/d95** geom=(modela,print) test pop=full density=curr iop(9/2=316000 #p rmp2/d95** geom=(modela,print) test pop=full density=curr iop(9/2=316000
test070.com	#p rmp2/d95v** geom=(modela,print) test
test071.com	#p ump2/d95** geom=(modela,print) test density=curr #p ump2/d95** geom=(modela,print) test density=curr iop(9/2=3210000,9/16 #p ump2/d95** geom=(modela,print) test density=curr iop(9/2=3210000,9/8= #p ump2/d95** geom=(modela,print) test density=curr iop(9/2=3210000,9/8=
test072.com	#p rmp2(rw)/d95** geom=(modela,print) test
test073.com	#P TEST RHF/6-31G* FORCE
test074.com	#p rhf/6-31g* test geom=modela scf=conventional #p restart
test075.com	#P TEST OPT RHF/6-31G* 5D #p test freq rhf/6-31g* 5d geom=check guess=read iop(11/43=2)
test076.com	#p rhf/3-21g scan test #p rhf/3-21g scan=restart test
test077.com	#p ump2/3-21g scan test #p ump2/3-21g scan=restart test
test078.com	#p rmp2/3-21g test opt=calchffc optcyc=2
test079.com	#p rhf/3-21G freq=cubic geom=modela
test080.com	#P TEST OPT RHF/6-31G* 5D #P TEST FREQ RHF/6-31G* 5D GEOM=CHECK GUESS=READ cphf=mo
test081.com	#P TEST FREQ UHF/3-21G cphf=mo
test082.com	#p rhf/3-21G freq geom=modela test
test083.com	#p rhf/6-31g* opt=tight test
test085.com	#p rhf/6-31g(df,pd) test force

	#p rhf/6-31g(df,pd) test freq
test087.com	#p rhf/gen 6d name=frisch units=au gfoldprint test scf=conventional #p rhf/chkbas 6d geom=check guess=read test scf=(direct,tight)

test088.com	#p GVB(2)/6-31g(d) 5d force guess=(cards,lowsym) test pop=full geom=modela
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,read) test pop=full geom=modela
	scf=direct
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,read,cards) test pop=full geom
	int=(berny,dsrys) scf=noincore
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,cards) test pop=full geom=modela
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,cards) test pop=full geom=modela
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,cards) test pop=full geom=modela
	noraff
	#p GVB(2)/6-31g(d) 5d force guess=(lowsym,cards) test pop=full geom=model
	iop(5/29=3)

test089.com	#P UHF/6-31G* Pop=NBORead test scf=conventional
test090.com	#p uhf/6-31g* freq geom=modela test #p uhf/6-31g* freq geom=modela test cphf=mo guess=read #p uhf/6-31g* freq geom=modela test int=direct guess=read #p uhf/6-31g* freq geom=modela test cphf=simult guess=read #p uhf/6-31g* freq geom=modela test int=direct guess=read cphf=simult
test091.com	#p nosymm dreiding opt=tight freq test constants=1998 #p symm=loose dreiding freq=numer geom=check test
test092.com	#p rhf/sto-3g test scf=tight nosymm #p rhf/sto-3g test massage scf=tight nosymm #p rhf/sto-3g test charge scf=tight nosymm
test093.com	#p rhf/sto-2g test force guess=huckel geom=(nodist,noang) #p rhf/sto-2g test force guess=huckel geom=(nodist,noang)
test094.com	#p rmp2/sto-3g opt=calcfc test geom=modela
test095.com	#p gvb(oss)/3-21g geom=modela test force
test096.com	#p ram1 freq test geom=modela use=l402 #p rhf/sto-3g fopt=readfc test geom=modela #p rhf/sto-3g fopt=mndofc test geom=modela #p freq test geom=modela int=am1 #p rhf/sto-3g fopt=readfc test geom=modela
test097.com	#p rhf/6-31G(df,p) 5d 7f force test geom=modela scf=conventional iop(7/2 #p rhf/6-31G(df,p) 5d 7f force test geom=modela int=dprdsrf scf=conventi #p rhf/6-31G(df,p) 5d 7f force test geom=modela int=dsrys scf=conventiona #p rhf/6-31G(df,p) 5d 7f force test geom=modela int=(berny,dsrys) scf=co
test098.com	#p rhf/6-31G(df,p) 5d 7f freq test geom=modela

	#p rhf/6-31G(df,p) 5d 7f freq test geom=modela iop(7/2=4000000) #p rhf/6-31G(df,p) 5d 7f freq test geom=modela int=dsrys #p rhf/6-31G(df,p) 5d 7f freq test geom=modela int=(berny,dsrys)
test099.com	#p ump4/d95 test #p ump4/d95 test tran=fulldirect #p ump4/d95 test tran=semidirect #p ump4/d95 test tran=full #p ump4/d95 test tran=(full,fulldirect) #p ump4/d95 test tran=(full,semidirect)
计算输入档	**计算执行路径**
test100.com	# TEST OPT=(fccards,enonly) RHF/6-31G* 5D # TEST force=enonly RHF/6-31G* 5D geom=check guess=read # TEST force=(enonly,restart) RHF/6-31G* 5D geom=check guess=read # TEST freq=enonly RHF/6-31G* 5D geom=check guess=read # TEST freq=(enonly,restart) RHF/6-31G* 5D geom=check guess=read
test101.com	#P TEST RHF/3-21G Polar #P TEST RHF/3-21G Polar=Numer #P TEST RHF/3-21G Polar=Enonly
test102.com	#p rmp2/3-21g test polar=numer #p rmp2/3-21g polar=enonly test #p rmp2/3-21g polar=(enonly,restart) test
test103.com	#p ump3/3-21g polar test geom=modela #p ump3/3-21g polar=restart test geom=modela int=reuse
test104.com	#P rhf/sto-3g LST #P rhf/sto-3g LST=restart guess=always
test105.com	#p rmp4/3-21g test geom=modela #p rmp4/3-21g test iop(8/30=1) geom=modela #p ump4/3-21g test geom=modela #p ump4/3-21g test iop(8/30=1) geom=modela
test106.com	#p test ump4sdq(full)/6-31g guess=alter #p test ump4sdq(full)/6-31g guess=alter use=l802
test107.com	#p test ump4sdq(full)/6-31g guess=alter #p test ump4sdq(full)/6-31g guess=alter use=l802
test108.com	#p test ump4sdq(full)/3-21g
test109.com	#P st4ccd/6-31G** test
test110.com	#P uccd+stccd/6-31G* test guess=alter #p uccd/6-31G* test guess=read scf=qc #p ump4sdtq/6-31G* test guess=read

test111.com	#p rmp2=rw/3-21g opt=fp geom=modela #p rmp2=rw/3-21g opt=(fp,restart) geom=modela test

test112.com	#p rqcisd/d95(df) 5d 7f force density=curr test tran=full iop(8/2=500000
	#p rqcisd/d95(df) 5d 7f force density=curr test iop1=nopacksort tran=ful
	iop(8/2=5000000,9/2=5000000)
	#p rqcisd/d95(df) 5d 7f force density=curr test tran=iabc iop(8/2=500000
	#p rqcisd=noincore/d95(df) 5d 7f force density=curr test tran=iabc
	iop(8/2=5000000,9/2=5000000)

test113.com	#p uqcisd/d95(df) 5d 7f force density=curr test extrabasis int=nobasistra
	tran=full iop(8/2=5000000,9/2=5000000)
	#p uqcisd/chkbas force density=curr test geom=check guess=read iop1=nopa
	tran=full iop(8/2=5000000,9/2=5000000)
	#p uqcisd/chkbas force density=curr test geom=check guess=read tran=iabc
	iop(8/2=12000000,9/2=12000000)
	#p uqcisd=noincore/chkbas force density=curr test geom=check guess=read
	iop(8/2=5000000,9/2=5000000)

test114.com	#p romp2/6-31g* geom=modela test #p romp2/6-31g* geom=modela test tran=conv
test115.com	#P blyp/sto-3g vshift=50 force test #P blyp/sto-3g vshift=50 force int=grid=50194
test116.com	#p rhf/6-31g* 5d test scf=tight nosymm #p rhf/6-31g* 5d test massage scf=tight nosymm #p rhf/6-31g* 5d test charge scf=tight nosymm
test117.com	#P TEST RHF/6-31G* FORCE scf=(qc,conventional) #P TEST RHF/6-31G* FORCE scf=(qc,direct)
test118.com	#P TEST UHF/6-31G* FORCE scf=(qc,conventional) #P TEST UHF/6-31G* FORCE scf=(qc,direct)
test119.com	# rhf/sto-3g opt=(ef,ts,calcall) test #T rhf/sto-3g opt=(ef,ts,restart,calcall) test #T rhf/sto-3g opt=(ef,ts,restart) test # rhf/sto-3g opt=(ef,enonly,ts) test #T rhf/sto-3g opt=(ef,enonly,ts,restart) test
test120.com	# rmp2=full/3-21g opt=(ef,ts,calcall) test #T rmp2=full/3-21g opt=(ef,ts,calcall,restart) test #T rmp2=full/3-21g opt=(ef,ts,restart) test # rmp2/3-21g opt=(ef,enonly,ts) test #T rmp2/3-21g opt=(ef,enonly,ts,restart) test
test121.com	# rqcisd(t,e4t)/gen test # rqcisd(t,fulltran)/gen test
test122.com	# uqcisd(t)/gen test guess(alter,mix) symm=noscf

	# uqcisd(t,fulltran)/gen test guess=(mix,alter) symm=noscf
test123.com	#P TEST MP4(SDTQ)/6-31G* int=intbuf=3200 tran=conv scf=conventional int=(rys1e,rys2e) guess=indo iop(3/2=582000,4/2=582000,5/2=582000,6/2=582 8/2=582000,8/10=101,9/2=582000)
test124.com	#P TEST FREQ UHF/6-31G* int=intbuf=3200 scf=conventional int=(rys1e, rys2e,berny,dsrys) guess=indo iop(3/2=583000,4/2=583000,5/2=583000, 6/2=215000,7/2=583000,8/2=583000,10/2=120000,11/2=583000)
test125.com	#p test mp4(sdtq)/6-31g* int=intbuf=3200 tran=conv iop(8/10=101) scf=conventional int=(rys1e,rys2e) guess=indo iop(3/2=870000,4/2=870000,5/2=870000,6/2=870000,8/2=870000,8/10=101,9/2=8
test130.com	#P TEST rhf/3-21G FREQ scf=qc noraff symm=noint #P TEST rhf/3-21G FREQ scf=(qc,tightlineq) raff #P TEST rhf/3-21G FREQ scf=(qc,direct)
test131.com	#P TEST FREQ UHF/3-21G scf=qc noraff symm=noint #P TEST FREQ UHF/3-21G scf=qc iop(3/11=3) #P TEST FREQ UHF/3-21G scf=(direct,qc)
test132.com	#p ump4sdtq=full/6-21G test guess=alter oldconst
test133.com	# RHF/3-21G freq test # RHF/3-21G test IRC=(rcfc,internal) geom=check guess=read
test134.com	#P TEST OPT RHF/6-31G* 5D SCF=Direct #P TEST FREQ RHF/6-31G* 5D GEOM=CHECK GUESS=READ SCF=Direct
test135.com	#P b3lyp/6-31g* test stable=(opt,qconly)
test136.com	#p rmp2/lp-31g opt test geom=modela
test137.com	#p rmp2=full/6-31G(df,p) 5d 7f force test geom=modela use=l804 tran=fulldirect iop(8/2=5000000,9/2=5000000,9/16=220) #p rmp2=(full,nodirect)/6-31G(df,p) 5d 7f test geom=modela mdv=981000 int=(rys1e,rys2e) force tran=old2pdm guess=indo iop(1/2=-1,2/2=-1) #p ump2=(full)/6-31G(df,p) 5d 7f force test geom=modela use=l804 tran=semidirect mdv=5000000 iop(1/2=-1,2/2=-1) #p ump2=(full,nodirect)/6-31G(df,p) 5d 7f test geom=modela int=(rys1e,rys2e) force tran=old2pdm guess=indo mdv=981000 iop(1/2=-1,2/2=-1)
test138.com	#P TEST OPT=CalcAll RHF/6-31G* 5D
test139.com	#p rmp2/D95(df,p) 5d 7f test geom=modela force density=curr mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(semidirect,maxdisk=6200000)/D95(df,p) 5d 7f test geom=modela fo density=curr guess=read extrabasis int=nobasistrans mdv=6500000 iop(1/2=-1,2/2=-1)

	#p rmp2=fulldirect/D95(df,p) 5d 7f test geom=modela density=curr guess=read force mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct,maxdisk=6200000)/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop(9/8=30,9/16=-8) mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct,maxdisk=6200000)/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop(9/8=20,9/16=-8) mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=semidirect=1/D95(df,p) 5d 7f test geom=modela density=curr guess=read mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2/D95(df,p) 5d 7f test geom=modela density=curr guess=read mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct)/D95(df,p) 5d 7f test geom=modela guess=read mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2/D95(df,p) 5d 7f test geom=modela guess=read mdv=6500000 iop(1/2= #p rmp2/D95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 mdv=5000000 iop(1/2=-1,2/2=-1) #p rmp2/D95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 tran=fulldirect #p rmp2/D95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 tran=semidirect extrabasis int=nobasistrans mdv=5000000 iop(1/2=-1,2/2=-1) #p rmp2=fulldirect/D95(df,p) 5d 7f test geom=modela density=curr guess=read force iop1=nopacksort mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct,maxdisk=6200000)/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop(9/8=30,9/16=-8) iop1=nopacksort mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct,maxdisk=6200000)/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop(9/8=20,9/16=-8) iop1=nopacksort mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=semidirect=1/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop1=nopacksort mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2/D95(df,p) 5d 7f test geom=modela density=curr guess=read iop1=nopacksor mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2=(direct)/D95(df,p) 5d 7f test geom=modela iop1=nopacksor guess=read mdv=6500000 iop(1/2=-1,2/2=-1) #p rmp2/D95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 iop1=nopacksort mdv=5000000 iop(1/2=-1,2/2=-1)
test140.com	#p rmp2=full/3-21g test polar scf=direct #p rmp2=full/3-21g polar=enonly test scf=direct #p rmp2=full/3-21g polar=(enonly,restart) test scf=direct

test141.com	#P ump4(fc)/6-31g* test
test142.com	#p rmp2=(direct,full)/3-21g test polar #p rmp2=(direct,full)/3-21g polar=enonly test #p rmp2=(direct,full)/3-21g polar=(enonly,restart) test
test143.com	#p rcis(icdiag,nstates=10) iop(9/23=1) tran=iabc test #p rcis(mo,root=4,50-50) geom=checkpoint guess=read iop(9/23=1) test tra #p rcis=(ao,50-50) geom=checkpoint guess=read test #p rcis=(direct,50-50) geom=checkpoint guess=read test #p rcis=direct geom=checkpoint guess=read test #p rcis=(direct,triplet) geom=checkpoint guess=read test
test144.com	#p ucis(mo,nstates=4) iop(9/23=1) test tran=iabc #p ucis(mo,read,root=4) iop(9/23=1) geom=checkpoint guess=read tran=iabc
test145.com	#p rcis=(nstate=3,mo,50-50,maxdavidson=14) test iop(9/43=-1) #p rcis=(nstate=8) geom=checkpoint test #p rcis=(root=8,direct,triplet) geom=checkpoint test guess=read
test146.com	#p 6-31G* ucis=(icdiag,alltrans) iop(9/23=1) test tran=iabc #P UHF/6-31G* CIS=mo TEST #P ucis=ao/6-31G* TEST #P ucis=direct/6-31G* TEST
test147.com	#P rcis=(mo,full)/6-31G* FORCE DENSITY=ALL POPU=FULL test #p rcis=(ao,full)/6-31g* force density=all popu=full geom=check test guess=read #p scf(direct) rcis=full/6-31g* force density=all popu=full geom=check test guess=read
test148.com	#P RCIS(MO,full) OPT TEST #P RCIS(AO,ALLTRANS,full) OPT GEOM=CHECK GUESS=READ DENSITY=ALL POP=REG TEST scf=conventional #P SCF(DIRECT) RCIS=full OPT GEOM=CHECK GUESS=READ TEST
test149.com	#P RCIS=full FREQ TEST
test150.com	#P rcis=(alltrans,50-50) sto-3g iop33(9=3) test #P sto-3g stable=repopt test #P test geom=check guess=read uhf/sto-3g stable use=1902 #P ucis=alltrans sto-3g iop33(9=3) test geom=check guess=read
test151.com	#P rhf/sto-3g test force #P rhf/sto-3g test force guess=read
test152.com	#p rhf/6-31g* test #p rhf/6-31g* guess=(read,local,lowsym,only) test
test153.com	#p scan rcis(icdiag) iop(9/23=1) test tran=iabc
test154.com	#P RHF/4-31G NOPOP NAME=INTQN test int=nosp scf=conventional

	#P RHF/4-31G NOPOP NAME=INTQN test geom=check guess=read int=rys2e scf=conventional #P RHF/4-31G NOPOP NAME=INTQN test geom=check guess=read scf=(direct,nofinal,tight)
test155.com	#p 6-31+G* freq rcis(full,mo) test #p 6-31+G* force rcis(mo,full) guess(read) geom(check) test #p 6-31+G* force rcis(ao,read,full) guess(read) geom(check) test #p 6-31+G* force scf(direct) rcis(read,full) guess(read) geom(check)test #p 6-31+G* force int(berny,dsrys) rcis(ao,read,full) guess(read)test geo
test156.com	#p 6-31+G* freq rcis(full,mo,triplet,root=4,nstates=6) test #p 6-31+G* force rcis(mo,triplet,root=4,nstates=6,full) guess(read) geom(check) test #p 6-31+G* force rcis(ao,read,root=4,nstates=6,full) guess(read) geom(check) test #p 6-31+G* force scf(direct) rcis(read,root=4,nstates=6,full) geom(check) test guess(read) #p 6-31+G* force int(berny,dsrys) rcis(ao,read,root=4,nstates=6,full) guess(read) geom(check) test
test157.com	#p 6-31+G* force ucis(full,icdiag,root=3,nstates=8) test #p 6-31+G* force ucis(mo,root=3,nstates=8,full) guess(read) geom(check) test #p 6-31+G* force ucis(ao,root=3,read,full) guess(read) geom(check) test #p 6-31+G* force scf(direct) ucis(read,root=3,full) guess(read) geom(check) test tran=iabc #p 6-31+G* force int(berny,dsrys) ucis(ao,read,root=3,full) guess(read) geom(check) test
test158.com	#P UCIS=full force 6-31G(df,p) 5d 7f TEST density=curr mdv=4000000 iop(1 #P UCIS=(ao,full) Force 6-31G(df,p) 5d 7f geom(check) guess(read) TEST int=(berny,dsrys) density=curr #P UCIS=(noincore,read,direct,full) Force 6-31G(df,p) 5d 7f geom(check) guess(read) TEST density=curr
test159.com	#p ump2=direct/d95(df,p) 5d 7f test geom=modela force density=curr extrabasis int=nobasistrans mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(semidirect,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela sc force density=curr guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(fulldirect)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(direct,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop(9/8=30,9/16=-8) mdv=7000000 iop(1/2=-1,2/2=- #p ump2=(direct,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop(9/8=20,9/16=-8) mdv=7000000 iop(1/2=-1,2/2=-

	#p ump2=(semidirect=1)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=semidirect/d95(df,p) 5d 7f test geom=modela density=curr guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(direct)/d95(df,p) 5d 7f test geom=modela guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=direct/d95(df,p) 5d 7f test geom=modela guess=read mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2/d95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 mdv=5000000 iop(1/2=-1,2/2=-1) #p ump2/d95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 tran=fulldirect #p ump2/d95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 tran=semidirect extrabasis int=nobasistrans mdv=5000000 iop(1/2=-1,2/2=-1) #p ump2=(semidirect,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela sc force density=curr guess=read iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2 #p ump2=(fulldirect)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(direct,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop(9/8=30,9/16=-8) iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(direct,maxdisk=6200000)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop(9/8=20,9/16=-8) iop1=nopacksort mdv=7000000 i #p ump2=(semidirect=1)/d95(df,p) 5d 7f test geom=modela force density=curr guess=read iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=semidirect/d95(df,p) 5d 7f test geom=modela density=curr guess=read iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=(direct)/d95(df,p) 5d 7f test geom=modela guess=read iop1=nopacksort mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2=direct/d95(df,p) 5d 7f test geom=modela guess=read iop1=nopackso mdv=7000000 iop(1/2=-1,2/2=-1) #p ump2/d95(df,p) 5d 7f test geom=modela guess=read force density=curr use=l804 iop1=nopacksort mdv=5000000 iop(1/2=-1,2/2=-
test160.com	#p cas(2,2)/6-31g** test scf=conventional force iop(5/5=5) guess=alter #p cas(2,2)/6-31g** test scf=conventional force guess=alter #p cas(2,2)/6-31g** test scf=incore force guess=alter #p cas(2,2)/6-31g** test force iop(5/5=2) guess=alter scf=noincore #p cas(2,2)/6-31g** test force iop(5/5=3) guess=alter #p cas(2,2,lanczos)/6-31g** test force iop(4/43=1) guess=alter
test161.com	#p uhf/sto-3g test pop=full scf=conventional guess=mix #p cas(4,uno,4,qc)/sto-3g test scf=conventional pop=full guess=read

test162.com	#p cas(4,4)/sto-3g test opt=(ts,z-matrix) guess=cards nosymm
test163.com	#p rqcisd=full/3-21g force test density=curr #p rqcisd=full/3-21g force test density=curr scf=direct
test164.com	#p cas(6,6)/6-31g* geom=modela test force pop=npa #p cas(6,6)/6-31g* geom=modela test force scf=direct pop=nbo #p cas(6,6)/6-31g* geom=modela test force scf=noincore
test165.com	#P RCIS TEST #P RCIS(read,add=9) guess=read geom=checkpoint test #P RCIS(root=7,read) Fopt=z-matrix guess=read geom=checkpoint test #P RCIS(root=7,read) guess=read geom=modify opt=z-matrix test
test166.com	#p scf=(tight,novaracc) uhf/6-31g* pop=nbodel test
test167.com	#p scf=(tight,novaracc) rhf/6-31g* test pop=nbodel
test168.com	#p rhf/sto-3g opt=ef pop=nbodel test
test169.com	#p uhf/sto-3g opt pop=nbodel test
test170.com	#P freq=noraman NOSYMM TEST uhf #P IRC=(STEPSIZE=5,READCARTESIANFC,READISOTOPES,MAXPOINTS=2) NOSYMM TEST uhf iop1=synch
test171.com	#P IRC=(STEPSIZE=5,calcfc,internal,MAXPOINTS=2) NOSYMM TEST uhf iop1=synch #P IRC=(STEPSIZE=5,calcfc,internal,MAXPOINTS=2,restart) NOSYMM TEST uhf iop1=synch
test172.com	#P IRC=(STEPSIZE=5,calcfc,cartesian,MAXPOINTS=2) NOSYMM TEST uhf iop1=synch
test175.com	# HF/6-31G* Test Geom=Connect

test176.com	#p rhf/chkbas geom=check freq=readfc
	#p rhf/chkbas guess=(check,only) density=(current,check) pop=full
	geom=check
	#p rhf/chkbas geom=check guess=read opt=readfc

test177.com	#P TEST RCCD/4-31G force density=curr
test178.com	#P RHF/6-31G** test pop=npa prop=fit
test179.com	#p rhf/lp-31G* 5d 10f force test geom=modela
test180.com	#p rhf/genecp 5d 7f test scf=tight geom=modela #p rhf/chkbas guess=read geom=check test scf=tight #p rhf/gen pseudo=old 5d 7f test scf=tight geom=modela #p rhf/gen pseudo=read 5d 7f test scf=tight geom=modela
test181.com	#p rhf/sto-3g scrf=(dipole,dielectric=80.0,a0=1.6) test geom=modela #p rhf/sto-3g scrf=(a0=1.6,dipole,dielectric=80.0) test geom=modela scf=

test182.com	#p uhf/sto-3g scrf=dipole test geom=modela #p uhf/sto-3g scrf=dipole test geom=modela scf=qc
test183.com	#p rhf/sto-3g scrf=dipole opt test #p rhf/sto-3g scrf=dipole opt test scf=qc
test184.com	#p rqcisd/3-21g scrf=dipole test iop1=synch #p rqcisd/3-21g scrf=(dipole,restart) test iop1=synch
test185.com	#p uhf/3-21g scrf=dipole test geom=modela #p ump2/3-21g scrf=(dipole,numer,chk) test geom=check guess=check
test186.com	# rbd/gen test # rbd(t)=fulltran/gen test # rbd(t)/gen test # rbd(t)/gen test scf=direct
test187.com	# ubd(t)/gen test guess(mix,alter) symm=noscf iop1=synch
test188.com	# ubd(t)/3-21g test iop1=synch # ubd(t)=fulltran/3-21g test iop1=synch scf=direct # ubd/3-21g test iop1=synch scf=direct
test189.com	#p rcndo test force #p rindo test force geom=check #p rmindo test force geom=check #p rmndo use=l402 test force geom=check #p ram1 use=l402 test force geom=check #p rpm3 use=l402 test force geom=check #p rpm3mm use=l402 test force geom=check #p int=mndo test force geom=check #p int=am1 test force geom=check #p int=pm3 test force geom=check #p int=pm3mm test force geom=check
test190.com	#p rqcisd/6-31g* 5d geom=modela test iop1=synch #p rqcisd(t)/6-31g* 5d geom=modela test iop1=synch
test191.com	#p uqcisd/6-31g* 5d geom=modela test iop1=synch #p uqcisd(t)/6-31g* 5d geom=modela test iop1=synch

test192.com	#p ump4/6-31g(df,p) 5d 7f test geom=modela trans=(incore,full)
	guess=mix mdv=5000000 iop(1/2=-1,2/2=-1)
	#p ump4=noincore/6-31g(df,p) 5d 7f test geom=modela scf=nopass
	trans=incore guess=read scf=nosymm mdv=5000000 iop(1/2=-1,2/2=-1)
	#p ump4/6-31g(df,p) 5d 7f test geom=modela trans=conventional guess=read
	scf=nosymm mdv=2000000 iop(1/2=-1,2/2=-1)
	#p ump4/6-31g(df,p) 5d 7f test geom=modela trans=fulldirect guess=read
	scf=nosymm mdv=3500000 iop(1/2=-1,2/2=-1)
	#p ump4/6-31g(df,p) 5d 7f test geom=modela trans=semidirect guess=read

	scf=nosymm mdv=4000000 iop(1/2=-1,2/2=-1)
test193.com	#p mp5/3-21g test geom=modela scf=direct iop1=synch
test194.com	#p uqcisd(tq)/gen test guess(mix,alter) symm=noscf iop1=synch
test195.com	#p bd(tq)/3-21g test iop1=synch scf=direct
test196.com	#p rmp3/6-31g* geom=modela test iop(8/9=3030)
test197.com	#p ump3/6-31g* geom=modela test iop(8/9=3030)
test198.com	#p rmp3=maxdisk=18000000/6-31g** test mdv=2000000 iop(1/2=-1,2/2=-1) #p rmp3=maxdisk=18000000/6-31g** test iop1=nopacksort mdv=2000000 iop(1/
test199.com	#p ump3/6-31g** maxdisk=12000000 test mdv=2000000 iop(1/2=-1,2/2=-1) #p ump3/6-31g** maxdisk=13000000 test iop1=nopacksort mdv=2000000 iop(1/
计算输入档	**计算执行路径**
test200.com	#p rhf/3-21g test geom=modela pop=mk #p rhf/3-21g pop=(mk,dipole) test geom=modela #p rhf/3-21g pop=(mk,atomdipole) test geom=modela #p rhf/3-21g test geom=modela pop=chelp #p rhf/3-21g test geom=modela pop=chelpg #p rhf/3-21g test geom=modela pop=(chelpg,readrad) #p rhf/3-21g test geom=modela pop=(chelpg,readatrad)
test201.com	#p test ucid/6-31g* density=curr #p test ucid/6-31g* density=curr force #p test ucisd/6-31g* density=curr #p test ucisd/6-31g* density=curr force #p test uccd/6-31g* density=curr #p test uccd/6-31g* density=curr force #p test uqcisd/6-31g* density=curr #p test uqcisd/6-31g* density=curr force
test202.com	#p cisd/3-21g test polar iop1=synch #p cisd/3-21g polar=(restart) test iop1=synch
test203.com	#p qcisd/6-31g* fopt=tight geom=modela iop1=synch tran=incore test #p qcisd/6-31g* freq polar geom=check guess=read iop1=synch tran=incore #p qcisd/6-31g* freq=restart polar geom=check guess=read iop1=synch tran
test204.com	#p rcid=full/3-21g freq=enonly geom=(modela,print) test iop1=synch
test205.com	#p cisd/3-21g test polar=enonly iop1=synch #p cisd/3-21g polar=(enonly,restart) test iop1=synch
test206.com	#p rmp2/3-21g freq=numer test iop1=synch #p rmp2/3-21g freq=(numer,restart) test iop1=synch
test207.com	#p rmp2/3-21g freq=enonly test iop1=synch #p rmp2/3-21g freq=(enonly,restart) test iop1=synch

test208.com	#p stable=icdiag/3-21g geom=modela test #p stable=mo/3-21g geom=modela iop1=synch test #p stable=ao/3-21g geom=modela iop1=synch test #p stable=direct/3-21g geom=modela iop1=synch test #p stable=(direct,noincore)/3-21g geom=modela iop1=synch test #p rhf/3-21g geom=modela iop1=synch test stable nosymm use=l902
test209.com	#p stable=icdiag/3-21g geom=modela test #p stable=mo/3-21g geom=modela iop1=synch test #p stable=ao/3-21g geom=modela iop1=synch test #p stable=direct/3-21g geom=modela iop1=synch test #p stable=(direct,noincore)/3-21g geom=modela iop1=synch test #p uhf/3-21g geom=modela iop1=synch test stable nosymm use=l902

test210.com	#p rhf/3-21G fopt scf=incore test mdv=4000000 iop(1/2=-1,2/2=-1)
	#p rhf/6-31g* fopt=readfc scf=direct guess=read geom=check test
	mdv=2000000 iop(1/2=-1,2/2=-1)

test211.com	# SP, RHF/STO-3G punch=archive trakio scf=conventional
test212.com	#p uhf sto-3g freq test scrf
test213.com	#p rhf 6-311g** freq test scrf scf=direct
test214.com	#p rhf/sto-3g scrf freq=(numer,step=5) test
test215.com	#p rhf sto-3g polar scrf test
test216.com	#p rhf sto-3g polar=numer test scrf
test217.com	#p rhf sto-3g polar=enonly scrf test
test218.com	#p rhf/sto-3g scrf freq=numer polar
test219.com	#p rhf 6-31g** freq test scrf 5d cphf=mo
test220.com	#p rhf sto-3g freq=(cubic,step=10) scrf test

test221.com	#p uhf/6-31g(df,p) 5d 7f scrf opt=tight geom=modela test mdv=3600000 iop
	#p uhf/6-31g(df,p) 5d 7f scrf freq scf=(incore,pass) geom=check guess=rea
	test mdv=8000000 iop(1/2=-1,2/2=-1)
	#p uhf/6-31g(df,p) 5d 7f scrf freq scf=noincore geom=check guess=read tes
	iop(1/2=-1,2/2=-1)
	#p uhf/6-31g(df,p) 5d 7f scrf freq geom=check guess=read test mdv=8000000 i
	#p uhf/6-31g(df,p) 5d 7f scrf freq geom=check guess=read cphf=mo
	test mdv=8000000 iop(1/2=-1,2/2=-1)

test222.com	#p rmp2/3-21g density=curr test geom=modela iop1=synch use=1804 #p ump2/3-21g density=curr test geom=modela iop1=synch use=1804 #p ump2/3-21g density=curr test geom=modela iop1=synch use=1804 #p ump2/3-21g density=curr test geom=modela iop1=synch use=1804 #p rmp2/3-21g density=curr test geom=modela iop1=synch

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#p ump2/3-21g density=curr test geom=modela iop1=synch
#p ump2/3-21g density=curr test geom=modela iop1=synch
#p ump2/3-21g density=curr test geom=modela iop1=synch
#p rmp2/3-21g force density=curr test geom=modela iop1=synch use=l804
#p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804
#p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804
#p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804
#p rmp2/3-21g force density=curr test geom=modela iop1=synch
#p ump2/3-21g force density=curr test geom=modela iop1=synch
#p ump2/3-21g force density=curr test geom=modela iop1=synch
#p ump2/3-21g force density=curr test geom=modela iop1=synch
#p rcid/3-21g density=curr test geom=modela iop1=synch
#p ucid/3-21g density=curr test geom=modela iop1=synch
#p ucid/3-21g density=curr test geom=modela iop1=synch
#p ucid/3-21g density=curr test geom=modela iop1=synch
#p rcid/3-21g force density=curr test geom=modela iop1=synch
#p ucid/3-21g force density=curr test geom=modela iop1=synch
#p ucid/3-21g force density=curr test geom=modela iop1=synch
#p ucid/3-21g force density=curr test geom=modela iop1=synch
#p rcisd/3-21g density=curr test geom=modela iop1=synch
#p ucisd/3-21g density=curr test geom=modela iop1=synch
#p ucisd/3-21g density=curr test geom=modela iop1=synch
#p ucisd/3-21g density=curr test geom=modela iop1=synch
#p rcisd/3-21g force density=curr test geom=modela iop1=synch
#p ucisd/3-21g force density=curr test geom=modela iop1=synch
#p ucisd/3-21g force density=curr test geom=modela iop1=synch
#p ucisd/3-21g force density=curr test geom=modela iop1=synch
#p rccd/3-21g density=curr test geom=modela iop1=synch
#p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1)
#p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1)
#p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1)
#p rccd/3-21g force density=curr test geom=modela iop1=synch
#p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1)
#p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1)
#p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1)
#p rqcisd/3-21g density=curr test geom=modela iop1=synch
#p uqcisd/3-21g density=curr test geom=modela iop1=synch
#p uqcisd/3-21g density=curr test geom=modela iop1=synch
#p uqcisd/3-21g density=curr test geom=modela iop1=synch
#p rqcisd/3-21g force density=curr test geom=modela iop1=synch
#p uqcisd/3-21g force density=curr test geom=modela iop1=synch
#p uqcisd/3-21g force density=curr test geom=modela iop1=synch
#p uqcisd/3-21g force density=curr test geom=modela iop1=synch
#p rccsd/3-21g density=curr test geom=modela iop1=synch
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	#p uccsd/3-21g density=curr test geom=modela iop1=synch #p uccsd/3-21g density=curr test geom=modela iop1=synch #p uccsd/3-21g density=curr test geom=modela iop1=synch #p rccsd/3-21g force density=curr test geom=modela iop1=synch #p uccsd/3-21g force density=curr test geom=modela iop1=synch #p uccsd/3-21g force density=curr test geom=modela iop1=synch #p uccsd/3-21g force density=curr test geom=modela iop1=synch
test223.com	#p rhf/sto-3g opt=coord test #p rhf/sto-3g opt geom=(coord,check,step=4) test #p rhf/sto-3g freq geom=check test mdv=2000000 iop(1/2=-1,2/2=-1)
test224.com	#p rhf/sto-3g opt=(cartes,calcall) test mdv=2000000 iop(1/2=-1,2/2=-1) #p rhf/sto-3g opt=(cartes,restart,calcall) test mdv=2000000 iop(1/2=-1,2
test225.com	#p rhf/sto-3g opt=(z-matrix,calcfc) test #p rhf/sto-3g test geom=check guess=read #p rhf/sto-3g scf=tight test geom=modify guess=read

test226.com	#p rmp2=incore/d95 test force mdv=5000000 iop(1/2=-1,2/2=-1)
	#p rmp2=fulldirect/d95 test force scf=incore mdv=3000000 iop(1/2=-1,2/2=
	#p rmp2=semidirect/d95 test force scf=incore mdv=3000000 iop(1/2=-1,2/2=
	#p rmp2=semidirect=4/d95 test force scf=incore iop(9/8=20) mdv=3000000 i
	#p rmp2=semidirect=3/d95 test nosymm force scf=incore iop(9/16=-4) mdv=3
	iop(1/2=-1,2/2=-1)
	#p rmp2/d95 test nosymm force scf=incore use=l804 mdv=3000000 iop(1/2=-1
	#p rmp2/d95 test nosymm force scf=incore use=l804 iop(11/17=-1) mdv=3000
	iop(1/2=-1,2/2=-1)

test227.com	#p ump2=incore/d95 test force mdv=5000000 iop(1/2=-1,2/2=-1)
	#p ump2=fulldirect/d95 test force scf=incore mdv=4000000 iop(1/2=-1,2/2=
	#p ump2=semidirect/d95 test force scf=incore mdv=4000000 iop(1/2=-1,2/2=
	#p ump2=semidirect=4/d95 test force scf=incore iop(9/8=20) mdv=4000000 i
	#p ump2=semidirect=3/d95 test nosymm force scf=incore iop(9/16=-4) mdv=4
	iop(1/2=-1,2/2=-1)
	#p ump2/d95 test nosymm force scf=incore use=l804 mdv=4000000 iop(1/2=-1
	#p ump2/d95 test nosymm force scf=incore use=l804 iop(11/17=-1) mdv=4000
	iop(1/2=-1,2/2=-1)

test228.com	#p rcis=(singlet,root=2)/d95 test force scf=incore mdv=2000000 iop(1/2=-
	#p rcis=(triplet,root=3,nstate=5,readwindow)/d95 test force scf=incore
	mdv=2000000 iop(1/2=-1,2/2=-1)

test229.com	#p ucis=incore/d95 test force scf=incore #p ucis=(root=2,nstate=5,readwindow)/d95 test force extrabasis int=nobas
test230.com	#p rmp2=stingy/d95(df,p) test freq
test231.com	#p ump2/d95(df,p) test freq scf=direct

test232.com	#p rhf/6-31g** volume test scf=(direct,tight) #p rhf/6-31g** volume=tight test scf=(direct,tight) #p rhf/6-31g** volume=tight iop(6/47=80) test scf=(direct,tight)
test233.com	#p rmp2/3-21g density=curr test geom=modela iop1=synch use=l804 iop(11/1 #p ump2/3-21g density=curr test geom=modela iop1=synch use=l804 iop(11/1 #p ump2/3-21g density=curr test geom=modela iop1=synch use=l804 iop(11/1 #p ump2/3-21g density=curr test geom=modela iop1=synch use=l804 iop(11/1 #p rmp2/3-21g density=curr test geom=modela iop1=synch #p ump2/3-21g density=curr test geom=modela iop1=synch #p ump2/3-21g density=curr test geom=modela iop1=synch #p ump2/3-21g density=curr test geom=modela iop1=synch #p rmp2/3-21g force density=curr test geom=modela iop1=synch use=l804 io #p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804 io #p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804 io #p ump2/3-21g force density=curr test geom=modela iop1=synch use=l804 io #p rmp2/3-21g force density=curr test geom=modela iop1=synch #p ump2/3-21g force density=curr test geom=modela iop1=synch #p ump2/3-21g force density=curr test geom=modela iop1=synch #p ump2/3-21g force density=curr test geom=modela iop1=synch #p rcid/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucid/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucid/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucid/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p rcid/3-21g force density=curr test geom=modela iop1=synch iop(11/17=1 #p ucid/3-21g force density=curr test geom=modela iop1=synch iop(11/17=1 #p ucid/3-21g force density=curr test geom=modela iop1=synch iop(11/17=1 #p ucid/3-21g force density=curr test geom=modela iop1=synch iop(11/17=1 #p rcisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p ucisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p rcisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p ucisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p ucisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p ucisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p rccd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1) iop(1 #p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1) iop(1 #p uccd/3-21g density=curr test geom=modela iop1=synch iop(9/19=1) iop(1 #p rccd/3-21g force density=curr test geom=modela iop1=synch iop(11/17=1 #p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1) #p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1) #p uccd/3-21g force density=curr test geom=modela iop1=synch iop(9/19=1)

	#p rqcisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uqcisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uqcisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uqcisd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p rqcisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17 #p uqcisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17 #p uqcisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17 #p uqcisd/3-21g force density=curr test geom=modela iop1=synch iop(11/17 #p rccsd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uccsd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uccsd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p uccsd/3-21g density=curr test geom=modela iop1=synch iop(11/17=1) #p rccsd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p uccsd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p uccsd/3-21g force density=curr test geom=modela iop1=synch iop(11/17= #p uccsd/3-21g force density=curr test geom=modela iop1=synch iop(11/17=
test234.com	#P uccsd(t,e4t)/gen test tran=iabc #P uccsd/gen test
test235.com	#P uccsd(t,e4t)/gen test tran=iabc #P uccsd/gen test
test236.com	#p RHF/3-21G freq test #p RHF/3-21G test IRC=(RCFC,internal) geom=check guess=read #p RHF/3-21G test IRC=(RESTART,internal,maxpoints=8) geom=check guess=rea #p RHF/3-21G test IRC=(RESTART,internal,maxpoints=9) geom=check guess=rea #p RHF/3-21G test IRC=(RESTART,internal,maxpoints=11) geom=check guess=r
test237.com	#p rhf/sto-3g test pop=(chelpg,readrad)
test238.com	#p rmp2(full)/3-21g freq test #p rmp2(full)/3-21g freq test scf=incore #p rmp2(full,stingy)/3-21g freq test scf=incore #p rmp2(full)/3-21g freq test scf=incore iop(8/23=3,11/13=22221) #p rmp2(full)/3-21g freq test scf=incore iop(8/23=3,11/13=20302) #p rmp2(full)/3-21g freq test scf=incore iop(8/23=3,8/18=2) #p rmp2(full)/3-21g freq test scf=incore iop(8/18=2)
test239.com	#p ump2(full)/3-21g freq test #p ump2(full)/3-21g freq test scf=incore #p ump2(full,stingy)/3-21g freq test scf=incore #p ump2(full)/3-21g freq test scf=incore iop(8/23=3,11/13=22221) #p ump2(full)/3-21g freq test scf=incore iop(8/23=3,11/13=20302) #p ump2(full)/3-21g freq test iop(8/23=3,8/18=2) #p ump2(full)/3-21g freq test iop(8/18=2)
test240.com	#p test rmp2=stingy/6-31g* freq scf=direct mdv=5000000 iop(1/2=-1,2/2=-1

test241.com	#p test ump2=stingy/6-31g* freq scf=direct mdv=5000000 iop(1/2=-1,2/2=-1)
test242.com	#p rhf/3-21g freq test
test243.com	#p rhf/3-21g freq test #p rhf/6-31g* opt=rcfc geom=(check,coord) test
test244.com	#p rhf/3-21g freq test #p rhf/6-31g* opt=rcfc geom=(check,coord) nosymm test
test245.com	#p rhf/3-21g freq test nosymm #p rhf/6-31g* opt=(cart,rcfc) geom=check nosymm test
test246.com	#p rhf/3-21g freq test nosymm #p rhf/3-21g opt=rcfc geom=(check,coord) nosymm test
test247.com	#p rhfs/6-31G(df,p) 5d 7f test geom=modela force #p rxalpha/6-31G(df,p) 5d 7f test geom=modela force #p rhfb/6-31G(df,p) 5d 7f test geom=modela force #p rsvwn5/6-31G(df,p) 5d 7f test geom=modela force #p rxavwn5/6-31G(df,p) 5d 7f test geom=modela force #p rbvwn5/6-31G(df,p) 5d 7f test geom=modela force scf=conventional #p rbvwn5/6-31G(df,p) 5d 7f test geom=modela scf=incore force mdv=6000000 i #p rbvwn5/6-31G(df,p) 5d 7f test geom=modela force #p rslyp/6-31G(df,p) 5d 7f test geom=modela force #p rxalyp/6-31G(df,p) 5d 7f test geom=modela force #p rblyp/6-31G(df,p) 5d 7f test geom=modela force #p rlsda/6-31G(df,p) 5d 7f test geom=modela force #p rbvwn/6-31G(df,p) 5d 7f test geom=modela force
test248.com	#p uhfs/6-31G(df,p) 5d 7f test geom=modela force #p uxalpha/6-31G(df,p) 5d 7f test geom=modela force #p uhfb/6-31G(df,p) 5d 7f test geom=modela force #p usvwn5/6-31G(df,p) 5d 7f test geom=modela force scf=conventional #p uxavwn5/6-31G(df,p) 5d 7f test geom=modela force #p ubvwn5/6-31G(df,p) 5d 7f test geom=modela force #p ubvwn5/6-31G(df,p) 5d 7f test geom=modela scf=incore force mdv=7000000 i #p ubvwn5/6-31G(df,p) 5d 7f test geom=modela force #p uslyp/6-31G(df,p) 5d 7f test geom=modela force #p uxalyp/6-31G(df,p) 5d 7f test geom=modela force #p ublyp/6-31G(df,p) 5d 7f test geom=modela force #p ulsda/6-31G(df,p) 5d 7f test geom=modela force #p ubvwn/6-31G(df,p) 5d 7f test geom=modela force
test249.com	#p rmp2(full)/3-21g freq nosymm test geom=modela #p rmp2(full)/3-21g freq nosymm test geom=modela iop(8/18=2)
test250.com	#p rmp2(fc)/3-21g freq nosymm test geom=modela
test251.com	#p ump2(full)/3-21g freq nosymm test

	#p ump2(full)/3-21g freq nosymm test iop(8/18=2)
test252.com	#p ump2(fc)/3-21g freq nosymm test
test253.com	#p ump2(fc)/3-21g freq nosymm test #P TEST FORCE rqcisd(full)/6-31G* 5d density=curr iop(11/17=1)
test254.com	#P TEST uqcisd(full)/6-31G* 5d Force density=curr #P TEST uqcisd(full)/6-31G* 5d Force density=curr iop(11/17=1)
test257.com	#p rhf/6-31g* 5d test geom=modela scf=tight cube=(density,read)
test258.com	#p rb3lyp/3-21g scrf geom=modela force test
test259.com	#p ublyp/3-21g vshift=50 scrf geom=modela scfcyc=128 force test
test260.com	#p rmp3/d95(d,p) force test
test261.com	#p ump3/d95(d,p) force test
test262.com	#p ump4/3-21g polar test geom=modela #p ump4/3-21g polar=restart test geom=modela int=reuse
test263.com	#p rmp3/3-21g density=curr test geom=modela iop1=synch #p ump3/3-21g density=curr test geom=modela iop1=synch #p ump3/3-21g density=curr test geom=modela iop1=synch #p ump3/3-21g density=curr test geom=modela iop1=synch #p rmp3/3-21g force density=curr test geom=modela iop1=synch #p ump3/3-21g force density=curr test geom=modela iop1=synch #p ump3/3-21g force density=curr test geom=modela iop1=synch #p ump3/3-21g force density=curr test geom=modela iop1=synch
test264.com	#p rhfs/3-21g geom=modela test freq Int=Grid=99302 scf=conventional #p rhfs/3-21g geom=modela test freq Int=Grid=99302 scf=incore #p rhfs/3-21g geom=modela test freq Int=Grid=99302 scf=noincore
test265.com	#p uhfs/3-21g geom=modela test freq Int=Grid=99302 #p uhfs/3-21g geom=modela test freq Int=Grid=99302 scf=incore #p uhfs/3-21g geom=modela test freq Int=Grid=99302 scf=noincore
test266.com	#P RHF/4-31G SCRF=OldPCM scf=tight Test nosymm iop(1/43=100)
test267.com	#p ublyp/3-21g geom=modela test freq Int=Grid=99302 #p ublyp/3-21g geom=modela test freq #p ublyp/3-21g geom=modela test freq scf=incore #p ublyp/3-21g geom=modela test freq scf=noincore
test268.com	#p ublyp/6-31g(df,p) 6d 10f geom=modela test freq Int=Grid=99302 scf=conventional mdv=9000000 iop(1/2=-1,2/2=-1) #p ublyp/6-31g(df,p) 6d 10f geom=modela test freq guess=read scf=conventional mdv=9000000 iop(1/2=-1,2/2=-1) #p ublyp/6-31g(df,p) 6d 10f geom=modela test freq scf=incore guess=read mdv=10000000 iop(1/2=-1,2/2=-1)

	#p ublyp/6-31g(df,p) 6d 10f geom=modela test freq scf=noincore guess=rea
	mdv=9000000 iop(1/2=-1,2/2=-1)

test269.com	#P UMP2/3-21g TEST SCRF=(numer,hexadecapole) SCF=Tight #P UMP2/3-21g TEST SCRF=(numer,hexadecapole) NOSYMM SCF=Tight
test270.com	#p rmp4dq=full/d95 density=curr test geom=modela #p rmp4dq=full/d95 force density=curr test geom=modela #p rmp4dq/d95 density=curr test geom=modela #p rmp4dq/d95 force density=curr test geom=modela #p rmp4sdq=full/d95 density=curr test geom=modela #p rmp4sdq=full/d95 force density=curr test geom=modela #p rmp4sdq/d95 density=curr test geom=modela #p rmp4sdq/d95 force density=curr test geom=modela
test271.com	#p ump4dq=full/3-21g density=current test #p ump4dq=full/3-21g force density=current test #p ump4dq/3-21g density=current test #p ump4dq/3-21g force density=current test #p ump4sdq=full/3-21g density=current test #p ump4sdq=full/3-21g force density=current test #p ump4sdq/3-21g density=current test #p ump4sdq/3-21g force density=current test
test272.com	#p rmp4dq/3-21g density=curr test geom=modela #p ump4dq/3-21g density=curr test geom=modela #p ump4dq/3-21g density=curr test geom=modela #p ump4dq/3-21g density=curr test geom=modela #p rmp4dq/3-21g force density=curr test geom=modela #p ump4dq/3-21g force density=curr test geom=modela #p ump4dq/3-21g force density=curr test geom=modela #p ump4dq/3-21g force density=curr test geom=modela #p rmp4sdq/3-21g density=curr test geom=modela #p ump4sdq/3-21g density=curr test geom=modela #p ump4sdq/3-21g density=curr test geom=modela #p ump4sdq/3-21g density=curr test geom=modela #p rmp4sdq/3-21g force density=curr test geom=modela #p ump4sdq/3-21g force density=curr test geom=modela #p ump4sdq/3-21g force density=curr test geom=modela #p ump4sdq/3-21g force density=curr test geom=modela

test273.com	#P UHF/STO-3G TEST SCF(InCore,Tight) SCRF=NUMER vshift iop(1/7=7)
	#P UHF/STO-3G TEST SCF(InCore,Tight) SCRF=(NUMER,quadrupole) vshift
	geom=check guess=read iop(1/7=7)
	#P UHF/STO-3G TEST SCF(InCore,Tight) SCRF=(NUMER,octapole) vshift
	geom=check guess=read iop(1/7=7)
	#P UHF/STO-3G TEST SCF(InCore,Tight) SCRF=(NUMER,hexadecapole) vshift

	geom=check guess=read iop(1/7=7)
	#P UHF/STO-3G TEST SCF(InCore,Tight) SCRF=(NUMER,hexadecapole,restart)
	geom=check guess=read iop(1/7=7) vshift

test274.com	#p rqcisd/6-31g** test mdv=4000000 iop(1/2=-1,2/2=-1)
test275.com	#p uqcisd/6-31g** test mdv=4000000 iop(1/2=-1,2/2=-1)

test276.com	#p rhfs/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rxalpha/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rhfb/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rxavwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rbvwn5/6-31G(df,p) 5d 7f test geom=modela scf=incore freq
	iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rbvwn5/6-31G(df,p) 5d 7f test geom=modela scf=direct freq
	iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rslyp/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rxalyp/6-31G(df,p) 5d 7f test geom=modela freq
	iop(3/76=0750002500,11/43=2) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rblyp/6-31G(df,p) 5d 7f test geom=modela freq
	iop(3/76=0750002500,11/43=2) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rlsda/6-31G(df,p) 5d 7f test geom=modela freq
	iop(3/76=0750002500,11/43=2) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p rbvwn/6-31G(df,p) 5d 7f test geom=modela freq
	iop(3/76=0750002500,11/43=2) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(10
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq nosymm scf=noincore
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1,10/29=3) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq iop(10/31=1) fmm
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq
	iop(10/29=2,10/31=1) fmm int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(10/31=
	mdv=7200000 iop(1/2=-1,2/2=-1)

	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore raff iop(10/31=1) iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff iop mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(10/31=1,10/29=3) iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(10/31=1) fmm mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(10/31=1) int=nogather mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore raff iop(10/31=1) int=nogather iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff iop(10/31=1) int=nogather mdv=7200000 iop(1/2=-1,2/2=-1) #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(10/31=1,10/29=3) int=nogather iop1=nodftj mdv=7200000 iop(1/2=-1,2/2 #p svwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(10/31=1) fmm int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)

test277.com	#p uhfs/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uxalpha/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uhfb/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p usvwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uxavwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn5/6-31G(df,p) 5d 7f test geom=modela scf=incore freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn5/6-31G(df,p) 5d 7f test geom=modela scf=direct freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uslyp/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uxalyp/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500,11/43=2) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ublyp/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500,11/
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ulsda/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500,11/
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn/6-31G(df,p) 5d 7f test geom=modela freq iop(3/76=0750002500,11/
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubecke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore iop(1

	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq nosymm scf=noincore
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1,10/29=3) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq iop(10/31=1) fmm
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p becke3p86/6-31G(df,p) 5d 7f test geom=modela freq
	iop(10/29=2,10/31=1) fmm int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore raff
	iop(10/31=1) iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff
	iop(10/31=1) mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1,10/29=3) iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq iop(10/31=1) fmm
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1) int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore raff
	iop(10/31=1) int=nogather iop1=nodftj mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore noraff
	iop(10/31=1) int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq scf=noincore
	iop(10/31=1,10/29=3) int=nogather iop1=nodftj mdv=7200000 iop(1/2=-1,2/2
	#p svwn5/6-31G(df,p) 5d 7f test geom=modela freq
	iop(10/31=1) fmm int=nogather mdv=7200000 iop(1/2=-1,2/2=-1)

test278.com	#p uhfs/6-31G(df,p) 5d 7f test geom=modela freq mdv=7200000 iop(1/2=-1,2
	#p uxalpha/6-31G(df,p) 5d 7f test geom=modela freq mdv=7200000 iop(1/2=-
	#p uhfb/6-31G(df,p) 5d 7f test geom=modela freq mdv=7200000 iop(1/2=-1,2
	#p usvwn5/6-31G(df,p) 5d 7f test geom=modela freq mdv=7200000 iop(1/2=-1
	#p uxavwn5/6-31G(df,p) 5d 7f test geom=modela freq
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn5/6-31G(df,p) 5d 7f test geom=modela scf=incore freq
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn5/6-31G(df,p) 5d 7f test geom=modela scf=direct freq
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p uslyp/6-31G(df,p) 5d 7f test geom=modela freq mdv=7200000 iop(1/2=-1,
	#p uxalyp/6-31G(df,p) 5d 7f test geom=modela freq iop(11/43=2)

	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ublyp/6-31G(df,p) 5d 7f test geom=modela freq iop(11/43=2)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ulsda/6-31G(df,p) 5d 7f test geom=modela freq iop(11/43=2)
	mdv=7200000 iop(1/2=-1,2/2=-1)
	#p ubvwn/6-31G(df,p) 5d 7f test geom=modela freq iop(11/43=2)
	mdv=7200000 iop(1/2=-1,2/2=-1)

test281.com	#p rblyp/6-31+G(df,p) 5d 7f stable=opt geom=modela iop(3/76=0850001500) s
	extrabasis int=nobasistrans
	#p ublyp/chkbas guess=read stable=opt geom=modela iop(3/76=0850001500)
	#p rblyp/6-31+G(df,p) 5d 7f stable=(noincore,opt) geom=modela iop(3/76=08
	#p ublyp/6-31+G(df,p) 5d 7f guess=read stable=(noincore,opt) geom=modela
	iop(3/76=0850001500)

test282.com	#p uhf/6-31G(df,p) 5d 7f force test geom=modela scf=conventional
	mdv=3000000 iop(1/2=-1,2/2=-1)
	#p uhf/6-31G(df,p) 5d 7f force test geom=modela int=dprdsrf
	scf=conventional
	#p uhf/6-31G(df,p) 5d 7f force test geom=modela int=dsrys
	scf=conventional
	#p uhf/6-31G(df,p) 5d 7f force test geom=modela int=(berny,dsrys)
	scf=conventional

test283.com	#p uhf/6-31G(df,p) 5d 7f freq test geom=modela mdv=4000000 iop(1/2=-1,2/ #p uhf/6-31G(df,p) 5d 7f freq test geom=modela mdv=5000000 iop(1/2=-1,2/ #p uhf/6-31G(df,p) 5d 7f freq test geom=modela int=dsrys #p uhf/6-31G(df,p) 5d 7f freq test geom=modela int=(berny,dsrys) #p uhf/6-31G(df,p) 5d 7f freq test geom=modela

test284.com	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) Test
	SCRF=(GradRho,UseMO,GasCavity)
	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) SCRF=(GradRho,GasCavity)
	Test
	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) SCRF=(GradRho,UseMO)
	Test
	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) Test
	SCRF=(IsoDensity,UseMO,GasCavity)
	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) SCRF=IsoDensity Test IOp(1/8
	#P RHF/6-311++G(2d,2p) 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM Test
	#P RHF/6-311++G(2d,2p) 6D SCRF=(GradVne,UseMO,GasCavity) Test
	#P RHF/6-311++G(2d,2p) 6D SCRF=(GradRho,GasCavity,UseMO) Test

test285.com	# HF/6-311G** 6D SCF=(DIRECT,TIGHT) OPT=TIGHT test # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=13003) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=23003) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=12003) GEOM=CHEC

	# HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=14003) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=13001) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=13002) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=23002) GEOM=CHEC # HF/6-311G** 6D SCF=(DIRECT,TIGHT) SCRF=OldPCM IOP(1/8=13004) GEOM=CHEC
test286.com	#p rhf/6-31g(df,p) 5d 7f test force mdv=5000000 iop(1/2=-1,2/2=-1) #p rhf/6-31g(df,p) 5d 7f test force scf=qc mdv=5000000 iop(1/2=-1,2/2=-1 #p rhf/6-31g(df,p) 5d 7f test freq mdv=5000000 iop(1/2=-1,2/2=-1)

test287.com	#p ubecke3lyp/6-31g(df,p) 5d 7f test force int=finegrid
	mdv=5000000 iop(1/2=-1,2/2=-1)
	#p ubecke3lyp/6-31g(df,p) 5d 7f test force int=finegrid scf=(qc,intrep)
	mdv=5000000 iop(1/2=-1,2/2=-1)
	#p ubecke3lyp/6-31g(df,p) 5d 7f test freq int=finegrid
	mdv=7500000 iop(1/2=-1,2/2=-1)

test288.com	#p rhf/6-311++G** 6d test mdv=5000000 iop(1/2=-1,2/2=-1)
	#p CAS(4,4)/6-311++G** 6D test Guess=(check,alter)
	mdv=5000000 iop(1/2=-1,2/2=-1)

test289.com	#p cas(2,2,rfo)/6-31g** test scf=tight guess=alter
test290.com	#p casscf(4,4)/sto-3g opt=conical test guess=alter nosymm #p casscf(4,4)/sto-3g opt=conical test guess=alter nosymm scf=conventiona #p casscf(4,4)/sto-3g opt=conical test guess=alter nosymm iop(10/50=3)
test292.com	#p rhf/6-311G(df,p) nmr test #p rhf/6-311G(df,p) nmr=all int=grid=99302 cphf=mo test #p rhf/6-311G(df,p) nmr=all int=grid=99302 test #p rhf/6-311G(df,p) nmr=all int=grid=99302 test mdv=6000000 iop(1/2=-1,2

test293.com	#p uhf/6-311G(df,p) nmr test
	#p uhf/6-311G(df,p) nmr=all int=grid=99302 cphf=mo test guess=read
	#p uhf/6-311G(df,p) nmr=all int=grid=99302 test guess=read
	#p uhf/6-311G(df,p) nmr=all int=grid=99302 test guess=read
	mdv=6000000 iop(1/2=-1,2/2=-1)

test294.com	#p uhf/3-21g opt=tight freq=noraman test geom=modela
test295.com	#p g1 test #p g1 test
test296.com	#p G1 geom=modela test #p G2 geom=modela test #p G2MP2 geom=modela test #p rhf/6-31g* opt freq geom=modela test #p g2=startmp2 test
test297.com	#p G1 geom=modela test #p G2 geom=modela test

	#p G2MP2 geom=modela test #p uhf/6-31g* opt freq geom=modela test #p g2=startmp2 test #p g2=restart test
test298.com	#p CBS-4O geom=modela test #p CBS-4M geom=modela test #p CBS-LQ geom=modela test #p CBS-Q geom=modela test #p CBS-QB3O geom=modela test #p CBS-QB3 geom=modela test
test299.com	#p CBS-4O geom=modela test #p CBS-4M geom=modela test #p CBS-LQ geom=modela test #p CBS-Q geom=modela test #p CBS-QB3O geom=modela test #p CBS-QB3 geom=modela test
计算输入档	**计算执行路径**
test300.com	#p cas(6,6)/d95 mp2 test iop(5/42=5) guess=cards
test301.com	#p rhf/sto-3g test #p cas(2,2,spin)/6-31g** 5d guess=read geom=check test
test302.com	#p hf/3-21g opt=qst2 test
test303.com	#p hf/3-21g opt=qst3 test
test304.com	#p cas(5,6)/d95 mp2 test iop(5/42=5) guess=cards

test305.com	#p rept=ovgf/gen tran=full test mdv=7000000 iop(1/2=-1,2/2=-1)
	#p ept=ovgf/chkbas test geom=check guess=read mdv=7000000 iop(1/2=-1,2/2
	#p ept=ovgf/chkbas test geom=check guess=read tran=ijab
	mdv=7000000 iop(1/2=-1,2/2=-1)

test306.com	#p ept/6-31g* test #p ept/6-31g* test tran=full
test307.com	#P EPT=ReadOrbitals/6-31G* test mdv=3000000 iop(1/2=-1,2/2=-1)
test308.com	#p mp2/6-31g* test mdv=5000000 iop(1/2=-1,2/2=-1)
test309.com	#p hf/3-21g nosymm opt=qst3 freq test
test310.com	#p hf/sto-3g opt=tight freq test
test311.com	#P RHF/6-311G** 6D opt=tight test scrf=scipcm
test312.com	#P RHF/6-311G** 6D force test scrf=scipcm
test313.com	#p rhf/sto-3g opt=(ts,calcfc) freq test #p rhf/sto-3g irc=(cartesian,rcfc) geom=check guess=read test

test314.com	#p rb3lyp/6-311G(df,p) nmr test #p rb3lyp/6-311G(df,p) nmr=all test guess=read
test315.com	#p ub3lyp/6-311G(df,p) nmr test extrabasis int=nobasistrans #p ub3lyp/chkbas nmr=all test guess=read geom=check
test316.com	#p rhf/6-31g* freq test #p g1(startmp2) opt=ts test #p g1 test opt=(ts,calcfc)
test317.com	#p freq test #p opt=(ts,rcfc) test geom=modify guess=read
test318.com	#p rhf/6-31g* 5d test geom=modela scf=tight cube=(cards,potential) #p rhf/6-31g* 5d test geom=modela scf=tight cube=(10,potential)

test319.com	#p rcis=(singlet,root=2)/d95(df,p) test freq
	extrabasis int=nobasistrans
	#p rcis=(singlet,root=2,direct)/d95(df,p) test freq
	guess=read
	#p rcis=(triplet,root=3,nstate=5,readwindow)/d95(df,p) test freq
	guess=read
	#p rcis=(triplet,root=3,nstate=5,readwindow,direct)/d95(df,p) test freq
	guess=read extrabasis int=nobasistrans

test320.com	#p ucis/d95(df,p) test freq
	#p ucis=direct/d95(df,p) test freq guess=read
	#p ucis=(root=2,nstate=5,readwindow)/d95(df,p) test freq
	guess=read
	#p ucis=(root=2,nstate=5,readwindow,direct)/d95(df,p) test freq
	guess=read

test321.com	#p rhf/6-31g* force test mdv=7000000 iop(1/2=-1,2/2=-1)
test322.com	#p RHF/STO-3G test opt freq #p rhf/sto-3g freq=numer test geom=check guess=read
test323.com	#p rhf/6-31g(2df,p) 5d 7f freq=(vcd,readiso) test #p rhf/6-31g(2df,p) 5d 7f polar=optrot test
test324.com	#p uhf/6-31g(df,p) test freq=(vcd,readiso) 5d 7f #p freq=(readiso,readfc) geom=allcheck test #p freq=readfc test #p uhf/chkbas polar=optrot geom=allcheck test guess=read
test325.com	#p rb3lyp/gen 5d 7f freq=(vcd,readiso) test #p rb3lyp/chkbas polar=optrot test geom=check guess=read
test326.com	#p rmp2/6-31g* tran=iajb test geom=modela iop(8/9=20000) #p rmp2/6-31g* tran=iajb test geom=modela iop(8/9=20020) #p rmp2/6-31g* tran=iajb test geom=modela iop(8/9=20030)

	#p rmp2/6-31g* tran=iabc test geom=modela iop(8/9=20000) #p rmp2/6-31g* tran=iabc test geom=modela iop(8/9=20020) #p rmp2/6-31g* tran=iabc test geom=modela iop(8/9=20030) #p rmp2/6-31g* tran=abcd test geom=modela iop(8/9=20000) #p rmp2/6-31g* tran=abcd test geom=modela iop(8/9=20020) #p rmp2/6-31g* tran=abcd test geom=modela iop(8/9=20030)
test327.com	#p ump2/6-31g* tran=iajb test geom=modela iop(8/9=20000) #p ump2/6-31g* tran=iajb test geom=modela iop(8/9=20020) #p ump2/6-31g* tran=iajb test geom=modela iop(8/9=20030) #p ump2/6-31g* tran=iabc test geom=modela iop(8/9=20000) #p ump2/6-31g* tran=iabc test geom=modela iop(8/9=20020) #p ump2/6-31g* tran=iabc test geom=modela iop(8/9=20030) #p ump2/6-31g* tran=abcd test geom=modela iop(8/9=20000) #p ump2/6-31g* tran=abcd test geom=modela iop(8/9=20020) #p ump2/6-31g* tran=abcd test geom=modela iop(8/9=20030)
test328.com	#p ROHF/sto-3g scf=tight test #p ROMP2/cc-pVDZ 5D test guess=read #p ROMP2/cc-pVDZ 5D test guess=read use=l804
test329.com	#p rb3lyp/6-31G(df,p) 5d 7f polar test geom=modela
test330.com	#p rohf/gen test units=au 6d 10f opt=z-matrix charge nosymm
test331.com	#p RHF/STO-3G FOPT=(CALCfc,TS) Test Freq #p RHF/STO-3G IRC=RCFC GUESS=READ test GEOM=CHECK
test332.com	#p rlsda/6-31g* units=au force test #p rlsda/6-31g* units=au force test int=fofcou geom=check #p rlsda/6-31g* units=au force test fmm=levels=5 geom=check #p rlsda/6-31g* units=au force test fmm=(levels=5,fmflg1=9) geom=check #p rlsda/6-31g* units=au force test fmm=boxlen=100 geom=check #p rlsda/6-31g* units=au force test fmm=boxlen=2000 geom=check
test333.com	#p rb3lyp/STO-3G test opt freq
test334.com	#p UHF/CC-PVDZ Freq TEST #p Freq=readfc geom=check TEST #p UHF/CC-PVDZ OPT=CALCALL TEST #p Freq=readfc geom=check TEST #p UHF/CC-PVDZ OPT=CALCALL TEST #p Freq=readfc geom=check TEST
test335.com	#p CBS-4O geom=modela test #p CBS-4M geom=modela test #p CBS-LQ geom=modela test #p CBS-Q geom=modela test #p CBS-QB3O geom=modela test

	#p CBS-QB3 geom=modela test #p G1 geom=modela test #p G2MP2 geom=modela test #p G2 geom=modela test #p G3 geom=modela test #p G3MP2 geom=modela test #p G3B3 geom=modela test #p G3MP2B3 geom=modela test
test336.com	#p HF/6-31g(df,pd) 5d 7f test #p rhf/6-31g(df,pd) 5d 7f test #p rhf/6-31g(df,pd) 5d 7f test #p HF/6-31g(df,pd) 5d 7f test nosymm
test337.com	#p rqcisd(t)/3-21g scan test
test338.com	#p rb3lyp/6-31g(df,pd) test opt
test339.com	#p rb3lyp/6-31g(df,pd) test opt
test340.com	#p rb3lyp/6-31g(df,pd) test force
test341.com	#p uhf/3-21g opt geom=modela test scf=symm guess=(alter,always)
test342.com	#p uhf/6-311g(df,pd) force test
test343.com	#p uhf/6-311g(df,pd) force test iop(4/15=3) alter symm=noscf
test344.com	#p freq rhf/6-31g* 5d test
test345.com	#p rhf/6-31g* 5d opt freq test
test346.com	#p rhf/6-31g(df,pd) 5d 7f test scf=tight
test347.com	#p rhf/6-31g(df,pd) 5d 7f test scf=tight
test348.com	#p rhf/6-31g(df) 5d 7f force test
test349.com	#p opt freq pm3 test
test350.com	#p opt freq dreiding geom=connectivity test
test351.com	#p rhf/6-31+g* 5d force test
test352.com	#p rhf/sto-3g opt=tight freq test
test353.com	#p opt=tight freq sto-3g test
test354.com	#p rlsda/3-21g units=au freq test #p rlsda/3-21g units=au freq test int=fofcou #p rlsda/3-21g units=au freq test fmm=levels=5 #p rlsda/3-21g units=au freq test fmm=(levels=5,fmflg1=9)
test355.com	#p nosym pop=full test #p casscf(10,10)/sto-3g guess=(read,alter) geom=allcheck test #p casscf(10,10,slater)/sto-3g guess=read geom=allcheck test#p casscf(10,

	guess=read geom=allcheck iop(4/46=3) test#p casscf(10,10,nroot=2)/sto-3g iop(4/46=1) geom=allcheck test #p casscf(10,10,nroot=3)/sto-3g guess=read iop(4/46=3) geom=allcheck tes #p casscf(10,10)/sto-3g guess=read geom=check test #p casscf(10,10)/sto-3g guess=read geom=allcheck iop(4/46=3) test #p casscf(10,10)/sto-3g guess=read geom=check test
test356.com	#p rhf/gen pseudo=read force test #p rhf/gen pseudo=read force test #p rhf/gen pseudo=read force test
test357.com	#p rhf/gen pseudo=read freq=noraman test #p rhf/gen pseudo=read freq=noraman test #p rhf/gen pseudo=read freq=noraman test
test358.com	#p rhf/lp-31g* force test
test359.com	#p rcis/3-21g opt=calchffc test geom=modela
test361.com	#p rhf/lp-31g test geom=modela aim
test362.com	#p rmp2=full/6-31+g* density=curr test iop(6/51=-1) #p rmp2=full/6-31+g* density=current test iop(6/51=10) geom=check guess=
test363.com	#p ump2=full/6-31+g* density=curr test iop(6/51=-1) #p ump2=full/6-31+g* density=current guess=read geom=check test iop(6/51 ! density=check guess=only
test364.com	#P HF/6-311G** SCF=Tight AIM symm=loose test
test365.com	#p ulsda/6-31g* 5d units=au force test #p ulsda/6-31g* 5d units=au force test int=fofcou geom=check #p ulsda/6-31g* 5d units=au force test fmm=levels=5 geom=check #p ulsda/6-31g* 5d units=au force test fmm=(levels=5,fmflg1=9) geom=chec
test366.com	#p ulsda/6-31g* 5d units=au freq test #p ulsda/6-31g* 5d units=au freq test int=fofcou #p ulsda/6-31g* 5d units=au freq test fmm=levels=5 #p ulsda/6-31g* 5d units=au freq test fmm=(levels=5,fmflg1=9)
test367.com	#p uhf/6-31g* 5d units=au force test #p uhf/6-31g* 5d units=au force test fmm=(levels=5) geom=check #p uhf/6-31g* 5d units=au force test fmm geom=check
test368.com	#p ub3lyp/6-31g* 5d units=au freq test #p ub3lyp/6-31g* 5d units=au freq test fmm=(levels=5) #p ub3lyp/6-31g* 5d units=au freq test fmm
test369.com	#p opt=tight freq oniom(mp2/genecp:blyp/genecp/auto) test #p freq oniom(mp2/chkbas:blyp/chkbas) test geom=allcheck guess=read
test370.com	#p freq oniom(mp2/lanl2dz:hf/lanl2mb) test

test371.com	#p opt freq oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	#p polar=numer oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	geom=allcheck guess=read
	#p polar=enonly oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	geom=allcheck guess=read
	#p freq=numer polar oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	geom=allcheck guess=read
	#p freq=enonly oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	geom=allcheck guess=read
	#p scf=tight oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
	geom=allcheck guess=read

test372.com	#p ub3lyp/6-31g* freq test int=ultrafine #p oniom(ub3lyp/6-31g*:uff) freq test int=ultrafine
test374.com	#p cas(4,4,npair=4)/sto-3g test pop=full scfcon=7 guess=(lowsym,cards) #p cas(4,4,npair=4)/6-31g* test pop=full opt scfcon=7 geom=check guess=(
test375.com	#p cas(12,10)/6-31+g* guess=cards nosym pop=full scfcon=7 test iop(4/46= #p cas(12,10)/6-31+g* geom=check guess=read nosym pop=full scfcon=7 iop(4/4

test376.com	#p cas(6,6,nofulldiag)/d95 test guess=cards
	iop(4/44=1,5/42=5,5/52=100,5/65=1,5/69=1)
	#p cas(6,6,nofulldiag)/d95 test geom=check guess=read
	iop(4/44=1,4/46=3,5/39=3,5/42=5,5/52=100,5/65=1,5/69=1)

test377.com	#P cas(3,3,nroot=2)/sto-3g test opt=(conical,z-matrix) nosymm
	iop(5/17=31000200,10/10=700008)
	#P cas(3,3,nroot=2)/sto-3g test freq nosymm pop=full scf=tight guess=rea
	iop(5/17=41000200,10/10=700007)
	#P nonstd
	1/10=4,29=2,30=1,38=11/1,3,6;
	2/15=1/2;
	3/25=1,31=1,116=101/1,2,3;
	4/5=1,17=3,18=3/1,5;
	5/5=2,6=12,17=31000200,28=2,32=2/10;
	8/6=4,10=90,11=11/1;
	11/31=1,42=1,45=1/1;
	10/6=1,10=700008,28=2,29=1,31=1/3;
	6/7=3,28=1/1;
	7/30=1/16;
	1/38=10,39=50/6(3);
	7/8=1,25=1,30=1,44=-1/16;
	1/10=4,30=1,38=10,39=50/3;
	99//99;
	3/25=1,31=1,116=101/1,2,3;
	4/5=5,16=2,17=3,18=3/1;

	5/5=2,6=12,17=31000200,23=1,28=2,32=2,38=4/10; 8/6=4,10=90,11=11/1; 11/31=1,42=1,45=1/1; 10/6=1,10=700008,28=2,29=1,31=1/3; 7/30=1/16; 1/38=10,39=50/6(-7); 7/8=1,25=1,30=1,44=-1/16; 1/10=4,30=1,38=10,39=50/3; 99//99;

test378.com	#p casscf(4,4)/sto-3g opt=conical test guess=alter nosymm
	iop(5/17=31000400,10/17=400,10/50=3,10/10=600008)

test379.com	#P nonstd 1/6=1,7=11,8=300,9=3,10=4,20=1,38=1,42=6,44=1,80=1/1,18; 2/15=1,17=6,18=5/2; 3/5=1,6=6,7=1,25=1,31=1,116=101/1,2,3; 4/17=3,18=3/1,5; 5/5=2,17=41000200,28=2,32=2,38=4,97=11/10; 8/6=4,11=11,23=2/1; 11/31=1,42=1,45=1/1; 10/6=1,10=700007,28=2,29=1,31=1,80=1,97=11,99=300/3(-3); 6/7=3,18=1,28=1/1; 7/10=1,25=1,30=1/1,2,3,16; 1/6=1,7=11,8=300,9=3,10=4,42=6,44=1,80=1/18(3); 3/5=1,6=6,7=1,25=1,31=1,39=1/1,3; 7/8=1,9=1,25=1,30=1,44=-1/16; 99//99; 3/5=1,6=6,7=1,25=1,31=1,116=101/1,2,3; 4/5=5,16=2,17=3,18=3/1; 5/5=2,17=41000200,23=1,28=2,32=2,38=4,97=11/10; 8/6=4,11=11,23=2/1; 11/31=1,42=1,45=1/1; 10/6=1,10=700007,28=2,29=1,31=1,80=1,97=11,99=300/3(-3); 7/10=1,25=1,30=1/1,2,3,16; 1/6=1,7=11,8=300,9=3,10=4,42=6,44=1,80=1/18(-7); 2/15=1/2; 3/5=1,6=6,7=1,25=1,31=1,39=1/1,3; 6/7=3,18=1,19=2,28=1/1; 7/8=1,9=1,25=1,30=1,44=-1/16; 99//99;
test380.com	#P nonstd 1/5=18,6=1,7=11,8=3000,9=1,10=4,38=1,42=20,44=1,80=1/1,18; 2/15=1,17=6,18=5/2; 3/25=1,31=1,116=101/1,2,3;

	4/17=3,18=3/1,5; 5/5=2,17=41000200,28=2,32=2,38=4,55=2,97=11/10; 8/6=4,11=11,23=2/1; 11/31=1,42=1,45=1/1; 10/6=1,10=700007,28=2,29=1,31=1,55=2,80=1,97=11,99=300/3; 6/7=3,18=1,28=1/1; 7/10=1,25=1,30=1/1,2,3,16; 1/5=18,6=1,7=11,8=3000,9=1,10=4,42=20,44=1,80=1/18(3); 3/25=1,31=1,39=1/1,3; 7/8=0,9=1,25=1,30=1,44=-1/16; 99//99; 3/25=1,31=1,116=101/1,2,3; 4/5=5,16=2,17=3,18=3/1; 5/5=2,17=41000200,23=1,28=2,32=2,38=4,55=2,97=11/10; 8/6=4,11=11,23=2/1; 11/31=1,42=1,45=1/1; 10/6=1,10=700007,28=2,29=1,31=1,55=2,80=1,97=11,99=300/3(-3); 7/10=1,25=1,30=1/1,2,3,16; 1/5=18,6=1,7=11,8=3000,9=1,10=4,42=20,44=1,80=1/18(-7); 3/25=1,31=1,39=1/1,3; 6/7=3,18=1,19=2,28=1/1; 7/8=0,9=1,25=1,30=1,44=-1/16; 99//99;
test381.com	#p AM1 use=1402 units=au pop=none test #p RHF Int=AM1 units=au sparse pop=none test #p RHF Int=AM1 units=au sparse=medium pop=none test #p RHF Int=AM1 units=au sparse=loose pop=none test
test382.com	#p SVWN/3-21g units=au test scf=tight force #p SVWN/3-21g units=au test scf=tight iop1=abelian force #p SVWN/3-21g units=au pop=none test scf=(tight,noincfock,novaracc) Sparse Guess=NoSparse force #p SVWN/3-21g units=au pop=none test scf=(tight,noincfock,novaracc) Sparse force #p SVWN/3-21g units=au pop=none test scf=(tight,noincfock,novaracc) Sparse fmm=print force #p SVWN/3-21g units=au pop=none test scf=(tight,noincfock,novaracc) Sparse=medium force #p SVWN/3-21g units=au pop=none test scf=(noincfock,novaracc) Sparse=loose
test383.com	#p ublyp/6-31g* units=au test scf=tight #p ublyp/6-31g* units=au pop=none test scf=(tight,noincfock,novaracc) Sparse Guess=NoSparse #p ublyp/6-31g* units=au pop=none test scf=(tight,noincfock,novaracc)

	Sparse #p ublyp/6-31g* units=au pop=none test scf=(tight,noincfock,novaracc) Sparse fmm=print

test384.com	#p ub3pw91/6-31g* units=au test scf=tight iop1=abelian fmm
	#p ub3pw91/6-31g* units=au pop=none test scf=(tight,noincfock,novaracc)
	Guess=NoSparse Sparse
	#p ub3pw91/6-31g* units=au pop=none test scf=(tight,noincfock,novaracc)
	Guess=NoSparse Sparse fmm

test385.com	#p ram1 opt=(big,rfo) test geom=(nodist,noangle,nodihed) nosymm
test386.com	#p ram1 opt=(gdiis,big) test geom=(nodist,noangle,nodihed) nosymm
test387.com	#p AM1 opt=(tight,small,gdiis) test
test388.com	#p AM1 opt=(big,tight) test
test389.com	#p AM1 opt=(tight,small,rfo) test
test390.com	# uhf/6-311g* nosym guess=(mix,alter) test scf=(tight,novaracc) #p cas(3,3,uno)/6-311g* pop=full guess=read geom=check iop(5/72=1,4/21=1 #p cas(3,3)/6-311g* pop=full guess=read geom=check iop(5/72=0,4/21=10) n #p cas(7,7)/6-311g* pop=full guess=read geom=check iop(5/72=1,4/21=10) n
test393.com	#P AM1 OPT=(big,Tight,addredund) Test iop(4/28=8)

test394.com	# uhf/3-21g
	opt=(path=5,bimolecular,noreact,noproduct,trustupdate,updatemethod=d2cor
	pop=none guess=always iop(1/8=30)

test395.com	#p ram1 use=l402 force test geom=(nodist,noangle,nodihed)
	#p rhf int=am1 force test geom=(nodist,noangle,nodihed,check)sparse pop=
	#p rhf int=am1 force test geom=(nodist,noangle,nodihed,check)
	sparse=medium pop=none scfcon=6

test396.com	#p rmp2/cc-pvtz test geom=modela
test397.com	#p rb3lyp/3-21g force test scf=novaracc
test398.com	#p EPT=(P3,ReadOrbitals,ForceSort) units=bohr 6-311G** iop33(9=1) test
test399.com	#P b3lyp td=nstates=6/6-31+g* 5d test #P b3lyp td=(triplet,nstates=6)/6-31+g* 5d test geom=check guess=read #P b3lyp td=(50-50,nstates=5)/6-31+g* 5d test geom=check guess=read #P ub3lyp td=nstates=5/6-31+g* 5d test geom=check guess=read
计算输入档	**计算执行路径**
test400.com	#P ub3lyp td=nstates=12/6-31+g* 5d test
test401.com	#p mPW1PW91 6-31g(d,p) opt=tight freq test
test402.com	#p lg1lyp 6-31g(d,p) opt=tight freq test

test403.com	#p B1LYP/6-31G(d,p) opt=tight freq test
test404.com	#p B1LYP/6-31G(d,p) SCRF=(CPCM,READ,SOLVENT=WATER) NOSYMM OPT=Z-matrix test
test405.com	#p pw91PW91 6-31g(d,p) opt=tight freq test
test406.com	#p G96PW91 6-31g(d,p) opt=tight freq test
test407.com	#p rhf/3-21g polar=optrot test geom=modela extrabasis int=nobasistrans #p rhf/3-21g freq=vcd test geom=modela extrabasis int=nobasistrans #p rhf/3-21g freq=nraman test geom=modela #p rhf/3-21g freq=(nraman,restart) test geom=modela #p rhf/3-21g freq=(vcd,nraman) test geom=modela #p rhf/3-21g freq=cubic polar test geom=modela
test408.com	#p ub3lyp/3-21g polar=optrot test geom=modela #p ub3lyp/3-21g freq=vcd test geom=modela #p ub3lyp/3-21g freq=raman test geom=modela #p ub3lyp/3-21g freq=nraman test geom=modela #p ub3lyp/3-21g freq=(nraman,restart) test geom=modela #p ub3lyp/3-21g freq=(vcd,raman) test geom=modela scf=qc extrabasis int= #p ub3lyp/3-21g freq=(vcd,nraman) test geom=modela scf=qc extrabasis int #p ub3lyp/3-21g freq=cubic polar test geom=modela
test409.com	#p rmp2/3-21g freq test geom=modela #p rmp2/3-21g freq=raman test geom=modela #p rmp2/3-21g freq=(raman,restart) test geom=modela #p rmp2/3-21g freq=cubic polar test geom=modela
test410.com	#p opt=tight freq oniom(hf/sto-3g:am1) test scfcon=10 cphf=conver=10 int #p freq=(numer,four) polar oniom(hf/sto-3g:am1) test geom=check guess=rea cphf=conver=10 int=acc2e=12 #p freq=enonly oniom(hf/sto-3g:am1) test geom=check guess=read scfcon=10
test411.com	#p ump2/d95(df,p) 5d 7f test geom=modela cbsextrap=pop extrabasis int=no mdv=8000000 iop(1/2=-1,2/2=-1)
test412.com	#P CBS-Q Test
test413.com	#p uhf/3-21g opt=(path=7,trustupdate,modredun,qst3) pop=none guess=alway
test414.com	#p mp2/6-31g* nmr=print 5d units=bohr test
test415.com	#p mp2/6-311G(df,pd) 5d 7f Units=Bohr NMR test #p mp2/6-311G(df,pd) 5d 7f Units=Bohr NMR test
test416.com	#p UMP2/STO-3G NMR Units=Bohr Test
test417.com	#p AM1 nosymm opt=ModRedundant test
test418.com	#p b3lyp/6-311G(df,pd) 5d 7f Units=Bohr NMR test #p b3lyp/6-311G(df,pd) 5d 7f Units=Bohr NMR test

test419.com	#p rhf/3-21g test guess=core scf=(tight,novaracc) geom=modela stable=(op #p uhf/3-21g test guess=core scf=(tight,fermi,novaracc) geom=modela stab #p rohf/3-21g test scf=(tight,novaracc) geom=modela
test420.com	#p MP2/6-311G(2df,p) force symm=loose MaxDisk=250000000 iop1=timestamp #p MP2/6-311G(2df,p) force symm=loose MaxDisk=250000000 iop1=nopacksort
test422.com	#p dreiding opt=(tight,nomicro) freq units=au test #p uff opt=(tight,nomicro) freq units=au test
test423.com	#p amber opt=tight freq test
test424.com	#P rmp2/6-31g* 5d freq test maxdisk=1gb #P rmp2/6-31g* 5d freq test maxdisk=1200mb iop1=nopacksort
test425.com	#p amber opt=(verytight,nomicro) freq test
test426.com	#p opt=(verytight,nomicro) freq amber test
test427.com	#p opt=(verytigh,nomicro) freq amber test
test428.com	#p opt=tight freq amber test
test429.com	# hf/6-31g* freq test #p NonStd 1/7=0,10=5,14=100,22=1,29=120002,38=1,39=1,42=8,44=3,54=1/1,15; 2/12=2,15=1,29=3/2; 3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3; 4/5=1/1; 5/5=2/2; 6/7=2,8=2,9=2,10=2,28=1/1; 7//1,2,3,16; 1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15; 2/15=1,29=3/2; 3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3; 4/5=5,16=2/1; 5/5=2/2; 7//1,2,3,16; 1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15(-5); 2/15=1,29=3/2; 3/5=1,6=6,7=1,11=9,30=1,39=0,31=1/1,2,3; 4/5=5,16=2/1; 5/5=2/2; 8/6=4,11=10/1; 11/6=1,8=1,9=11,15=111,16=11/1,2,10; 10/6=1,9=1/2; 7/10=1,25=1,45=2/1,2,3,16; 1/10=4,14=100,22=1,30=1,39=1,42=8,44=3,54=1/15(-14); 7/8=1,10=1,25=11,45=2/16;

	1/10=4,14=100,22=1,30=0,42=8,44=3,54=1/15(-16); 6/7=2,8=2,9=2,10=2,18=1,28=1/1; 99/9=1/99; #p NonStd 1/7=0,10=4,14=100,22=1,29=120000,38=1,39=1,42=8,44=3,54=1/1,15; 2/12=2,15=1,29=3/2; 3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3; 4/5=1/1; 5/5=2/2; 6/7=2,8=2,9=2,10=2,28=1/1; 8/6=4,11=10/1; 11/6=1,8=1,9=11,15=111,16=11/1,2,10; 10/6=1,9=1/2; 7/10=1,25=1/1,2,3,16; 1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15; 2/15=1,29=3/2; 3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3; 4/5=5,16=2/1; 5/5=2/2; 7//1,2,3,16; 1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15(-5); 2/15=1,29=3/2; 3/5=1,6=6,7=1,11=9,30=1,39=0,31=1/1,2,3; 4/5=5,16=2/1; 5/5=2/2; 8/6=4,11=10/1; 11/6=1,8=1,9=11,15=111,16=11/1,2,10; 10/6=1,9=1/2; 7/10=1,25=1,45=1/1,2,3,16; 1/10=4,14=100,22=1,30=1,39=1,42=8,44=3,54=1/15(-14); 7/8=1,10=1,25=11,45=1/16; 1/10=4,14=100,22=1,30=0,42=8,44=3,54=1/15(-16); 6/7=2,8=2,9=2,10=2,18=1,28=1/1; 99/9=1/99; #p NonStd 1/7=0,10=4,14=100,22=1,29=120000,38=1,39=1,42=8,44=3,54=1/1,15; 2/12=2,15=1,29=3/2; 3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3; 4//1; 5/5=2/2; 6/7=2,8=2,9=2,10=2,28=1/1; 8/6=4,11=10/1; 11/6=1,8=1,9=11,15=111,16=11/1,2,10; 10/6=1,9=1/2;

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7/10=1,25=1/1,2,3,16;
1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15;
2/15=1,29=3/2;
3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3;
4/5=5,16=2/1;
5/5=2/2;
7//1,2,3,16;
1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15(-5);
2/15=1,29=3/2;
3/5=1,6=6,7=1,11=9,30=1,39=0,31=1/1,2,3;
4/5=5,16=2/1;
5/5=2/2;
8/6=4,11=10/1;
11/6=1,8=1,9=11,15=111,16=11/1,2,10;
10/6=1,9=1/2;
7/10=1,25=1,45=1/1,2,3,16;
1/10=4,14=100,22=1,30=1,39=1,42=8,44=3,54=1/15(-14);
7/8=1,10=1,25=11,45=1/16;
1/10=4,14=100,22=1,30=0,42=8,44=3,54=1/15(-16);
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
99/9=1/99;
#p NonStd
1/7=0,10=7,14=100,22=1,30=1,35=1,39=1,42=8,44=3,54=1/15(1);
2/15=1,29=3/2(7);
2/15=1,29=3/2;
3/5=1,6=6,7=1,11=9,25=20,30=1,31=1/1,2,3;
4/5=5,16=2/1;
5/5=2/2;
7//1,2,3,16;
1/22=1,14=100,30=1,39=1,42=8,44=3,54=1/15(-5);
2/15=1,29=3/2;
3/5=1,6=6,7=1,11=9,30=1,39=0,31=1/1,2,3;
4/5=5,16=2/1;
5/5=2/2;
8/6=4,11=10/1;
11/6=1,8=1,9=11,15=111,16=11/1,2,10;
10/6=1,9=1/2;
7/10=1,25=1,45=1/1,2,3,16;
1/10=4,14=100,22=1,30=1,39=1,42=8,44=3,54=1/15(-14);
7/8=1,10=1,25=11,45=1/16;
1/10=4,14=100,22=1,30=0,42=8,44=3,54=1/15(-16);
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
99/9=1/99;
```

test430.com	# irc=(calcfc,maxpoints=1,downhill) test # irc=(calcfc,reverse,maxpoints=1,phase=(3,1,2)) test
test431.com	#p opt=(tight,nomicro) freq amber geom=(nodist,noangle,nodihed) test
test432.com	#p opt freq amber geom=(nodist,noangle,nodihed) test
test433.com	#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(iefpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(iefpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G** scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* NOSYMM scrf=(cpcm,read) test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(iefpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=5000000 iop(1/2= #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* NOSYMM scrf=(dpcm,read) test scf=tight #p HF/gen pseudo=read gfinput scrf=(dpcm,read) NOSYMM test scf=tight #p HF/gen pseudo=read gfinput scrf=(cpcm,read) NOSYMM test scf=tight

	#p HF/gen 6d pseudo=read NOSYMM scrf=(cpcm,read) test scf=tight #p HF/gen pseudo=read 6d scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* NOSYMM scrf=(dpcm,read) test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight mdv=6000000 iop(1/2= #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM iop(2/15=3) test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=8000000 iop(1/2= #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight mdv=5000000 iop(1/2= #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=5000000 iop(1/2= #p HF/6-31+g* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=5000000 iop(1/2 #p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31+G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/LANL2DZ scrf=(dpcm,read) NOSYMM extrabasis gfinput test scf=tight #p HF/LANL2DZ scrf=(dpcm,read) NOSYMM extrabasis gfinput test scf=tight #p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31+G* scrf=(iefpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM opt test #p HF/6-31G* scrf=(iefpcm,read) NOSYMM opt test #p HF/6-31G* scrf=(ivcpcm,read) NOSYMM opt test
test434.com	#p rhf/lp-31g* opt=tight freq test geom=modela #p rhf/lp-31g* freq=numer test geom=check guess=read
test435.com	#p cbs-qb3 test opt=tight int=ultrafine
test436.com	#p uhf/sto-3g guess=(alter) stable=opt test
test437.com	#p zindo=(window=(22,46),nstates=40) test
test438.com	#p b3lyp 6-31G* td(nstates=10) test
test439.com	#P RHF/6-31+g* opt TEST scfcon=7 #P RHF/6-31+g* force TEST geom=allcheck iop(3/59=3)
test440.com	#p test freq=hindered
test441.com	#p test freq=hinderedrotor

	#p test freq=(readfc,readhindrot) #p test freq=(readfc,readhindrot,readisotopes)
test442.com	#p dreiding freq=hindrot geom=(nodist,noang,nodihed) test
test443.com	#p opt=tight freq oniom(b3lyp/lanl2dz:dreiding) test #p opt=tight freq oniom(b3lyp/lanl2dz:dreiding) test nosymm
test444.com	#p pbepbe/6-31g** test #p pbepbe/6-31g** test geom=modela freq #p pbepbe/6-31g** test geom=modela freq #p pbepbe/6-31g** test geom=modela freq #p pbepbe/6-31g** test geom=modela freq
test445.com	#p test gen 6d bpw91 opt freq
test446.com	#p mpw1pw91/6-311+g** opt=tight freq test
test447.com	#p mpw1pw91/6-311+g* opt=tight freq test int=ultrafine
test448.com	#p opt amber test mdv=2000000 iop(1/2=-1,2/2=-1)
test449.com	#p rccsd(t)/sto-3g test geom=modela #p rqcisd/sto-3g force test geom=modela
test450.com	#p ccsd(t)/d95 units=au test mdv=2000000 iop(1/2=-1,2/2=-1) #p bd(t,e4t)/d95 units=au test mdv=2000000 iop(1/2=-1,2/2=-1)
test451.com	#p uqcisd/sto-3g guess=alter force test #p uccsd(t)/sto-3g guess=alter test
test452.com	#p hf/sto-3g opt=(ts,calcall,z-matrix) test #p ircmax(zero,maxpoints=10,hf/6-31g*:hf/sto-3g) geom=check guess=read t
test453.com	#p hf/sto-3g opt=(ts,calcall) test #p ircmax(calcall,hf/6-31g*:hf/sto-3g) geom=check guess=read test nosymm
test454.com	#p rhf/3-21g freq test scrf geom=modela
test455.com	#p uhf/3-21g freq test scrf geom=modela

test456.com	#p blyp/3-21g units=au test scf=tight force
	#p blyp/3-21g units=au test scf=tight iop1=abelian force
	#p blyp/3-21g units=au pop=none test scf=(tight,noincfock,novaracc)
	Sparse Guess=NoSparse force
	#p blyp/3-21g units=au pop=none test scf=(tight,noincfock,novaracc)
	Sparse force
	#p blyp/3-21g units=au pop=none test scf=(tight,noincfock,novaracc)
	Sparse fmm=print force
	#p blyp/3-21g units=au pop=none test scf=(tight,noincfock,novaracc)
	Sparse=medium force
	#p blyp/3-21g units=au pop=none test scf=(noincfock,novaracc) Sparse=loo

test457.com	#P td=50-50/6-31G* test

	#P td(50-50)/6-31G* scrf=(iefpcm,read) test #P utd(50-50)/6-31G* scrf=(iefpcm,read) test
test458.com	#p td=(full,sos)/3-21g geom=modela test #p td=(full,sos,eqsolv)/3-21g geom=modela test scrf=iefpcm #p td=(full,sos)/3-21g geom=modela test scrf=iefpcm
test459.com	#p rhf/3-21g polar geom=modela test #p rhf/3-21g polar geom=modela test cphf=xy #p rhf/3-21g polar geom=modela test cphf=rdfreq #p rhf/3-21g polar geom=modela test cphf=rdfreq #p rhf/3-21g polar geom=modela test scrf=iefpcm #p rhf/3-21g polar geom=modela test cphf=xy scrf=iefpcm #p rhf/3-21g polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefpcm #p rhf/3-21g polar geom=modela test cphf=rdfreq scrf=iefpcm #p rhf/3-21g polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefpcm #p rhf/3-21g polar geom=modela test cphf=rdfreq scrf=iefpcm
test460.com	#p td=(full,sos) b3lyp/6-31g* 5d geom=modela test #p td=(full,sos,eqsolv) b3lyp/6-31g* 5d geom=modela test scrf=iefpcm #p td=(full,sos) b3lyp/6-31g* 5d geom=modela test scrf=iefpcm
test461.com	#p rb3lyp/6-31g* 5d polar geom=modela test #p rb3lyp/6-31g* 5d polar geom=modela test cphf=xy #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq #p rb3lyp/6-31g* 5d polar geom=modela test scrf=iefpcm #p rb3lyp/6-31g* 5d polar geom=modela test cphf=xy scrf=iefpcm #p rb3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm #p rb3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm
test462.com	#p rb3lyp/6-31g* 5d polar geom=modela test scf=noincore #p rb3lyp/6-31g* 5d polar geom=modela test cphf=xy scf=noincore #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scf=noincore #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scf=noincore #p rb3lyp/6-31g* 5d polar geom=modela test scrf=iefpcm scf=noincore #p rb3lyp/6-31g* 5d polar geom=modela test cphf=xy scrf=iefpcm scf=noinc #p rb3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm scf=no #p rb3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p rb3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm scf=no
test463.com	#P rb3lyp/6-31G** test polar int=ultrafine #P ub3lyp/6-31G** test scf=(tight,novaracc,dsymm) stable=opt int=ultrafi #P ub3lyp/6-31G** test polar geom=check guess=read int=ultrafine

test464.com	#p rhf/6-31g* 5d opt freq scrf=(iefpcm,solvent=water) test
test465.com	#p uhf/6-31g* 5d opt freq scrf=iefpcm test
test466.com	#p B3LYP/6-31+G* test Opt Freq int=ultrafinegrid
test467.com	#P CCSD/Gen Scan Test scf=(nosymm,xqc) geom=nocrowd
test468.com	#p b3lyp/cep-121g opt=tight freq test
test469.com	#p opt freq test 3-21g*
test470.com	#p uvsxc/6-31g* int=ultrafine opt=tight freq test
test471.com	#p cis=root=2/3-21g geom=modela opt freq optcyc=100 test
test472.com	#p cis=(root=2,50-50)/3-21g geom=modela opt freq optcyc=100 test
test473.com	#p test pbepbe/3-21g opt=(addredundant) pbc=cellrange=80 int=ultrafine
test474.com	#p test lsda/sto-3g opt=(tight,addredundant) fmm=levels=2 int=ultrafine
test475.com	#p test lsda/sto-3g opt=(tight,addredundant) fmm int=ultrafine
test476.com	#p ub3lyp/lp-31g* 5d test nmr geom=modela #p ump2/lp-31g* 5d test nmr geom=modela
test477.com	#p rvsxc/3-21g opt=tight freq test int=ultrafine #p rvsxc/3-21g opt=tight freq test fmm int=ultrafine
test478.com	#p uvsxc/3-21g test int=ultrafine opt=tight freq #p uvsxc/3-21g opt=(readfc,tight) freq test int=ultrafine guess=read geom=allcheck fmm
test479.com	#P TEST polar=cubic b3lyp/6-31G*
test480.com	#P TEST polar=cubic mp2/6-31G*
test481.com	#p ub3lyp/6-31g* 5d polar geom=modela test #p ub3lyp/6-31g* 5d polar geom=modela test cphf=xy #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq #p ub3lyp/6-31g* 5d polar geom=modela test scrf=iefpcm #p ub3lyp/6-31g* 5d polar geom=modela test cphf=xy scrf=iefpcm #p ub3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm #p ub3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm
test482.com	#p ub3lyp/6-31g* 5d polar geom=modela test scf=noincore #p ub3lyp/6-31g* 5d polar geom=modela test cphf=xy scf=noincore #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scf=noincore #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scf=noincore #p ub3lyp/6-31g* 5d polar geom=modela test scrf=iefpcm scf=noincore #p ub3lyp/6-31g* 5d polar geom=modela test cphf=xy scrf=iefpcm scf=noinc

	#p ub3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm scf=no #p ub3lyp/6-31g* 5d polar geom=modela test cphf=(rdfreq,eqsolv) scrf=iefp #p ub3lyp/6-31g* 5d polar geom=modela test cphf=rdfreq scrf=iefpcm scf=no
test483.com	#p rb3lyp/6-31g* opt freq geom=modela scrf=(iefpcm,read) test nosymm
test484.com	#p HF/STO-3G Scan Units=(Au,Deg) test #p HF/STO-3G Scan test #p HF/STO-3G Scan Units=(Au,Deg) test #p HF/STO-3G Scan test
test485.com	#p oniom(HF/6-31G*:amber) opt test
test487.com	#p opt test rhf/6-31g*
test488.com	#p rhf/freq=(vibrot,anharm,readanh) test
test489.com	#p ubb95/6-31g* int=ultrafine opt freq test #p ub1b95/6-31g* int=ultrafine opt=readfc freq test guess=read geom=check
test490.com	#p rhf/sto-3g* test scf=(tight,novaracc) units=au force #p rhf/sto-3g* test scf=(tight,novaracc) units=au force #p rhf/sto-3g* test scf=(tight,novaracc) units=au force iop1=abelian #p rhf/sto-3g* test scf=(tight,novaracc) units=au force iop1=abelian #p rhf/sto-3g* test scf=(tight,novaracc) units=au force iop(5/17=2000) #p rhf/sto-3g* test scf=(tight,novaracc) units=au force iop(5/17=2000) #p rhf/sto-3g* test scf=(tight,novaracc) units=au force scf=qc #p rhf/sto-3g* test scf=(tight,novaracc) units=au force scf=(qc,intrep)
test491.com	#p test oniom(hf/genecp:pm3) opt freq

test492.com	#p mp2/sto-3g
	bomd=(nsample=-1,ntraj=1,step=500,readmwvel,update=5,maxpoint=20,rtemp=29
	pop=none scf=(qc,maxcycles=1500) nosymm test

test493.com	#P hf/3-21g* opt test
test494.com	#p td(full,sos)/sto-5g test #p rhf/sto-3g test td(full,singlet,nstates=10) #p pbe1pbe/sto-3g test td(full,singlet,nstates=10)
test495.com	#p oniom(mp2/lanl2dz:hf/lanl2mb)=svalue scf=tight test
test496.com	#p oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb)=svalue scf=tight test
test497.com	#p Mp2/6-31G(d) NMR test
test498.com	#p uhf int=indo admp=(maxpoint=10,nke=1000) test
test499.com	#p lsda/sto-3g admp test #p lsda/sto-3g admp=restart test
计算输入档	**计算执行路径**

test500.com	#p lsda/sto-3g admp=lowdin test
test501.com	#p b3lyp/6-31g* admp geom=modela test
test502.com	#p b3lyp/6-31g* admp=(lowdin,dke=100) geom=modela test
test503.com	#p admp=emass=-1000 oniom(hf:uff) test #p admp=(restart,emass=-1000) oniom(hf:uff) test
test508.com	#p b3lyp/6-31g* units=au force test #p b3lyp/6-31g* units=au force test fmm #p b3lyp/6-31g* units=au force test fmm=(levels=5,fmflg1=9)
test509.com	#p ub3lyp/6-31g* 5d units=au force test #p ub3lyp/6-31g* 5d units=au force test fmm #p ub3lyp/6-31g* 5d units=au force test fmm=(levels=5,fmflg1=9)
test510.com	#p b3lyp/6-31g* units=au freq test #p b3lyp/6-31g* units=au freq test fmm #p b3lyp/6-31g* units=au freq test fmm=(levels=5,fmflg1=9)
test511.com	#p ub3lyp/6-31g* 5d units=au freq test #p ub3lyp/6-31g* 5d units=au freq test fmm #p ub3lyp/6-31g* 5d units=au freq test fmm=(levels=5,fmflg1=9)
test512.com	#p opt=tight freq oniom(hf/lanl2dz:dreiding=qeq) test #p opt=(tight,restart) freq oniom(hf/lanl2dz:dreiding=qeq) test #p opt=tight freq oniom(hf/lanl2dz:dreiding=qeq) test nosymm #p opt=(tight,restart) freq oniom(hf/lanl2dz:dreiding=qeq) test nosymm
test513.com	#p rhf/3-21g force test fmm iop(11/43=2) #p rhf/3-21g freq test fmm geom=allcheck guess=read
test514.com	#p rbd/6-31g** 5d units=au extrabasis int=nobasistrans test
test515.com	#p ubd/6-31g** 5d units=au extrabasis int=nobasistrans test
test517.com	#p HF/6-311+G(2d,2p) freq=vibrot scf(conver=10) test #p HF/6-311+G(2d,2p) freq=(readfc,vibrot) geom=allcheck test #p HF/6-311+G(2d,2p) freq=(vibrot,anharm) scf(conver=10) test #p HF/6-311+G(2d,2p) freq=(vibrot,anharm,restart) scf(conver=10)test
test518.com	#p rb3lyp/6-31g* 5d opt freq scrf=cpcm test geom=modela nosymm #p rb3lyp/6-31g* 5d polar scrf=check test geom=allcheck guess=read nosymm #p rb3lyp/6-31g* 5d polar=numer scrf=check test geom=allcheck guess=read nosymm #p rb3lyp/6-31g* 5d freq=numer polar scrf=check test geom=allcheck nosymm guess=read
test519.com	#p opt freq oniom(mp2/lanl2dz:hf/lanl2mb) test #p polar=numer oniom(mp2/lanl2dz:hf/lanl2mb) test geom=allcheck guess=rea

	#p polar=enonly oniom(mp2/lanl2dz:hf/lanl2mb) test geom=allcheck guess=r #p freq=numer polar oniom(mp2/lanl2dz:hf/lanl2mb) test geom=allcheck gue #p freq=enonly oniom(mp2/lanl2dz:hf/lanl2mb) test geom=allcheck guess=re
test520.com	#p ub3lyp/6-31g* 5d opt freq scrf=cpcm test geom=modela nosymm #p ub3lyp/6-31g* 5d polar scrf=check test geom=allcheck guess=read nosym #p ub3lyp/6-31g* 5d polar=numer scrf=check test geom=allcheck guess=read #p ub3lyp/6-31g* 5d freq=numer polar scrf=check test geom=allcheck nosym
test521.com	#p rmp2/6-31g* 5d opt freq scrf test geom=modela nosymm #p rmp2/6-31g* 5d polar scrf=check test geom=allcheck guess=read nosymm #p rmp2/6-31g* 5d polar=numer scrf=check test geom=allcheck guess=read nosymm #p rmp2/6-31g* 5d freq=numer polar scrf=check test geom=allcheck nosymm guess=read
test522.com	#p ump2/6-31g* 5d opt freq scrf=read test geom=modela nosymm #p ump2/6-31g* 5d polar scrf=check test geom=allcheck guess=read nosymm #p ump2/6-31g* 5d polar=numer scrf=check test geom=allcheck guess=read n #p ump2/6-31g* 5d freq=numer polar scrf=check test geom=allcheck nosymm
test523.com	#p opt freq oniom(qcisd/lanl2dz:mp2/lanl2mb) test #p polar=numer oniom(qcisd/lanl2dz:mp2/lanl2mb) test geom=allcheck guess #p polar=enonly oniom(qcisd/lanl2dz:mp2/lanl2mb) test geom=allcheck gues #p freq=enonly oniom(qcisd/lanl2dz:mp2/lanl2mb) test geom=allcheck guess
test524.com	#p opt freq oniom(b3lyp/lanl2dz:mp2/lanl2dz:hf/lanl2mb) test
test525.com	#p rhf/sto-3g nmr test geom=modela scf=tight nosymm #p rhf/sto-3g test massage geom=modela scf=tight nmr nosymm #p rhf/sto-3g test geom=modela charge scf=tight nmr nosymm
test526.com	#p rmp2/3-21g nmr test geom=modela scf=tight nosymm #p rmp2/3-21g test massage geom=modela scf=tight nmr nosymm #p rmp2/3-21g test geom=modela charge scf=tight nmr nosymm
test527.com	#p lsda/3-21G pbc=gammaonly pop=min force test #p lsda/3-21G pbc=nrecip=1 pop=min force test #p lsda/3-21G pbc=nrecip=16 pop=min force test #p ulsda/3-21G pbc=nrecip=1 pop=min force test #p ulsda/3-21G pbc=nrecip=16 pop=min force test #p ulsda/3-21G pbc=nrecip=16 guess=mix pop=min force test

test528.com	#p ONIOM(RHF/6-31G(d):AM1 sparse:AMBER=softfirst) pop=none test
	scf=(tight,xqc,fermi,novaracc)

test529.com	#p lsda/sto-3g force geom=modred pbc=gammaonly
test533.com	#p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974

	#p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(ndamp=30,tight,fermi,novaracc,xqc) int=grid #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/6-311++g test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,novaracc) int=grid=99974 symm=noscf #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,novaracc) int=grid=99974 symm=noscf #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 symm=n #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc,xqc) int=grid=99974 sy #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974

	#p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p ub3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974 #p rb3lyp/3-21g 5d test scf=(tight,fermi,novaracc) int=grid=99974
test534.com	#p b3lyp/gen prop pseudo=read test pop=full int=grid=199302

test535.com	#p lsda/sto-3g opt=(maxcyc=10,tight,addredundant) fmm=levels=2
	scf=(novaracc,vshift=-1)

test536.com	#p lsda/6-311+G(d,p)/auto opt=tight int=ultrafine scfcon=8 test
test538.com	#p rlsda/3-21g force test geom=modela #p rlsda/3-21g force test geom=modela int=fofcou #p rlsda/3-21g force test geom=modela fmm #p rlsda/3-21g freq test geom=modela #p rlsda/3-21g freq test geom=modela int=fofcou #p rlsda/3-21g freq test geom=modela fmm
test539.com	#p rb3lyp/3-21g force test geom=modela #p rb3lyp/3-21g force test geom=modela fmm #p rb3lyp/3-21g freq test geom=modela #p rb3lyp/3-21g freq test geom=modela fmm
test540.com	#p ulsda/3-21g force test geom=modela #p ulsda/3-21g force test geom=modela int=fofcou #p ulsda/3-21g force test geom=modela fmm #p ulsda/3-21g freq test geom=modela #p ulsda/3-21g freq test geom=modela int=fofcou #p ulsda/3-21g freq test geom=modela fmm
test541.com	#p ub3lyp/3-21g force test geom=modela #p ub3lyp/3-21g force test geom=modela fmm #p ub3lyp/3-21g freq test geom=modela #p ub3lyp/3-21g freq test geom=modela fmm
test542.com	#p rlsda/3-21g force test geom=modela #p rlsda/3-21g/dga1 force test geom=modela
test543.com	#p ulsda/3-21g force test geom=modela #p ulsda/3-21g/dga1 force test geom=modela
test544.com	#p rhf/sto-3g scf=tight test geom=modred #p rhf/sto-3g pbc=nrecip=256 guess=read scf=tight test geom=check
test545.com	#p uhf/6-311g force test units=bohr

test546.com	#p hcth/6-31g* opt=(tight,calcfc) freq geom=(modela,print) int=ultrafine
test547.com	#p hcth/6-31g* opt=(tight,calcfc) freq geom=(modela,print) int=ultrafine
test552.com	#p rhf/3-21g nmr pop=ncs geom=modela test #p rhf/3-21g nmr pop=ncsdiag geom=modela test #p rhf/3-21g nmr pop=ncsall geom=modela test
test553.com	#p b3lyp/6-31g(df,pd) 5d 7f force test
test554.com	#p oniom=(hf/3-21g:amber)=scale=3 test opt freq
test557.com	#p rhf/3-21g freq=raman geom=modela test cphf=rdfreq
test558.com	#p rb3lyp/3-21g freq=raman geom=modela test cphf=rdfreq
test559.com	#p rhf/3-21g counter=2 test opt freq #p rhf/3-21g counter=2 test freq=numer polar geom=allcheck guess=read #p rhf/3-21g counter=2 test freq=enonly geom=allcheck guess=read
test560.com	#p rmp2/3-21g counter=2 test opt freq #p rmp2/3-21g counter=2 test freq=numer polar geom=allcheck guess=read #p rmp2/3-21g counter=2 test freq=enonly geom=allcheck guess=read
test561.com	#p rb3lyp/3-21g counter=2 test opt freq #p rb3lyp/3-21g counter=2 test freq=numer polar geom=allcheck guess=read #p rb3lyp/3-21g counter=2 test freq=enonly geom=allcheck guess=read
test562.com	#p uhf/3-21g counter=2 test scf=tight opt freq
test563.com	#p mp2/6-31G Counterpoise=2 test opt
test564.com	#p rhf/3-21g Counterpoise=3 opt freq test
test565.com	#p gen scf=tight units=bohr test int=dkh iop(3/93=1) #p rhf/chkbas scf=tight geom=check guess=read test int=dkh
test566.com	#P ub3lyp/6-311g* scf=(tight,novaracc) int=dkh test #p ub3lyp/chkbas geom=check guess=read scf=tight int=dkh iop(3/93=1)
test567.com	#p ump2/6-311+g(2df,p) test opt #p ump2/6-311+g(2df,p) test freq geom=check guess=read
test568.com	#P blyp td=nstates=12/6-31+g* 5d test #P blyp td=(nstates=12,read)/6-31+g* 5d test geom=check guess=read iop(9 #P blyp td=(triplet,nstates=6)/6-31+g* 5d test geom=check guess=read #P blyp td=(triplet,add=3)/6-31+g* 5d test geom=check guess=read iop(9/7 #P blyp td=(50-50,nstates=5)/6-31+g* 5d test geom=check guess=read #P blyp td=(50-50,read)/6-31+g* 5d test geom=check guess=read
test569.com	#P ublyp td=nstates=12/6-31+g* 5d test #P ublyp td=add=4/6-31+g* 5d test geom=check guess=read #P ublyp td=add=2/6-31+g* 5d test geom=check guess=read iop(9/70=1)
test570.com	#p rb3lyp/3-21g counter=2 test opt=(tight,calcall) freq int=ultrafine

	#p rb3lyp/3-21g counter=2 test freq=numer polar geom=allcheck guess=read #p rb3lyp/3-21g counter=2 test freq=enonly geom=allcheck guess=read int=
test571.com	#p AM1 freq use=l402 test #p AM1 opt=rcfc scrf=cosmo test geom=allcheck
test572.com	#p rhf/lp-31G test nmr=suscep nosymm
test573.com	#p rhf/6-31g(df,pd) 5d 7f geom=modela nmr=suscep
test574.com	#p rblyp/3-21g force test scf=novaracc #p rblyp/3-21g/dga1 force test scf=novaracc geom=check #p rblyp/3-21g/dga1 force test scf=novaracc geom=check fmm #p rblyp/3-21g/auto force test scf=novaracc geom=check #p rblyp/3-21g/auto force test scf=novaracc geom=check denfit=iter #p rblyp/3-21g/auto force test scf=novaracc geom=check int=usepcw #p rblyp/3-21g/auto force test scf=novaracc geom=check int=revdist

test575.com	#p b3lyp/cep-31G**/dga1 counterpoise=2 nosymm opt freq Test extrabasis in
	#p b3lyp/cep-31G**/dga1 counterpoise=2 nosymm opt=restart freq Test extra
	int=nobasistrans 5d
	#p b3lyp/chkbas counterpoise=2 nosymm Test geom=allcheck guess=read forc

test576.com	#p oniom(hf/6-31g**:hf/sto-3g)=compress opt freq test 5d #p oniom(hf/6-31g**:hf/sto-3g)=compress freq test geom=check guess=read #p oniom(hf/6-31g**:hf/sto-3g)=nocompress freq test geom=check guess=rea

test577.com	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=compress opt freq test 5d
	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=compress freq test geom=check
	iop(11/43=2)
	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=nocompress freq test geom=chec

test578.com	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1) force test 5d
	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=compress freq test geom=check
	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=compress freq test geom=check
	iop(11/43=4)
	#p oniom(b3lyp/6-31g**:blyp/6-31g**/dga1)=nocompress freq test geom=chec

test579.com	#p oniom(hf/sto-3g:blyp/sto-3g/dga1)=compress freq test 5d field=z+100
	#p oniom(hf/sto-3g:blyp/sto-3g/dga1)=compress freq test 5d field=z+100 i
	geom=check guess=read
	#p oniom(hf/sto-3g:blyp/sto-3g/dga1)=nocompress freq test 5d field=z+100
	geom=check guess=read
	#p oniom(hf/sto-3g:blyp/sto-3g/dga1)=nocompress freq test 5d field=z+100
	geom=check guess=read

test580.com	#p oniom(cis=(direct)/6-31g*:hf/sto-3g) force test 5d extrabasis int=nob
	#p oniom(cis=(direct,read)/chkbas:hf/chkbas)=compress freq test
	geom=allcheck guess=read
	#p oniom(cis=(direct,read)/chkbas:hf/chkbas)=compress freq test iop(11/4

	geom=allcheck guess=read
	#p oniom(cis=(direct,read)/chkbas:hf/chkbas)=nocompress freq test
	geom=allcheck guess=read
	#p oniom(cis=(direct,read)/chkbas:hf/chkbas)=nocompress freq test iop(11/
	geom=allcheck guess=read

test581.com	#p oniom(mp2/6-31g**:hf/sto-3g)=compress opt freq test 5d extrabasis int= #p oniom(mp2/chkbas:hf/chkbas)=compress freq test geom=check guess=read #p oniom(mp2/chkbas:hf/chkbas)=nocompress freq test geom=check guess=rea #p oniom(mp2/chkbas:hf/chkbas)=nocompress freq test geom=check guess=rea
test582.com	#p oniom(mp2/6-31g**:hf/sto-3g)=compress force test 5d extrabasis int=no #p oniom(mp2/chkbas:hf/chkbas)=compress freq test geom=allcheck guess=rea #p oniom(mp2/chkbas:hf/chkbas)=compress freq test geom=allcheck guess=rea #p oniom(mp2/chkbas:hf/chkbas)=nocompress freq test geom=check guess=rea
test583.com	#p b3lyp/6-31G* bomd=(maxpoint=10,update=4) test counter=2
test584.com	#p oniom(b3lyp/6-31G*:uff) bomd=(maxpoint=22,update=5) test
test585.com	#p opt=tight freq oniom(b3lyp/lanl2dz:dreiding=softfirst) test #p opt=(tight,restart) freq oniom(b3lyp/lanl2dz:dreiding=softfirst) test
test586.com	#p b3lyp/lp-31G* 6d opt test
test587.com	#p pbepbe/3-21g opt test int=ultrafine #p pbepbe/3-21g opt test int=ultrafine #p pbepbe/3-21g opt test int=ultrafine
test588.com	#p pbepbe/lanl2dz opt=(modred,expert) test
test589.com	#p lsda/gen pseudo=lanl1 opt=(modred,expert) units=au test
test590.com	#p lsda/gen/auto opt=(modred,expert) test
test592.com	#p ub3lyp/6-31g(df,pd) 5d 7f nmr=suscep int=ultrafine cphf=ultrafine tes
test593.com	#p ub3lyp/lp-31g 5d 7f nmr=suscep int=ultrafine cphf=ultrafine test extra
test594.com	#p ub3lyp/lp-31g** geom=modela test nmr=suscep
test595.com	#p dreiding opt test #p uff opt test
test596.com	#P oniom(b3lyp/3-21g:amber) geom=connectivity test opt=loose

test597.com	#P oniom(blyp/3-21g/dga1:amber) geom=connectivity test opt=loose scf=nova
	#P oniom(blyp/3-21g/dga1:amber)=embed geom=check guess=read test opt=(rea
	scf=novaracc

test598.com	#P oniom(b3lyp/3-21g:amber) geom=connectivity test opt=loose
test599.com	#p rhf/3-21g scf=(tight,novaracc) test units=au #p rhf/3-21g scf=(tight,novaracc) test units=au guess=indo #p rhf/3-21g scf=(tight,novaracc) test units=au guess=(only,save)

	#p rhf/3-21g scf=(tight,novaracc) test units=au guess=read #p rhf/3-21g scf=(tight,novaracc) test units=au guess=(only,save,indo) #p rhf/3-21g scf=(tight,novaracc) test units=au guess=read
计算输入档	计算执行路径
test600.com	#p hf/3-21g sparse test force geom=nocrowd
test601.com	#p pbepbe/3-21g sparse test force
test602.com	#p pbepbe/3-21g opt test optcyc=3

test603.com	#p lsda/sto-3g admp(maxpoint=10,emass=-1000,bandgap) test
	#p lsda/sto-3g admp(maxpoint=10,lowdin,emass=-1000,bandgap) test
	!#p lsda/sto-3g admp(maxpoint=10,emass=-1000,bandgap) test sparse=20
	#p lsda/sto-3g admp(maxpoint=10,bandgap) test
	#p lsda/sto-3g admp(maxpoint=10,lowdin,bandgap) test
	!#p lsda/sto-3g admp(maxpoint=10,bandgap) test sparse=20
	#p lsda/sto-3g admp=bandgap test geom=rharm
	#p lsda/sto-3g admp(maxpoint=10,cholesky,bandgap) test geom=rharm
	#p lsda/sto-3g admp(maxpoint=10,cholesky,restart,bandgap) test geom=rhar
	#p lsda/sto-3g admp(maxpoint=10,cholesky,bandgap) field=z+123 test geom=
	#p lsda/sto-3g admp(maxpoint=10,cholesky,nke=51279,bandgap) test
	iop(1/80=1000000,1/81=1,1/82=300,1/89=1)
	#p lsda/sto-3g admp=(bandgap,nke=51279) test iop(1/80=1200100,1/81=1,1/8
	#p lsda/sto-3g admp=(bandgap,nke=51279) test iop(1/80=-1200210,1/81=1,1/
	#p lsda/sto-3g admp(maxpoint=10,emass=-1000,bandgap) oniom(hf:uff) test
	#p admp(maxpoint=5,emass=-1000,bandgap) oniom(b3lyp/3-21G*:uff) test
	#p admp(maxpoint=5,bandgap) oniom(b3lyp/3-21G*:uff) test
	#p admp(maxpoint=5,bandgap) oniom(b3lyp/3-21G*:uff) field = z+123 test
	#p admp(maxpoint=5,emass=-1000,bandgap) oniom(b3lyp/3-21G*:uff) test geo
	#p lsda/sto-3g admp(maxpoint=10,cholesky,bandgap) test

test605.com	#p oniom=(hf/lanl2dz:am1:amber) opt geom=connect test optcyc=3
test606.com	#p oniom(ccsd(t)/3-21g:am1) sym=loose test
test607.com	#P oniom(hf:UFF) opt freq TEST NOSYMM geom=connect #P oniom(hf:UFF) freq=numer polar TEST NOSYMM geom=allcheck
test608.com	#p opt=tight freq oniom(blyp/3-21g:uff) test #p freq=numer polar oniom(blyp/3-21g:uff) test geom=allcheck guess=read
test609.com	#p oniom(hf:amber) geom=connectivity test opt freq #p oniom(hf:amber) geom=connectivity test opt freq nosymm
test610.com	#p oniom(hf:amber) geom=connectivity test opt=nomicro freq #p oniom(hf:amber) geom=connectivity test opt=nomicro freq nosymm
test611.com	#p oniom(hf:amber) geom=connectivity test opt=tight freq #p oniom(hf:amber) geom=connectivity test opt=tight freq nosymm

test612.com	#p oniom(hf:amber) geom=connectivity test opt=tight freq #p oniom(hf:amber) geom=connectivity test opt=tight freq nosymm
test613.com	#p oniom(hf:amber)=embed geom=connectivity test opt=tight freq #p oniom(hf:amber)=embed geom=connectivity test opt=tight freq nosymm
test614.com	#p hf/sto-3g scf=tight nosymm scrf(dpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(dpcm,read) test #p cas(4,3,nroot=1)/sto-3g guess=(read) nosymm scrf(dpcm,read) test #p hf/sto-3g scf=tight nosymm scrf(cpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(cpcm,read) test #p cas(4,3,nroot=1)/sto-3g guess=(read) nosymm scrf(cpcm,read) test #p hf/sto-3g scf=tight nosymm scrf(iefpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(iefpcm,read) test #p cas(4,3,nroot=1)/sto-3g guess=(read) nosymm scrf(iefpcm,read) test
test615.com	#p hf/sto-3g scf=tight nosymm scrf(dpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(dpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(dpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(dpcm,read) test #p hf/sto-3g scf=tight nosymm scrf(cpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(cpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(cpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(cpcm,read) test #p hf/sto-3g scf=tight nosymm scrf(iefpcm,read) test #p cas(4,3)/sto-3g guess=(read) nosymm scrf(iefpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(iefpcm,read) test #p cas(4,3,nroot=2)/sto-3g guess=(read) nosymm scrf(iefpcm,read) test
test616.com	#p hf/sto-3g scf=tight nosymm population(full) scrf(iefpcm,read) test #p cas(6,4)/sto-3g guess=(read) nosymm force scrf(iefpcm,read) test #p hf/sto-3g scf=tight nosymm scrf(iefpcm,read) test #p cas(6,4)/sto-3g guess=(read) nosymm force=enonly iop(1/39=-1) scrf(ie
test617.com	#p force amber=hardfirst test geom=connectivity
test618.com	#p opt amber=hardfirst test geom=connectivity #p force amber test geom=allcheck #p opt amber test geom=allcheck

test619.com	#P rlsda/6-31g**/dga1 5d opt test mdv=4194304 iop(1/2=-1,2/2=-1)
	#P Geom=AllCheck Guess=Read SCRF=Check Test GenChk RSVWN/chkbas/chkbas F
	mdv=4194304 iop(1/2=-1,2/2=-1)
	#p rlsda/chkbas/chkbas freq=numer polar geom=allcheck guess=read test

test620.com	#P ulsda/6-31g**/dga1 5d stable=opt test #p ulsda/chkbas/chkbas opt freq scf=idsymm geom=allcheck guess=read test #p ulsda/chkbas/chkbas freq=numer polar geom=allcheck guess=read test

test622.com	#p hf/6-31G(d) freq=(anharm,readanharm) test
test624.com	#p ept/6-31G* test #p ept=(ovgf,readorbitals)/6-31G* guess=read test
test625.com	#p ept=(ovgf+p3,readorbitals)/6-31G* test #p ept=(ovgf+p3,readorbitals)/6-31G* test #p ept=readorbitals/6-31G* test #p ept=readorbitals/6-31G* test
test626.com	#p ub3lyp/6-311+G** test Freq=(vcd,vibrot) #p rearchive output=pickett test #p rearchive output=(pickett,read) test #p rhf/3-21g freq=(vcd,vibrot) test geom=modela output=pickett #p ub3lyp/6-31G* test nmr output=pickett #p ub3lyp/6-31G* test Freq=(vcd,vibrot) output=pickett #p uhf/sto-3g geom=modela test output=pickett #p uhf/sto-3g test output=pickett #p rearchive output=(pickett,readatom) test

test627.com	#P ROHF/STO-3G test scf=tight
	#P CASSCF(4,4)/STO-3G guess=read geom=check test
	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=3)/STO-3G guess=read geom=check te
	scfcyc=3 iop(5/13=1,5/106=1)
	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=3)/STO-3G geom=check test guess=re
	iop(5/106=3)
	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=6)/STO-3G guess=read geom=check te
	iop(5/106=3)

test628.com	#P rhf/STO-3G nosym test scf=tight #P cas(8,8,rasscf(4,2,4,2))/STO-3G nosym test guess=(read,alter) geom=ch #P cas(8,8,lanczos,rasscf(4,2,4,2))/STO-3G nosym test guess=read geom=ch
test629.com	#p rhf/sto-3g test nmr=spinspin #p b3lyp/sto-3g test nmr=spinspin
test630.com	#p ub3lyp/6-31g(df,pd) 5d 7f test nmr=spinspin extrabasis int=nobasistra

test631.com	# SAC-CI(Singlet=(NState=(2,2,2,2),NonVariational),
	Triplet=(NState=(2,2,2,2),NonVariational),
	CationDoublet=(NState=(3,0,1,1),NonVariational),
	AnionDoublet=(NState=(2,0,1,2),NonVariational),FullActive,SD-R,
	NoLinkedSelection,NoUnLinkedSelection)/D95 Unit=Bohr Test

test632.com	# SAC-CI(Singlet=(NState=(4,2,4,2),NonVariational,Density),
	Triplet=(NState=(4,2,4,2),NonVariational,Density),
	CationDoublet=(NState=(1,0,1,1),NonVariational,Density),
	SD-R,AllProperties)/D95(d,p) ExtraBasis Unit=Bohr Test

test633.com	# SAC-CI(Singlet=(Nstate=(0,0,0,0,0,2,0,0)),SelecCISOnly,LevelOne)

	/Gen Massage Symm=On test # SAC-CI(Singlet=(Nstate=(0,0,0,0,0,2,0,0)),SelecCISOnly,LevelTwo) /Gen Massage Symm=On test # SAC-CI(Singlet=(Nstate=(0,0,0,0,0,2,0,0)),SelecCISOnly,LevelThree) /Gen Massage Symm=On test # SAC-CI(Singlet=(Nstate=(0,0,0,0,0,2,0,0)),LevelThree) /Gen Massage Symm=On test

test634.com	# SAC-CI(Singlet=(NState=(2,3,3,1,2,2,2,5)),
	Triplet=(NState=(2,3,3,1,2,2,2,5)),
	CationDoublet=(NState=(2,0,0,1,0,1,1,1)))
	/Gen Massage Symm=On test

test635.com	# SAC-CI(LevelOne, Singlet=(NState=(2,3,3,1,2,2,2,5)),
	Triplet=(NState=(2,3,3,1,2,2,2,5)),CationDoublet=(NState=(2,0,0,1,0,1,1,
	/Gen Massage Symm=On test
	# SAC-CI(LevelTwo,Singlet=(NState=(2,3,3,1,2,2,2,5)),
	Triplet=(NState=(2,3,3,1,2,2,2,5)),CationDoublet=(NState=(2,0,0,1,0,1,1,
	/Gen Massage Symm=On test
	# SAC-CI(LevelThree,Singlet=(NState=(2,3,3,1,2,2,2,5)),
	Triplet=(NState=(2,3,3,1,2,2,2,5)),CationDoublet=(NState=(2,0,0,1,0,1,1,
	/Gen Massage Symm=On test

test636.com	# SAC-CI(LevelOne,Singlet=(NState=(0,0,1,0,2,2,1,0)),
	Triplet=(NState=(2,0,1,0,2,2,1,0)),CationDoublet=(NState=(1,0,1,0,0,1,1,
	AnionDoublet=(NState=(1,0,1,0,0,1,1,0)))/D95(d,p) ExtraBasis test
	# SAC-CI(LevelTwo,Singlet=(NState=(0,0,1,0,2,2,1,0)),
	Triplet=(NState=(2,0,1,0,2,2,1,0)),CationDoublet=(NState=(1,0,1,0,0,1,1,
	AnionDoublet=(NState=(1,0,1,0,0,1,1,0)))/D95(d,p) ExtraBasis test
	# SAC-CI(LevelThree,Singlet=(NState=(0,0,1,0,2,2,1,0)),
	Triplet=(NState=(2,0,1,0,2,2,1,0)),CationDoublet=(NState=(1,0,1,0,0,1,1,
	AnionDoublet=(NState=(1,0,1,0,0,1,1,0)))/D95(d,p) ExtraBasis test

test637.com	# SAC-CI(Singlet=(NState=(0,0,0,0,0,4,4,1)), LevelOne,Window=(25,244))/Gen Test

test638.com	# SAC-CI(Singlet=(NState=(0,1)),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))/D95(d) Opt test
	# SAC-CI(SacOnly,TargetState=(SpinState=Singlet,Symmetry=1,Root=0))
	/D95(d) Opt test

test639.com	# SAC-CI(CationDoublet=(NState=(0,0,1,0)),macro=1,
	TargetState=(SpinState=CationDoublet,Symmetry=3,Root=1))/D95(d,p) Opt te
	# SAC-CI(CationDoublet=(NState=(1,0,0,0)),macro=1,
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1))/D95(d,p) Opt te

test640.com	# SAC-CI(LevelTwo,Singlet=(NState=(1,4,0,0)))/LANL2DZ test

	# SAC-CI(LevelTwo,Singlet=(NState=(2,4,0,0)),WithoutDegeneracy)/LANL2DZ

test641.com	# SAC-CI(Singlet=(NState=(0,1,1,0))Triplet=(NState=(0,0,1,0))
	CationDoublet=(NState=(1,1,1,1)),LevelTwo)/TZV Extrabasis test

test642.com	# SAC-CI(Singlet=(NState=1),LMO=Pipek-Mezey)/D95 test # SAC-CI(Singlet=(NState=(0,1)))/D95 test

test643.com	# SAC-CI(Singlet=(NState=(2,1,1,1),NoTransitionDensity),
	Triplet=(NState=(1,1,1,2),NoTransitionDensity),
	FullUnlinked,ReadWindow)/6-31G* test
	# SAC-CI(Singlet=(NState=(2,1,1,1),NonVariational,
	NoTransitionDensity,InCoreDiag),Triplet=(NState=(1,1,1,2),NonVariational,
	NoTransitionDensity,InCoreDiag),
	NoLinkedSelection,NoUnlinkedSelection,ReadWindow)/6-31G* test
	# SAC-CI(Singlet=(NState=(2,1,1,1),NonVariational,
	NoTransitionDensity,InCoreDiag),
	Triplet=(NState=(1,1,1,2),NonVariational,
	NoTransitionDensity,InCoreDiag),InCoreSAC,ReadWindow)/6-31G* test
	# SAC-CI(Singlet=(NState=(3,0,2,0),NoTransitionDensity),
	FullActive,FullUnlinked)/Gen 6d Unit=Bohr test
	# SAC-CI(Singlet=(NState=(3,0,2,0),NoTransitionDensity,InCoreDiag),
	NoLinkedSelection,NoUnlinkedSelection,FullActive)/Gen 6d Unit=Bohr test
	# SAC-CI(Singlet=(NState=(3,0,2,0),NoTransitionDensity,InCoreDiag),
	InCoreSAC,FullActive)/Gen 6d Unit=Bohr test

test644.com	# SAC-CI(BeforeGSUM,
	Singlet=(NState=(1,0,1,0,0,1,1,0),InCoreDiag),
	FullActive)/D95(d) Unit=Bohr CPHF=Canonical test
	# SAC-CI(CalcGSUM,
	Singlet=(NState=(1,0,1,0,0,1,1,0),InCoreDiag),
	FullActive)/D95(d) SCAN Unit=Bohr CPHF=Canonical test
	# SAC-CI(AfterGSUM,
	Singlet=(NState=(1,0,1,0,0,1,1,0),InCoreDiag),
	FullActive,MaxItSAC=40)
	/D95(d) SCAN Unit=Bohr CPHF=Canonical test

test645.com	# SAC-CI(Quartet=(NState=(2,2,1,1,2,2,1,1)),
	Quintet=(NState=(3,1,2,2,2,2,2,2)),
	Sextet=(NState=(1,0,1,1,0,1,0,0)),
	Septet=(NState=(0,0,0,0,0,1,0,0)),
	NoLinkedSelection,NoUnlinkedSelection,Window=(3,15))/D95 ExtraBasis test
	# SAC-CI(Quartet=(NState=(2,2,1,1,2,2,1,1),NonVariational),
	Quintet=(NState=(3,1,2,2,2,2,2,2),NonVariational),
	Sextet=(NState=(1,0,1,1,0,1,0,0),NonVariational),
	Septet=(NState=(0,0,0,0,0,1,0,0),NonVariational),
	NoLinkedSelection,NoUnlinkedSelection,Window=(3,15))/D95 ExtraBasis test

test646.com	# SAC-CI(General-R,
	Singlet=(NState=1),
	Triplet=(NState=1),
	CationDoublet=(NState=1),
	AnionDoublet=(NState=1),
	Quartet=(NState=(2,2,1,1,2,2,1,1)),
	Quintet=(NState=(3,1,2,2,2,2,2,2)),
	Sextet=(NState=(1,0,1,1,0,1,0,0)),
	Septet=(NState=(0,0,0,0,0,1,0,0)),
	Window=(3,15),MaxItDiag=100)
	/D95 ExtraBasis test

test647.com	# SAC-CI(Singlet=(NState=(0,1,0,0)),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
	General-R) /D95** Opt CPHF=Canonical test
	# SAC-CI(Singlet=(NState=(0,1,0,0),MaxR=2),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
	General-R) /D95** Opt CPHF=Canonical test
	# SAC-CI(SacOnly,
	TargetState=(SpinState=Singlet,Symmetry=1,Root=0))
	/D95** Opt CPHF=Canonical test

test648.com	# SAC-CI(Quartet=(NState=(0,1,0,0,0,0,0,0)),
	TargetState=(SpinState=Quartet,Symmetry=2,Root=1))
	/D95** Opt CPHF=Canonical test
	# SAC-CI(Quartet=(NState=(0,0,0,0,1,0,0,0)),
	TargetState=(SpinState=Quartet,Symmetry=5,Root=1),
	CutoffDIISZVec=1.0d-3) /D95** Opt CPHF=Canonical test
	# SAC-CI(Quartet=(NState=(0,1,0,0,0,0,0,0)),
	TargetState=(SpinState=Quartet,Symmetry=2,Root=1),
	General-R) /D95** Opt CPHF=Canonical test
	# SAC-CI(Quartet=(NState=(0,0,0,0,1,0,0,0)),
	Targetstate=(SpinState=Quartet,Symmetry=5,Root=1),
	General-R,CutoffDIISZVec=1.0d-3) /D95** Opt CPHF=Canonical test

test649.com	# SAC-CI(Singlet=(NState=(0,1)),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/D95 Force Pop=Full test
	# SAC-CI(Triplet=(NState=(0,1)),
	TargetState=(SpinState=Triplet,Symmetry=2,Root=1))
	/D95 Force Pop=Full test
	# SAC-CI(CationDoublet=(NState=(1,0)),
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1))
	/D95 Force Pop=Full test

test650.com	# SAC-CI(Singlet=(NState=3,Density),

	Triplet=(NState=3,Density), CationDoublet=(NState=2,Density), AnionDoublet=(NState=(5,0,5,5),Density), AllProperties,MaxItDiag=100)/cc-pVDZ ExtraBasis test

test651.com	# SAC-CI(Singlet=(NState=(0,1)),macro=2,
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/D95(d) Opt test
	# SAC-CI(Triplet=(NState=(0,1)),macro=3,
	TargetState=(SpinState=Triplet,Symmetry=2,Root=1))
	/D95(d) Opt test
	# SAC-CI(SACOnly,TargetState=(SpinState=Singlet,Symmetry=1,Root=0))
	/D95(d) Opt test

test652.com	# SAC-CI(CationDoublet=(NState=(0,0,0,1),SpinDensity))/D95 test # SAC-CI(CationDoublet=(NState=(0,0,1,0),SpinDensity))/D95 test # SAC-CI(CationDoublet=(NState=(0,0,1,0),SpinDensity))/D95 test
test653.com	# SAC-CI(Singlet=(NState=(2,0,0,0)),LevelOne)/Gen 5D test # SAC-CI(Singlet=(NState=(2,0,0,0)),LevelOne)/Gen 5D test

test654.com	# SAC-CI(Singlet=(NState=(0,1,0,0),Variational,Iterative),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/D95 Opt test
	# SAC-CI(Singlet=(NState=(0,1,0,0),Variational,InCoreDiag),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
	InCoreSAC)/D95 Opt test
	# SAC-CI(Singlet=(NState=(0,1,0,0),NonVariational,Iterative),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/D95 Opt test
	# SAC-CI(Singlet=(NState=(0,1,0,0),NonVariational,InCoreDiag),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
	InCoreSAC)/D95 Opt test

test655.com	# SAC-CI(Triplet=(NState=(0,0,1,0),Variational,Iterative),
	TargetState=(SpinState=Triplet,Symmetry=3,Root=1))
	/D95 Opt test
	# SAC-CI(Triplet=(NState=(0,0,1,0),Variational,InCoreDiag),
	TargetState=(SpinState=Triplet,Symmetry=3,Root=1),
	InCoreSAC)/D95 Opt test
	# SAC-CI(Triplet=(NState=(0,0,1,0),NonVariational,Iterative),
	TargetState=(SpinState=Triplet,Symmetry=3,Root=1))
	/D95 Opt test
	# SAC-CI(Triplet=(NState=(0,0,1,0),NonVariational,InCoreDiag),
	TargetState=(SpinState=Triplet,Symmetry=3,Root=1),
	InCoreSAC)/D95 Opt test

test656.com	# SAC-CI(CationDoublet=(NState=(1,0,0,0),Variational,Iterative),
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1))
	/D95 Opt test
	# SAC-CI(CationDoublet=(NState=(1,0,0,0),Variational,InCoreDiag)
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1),
	InCoreSAC)/D95 Opt test
	# SAC-CI(CationDoublet=(NState=(1,0,0,0),NonVariational,Iterative),
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1))
	/D95 Opt test
	# SAC-CI(CationDoublet=(NState=(1,0,0,0),NonVariational,InCoreDiag),
	TargetState=(SpinState=CationDoublet,Symmetry=1,Root=1),
	InCoreSAC)/D95 Opt test

test657.com	# SAC-CI(AnionDoublet=(NState=(0,0,1,0),Variational,Iterative),
	Targetstate=(SpinState=AnionDoublet,Symmetry=3,Root=1))
	/D95 Opt test
	# SAC-CI(AnionDoublet=(NState=(0,0,1,0),Variational,InCoreDiag),
	Targetstate=(SpinState=AnionDoublet,Symmetry=3,Root=1),
	InCoreSAC)/D95 Opt test
	# SAC-CI(AnionDoublet=(NState=(0,0,1,0),NonVariational,Iterative),
	Targetstate=(SpinState=AnionDoublet,Symmetry=3,Root=1))
	/D95 Opt test
	# SAC-CI(AnionDoublet=(NState=(0,0,1,0),NonVariational,InCoreDiag),
	Targetstate=(SpinState=AnionDoublet,Symmetry=3,Root=1),
	InCoreSAC)/D95 Opt test

test658.com	# SAC-CI(Singlet=(NState=(0,1),Variational),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/3-21G Opt CPHF=Canonical test
	# SAC-CI(Singlet=(NState=1,Variational),
	TargetState=(SpinState=Singlet,Symmetry=1,Root=1),
	LMO=PM,CutoffDIISZVec=1.0d-3)/3-21G Opt Nosymmetry test
	# SAC-CI(Singlet=(NState=(0,1),NonVariational),
	TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
	/3-21G Opt CPHF=Canonical test
	# SAC-CI(Singlet=(NState=1,NonVariational),
	TargetState=(SpinState=Singlet,Symmetry=1,Root=1),
	LMO=PM,CutoffDIISZVec=1.0d-3)/3-21G Opt Nosymmetry test

test659.com	# SAC-CI(Singlet=(NState=1,Variational),
	LMO=PM,BGSUM)/3-21G Nosymmetry test
	# SAC-CI(Singlet=(NState=1,Variational),
	CGSUM)/3-21G Nosymmetry test
	# SAC-CI(Singlet=(NState=1,Variational),
	CGSUM)/3-21G Nosymmetry test
	# SAC-CI(Singlet=(NState=1,Variational),

	TargetState=(SpinState=Singlet,Symmetry=1,Root=1),
	AGSUM)/3-21G Opt=ModRedundant Nosymmetry test
	# SAC-CI(Singlet=(NState=1,NonVariational),
	TargetState=(SpinState=Singlet,Symmetry=1,Root=1),
	AGSUM)/3-21G Opt=ModRedundant Nosymmetry test

test660.com	# SAC-CI(Full,Quartet=(NState=(0,1,0,0,0,0,0,0),Variational),
	Targetstate=(SpinState=Quartet,Symmetry=2,Root=1))
	/D95 Opt test
	# SAC-CI(Full,Quartet=(NState=(0,1,0,0,0,0,0,0),Variational,InCoreDiag),
	Targetstate=(SpinState=Quartet,Symmetry=2,Root=1),
	InCoreSAC)/D95 Opt test
	# SAC-CI(Full,Quartet=(NState=(0,1,0,0,0,0,0,0),NonVariational,Iterative)
	Targetstate=(SpinState=Quartet,Symmetry=2,Root=1))
	/D95 Opt test
	# SAC-CI(Full,Quartet=(NState=(0,1,0,0,0,0,0,0),NonVariational,InCoreDia
	Targetstate=(SpinState=Quartet,Symmetry=2,Root=1),
	InCoreSAC)/D95 Opt test

test661.com	# SAC-CI(AnionDoublet=(NState=(0,2,0,0),MaxR=4),
	TargetState=(SpinState=AnionDoublet,Symmetry=2,Root=2),
	General-R,MaxItDiag=100)/D95** Opt test

test663.com	# SAC-CI(Singlet=(NState=1),
	Targetstate=(SpinState=Singlet,Symmetry=1,Root=1),
	LMO=PM,General-R)/3-21G Opt Nosymmetry

test664.com	# SAC-CI(CationDoublet=(NState=1,Variational,Iterative), SD-R,RefCISD)/D95 test

test665.com	# SAC-CI(CationDoublet=(NState=3),
	TransitionFrom=(SpinState=CationDoublet,Symmetry=1,Root=2),
	FullActive)/D95 Unit=Bohr test

test666.com	# SAC-CI(Singlet=(NState=3),
	TransitionFrom=(SpinState=Singlet,symmetry=1,root=2),
	FullActive)/D95 Unit=Bohr test

test667.com	# SAC-CI(CationDoublet=(NState=(10,0,1,1),MaxR=3), General-R,FullRGeneration,MaxItDiag=300)/D95** test

test668.com	# SAC-CI(Singlet=(NState=3),TransitionFrom=(SpinState=Singlet,
	Symmetry=1,Root=2), General-R,MaxItDiag=256)/D95 Unit=Bohr test

test669.com	# SAC-CI(Aniondoublet=(NState=1))/D95 ROHF test
test670.com	# SAC-CI(Triplet=(NState=1))/D95 ROHF test
test671.com	# SAC-CI(Cationdoublet=(NState=1))/D95 ROHF test
test672.com	# SAC-CI(CationDoublet=(NState=1,NonVariational))/D95 ROHF test

test673.com	# SAC-CI(AnionDoublet=(NState=1),General-R)/D95 ROHF test
test674.com	# SAC-CI(CationDoublet=(NState=1),General-R)/D95 ROHF test
test675.com	# SAC-CI(Cationdoublet=(NState=1,NonVariational),General-R)/D95 ROHF tes
test676.com	#p lsda/sto-3g/auto admp=maxpoint=3 test
test677.com	#p B3LYP gen freq test #p B3LYP gen freq test int=beckeweight
test678.com	#P test ONIOM(mp2/6-311g**:b3lyp/6-31g*:hf/3-21g) nmr
test679.com	#P test ONIOM(b3lyp/6-311g**:b3lyp/6-31g*:hf/3-21g) polar cphf=rdfreq
test680.com	#P test ONIOM(b3lyp/6-311g**:b3lyp/6-31g*:hf/3-21g) nmr=spin
test681.com	#p freq=raman cphf=rdfreq oniom(b3lyp/6-31g*:hf/3-21g) test
test682.com	#P ONIOM(mp2/6-311g**:b3lyp/6-31g*:hf/3-21g) freq=raman test
test683.com	#P ccsd/6-31g* 5d opt freq test #p ccsd/6-31g* 5d force tran=iabc geom=allcheck guess=read #p ccsd=noincore/6-31g* 5d force tran=iabc geom=allcheck guess=read #p ccsd/6-31g* 5d force tran=iabc geom=allcheck guess=read extrabasis in
test684.com	#p ccsd/6-31g* 5d opt freq test #p ccsd/6-31g* 5d force tran=iabc geom=allcheck guess=read #p ccsd=noincore/6-31g* 5d force tran=iabc geom=allcheck guess=read
test685.com	#p uff=softonly opt=tight geom=connect nosym test #p uff=softonly opt=(calcall,nomicro,tight) geom=connect nosym test #p uff=softonly opt=(nomicro,tight) geom=connect nosym test #p ccsd/6-31g* 5d force tran=iabc geom=allcheck guess=read extrabasis in
test686.com	#p cis(d)/3-21g test geom=modela #p cis(d,triplet)/3-21g test geom=modela
test687.com	#p cis(d)/3-21g test geom=modela
test688.com	#p rb3lyp/6-311+g(d,p) test polar=optrot cphf=rdfreq #p rb3lyp/6-311+g(d,p) test polar=optrot cphf=rdfreq scrf=solvent=ccl4 geom=check guess=read #p rb3lyp/6-311+g(d,p) test polar=optrot cphf=rdfreq scrf geom=check gue
test689.com	#SAC-CI(Singlet=(NState=1), FullActive,BGSUM)/D95 Nosymmetry test #SAC-CI(Singlet=(NState=1), FullActive,CGSUM)/D95 Nosymmetry test #SAC-CI(Singlet=(NState=1), FullActive,CGSUM)/D95 Nosymmetry test #SAC-CI(Singlet=(NState=1), TargetState=(SpinState=Singlet,Symmetry=1,Ro FullActive,AGSUM)/D95 Opt Nosymmetry test #SAC-CI(Singlet=(NState=1), TargetState=(SpinState=Singlet,Symmetry=1,Ro FullActive,AGSUM)/D95 Geom=Chk Freq Nosymmetry test
test690.com	#p b3lyp/6-31g(d) scrf=(iefpcm,read) test scf=tight

	mdv=5242880 iop(1/2=-1,2/2=-1)
	#p b3lyp/6-31g(d) scrf=(iefpcm,read) test scf=tight
	mdv=5242880 iop(1/2=-1,2/2=-1)
	#p b3lyp/6-31g(d) scrf=(iefpcm,read) test scf=tight
	mdv=5242880 iop(1/2=-1,2/2=-1)
	#p b3lyp/6-31g(d) scrf=(iefpcm,read) test scf=tight
	mdv=5242880 iop(1/2=-1,2/2=-1)

test691.com	#p b3lyp/6-31G(d,p) scrf=(iefpcm,read) nosym scf=tight test #p b3lyp/6-31G(d,p) scrf=(iefpcm,read) nosym test scf=tight
test692.com	#p rblyp/6-31g*/dga1 5d geom=modela opt=tight freq scrf=dipole int=ultra #p rblyp/6-31g*/dga1 5d geom=check freq=numer polar scrf=dipole int=ultra
test693.com	#p ublyp/6-31g*/dga1 5d geom=modela opt=tight freq scrf=dipole int=ultra #p ublyp/6-31g*/dga1 5d geom=check freq=numer polar scrf=dipole int=ultra
test694.com	#p rblyp/6-31g*/dga1 5d geom=modela opt freq scrf int=ultrafine test #p rblyp/6-31g*/dga1 5d geom=check freq=numer polar scrf int=ultrafine te
test695.com	#p ublyp/6-31g*/dga1 5d geom=modela opt freq scrf int=ultrafine test #p ublyp/6-31g*/dga1 5d geom=check freq=numer polar scrf int=ultrafine te
test696.com	#p tpsstpss/6-31g* opt=(tight,calcfc) freq geom=(modela,print) int=ultra
test697.com	#p tpsstpss/6-31g* opt=(tight,calcfc) freq geom=(modela,print) int=ultra
test698.com	#p BVP86/SVP/Auto opt freq scrf=cosmo int=ultrafine test
test699.com	#p opt freq=noraman oniom(ub3lyp/genecp:uhf/genecp) test
计算输入档	**计算执行路径**
test700.com	#p hse2pbe/6-31g* pop=min scf=tight test
test701.com	#p hse2pbe/6-31g* scf=tight test opt
test702.com	#p pbeh1pbe/6-31g* test opt
test703.com	#p oniom(b3lyp/6-31g**:blyp/lp-31g**/auto)=compress opt freq test 5d #p oniom(b3lyp/6-31g**:blyp/lp-31g**/auto)=compress freq test geom=check iop(11/43=2) #p oniom(b3lyp/6-31g**:blyp/lp-31g**/auto)=nocompress freq test geom=che
test704.com	#p oniom(mp2/lp-31g**:hf/lanl2mb)=compress opt freq test 5d extrabasis i #p oniom(mp2/chkbas:hf/chkbas)=compress freq test geom=check guess=read #p oniom(mp2/chkbas:hf/chkbas)=nocompress freq test geom=check guess=rea #p oniom(mp2/chkbas:hf/chkbas)=nocompress freq test geom=check guess=rea
test705.com	#p oniom(cis=(direct)/6-31g*:hf/lp-31g*) force test 5d extrabasis int=no #p oniom(cis=(direct,read)/chkbas:hf/chkbas)=compress freq test geom=allcheck guess=read #p oniom(cis=(direct,read)/chkbas:hf/chkbas)=compress freq test iop(11/4 geom=allcheck guess=read

	#p oniom(cis=(direct,read)/chkbas:hf/chkbas)=nocompress freq test geom=allcheck guess=read #p oniom(cis=(direct,read)/chkbas:hf/chkbas)=nocompress freq test iop(11/ geom=allcheck guess=read

test706.com	#P oniom(b3lyp/3-21g:amber) geom=connectivity noarchive opt=(calcfc,quadr scf=novaracc
	freq=(nodiagfull,selectnm) int=ultrafine

test707.com	#p hf/3-21g force geom=modred test
test708.com	#p pbe1pbe/3-21g force test int=ultrafine #p pbe1pbe/3-21g force test int=ultrafine #p pbe1pbe/3-21g force test int=ultrafine
test709.com	#p ub3lyp/3-21g force test scf=novaracc
test710.com	#p HF/STO-3G OPT=TIGHT FREQ=ANHARM test
test711.com	#p HF/STO-3G FREQ test #p HF/STO-3G FREQ=(READFC,ANHARM,READANHARM) test
test712.com	#p rhf/3-21g freq=nnroa test
test713.com	#p b3lyp/3-21g freq=nnroa test
test714.com	#p rhf/3-21g freq=roa test cphf=rdfreq #p rhf/3-21g freq=(nnroa,four) test cphf=(rdfreq,nostatic)
test715.com	#p b3lyp/3-21g freq=roa test cphf=rdfreq int=ultrafine #p b3lyp/3-21g freq=(nnroa,fourpoint) test cphf=(rdfreq,nostatic) int=ul
test716.com	#p rtpsstpss/6-31g* 5d opt freq test
test717.com	#p utpsstpss/6-31g* 5d opt freq test
test718.com	#p b3lyp/6-31g* 5d test freq=roa cphf=rdfreq int=ultrafine
test719.com	#p RB3LYP/sdd opt freq scrf=cpcm test #p RB3LYP/sdd freq=numer polar geom=check guess=read scrf=cpcm test #p RB3LYP/sdd opt=readfc freq geom=check guess=read scrf=(iefpcm,solvent= #p RB3LYP/sdd freq=numer polar geom=check guess=read scrf=(iefpcm,solvent=
test720.com	#p ub3lyp/sdd opt freq scrf=cpcm test scf=(fermi,xqc) #p uB3LYP/sdd freq=numer polar geom=check guess=always scrf=(cpcm,check) scf=(intrep,fermi,xqc) #p uB3LYP/sdd opt freq geom=check guess=read scrf=(iefpcm,solvent=cycloh optcyc=40 scf=(fermi,intrep,xqc) #p uB3LYP/sdd freq=numer polar geom=check guess=always scrf=(iefpcm,solvent=cyclohexane,check) test scf=(xqc,fermi,intrep)

test722.com	#p dreiding=(softonly) geom=connectivity nosym
test723.com	#p dreiding=(softonly) geom=connectivity nosym
test724.com	#P ROMP2/CBSB3 CBSExtrap=NMin=10 test
test725.com	#p ONIOM(CAS(4,4)/6-31g*:CAS(4,4)/STO-3G) Guess=Alter Opt=Conical Test N
test726.com	#p external=extuffex opt=(tight,nomicro) nosym test
test727.com	#p b3lyp/6-311G(df,pd) 5d 7f Units=Bohr NMR test scrf #p b3lyp/6-311G(df,pd) 5d 7f Units=Bohr NMR test scrf
test729.com	#p rb3lyp/6-31G(d) td(singlet) geom(modela) density(current) force test #p rblyp/6-31G(d) td(singlet) geom(modela) density(current) force test #p rblyp/6-31G(d)/auto td(singlet) geom(modela) density(current) force t
test730.com	#p rb3lyp/6-31G(d) td(triplet) geom(modela) density(current) force test #p rblyp/6-31G(d) td(triplet) geom(modela) density(current) force test #p rblyp/6-31G(d)/auto td(triplet) geom(modela) density(current) force t
test731.com	#p ub3lyp/6-31G(d) td geom(modela) density(current) force test #p ublyp/6-31G(d) td geom(modela) density(current) force test #p ublyp/6-31G(d)/auto td geom(modela) density(current) force test
test732.com	#p rb3lyp/3-21g td=singlet force density=curr test geom=modela #p rb3lyp/3-21g td=triplet force density=curr test geom=modela #p ub3lyp/3-21g td force density=curr test geom=modela #p ub3lyp/3-21g td=root=2 force density=curr test geom=modela #p ub3lyp/3-21g td force density=curr test geom=modela #p ub3lyp/3-21g td force density=curr test geom=modela #p rblyp/3-21g td=singlet force density=curr test geom=modela #p rblyp/3-21g td=triplet force density=curr test geom=modela #p ublyp/3-21g td force density=curr test geom=modela #p ublyp/3-21g td=root=2 force density=curr test geom=modela #p ublyp/3-21g td force density=curr test geom=modela #p ublyp/3-21g td force density=curr test geom=modela #p rblyp/3-21g/auto td=singlet force density=curr test geom=modela #p rblyp/3-21g/auto td=triplet force density=curr test geom=modela #p ublyp/3-21g/auto td force density=curr test geom=modela #p ublyp/3-21g/auto td=root=2 force density=curr test geom=modela #p ublyp/3-21g/auto td force density=curr test geom=modela #p ublyp/3-21g/auto td force density=curr test geom=modela

test733.com	#P ROHF/STO-3G test scf=tight
	#P CASSCF(4,4)/STO-3G guess=read geom=check test
	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=3,slater)/STO-3G guess=read geom=che
	scfcyc=3 iop(5/13=1,5/106=1)
	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=3,slater)/STO-3G geom=check test gue
	iop(5/106=3)

	#P CASSCF(22,22,rasscf(1,9,1,9),nroot=6,slater)/STO-3G guess=read geom=che
	iop(5/106=3)

test734.com	#p cndo test force #p cndo test force scf=conventional #p cndo test force use=l402
test735.com	#p hf/sto-3g irc(calcfc) use=l123 test
test736.com	#p opt=quadmac test oniom(b3lyp/6-311g(d,p):pm6:uff) geom=connectivity
test737.com	#p int=aml test scf(tight) force scrf(read)
test738.com	#p uhf/d95++** scrf=(iefpcm,read,solvent=water) test
test739.com	#p zindo scrf(cpcm) geom(modela) test #p zindo scrf(cpcm,read) geom(modela) test #p zindo(eqsolv) scrf(cpcm) geom(modela) test #p zindo(eqsolv) scrf(cpcm,read) geom(modela) test #p zindo scrf(pcm) geom(modela) test #p zindo scrf(read) geom(modela) test #p zindo(eqsolv) scrf(pcm) geom(modela) test #p zindo(eqsolv) scrf(read) geom(modela) test
test740.com	#p ehtsc=read test scf=tight #p ehtsc=chk test scf=tight geom=check guess=read #p ehtsc=chk test scf=tight geom=check
test741.com	#p cas(4,4)/6-31g(d,p) test BOMD=(gradientonly,maxpoint=10,readmwvel)
test742.com	#p HF/6-31G(d) freq=(temp=200,anharm) test #p HF/6-31G(d) geom=checkpoint freq=(readfc,temp=200,anharm,readanharm)
test744.com	#p oniom(hf:amber) geom=connectivity test opt=tight freq
test745.com	#p oniom(hf:amber)=embed geom=connectivity test opt=tight freq
test748.com	#p bmk 6-311G(d,p) opt(tight) int(grid=ultrafine) freq test
test749.com	#p bmk 6-311G(d,p) opt(tight) int(grid=ultrafine) freq test
test750.com	#p pbe1pbe/6-31G(d) test nosymm scrf(pcm) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,dovac) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,skipvac) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(read) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,dovac,check) geom(check) scf(t #p pbe1pbe/6-31G(d) test nosymm scrf(self,skipvac,check) geom(check) scf
test751.com	#p pbe1pbe/6-31G(d) test nosymm scrf(pcm) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,dovac) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,skipvac) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(read) geom(check) scf(tight) #p pbe1pbe/6-31G(d) test nosymm scrf(self,dovac,check) geom(check) scf(t

	#p pbe1pbe/6-31G(d) test nosymm scrf(self,skipvac,check) geom(check) scf

test752.com	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm density(all)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1,eqsolv) test nosymm scrf(read) d
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf(read) density(
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)

test753.com	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1) test nosymm density(all)
	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1,eqsolv) test nosymm scrf(r
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1) test nosymm scrf(read)
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1) test nosymm scrf=(self,
	density(all)
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1) test nosymm scrf=(self,
	density(all)
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(triplet,nstates=1,root=1) test nosymm scrf=(self,
	density(all)
	geom(check) guess(check)

test754.com	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm density(all)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1,eqsolv) test nosymm scrf(read) d
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf(read) density(
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)
	#p pbe1pbe/6-31G(d) td(nstates=1,root=1) test nosymm scrf=(self,skipvac,r
	geom(check) guess(check)

test755.com	#p HSE2PBE/6-31G* Opt freq test int=ultrafine #p HSE2PBE/6-31G* Opt freq test int=ultrafine geom=modela
test756.com	#p PBEH1PBE/6-31G* Opt freq int=ultrafine #p pbeh1pbe/6-31G* Opt freq test int=ultrafine geom=modela

test757.com	#p rhf/sto-3g test td(full,singlet,sos) nosymm #p rhf/sto-3g test td(full,singlet,sos) #p rhf/sto-3g test td(full,singlet,sos) nosymm
test758.com	#p rb3lyp/aug-cc-pvtz geom=modela nmr=mixed test
test759.com	#p rhf/sto-3g test nmr=igaim IOp(10/46=6) cphf=(conver=10,rdfreq) #p rhf/sto-3g test nmr=igaim IOp(10/46=4) cphf=(conver=10,rdfreq) #p rhf/sto-3g test nmr=igaim IOp(10/46=5) cphf=(conver=10,rdfreq) #p rhf/sto-3g test nmr=igaim IOp(10/46=3) cphf=(conver=10,rdfreq)
test760.com	#p uhf/sto-3g test nmr=igaim IOp(10/46=6) cphf=(conver=10,rdfreq) #p uhf/sto-3g test nmr=igaim IOp(10/46=4) cphf=(conver=10,rdfreq) #p uhf/sto-3g test nmr=igaim IOp(10/46=5) cphf=(conver=10,rdfreq)
test761.com	#p b3lyp/6-31G* test nmr=igaim IOp(10/46=6) cphf=(sg1,conver=10,rdfreq) #p b3lyp/6-31G* test nmr=igaim IOp(10/46=4) cphf=(sg1,conver=10,rdfreq) #p b3lyp/6-31G* test nmr=igaim IOp(10/46=5) cphf=(sg1,conver=10,rdfreq) #p b3lyp/6-31G* test nmr=igaim IOp(10/46=3) cphf=(sg1,conver=10,rdfreq)
test762.com	#p rhf/aug-cc-pVDZ test nmr=igaim IOp(10/46=6) cphf=(conver=10,rdfreq)

test763.com	#p hf 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p hf 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p hf 6-31G(d) scrf(read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p hf 6-31G(d) scrf(read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)

test764.com	#p hf 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela) mdv=8388608 i #p hf 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela) mdv=8388608 i #p hf 6-31G(d) scrf(read) nmr(giao) test geom(modela) mdv=8388608 iop(1/ #p hf 6-31G(d) scrf(read) nmr(giao) test geom(modela) mdv=8388608 iop(1/

test765.com	#p mp2(full) 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p mp2(full) 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p mp2(full) 6-31G(d) scrf(read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p mp2(full) 6-31G(d) scrf(read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)

test766.com	#p ump2(full) 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)
	#p ump2(full) 6-31G(d) scrf(cpcm,read) nmr(giao) test geom(modela)
	mdv=8388608 iop(1/2=-1,2/2=-1)

	#p ump2(full) 6-31G(d) scrf(read) nmr(giao) test geom(modela) mdv=8388608 iop(1/2=-1,2/2=-1) #p ump2(full) 6-31G(d) scrf(read) nmr(giao) test geom(modela) mdv=8388608 iop(1/2=-1,2/2=-1)
test769.com	#p freq=noraman oniom(external="mygau g09 b3lyp 6-311G\(d\,p\)":uff=qeq) geom=connectivity test
test770.com	#P hse2pbe/6-31G** 5d test td=(nstates=6,50-50)
test771.com	#p wlu geom=modela test #p wlu=(saveamp,readamp) geom=modela test
test774.com	#p ghf/gen pseudo=read 5d 7F freq=numer polar scf=novaracc test
test775.com	#p ONIOM(hf/sto-3g:uff) freq=(noraman,printfrozen) test #p ONIOM(hf/sto-3g:uff) freq=readfc test geom=check #p ONIOM(hf/sto-3g:uff) freq test geom=check nosymm
test776.com	#p ONIOM(HF/3-21G:UFF) NoSymm Freq=(NFreq=5,noraman) Geom=Connect test #p ONIOM(HF/3-21G:UFF) Freq=(NFreq=5,noraman) Geom=check
test777.com	#p oniom(hf/3-21g:uff) freq test
test778.com	#p ONIOM(HF/3-21G:UFF) NoSymm Freq=(NFreq=2,noraman) Geom=Connect
test779.com	#p thcthhyb/6-31g* 5d freq=raman test int=ultrafine cphf=finegrid
test780.com	#P UBP86/6-311G* test guess=(fragment=8,only) pop=none #P UBP86/6-311G*/auto test guess=read scf=(tight,novaracc) stable=(opt,qcon
test781.com	#P UBP86/6-311G* test guess=(fragment=8) pop=none #P UBP86/6-311G*/auto test guess=read scf=(tight,novaracc) stable=(opt,qcon
test782.com	#p cam-b3lyp/6-311G(d,p) geom(modela) opt freq test #p cam-b3lyp/6-31+G(d) 5d td(fc,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p cam-b3lyp/6-31+G(d) 5d td(fc,nstates=2,root=1,triplet) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p cam-b3lyp/6-311G(d,p) geom=check guess=read opt=readfc freq test #p cam-b3lyp/6-31+G(d) 5d td(fc,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test
test783.com	#p lc-blyp/6-311G(d,p) geom(modela) opt freq test #p lc-blyp/6-31+G(d) 5d td(full,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p lc-blyp/6-31+G(d) 5d td(full,nstates=2,root=1,triplet) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p lc-blyp/6-311G(d,p) geom=check guess=read opt=readfc freq test #p lc-blyp/6-31+G(d) 5d td(full,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test

test785.com	#p hseh1pbe/6-311G(d,p) geom(modela) opt freq test
	#p hseh1pbe/6-31+G(d) 5d td(full,nstates=2,root=1)
	geom(check) guess(check) int(grid=ultrafine) test force density(all)
	#p hseh1pbe/6-31+G(d) 5d td(full,nstates=2,root=1,triplet)
	geom(check) guess(check) int(grid=ultrafine) test force density(all)
	#p hseh1pbe/6-311G(d,p) geom=check guess=read opt=readfc freq test
	#p hseh1pbe/6-31+G(d) 5d td(full,nstates=2,root=1)
	geom(check) guess(check) int(grid=ultrafine) test force density(all)

test786.com	#p b3lyp/6-311G(d,p) geom(modela) opt freq test #p b3lyp/6-31+G(d) 5d td(full,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p b3lyp/6-31+G(d) 5d td(full,nstates=2,root=1,triplet) force geom(check) guess(check) density(all) int(grid=ultrafine) test #p b3lyp/6-311G(d,p) geom=check guess=read opt=readfc freq test #p b3lyp/6-31+G(d) 5d td(full,nstates=2,root=1) force geom(check) guess(check) density(all) int(grid=ultrafine) test
test787.com	#p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(iefpcm) NOSYMM test scf=tight #p HF/6-31G* scrf=iefpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm) NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G** scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* NOSYMM scrf=cpcm test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=cpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(iefpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=cpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight #p HF/6-31G* scrf=dpcm NOSYMM test scf=tight #p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight

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#p HF/6-31G* scrf=dpcm NOSYMM test scf=tight
#p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=dpcm NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=dpcm NOSYMM test scf=tight mdv=5000000 iop(1/2=-1,2/2=
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=(cpcm) NOSYMM test scf=tight
#p HF/6-31G* NOSYMM scrf=(dpcm,read) test scf=tight
#p HF/gen pseudo=read gfinput scrf=(dpcm) NOSYMM test scf=tight
#p HF/gen pseudo=read gfinput scrf=(cpcm,read) NOSYMM test scf=tight
#p HF/6-31G* NOSYMM scrf=(dpcm) test scf=tight
#p HF/gen 6d pseudo=read NOSYMM scrf=(cpcm,read) test scf=tight
#p HF/gen pseudo=read 6d scrf=dpcm NOSYMM test scf=tight
#p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=cpcm NOSYMM test scf=tight
#p HF/6-31G* NOSYMM scrf=(dpcm,read) test scf=tight
#p HF/6-31G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(cpcm,read) NOSYMM test scf=tight mdv=6000000 iop(1/2=
#p HF/6-31G* scrf=(cpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM iop(2/15=3) test scf=tight
#p HF/6-31G* scrf=(cpcm) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=8000000 iop(1/2=
#p HF/6-31G* scrf=(cpcm) NOSYMM test scf=tight mdv=5000000 iop(1/2=-1,2/
#p HF/6-31G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31G* scrf=(dpcm) NOSYMM test scf=tight mdv=5000000 iop(1/2=-1,2/
#p HF/6-31+g* scrf=(cpcm) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(dpcm,read) NOSYMM test scf=tight mdv=5000000 iop(1/2
#p HF/6-31+G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(cpcm,read) NOSYMM test scf=tight
#p HF/LANL2DZ scrf=(dpcm) NOSYMM extrabasis gfinput test scf=tight
#p HF/LANL2DZ scrf=(dpcm) NOSYMM extrabasis gfinput test scf=tight
#p HF/6-31+G* scrf=(dpcm) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(iefpcm,read) NOSYMM test scf=tight
#p HF/6-31+G* scrf=(dpcm) NOSYMM test scf=tight
!#p HF/6-31G* scrf=dpcm NOSYMM opt test
#p HF/6-31G* scrf=cpcm NOSYMM opt test
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	#p HF/6-31G* scrf=iefpcm NOSYMM opt test #p HF/6-31G* scrf=ivcpcm NOSYMM opt test

test788.com	#p oniom(b3lyp/6-311g**:blyp/6-31g*)=compress freq=raman test 5d cphf=rd
	int=ultrafine cphf=ultrafine

test789.com	#p oniom(b3lyp:hf:amber)=scale=20 test opt iop(1/52=1212013)
test790.com	#p am1 force(enonly,step=1) scrf(cpcm) geom(modela) test scfcon=10 #p am1 force scrf(cpcm) geom(modela) test scfcon=10 #p am1 force scrf(cpcm,read) geom(modela) test scfcon=10 #p am1 force(enonly,step=1) scrf(pcm) geom(modela) test scfcon=10 #p am1 force scrf(pcm) geom(modela) test scfcon=10 #p am1 force scrf(read) geom(modela) test scfcon=10
test791.com	#p oniom(hf:uff)=scale=5 freq=raman test geom=connect #p oniom(hf:uff)=(scale=5,nocompress) freq=raman test geom=check guess=r #p oniom(hf:uff)=(scale=5) freq=raman test geom=check guess=read nosymm #p oniom(hf:uff)=(scale=5,nocompress) freq=raman test geom=check guess=r
test792.com	#p force oniom(b3lyp/6-31g(d):amber=hardfirst)=embed test 5d geom=connec #p freq=(vcd,raman) oniom(b3lyp/6-31g(d):amber)=embed test 5d geom=check
test799.com	#p bd(full)/6-31g* 5d geom=modela opt test #p bd=(full,read)/6-31g* 5d geom=allcheck force use=l916 test #p bd=(full,read)/6-31g* 5d geom=allcheck freq polar test
计算输入档	计算执行路径
test800.com	#p bd(full)/6-31g* 5d geom=modela opt test #p bd=(full,read)/6-31g* 5d geom=allcheck force use=l916 test #p bd=(full,read)/6-31g* 5d geom=allcheck freq polar test
test801.com	#p pbe1pbe/3-21g force test int=ultrafine #p pbe1pbe/3-21g force test int=ultrafine #p pbe1pbe/3-21g force test int=ultrafine
test802.com	#p hse1pbe/3-21g force test int=ultrafine #p hse1pbe/3-21g force test int=ultrafine #p hse1pbe/3-21g force test int=ultrafine
test803.com	#p LC-wPBE/6-311G(df,p) 5d 7f opt(tight) freq(noraman) geom(modela) int(gri
test804.com	#p LC-wPBE/6-311G(df,p) 5d 7f opt(tight) freq(noraman) geom(modela) int(gri
test805.com	#p ONIOM(RHF/6-31G(d):hf/sto-3g:uff)=scalecharge=5 test freq=noraman 5d
test806.com	#p hf/3-21g opt=tight freq=hindered geom=connectivity test
test807.com	#p tpsstpss/6-311g(d) 5d 7f freq=hindered geom=connectivity test
test808.com	#p dreiding=softonly geom=connectivity iop33(4=2) test
test809.com	#p dreiding=softonly iop33(4=2) test

test810.com	#p dreiding=softonly iop33(4=2) test
test811.com	#p dreiding=softonly geom=connectivity iop33(4=2) test

test813.com	#p uhf/6-31g* 5d freq nosymm test geom=modela scfcon=10 cphf=conver=10 i
	#p uhf/6-31g* 5d freq nosymm test geom=modela iop(4/115=100)scfcon=10 cp
	int=acc2e=12
	#p uhf/6-31g* 5d freq=(numer,four) polar nosymm test geom=modela iop(4/1
	scfcon=10 cphf=conver=10 int=acc2e=12

test814.com	#p uhf/3-21g complex freq=(numer,four) polar nosymm test geom=modela iop
	scfcon=10 cphf=conver=10 int=acc2e=12

test815.com	#p ghf/3-21g freq=(numer,four) polar nosymm test geom=modela iop(4/115=1
test816.com	#p blyp/6-31G(df)/auto 5d 7f force fmm test geom(modela) #p blyp/6-31G(df)/auto 5d 7f freq fmm test geom(modela)
test817.com	#p rm05/6-31G(df,p) 5d 7f test geom=modela force #p rm05/6-31G(df,p) 5d 7f test geom=modela freq #p rm052x/6-31G(df,p) 5d 7f test geom=modela force #p rm052x/6-31G(df,p) 5d 7f test geom=modela freq #p um05/6-31G(df,p) 5d 7f test geom=modela force #p um05/6-31G(df,p) 5d 7f test geom=modela freq #p um052x/6-31G(df,p) 5d 7f test geom=modela force #p um052x/6-31G(df,p) 5d 7f test geom=modela freq
test818.com	#p hse1pbe/lp-31g* 5d test int=ultrafine opt=(tight,addredundant)
test819.com	#p HF/sto-3g freq=numer int(grid=ultrafine)
test820.com	#p svwn5/sto-3g int(grid=ultrafine) freq=numer pbc=nrecip=-100
test821.com	#p svwn5/sto-3g Int(Grid=UltraFine) freq=numer pbc=nrecip=-24
test822.com	#p ghf/3-21g freq=(numer,four) polar nosymm test geom=modela iop(4/115=1
test823.com	#p CCSD=FC1 Opt Gen test
test824.com	#p oniom(hf:amber)=nocompress geom=connectivity test opt=(calcall,quadma
test825.com	#p oniom(hf:amber)=embed geom=connectivity test opt=(maxcyc=100,calcfc)
test826.com	#p oniom(hf:amber)=embed geom=connectivity test opt=(maxcyc=100,calcall,t
test827.com	#P HSE1PBE 6-311+G Int(Grid=UltraFine) scf=tight test #P HSE1PBE 6-311+G Int(Grid=UltraFine) scf=tight test symm=noscf #P HSE1PBE 6-311+G Int(Grid=UltraFine) scf=tight test nosymm
test828.com	#p freq=roa cphf=rdfreq oniom(b3lyp/6-31g*:blyp/3-21g) test
test829.com	#p ONIOM(b3lyp/6-31G(d):uff)=scalecharge=5 test freq=roa cphf=rdfreq 5d
test832.com	#p oniom(b3lyp/6-31G(d):uff) scrf=(oniompcm=A,read) 5d 7f test int(grid= #p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=A,restart) 5d 7f test int(gri

	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=B,modify) 5d 7f test int(grid=
	geom(check)
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=C,modify) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=C,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test833.com	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=A,read) 5d 7f
	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=A,restart) 5d
	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(modify,oniompcm=B) 5d
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=C,modify) 5d
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=C,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scr(oniompcm=X,check) 5d 7f
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test834.com	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=A,read) 5d 7f test
	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=A,restart) 5d 7f test
	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=B,modify) 5d 7f test
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=C,modify) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=C,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test835.com	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=A,read) 5d 7f

	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=A,restart) 5d
	int(grid=ultrafine)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=B,modify) 5d
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=C,modify) 5d
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=C,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(b3lyp/6-31G(d):uff)=(embed,scale=5) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test836.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=A,read) 5d 7f
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=B,modify) 5d
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=C,modify) 5d
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=C,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test837.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=A,read) 5d 7f
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=A,restart) 5d
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=B,modify) 5d
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=C,modify) 5d
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=C,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=X,check) 5d 7
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq

	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto) scrf(oniompcm=X,check) 5d 7 int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test838.com	#p oniom(b3lyp/6-31G(d):am1) scrf(oniompcm=C,read) 5d 7f test
	int(grid=ultrafine) opt(tight)
	#p oniom(b3lyp/6-31G(d):am1) scrf(oniompcm=C,check) 5d 7f test
	int(grid=ultrafine) opt(tight,restart)
	#p oniom(b3lyp/6-31G(d):am1) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,readfc)
	#p oniom(b3lyp/6-31G(d):am1) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart)

test839.com	#p oniom(am1:uff) scrf(oniompcm=C,read) 5d 7f test
	int(grid=ultrafine) opt(tight)
	#p oniom(am1:uff) scrf(oniompcm=C,check) 5d 7f test
	int(grid=ultrafine) opt(tight,restart)
	#p oniom(am1:uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,readfc)
	#p oniom(am1:uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart)

test840.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=A,read) 5
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=A,restart
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=B,modify)
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=C,modify)
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=C,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=X,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=X,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test841.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 7f test int(grid=ultrafine) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 5d 7f test int(grid=ultrafine) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 5d 7f test

	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w disappear. int(grid=ultrafine) geom(check) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 5d 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(oni 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(oni 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(oni 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test842.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=A,read) 5
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=A,restart)
	int(grid=ultrafine)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=B,modify)
	! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w
	disappear.
	int(grid=ultrafine) geom(check)
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=C,modify)
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=C,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=X,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq
	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff) scrf(oniompcm=X,check) 5
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test843.com	#p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 7f test int(grid=ultrafine) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 5d 7f test int(grid=ultrafine) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on 5d 7f test ! int(grid=ultrafine) geom(check) guess(check) --- guess(check) is broken w disappear. int(grid=ultrafine) geom(check) #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(on

	5d 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(oni 7f test int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(ch int(grid=ultrafine) geom(check) guess(check) opt(tight,calcfc) freq #p oniom(mp2(full)/6-31G(d):blyp/3-21G/auto:uff)=(embed,scale=5) scrf(ch int(grid=ultrafine) geom(check) guess(check) opt(tight,restart) freq

test844.com	#p oniom(b3lyp/6-31G(d):am1:uff) scrf(oniompcm=C,read) 5d 7f test
	int(grid=ultrafine) opt(tight)
	#p oniom(b3lyp/6-31G(d):am1:uff) scrf(oniompcm=C,check) 5d 7f test
	int(grid=ultrafine) opt(tight,restart)
	#p oniom(b3lyp/6-31G(d):am1:uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,readfc)
	#p oniom(b3lyp/6-31G(d):am1:uff) scrf(oniompcm=X,check) 5d 7f test
	int(grid=ultrafine) geom(check) guess(check) opt(tight,restart)

test845.com	#p uhf/6-31g(df,p) test freq=(vcd,readiso) 5d 7f #p uhf/6-31g(df,p) test freq=roa 5d 7f cphf=rdfreq geom=allcheck guess=r #p uhf/6-31g(df,p) test freq=(roa,vcd) 5d 7f cphf=rdfreq geom=allcheck g

test848.com	#p rhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,grid=ultra
	int=ultrafinegrid scf(conver=10) field=Y-50 scrf(cpcm,read) int=acc2e=12
	#p rhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,grid=ultra
	int=ultrafinegrid scf(noincore,conver=10) int=fofcou field=Y-50 scrf(cpc
	int=acc2e=12
	#p rhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic,
	iop(10/49=112) int=ultrafinegrid scf(noincore,conver=10) int(fofcou) fie
	scrf(cpcm,read)
	int=acc2e=12
	#p rhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic,
	iop(10/49=113,11/6=1,11/24=10) int=ultrafinegrid scf(noincore,conver=10)
	int=acc2e=12 field=Y-50 scrf(cpcm,read)

test849.com	#p uhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostatic,g nosymm int=ultrafinegrid scf(conver=10) field=Y-50 scrf(cpcm,read) int=acc2e=12 #p uhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostatic,g nosymm int=ultrafinegrid scf(noincore,conver=10) int(fofcou) field=Y-50 scrf(cp int=acc2e=12 #p uhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic, nosymm iop(10/49=112) int=ultrafinegrid scf(noincore,conver=10) int(fofcou) fie

	scrf(cpcm,read) int=acc2e=12 #p uhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic, nosymm iop(10/49=113,11/6=1,11/24=10) int=ultrafinegrid scf(noincore,conver=10) field=Y-50 scrf(cpcm,read) int=acc2e=12

test850.com	#p rhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,grid=ultra
	int=ultrafinegrid scf(conver=10) field=Y-50 scrf=read int=acc2e=12
	#p rhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,grid=ultra
	int=ultrafinegrid scf(noincore,conver=10) int=fofcou field=Y-50 scrf=rea
	#p rhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic,
	iop(10/49=112) int=ultrafinegrid scf(noincore,conver=10) int(fofcou) fie
	int=acc2e=12
	#p rhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic,
	iop(10/49=113,11/6=1,11/24=10) int=ultrafinegrid scf(noincore,conver=10)
	field=Y-50 scrf=read int=acc2e=12

test851.com	#p uhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostatic,g nosymm int=ultrafinegrid scf(conver=10) field=Y-50 scrf(read) int=acc2e=12 #p uhf/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostatic,g nosymm int=ultrafinegrid scf(noincore,conver=10) int(fofcou) field=Y-50 scrf(rea #p uhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic, nosymm iop(10/49=112) int=ultrafinegrid scf(noincore,conver=10) int(fofcou) fiel int=acc2e=12 #p uhf/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostatic, nosymm iop(10/49=113,11/6=1,11/24=10) int=ultrafinegrid scf(noincore,conver=10) field=Y-50 scrf(read) int=acc2e=12 #p ub3lyp/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostati nosymm int=ultrafinegrid scf(conver=10) field=Y-50 scrf(read) int=acc2e=12 #p ub3lyp/6-31G(df,p) 5d 7f test freq=roa cphf=(rdfreq,conver=10,nostati nosymm int=ultrafinegrid scf(noincore,conver=10) int(fofcou) field=Y-50 scrf(rea #p ub3lyp/6-31G(df,p) 5d 7f test freq=(roa) cphf=(rdfreq,conver=10,nostati nosymm iop(10/49=112) int=ultrafinegrid scf(noincore,conver=10) int(fofcou) fiel int=acc2e=12
test852.com	#p b2plyp=incore/6-31G(d) 5d 7f test force density=current int=ultrafine

	#p b2plyp=fulldirect/6-31G(d) 5d 7f test force density=current int=ultra
	#p b2plyp(fc,semidirect)/6-31G(d) 5d 7f test force density=current int=ultr
	#p b2plyp=fulldirect/6-31G(d) 5d 7f test force density=current int=ultra
	#p b2plyp=semidirect=-4/6-31G(d) 5d 7f test force density=current int=ultr
	#p b2plyp=semidirect=-7/6-31G(d) 5d 7f test force density=current int=ultr
	#p iop(9/8=10) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre
	geom=modela
	#p iop(9/8=20) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre
	geom=modela
	#p iop(9/8=20) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre
	geom=modela
	#p iop(9/8=200) b2plyp=fulldirect/6-31G(d) 5d 7f test force density=curr
	geom=modela
	#p iop(9/8=200) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curr
	geom=modela

test853.com	#p b2plyp=(incore,full)/6-31G(d) 5d 7f test force density=current int=ultr
	#p b2plyp=(fulldirect,full)/6-31G(d) 5d 7f test force density=current in
	geom=modela
	#p b2plyp(full,semidirect)/6-31G(d) 5d 7f test force density=current int
	geom=modela
	#p b2plyp=(full,fulldirect)/6-31G(d) 5d 7f test force density=current in
	geom=modela
	#p b2plyp=(full,semidirect=-4)/6-31G(d) 5d 7f test force density=current
	geom=modela
	#p b2plyp=(semidirect=-7,full)/6-31G(d) 5d 7f test force density=current
	geom=modela
	#p iop(9/8=10) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=20) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=20) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=200) b2plyp=(fulldirect,full)/6-31G(d) 5d 7f test force densi
	int=ultrafine geom=modela
	#p iop(9/8=200) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densi
	int=ultrafine geom=modela

test854.com	#p b2plyp=incore/6-31G(d) 5d 7f test force density=current int=ultrafine #p b2plyp=fulldirect/6-31G(d) 5d 7f test force density=current int=ultra #p b2plyp(fc,semidirect)/6-31G(d) 5d 7f test force density=current int=ultr #p b2plyp=fulldirect/6-31G(d) 5d 7f test force density=current int=ultra #p b2plyp=semidirect=-4/6-31G(d) 5d 7f test force density=current int=ultr #p b2plyp=semidirect=-7/6-31G(d) 5d 7f test force density=current int=ultr #p iop(9/8=10) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre

	geom=modela
	#p iop(9/8=20) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre
	geom=modela
	#p iop(9/8=20) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curre
	geom=modela
	#p iop(9/8=200) b2plyp=fulldirect/6-31G(d) 5d 7f test force density=curr
	geom=modela
	#p iop(9/8=200) b2plyp=semidirect/6-31G(d) 5d 7f test force density=curr
	geom=modela

test855.com	#p b2plyp=(incore,full)/6-31G(d) 5d 7f test force density=current int=ultr
	#p b2plyp=(fulldirect,full)/6-31G(d) 5d 7f test force density=current in
	geom=modela
	#p b2plyp(full,semidirect)/6-31G(d) 5d 7f test force density=current int
	geom=modela
	#p b2plyp=(full,fulldirect)/6-31G(d) 5d 7f test force density=current in
	geom=modela
	#p b2plyp=(full,semidirect=-4)/6-31G(d) 5d 7f test force density=current
	geom=modela
	#p b2plyp=(semidirect=-7,full)/6-31G(d) 5d 7f test force density=current
	geom=modela
	#p iop(9/8=10) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=20) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=20) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densit
	int=ultrafine geom=modela
	#p iop(9/8=200) b2plyp=(fulldirect,full)/6-31G(d) 5d 7f test force densi
	int=ultrafine geom=modela
	#p iop(9/8=200) b2plyp=(semidirect,full)/6-31G(d) 5d 7f test force densi
	int=ultrafine geom=modela

test857.com	#p freq=sort oniom(hf/3-21g:hf/sto-3g:uff) geom=connectivity test #p freq=(model,readfc) oniom(hf/3-21g:hf/sto-3g:uff) geom=check test #p freq=(middle,readfc) oniom(hf/3-21g:hf/sto-3g:uff) geom=check test
test858.com	#p UFF=QEq Freq test
test859.com	#p eomccsd(full,ncis=20,nstate=10,lrtrans)/sto-3g units=bohr test
test860.com	#p eomccsd=ncis=10/6-311++g(d,p) test
test861.com	#p eomccsd=(ncis=10,lrtrans)/6-311++g(d,p) test
test862.com	#p pm6 test force #p pm6 test force scf=noincore geom=check

	#p pm6 test stable=nstate=20 geom=check #p pm6 test stable=(noincore,nstate=20) scf=noincore geom=check #p pm6 test freq geom=check #p pm6 test freq scf=noincore geom=check
test863.com	#p pm6 test freq
test864.com	#p hf/sto-3g opt freq=(anharm,vibrot) test
test867.com	#p hf/sto-3g* freq=noraman test scf=conver=10 int=acc2e=12 cphf=conver=1 #p hf/sto-3g* freq=(numer,four) polar test scf=conver=10 int=acc2e=12 geom=check guess=read
test868.com	#p cis/sto-3g* freq=noraman test scf=conver=10 int=acc2e=12 cphf=conver= #p CIS/sto-3g* freq=(numer,four) polar test scf=conver=10 int=acc2e=12 geom=check guess=read
test869.com	#p mp2/sto-3g* freq=noraman test scf=conver=10 int=acc2e=12 cphf=conver= #p mp2/sto-3g* freq=(numer,four) polar test scf=conver=10 int=acc2e=12 geom=check guess=read
test870.com	#p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p rpm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight #p upm6 test scf=tight

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#p upm6 test scf=tight symm=noscf
#p upm6 test scf=tight
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#p upm6 test scf=tight
#p upm6 test scf=tight
#p rpm6 test scf=tight
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#p upm6 test scf=tight symm=noscf
#p upm6 test scf=tight
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test871.com	#p pm6 test force scf=xqc #p pm6 test force scf=noincore geom=check guess=read #p pm6 test stable=nstate=20 geom=check guess=read #p pm6 test stable=(noincore,nstate=20) scf=noincore geom=check guess=rea #p pm6 test freq geom=check guess=read #p pm6 test freq scf=noincore geom=check guess=read
test872.com	#p dftba test opt freq
test873.com	#p dftba test opt freq
test874.com	#p dftba test force #p dftba=chk test freq geom=check guess=read
test875.com	#p pm6 freq test #p pm6 force test scrf=(cpcm,solvent=cyclohexane) geom=check guess=read #p pm6 freq test scrf=(cpcm,solvent=cyclohexane) geom=check guess=read #p pm6 force test scrf=solvent=cyclohexane geom=check guess=read #p pm6 freq test scrf=solvent=cyclohexane geom=check guess=read

test876.com	#p pm6 opt=(z-matrix,tight) freq test
	#p pm6 opt=(z-matrix,tight,readfc) freq test scrf=(solvent=acetonitrile,
	geom=check guess=read
	#p pm6 opt=(z-matrix,tight,readfc) freq test scrf=(solvent=acetonitrile)
	guess=read

test877.com	#p eomccsd(nstate=3,lrtrans)/6-31g** 5d units=bohr test #p eomccsd(nstate=6,lrtrans,readamp)/6-31g** 5d units=bohr test geom=che

test878.com	#p eomccsd(nstate=3,lrtrans)/6-31g** 5d units=bohr test
	#p eomccsd(nstate=6,50-50,newcis,lrtrans,readamp)/6-31g** 5d units=bohr
	guess=read

test879.com	#p eomccsd(nstate=3,lrtrans)/6-31g** 5d units=bohr test #p eomccsd(nstate=6,lrtrans,readamp)/6-31g** 5d units=bohr test geom=che
test880.com	#p rccsd=saveamp/6-31g* test geom=modela #p rccsd=(readamp,saveamp)/aug-cc-pvtz test geom=check guess=read #p rccsd=(readamp,full,saveamp)/6-31g** test geom=check guess=read #p rccsd=(readamp)/6-31g** test geom=check guess=read
test881.com	#p uccsd=saveamp/6-31g* test geom=modela #p uccsd=(readamp,saveamp)/aug-cc-pvtz test geom=check guess=read #p uccsd=(readamp,full,saveamp)/6-31g** test geom=check guess=read #p uccsd=(readamp)/6-31g** test geom=check guess=read
test882.com	#p roccsd=saveamp/6-31g* test geom=modela #p roccsd=(readamp,saveamp)/aug-cc-pvtz test geom=check guess=read #p roccsd=(readamp,full,saveamp)/6-31g** test geom=check guess=read #p roccsd=(readamp)/6-31g** test geom=check guess=read

test883.com	#p wlro geom=modela test #p wlro=(saveamp,readamp) geom=modela test
test884.com	#p wlbd=nosaveamp geom=modela test #p wlbd geom=modela test

test885.com	#p opt=tight freq oniom(b2plyp/6-31g*:b3lyp/3-21g) test int=ultrafine
	#p freq=numer polar oniom(b2plyp/6-31g*:b3lyp/3-21g) test geom=allcheck
	int=ultrafine

test887.com	#p m06/6-311G(d,p) opt freq(raman) geom(modela) test #p m062x/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p m06hf/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p m06l/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p td(nstates=4,root=1) m06/6-311G(d,p) opt geom(check) guess(check) tes #p td(nstates=4,root=1) m062x/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=4,root=1) m06hf/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=4,root=1) m06l/6-311G(d,p) opt geom(check) guess(check) te
test888.com	#p m06/6-311G(d,p) opt freq(raman) geom(modela) test #p m062x/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p m06hf/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p m06l/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p td(nstates=4,root=1) m06/6-311G(d,p) opt geom(check) guess(check) tes #p td(nstates=4,root=1) m062x/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=4,root=1) m06hf/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=4,root=1) m06l/6-311G(d,p) opt geom(check) guess(check) te
test889.com	#p hf/6-31G(d) 5d scrf(read,solvent=methanol) geom(modela) opt freq test #p hf/6-31G(d) 5d scrf(solvent=generic) geom(modela) opt freq test #p hf/6-31G(d) 5d scrf(solvent=generic) geom(modela) opt freq test #p hf/6-31G(d) 5d scrf(modify) geom(modela) opt freq test
test890.com	#p b3lyp/6-311G(d,p) td(nstates=1,root=1,eqsolv) density(current) geom(m test #p b3lyp/6-311G(d,p) td(nstates=1,root=1,eqsolv) density(current) geom(ch scrf(statespecificperturbation) test #p b3lyp/6-311G(d,p) td(nstates=1,root=1,eqsolv) density(current) geom(ch scrf(selfconsistent) test
test891.com	#p pm6 freq test iop(10/73=-6)
test892.com	#p restart
test893.com	#p pm6 freq test iop(10/73=-6)
test894.com	#p restart
test895.com	#p ub3lyp/6-31g* 5d test freq=roa cphf=rdfreq iop(10/73=-5)
test896.com	#p restart

test897.com	#p restart
test898.com	#p test pm6 freq=savenm #p test pm6 irc(maxpoints=5,rcfc,report=read)
test899.com	#p test pm6 irc(forward,maxpoints=5,eulerpc,calcfc,report,recorr=always)
计算输入档	计算执行路径
test900.com	#p test pm6 irc(reverse,maxpoints=5,eulerpc,calcfc,report,recorr=always)
test901.com	#P B3LYP/6-311+g(d,p) Int=UltraFine Freq=SaveNM test #P B3LYP/6-311+g(d,p) Int=UltraFine Freq=SaveNM test #P Freq=(FC,ReadFCHT,VibRot,ReadFC,Emission) Geom=Check NoSymm
test902.com	#P B3LYP/6-31+g(d,p) Int=UltraFine Freq=SaveNM Test #P B3LYP/6-31+g(d,p) Int=UltraFine Freq=SaveNM Test #P Freq=(ReadFC,FC,ReadFCHT,VibRot) Geom=Check NoSymm
test903.com	#p wB97/6-311G(d,p) opt freq(raman) geom(modela) test #p wB97X/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p wB97XD/6-311G(d,p) opt freq(raman) geom(check) guess(check) test #p td(nstates=4,root=1) wB97/6-311G(d,p) opt geom(check) guess(check) te #p td(nstates=4,root=1) wB97X/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=4,root=1) wB97XD/6-311G(d,p) opt geom(check) guess(check)
test904.com	#p wB97/6-311G(d,p) opt(calcfc) freq(raman) geom(modela) test #p wB97X/6-311G(d,p) opt(calcfc) freq(raman) geom(check) guess(check) te #p wB97XD/6-311G(d,p) opt(calcfc) freq(raman) geom(check) guess(check) t #p td(nstates=3,root=1) wB97/6-311G(d,p) opt geom(check) test #p td(nstates=3,root=1) wB97X/6-311G(d,p) opt geom(check) guess(check) t #p td(nstates=3,root=1) wB97XD/6-311G(d,p) opt geom(check) guess(check)

test905.com	#p hf/sto-3g nosymm scf(tight) scrf(smd,solvent=water) test
	#p hf/sto-3g nosymm scf(tight) scrf(check,solvent=fluorobenzene) test ge
	guess(check)
	#p hf/sto-3g nosymm scf(tight) scrf(check,solvent=water) test
	#p hf/sto-3g nosymm scf(tight) scrf(check,solvent=fluorobenzene) test ge
	guess(check)
	#p hf/sto-3g nosymm scf(tight) scrf(check,solvent=water) test
	#p hf/sto-3g nosymm scf(tight) scrf(check,solvent=fluorobenzene) test ge
	guess(check)

test906.com	#p b3lyp/6-31G(d) opt(calcfc) freq test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=fluorobenzene) test int=ult
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=water) test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) guess(check) opt(readfc) freq scrf(smd,solve
	test int=ultrafine
	#p b3lyp/6-31(d) geom(check) guess(check) opt(readfc) freq scrf(smd,solv
	int=ultrafine

test907.com	#p b3lyp/6-31G(d) opt(calcfc) freq test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=fluorobenzene) test int=ult
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=water) test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) guess(check) opt(readfc) freq
	scrf(smd,solvent=fluorobenzene) test int=ultrafine
	#p b3lyp/6-31(d) geom(check) guess(check) opt(readfc) freq scrf(smd,solv
	int=ultrafine

test908.com	#p opt=modredundant freq hf/3-21g geom=connectivity test
test909.com	#p eomccsd(nstate=4,50-50,lrtrans)/6-31g** 5d units=bohr test #p eomccsd(nstate=6,50-50,newcis,lrtrans,readamp)/6-31g** 5d test geom=c
test910.com	#p eomccsd=lrtrans/6-31g* test geom=modela #p eomccsd=(readamp,lrtrans)/aug-cc-pvdz test geom=check guess=read #p eomccsd=(readamp,full,lrtrans)/6-31g** test geom=check guess=read #p eomccsd=(readamp,lrtrans)/6-31g** test geom=check guess=read
test911.com	#p eomccsd=(lrtrans,singlet,triplet)/6-31g* test geom=modela #p eomccsd=(readamp,lrtrans,singlet,triplet)/aug-cc-pvdz test geom=check #p eomccsd=(readamp,full,lrtrans,singlet,triplet)/6-31g** test geom=chec #p eomccsd=(readamp,lrtrans,singlet,triplet)/6-31g** test geom=check gue
test912.com	#p eomccsd=lrtrans/6-31g* test geom=modela #p eomccsd=(readamp,lrtrans)/aug-cc-pvdz test geom=check guess=read #p eomccsd=(readamp,full,lrtrans)/6-31g** test geom=check guess=read #p eomccsd=(readamp,lrtrans)/6-31g** test geom=check guess=read
test913.com	#p oniom(mp2/3-21g:pm6) scrf(smd,oniompcm=C) test force #p oniom(mp2/3-21g:pm6) scrf(smd,oniompcm=C) test freq geom=check guess= #p oniom(mp2/3-21g:pm6) scrf=smd test force geom=check guess=read #p oniom(mp2/3-21g:pm6) scrf=smd test freq geom=check guess=read
test914.com	#p oniom(mp2/3-21g:hf/sto-3g) scrf(smd,oniompcm=C) test force #p oniom(mp2/3-21g:hf/sto-3g) scrf(smd,oniompcm=C) test freq geom=check #p oniom(mp2/3-21g:hf/sto-3g) scrf=smd test force geom=check guess=read #p oniom(mp2/3-21g:hf/sto-3g) scrf=smd test freq geom=check guess=read
test915.com	#p oniom(pm6:uff) scrf(smd,oniompcm=C) test force #p oniom(pm6:uff) scrf(smd,oniompcm=C) test freq geom=check guess=read #p oniom(pm6:uff) scrf=smd test force geom=check guess=read #p oniom(pm6:uff) scrf=smd test freq geom=check guess=read
test916.com	#p oniom(hf/3-21g:uff)=embed scrf(smd,oniompcm=C) test force #p oniom(hf/3-21g:uff)=embed scrf(smd,oniompcm=C) test freq geom=check g #p oniom(hf/3-21g:uff)=embed scrf=smd test force geom=check guess=read #p oniom(hf/3-21g:uff)=embed scrf=smd test freq geom=check guess=read
test917.com	#p b3lyp/6-31G(d) opt(calcfc) freq test int=ultrafine #p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=fluorobenzene) test guess

	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=water) test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) guess(check) opt(readfc)
	freq scrf(smd,solvent=fluorobenzene) test int=ultrafine
	#p b3lyp/6-31(d) geom(check) guess(check) opt(readfc) freq scrf(smd,solv
	int=ultrafine

test918.com	#p b3lyp/6-31G(d) opt(calcfc) freq test int=ultrafine
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=fluorobenzene) test guess
	int=ultrafine
	#p b3lyp/6-31G(d) geom(check) scrf(smd,solvent=water) test guess=read
	int=ultrafine
	#p b3lyp/6-31G(d) geom(check) guess(check) opt(readfc) freq scrf(smd,solve
	test int=ultrafine
	#p b3lyp/6-31(d) geom(check) guess(check) opt(calcfc) freq scrf(smd,solv
	int=ultrafine

test919.com	#p oniom(hf/sto-3g:uff) scrf(smd,oniompcm=C) test force #p oniom(hf/sto-3g:uff) scrf(smd,oniompcm=C) test freq=noraman geom=chec #p oniom(hf/sto-3g:uff) scrf=smd test force geom=check guess=read #p oniom(hf/sto-3g:uff) scrf=smd test freq=noraman geom=check guess=read

References

Abegg74	P. W. Abegg and T.-K. Ha, "Ab initio calculation of spin-orbit-coupling constant from Gaussian lobe SCF molecular wavefunctions," *Mol. Phys.*, **27** (1974) 763-67.
Abegg75	P. W. Abegg, "Ab initio calculation of spin-orbit-coupling constants for Gaussian lobe and Gaussian-type wave-functions," *Mol. Phys.*, **30** (1975) 579-96.
Abraham93	M. H. Abraham, "Scales of solute hydrogen-bonding: their construction and application to physicochemical and biochemical processes," *Chem. Soc. Reviews*, **22** (1993) 73.
Adamo90	C. Adamo, M. Cossi, N. Rega, and V. Barone, in *Theoretical Biochemistry: Processes and Properties of Biological Systems*, *Theoretical and Computational Chemistry*, Vol. 9 (Elsevier, New York, 1990).
Adamo97	C. Adamo and V. Barone, "Toward reliable adiabatic connection models free from adjustable parameters," *Chem. Phys. Lett.*, **274** (1997) 242-50.

Adamo98	C. Adamo and V. Barone, “Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models,” *J. Chem. Phys.*, **108** (1998) 664-75.
Adamo98a	C. Adamo and V. Barone, “Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods,” *J. Comp. Chem.*, **19** (1998) 418-29.
Adamo99a	C. Adamo and V. Barone, “Toward reliable density functional methods without adjustable parameters: The PBE0 model,” *J. Chem. Phys.*, **110** (1999) 6158-69.
Almlof82	J. Almlöf, K. Korsell, and K. Fægri Jr., “Principles for a direct SCF approach to LCAO-MO ab-initio calculations,” *J. Comp. Chem.*, **3** (1982) 385-99.
Amos82	R. D. Amos, “Electric and Magnetic Properties of CO, HF, HCl and CH3F,” *Chem. Phys. Lett.*, **87** (1982) 23-26.
Amos84	R. D. Amos, “Dipole-moment derivatives of H2O and H2S,” *Chem. Phys. Lett.*, **108** (1984) 185-90.
Anders93	E. Anders, R. Koch, and P. Freunscht, “Optimization and application of lithium parameters for PM3,” *J. Comp. Chem.*, **14** (1993) 1301-12.
Anderson86	W. P. Anderson, W. D. Edwards, and M. C. Zerner, “Calculated Spectra of Hydrated Ions of the First Transition-Metal Series,” *Inorganic Chem.*, **25** (1986) 2728-32.
Andrae90	D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, and H. Preuss, “Energy-adjusted ab initio pseudopotentials for the 2nd and 3rd row transition-elements,” *Theor. Chem. Acc.*, **77** (1990) 123-41.
Andzelm92	J. Andzelm and E. Wimmer, “Density functional Gaussian-type-orbital approach to molecular geometries, vibrations, and reaction energies,” *J. Chem. Phys.*, **96** (1992) 1280-303.
Atkins69	P. W. Atkins and L. D. Barron, “Rayleigh Scattering of Polarized Photons by Molecules,” *Mol. Phys.*, **16** (1969) 453.
Austin02	A. J. Austin, M. J. Frisch, J. A. Montgomery Jr., and G. A. Petersson, “An overlap criterion for selection of core orbitals,” *Theor. Chem. Acc.*, **107** (2002) 180-86.

Autschbach02	J. Autschbach, T. Ziegler, S. J. A. van Gisbergen, and E. J. Baerends, “Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules,” *J. Chem. Phys.*, **116** (2002) 6930-40.
Ayala97	P. Y. Ayala and H. B. Schlegel, “A combined method for determining reaction paths, minima and transition state geometries,” *J. Chem. Phys.*, **107** (1997) 375-84.
Ayala98	P. Y. Ayala and H. B. Schlegel, “Identification and treatment of internal rotation in normal mode vibrational analysis,” *J. Chem. Phys.*, **108** (1998) 2314-25.
Baboul97	A. G. Baboul and H. B. Schlegel, “Improved Method for Calculating Projected Frequencies along a Reaction Path,” *J. Chem. Phys.*, **107** (1997) 9413-17.
Baboul99	A. G. Baboul, L. A. Curtiss, P. C. Redfern, and K. Raghavachari, “Gaussian-3 theory using density functional geometries and zero-point energies,” *J. Chem. Phys.*, **110** (1999) 7650-57.
Bacon79	A. D. Bacon and M. C. Zerner, “An Intermediate Neglect of Differential Overlap Theory for Transition Metal Complexes: Fe, Co, and Cu Chlorides,” *Theor. Chem. Acc.*, **53** (1979) 21-54.
Bacskay81	G. B. Bacskay, “A Quadratically Convergent Hartree-Fock (QC-SCF) Method. Application to Closed Systems,” *Chem. Phys.*, **61** (1981) 385-404.
Bak93	K. L. Bak, P. Jørgensen, T. Helgaker, K. Ruud, and H. J. A. Jensen, “Gauge-Origin Independent Multiconfigurational Self-Consistent-Field Theory for Vibrational Circular-Dichroism,” *J. Chem. Phys.*, **98** (1993) 8873-87.
Bak94	K. L. Bak, P. Jørgensen, T. Helgaker, and K. Ruud, “Basis Set Convergence and Correlation Effects in Vibrational Circular Dichroism Calculations Using London Atomic Orbitals,” *Faraday Discuss.*, **99** (1994) 121.
Bak95	K. L. Bak, A. E. Hansen, K. Ruud, T. Helgaker, J. Olsen, and P. Jørgensen, “Ab Initio Calculation of Electronic Circular-Dichroism for trans-Cyclooctene Using London Atomic Orbitals,” *Theor. Chem. Acc.*, **90** (1995) 441-58.
Baker86	J. Baker, “An algorithm for the location of

	transition-states," *J. Comp. Chem.*, **7** (1986) 385-95.
Baker87	J. Baker, "An algorithm for geometry optimization without analytical gradients," *J. Comp. Chem.*, **8** (1987) 563-74.
Baker93	J. Baker, "Techniques for geometry optimization - a comparison of cartesian and natural internal coordinates," *J. Comp. Chem.*, **14** (1993) 1085-100.
Bakken99	V. Bakken, J. M. Millam, and H. B. Schlegel, "Ab initio classical trajectories on the Born-Oppenheimer Surface: Updating methods for Hessian-Based Integrators," *J. Chem. Phys.*, **111** (1999) 8773-77.
Banerjee85	A. Banerjee, N. Adams, J. Simons, and R. Shepard, "Search for Stationary Points on Surfaces," *J. Phys. Chem.*, **89** (1985) 52-57.
Barnes09	E. C. F. Barnes, M.J., G. A. Petersson, and J. M. L. Martin, (2009) in prep.
Barone02	V. Barone, J. E. Peralta, R. H. Contreras, and J. P. Snyder, "DFT Calculation of NMR JFF Spin-Spin Coupling Constants in Fluorinated Pyridines," *J. Phys. Chem. A*, **106** (2002) 5607-12.
Barone03	V. Barone, M. Cossi, N. Rega, and G. Scalmani, "Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model," *J. Comp. Chem.*, **24** (2003) 669-81.
Barone04	V. Barone, "Vibrational zero-point energies and thermodynamic functions beyond the harmonic approximation," *J. Chem. Phys.*, **120** (2004) 3059-65.
Barone05	V. Barone, "Anharmonic vibrational properties by a fully automated second-order perturbative approach," *J. Chem. Phys.*, **122** (2005) 014108: 1-10.
Barone09	V. Barone, J. Bloino, M. Biczysko, and F. Santoro, "Fully integrated approach to compute vibrationally resolved optical spectra: From small molecules to macrosystems," *J. Chem. Theory and Comput.*, **5** (2009) 540-54.
Barone94	V. Barone, "Characterization of the potential energy surface of the HO2 molecular system by a density functional approach," *J. Chem. Phys.*, **101** (1994) 10666-76.
Barone95	V. Barone and C. Minichino, "From concepts to

	algorithms for the treatment of large-amplitude internal motions and unimolecular reactions," *J. Mol. Struct. (Theochem)*, **330** (1995) 365-76.
Barone96	V. Barone, "Electronic, vibrational and environmental effects on the hyperfine coupling constants of nitroside radicals. H2NO as a case study," *Chem. Phys. Lett.*, **262** (1996) 201-06.
Barone96a	V. Barone, in *Recent Advances in Density Functional Methods, Part I*, Ed. D. P. Chong (World Scientific Publ. Co., Singapore, 1996).
Barone97	V. Barone, M. Cossi, and J. Tomasi, "A new definition of cavities for the computation of solvation free energies by the polarizable continuum model," *J. Chem. Phys.*, **107** (1997) 3210-21.
Barone98	V. Barone and M. Cossi, "Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model," *J. Phys. Chem. A*, **102** (1998) 1995-2001.
Barone98a	V. Barone, M. Cossi, and J. Tomasi, "Geometry optimization of molecular structures in solution by the polarizable continuum model," *J. Comp. Chem.*, **19** (1998) 404-17.
Barron04	L. D. Barron, *Molecular Light Scattering and Optical Activity*, 2nd ed. (Cambridge University Press, Cambridge, UK, 2004).
Barron71	L. D. Barron and A. D. Buckingham, "Rayleigh and Raman Scattering from Optically Active Molecules," *Mol. Phys.*, **20** (1971) 1111.
Bartlett78	R. J. Bartlett and G. D. Purvis III, "Many-body perturbation-theory, coupled-pair many-electron theory, and importance of quadruple excitations for correlation problem," *Int. J. Quantum Chem.*, **14** (1978) 561-81.
Barysz01	M. Barysz and A. J. Sadlej, "Two-component methods of relativistic quantum chemistry: From the Douglas-Kroll approximation to the exact two-component formalism," *J. Mol. Struct. (Theochem)*, **573** (2001) 181-200.
Bauernschmitt96	R. Bauernschmitt and R. Ahlrichs, "Stability analysis for solutions of the closed shell Kohn-Sham equation," *J. Chem. Phys.*, **104** (1996) 9047-52.
Bauernschmitt96a	R. Bauernschmitt and R. Ahlrichs, "Treatment of

	electronic excitations within the adiabatic approximation of time dependent density functional theory," *Chem. Phys. Lett.*, **256** (1996) 454-64.
Bearpark94	M. J. Bearpark, M. A. Robb, and H. B. Schlegel, "A Direct Method for the Location of the Lowest Energy Point on a Potential Surface Crossing," *Chem. Phys. Lett.*, **223** (1994) 269-74.
Becke88b	A. D. Becke, "Density-functional exchange-energy approximation with correct asymptotic-behavior," *Phys. Rev. A*, **38** (1988) 3098-100.
Becke89a	A. D. Becke and M. R. Roussel, "Exchange holes in inhomogeneous systems: A coordinate-space model," *Phys. Rev. A*, **39** (1989) 3761-67.
Becke92	A. D. Becke, "Density-functional thermochemistry. I. The effect of the exchange-only gradient correction," *J. Chem. Phys.*, **96** (1992) 2155-60.
Becke92a	A. D. Becke, "Density-functional thermochemistry. II. The effect of the Perdew-Wang generalized-gradient correlation correction," *J. Chem. Phys.*, **97** (1992) 9173-77.
Becke93	A. D. Becke, "A new mixing of Hartree-Fock and local density-functional theories," *J. Chem. Phys.*, **98** (1993) 1372-77.
Becke93a	A. D. Becke, "Density-functional thermochemistry. III. The role of exact exchange," *J. Chem. Phys.*, **98** (1993) 5648-52.
Becke96	A. D. Becke, "Density-functional thermochemistry. IV. A new dynamical correlation functional and implications for exact-exchange mixing," *J. Chem. Phys.*, **104** (1996) 1040-46.
Becke97	A. D. Becke, "Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals," *J. Chem. Phys.*, **107** (1997) 8554-60.
Benson68	S. W. Benson, *Thermochemical Kinetics* (Wiley and Sons, New York, 1968).
Berger97	R. Berger and M. Klessinger, "Algorithms for exact counting of energy levels of spectroscopic transitions at different temperatures," *J. Comp. Chem.*, **18** (1997) 1312-19.
Berger98	R. Berger, C. Fischer, and M. Klessinger, "Calculation

	of the vibronic fine structure in electronic spectra at higher temperatures. 1. Benzene and pyrazine," *J. Phys. Chem. A*, **102** (1998) 7157-67.
Bergner93	A. Bergner, M. Dolg, W. Kuechle, H. Stoll, and H. Preuss, "Ab-initio energy-adjusted pseudopotentials for elements of groups 13-17," *Mol. Phys.*, **80** (1993) 1431-41.
Bernardi84	F. Bernardi, A. Bottini, J. J. W. McDougall, M. A. Robb, and H. B. Schlegel, "MCSCF gradient calculation of transition structures in organic reactions," *Far. Symp. Chem. Soc.*, **19** (1984) 137-47.
Bernardi88	F. Bernardi, A. Bottoni, M. J. Field, M. F. Guest, I. H. Hillier, M. A. Robb, and A. Venturini, "MC-SCF Study of the Diels-Alder Reaction Between Ethylene and Butadiene," *J. Am. Chem. Soc.*, **110** (1988) 3050-55.
Bernardi88a	F. Bernardi, A. Bottoni, M. Olivucci, M. A. Robb, H. B. Schlegel, and G. Tonachini, "Do Supra-Antara Paths Really Exist for 2+2 Cycloaddition Reactions? Analytical Computation of the MC-SCF Hessians for Transition States of C2H4 with C2H4, Singlet O2, and Ketene," *J. Am. Chem. Soc.*, **110** (1988) 5993-95.
Bernardi90	F. Bernardi, A. Bottoni, M. A. Robb, and A. Venturini, "MC-SCF study of the cycloaddition reaction between ketene and ethylene," *J. Am. Chem. Soc.*, **112** (1990) 2106-14.
Bernardi92	F. Bernardi, M. Olivucci, I. Palmer, and M. A. Robb, "An MC-SCF study of the thermal and photochemical cycloaddition of Dewar benzene," *J. Organic Chem.*, **57** (1992) 5081-87.
Bernardi96	F. Bernardi, M. A. Robb, and M. Olivucci, "Potential energy surface crossings in organic photochemistry," *Chem. Soc. Reviews*, **25** (1996) 321.
Besler90	B. H. Besler, K. M. Merz Jr., and P. A. Kollman, "Atomic charges derived from semiempirical methods," *J. Comp. Chem.*, **11** (1990) 431-39.
Bingham75	R. C. Bingham, M. J. S. Dewar, and D. H. Lo, "Ground-states of molecules. 25. MINDO-3 - Improved version of MINDO semiempirical SCF-MO method," *J. Am. Chem. Soc.*, **97** (1975) 1285-93.
Binkley80a	J. S. Binkley, J. A. Pople, and W. J. Hehre, "Self-Consistent Molecular Orbital Methods. 21. Small

	Split-Valence Basis Sets for First-Row Elements," *J. Am. Chem. Soc.*, **102** (1980) 939-47.
Binning90	R. C. Binning Jr. and L. A. Curtiss, "Compact contracted basis-sets for 3rd-row atoms - GA-KR," *J. Comp. Chem.*, **11** (1990) 1206-16.
Blaudeau97	J.-P. Blaudeau, M. P. McGrath, L. A. Curtiss, and L. Radom, "Extension of Gaussian-2 (G2) theory to molecules containing third-row atoms K and Ca," *J. Chem. Phys.*, **107** (1997) 5016-21.
Bobrowicz77	F. W. Bobrowicz and W. A. Goddard III, in *Methods of Electronic Structure Theory*, Ed. H. F. Schaefer III, *Modern Theoretical Chemistry*, Vol. 3 (Plenum, New York, 1977) 79-126.
Boese00	A. D. Boese, N. L. Doltsinis, N. C. Handy, and M. Sprik, "New generalized gradient approximation functionals," *J. Chem. Phys.*, **112** (2000) 1670-78.
Boese01	A. D. Boese and N. C. Handy, "A new parametrization of exchange-correlation generalized gradient approximation functionals," *J. Chem. Phys.*, **114** (2001) 5497-503.
Boese02	A. D. Boese and N. C. Handy, "New exchange-correlation density functionals: The role of the kinetic-energy density," *J. Chem. Phys.*, **116** (2002) 9559-69.
Boese04	A. D. Boese and J. M. L. Martin, "Development of Density Functionals for Thermochemical Kinetics," *J. Chem. Phys.*, **121** (2004) 3405-16.
Bofill89	J. M. Bofill and P. Pulay, "The unrestricted natural orbital-complete active space (UNO-CAS) method: An inexpensive alternative to the complete active space-self-consistent-field (CAS-SCF) method," *J. Chem. Phys.*, **90** (1989) 3637-46.
Bofill94	J. M. Bofill, "Updated Hessian matrix and the restricted step method for locating transition structures," *J. Comp. Chem.*, **15** (1994) 1-11.
Bofill95	J. M. Bofill and M. Comajuan, "Analysis of the updated Hessian matrices for locating transition structures," *J. Comp. Chem.*, **16** (1995) 1326-38.
Bohmann97	J. A. Bohmann, F. Weinhold, and T. C. Farrar, "Natural Chemical Shielding Analysis of Nuclear Magnetic Resonance Shielding Tensors from Gauge-Including Atomic Orbital Calculations," *J. Chem. Phys.*, **107**

	(1997) 1173-84.
Bolton98	K. Bolton, W. L. Hase, and G. H. Peslherbe, in *Modern Methods for Multidimensional Dynamics Computation in Chemistry*, Ed. D. L. Thompson (World Scientific, Singapore, 1998) 143.
Borrelli03	R. Borrelli and A. Peluso, "Dynamics of radiationless transitions in large molecular systems: A Franck-Condon-based method accounting for displacements and rotations of all the normal coordinates," *J. Chem. Phys.*, **119** (2003) 8437-48.
Boys60	S. F. Boys, "Construction of Molecular Orbitals to be Approximately Invariant for Changes from One Molecule to Another," *Rev. Mod. Phys.*, **32** (1960) 296-99.
Boys66	S. F. Boys, in *Quantum Theory of Atoms, Molecules and the Solid State*, Ed. P.-O. Löwdin (Academic Press, New York, 1966) 253.
Boys70	S. F. Boys and F. Bernardi, "Calculation of Small Molecular Interactions by Differences of Separate Total Energies - Some Procedures with Reduced Errors," *Mol. Phys.*, **19** (1970) 553.
Breneman90	C. M. Breneman and K. B. Wiberg, "Determining atom-centered monopoles from molecular electrostatic potentials - the need for high sampling density in formamide conformational-analysis," *J. Comp. Chem.*, **11** (1990) 361-73.
Buckingham67	A. D. Buckingham, in *Advances in Chemical Physics*, Ed. I. Prigogine, Vol. 12 (Wiley Interscience, New York, 1967) 107.
Buckingham68	A. D. Buckingham and G. C. Longuet-Higgins, "Quadrupole Moments of Dipolar Molecules," *Mol. Phys.*, **14** (1968) 63.
Bunker71	D. L. Bunker, "Classical Trajectory Methods," *Meth. Comp. Phys.*, **10** (1971) 287.
Burant96	J. C. Burant, M. C. Strain, G. E. Scuseria, and M. J. Frisch, "Kohn-Sham Analytic Energy Second Derivatives with the Gaussian Very Fast Multipole Method (GvFMM)," *Chem. Phys. Lett.*, **258** (1996) 45-52.
Burant96a	J. C. Burant, M. C. Strain, G. E. Scuseria, and M. J. Frisch, "Analytic Energy Gradients for the Gaussian Very Fast Multipole Method (GvFMM)," *Chem. Phys. Lett.*, **248** (1996) 43-49.

Burant96b	J. C. Burant, G. E. Scuseria, and M. J. Frisch, “Linear scaling method for Hartree-Fock exchange calculations of large molecules,” *J. Chem. Phys.*, **105** (1996) 8969-72.
Burke98	K. Burke, J. P. Perdew, and Y. Wang, in *Electronic Density Functional Theory: Recent Progress and New Directions*, Ed. J. F. Dobson, G. Vignale, and M. P. Das (Plenum, 1998).
Califano76	S. Califano, *Vibrational States* (Wiley, London, 1976).
Cammi00	R. Cammi, B. Mennucci, and J. Tomasi, “Fast evaluation of geometries and properties of excited molecules in solution: A Tamm-Dancoff model with application to 4-dimethylaminobenzonitrile,” *J. Phys. Chem. A*, **104** (2000) 5631-37.
Cammi00a	R. Cammi, C. Cappelli, S. Corni, and J. Tomasi, “On the calculation of infrared intensities in solution within the polarizable continuum model,” *J. Phys. Chem. A*, **104** (2000) 9874-79.
Cammi99	R. Cammi, B. Mennucci, and J. Tomasi, “Second-order Møller-Plesset analytical derivatives for the polarizable continuum model using the relaxed density approach,” *J. Phys. Chem. A*, **103** (1999) 9100-08.
Cances01	E. Cancès and B. Mennucci, “Comment on ‘Reaction field treatment of charge penetration ‘,” *J. Chem. Phys.*, **114** (2001) 4744-45.
Cances97	E. Cancès, B. Mennucci, and J. Tomasi, “A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anistropic dielectrics,” *J. Chem. Phys.*, **107** (1997) 3032-41.
Cao01	X. Y. Cao and M. Dolg, “Valence basis sets for relativistic energy-consistent small-core lanthanide pseudopotentials,” *J. Chem. Phys.*, **115** (2001) 7348-55.
Cao02	X. Y. Cao and M. Dolg, “Segmented contraction scheme for small-core lanthanide pseudopotential basis sets,” *J. Mol. Struct. (Theochem)*, **581** (2002) 139-47.
Cappelli02	C. Cappelli, S. Corni, B. Mennucci, R. Cammi, and J. Tomasi, “Vibrational Circular Dichroism within the Polarizable Continuum Model: A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(-)-3-Butyn-2-ol in CCl4 Solution,” *J. Phys. Chem.*

	A, **106** (2002) 12331-39.
Car85	R. Car and M. Parrinello, "Unified Approach for Molecular-Dynamics and Density-Functional Theory," *Phys. Rev. Lett.*, **55** (1985) 2471-74.
Caricato06	M. Caricato, B. Mennucci, J. Tomasi, F. Ingrosso, R. Cammi, S. Corni, and G. Scalmani, "Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory," *J. Chem. Phys.*, **124** (2006) 124520.
Carpenter87	J. E. Carpenter, *Extension of Lewis structure concepts to open-shell and excited-state molecular species*, Ph. D. thesis, University of Wisconsin, Madison, WI, 1987.
Carpenter88	J. E. Carpenter and F. Weinhold, "Analysis of the geometry of the hydroxymethyl radical by the different hybrids for different spins natural bond orbital procedure," *J. Mol. Struct. (Theochem)*, **46** (1988) 41-62.
Carsky91	P. Cársky and E. Hubak, "Restricted Hartree-Fock and Unrestricted Hartree-Fock as reference states in many-body perturbation-theory: A critical comparison of the two approaches," *Theor. Chem. Acc.*, **80** (1991) 407-25.
Casida98	M. E. Casida, C. Jamorski, K. C. Casida, and D. R. Salahub, "Molecular excitation energies to high-lying bound states from time-dependent density-functional response theory: Characterization and correction of the time-dependent local density approximation ionization threshold," *J. Chem. Phys.*, **108** (1998) 4439-49.
Cederbaum75	L. S. Cederbaum, "One-body Green's function for atoms and molecules: theory and application," *J. Phys. B*, **8** (1975) 290-303.
Cederbaum77	L. S. Cederbaum and W. Domcke, in *Advances in Chemical Physics*, Ed. I. Prigogine and S. A. Rice, Vol. 36 (Wiley & Sons, New York, 1977) 205.
Cerjan81	C. J. Cerjan and W. H. Miller, "On Finding Transition States," *J. Chem. Phys.*, **75** (1981) 2800-06.
Chai08	J.-D. Chai and M. Head-Gordon, "Systematic optimization of long-range corrected hybrid density functionals," *J. Chem. Phys.*, **128** (2008) 084106.
Chai08a	J.-D. Chai and M. Head-Gordon, "Long-range corrected

	hybrid density functionals with damped atom-atom dispersion corrections," *Phys. Chem. Chem. Phys.*, **10** (2008) 6615-20.
Charney79	E. Charney, *The Molecular Basis of Optical Activity* (Wiley, New York, 1979).
Cheeseman09	J. R. Cheeseman, G. S. Scalmani, and M. J. Frisch, "Analytic Vibrational Raman Optical Activity Intensities," *J. Chem. Theory and Comput.*, (2009) to be submitted.
Cheeseman96	J. R. Cheeseman, G. W. Trucks, T. A. Keith, and M. J. Frisch, "A Comparison of Models for Calculating Nuclear Magnetic Resonance Shielding Tensors," *J. Chem. Phys.*, **104** (1996) 5497-509.
Cheeseman96a	J. R. Cheeseman, M. J. Frisch, F. J. Devlin, and P. J. Stephens, "Ab Initio Calculation of Atomic Axial Tensors and Vibrational Rotational Strengths Using Density Functional Theory," *Chem. Phys. Lett.*, **252** (1996) 211-20.
Chen94	W. Chen, W. L. Hase, and H. B. Schlegel, "Ab initio classical trajectory study of H2C --> H2 + CO dissociation," *Chem. Phys. Lett.*, **228** (1994) 436-42.
Chipman00	D. M. Chipman, "Reaction field treatment of charge penetration," *J. Chem. Phys.*, **112** (2000) 5558-65.
Chirlian87	L. E. Chirlian and M. M. Francl, "Atomic charges derived from electrostatic potentials - a detailed study," *J. Comp. Chem.*, **8** (1987) 894-905.
Cimiraglia80	R. Cimiraglia, M. Persico, and J. Tomasi, "Roto-electronic and spin-orbit couplings in the predissociation of HNO - a theoretical calculation," *Chem. Phys. Lett.*, **76** (1980) 169-71.
Cioslowski89	J. Cioslowski, "A New Population Analysis Based on Atomic Polar Tensors," *J. Am. Chem. Soc.*, **111** (1989) 8333-36.
Cizek69	J. Cizek, in *Advances in Chemical Physics*, Ed. P. C. Hariharan, Vol. 14 (Wiley Interscience, New York, 1969) 35.
Clabo88	D. A. Clabo, W. D. Allen, R. B. Remington, Y. Yamaguchi, and H. F. Schaefer III, "A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods -

	asymmetric-top molecules," *Chem. Phys.*, **123** (1988) 187-239.
Clark83	T. Clark, J. Chandrasekhar, G. W. Spitznagel, and P. v. R. Schleyer, "Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F," *J. Comp. Chem.*, **4** (1983) 294-301.
Clemente08	F. Clemente, T. Vreven, and M. J. Frisch, in *Quantum Biochemistry*, Ed. C. Matta (Wiley VCH, 2008).
Clifford96	S. Clifford, M. J. Bearpark, and M. A. Robb, "A hybrid MC-SCF method: Generalized valence bond (GVB) with complete active space SCF (CASSCF)," *Chem. Phys. Lett.*, **255** (1996) 320-26.
Cohen01	A. J. Cohen and N. C. Handy, "Dynamic correlation," *Mol. Phys.*, **99** (2001) 607-15.
Cohen86	E. R. Cohen and B. N. Taylor, *The 1986 Adjustment of the Fundamental Physical Constants*, *CODATA Bulletin* (Pergamon, Elmsford, NY, 1986).
Collins76	J. B. Collins, P. v. R. Schleyer, J. S. Binkley, and J. A. Pople, "Self-Consistent Molecular Orbital Methods. 17. Geometries and binding energies of second-row molecules. A comparison of three basis sets," *J. Chem. Phys.*, **64** (1976) 5142-51.
Collins02	M. A. Collins, "Molecular potential-energy surfaces for chemical reaction dynamics," *Theor. Chem. Acc.*, **108** (2002) 313-24.
Condon37	E. U. Condon, "Theories of optical rotatory power," *Rev. Mod. Phys.*, **9** (1937) 432-57.
Constyear73	*Pure and Applied Chemistry*, **2** (1973) 717.
Constyear79	*Pure and Applied Chemistry*, **51** (1979) 1.
Cornell95	W. D. Cornell, P. Cieplak, C. I. Bayly, I. R. Gould, K. M. Merz Jr., D. M. Ferguson, D. C. Spellmeyer, T. Fox, J. W. Caldwell, and P. A. Kollman, "A second generation force-field for the simulation of proteins, nucleic-acids, and organic-molecules," *J. Am. Chem. Soc.*, **117** (1995) 5179-97.
Cossi00	M. Cossi and V. Barone, "Solvent effect on vertical electronic transitions by the polarizable continuum model," *J. Chem. Phys.*, **112** (2000) 2427-35.
Cossi01	M. Cossi and V. Barone, "Time-dependent density

	functional theory for molecules in liquid solutions," *J. Chem. Phys.*, **115** (2001) 4708-17.
Cossi01a	M. Cossi, N. Rega, G. Scalmani, and V. Barone, "Polarizable dielectric model of solvation with inclusion of charge penetration effects," *J. Chem. Phys.*, **114** (2001) 5691-701.
Cossi02	M. Cossi, G. Scalmani, N. Rega, and V. Barone, "New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution," *J. Chem. Phys.*, **117** (2002) 43-54.
Cossi03	M. Cossi, N. Rega, G. Scalmani, and V. Barone, "Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model," *J. Comp. Chem.*, **24** (2003) 669-81.
Cossi96	M. Cossi, V. Barone, R. Cammi, and J. Tomasi, "Ab initio study of solvated molecules: A new implementation of the polarizable continuum model," *Chem. Phys. Lett.*, **255** (1996) 327-35.
Cossi98	M. Cossi, V. Barone, B. Mennucci, and J. Tomasi, "Ab initio study of ionic solutions by a polarizable continuum dielectric model," *Chem. Phys. Lett.*, **286** (1998) 253-60.
Cossi99	M. Cossi, V. Barone, and M. A. Robb, "A direct procedure for the evaluation of solvent effects in MC-SCF calculations," *J. Chem. Phys.*, **111** (1999) 5295-302.
Coutsias04	E. A. Coutsias, C. Seok, and K. A. Dill, "Using quaternions to calculate RMSD," *J. Comp. Chem.*, **25** (2004) 1849-57.
CRC80	*CRC Handbook of Chemistry and Physics*, 60th ed., Ed. D. R. Lide (CRC Press, Boca Raton, FL, 1980).
Csaszar84	P. Csaszar and P. Pulay, "Geometry optimization by direct inversion in the iterative subspace," *J. Mol. Struct. (Theochem)*, **114** (1984) 31-34.
Cundari93	T. R. Cundari and W. J. Stevens, "Effective core potential methods for the lanthanides," *J. Chem. Phys.*, **98** (1993) 5555-65.
Curl65	R. F. Curl Jr., "Relationship between Electron Spin Rotation Coupling Constants and G-Tensor Components," *Mol. Phys.*, **9** (1965) 585.

Curtiss07	L. A. Curtiss, P. C. Redfern, and K. Raghavachari, “Gaussian-4 theory,” *J. Chem. Phys.*, **126** (2007) 084108.
Curtiss07a	L. A. Curtiss, P. C. Redfern, and K. Raghavachari, “Gaussian-4 theory using reduced order perturbation theory,” *J. Chem. Phys.*, **127** (2007) 124105.
Curtiss90	L. A. Curtiss, C. Jones, G. W. Trucks, K. Raghavachari, and J. A. Pople, “Gaussian-1 theory of molecular energies for second-row compounds,” *J. Chem. Phys.*, **93** (1990) 2537-45.
Curtiss91	L. A. Curtiss, K. Raghavachari, G. W. Trucks, and J. A. Pople, “Gaussian-2 theory for molecular energies of first- and second-row compounds,” *J. Chem. Phys.*, **94** (1991) 7221-30.
Curtiss93	L. A. Curtiss, K. Raghavachari, and J. A. Pople, “Gaussian-2 theory using reduced Møller-Plesset orders,” *J. Chem. Phys.*, **98** (1993) 1293-98.
Curtiss95	L. A. Curtiss, M. P. McGrath, J.-P. Blaudeau, N. E. Davis, R. C. Binning Jr., and L. Radom, “Extension of Gaussian-2 theory to molecules containing third-row atoms Ga-Kr,” *J. Chem. Phys.*, **103** (1995) 6104-13.
Curtiss98	L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolov, and J. A. Pople, “Gaussian-3 (G3) theory for molecules containing first and second-row atoms,” *J. Chem. Phys.*, **109** (1998) 7764-76.
Curtiss99	L. A. Curtiss, P. C. Redfern, K. Raghavachari, V. Rassolov, and J. A. Pople, “Gaussian-3 theory using reduced Møller-Plesset order,” *J. Chem. Phys.*, **110** (1999) 4703-09.
daCosta87	H. F. M. da Costa, M. Trsic, and J. R. Mohallem, “Universal Gaussian and Slater-type basis-sets for atoms He to Ar based on an integral version of the Hartree-Fock equations,” *Mol. Phys.*, **62** (1987) 91-95.
Daniels97	A. D. Daniels, J. M. Millam, and G. E. Scuseria, “Semiempirical methods with conjugate gradient density matrix search to replace diagonalization for molecular systems containing thousands of atoms,” *J. Chem. Phys.*, **107** (1997) 425-31.
Dapprich99	S. Dapprich, I. Komáromi, K. S. Byun, K. Morokuma, and M. J. Frisch, “A New ONIOM Implementation in Gaussian 98. 1. The Calculation of Energies, Gradients and

	Vibrational Frequencies and Electric Field Derivatives," *J. Mol. Struct. (Theochem)*, **462** (1999) 1-21.
daSilva89	A. B. F. da Silva, H. F. M. da Costa, and M. Trsic, "Universal Gaussian and Slater-type bases for atoms H to Xe based on the generator-coordinate Hartree-Fock method .1. Ground and certain low-lying excited-states of the neutral atoms," *Mol. Phys.*, **68** (1989) 433-45.
Davidson96	E. R. Davidson, "Comment on "Comment on Dunning's correlation-consistent basis sets"," *Chem. Phys. Lett.*, **260** (1996) 514-18.
Davis81	L. P. Davis, et. al., "MNDO calculations for compounds containing aluminum and boron," *J. Comp. Chem.*, **2** (1981) 433-45.
deCastro98	E. V. R. de Castro and F. E. Jorge, "Accurate universal gaussian basis set for all atoms of the periodic table," *J. Chem. Phys.*, **108** (1998) 5225-29.
deJong01	W. A. deJong, R. J. Harrison, and D. A. Dixon, "Parallel Douglas-Kroll energy and gradients in NWChem: Estimating scalar relativistic effects using Douglas-Kroll contracted basis sets," *J. Chem. Phys.*, **114** (2001) 48-53.
Deng06	W. Deng, J. R. Cheeseman, and M. J. Frisch, "Calculation of Nuclear Spin-Spin Coupling Constants of Molecules with First and Second Row Atoms in Study of Basis Set Dependence," *J. Chem. Theory and Comput.*, **2** (2006) 1028-37.
Dewar77	M. J. S. Dewar and W. Thiel, "Ground-States of Molecules. 38. The MNDO Method: Approximations and Parameters," *J. Am. Chem. Soc.*, **99** (1977) 4899-907.
Dewar78	M. J. S. Dewar and H. S. Rzepa, "Ground-states of molecules. 45. MNDO results for molecules containing beryllium," *J. Am. Chem. Soc.*, **100** (1978) 777-84.
Dewar78a	M. J. S. Dewar, M. L. McKee, and H. S. Rzepa, "MNDO parameters for 3rd period elements," *J. Am. Chem. Soc.*, **100** (1978) 3607-07.
Dewar83	M. J. S. Dewar and M. L. McKee, "Ground-states of molecules. 56. MNDO calculations for molecules containing sulfur," *J. Comp. Chem.*, **4** (1983) 84-103.
Dewar83a	M. J. S. Dewar and E. F. Healy, "Ground-states of molecules. 64. MNDO calculations for compounds

	containing bromine," *J. Comp. Chem.*, **4** (1983) 542-51.
Dewar84	M. J. S. Dewar, G. L. Grady, and J. J. P. Stewart, "Ground-states of molecules. 68. MNDO calculations for compounds containing tin," *J. Am. Chem. Soc.*, **106** (1984) 6771-73.
Dewar85	M. J. S. Dewar, E. G. Zoebisch, and E. F. Healy, "AM1: A New General Purpose Quantum Mechanical Molecular Model," *J. Am. Chem. Soc.*, **107** (1985) 3902-09.
Dewar85a	M. J. S. Dewar, et. al., "Ground-states of molecules. 74. MNDO calculations for compounds containing mercury," *Organometallics*, **4** (1985) 1964-66.
Dewar86	M. J. S. Dewar and C. H. Reynolds, "An improved set of MNDO parameters for sulfur," *J. Comp. Chem.*, **7** (1986) 140-43.
Dewar88	M. J. S. Dewar, C. Jie, and E. G. Zoebisch, "AM1 calculations for compounds containing boron," *Organometallics*, **7** (1988) 513-21.
Dewar88a	M. J. S. Dewar and K. M. Merz Jr., "AM1 parameters for zinc," *Organometallics*, **7** (1988) 522-24.
Dewar89	M. J. S. Dewar and C. Jie, "AM1 parameters for phosphorus," *J. Mol. Struct. (Theochem)*, **187** (1989) 1.
Dewar90	M. J. S. Dewar and Y.-C. Yuan, "AM1 parameters for sulfur," *Inorganic Chem.*, **29** (1990) 3881-90.
Dewar90a	M. J. S. Dewar and A. J. Holder, "AM1 parameters for aluminum," *Organometallics*, **9** (1990) 508-11.
Diercksen81	G. H. F. Diercksen, B. O. Roos, and A. J. Sadlej, "Legitimate calculation of 1st-order molecular-properties in the case of limited CI functions - dipole-moments," *Chem. Phys.*, **59** (1981) 29-39.
Diercksen81a	G. H. F. Diercksen and A. J. Sadlej, "Perturbation-theory of the electron correlation-effects for atomic and molecular-properties - 2nd-order and 3rd-order correlation corrections to molecular dipole-moments and polarizabilities," *J. Chem. Phys.*, **75** (1981) 1253-66.
Dierksen04	M. Dierksen and S. Grimme, "Density functional calculations of the vibronic structure of electronic absorption spectra," *J. Chem. Phys.*, **120** (2004)

	3544-54.
Dierksen04a	M. Dierksen and S. Grimme, “The vibronic structure of electronic absorption spectra of large molecules: A time-dependent density functional study on the influence of ‘Exact‘ Hartree-Fock exchange,” *J. Phys. Chem. A*, **108** (2004) 10225-37.
Dierksen05	M. Dierksen and S. Grimme, “An efficient approach for the calculation of Franck-Condon integrals of large molecules,” *J. Chem. Phys.*, **122** (2005) 244101.
Ditchfield71	R. Ditchfield, W. J. Hehre, and J. A. Pople, “Self-Consistent Molecular Orbital Methods. 9. Extended Gaussian-type basis for molecular-orbital studies of organic molecules,” *J. Chem. Phys.*, **54** (1971) 724.
Ditchfield74	R. Ditchfield, “Self-consistent perturbation theory of diamagnetism. 1. Gauge-invariant LCAO method for N.M.R. chemical shifts,” *Mol. Phys.*, **27** (1974) 789-807.
Dobbs86	K. D. Dobbs and W. J. Hehre, “Molecular-orbital theory of the properties of inorganic and organometallic compounds. 4. Extended basis-sets for 3rd row and 4th row, main-group elements,” *J. Comp. Chem.*, **7** (1986) 359-78.
Dobbs87	K. D. Dobbs and W. J. Hehre, “Molecular-orbital theory of the properties of inorganic and organometallic compounds. 5. Extended basis-sets for 1st-row transition-metals,” *J. Comp. Chem.*, **8** (1987) 861-79.
Dobbs87a	K. D. Dobbs and W. J. Hehre, “Molecular-orbital theory of the properties of inorganic and organometallic compounds. 6. Extended basis-sets for 2nd-row transition-metals,” *J. Comp. Chem.*, **8** (1987) 880-93.
Dodds77	J. L. Dodds, R. McWeeny, W. T. Raynes, and J. P. Riley, “SCF theory for multiple perturbations,” *Mol. Phys.*, **33** (1977) 611-17.
Dodds77a	J. L. Dodds, R. McWeeny, and A. J. Sadlej, “Self-consistent perturbation theory: Generalization for perturbation-dependent non-orthogonal basis set,” *Mol. Phys.*, **34** (1977) 1779-91.
Doktorov77	E. V. Doktorov, I. A. Malkin, and V. I. Manko, “Dynamical symmetry of vibronic transitions in polyatomic-molecules and Franck-Condon principle.

	2. ,” *J. Mol. Spec.*, **64** (1977) 302-26.
Dolg87	M. Dolg, U. Wedig, H. Stoll, and H. Preuss, “Energy-adjusted ab initio pseudopotentials for the first row transition elements,” *J. Chem. Phys.*, **86** (1987) 866-72.
Dolg89	M. Dolg, H. Stoll, and H. Preuss, “Energy-adjusted ab initio pseudopotentials for the rare earth elements,” *J. Chem. Phys.*, **90** (1989) 1730-34.
Dolg89a	M. Dolg, H. Stoll, A. Savin, and H. Preuss, “Energy-adjusted pseudopotentials for the rare-earth elements,” *Theor. Chem. Acc.*, **75** (1989) 173-94.
Dolg91	M. Dolg, P. Fulde, W. Kuechle, C.-S. Neumann, and H. Stoll, “Ground state calculations of di-pi-cyclooctatetraene cerium,” *J. Chem. Phys.*, **94** (1991) 3011-17.
Dolg92	M. Dolg, H. Stoll, H.-J. Flad, and H. Preuss, “Ab initio pseudopotential study of Yb and YbO,” *J. Chem. Phys.*, **97** (1992) 1162-73.
Dolg93	M. Dolg, H. Stoll, and H. Preuss, “A combination of quasi-relativistic pseudopotential and ligand-field calculations for lanthanoid compounds,” *Theor. Chem. Acc.*, **85** (1993) 441-50.
Dolg93a	M. Dolg, H. Stoll, H. Preuss, and R. M. Pitzer, “Relativistic and correlation-effects for element 105 (Hahnium, Ha) - a comparative-study of M and MO (M = NB, TA, HA) using energy-adjusted ab initio pseudopotentials,” *J. Phys. Chem.*, **97** (1993) 5852-59.
Douglas74	M. Douglas and N. M. Kroll, “Quantum electrodynamical corrections to fine-structure of helium,” *Ann. Phys. (NY)*, **82** (1974) 89-155.
Dukor00	R. K. Dukor and L. A. Nafie, in *Encyclopedia of Analytical Chemistry: Instrumentation and Applications*, Ed. R. A. Meyers (Wiley & Sons, Chichester, 2000) 662-76.
Dunlap00	B. I. Dunlap, “Robust and variational fitting: Removing the four-center integrals from center stage in quantum chemistry,” *J. Mol. Struct. (Theochem)*, **529** (2000) 37-40.
Dunlap83	B. I. Dunlap, “Fitting the Coulomb Potential Variationally in X-Alpha Molecular Calculations,” *J. Chem. Phys.*, **78** (1983) 3140-42.

Dunning76	T. H. Dunning Jr. and P. J. Hay, in *Modern Theoretical Chemistry*, Ed. H. F. Schaefer III, Vol. 3 (Plenum, New York, 1976) 1-28.
Dunning89	T. H. Dunning Jr., "Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen," *J. Chem. Phys.*, **90** (1989) 1007-23.
Dupuis76	M. Dupuis, J. Rys, and H. F. King, "Evaluation of molecular integrals over Gaussian basis functions," *J. Chem. Phys.*, **65** (1976) 111-16.
Dykstra77	C. E. Dykstra, "Examination of Brueckner condition for selection of molecular-orbitals in correlated wavefunctions," *Chem. Phys. Lett.*, **45** (1977) 466-69.
Dykstra84	C. E. Dykstra and P. G. Jasien, "Derivative Hartree-Fock theory to all orders," *Chem. Phys. Lett.*, **109** (1984) 388-93.
Eade81	R. H. A. Eade and M. A. Robb, "Direct minimization in MC SCF theory - the Quasi-Newton method," *Chem. Phys. Lett.*, **83** (1981) 362-68.
Easton96	R. E. Easton, D. J. Giesen, A. Welch, C. J. Cramer, and D. G. Truhlar, "The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges," *Theor. Chem. Acc.*, **93** (1996) 281-301.
Ehara02	M. Ehara, M. Ishida, K. Toyota, and H. Nakatsuji, in *Reviews in Modern Quantum Chemistry*, Ed. K. D. Sen (World Scientific, Singapore, 2002) 293.
Eichkorn95	K. Eichkorn, O. Treutler, H. Ohm, M. Haser, and R. Ahlrichs, "Auxiliary basis-sets to approximate Coulomb potentials," *Chem. Phys. Lett.*, **240** (1995) 283-89.
Eichkorn97	K. Eichkorn, F. Weigend, O. Treutler, and R. Ahlrichs, "Auxiliary basis sets for main row atoms and transition metals and their use to approximate Coulomb potentials," *Theor. Chem. Acc.*, **97** (1997) 119-24.
Elstner98	M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, "Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties," *Phys. Rev. B*, **58** (1998) 7260-68.

Ernzerhof98	M. Ernzerhof and J. P. Perdew, “Generalized gradient approximation to the angle- and system-averaged exchange hole,” *J. Chem. Phys.*, **109** (1998)
Eyring35	H. Eyring, “The activated complex in chemical reactions,” *J. Chem. Phys.*, **3** (1935) 107-15.
Eyring44	H. Eyring, J. Walter, and G. E. Kimball, *Quantum Chemistry* (Wiley, New York, 1944).
Farkas95	Ö. Farkas, PhD (CsC) thesis, Eötvös Loránd University and Hungarian Academy of Sciences, Budapest, 1995 (in Hungarian).
Farkas98	Ö. Farkas and H. B. Schlegel, “Methods for geometry optimization of large molecules. I. An O(N2) algorithm for solving systems of linear equations for the transformation of coordinates and forces,” *J. Chem. Phys.*, **109** (1998) 7100-04.
Farkas99	Ö. Farkas and H. B. Schlegel, “Methods for optimizing large molecules. II. Quadratic search,” *J. Chem. Phys.*, **111** (1999) 10806-14.
Ferreira01	A. M. Ferreira, G. Seabra, O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz, in *Quantum-Mechanical Prediction of Thermochemical Data*, Ed. J. Cioslowski, *Understanding Chemical Reactivity*, Vol. 22 (Kluwer Academic, Dordrecht, 2001) 131-60.
Fitzpatrick86	N. J. Fitzpatrick and G. H. Murphy, “Double Zeta-D Radial Wave-Functions for Transition-Elements,” *Inorg. Chim. Acta*, **111** (1986) 139-40.
Fletcher63	R. Fletcher and M. J. D. Powell, “A Rapidly Convergent Descent Method for Minimization,” *Comput. J.*, **6** (1963) 163-68.
Fletcher80	R. Fletcher, *Practical Methods of Optimization* (Wiley, New York, 1980).
Floris89	F. Florsi and J. Tomasi, “Evaluation of the dispersion contribution to the solvation energy. A simple computational model in the continuum approximation,” *J. Comp. Chem.*, **10** (1989) 616.
Floris91	F. Florsi, J. Tomasi, and J. L. Pascual-Ahuir, “Dispersion and repulsion contributions to the solvation energy: Refinements to a simple computational model in the continuum approximation,” *J. Comp. Chem.*, **12** (1991) 784.

Fogarasi92	G. Fogarasi, X. Zhou, P. Taylor, and P. Pulay, “The calculation of ab initio molecular geometries: Efficient optimization by natural internal coordinates and empirical correction by offset forces,” *J. Am. Chem. Soc.*, **114** (1992) 8191-201.
Foresman92	J. B. Foresman, M. Head-Gordon, J. A. Pople, and M. J. Frisch, “Toward a Systematic Molecular Orbital Theory for Excited States,” *J. Phys. Chem.*, **96** (1992) 135-49.
Foresman93	J. B. Foresman and H. B. Schlegel, in *Recent experimental and computational advances in molecular spectroscopy*, Ed. R. Fausto and J. M. Hollas, *NATO-ASI Series C, vol. 406* (Kluwer Academic, The Netherlands, 1993) 11-26.
Foresman96	J. B. Foresman, T. A. Keith, K. B. Wiberg, J. Snoonian, and M. J. Frisch, “Solvent Effects 5. The Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on ab initio Reaction Field Calculations,” *J. Phys. Chem.*, **100** (1996) 16098-104.
Foresman96b	J. B. Foresman and Æ. Frisch, *Exploring Chemistry with Electronic Structure Methods*, 2nd ed. (Gaussian, Inc., Pittsburgh, PA, 1996).
Foster60	J. M. Foster and S. F. Boys, “Canonical configurational interaction procedure,” *Rev. Mod. Phys.*, **32** (1960) 300-02.
Foster80	J. P. Foster and F. Weinhold, “Natural hybrid orbitals,” *J. Am. Chem. Soc.*, **102** (1980) 7211-18.
Francl82	M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, D. J. DeFrees, J. A. Pople, and M. S. Gordon, “Self-Consistent Molecular Orbital Methods. 23. A polarization-type basis set for 2nd-row elements,” *J. Chem. Phys.*, **77** (1982) 3654-65.
Frauenheim00	T. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai, and R. Scholz, “A self-consistent charge density-functional based tight-binding method for predictive materials simulations in physics, chemistry and biology,” *Physica Stat. Sol. B*, **217** (2000) 41-62.
Frauenheim02	T. Frauenheim, G. Seifert, M. Elstner, T. Niehaus, C. Kohler, M. Amkreutz, M. Sternberg, Z. Hajnal, A. D. Carlo, and S. Suhai, “Atomistic simulations of complex materials: ground-state and excited-state

	properties," *J. Phys.: Condens. Matter*, **14** (2002) 3015-47.
Frisch09	M. J. Frisch, G. Scalmani, T. Vreven, and G. Zheng, "Analytic second derivatives for semiempirical models based on MNDO," *(for Mol. Phys.)*, (2009)
Frisch84	M. J. Frisch, J. A. Pople, and J. S. Binkley, "Self-Consistent Molecular Orbital Methods. 25. Supplementary Functions for Gaussian Basis Sets," *J. Chem. Phys.*, **80** (1984) 3265-69.
Frisch86a	M. J. Frisch, Y. Yamaguchi, J. Gaw, H. F. Schaefer III, and J. S. Binkley, "Analytic Raman intensities from molecular electronic wave functions," *J. Chem. Phys.*, **84** (1986) 531-32.
Frisch90a	M. J. Frisch, M. Head-Gordon, and J. A. Pople, "Direct analytic SCF second derivatives and electric field properties," *Chem. Phys.*, **141** (1990) 189-96.
Frisch90b	M. J. Frisch, M. Head-Gordon, and J. A. Pople, "Direct MP2 gradient method," *Chem. Phys. Lett.*, **166** (1990) 275-80.
Frisch90c	M. J. Frisch, M. Head-Gordon, and J. A. Pople, "Semi-direct algorithms for the MP2 energy and gradient," *Chem. Phys. Lett.*, **166** (1990) 281-89.
Frisch92	M. J. Frisch, I. N. Ragazos, M. A. Robb, and H. B. Schlegel, "An Evaluation of 3 Direct MC-SCF Procedures," *Chem. Phys. Lett.*, **189** (1992) 524-28.
Fuentealba82	P. Fuentealba, H. Preuss, H. Stoll, and L. v. Szentpaly, "A Proper Account of Core-polarization with Pseudopotentials - Single Valence-Electron Alkali Compounds," *Chem. Phys. Lett.*, **89** (1982) 418-22.
Fuentealba83	P. Fuentealba, H. Stoll, L. v. Szentpaly, P. Schwerdtfeger, and H. Preuss, "On the reliability of semi-empirical pseudopotentials - simulation of Hartree-Fock and Dirac-Fock results," *J. Phys. B*, **16** (1983) L323-L28.
Fuentealba85	P. Fuentealba, L. v. Szentpaly, H. Preuss, and H. Stoll, "Pseudopotential calculations for alkaline-earth atoms," *J. Phys. B*, **18** (1985) 1287-96.
Fukui81	K. Fukui, "The path of chemical-reactions - The IRC approach," *Acc. Chem. Res.*, **14** (1981) 363-68.
Furche02	F. Furche and R. Ahlrichs, "Adiabatic time-dependent

	density functional methods for excited state properties," *J. Chem. Phys.*, **117** (2002) 7433-47.
G03	M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Rob, J. R. Cheeseman, J. A. Montgomery Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian 03* (Gaussian, Inc., Wallingford, CT, 2003).
G70	W. J. Hehre, W. A. Lathan, R. Ditchfield, M. D. Newton, and J. A. Pople, *Gaussian 70* (Quantum Chemistry Program Exchange, Program No. 237, 1970).
G76	J. S. Binkley, R. A. Whiteside, P. C. Hariharan, R. Seeger, J. A. Pople, W. J. Hehre, and M. D. Newton, *Gaussian 76* (Carnegie-Mellon University, Pittsburgh, PA, 1976).
G80	J. S. Binkley, R. A. Whiteside, R. Krishnan, R. Seeger, D. J. Defrees, H. B. Schlegel, S. Topiol, L. R. Kahn, and J. A. Pople, *Gaussian 80* (Carnegie-Mellon Quantum Chemistry Publishing Unit, Pittsburgh, PA, 1980).
G82	J. S. Binkley, M. J. Frisch, D. J. Defrees, R. Krishnan, R. A. Whiteside, H. B. Schlegel, E. M. Fluder, and J. A. Pople, *Gaussian 82* (Carnegie-Mellon Quantum Chemistry Publishing Unit, Pittsburgh, PA, 1982).
G86	M. J. Frisch, J. S. Binkley, H. B. Schlegel, K. Raghavachari, C. F. Melius, R. L. Martin, J. J. P. Stewart, F. W. Bobrowicz, C. M. Rohlfing, L. R. Kahn, D. J. Defrees, R. Seeger, R. A. Whiteside, D. J. Fox,

	E. M. Fluder, and J. A. Pople, *Gaussian 86* (Gaussian, Inc., Pittsburgh, PA, 1986).
G88	M. J. Frisch, M. Head-Gordon, H. B. Schlegel, K. Raghavachari, J. S. Binkley, C. Gonzalez, D. J. Defrees, D. J. Fox, R. A. Whiteside, R. Seeger, C. F. Melius, J. Baker, L. R. Kahn, J. J. P. Stewart, E. M. Fluder, S. Topiol, and J. A. Pople, *Gaussian 88* (Gaussian, Inc., Pittsburgh, PA, 1988).
G90	M. J. Frisch, M. Head-Gordon, G. W. Trucks, J. B. Foresman, K. Raghavachari, H. B. Schlegel, M. Robb, J. S. Binkley, C. Gonzalez, D. J. Defrees, D. J. Fox, R. A. Whiteside, R. Seeger, C. F. Melius, J. Baker, L. R. Kahn, J. J. P. Stewart, E. M. Fluder, S. Topiol, and J. A. Pople, *Gaussian 90* (Gaussian, Inc., Pittsburgh, PA, 1990).
G92	M. J. Frisch, G. W. Trucks, M. Head-Gordon, P. M. W. Gill, M. W. Wong, J. B. Foresman, B. G. Johnson, H. B. Schlegel, M. A. Robb, E. S. Replogle, R. Gomperts, J. L. Andres, K. Raghavachari, J. S. Binkley, C. Gonzalez, R. L. Martin, D. J. Fox, D. J. Defrees, J. Baker, J. J. P. Stewart, and J. A. Pople, *Gaussian 92* (Gaussian, Inc., Pittsburgh, PA, 1992).
G92DFT	M. J. Frisch, G. W. Trucks, H. B. Schlegel, P. M. W. Gill, B. G. Johnson, M. W. Wong, J. B. Foresman, M. A. Robb, M. Head-Gordon, E. S. Replogle, R. Gomperts, J. L. Andres, K. Raghavachari, J. S. Binkley, C. Gonzalez, R. L. Martin, D. J. Fox, D. J. Defrees, J. Baker, J. J. P. Stewart, and J. A. Pople, *Gaussian 92/DFT* (Gaussian, Inc., Pittsburgh, PA, 1993).
G94	M. J. Frisch, G. W. Trucks, H. B. Schlegel, P. M. W. Gill, B. G. Johnson, M. A. Robb, J. R. Cheeseman, T. A. Keith, G. A. Petersson, J. A. Montgomery Jr., K. Raghavachari, M. A. Al-Laham, V. G. Zakrzewski, J. V. Ortiz, J. B. Foresman, J. Cioslowski, B. B. Stefanov, A. Nanayakkara, M. Challacombe, C. Y. Peng, P. Y. Ayala, W. Chen, M. W. Wong, J. L. Andres, E. S. Replogle, R. Gomperts, R. L. Martin, D. J. Fox, J. S. Binkley, D. J. Defrees, J. Baker, J. P. Stewart, M. Head-Gordon, C. Gonzalez, and J. A. Pople, *Gaussian 94* (Gaussian, Inc., Pittsburgh, PA, 1995).
G98	M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski,

	J. A. Montgomery Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, *Gaussian 98* (Gaussian, Inc., Pittsburgh, PA, 1998).
Garrett80	B. C. Garrett, D. G. Truhlar, R. S. Grev, and A. W. Magnusson, “Improved treatment of threshold contributions in variational transition-state theory,” *J. Phys. Chem.*, **84** (1980) 1730-48.
Gauss88	J. Gauss and D. Cremer, “Analytical evaluation of energy gradients in quadratic configuration-interaction theory,” *Chem. Phys. Lett.*, **150** (1988) 280-86.
Gauss92	J. Gauss, “Calculation of NMR chemical shifts at second-order many-body perturbation theory using gauge-including atomic orbitals,” *Chem. Phys. Lett.*, **191** (1992) 614-20.
Gauss93	J. Gauss, “Effects of Electron Correlation in the Calculation of Nuclear- Magnetic-Resonance Chemical-Shifts,” *J. Chem. Phys.*, **99** (1993) 3629-43.
Gauss95	J. Gauss, “Accurate Calculation of NMR Chemical-Shifts,” *Phys. Chem. Chem. Phys.*, **99** (1995) 1001-08.
Gauss96	J. Gauss, K. Ruud, and T. Helgaker, “Perturbation-dependent atomic orbitals for the calculation of spin-rotation constants and rotational g tensors,” *J. Chem. Phys.*, **105** (1996) 2804-12.
Gerratt68	J. Gerratt and I. M. Mills, “Force constants and dipole-moment derivatives of molecules from perturbed Hartree-Fock calculations. I.,” *J. Chem. Phys.*, **49** (1968) 1719.
Gill92	P. M. W. Gill, B. G. Johnson, J. A. Pople, and M. J.

	Frisch, “The performance of the Becke-Lee-Yang-Parr (B-LYP) density functional theory with various basis sets,” *Chem. Phys. Lett.*, **197** (1992) 499-505.
Gill94	P. M. W. Gill, in *Advances in Quantum Chemistry*, Vol. 25 (Academic Press, San Diego, CA, 1994) 141-205.
Gill96	P. M. W. Gill, “A new gradient-corrected exchange functional,” *Mol. Phys.*, **89** (1996) 433-45.
Godbout92	N. Godbout, D. R. Salahub, J. Andzelm, and E. Wimmer, “Optimization of Gaussian-type basis sets for local spin density functional calculations. Part I. Boron through neon, optimization technique and validation,” *Can. J. Chem.*, **70** (1992) 560-71.
Goddard78	W. A. Goddard III and L. B. Harding, in *Annual Review of Physical Chemistry*, Ed. B. S. Rabinovitch, Vol. 29 (Annual Reviews, Inc., Palo Alto, CA, 1978) 363-96.
Golab83	J. T. Golab, D. L. Yeager, and P. Jørgensen, “Proper characterization of MC SCF stationary-points,” *Chem. Phys.*, **78** (1983) 175-99.
Gonzalez89	C. Gonzalez and H. B. Schlegel, “An Improved Algorithm for Reaction Path Following,” *J. Chem. Phys.*, **90** (1989) 2154-61.
Gonzalez90	C. Gonzalez and H. B. Schlegel, “Reaction Path Following in Mass-Weighted Internal Coordinates,” *J. Phys. Chem.*, **94** (1990) 5523-27.
Gordon80	M. S. Gordon, “The isomers of silacyclopropane,” *Chem. Phys. Lett.*, **76** (1980) 163-68.
Gordon82	M. S. Gordon, J. S. Binkley, J. A. Pople, W. J. Pietro, and W. J. Hehre, “Self-Consistent Molecular Orbital Methods. 22. Small Split-Valence Basis Sets for Second-Row Elements,” *J. Am. Chem. Soc.*, **104** (1982) 2797-803.
Gready77	J. E. Gready, G. B. Bacskay, and N. S. Hush, “Finite-field Method Calculations. III. Dipole moment gradients, polarisability gradients and field-induced shifts in bond lengths, vibrational levels, spectroscopic constants and dipole functions -- Application to LiH,” *Chem. Phys.*, **24** (1977) 333-41.
Greengard87	L. Greengard and V. Rokhlin, “A fast algorithm for particle simulations,” *J. Comp. Phys.*, **73** (1987) 325-48.

Greengard88	L. Greengard, *The Rapid Evaluation of Potential Fields in Particle Systems* (MIT Press, Cambridge, MA, 1988).
Greengard94	L. Greengard, "Fast algorithms for classical physics," *Science*, **265** (1994) 909-14.
Grimme06	S. Grimme, "Semiempirical GGA-type density functional constructed with a long-range dispersion correction," *J. Comp. Chem.*, **27** (2006) 1787-99.
Grimme06a	S. Grimme, "Semiempirical hybrid density functional with perturbative second-order correlation," *J. Chem. Phys.*, **124** (2006) 034108.
Haeussermann93	U. Haeussermann, M. Dolg, H. Stoll, and H. Preuss, "Accuracy of energy-adjusted quasi-relativistic ab initio pseudopotentials - all-electron and pseudopotential benchmark calculations for HG, HGH and their cations," *Mol. Phys.*, **78** (1993) 1211-24.
Halgren77	T. A. Halgren and W. N. Lipscomb, "The Synchronous Transit Method for Determining Reaction Pathways and Locating Transition States," *Chem. Phys. Lett.*, **49** (1977) 225-32.
Hall84	G. G. Hall and C. M. Smith, "Fitting electron-densities of molecules," *Int. J. Quantum Chem.*, **25** (1984) 881-90.
Hamilton88	T. P. Hamilton and P. Pulay, "UHF natural orbitals for defining and starting MC-SCF calculations," *J. Chem. Phys.*, **88** (1988) 4926-33.
Hamprecht98	F. A. Hamprecht, A. Cohen, D. J. Tozer, and N. C. Handy, "Development and assessment of new exchange-correlation functionals," *J. Chem. Phys.*, **109** (1998) 6264-71.
Handy01	N. C. Handy and A. J. Cohen, "Left-right correlation energy," *Mol. Phys.*, **99** (2001) 403-12.
Handy84	N. C. Handy and H. F. Schaefer III, "On the evaluation of analytic energy derivatives for correlated wave-functions," *J. Chem. Phys.*, **81** (1984) 5031-33.
Handy89	N. C. Handy, J. A. Pople, M. Head-Gordon, K. Raghavachari, and G. W. Trucks, "Size-consistent Brueckner theory limited to double substitutions," *Chem. Phys. Lett.*, **164** (1989) 185-92.
Hansen99	A. E. Hansen and K. L. Bak, "Ab initio calculations of electronic circular dichroism," *ENANTIOMER*, **4** (1999) 455-76.

Hanson87	L. K. Hanson, J. Fajer, M. A. Thompson, and M. C. Zerner, “Electrochromic Effects of Charge Separation in Bacterial Photosynthesis - Theoretical Models,” *J. Am. Chem. Soc.*, **109** (1987) 4728-30.
Hariharan73	P. C. Hariharan and J. A. Pople, “Influence of polarization functions on molecular-orbital hydrogenation energies,” *Theor. Chem. Acc.*, **28** (1973) 213-22.
Hariharan74	P. C. Hariharan and J. A. Pople, “Accuracy of AH equilibrium geometries by single determinant molecular-orbital theory,” *Mol. Phys.*, **27** (1974) 209-14.
Harris85	J. Harris, “Simplified method for calculating the energy of weakly interacting fragments,” *Phys. Rev. B*, **31** (1985) 1770-79.
Hase91	*Advances in Classical Trajectory Methods*, Vol. 1-3, Ed. W. L. Hase (JAI, Stamford, CT, 1991).
Hase96	W. L. Hase, R. J. Duchovic, X. Hu, A. Komornicki, K. F. Lim, D.-H. Lu, G. H. Peslherbe, K. N. Swamy, S. R. V. Linde, A. Varandas, H. Wang, and R. J. Wolfe, “VENUS96: A General Chemical Dynamics Computer Program,” *QCPE*, **16** (1996) 671.
Hay77	P. J. Hay, “Gaussian basis sets for molecular calculations - representation of 3D orbitals in transition-metal atoms,” *J. Chem. Phys.*, **66** (1977) 4377-84.
Hay85	P. J. Hay and W. R. Wadt, “Ab initio effective core potentials for molecular calculations - potentials for the transition-metal atoms Sc to Hg,” *J. Chem. Phys.*, **82** (1985) 270-83.
Hay85a	P. J. Hay and W. R. Wadt, “Ab initio effective core potentials for molecular calculations - potentials for K to Au including the outermost core orbitals,” *J. Chem. Phys.*, **82** (1985) 299-310.
Head-Gordon88	M. Head-Gordon and J. A. Pople, “A Method for Two-Electron Gaussian Integral and Integral Derivative Evaluation Using Recurrence Relations,” *J. Chem. Phys.*, **89** (1988) 5777-86.
Head-Gordon88a	M. Head-Gordon, J. A. Pople, and M. J. Frisch, “MP2 energy evaluation by direct methods,” *Chem. Phys. Lett.*, **153** (1988) 503-06.

Head-Gordon94	M. Head-Gordon and T. Head-Gordon, “Analytic MP2 Frequencies Without Fifth Order Storage: Theory and Application to Bifurcated Hydrogen Bonds in the Water Hexamer,” *Chem. Phys. Lett.*, **220** (1994) 122-28.
Head-Gordon94a	M. Head-Gordon, R. J. Rico, M. Oumi, and T. J. Lee, “A Doubles Correction to Electronic Excited-States from Configuration-Interaction in the Space of Single Substitutions,” *Chem. Phys. Lett.*, **219** (1994) 21-29.
Head-Gordon95	M. Head-Gordon, D. Maurice, and M. Oumi, “A Perturbative Correction to Restricted Open-Shell Configuration-Interaction with Single Substitutions for Excited-States of Radicals,” *Chem. Phys. Lett.*, **246** (1995) 114-21.
Hegarty79	D. Hegarty and M. A. Robb, “Application of unitary group-methods to configuration-interaction calculations,” *Mol. Phys.*, **38** (1979) 1795-812.
Hehre69	W. J. Hehre, R. F. Stewart, and J. A. Pople, “Self-Consistent Molecular Orbital Methods. 1. Use of Gaussian expansions of Slater-type atomic orbitals,” *J. Chem. Phys.*, **51** (1969) 2657-64.
Hehre72	W. J. Hehre, R. Ditchfield, and J. A. Pople, “Self-Consistent Molecular Orbital Methods. 12. Further extensions of Gaussian-type basis sets for use in molecular-orbital studies of organic-molecules,” *J. Chem. Phys.*, **56** (1972) 2257.
Helgaker00	T. Helgaker, M. Watson, and N. C. Handy, “Analytical calculation of nuclear magnetic resonance indirect spin-spin coupling constants at the generalized gradient approximation and hybrid levels of density-functional theory,” *J. Chem. Phys.*, **113** (2000) 9402-09.
Helgaker90	T. Helgaker, E. Uggerud, and H. J. A. Jensen, “Integration of the Classical Equations of Motion on ab initio Molecular-Potential Energy Surfaces Using Gradients and Hessians - Application to Translational Energy-Release Upon Fragmentation,” *Chem. Phys. Lett.*, **173** (1990) 145-50.
Helgaker91	T. Helgaker and P. Jørgensen, “An Electronic Hamiltonian for Origin Independent Calculations of Magnetic-Properties,” *J. Chem. Phys.*, **95** (1991) 2595-601.

Helgaker94	T. Helgaker, K. Ruud, K. L. Bak, P. Jørgensen, and J. Olsen, “Vibrational Raman Optical-Activity Calculations Using London Atomic Orbitals,” *Faraday Discuss.*, **99** (1994) 165-80.
Henderson09	T. M. Henderson, A. F. Izmaylov, G. Scalmani, and G. E. Scuseria, “Can short-range hybrids describe long-range-dependent properties?,” *J. Chem. Phys.*, **131** (2009) 044108.
Herzberg33	G. Herzberg and E. Teller, “Fluctuation structure of electron transfer in multiatomic molecules,” *Z. Phys. Chemie*, **21** (1933) 410.
Hess85	B. A. Hess, “Applicability of the no-pair equation with free-particle projection operators to atomic and molecular-structure calculations,” *Phys. Rev. A*, **32** (1985) 756-63.
Hess86	B. A. Hess, “Relativistic electronic-structure calculations employing a 2-component no-pair formalism with external-field projection operators,” *Phys. Rev. A*, **33** (1986) 3742-48.
Heyd03	J. Heyd, G. Scuseria, and M. Ernzerhof, “Hybrid functionals based on a screened Coulomb potential,” *J. Chem. Phys.*, **118** (2003) 8207-15.
Heyd04	J. Heyd and G. Scuseria, “Efficient hybrid density functional calculations in solids: The HS-Ernzerhof screened Coulomb hybrid functional,” *J. Chem. Phys.*, **121** (2004) 1187-92.
Heyd04a	J. Heyd and G. E. Scuseria, “Assessment and validation of a screened Coulomb hybrid density functional,” *J. Chem. Phys.*, **120** (2004) 7274.
Heyd05	J. Heyd, J. E. Peralta, G. E. Scuseria, and R. L. Martin, “Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional,” *J. Chem. Phys.*, **123** (2005) 174101: 1-8.
Heyd06	J. Heyd, G. E. Scuseria, and M. Ernzerhof, “Erratum: ″Hybrid functionals based on a screened Coulomb potential″,” *J. Chem. Phys.*, **124** (2006) 219906.
Hirota85	E. Hirota, *High-Resolution Spectroscopy of Transient Molecules*, *Springer Series in Chemical Physics, Vol. 40* (Springer-Verlag, Berlin, 1985).
Hirota94	E. Hirota, J. M. Brown, J. T. Hougen, T. Shida, and N. Hirota, “Symbols for fine and hyperfine-structure

	parameters," *Pure & Appl. Chem.*, **66** (1994) 571-76.
Hirshfeld77	F. L. Hirshfeld, "Bonded-atom fragments for describing molecular charge densities," *Theor. Chem. Acc.*, **44** (1977) 129-38.
Hoe01	W.-M. Hoe, A. Cohen, and N. C. Handy, "Assessment of a new local exchange functional OPTX," *Chem. Phys. Lett.*, **341** (2001) 319-28.
Hoffmann63	R. Hoffmann, "An Extended Huckel Theory. I. Hydrocarbons," *J. Chem. Phys.*, **39** (1963) 1397.
Hoffmann64	R. Hoffmann, "An Extended Huckel Theory. II. Sigma Orbitals in the Azines," *J. Chem. Phys.*, **40** (1964) 2745.
Hoffmann64a	R. Hoffmann, "An Extended Huckel Theory. III. Compounds of Boron and Nitrogen," *J. Chem. Phys.*, **40** (1964) 2474.
Hoffmann64b	R. Hoffmann, "An Extended Huckel Theory. IV. Carbonium Ions," *J. Chem. Phys.*, **40** (1964) 2480.
Hoffmann66	R. Hoffmann, "Extended Huckel Theory. V. Cumulenes, Polyenes, Polyacetylenes and Cn," *Tetrahedron*, **22** (1966) 521.
Hohenberg64	P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," *Phys. Rev.*, **136** (1964) B864-B71.
Hratchian02	H. P. Hratchian and H. B. Schlegel, "Following reaction pathways using a damped classical trajectory algorithm," *J. Phys. Chem. A*, **106** (2002) 165-69.
Hratchian04a	H. P. Hratchian and H. B. Schlegel, "Accurate reaction paths using a Hessian based predictor-corrector integrator," *J. Chem. Phys.*, **120** (2004) 9918-24.
Hratchian05a	H. P. Hratchian and H. B. Schlegel, in *Theory and Applications of Computational Chemistry: The First 40 Years*, Ed. C. E. Dykstra, G. Frenking, K. S. Kim, and G. Scuseria (Elsevier, Amsterdam, 2005) 195-249.
Hratchian05b	H. P. Hratchian and H. B. Schlegel, "Using Hessian updating to increase the efficiency of a Hessian based predictor-corrector reaction path following method," *J. Chem. Theory and Comput.*, **1** (2005) 61-69.
Humbel96	S. Humbel, S. Sieber, and K. Morokuma, "The IMOMO method: Integration of different levels of molecular orbital approximations for geometry optimization of large systems: Test for n-butane conformation and SN2

	reaction: RCI+Cl-," *J. Chem. Phys.*, **105** (1996) 1959-67.
Igel-Mann88	G. Igel-Mann, H. Stoll, and H. Preuss, "Pseudopotentials for main group elements (IIIA through VIIA)," *Mol. Phys.*, **65** (1988) 1321-28.
Iikura01	H. Iikura, T. Tsuneda, T. Yanai, and K. Hirao, "Long-range correction scheme for generalized-gradient-approximation exchange functionals," *J. Chem. Phys.*, **115** (2001) 3540-44.
Improta06	R. Improta, V. Barone, G. Scalmani, and M. J. Frisch, "A state-specific polarizable continuum model time dependent density functional method for excited state calculations in solution," *J. Chem. Phys.*, **125** (2006) 054103: 1-9.
Improta07	R. Improta, G. Scalmani, M. J. Frisch, and V. Barone, "Toward effective and reliable fluorescence energies in solution by a new State Specific Polarizable Continuum Model Time Dependent Density Functional Theory Approach," *J. Chem. Phys.*, **127** (2007) 074504: 1-9.
Ishida01	M. Ishida, K. Toyota, M. Ehara, and H. Nakatsuji, "Analytical energy gradients of the excited, ionized and electron-attached states calculated by the SAC-CI general-R method," *Chem. Phys. Lett.*, **347** (2001) 493-98.
Ishida01a	M. Ishida, K. Toyota, M. Ehara, and H. Nakatsuji, "Analytical energy gradient of high-spin multiplet state calculated by the SAC-CI method," *Chem. Phys. Lett.*, **350** (2001) 351-58.
Iyengar01	S. S. Iyengar, H. B. Schlegel, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, "Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. II. Generalizations based on mass-weighting, idempotency, energy conservation and choice of initial conditions," *J. Chem. Phys.*, **115** (2001) 10291-302.
Izmaylov06	A. F. Izmaylov, G. Scuseria, and M. J. Frisch, "Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems," *J. Chem. Phys.*, **125** (2006) 104103: 1-8.
Jankowiak07	H.-C. Jankowiak, J. L. Stuber, and R. Berger, "Vibronic transitions in large molecular systems: rigorous

	prescreening conditions for Franck-Condon factors," *J. Chem. Phys.*, **127** (2007) 234101.
Jansen89	G. Jansen and B. A. Hess, "Revision of the Douglas-Kroll transformation," *Phys. Rev. A*, **39** (1989) 6016-17.
Johnson93	B. G. Johnson, P. M. W. Gill, and J. A. Pople, "Computing Molecular Electrostatic Potentials with the PRISM Algorithm," *Chem. Phys. Lett.*, **206** (1993) 239-46.
Johnson93a	B. G. Johnson and M. J. Frisch, "Analytic second derivatives of the gradient-corrected density functional energy: Effect of quadrature weight derivatives," *Chem. Phys. Lett.*, **216** (1993) 133-40.
Johnson94	B. G. Johnson and M. J. Frisch, "An implementation of analytic second derivatives of the gradient-corrected density functional energy," *J. Chem. Phys.*, **100** (1994) 7429-42.
Jorge97	F. E. Jorge, E. V. R. de Castro, and A. B. F. da Silva, "A universal Gaussian basis set for atoms Cerium through Lawrencium generated with the generator coordinate Hartree-Fock method," *J. Comp. Chem.*, **18** (1997) 1565-69.
Jorge97a	F. E. Jorge, E. V. R. de Castro, and A. B. F. da Silva, "Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree-Fock method," *Chem. Phys.*, **216** (1997) 317-21.
Jorgensen88	P. Jørgensen, H. J. A. Jensen, and J. Olsen, "Linear Response Calculations for Large-Scale Multiconfiguration Self-Consistent Field Wave-Functions," *J. Chem. Phys.*, **89** (1988) 3654-61.
Kallay04	M. Kállay and J. Gauss, "Calculation of excited-state properties using general coupled-cluster and configuration-interaction models," *J. Chem. Phys.*, **121** (2004) 9257.
Karna91	S. P. Karna and M. Dupuis, "Frequency-Dependent Nonlinear Optical-Properties of Molecules - Formulation and Implementation in the Hondo Program," *J. Comp. Chem.*, **12** (1991) 487-504.
Kaupp91	M. Kaupp, P. v. R. Schleyer, H. Stoll, and H. Preuss, "Pseudopotential approaches to CA, SR, and BA

	hydrides. Why are some alkaline-earth MX2 compounds bent?," *J. Chem. Phys.*, **94** (1991) 1360-66.
Keith92	T. A. Keith and R. F. W. Bader, "Calculation of magnetic response properties using atoms in molecules," *Chem. Phys. Lett.*, **194** (1992) 1-8.
Keith93	T. A. Keith and R. F. W. Bader, "Calculation of magnetic response properties using a continuous set of gauge transformations," *Chem. Phys. Lett.*, **210** (1993) 223-31.
Kendall92	R. A. Kendall, T. H. Dunning Jr., and R. J. Harrison, "Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions," *J. Chem. Phys.*, **96** (1992) 6796-806.
King76	H. F. King and M. Dupuis, "Numerical Integration Using Rys Polynomials," *J. Comp. Phys.*, **21** (1976) 144-65.
Kirkwood34	J. G. Kirkwood, "Theory of Solutions of Molecules Containing Widely Separated Charges with Special Application to Zwitterions," *J. Chem. Phys.*, **2** (1934) 351.
Klene00	M. Klene, M. A. Robb, M. J. Frisch, and P. Celani, "Parallel implementation of the CI-vector evaluation in full CI/CAS-SCF," *J. Chem. Phys.*, **113** (2000) 5653-65.
Klene03	M. Klene, M. A. Robb, L. Blancafort, and M. J. Frisch, "A New Efficient Approach to the Direct RASSCF Method," *J. Chem. Phys.*, **119** (2003) 713-28.
Knowles91	P. J. Knowles, J. S. Andrews, R. D. Amos, N. C. Handy, and J. A. Pople, "Restricted Møller-Plesset theory for open shell molecules," *Chem. Phys. Lett.*, **186** (1991) 130-36.
Kobayashi91	R. Kobayashi, N. C. Handy, R. D. Amos, G. W. Trucks, M. J. Frisch, and J. A. Pople, "Gradient theory applied to the Brueckner doubles method," *J. Chem. Phys.*, **95** (1991) 6723-33.
Koch90	H. Koch and P. Jørgensen, "Coupled cluster response functions," *J. Chem. Phys.*, **93** (1990) 3333-44.
Koch94a	H. Koch, R. Kobayashi, A. Sánchez de Merás, and P. Jørgensen, "Calculation of size-intensive transition moments from the coupled cluster singles and doubles linear response function," *J. Chem. Phys.*, **100** (1994) 4393.

Kohn65	W. Kohn and L. J. Sham, “Self-Consistent Equations Including Exchange and Correlation Effects,” *Phys. Rev.*, **140** (1965) A1133-A38.
Komornicki79	A. Komornicki and R. L. Jaffe, “Ab initio investigation of the structure, vibrational frequencies, and intensities of HO2 and HOCl,” *J. Chem. Phys.*, **71** (1979) 2150-55.
Kondru98	R. K. Kondru, P. Wipf, and D. N. Beratan, “Theory-assisted determination of absolute stereochemistry for complex natural products via computation of molar rotation angles,” *J. Am. Chem. Soc.*, **120** (1998) 2204-05.
Koseki92	S. Koseki, M. W. Schmidt, and M. S. Gordon, “MCSCF/6-31G(d,p) calculations of one-electron spin-orbit-coupling constants in diatomic-molecules,” *J. Phys. Chem.*, **96** (1992) 10768-72.
Koseki95	S. Koseki, M. S. Gordon, M. W. Schmidt, and N. Matsunaga, “Main-group effective nuclear charges for spin-orbit calculations,” *J. Phys. Chem.*, **99** (1995) 12764-72.
Koseki98	S. Koseki, M. W. Schmidt, and M. S. Gordon, “Effective nuclear charges for the first- through third-row transition metal elements in spin-orbit calculations,” *J. Phys. Chem. A*, **102** (1998) 10430-35.
Krack98	M. Krack and A. M. Köster, “An adaptive numerical integrator for molecular integrals,” *J. Chem. Phys.*, **108** (1998) 3226-34.
Krieger01	J. B. Krieger, J. Q. Chen, and S. Kurth, in *Density Functional Theory and its Application to Materials*, Ed. V. VanDoren, C. VanAlsenoy, and P. Geerlings, *A.I.P. Conference Proceedings*, Vol. 577 (A.I.P., New York, 2001) 48-69.
Krieger99	J. B. Krieger, J. Q. Chen, G. J. Iafrate, and A. Savin, in *Electron Correlations and Materials Properties*, Ed. A. Gonis, N. Kioussis, and M. Ciftan (Kluwer Academic, New York, 1999) 463-77.
Krukau06	A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, and G. E. Scuseria, “Influence of the exchange screening parameter on the performance of screened hybrid functionals,” *J. Chem. Phys.*, **125** (2006) 224106.
Kudin02	K. N. Kudin, G. E. Scuseria, and E. Cancès, “A black-box

	self-consistent field convergence algorithm: One step closer," *J. Chem. Phys.*, **116** (2002) 8255-61.
Kuechle91	W. Kuechle, M. Dolg, H. Stoll, and H. Preuss, "Ab initio pseudopotentials for HG through RN. 1. Parameter sets and atomic calculations," *Mol. Phys.*, **74** (1991) 1245-63.
Kuechle94	W. Kuechle, M. Dolg, H. Stoll, and H. Preuss, "Energy-adjusted pseudopotentials for the actinides. Parameter sets and test calculations for thorium and thorium molecules," *J. Chem. Phys.*, **100** (1994) 7535-42.
Kupka86	H. Kupka and P. H. Cribb, "Multidimensional Franck-Condon integrals and Duschinsky mixing effects," *J. Chem. Phys.*, **85** (1986) 1303-15.
Labanowski91	*Density Functional Methods in Chemistry*, Ed. J. K. Labanowski and J. W. Andzelm (Springer-Verlag, New York, 1991).
Lami04	A. Lami, C. Petrongolo, and F. Santoro, in *Conical Intersections: Electronic Structure, Dynamics & Spectroscopy*, Ed. W. Domcke, D. R. Yarkony, and H. Koppel (World Scientific, Singapore, 2004).
Lauderdale91	W. J. Lauderdale, J. F. Stanton, J. Gauss, J. D. Watts, and R. J. Bartlett, "Many-body perturbation theory with a restricted open-shell Hartree-Fock reference," *Chem. Phys. Lett.*, **187** (1991)
Lauderdale92	W. J. Lauderdale, J. F. Stanton, J. Gauss, J. D. Watts, and R. J. Bartlett, "Restricted open-shell Hartree-Fock based many-body perturbation theory: Theory and application of energy and gradient calculations," *J. Chem. Phys.*, **97** (1992)
Lebedev75	V. I. Lebedev, "Weights and Nodes of Gauss-Markov Quadrature Formulas of Orders 9 to 17 for the Sphere that are Invariant under the Octahedron Group with Inversion," *Zh. Vychisl. Mat. Mat. Fiz.*, **15** (1975) 48-54.
Lebedev76	V. I. Lebedev, "Quadratures on a Sphere," *Zh. Vychisl. Mat. Mat. Fiz.*, **16** (1976) 293-306.
Lebedev80	V. I. Lebedev, in *Theory of Cubature Formulas and Computational Mathematics*, Ed. S. L. Sobolev (Nauka, Novosibirsk, 1980) 75-82 [in Russian].
Lebedev92	V. I. Lebedev and L. Skorokhodov, "Quadrature formulas

	of orders 41,47 and 53 for the sphere," *Russian Acad. Sci. Dokl. Math.*, **45** (1992) 587-92.
Lee88	C. Lee, W. Yang, and R. G. Parr, "Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density," *Phys. Rev. B*, **37** (1988) 785-89.
Lee89	T. J. Lee and P. R. Taylor, "A diagnostic for determining the quality of single-reference electron correlation methods," *Int. J. Quantum Chem., Quant. Chem. Symp.*, **S23** (1989) 199-207.
Lee90	T. J. Lee, A. P. Rendell, and P. R. Taylor, "Comparison of the Quadratic Configuration Interaction and Coupled-Cluster Approaches to Electron Correlation Including the Effect of Triple Excitations," *J. Phys. Chem.*, **94** (1990) 5463-68.
Leininger96	T. Leininger, A. Nicklass, H. Stoll, M. Dolg, and P. Schwerdtfeger, "The accuracy of the pseudopotential approximation. II. A comparison of various core sizes for indium pseudopotentials in calculations for spectroscopic constants of InH, InF, and InCI," *J. Chem. Phys.*, **105** (1996) 1052-59.
Li00	X. Li, J. M. Millam, and H. B. Schlegel, "Ab initio molecular dynamics studies of the photodissociation of formaldehyde, H2CO --> H2+CO: Direct classical trajectory calculations by MP2 and density functional theory," *J. Chem. Phys.*, **113** (2000) 10062-67.
Li06	X. Li and M. J. Frisch, "Energy-represented DIIS within a hybrid geometry optimization method," *J. Chem. Theory and Comput.*, **2** (2006) 835-39.
Liang05	J. Liang and H. Y. Li, "Calculation of the multimode Franck-Condon factors based on the coherent state method," *Mol. Phys.*, **103** (2005) 3337-42.
Lin74	S. H. Lin and H. Eyring, "Study of Franck-Condon and Herzberg-Teller approximations," *Proceedings of the National Acad. of Sciences*, **71** (1974) 3802-04.
Linderberg04	J. Linderberg and Y. Öhrn, *Propagators in Quantum Chemistry*, 2nd ed. (Wiley & Sons, Hoboken, NJ, 2004).
Lippert97	G. Lippert, J. Hutter, and M. Parrinello, "A hybrid Gaussian and plane wave density functional scheme," *Mol. Phys.*, **92** (1997) 477-87.
Lippert99	G. Lippert, J. Hutter, and M. Parrinello, "The Gaussian

	and augmented-plane-wave density functional method for ab initio molecular dynamics simulations," *Theor. Chem. Acc.*, **103** (1999) 124-40.
London37	F. London, "The quantic theory of inter-atomic currents in aromatic combinations," *J. Phys. Radium*, **8** (1937) 397-409.
Lundberg09	M. Lundberg, T. Kawatsu, T. Vreven, M. J. Frisch, and K. Morokuma, "Transition States in the Protein Environment -- ONIOM QM:MM Modeling of Isopenicillin N Synthesis," *J. Chem. Theory and Comput.*, **5** (2009) 222-34.
Macbeth	W. Shakespeare, *Macbeth*, III.iv.40-107 (London, c.1606-1611).
Malick98	D. K. Malick, G. A. Petersson, and J. A. Montgomery Jr., "Transition states for chemical reactions. I. Geometry and classical barrier height," *J. Chem. Phys.*, **108** (1998) 5704-13.
Marenich09	A. V. Marenich, C. J. Cramer, and D. G. Truhlar, "Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions," *J. Phys. Chem. B*, **113** (2009) 6378-96.
Martin03	R. L. Martin, "Natural transition orbitals," *J. Chem. Phys.*, **118** (2003) 4775-77.
Martin99	J. M. L. Martin and G. de Oliveira, "Towards standard methods for benchmark quality ab initio thermochemistry - W1 and W2 theory," *J. Chem. Phys.*, **111** (1999) 1843-56.
Martyna91	G. Martyna, C. Cheng, and M. L. Klein, "Electronic States and Dynamic Behavior of Lixen and Csxen Clusters," *J. Chem. Phys.*, **95** (1991) 1318-36.
Maseras95	F. Maseras and K. Morokuma, "IMOMM - A new integrated ab-initio plus molecular mechanics geometry optimization scheme of equilibrium structures and transition-states," *J. Comp. Chem.*, **16** (1995) 1170-79.
Matsubara96	T. Matsubara, S. Sieber, and K. Morokuma, "A Test of the New "Integrated MO + MM" (IMOMM) Method for the Conformational Energy of Ethane and n-Butane," *Int. J. Quantum Chem.*, **60** (1996) 1101-09.
Mayo90	S. L. Mayo, B. D. Olafson, and W. A. Goddard III, "Dreiding - A generic force-field for molecular simulations," *J. Phys. Chem.*, **94** (1990) 8897-909.

McClurg97	R. B. McClurg, R. C. Flagan, and W. A. Goddard III, “The hindered rotor density-of-states interpolation function,” *J. Chem. Phys.*, **106** (1997) 6675.
McClurg99	R. B. McClurg, “Comment on: ’The hindered rotor density-of-states interpolation function’ [J. Chem. Phys. 106, 6675 (1997)] and ’The hindered rotor density-of-states’ [J. Chem. Phys. 108, 2314 (1998)],” *J. Chem. Phys.*, **111** (1999) 7163.
McDouall88	J. J. McDouall, K. Peasley, and M. A. Robb, “A Simple MC-SCF Perturbation Theory: Orthogonal Valence Bond Møller-Plesset 2 (OVB-MP2),” *Chem. Phys. Lett.*, **148** (1988) 183-89.
McGrath91	M. P. McGrath and L. Radom, “Extension of Gaussian-1 (G1) theory to bromine-containing molecules,” *J. Chem. Phys.*, **94** (1991) 511-16.
McLaren63	A. D. McLaren, “Optimal Numerical Integration on a Sphere,” *Math. Comp.*, **17** (1963) 361-83.
McLean80	A. D. McLean and G. S. Chandler, “Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18,” *J. Chem. Phys.*, **72** (1980) 5639-48.
McQuarrie73	D. A. McQuarrie, *Statistical Thermodynamics* (Harper and Row, New York, 1973).
McWeeny60	R. McWeeny, “Some recent advances in density matrix theory,” *Rev. Mod. Phys.*, **32** (1960) 335-69.
McWeeny62	R. McWeeny, “Perturbation Theory for Fock-Dirac Density Matrix,” *Phys. Rev.*, **126** (1962) 1028.
McWeeny68	R. McWeeny and G. Dierksen, “Self-consistent perturbation theory. 2. Extension to open shells,” *J. Chem. Phys.*, **49** (1968) 4852.
Mennucci02	B. Mennucci, J. Tomasi, R. Cammi, J. R. Cheeseman, M. J. Frisch, F. J. Devlin, S. Gabriel, and P. J. Stephens, “Polarizable continuum model (PCM) calculations of solvent effects on optical rotations of chiral molecules,” *J. Phys. Chem. A*, **106** (2002) 6102-13.
Mennucci97	B. Mennucci and J. Tomasi, “Continuum solvation models: A new approach to the problem of solute’s charge distribution and cavity boundaries,” *J. Chem. Phys.*, **106** (1997) 5151-58.
Mennucci97a	B. Mennucci, E. Cancès, and J. Tomasi, “Evaluation of Solvent Effects in Isotropic and Anisotropic

	Dielectrics, and in Ionic Solutions with a Unified Integral Equation Method: Theoretical Bases, Computational Implementation and Numerical Applications," *J. Phys. Chem. B*, **101** (1997) 10506-17.
Miehlich89	B. Miehlich, A. Savin, H. Stoll, and H. Preuss, "Results obtained with the correlation-energy density functionals of Becke and Lee, Yang and Parr," *Chem. Phys. Lett.*, **157** (1989) 200-06.
Miertus81	S. Miertuš, E. Scrocco, and J. Tomasi, "Electrostatic Interaction of a Solute with a Continuum. A Direct Utilization of ab initio Molecular Potentials for the Prevision of Solvent Effects," *Chem. Phys.*, **55** (1981) 117-29.
Miertus82	S. Miertuš and J. Tomasi, "Approximate Evaluations of the Electrostatic Free Energy and Internal Energy Changes in Solution Processes," *Chem. Phys.*, **65** (1982) 239-45.
Millam97	J. M. Millam and G. E. Scuseria, "Linear scaling conjugate gradient density matrix search as an alternative to diagonalization for first principles electronic structure calculations," *J. Chem. Phys.*, **106** (1997) 5569-77.
Millam99	J. M. Millam, V. Bakken, W. Chen, W. L. Hase, and H. B. Schlegel, "Ab initio classical trajectories on the Born-Oppenheimer Surface: Hessian-Based Integrators using Fifth Order Polynomial and Rational Function Fits," *J. Chem. Phys.*, **111** (1999) 3800-05.
Miller80	W. H. Miller, N. C. Handy, and J. E. Adams, "Reaction-path Hamiltonian for polyatomic-molecules," *J. Chem. Phys.*, **72** (1980) 99-112.
Miller81	W. H. Miller, in *Potential Energy Surfaces and Dynamical Calculations*, Ed. D. G. Truhlar (Plenum, New York, 1981) 265.
Miller88	W. H. Miller, B. A. Ruf, and Y. T. Chang, "A diabatic reaction path Hamiltonian," *J. Chem. Phys.*, **89** (1988) 6298-304.
Miller90	W. H. Miller, R. Hernandez, N. C. Handy, D. Jayatilaka, and A. Willets, "Ab initio calculation of anharmonic constants for a transition-state, with application to semiclassical transition-state tunneling

	probabilities," *Chem. Phys. Lett.*, **172** (1990) 62-68.
Mills93	*Quantities, Units and Symbols in Physical Chemistry*, 2nd ed., Ed. I. Mills, T. Cvitaš, K. Homann, N. Kállay, and K. Kuchitsu (Blackwell, Oxford; dist. CRC Press, Boca Raton, 1993).
Minichino94	C. Minichino and V. Barone, "From concepts to algorithms for the characterization of reaction mechanisms. H2CS as a case study," *J. Chem. Phys.*, **100** (1994) 3717-41.
Mo03	S. J. Mo, T. Vreven, B. Mennucci, K. Morokuma, and J. Tomasi, "Theoretical study of the SN2 reaction of Cl-(H2O) + CH3Cl using our own N-layered integrated molecular orbital and molecular mechanics polarizable continuum model method (ONIOM-PCM)," *Theor. Chem. Acc.*, **111** (2003) 154-61.
Mohallem86	J. R. Mohallem, R. M. Dreizler, and M. Trsic, "A Griffin-Hill-Wheeler version of the Hartree-Fock equations," *Int. J. Quantum Chem., Quant. Chem. Symp.*, **30 (S20)** (1986) 45-55.
Mohallem87	J. R. Mohallem and M. Trsic, "A universal Gaussian basis set for atoms Li through Ne based on a generator coordinate version of the Hartree-Fock equations," *J. Chem. Phys.*, **86** (1987) 5043-44.
Mohr00	P. J. Mohr and B. N. Taylor, "CODATA Recommended Values of the Fundamental Physical Constants: 1998," *Rev. Mod. Phys.*, **72** (2000) 351-495.
Mohr08	P. J. Mohr, B. N. Taylor, and D. B. Newell, "CODATA Recommended Values of the Fundamental Physical Constants: 2006," *Rev. Mod. Phys.*, **80** (2008) 633-730.
Moller34	C. Møller and M. S. Plesset, "Note on an approximation treatment for many-electron systems," *Phys. Rev.*, **46** (1934) 0618-22.
Montgomery00	J. A. Montgomery Jr., M. J. Frisch, J. W. Ochterski, and G. A. Petersson, "A complete basis set model chemistry. VII. Use of the minimum population localization method," *J. Chem. Phys.*, **112** (2000) 6532-42.
Montgomery94	J. A. Montgomery Jr., J. W. Ochterski, and G. A. Petersson, "A complete basis set model chemistry. IV. An improved atomic pair natural orbital method," *J. Chem. Phys.*, **101** (1994) 5900-09.
Montgomery99	J. A. Montgomery Jr., M. J. Frisch, J. W. Ochterski, and

	G. A. Petersson, “A complete basis set model chemistry. VI. Use of density functional geometries and frequencies,” *J. Chem. Phys.*, **110** (1999) 2822-27.
Morokuma01	K. Morokuma, D. G. Musaev, T. Vreven, H. Basch, M. Torrent, and D. V. Khoroshun, “Model Studies of the Structures, Reactivities, and Reaction Mechanisms of Metalloenzymes,” *IBM J. Res. & Dev.*, **45** (2001) 367-95.
Mulliken55	R. S. Mulliken, “Electronic Population Analysis on LCAO-MO Molecular Wave Functions,” *J. Chem. Phys.*, **23** (1955) 1833-40.
Murtaugh70	B. A. Murtaugh and R. W. H. Sargent, “Computational Experience with Quadratically Convergent Minimization Methods,” *Comput. J.*, **13** (1970) 185-94.
Nakajima97	T. Nakajima and H. Nakatsuji, “Analytical energy gradient of the ground, excited, ionized and electron-attached states calculated by the SAC/SAC-CI method,” *Chem. Phys. Lett.*, **280** (1997) 79-84.
Nakajima99	T. Nakajima and H. Nakatsuji, “Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SAC-CI (configuration interaction) method,” *Chem. Phys.*, **242** (1999) 177-93.
Nakatsuji78	H. Nakatsuji and K. Hirao, “Cluster expansion of the wavefunction: Symmetry-adapted-cluster expansion, its variational determination, and extension of open-shell orbital theory,” *J. Chem. Phys.*, **68** (1978) 2053-65.
Nakatsuji79	H. Nakatsuji, “Cluster expansion of the wavefunction: Calculation of electron correlations in ground and excited states by SAC and SAC CI theories,” *Chem. Phys. Lett.*, **67** (1979) 334-42.
Nakatsuji79a	H. Nakatsuji, “Cluster expansion of the wavefunction: Electron correlations in ground and excited states by SAC (Symmetry-Adapted-Cluster) and SAC CI theories,” *Chem. Phys. Lett.*, **67** (1979) 329-33.
Nakatsuji91	H. Nakatsuji, “Description of 2-electron and many-electron processes by the SAC-CI method,” *Chem. Phys. Lett.*, **177** (1991) 331-37.
Nakatsuji91a	H. Nakatsuji, “Exponentially generated configuration interaction theory. Descriptions of excited, ionized and electron attached states,” *J. Chem. Phys.*, **94** (1991) 6716-27.

Nakatsuji93	H. Nakatsuji and M. Ehara, “Symmetry-adapted cluster-configuration interaction method applied to high-spin multiplicity,” *J. Chem. Phys.*, **98** (1993) 7179-84.
Nakatsuji96	H. Nakatsuji, “Dipped adcluster model for chemisorption and catalytic reactions,” *Prog. Surf. Sci.*, **54** (1996) 1.
Nakatsuji97	H. Nakatsuji, in *Computational Chemistry: Reviews of Current Trends*, Ed. J. Leszczynski, Vol. 2 (World Scientific, Singapore, 1997) 62-124.
Neese01	F. Neese, “Prediction of electron paramagnetic resonance g values using coupled perturbed Hartree-Fock and Kohn-Sham theory,” *J. Chem. Phys.*, **115** (2001) 11080-96.
Nicklass95	A. Nicklass, M. Dolg, H. Stoll, and H. Preuss, “Ab initio energy-adjusted pseudopotentials for the noble gases Ne through Xe: Calculation of atomic dipole and quadrupole polarizabilities,” *J. Chem. Phys.*, **102** (1995) 8942-52.
Nyden81	M. R. Nyden and G. A. Petersson, “Complete basis set correlation energies. I. The asymptotic convergence of pair natural orbital expansions,” *J. Chem. Phys.*, **75** (1981) 1843-62.
Ochterski96	J. W. Ochterski, G. A. Petersson, and J. A. Montgomery Jr., “A complete basis set model chemistry. V. Extensions to six or more heavy atoms,” *J. Chem. Phys.*, **104** (1996) 2598-619.
Ohrn81	Y. Öhrn and G. Born, in *Advances in Quantum Chemistry*, Ed. P.-O. Löwdin, Vol. 13 (Academic Press, San Diego, CA, 1981) 1-88.
Olsen85	J. Olsen and P. Jørgensen, “Linear and Nonlinear Response Functions for an Exact State and for an MCSCF State,” *J. Chem. Phys.*, **82** (1985) 3235-64.
Olsen88	J. Olsen, B. O. Roos, P. Jørgensen, and H. J. A. Jensen, “Determinant Based Configuration-Interaction Algorithms for Complete and Restricted Configuration-Interaction Spaces,” *J. Chem. Phys.*, **89** (1988) 2185-92.
Olsen95	J. Olsen, K. L. Bak, K. Ruud, T. Helgaker, and P. Jørgensen, “Orbital Connections for Perturbation-Dependent Basis-Sets,” *Theor. Chem.*

	Acc., **90** (1995) 421-39.
Onsager36	L. Onsager, "Electric Moments of Molecules in Liquids," *J. Am. Chem. Soc.*, **58** (1936) 1486-93.
Orlandi73	G. Orlandi and W. Siebrand, "Theory of vibronic intensity borrowing - Comparison of Herzberg-Teller and Born-Oppenheimer coupling," *J. Chem. Phys.*, **58** (1973) 4513-23.
Ortiz88	J. V. Ortiz, "Electron binding energies of anionic alkali metal atoms from partial fourth order electron propagator theory calculations," *J. Chem. Phys.*, **89** (1988) 6348-52.
Ortiz88a	J. V. Ortiz, "Partial fourth order electron propagator theory," *Int. J. Quantum Chem., Quant. Chem. Symp.*, **34 (S22)** (1988) 431-36.
Ortiz89	J. V. Ortiz, "Electron propagator calculations with nondiagonal partial 4th-order self-energies and unrestricted Hartree-Fock reference states," *Int. J. Quantum Chem., Quant. Chem. Symp.*, **S23** (1989) 321-32.
Ortiz96	J. V. Ortiz, "Partial third-order quasiparticle theory: Comparisons for closed-shell ionization energies and an application to the Borazine photoelectron spectrum," *J. Chem. Phys.*, **104** (1996) 7599-605.
Ortiz97	J. V. Ortiz, V. G. Zakrzewski, and O. Dolgounircheva, in *Conceptual Perspectives in Quantum Chemistry*, Ed. J.-L. Calais and E. Kryachko (Kluwer Academic, Dordrecht, 1997) 465-518.
Osamura81	Y. Osamura, Y. Yamaguchi, and H. F. Schaefer III, "Analytic configuration-interaction (CI) gradient techniques for potential-energy hypersurfaces - a method for openshell molecular wave-functions," *J. Chem. Phys.*, **75** (1981) 2919-22.
Osamura82	Y. Osamura, Y. Yamaguchi, and H. F. Schaefer III, "Generalization of analytic configuration-interaction (CI) gradient techniques for potential-energy hypersurfaces, including a solution to the coupled perturbed Hartree-Fock equations for multiconfiguration SCF molecular wave-functions," *J. Chem. Phys.*, **77** (1982) 383-90.
Otte07	N. Otte, M. Scholten, and W. Thiel, "Looking at self-consistent-charge density functional tight

	binding from a semiempirical perspective," *J. Phys. Chem. A*, **111** (2007) 5751-55.
Page88	M. Page and J. W. McIver Jr., "On evaluating the reaction path Hamiltonian," *J. Chem. Phys.*, **88** (1988) 922-35.
Page90	M. Page, C. Doubleday Jr., and J. W. McIver Jr., "Following steepest descent reaction paths - the use of higher energy derivatives with ab initio electronic-structure methods," *J. Chem. Phys.*, **93** (1990) 5634-42.
Palmer94	I. J. Palmer, F. Bernardi, M. Olivucci, I. N. Ragazos, and M. A. Robb, "An MC-SCF study of the (photochemical) Paterno-Buchi reaction," *J. Am. Chem. Soc.*, **116** (1994) 2121-32.
Papousek82	D. Papousek and M. R. Aliev, in *Molecular Vibrational Spectra*, Ed. J. R. Durig (Elsevier, New York, 1982).
Parr89	R. G. Parr and W. Yang, *Density-functional theory of atoms and molecules* (Oxford Univ. Press, Oxford, 1989).
Parthiban01	S. Parthiban and J. M. L. Martin, "Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities," *J. Chem. Phys.*, **114** (2001) 6014-29.
Pascual-Ahuir94	J. L. Pascual-Ahuir, E. Silla, and I. Tuñón, "GEPOL: An improved description of molecular-surfaces. 3. A new algorithm for the computation of a solvent-excluding surface," *J. Comp. Chem.*, **15** (1994) 1127-38.
Pedersen95	T. B. Pedersen and A. E. Hansen, "Ab initio calculation and display of the rotatory strength tensor in the random phase approximation. Method and model studies," *Chem. Phys. Lett.*, **246** (1995) 1-8.
Peluso97	A. Peluso, F. Santoro, and G. del Re, "Vibronic coupling in electronic transitions with significant Duschinsky effect," *Int. J. Quantum Chem.*, **63** (1997) 233-44.
Peng93	C. Peng and H. B. Schlegel, "Combining Synchronous Transit and Quasi-Newton Methods for Finding Transition States," *Israel J. Chem.*, **33** (1993) 449-54.
Peng96	C. Peng, P. Y. Ayala, H. B. Schlegel, and M. J. Frisch, "Using redundant internal coordinates to optimize equilibrium geometries and transition states," *J. Comp. Chem.*, **17** (1996) 49-56.

Peralta03	J. E. Peralta, G. E. Scuseria, J. R. Cheeseman, and M. J. Frisch, “Basis set dependence of NMR Spin-Spin Couplings in Density Functional Theory Calculations: First row and hydrogen atoms,” *Chem. Phys. Lett.*, **375** (2003) 452-58.
Perdew81	J. P. Perdew and A. Zunger, “Self-interaction correction to density-functional approximations for many-electron systems,” *Phys. Rev. B*, **23** (1981) 5048-79.
Perdew86	J. P. Perdew, “Density-functional approximation for the correlation energy of the inhomogeneous electron gas,” *Phys. Rev. B*, **33** (1986) 8822-24.
Perdew91	J. P. Perdew, in *Electronic Structure of Solids ‘91*, Ed. P. Ziesche and H. Eschrig (Akademie Verlag, Berlin, 1991) 11.
Perdew92	J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, “Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation,” *Phys. Rev. B*, **46** (1992) 6671-87.
Perdew92a	J. P. Perdew and Y. Wang, “Accurate and Simple Analytic Representation of the Electron Gas Correlation Energy,” *Phys. Rev. B*, **45** (1992) 13244-49.
Perdew93a	J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, “Erratum: Atoms, molecules, solids, and surfaces - Applications of the generalized gradient approximation for exchange and correlation,” *Phys. Rev. B*, **48** (1993) 4978.
Perdew96	J. P. Perdew, K. Burke, and Y. Wang, “Generalized gradient approximation for the exchange-correlation hole of a many-electron system,” *Phys. Rev. B*, **54** (1996) 16533-39.
Perdew96a	J. P. Perdew, K. Burke, and M. Ernzerhof, “Generalized gradient approximation made simple,” *Phys. Rev. Lett.*, **77** (1996) 3865-68.
Perdew97	J. P. Perdew, K. Burke, and M. Ernzerhof, “Errata: Generalized gradient approximation made simple,” *Phys. Rev. Lett.*, **78** (1997) 1396.
Perdew99	J. P. Perdew, S. Kurth, A. Zupan, and P. Blaha, “Accurate density functional with correct formal properties: A step beyond the generalized gradient

	approximation," *Phys. Rev. Lett.*, **82** (1999) 2544-47.
Peterson94	K. A. Peterson, D. E. Woon, and T. H. Dunning Jr., "Benchmark calculations with correlated molecular wave functions. IV. The classical barrier height of the H+H2 ® H2+H reaction," *J. Chem. Phys.*, **100** (1994) 7410-15.
Petersson88	G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Al-Laham, W. A. Shirley, and J. Mantzaris, "A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row atoms," *J. Chem. Phys.*, **89** (1988) 2193-218.
Petersson91	G. A. Petersson and M. A. Al-Laham, "A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms," *J. Chem. Phys.*, **94** (1991) 6081-90.
Petersson91a	G. A. Petersson, T. G. Tensfeldt, and J. A. Montgomery Jr., "A complete basis set model chemistry. III. The complete basis set-quadratic configuration interaction family of methods," *J. Chem. Phys.*, **94** (1991) 6091-101.
Petersson98	G. A. Petersson, in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, Ed. K. K. Irikura and D. J. Frurip, *ACS Symposium Series*, Vol. 677 (ACS, Washington, D.C., 1998) 237.
Petersson98a	G. A. Petersson, D. K. Malick, W. G. Wilson, J. W. Ochterski, J. A. Montgomery Jr., and M. J. Frisch, "Calibration and comparison of the Gaussian-2, complete basis set, and density functional methods for computational thermochemistry," *J. Chem. Phys.*, **109** (1998) 10570-79.
Pickett91	H. M. Pickett, "The Fitting and Prediction of Vibration-Rotation Spectra with Spin Interactions," *J. Mol. Spec.*, **148** (1991) 371-77.
Pierotti76	R. A. Pierotti, "A scaled particle theory of aqueous and nonaqueous solutions," *Chem. Rev.*, **76** (1976) 717.
Pietro82	W. J. Pietro, M. M. Francl, W. J. Hehre, D. J. Defrees, J. A. Pople, and J. S. Binkley, "Self-Consistent Molecular Orbital Methods. 24. Supplemented small split-valence basis-sets for 2nd-row elements," *J. Am. Chem. Soc.*, **104** (1982) 5039-48.
Pipek89	J. Pipek and P. G. Mezey, "A fast intrinsic localization procedure applicable for ab initio and

	semiempirical linear combination of atomic orbital wave functions," *J. Chem. Phys.*, **90** (1989) 4916-26.
Pople54	J. A. Pople and R. K. Nesbet, "Self-Consistent Orbitals for Radicals," *J. Chem. Phys.*, **22** (1954) 571-72.
Pople67	J. A. Pople, D. Beveridge, and P. Dobosh, "Approximate self-consistent molecular-orbital theory. 5. Intermediate neglect of differential overlap," *J. Chem. Phys.*, **47** (1967) 2026-33.
Pople67a	J. A. Pople and M. S. Gordon, "Molecular orbital theory of electronic structure of organic compounds. 1. Substituent effects and dipole methods," *J. Am. Chem. Soc.*, **89** (1967) 4253.
Pople76	J. A. Pople, J. S. Binkley, and R. Seeger, "Theoretical Models Incorporating Electron Correlation," *Int. J. Quantum Chem.*, **Suppl. Y-10** (1976) 1-19.
Pople77	J. A. Pople, R. Seeger, and R. Krishnan, "Variational Configuration Interaction Methods and Comparison with Perturbation Theory," *Int. J. Quantum Chem.*, **Suppl. Y-11** (1977) 149-63.
Pople78	J. A. Pople, R. Krishnan, H. B. Schlegel, and J. S. Binkley, "Electron Correlation Theories and Their Application to the Study of Simple Reaction Potential Surfaces," *Int. J. Quantum Chem.*, **14** (1978) 545-60.
Pople79	J. A. Pople, K. Raghavachari, H. B. Schlegel, and J. S. Binkley, "Derivative Studies in Hartree-Fock and Møller-Plesset Theories," *Int. J. Quantum Chem., Quant. Chem. Symp.*, **S13** (1979) 225-41.
Pople87	J. A. Pople, M. Head-Gordon, and K. Raghavachari, "Quadratic configuration interaction - a general technique for determining electron correlation energies," *J. Chem. Phys.*, **87** (1987) 5968-75.
Pople89	J. A. Pople, M. Head-Gordon, D. J. Fox, K. Raghavachari, and L. A. Curtiss, "Gaussian-1 theory: A general procedure for prediction of molecular energies," *J. Chem. Phys.*, **90** (1989) 5622-29.
Pople92	J. A. Pople, P. M. W. Gill, and B. G. Johnson, "Kohn-Sham density-functional theory within a finite basis set," *Chem. Phys. Lett.*, **199** (1992) 557-60.
Porezag95	D. Porezag, T. Frauenheim, T. Köhler, G. Seifert, and R. Kaschner, "Construction of tight-binding-like potentials on the basis of density-functional theory:

	Application to carbon," *Phys. Rev. B*, **51** (1995) 12947-57.
Pulay72	P. Pulay and W. Meyer, "Force constants and dipole-moment derivatives of ammonia from Hartree-Fock calculations," *J. Chem. Phys.*, **57** (1972) 3337.
Pulay79	P. Pulay, G. Fogarasi, F. Pang, and J. E. Boggs, "Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole-moment derivatives," *J. Am. Chem. Soc.*, **101** (1979) 2550-60.
Pulay82	P. Pulay, "Improved SCF convergence acceleration," *J. Comp. Chem.*, **3** (1982) 556-60.
Pulay83	P. Pulay, "2nd and 3rd derivatives of variational energy expressions - application to multi-configurational self-consistent field wave-functions," *J. Chem. Phys.*, **78** (1983) 5043-51.
Pulay92	P. Pulay and G. Fogarasi, "Geometry optimization in redundant internal coordinates," *J. Chem. Phys.*, **96** (1992) 2856-60.
Purvis82	G. D. Purvis III and R. J. Bartlett, "A full coupled-cluster singles and doubles model - the inclusion of disconnected triples," *J. Chem. Phys.*, **76** (1982) 1910-18.
Pyykko81	P. Pyykko and L. L. Lohr, "Relativistically Parameterized Extended Huckel Calculations. 3. Structure and Bonding for Some Compounds of Uranium and Other Heavy-Elements," *Inorganic Chem.*, **20** (1981) 1950-59.
Pyykko84	P. Pyykko and L. Laaksonen, "Relativistically Parameterized Extended Huckel Calculations. 8. Double-Zeta Parameters for the Actinoids Th, Pa, U, Np, Pu, and Am and an Application on Uranyl," *J. Phys. Chem.*, **88** (1984) 4892-95.
Rabuck99	A. Rabuck and G. E. Scuseria, "Improving self-consistent field convergence by varying occupation numbers," *J. Chem. Phys.*, **110** (1999) 695-700.
Raff85	L. M. Raff and D. L. Thompson, in *Theory of Chemical Reaction Dynamics*, Ed. M. Baer (CRC, Boca Raton, FL, 1985).
Raffenetti73	R. C. Raffenetti, "Pre-processing Two-Electron

	Integrals for Efficient Utilization in Many-Electron Self-Consistent Field Calculations," *Chem. Phys. Lett.*, **20** (1973) 335-38.
Ragazos92	I. N. Ragazos, M. A. Robb, F. Bernardi, and M. Olivucci, "Optimization and Characterization of the Lowest Energy Point on a Conical Intersection using an MC-SCF Lagrangian," *Chem. Phys. Lett.*, **197** (1992) 217-23.
Raghavachari78	K. Raghavachari and J. A. Pople, "Approximate 4th-order perturbation-theory of electron correlation energy," *Int. J. Quantum Chem.*, **14** (1978) 91-100.
Raghavachari80	K. Raghavachari, M. J. Frisch, and J. A. Pople, "Contribution of triple substitutions to the electron correlation energy in fourth-order perturbation theory," *Chem. Phys. Lett.*, **72** (1980) 4244-45.
Raghavachari80a	K. Raghavachari, H. B. Schlegel, and J. A. Pople, "Derivative studies in configuration-interaction theory," *J. Chem. Phys.*, **72** (1980) 4654-55.
Raghavachari80b	K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, "Self-Consistent Molecular Orbital Methods. 20. Basis set for correlated wave-functions," *J. Chem. Phys.*, **72** (1980) 650-54.
Raghavachari81	K. Raghavachari and J. A. Pople, "Calculation of one-electron properties using limited configuration-interaction techniques," *Int. J. Quantum Chem.*, **20** (1981) 1067-71.
Raghavachari89	K. Raghavachari and G. W. Trucks, "Highly correlated systems: Excitation energies of first row transition metals Sc-Cu," *J. Chem. Phys.*, **91** (1989) 1062-65.
Raghavachari90	K. Raghavachari, J. A. Pople, E. S. Replogle, and M. Head-Gordon, "Fifth Order Møller-Plesset Perturbation Theory: Comparison of Existing Correlation Methods and Implementation of New Methods Correct to Fifth Order," *J. Phys. Chem.*, **94** (1990) 5579-86.
Rappe81	A. K. Rappé, T. Smedly, and W. A. Goddard III, "The Shape and Hamiltonian Consistent (SHC) Effective Potentials," *J. Phys. Chem.*, **85** (1981) 1662-66.
Rappe91	A. K. Rappé and W. A. Goddard III, "Charge equilibration for molecular-dynamics simulations," *J. Phys. Chem.*, **95** (1991) 3358-63.
Rappe92	A. K. Rappé, C. J. Casewit, K. S. Colwell, W. A. G. III, and W. M. Skiff, "UFF, a full periodic-table

	force-field for molecular mechanics and molecular-dynamics simulations," *J. Am. Chem. Soc.*, **114** (1992) 10024-35.
Rassolov01	V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern, and L. A. Curtiss, "6-31G* Basis Set for Third-Row Atoms," *J. Comp. Chem.*, **22** (2001) 976-84.
Rassolov98	V. A. Rassolov, J. A. Pople, M. A. Ratner, and T. L. Windus, "6-31G* basis set for atoms K through Zn," *J. Chem. Phys.*, **109** (1998) 1223-29.
Reed83a	A. E. Reed and F. Weinhold, "Natural bond orbital analysis of near-Hartree-Fock water dimer," *J. Chem. Phys.*, **78** (1983) 4066-73.
Reed85	A. E. Reed, R. B. Weinstock, and F. Weinhold, "Natural-population analysis," *J. Chem. Phys.*, **83** (1985) 735-46.
Reed85a	A. E. Reed and F. Weinhold, "Natural Localized Molecular Orbitals," *J. Chem. Phys.*, **83** (1985) 1736-40.
Reed88	A. E. Reed, L. A. Curtiss, and F. Weinhold, "Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint," *Chem. Rev.*, **88** (1988) 899-926.
Rega96	N. Rega, M. Cossi, and V. Barone, "Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution," *J. Chem. Phys.*, **105** (1996) 11060-67.
Repasky02	M. P. Repasky, J. Chandrasekhar, and W. L. Jorgensen, "PDDG/PM3 and PDDG/MNDO: Improved semiempirical methods," *J. Comp. Chem.*, **23** (2002) 1601-22.
Rey98	J. Rey and A. Savin, "Virtual space level shifting and correlation energies," *Int. J. Quantum Chem.*, **69** (1998) 581-90.
Ricca95	A. Ricca and C. W. Bauschlicher Jr., "Successive H2O binding energies for Fe(H2O)N+," *J. Phys. Chem.*, **99** (1995) 9003-07.
Rice90	J. E. Rice, R. D. Amos, S. M. Colwell, N. C. Handy, and J. Sanz, "Frequency-Dependent Hyperpolarizabilities with Application to Formaldehyde and Methyl-Fluoride," *J. Chem. Phys.*, **93** (1990) 8828-39.
Rice91	J. E. Rice and N. C. Handy, "The Calculation of

	Frequency-Dependent Polarizabilities as Pseudo-Energy Derivatives," *J. Chem. Phys.*, **94** (1991) 4959-71.
Rice92	J. E. Rice and N. C. Handy, "The Calculation of Frequency-Dependent Hyperpolarizabilities Including Electron Correlation-Effects," *Int. J. Quantum Chem.*, **43** (1992) 91-118.
Ridley73	J. E. Ridley and M. C. Zerner, "An Intermediate Neglect of Differential Overlap Technique for Spectroscopy: Pyrrole and the Azines," *Theor. Chem. Acc.*, **32** (1973) 111-34.
Ridley76	J. E. Ridley and M. C. Zerner, "Triplet states via Intermediate Neglect of Differential Overlap: Benzene, Pyridine, and Diazines," *Theor. Chem. Acc.*, **42** (1976) 223-36.
Ritchie85	J. P. Ritchie, "Electron density distribution analysis for nitromethane, nitromethide, and nitramide," *J. Am. Chem. Soc.*, **107** (1985) 1829-37.
Ritchie87	J. P. Ritchie and S. M. Bachrach, "Some methods and applications of electron density distribution analysis," *J. Comp. Chem.*, **8** (1987) 499-509.
Robb90	M. A. Robb and U. Niazi, *Reports in Molecular Theory*, **1** (1990) 23.
Roothaan51	C. C. J. Roothaan, "New Developments in Molecular Orbital Theory," *Rev. Mod. Phys.*, **23** (1951) 69.
Rosenfeld28	L. Z. Rosenfeld, *Physik*, **52** (1928) 161.
Ruud02	K. Ruud and T. Helgaker, "Optical rotation studied by density-functional and coupled-cluster methods," *Chem. Phys. Lett.*, **352** (2002) 533-39.
Ruud02a	K. Ruud, T. Helgaker, and P. Bour, "Gauge-origin independent density-functional theory calculations of vibrational Raman optical activity," *J. Phys. Chem. A*, **106** (2002) 7448-55.
Ruud93	K. Ruud, T. Helgaker, K. L. Bak, P. Jørgensen, and H. J. A. Jensen, "Hartree-Fock Limit Magnetizabilities from London Orbitals," *J. Chem. Phys.*, **99** (1993) 3847-59.
Rys83	J. Rys, M. Dupuis, and H. F. King, "Computation of electron repulsion integrals using the Rys quadrature method," *J. Comp. Chem.*, **4** (1983) 154-57.
Saebo89	S. Saebø and J. Almlöf, "Avoiding the integral storage

	bottleneck in LCAO calculations of electron correlation," *Chem. Phys. Lett.*, **154** (1989) 83-89.
Salahub89	*The Challenge of d and f Electrons*, Ed. D. R. Salahub and M. C. Zerner (ACS, Washington, D.C., 1989).
Salter89	E. A. Salter, G. W. Trucks, and R. J. Bartlett, "Analytic Energy Derivatives in Many-Body Methods. I. First Derivatives," *J. Chem. Phys.*, **90** (1989) 1752-66.
Santoro07	F. Santoro, R. Improta, A. Lami, J. Bloino, and V. Barone, "Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution," *J. Chem. Phys.*, **126** (2007) 084509 1-13.
Santoro07a	F. Santoro, A. Lami, R. Improta, and V. Barone, "Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution," *J. Chem. Phys.*, **126** (2007) 184102.
Santoro08	F. Santoro, A. Lami, R. Improta, J. Bloino, and V. Barone, "Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect: The Qx band of porphyrin as a case study," *J. Chem. Phys.*, **128** (2008) 224311.
Sattelmeyer06	K. W. Sattelmeyer, J. Tirado-Rives, and W. L. Jorgensen, "Comparison of SCC-DFTB and NDDO-based semiempirical molecular orbital methods for organic molecules," *J. Phys. Chem. A*, **110** (2006) 13551-59.
Scalmani06	G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi, and V. Barone, "Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model," *J. Chem. Phys.*, **124** (2006) 094107: 1-15.
Scalmani09	G. Scalmani and M. J. Frisch, "A continuous surface charge formalism for the polarizable continuum model of solvation," (2009) in prep.
Schaefer92	A. Schaefer, H. Horn, and R. Ahlrichs, "Fully optimized contracted Gaussian-basis sets for atoms Li to Kr," *J. Chem. Phys.*, **97** (1992) 2571-77.
Schaefer94	A. Schaefer, C. Huber, and R. Ahlrichs, "Fully optimized contracted Gaussian-basis sets of triple zeta valence quality for atoms Li to Kr," *J. Chem. Phys.*,

	100 (1994) 5829-35.
Schlegel01	H. B. Schlegel, J. M. Millam, S. S. Iyengar, G. A. Voth, G. E. Scuseria, A. D. Daniels, and M. J. Frisch, "Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals," *J. Chem. Phys.*, **114** (2001) 9758-63.
Schlegel02	H. B. Schlegel, S. S. Iyengar, X. Li, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, "Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with Born-Oppenheimer dynamics," *J. Chem. Phys.*, **117** (2002) 8694-704.
Schlegel82	H. B. Schlegel, "Optimization of Equilibrium Geometries and Transition Structures," *J. Comp. Chem.*, **3** (1982) 214-18.
Schlegel82a	H. B. Schlegel and M. A. Robb, "MC SCF gradient optimization of the H2CO --> H2 + CO transition structure," *Chem. Phys. Lett.*, **93** (1982) 43-46.
Schlegel84	H. B. Schlegel, J. S. Binkley, and J. A. Pople, "First and Second Derivatives of Two Electron Integrals over Cartesian Gaussians using Rys Polynomials," *J. Chem. Phys.*, **80** (1984) 1976-81.
Schlegel84a	H. B. Schlegel, "Estimating the Hessian for gradient-type geometry optimizations," *Theor. Chem. Acc.*, **66** (1984) 333-40.
Schlegel89	H. B. Schlegel, in *New Theoretical Concepts for Understanding Organic Reactions*, Ed. J. Bertran and I. G. Csizmadia, *NATO-ASI series C, vol. 267* (Kluwer Academic, The Netherlands, 1989) 33-53.
Schlegel91	H. B. Schlegel and M. J. Frisch, in *Theoretical and Computational Models for Organic Chemistry*, Ed. J. S. Formosinho, I. G. Csizmadia, and L. G. Arnaut, *NATO-ASI Series C, vol. 339* (Kluwer Academic, The Netherlands, 1991) 5-33.
Schlegel91a	H. B. Schlegel and J. J. McDouall, in *Computational Advances in Organic Chemistry*, Ed. C. Ögretir and I. G. Csizmadia (Kluwer Academic, The Netherlands, 1991) 167-85.
Schlegel95	H. B. Schlegel, in *Modern Electronic Structure Theory*, Ed. D. R. Yarkony (World Scientific Publishing, Singapore, 1995) 459-500.

Schlegel95a	H. B. Schlegel and M. J. Frisch, “Transformation between Cartesian and Pure Spherical Harmonic Gaussians,” *Int. J. Quantum Chem.*, **54** (1995) 83-87.
Schmider98	H. L. Schmider and A. D. Becke, “Optimized density functionals from the extended G2 test set,” *J. Chem. Phys.*, **108** (1998) 9624-31.
Schwabe06	T. Schwabe and S. Grimme, “Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects,” *Phys. Chem. Chem. Phys.*, **8** (2006) 4398.
Schwabe07	T. Schwabe and S. Grimme, “Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability,” *Phys. Chem. Chem. Phys.*, **9** (2007) 3397.
Schwartz98	M. Schwartz, P. Marshall, R. J. Berry, C. J. Ehlers, and G. A. Petersson, “Computational study of the kinetics of hydrogen abstraction from fluoromethanes by the hydroxyl radical,” *J. Phys. Chem. A*, **102** (1998) 10074-81.
Schwerdtfeger89	P. Schwerdtfeger, M. Dolg, W. H. E. Schwarz, G. A. Bowmaker, and P. D. W. Boyd, “Relativistic effects in gold chemistry. 1. Diatomic gold compounds,” *J. Chem. Phys.*, **91** (1989) 1762-74.
Scuseria88	G. E. Scuseria, C. L. Janssen, and H. F. Schaefer III, “An efficient reformulation of the closed-shell coupled cluster single and double excitation (CCSD) equations,” *J. Chem. Phys.*, **89** (1988) 7382-87.
Scuseria89	G. E. Scuseria and H. F. Schaefer III, “Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration-interaction (QCISD)?,” *J. Chem. Phys.*, **90** (1989) 3700-03.
Scuseria92	G. E. Scuseria, “Comparison of coupled-cluster results with a hybrid of Hartree-Fock and density functional theory,” *J. Chem. Phys.*, **97** (1992) 7528-30.
Seeger76	R. Seeger and J. A. Pople, “Self-Consistent Molecular Orbital Methods. 16. Numerically stable direct energy minimization procedures for solution of Hartree-Fock equations,” *J. Chem. Phys.*, **65** (1976) 265-71.
Seeger77	R. Seeger and J. A. Pople, “Self-Consistent Molecular Orbital Methods. 28. Constraints and Stability in Hartree-Fock Theory,” *J. Chem. Phys.*, **66** (1977)

	3045-50.
Segal66	G. Segal and J. Pople, “Approximate self-consistent molecular orbital theory. 3. CNDO results for AB2 and AB3 systems,” *J. Chem. Phys.*, **44** (1966) 3289-96.
Sekino86	H. Sekino and R. J. Bartlett, “Frequency-Dependent Nonlinear Optical-Properties of Molecules,” *J. Chem. Phys.*, **85** (1986) 976-89.
Sharp64	T. E. Sharp and H. M. Rosenstock, “Franck-Condon factors for polyatomic molecules,” *J. Chem. Phys.*, **41** (1964) 3453.
Siegbahn84	P. E. M. Siegbahn, “A new direct CI method for large CI expansions in a small orbital space,” *Chem. Phys. Lett.*, **109** (1984) 417-23.
Silver78	D. M. Silver, S. Wilson, and W. C. Nieuwpoort, “Universal basis sets and transferability of integrals,” *Int. J. Quantum Chem.*, **14** (1978) 635-39.
Silver78a	D. M. Silver and W. C. Nieuwpoort, “Universal atomic basis sets,” *Chem. Phys. Lett.*, **57** (1978) 421-22.
Simon96	S. Simon, M. Duran, and J. J. Dannenberg, “How does basis set superposition error change the potential surfaces for hydrogen bonded dimers?,” *J. Chem. Phys.*, **105** (1996) 11024-31.
Simons83	J. Simons, P. Jørgensen, H. Taylor, and J. Ozment, “Walking on Potential Energy Surfaces,” *J. Phys. Chem.*, **87** (1983) 2745-53.
Singh84	U. C. Singh and P. A. Kollman, “An approach to computing electrostatic charges for molecules,” *J. Comp. Chem.*, **5** (1984) 129-45.
Skodje82	R. T. Skodje, D. G. Truhlar, and B. C. Garrett, “Vibrationally adiabatic models for reactive tunneling,” *J. Chem. Phys.*, **77** (1982) 5955-76.
Slater74	J. C. Slater, *The Self-Consistent Field for Molecular and Solids*, *Quantum Theory of Molecular and Solids, Vol. 4* (McGraw-Hill, New York, 1974).
Small71	G. J. Small, “Herzberg-Teller vibronic coupling and Duschinsky effect,” *J. Chem. Phys.*, **54** (1971) 3300.
Smith86	C. M. Smith and G. G. Hall, “Approximation of electron-densities,” *Theor. Chem. Acc.*, **69** (1986) 63-69.
Sosa92	C. Sosa, J. Andzelm, B. C. Elkin, E. Wimmer, K. D. Dobbs,

	and D. A. Dixon, “A Local Density Functional Study of the Structure and Vibrational Frequencies of Molecular Transition-Metal Compounds,” *J. Phys. Chem.*, **96** (1992) 6630-36.
Sosa93a	C. Sosa and C. Lee, “Density-functional description of transition structures using nonlocal corrections: Silylene insertion reactions into the hydrogen molecule,” *J. Chem. Phys.*, **98** (1993) 8004-11.
Stanton93	J. F. Stanton and R. J. Bartlett, “Equation of motion coupled-cluster method: A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties,” *J. Chem. Phys.*, **98** (1993) 7029-39.
Stephens01	P. J. Stephens, F. J. Devlin, J. R. Cheeseman, and M. J. Frisch, “Calculation of optical rotation using density functional theory,” *J. Phys. Chem. A*, **105** (2001) 5356-71.
Stephens02a	P. J. Stephens, F. J. Devlin, J. R. Cheeseman, M. J. Frisch, and C. Rosini, “Determination of Absolute Configuration Using Optical Rotation Calculated Using Density Functional Theory,” *Org. Lett.*, **4** (2002) 4595-98.
Stephens03	P. J. Stephens, F. J. Devlin, J. R. Cheeseman, M. J. Frisch, O. Bortolini, and P. Besse, “Determination of Absolute Configuration Using Ab Initio Calculation of Optical Rotation,” *Chirality*, **15** (2003) S57-S64.
Stephens05	P. J. Stephens, D. M. McCann, J. R. Cheeseman, and M. J. Frisch, “Determination of absolute configurations of chiral molecules using ab initio time-dependent density functional theory calculations of optical rotation: How reliable are absolute configurations obtained for molecules with small rotations?,” *Chirality*, **17** (2005) S52-S64.
Stephens08	J. P. Stephens, J. J. Pan, F. J. Devlin, and J. R. Cheeseman, “Determination of the Absolute Configurations of Natural Products Using TDDFT Optical Rotation Calculations: The Iridoid Oruwacin,” *J. Natural Prod.*, **71** (2008) 285-88.
Stephens94	P. J. Stephens, F. J. Devlin, M. J. Frisch, and C. F. Chabalowski, “Ab initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields,” *J. Phys. Chem.*, **98** (1994)

	11623-27.
Stephens94a	P. J. Stephens, F. J. Devlin, C. S. Ashvar, C. F. Chabalowski, and M. J. Frisch, “Theoretical Calculation of Vibrational Circular Dichroism Spectra,” *Faraday Discuss.*, **99** (1994) 103-19.
Stevens63	R. M. Stevens, R. M. Pitzer, and W. N. Lipscomb, “Perturbed Hartree-Fock calculations. 1. Magnetic susceptibility and shielding in LiH molecule,” *J. Chem. Phys.*, **38** (1963) 550.
Stevens84	W. J. Stevens, H. Basch, and M. Krauss, “Compact effective potentials and efficient shared-exponent basis-sets for the 1st-row and 2nd-row atoms,” *J. Chem. Phys.*, **81** (1984) 6026-33.
Stevens92	W. J. Stevens, M. Krauss, H. Basch, and P. G. Jasien, “Relativistic compact effective potentials and efficient, shared-exponent basis-sets for the 3rd-row, 4th-row, and 5th-row atoms,” *Can. J. Chem.*, **70** (1992) 612-30.
Stewart07	J. J. P. Stewart, “Optimization of parameters for semiempirical methods. V. Modification of NDDO approximations and application to 70 elements,” *J. Mol. Model.*, **13** (2007) 1173-213.
Stewart89	J. J. P. Stewart, “Optimization of parameters for semiempirical methods. I. Method,” *J. Comp. Chem.*, **10** (1989) 209-20.
Stewart89a	J. J. P. Stewart, “Optimization of parameters for semiempirical methods. II. Applications,” *J. Comp. Chem.*, **10** (1989) 221-64.
Stoll84	H. Stoll, P. Fuentealba, P. Schwerdtfeger, J. Flad, L. v. Szentpaly, and H. Preuss, “Cu and Ag as one-valence-electron atoms - CI results and quadrupole corrections of Cu2, Ag2, CuH, and AgH,” *J. Chem. Phys.*, **81** (1984) 2732-36.
Strain96	M. C. Strain, G. E. Scuseria, and M. J. Frisch, “Achieving Linear Scaling for the Electronic Quantum Coulomb Problem,” *Science*, **271** (1996) 51-53.
Stratmann96	R. E. Stratmann, G. E. Scuseria, and M. J. Frisch, “Achieving linear scaling in exchange-correlation density functional quadratures,” *Chem. Phys. Lett.*, **257** (1996) 213-23.
Stratmann97	R. E. Stratmann, J. C. Burant, G. E. Scuseria, and M.

	J. Frisch, “Improving harmonic vibrational frequencies calculations in density functional theory,” *J. Chem. Phys.*, **106** (1997) 10175-83.
Stratmann98	R. E. Stratmann, G. E. Scuseria, and M. J. Frisch, “An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules,” *J. Chem. Phys.*, **109** (1998) 8218-24.
Svensson96	M. Svensson, S. Humbel, R. D. J. Froese, T. Matsubara, S. Sieber, and K. Morokuma, “ONIOM: A multi-layered integrated MO+MM method for geometry optimizations and single point energy predictions. A test for Diels-Alder reactions and Pt(P(t-Bu)3)2+H2 oxidative addition,” *J. Phys. Chem.*, **100** (1996) 19357-63.
Svensson96a	M. Svensson, S. Humbel, and K. Morokuma, “Energetics using the single point IMOMO (integrated molecular orbital plus molecular orbital) calculations: Choices of computational levels and model system,” *J. Chem. Phys.*, **105** (1996) 3654-61.
Sychrovsky00	V. Sychrovsky, J. Gräfenstein, and D. Cremer, “Nuclear magnetic resonance spin-spin coupling constants from coupled perturbed density functional theory,” *J. Chem. Phys.*, **113** (2000) 3530-47.
Szentpaly82	L. v. Szentpaly, P. Fuentealba, H. Preuss, and H. Stoll, “Pseudopotential calculations on Rb+2, Cs+2, RbH+, CsH+ and the mixed alkali dimer ions ” *Chem. Phys. Lett.*, **93** (1982) 555-59.
Tao03	J. M. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, “Climbing the density functional ladder: Nonempirical meta-generalized gradient approximation designed for molecules and solids,” *Phys. Rev. Lett.*, **91** (2003) 146401.
Tawada04	Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai, and K. Hirao, “A long-range-corrected time-dependent density functional theory,” *J. Chem. Phys.*, **120** (2004) 8425.
Taylor87	P. R. Taylor, “Integral processing in beyond-Hartree-Fock calculations,” *Int. J. Quantum Chem.*, **31** (1987) 521-34.
Thiel92	W. Thiel and A. A. Voityuk, “Extension of the MNDO formalism to d orbitals: Integral approximations and preliminary numerical results,” *Theor. Chem. Acc.*, **81**

	(1992) 391-404.
Thiel96	W. Thiel and A. A. Voityuk, “Extension of MNDO to d orbitals: Parameters and results for the second-row elements and for the zinc group,” *J. Phys. Chem.*, **100** (1996) 616-26.
Thompson91	M. A. Thompson and M. C. Zerner, “A Theoretical Examination of the Electronic Structure and Spectroscopy of the Photosynthetic Reaction Center from Rhodopseudomonas viridis,” *J. Am. Chem. Soc.*, **113** (1991) 8210-15.
Thompson98	D. L. Thompson, in *Encyclopedia of Computational Chemistry*, Ed. P. v. R. Schleyer, N. L. Allinger, P. A. Kollman, T. Clark, H. F. Schaefer III, J. Gasteiger, and P. R. Schreiner (Wiley, Chichester, 1998) 3056-73.
Thorvaldsen08	A. J. Thorvaldsen, K. Ruud, K. Kristensen, P. Jørgensen, and S. Coriani, “A density matrix-based quasienergy formulation of the Kohn-Sham density functional response theory using perturbation- and time-dependent basis sets,” *J. Chem. Phys.*, **129** (2008) 214108.
Tirado-Rives08	J. Tirado-Rives and W. L. Jorgensen, “Performance of B3LYP density functional methods for a large set of organic molecules,” *J. Chem. Theory and Comput.*, **4** (2008) 297-306.
Tomasi02	J. Tomasi, R. Cammi, B. Mennucci, C. Cappelli, and S. Corni, “Molecular properties in solution described with a continuum solvation model,” *Phys. Chem. Chem. Phys.*, **4** (2002) 5697-712.
Tomasi05	J. Tomasi, B. Mennucci, and R. Cammi, “Quantum mechanical continuum solvation models,” *Chem. Rev.*, **105** (2005) 2999-3093.
Tomasi99	J. Tomasi, B. Mennucci, and E. Cancès, “The IEF version of the PCM solvation method: An overview of a new method addressed to study molecular solutes at the QM ab initio level,” *J. Mol. Struct. (Theochem)*, **464** (1999) 211-26.
Tonachini90	G. Tonachini, H. B. Schlegel, F. Bernardi, and M. A. Robb, “MC-SCF Study of the Addition Reaction of the 1Dg Oxygen Molecule to Ethene,” *J. Am. Chem. Soc.*, **112** (1990) 483-91.
Torrent02	M. Torrent, T. Vreven, D. G. Musaev, K. Morokuma, Ö. Farkas, and H. B. Schlegel, “Effects of the protein environment on the structure and energetics of active

	sites of metalloenzymes: ONIOM study of methane monooxygenase and ribonucleotide reductase," *J. Am. Chem. Soc.*, **124** (2002) 192-93.
Toulouse02	J. Toulouse, A. Savin, and C. Adamo, "Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Krieger-Chen-Iafrate-Savin model," *J. Chem. Phys.*, **117** (2002) 10465-73.
Toyota02	K. Toyota, M. Ehara, and H. Nakatsuji, "Elimination of singularities in molecular orbital derivatives: Minimum orbital-deformation (MOD) method," *Chem. Phys. Lett.*, **356** (2002) 1-6.
Toyota03	K. Toyota, I. Mayumi, M. Ehara, M. J. Frisch, and H. Nakatsuji, "Singularity-free analytical energy gradients for the SAC/SAC-CI method: Coupled perturbed minimum orbital-deformation (CPMOD) approach," *Chem. Phys. Lett.*, **367** (2003) 730-36.
Trucks88	G. W. Trucks, J. D. Watts, E. A. Salter, and R. J. Bartlett, "Analytical MBPT(4) Gradients," *Chem. Phys. Lett.*, **153** (1988) 490-95.
Trucks88a	G. W. Trucks, E. A. Salter, C. Sosa, and R. J. Bartlett, "Theory and Implementation of the MBPT Density Matrix: An Application to One-Electron Properties," *Chem. Phys. Lett.*, **147** (1988) 359-66.
Truhlar70	D. G. Truhlar, "Adiabatic theory of chemical reactions," *J. Chem. Phys.*, **53** (1970) 2041.
Truhlar71	D. G. Truhlar and A. Kuppermann, "Exact tunneling calculations," *J. Am. Chem. Soc.*, **93** (1971) 1840.
Tubert-Brohman04	I. Tubert-Brohman, C. R. W. Guimaraes, M. P. Repasky, and W. L. Jorgensen, "Extension of the PDDG/PM3 and PDDG/MNDO Semiempirical Molecular Orbital Methods to the Halogens," *J. Comp. Chem.*, **25** (2004) 138-50.
Tubert-Brohman05	I. Tubert-Brohman, C. R. W. Guimaraes, and W. L. Jorgensen, "Extension of the PDDG/PM3 Semiempirical Molecular Orbit Method to Sulfur, Silicon, and Phosphorus," *J. Chem. Theory and Comput.*, **1** (2005) 817-23.
Uggerud92	E. Uggerud and T. Helgaker, "Dynamics of the Reaction CH2OH+ --> CHO+ + H2. Translational Energy-Release from ab initio Trajectory Calculations," *J. Am. Chem. Soc.*, **114** (1992) 4265-68.

VanCaillie00	C. Van Caillie and R. D. Amos, “Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals,” *Chem. Phys. Lett.*, **317** (2000) 159-64.
VanCaillie99	C. Van Caillie and R. D. Amos, “Geometric derivatives of excitation energies using SCF and DFT,” *Chem. Phys. Lett.*, **308** (1999) 249-55.
VanVoorhis98	T. Van Voorhis and G. E. Scuseria, “A never form for the exchange-correlation energy functional,” *J. Chem. Phys.*, **109** (1998) 400-10.
Visscher97	L. Visscher and K. G. Dyall, “Dirac-Fock atomic electronic structure calculations using different nuclear charge distributions,” *Atomic Data and Nuclear Data Tables*, **67** (1997) 207-24.
vonNiessen84	W. von Niessen, J. Schirmer, and L. S. Cederbaum, “Computational methods for the one-particle Green’s function,” *Comp. Phys. Rep.*, **1** (1984) 57-125.
Vosko80	S. H. Vosko, L. Wilk, and M. Nusair, “Accurate spin-dependent electron liquid correlation energies for local spin density calculations: A critical analysis,” *Can. J. Phys.*, **58** (1980) 1200-11.
Vreven00	T. Vreven and K. Morokuma, “On the application of the IMOMO (Integrated Molecular Orbital + Molecular Orbital) method,” *J. Comp. Chem.*, **21** (2000) 1419-32.
Vreven01	T. Vreven, B. Mennucci, C. O. da Silva, K. Morokuma, and J. Tomasi, “The ONIOM-PCM method: Combining the hybrid molecular orbital method and the polarizable continuum model for solvation. Application to the geometry and properties of a merocyanine in solution,” *J. Chem. Phys.*, **115** (2001) 62-72.
Vreven03	T. Vreven, K. Morokuma, Ö. Farkas, H. B. Schlegel, and M. J. Frisch, “Geometry optimization with QM/MM, ONIOM and other combined methods. I. Microiterations and constraints,” *J. Comp. Chem.*, **24** (2003) 760-69.
Vreven06	T. Vreven, K. S. Byun, I. Komáromi, S. Dapprich, J. A. Montgomery Jr., K. Morokuma, and M. J. Frisch, “Combining quantum mechanics methods with molecular mechanics methods in ONIOM,” *J. Chem. Theory and Comput.*, **2** (2006) 815-26.
Vreven06a	T. Vreven, M. J. Frisch, K. N. Kudin, H. B. Schlegel, and K. Morokuma, “Geometry optimization with QM/MM

	Methods. II. Explicit Quadratic Coupling," *Mol. Phys.*, **104** (2006) 701-14.
Vreven06b	T. Vreven and K. Morokuma, in *Annual Reports in Computational Chemistry*, Ed. D. C. Spellmeyer, Vol. 2 (Elsevier, 2006) 35 - 51.
Vreven08	T. Vreven and K. Morokuma, in *Continuum Solvation Models in Chemical Physics: From Theory to Applications*, Ed. B. Mennucci and R. Cammi (Wiley, 2008).
Vreven97	T. Vreven, F. Bernardi, M. Garavelli, M. Olivucci, M. A. Robb, and H. B. Schlegel, "Ab initio photoisomerization dynamics of a simple retinal chromophore model," *J. Am. Chem. Soc.*, **119** (1997) 12687-88.
Vydrov06	O. A. Vydrov and G. E. Scuseria, "Assessment of a long range corrected hybrid functional," *J. Chem. Phys.*, **125** (2006) 234109.
Vydrov06a	O. A. Vydrov, J. Heyd, A. Krukau, and G. E. Scuseria, "Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals," *J. Chem. Phys.*, **125** (2006) 074106.
Vydrov07	O. A. Vydrov, G. E. Scuseria, and J. P. Perdew, "Tests of functionals for systems with fractional electron number," *J. Chem. Phys.*, **126** (2007) 154109.
Wachters70	A. J. H. Wachters, "Gaussian basis set for molecular wavefunctions containing third-row atoms," *J. Chem. Phys.*, **52** (1970) 1033.
Wadt85	W. R. Wadt and P. J. Hay, "Ab initio effective core potentials for molecular calculations - potentials for main group elements Na to Bi," *J. Chem. Phys.*, **82** (1985) 284-98.
Walker70	T. E. H. Walker, "Molecular spin-orbit coupling constants. Role of core polarization," *J. Chem. Phys.*, **52** (1970) 1311.
Watts93	J. D. Watts, J. Gauss, and R. J. Bartlett, "Coupled-cluster methods with noniterative triple excitations for restricted open-shell Hartree-Fock and other general single determinant reference functions. Energies and analytical gradients," *J. Chem. Phys.*, **98** (1993)
Weber03	J. Weber and G. Hohlneicher, "Franck-Condon factors

	for polyatomic molecules," *Mol. Phys.*, **101** (2003) 2125-44.
Wedig86	U. Wedig, M. Dolg, H. Stoll, and H. Preuss, in *Quantum Chemistry: The Challenge of Transition Metals and Coordination Chemistry*, Ed. A. Veillard, Reidel, and Dordrecht (1986) 79.
Weigend03	F. Weigend, F. Furche, and R. Ahlrichs, "Gaussian basis sets of quadruple zeta valence quality for atoms H-Kr," *J. Chem. Phys.*, **119** (2003) 12753-62.
Weigend05	F. Weigend and R. Ahlrichs, "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy," *Phys. Chem. Chem. Phys.*, **7** (2005) 3297-305.
Weigend06	F. Weigend, "Accurate Coulomb-fitting basis sets for H to Rn," *Phys. Chem. Chem. Phys.*, **8** (2006) 1057-65.
Weinhold88	F. Weinhold and J. E. Carpenter, in *The Structure of Small Molecules and Ions*, Ed. R. Naaman and Z. Vager (Plenum, 1988) 227-36.
Wiberg92	K. B. Wiberg, C. M. Hadad, T. J. LePage, C. M. Breneman, and M. J. Frisch, "An Analysis of the Effect of Electron Correlation on Charge Density Distributions," *J. Phys. Chem.*, **96** (1992) 671-79.
Wilson01a	P. J. Wilson, T. J. Bradley, and D. J. Tozer, "Hybrid exchange-correlation functional determined from thermochemical data and ab initio potentials," *J. Chem. Phys.*, **115** (2001) 9233-42.
Wilson05	S. M. Wilson, K. B. Wiberg, J. R. Cheeseman, M. J. Frisch, and P. H. Vaccaro, "Nonresonant optical activity of isolated organic molecules," *J. Phys. Chem. A*, **109** (2005) 11752-64.
Wilson96	A. K. Wilson, T. van Mourik, and T. H. Dunning Jr., "Gaussian Basis Sets for use in Correlated Molecular Calculations. VI. Sextuple zeta correlation consistent basis sets for boron through neon," *J. Mol. Struct. (Theochem)*, **388** (1996) 339-49.
Wolinski80	K. Wolinski and A. Sadlej, "Self-consistent perturbation theory: Open-shell states in perturbation-dependent non-orthogonal basis sets," *Mol. Phys.*, **41** (1980) 1419-30.
Wolinski90	K. Wolinski, J. F. Hilton, and P. Pulay, "Efficient Implementation of the Gauge-Independent Atomic Orbital

	Method for NMR Chemical Shift Calculations," *J. Am. Chem. Soc.*, **112** (1990) 8251-60.
Wong91	M. W. Wong, M. J. Frisch, and K. B. Wiberg, "Solvent Effects 1. The Mediation of Electrostatic Effects by Solvents," *J. Am. Chem. Soc.*, **113** (1991) 4776-82.
Wong91a	M. W. Wong, K. B. Wiberg, and M. J. Frisch, "Hartree-Fock Second Derivatives and Electric Field Properties in a Solvent Reaction Field - Theory and Application," *J. Chem. Phys.*, **95** (1991) 8991-98.
Wong92	M. W. Wong, K. B. Wiberg, and M. J. Frisch, "Solvent Effects 2. Medium Effect on the Structure, Energy, Charge Density, and Vibrational Frequencies of Sulfamic Acid," *J. Am. Chem. Soc.*, **114** (1992) 523-29.
Wong92a	M. W. Wong, K. B. Wiberg, and M. J. Frisch, "Solvent Effects 3. Tautomeric Equilibria of Formamide and 2-Pyridone in the Gas Phase and Solution: An ab initio SCRF Study," *J. Am. Chem. Soc.*, **114** (1992) 1645-52.
Wood06	G. P. F. Wood, L. Radom, G. A. Petersson, E. C. Barnes, M. J. Frisch, and J. A. Montgomery Jr. , "A restricted-open-shell complete-basis-set model chemistry," *J. Chem. Phys.*, **125** (2006) 094106: 1-16.
Woon93	D. E. Woon and T. H. Dunning Jr., "Gaussian-basis sets for use in correlated molecular calculations. 3. The atoms aluminum through argon," *J. Chem. Phys.*, **98** (1993) 1358-71.
Xu04	X. Xu and W. A. Goddard III, "The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties," *Proc. Natl. Acad. Sci. USA*, **101** (2004) 2673-77.
Yamaguchi86	Y. Yamaguchi, M. J. Frisch, J. Gaw, H. F. Schaefer III, and J. S. Binkley, "Analytic computation and basis set dependence of Intensities of Infrared Spectra," *J. Chem. Phys.*, **84** (1986) 2262-78.
Yamamoto96	N. Yamamoto, T. Vreven, M. A. Robb, M. J. Frisch, and H. B. Schlegel, "A Direct Derivative MC-SCF Procedure," *Chem. Phys. Lett.*, **250** (1996) 373-78.
Yanai04	T. Yanai, D. Tew, and N. Handy, "A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP)," *Chem. Phys. Lett.*, **393** (2004) 51-57.

York99	D. M. York and M. Karplus, “Smooth solvation potential based on the conductor-like screening model,” *J. Phys. Chem. A*, **103** (1999) 11060-79.
Zakrzewski93	V. G. Zakrzewski and W. von Niessen, “Vectorizable algorithm for Green function and many-body perturbation methods,” *J. Comp. Chem.*, **14** (1993) 13-18.
Zakrzewski94a	V. G. Zakrzewski and J. V. Ortiz, “Semidirect algorithms in electron propagator calculations,” *Int. J. Quantum Chem., Quant. Chem. Symp.*, **S28** (1994) 23-27.
Zakrzewski95	V. G. Zakrzewski and J. V. Ortiz, “Semidirect algorithms for third-order electron propagator calculations,” *Int. J. Quantum Chem.*, **53** (1995) 583-90.
Zakrzewski96	V. G. Zakrzewski, J. V. Ortiz, J. A. Nichols, D. Heryadi, D. L. Yeager, and J. T. Golab, “Comparison of perturbative and multiconfigurational electron propagator methods,” *Int. J. Quant. Chem.*, **60** (1996) 29-36.
Zerner80	M. C. Zerner, G. H. Lowe, R. F. Kirchner, and U. T. Mueller-Westerhoff, “An Intermediate Neglect of Differential Overlap Technique for Spectroscopy of Transition-Metal Complexes. Ferrocene,” *J. Am. Chem. Soc.*, **102** (1980) 589-99.
Zerner82	M. C. Zerner, P. Correa de Mello, and M. Hehenberger, “Converging SCF Calculations on Excited States,” *Int. J. Quantum Chem.*, **21** (1982) 251-59.
Zerner91	M. C. Zerner, in *Reviews of Computational Chemistry*, Ed. K. B. Lipkowitz and D. B. Boyd, Vol. 2 (VCH Publishing, New York, 1991) 313-66.
Zhao05	Y. Zhao, N. E. Schultz, and D. G. Truhlar, “Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions,” *J. Chem. Phys.*, **123** (2005)
Zhao06	Y. Zhao, N. E. Schultz, and D. G. Truhlar, “Design of density functionals by combining the method of constraint satisfaction with parametrization for thermochemistry, thermochemical kinetics, and noncovalent interactions,” *J. Chem. Theory and Comput.*, **2** (2006) 364-82.
Zhao06a	Y. Zhao and D. G. Truhlar, “A new local density functional for main-group thermochemistry, transition

	metal bonding, thermochemical kinetics, and noncovalent interactions," *J. Chem. Phys.*, **125** (2006), 194101: 1-18.
Zhao06b	Y. Zhao and D. G. Truhlar, "Comparative DFT study of van der Waals complexes: Rare-gas dimers, alkaline-earth dimers, zinc dimer, and zinc-rare-gas dimers," *J. Phys. Chem.*, **110** (2006) 5121-29.
Zhao06c	Y. Zhao and D. G. Truhlar, "Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States," *J. Phys. Chem. A*, **110** (2006) 13126-30.
Zhao08	Y. Zhao and D. G. Truhlar, "The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals," *Theor. Chem. Acc.*, **120** (2008) 215-41.
Zheng05	G. Zheng, S. Irle, and K. Morokuma, "Performance of the DFTB method in comparison to DFT and semiempirical methods for geometries and energies of C20-C86 fullerene isomers," *Chem. Phys. Lett.*, **412** (2005) 210-16.
Zheng07	G. Zheng, H. Witek, P. Bobadova-Parvanova, S. Irle, D. G. Musaev, R. Prabhakar, K. Morokuma, M. Lundberg, M. Elstner, C. Kohler, and T. Frauenheim, "Parameter calibration of transition-metal elements for the spin-polarized self-consistent-charge density-functional tight-binding (DFTB) method: Sc, Ti, Fe, Co and Ni," *J. Chem. Theory and Comput.*, **3** (2007) 1349-67.
Zhixing89	C. Zhixing, "Rotation procedure in intrinsic reaction coordinate calculations," *Theor. Chim. Acta.*, **75** (1989) 481-84.

分子力學方法

描述

Gaussian 程式裡有三種分子力學方法可用。分子力學方法的程式實做是要在 ONIOM 計算中使用，但也可以獨立使用。這些關鍵字不應和任何基底函數關鍵字合用。

有三種力場可用：

Amber: 文獻 [Cornell95]中描述的 Amber 力場。實際使用的力場參數 (parm96.dat) 已從原始發表的論文稍微做了更新。現在使用的參數版本來自 Amber 網頁 (amber.scripps.edu)。

Dreiding: 文獻[Mayo90].中描述的 Dreiding 力場。

UFF: 文獻[Rappe92].描述的 UFF 力場。

分子力學分子系統設定

分子力學計算以原子類型決定建構力場的功能和參數。對某一元素，例如碳，會有許多不同的分子力學原子類型。根據每個原子的軌域混成，化學環境等等面向，決定採用哪一種原子類型來描述在分子中的這個原子。

UFF 和 Dreiding 分子力學計算中，Gaussian 程式會嘗試自動設定每一個原子的原子類型。但是 Amber 計算中，所有原子的原子類型必須在分子設定段落中明確指定，例如

C-CT *設定一個 SP3 脂肪族（aliphatic）碳原子，以 Amber CT 關鍵字表示*
C-CT-0.32 *設定一個 SP3 脂肪族（aliphatic）碳原子，附帶部份電荷 +0.32*
O-O--0.5 *設定一個 羰基氧原子，附帶部份電荷 -0.5.*

原子類型的設定是在元素符號後加一連字元，後面接上原子類型關鍵字。原子類型的定義和其關鍵字請參考 Amber 論文 [Cornell95] 。

前面範例的第二和第三行顯示，可以設定原子的部份電荷，當作原子設定資料的第三部份，以連字元做區隔。部份原子（點）電荷用來計算靜電作用。Gaussian 程式可用 QEq 公式[Rappe91] 自動設定這些電荷。可用設定 MM 關鍵字選項 QEq 的方式執行，例如：Dreiding=QEq。注意，這些電荷和分子幾何結構有關，並且在計算工作開始的時候計算的；但是，在幾何優選計算過程中，或其它造成幾何結構改變的程序中，這些原子電荷的數值並沒有隨著幾何結構的改變而更新。

若有需要，也可採用 UFF 和 Dreiding 力場的原子類型和電荷。要注意的是只對完善定義的分子系統， UFF 和 Dreiding 原子類型的自動設定才是可靠的，因此為了保險起見，最好是由使用者做明確設定原子型和電荷。

當使用 MM 方法時，特別是修改了力場項或定義新的力場作用（見以下討論）時，常需使用選項 Geom=Connectivity 明確定原子間的連接關係。注意，程式 GaussView 建構輸入檔案時會自動包含這個輸入資料段落。

電荷設定有關的選項

除非在分子系統設定段落內設定，使用任何分子力學力場時，不會預設任何原子的電荷。可用選項可在最初的結構上估計原子電荷，採用 QEq 計算方法 [Rappe91]，並以下列力學關鍵字控制：

QEq
利用 QEq 方法設定原子電荷。

UnTyped
只對在輸入檔案中沒有設定原子類型的原子才用 QEq 方法設定該原子的原子電荷。

UnCharged
對所有電荷為零的原子以 QEq 方法設定原子電荷（亦即，在輸入檔案中沒有設定原子類型或有原子類型但是沒有電荷的原子）。

參數優先選項

術語解釋: 上述幾種 Gaussian 內建的分子力場都有內建的參數組：稱為 *hard-wired* 參數。而 *Soft* 參數是由使用者對目前的計算工作，在輸入檔案內設定的參數，或是由稍早完成的計算工作的檢查檔中讀取的參數。若使用者在輸入檔中沒有提供相關的關鍵字，程式只會使用內建的力學參數。這個課題會在後面的 “普通分子力學力場設定” 章節中詳細說明。

HardFirst
從輸入檔中讀取額外的力學參數，若讀取的參數中有和內建參數重複，內建的參數優先採用。因此只有缺乏對應的內建參數時，才會用到讀入的參數。注意，和內建參數做萬用字元相符（wildcards matches）的結果優先於讀入的參數，即使後者含有完全相同的項目。若要取代符合的內建參數，應用 SoftFirst 選項。

SoftFirst
從輸入檔案中讀入額外的力學參數，讀入的參數比內建的參數優先採用。

SoftOnly
從輸入檔案中讀入力學參數，忽略內建的參數。

參數組多重相符的處理

因為參數可用萬用字元做設定，有可能同一個分子結構可符合多種參數組的設定。預設的處理方式是若力場指定上有任何疑義，計算工做就中斷。以下選項設定遇到這種情況的處理方式：

FirstEquiv
若要的參數有兩種相符的項，採用最先找到的。

LastEquiv
若要的參數有兩種相符的項，採用最後找到的。

從檢查檔讀取 MM 參數

預設的作法，用選項 Geom=Check 或 Geom=AllCheck 從檢查檔讀取分子幾何結構時，同時會讀取檢查檔內任何非標準 (soft) 分子力學參數。這些讀進的參數會比對應的內建參數優採用，除非設定 HardFirst 選項。以下選項也可用來改變這預設的作法。

ChkParameters
只從檢查檔中讀入分子力學參數。檢查檔中任何非內建參數都比內建參數優先採用，除非同時指定 HardFirst 選項。不能和 Geom=Check 或 Geom=AllCheck 合用。

NewParameters
讀進幾何結構時忽略檢查檔內任何分子力學參數。

Modify
將檢查檔內任何非內建分子力場參數和內建分子力場參數（由前述選項共治）組合後，讀進額外的參數設定和修改資料。這選項和 Geom=Modify 的作用方式類似。

印出 MM 參數

Print
預設的作法，設定 #P 時只印出對能量的貢獻（即，鍵結拉長，彎曲，靜電作用，等等）。選項 Print 將印出能量貢獻，最初幾何結構的力場參數，後在續幾何結構的能量貢獻（因為這些參數值不變）。另外還會印出 ONIOM 的兩組參數，因為模型系統和真實系統會設定不同的參數（即，在區塊邊緣上，氫原子取代一個連接的碳原子）。

注意，會印出系統中所有原子的分子力學參數，但印出的格式不適合當作輸入。在 Gaussian 程式主目錄區有內建參數檔案，所用的格式適合當作輸入

（amber.prm，uff.prm，等等），目錄區內還有非內建分子力場參數檔案（amber98.prm 和 oplsaa.prm）。印出目前計算工作所有原子的分子力學參數仍然有用，因為其中涉及決定將哪些參數設定到各鍵結，雙面角等等的複雜規則。

可用方法

解析能量、 梯度和頻率。

相關的關鍵字

ONIOM, Geom=Connectivity

普通分子力學力場設定

Gaussian 提供使用者極大的彈性對分子力學力場做修改或客製化。這個章節討論分子力學力場的修改和客製化。首先提供所需的背景知識，以便了解力場函數和參數的輸入資料。

基本分子力場位能函數通常形式：

$$E^{total} = \underbrace{\sum_{bonds} K_r (r - r_{eq})^2}_{\text{stretch terms}} + \underbrace{\sum_{angles} K_\theta (\theta - \theta_{eq})^2}_{\text{bend terms}} + \underbrace{\sum_{dihedrals} \frac{V_n}{2}[1 + \cos(n\phi - \gamma)]}_{\text{torsional terms}} + \underbrace{\sum_{i<j} \left[\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{\varepsilon r_{ij}} \right]}_{\text{non-bonded interactions}}$$

Molecular Mechanics Potential Function

如註釋所示，這展開式包含的項有拉長項（鍵結），彎曲項（鍵角），和扭轉項（雙面角），以及非鍵結作用項。方程式中個別函數的形式來自 Amber 力場，這力場使用簡單諧和函數表示拉長和彎曲，餘弦函數代表扭轉，和標準的靜電作用及凡瓦作用位能。別的力場使用不同的函數形式，有些含有 Amber 力場所沒有的額外位能函數項，像是電雙極相互作用或拉長--彎曲偶合作用。

為了要計算分子力學力場函數，Gaussian 需要知道分子系統中具有哪些結構--拉長，彎曲和扭轉，以及代表這些能量貢獻的函數形式及參數。結構可從分子中的原子連接關係確定。預設的作法， Gaussian 決定哪些原子是鍵結的，這些鍵結對應的鍵結度（單鍵，雙鍵，等等）。當分子幾何結構合理，鍵結度清楚定義，Gaussian 程式都能正確的完成這是別工作。但是，若計算工作從一近似的分子幾何開始，或當鍵結度不易確認時，比較安全的作法是在輸入檔中明確設定原子的連接關係，使用關鍵字 Geom=Connectivity （見 Geom 關鍵字的討論）。

這章節剩餘的部份將討論分子力場函數和其參數，後面的章節將列出所有可用函數的定義。

檢視 MM 函數。 檢視 Gaussian 分子力場計算工作的輸出檔是討論這課題很好的方式。這裡是甲烷的 Amber 計算的輸入檔：

```
#P Amber Geom=Connectivity IOp(4/33=3)

Methane

0 1
C-CT--0.4 -0.85 0.42 0.00
H-HC-0.1 -0.50 -0.57 0.00
H-HC-0.1 -0.50 0.93 0.87
H-HC-0.1 -0.50 0.93 -0.87
H-HC-0.1 -1.92 0.42 0.00
```

注意，碳原子的原子類型是 CT ，氫原子的原子類型是 HC。每個原子上還設定了部份電荷。

計算路徑中使用 IOp(4/33=3) ，產生以下這段輸出資料：

```
 Atomic parameters:                                          單元子的分子力學函數
Center VDW
1          1.9080 .1094000
2          1.4870 .0157000
3          1.4870 .0157000
4          1.4870 .0157000
5          1.4870 .0157000
Molecular mechanics terms:                                  雙原子或多原子的分子力學函數
NBDir 3 1 0 0                                               非鍵結作用主程式
HrmStr1 1-2 340.00 1.0900                                   拉長項
HrmStr1 1-3 340.00 1.0900
HrmStr1 1-4 340.00 1.0900
HrmStr1 1-5 340.00 1.0900
HrmBnd1 2-1-3 35.00 109.50                                  彎曲項
HrmBnd1 2-1-4 35.00 109.50
HrmBnd1 2-1-5 35.00 109.50
HrmBnd1 3-1-4 35.00 109.50
HrmBnd1 3-1-5 35.00 109.50
HrmBnd1 4-1-5 35.00 109.50 NBPair 2-1 3 1 0 0 -1.000 -1.000 鄰近原子非鍵結作用
```

```
NBPair 3-1 3 1 0 0 -1.000 -1.000
NBPair 3-2 3 1 0 0 -1.000 -1.000
NBPair 4-1 3 1 0 0 -1.000 -1.000
NBPair 4-2 3 1 0 0 -1.000 -1.000
NBPair 4-3 3 1 0 0 -1.000 -1.000
NBPair 5-1 3 1 0 0 -1.000 -1.000
NBPair 5-2 3 1 0 0 -1.000 -1.000
NBPair 5-3 3 1 0 0 -1.000 -1.000
NBPair 5-4 3 1 0 0 -1.000 -1.000
```

原子參數

某些分子力學函數只和原子的原子類型有關。在此範例中，Amber 有每個原子的煩得瓦作用項，其數值列印在標題 Atomic parameters 之下。原子中心編號對應分子系統設定段落中的原子位置。DREIDING 和 UFF 力場只包含這種類型的函數項。

分子力學項

分子力學項端落列出總能量函數內描述涉及多原子相互作用的能量項。例如，涉及每一對鍵結原子（1-2，2-3 和 1-4）的拉長項，經由函數 HrmStr1 計算，使用力常數的數值 340 kcal/(mol-Å^2) 和平衡鍵長 1.09 埃。這些參數值由原子中心 1 和 2 的原子類型決定：分別是：CT 和 HC。

特定函數和參數的選擇是根據以下規則：從原子連接關係，程式得知原子中心 1 和 2 間有一鍵結。Amber 力場對每一對鍵結原子提供一拉長項函數，各種函數和參數都放在程式裡的內存表單內。在最簡單的情形，Gaussian 藉由兩個原子類型查表，找出對應的能量函數和參數。在這個粒子中，使用到表中項目

```
HrmStr1 CT HC 340 1.09
```

因為這項目對應甲烷 C-H 鍵的兩個原子類型。這項目設定的力常數和平衡鍵長將用於計算。在以下參考資料章節中查詢這個函數的時候，會發現真正計算的函數是 ForceC*(R - R_{eq})^2 ，這裡 ForceC 勢利常數，R_{eq} 是平衡鍵長，R 是鍵長。在這個奮力，這函數變成 340.0*(R - 1.09)^2。

清單中的能量項包括所有鍵結的成對原子的拉長項，以及對應所有鍵角的彎曲項。

非鍵節作用項

清單中剩下的項對應非鍵結作用：由非鍵結的原子之間的相互作用對位能的貢獻。在討論個別作用的細節前，先看看這些項要如何計算。

通常，非鍵結項由所有可能的成對原子構成，因此這項的數量和分子系統內原子數量的平方成正比。但是，在空間上彼此相鄰的原子，根據期間分隔的鍵結數目，其相互作用通常會降低。典型的情況，相隔一和兩個鍵結原子間的相互作用會降為零（因為這些相互作用已包含在拉長和彎曲項內）。同樣的，間隔三個鍵結原

子間的相互作用要乘上一個幅度因子，這幅度因子的值在零與一之間，和力場有關。很明顯的是，對於大型分子系統，非鍵結作用項的清單會變得很長。在大部分分子力學程式中，採用一個距離門檻，使這清單的大小在可操控的範圍之內。Gaussian 程式採用較少見的方式對非鍵結作用做有效的處理。

分子系統的非鍵結作用總能量可寫成以下形式：

$$E^{NB} = \sum_{i}^{N}\sum_{j}^{j<i}\left[s_{ij}^{vdW}E_{ij}^{vdW} + s_{ij}^{Q}E_{ij}^{Q}\right]$$

$$= \underbrace{\sum_{i}^{N}\sum_{j}^{j<i}\left[E_{ij}^{vdW} + E_{ij}^{Q}\right]}_{\text{all pairs}} - \underbrace{\sum_{i}^{N}\sum_{j}^{j<i}\left[(1-s_{ij}^{vdW})E_{ij}^{vdW} + (1-s_{ij}^{Q})E_{ij}^{Q}\right]}_{\text{“overcounted” pairs}}$$

Total Non-Bonded Energy Expression

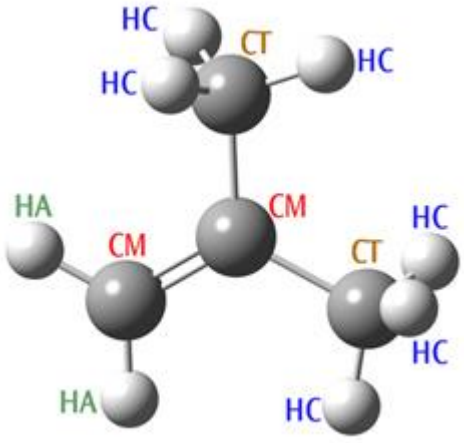
這裡 E^{vdW} 和 E^{Q} 分別是兩原子中心間的凡得瓦和靜電作用位能，對應的 s 職事相關的幅度因子。

第一個方程式是非鍵結作用的一般形式，第二個方程式是另一種表示方式，明確列出所有可能的非鍵結相互作用（不論距離），計算時不用幅度因子（第一項）和刪除多算的原子對作用（第二項）。

這重新組織的方程是有顯著的計算優勢。第一項可用很有效的方式處理，像是線性增長或其他技巧。而且，第二項中大部分的原子對的交互作用是零（若分子系統不是太小），因大部份的分子對的幅度因子 s_{ij} 都是 1。程式只需維持一個原子對清單，清單中的原子對在第二項中提供非零相互作用的貢獻。結果這高效能的計算方法沒有使用門檻值做篩選，只需維持一個清單，這清單的大小和分子系統的大小成線性正比關係。

函數 NBDir 和 NBTerm 用來成這兩個非鍵結作用項。如前面甲烷計算工作的輸出檔案所示，單一 NBDir 函數描述所有成對原子之間的相互作用，也就是第二型方程式的第一項，各種 NBTerm 項目夠成方程式中的第二項。這些函數最後兩個參數分別是凡得瓦和庫侖作用的幅度因子。在甲烷的範例中，所有項的幅度因子都是 1 ，因為甲烷中沒有任何兩個原子相距兩個鍵結以上，於是非鍵結作用的最後一項就是零。

設定缺少的參數 考慮以下分子：2-methylpropene 2-甲基丙烯。我們將建立這分子的 Amber 計算，設定 SP2 混成碳原子為原子類型 CM，SP3 混成碳原子為 CT。



2-MethylPropene

```
# Amber

2-methylpropene

0 1
 C-CM -2.53 0.19 0.00
 H-HA -2.00 -0.73 0.00
 H-HA -3.60 0.19 0.00
 C-CM -1.86 1.37 0.00
 C-CT -2.63 2.70 0.00
 H-HC -1.93 3.51 0.07
 H-HC -3.24 2.76 -0.88
 H-HC -3.24 2.76 0.85
 C-CT -0.32 1.37 0.00
 H-HC 0.03 1.87 -0.83
 H-HC 0.03 1.87 0.81
 H-HC 0.03 0.36 -0.00
```

執行這個計算後，程式產生以下錯誤訊息：

```
 Angle bend undefined between atoms 2 1 3
 Angle bend undefined between atoms 5 4 9
 MM function not complete
```

原子 2-1-3 對應類型 HA-CM-HA，原子 5-4-9 對應 CT-CM-CT。雖然原子類型和次序在化學上市合理的，但在程式內建的分子力學函數表中卻沒有這些彎曲項。原因是 Amber 力場主要是為生物化學分子系統發展設計的，在這些分子中，這樣特定的原子類型序列並不會出現。因此 Amber 對這樣的原子類型序列沒有定義對應的力學參數。注意，Gaussian 程式只對所有拉長和彎曲檢查是否有對應的函數可用，若內建的位能表單中沒有這個項目，扭轉和其他項就從總位能函數中忽略。

加入和更換參數

當沒有內建的參數可用，不論是從不完整的函數表，或是引進新的原子類型，都需要在輸入檔中設定。決定採用哪種適當的參數是很有挑戰性的工作。這些參數常可從文獻中找到，否則，需要從實驗數據或準確計算數據中推導（這主題已超過本章結得範圍）。

要設定新參數，使用關鍵字 Amber=HardFirst ，然後將新參數的定義加入輸入檔中的一個獨立的段落。在這個範例中，對缺少的原子類型序列定義 HrmBnd1 函數。這 2-甲基丙烯計算工作的輸入檔變成：

```
# Amber=HardFirst

2-methylpropene

0 1
 C-CM -2.53 0.19 0.00
 分子系統設定段落其餘部份...
HrmBnd1 CT CM CT 70.0 120.0
HrmBnd1 HA CM HA 40.0 120.0
```

這範例中使用的參數職事根據 Amber 參數做的粗略猜測。HardFirst 選項指示先檢查各函數項的 Amber 內建參數表，若沒有找到相符的項目，才會使用輸入檔內定義的函數項目。SoftFirst 選項指示取代內建參數組的參數。注意，設定 HardFirst 和 SoftFirst 選項的次序只有當一個或多個函數在兩組參數清單內都有定義得時候才會有影響。最後，選項 SoftOnly 表示輸入檔內江提供完整的力場定義，完全忽略內建的參數組。

此用外部參數檔

使用 Gaussian 程式內含檔案的機制，可以將輸入檔內的力場函數項用外部檔案的分子力場函數項目所取代，即，@oplsaa.prm。 各種力場的參數檔案放在 Gaussian 程式主目錄區內（即，$g09root/g09）。若要經由外部檔案設定整個力場，可用類似以下輸入檔：

```
# UFF=SoftOnly

Read-in force field example

molecule specification
@$g09root/g09/oplsaa.prm
```

注意，因為整個力場和讀進的函數及參數有關，和任何內建的函數項目及參數無關，計算路徑內設定的分子力學關鍵字的選擇就無關緊要(換句話說，設定 Amber 或 UFF 結果是一樣的）。

函數設定內的萬用字元

輸入檔中函數的數定可用萬用字元。例如，這 Amber 彎曲函數設定所有中心碳原子為原子類型 CM 的彎曲函數使用相同的參數值：

```
HrmBnd1 * CM * 70.0 120.0
```

使用者也可萬用字元及其它較特定的項目輸入檔內加入一個較廣義的項目：

```
HrmBnd1 * CM * 70.0 120.0
HrmBnd1 HA CM HA 40.0 120.0
```

預設的作法，程式對特定的結構（這裡是指以 CM 探源紫薇中心的鍵角）採用最特定的能量函數項目。項目中萬用字元的數目決定這項目相對的特定程度。若有不同的項目恰巧有相同的特定程度，程式將會中斷執行，並印出多重相符項目的錯誤訊息。這時使用者需引導程式選澤地一個或最後一個相符的項目，分別採用選項 FirstEquiv 或 LastEquiv。注意，出現多重相符項目錯誤訊息通常表示內建參數組有不一致的地方，需要做進一步調查並排除錯誤。

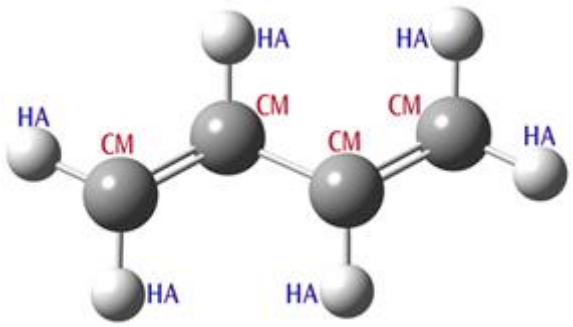
注意，萬用字元/項目的特定性並不影響是否要從內建或外部參數組中選用項目。因此，當指定 SoftFirst 選項時，輸入檔案內有一個項目用了三個萬用字元，程式將會採用這個能量項目，即使在內建函數組中包含完全相符的原子類型序列組合。

部份結構：使用鍵結度和結構特性選擇參數

子結構提供一種機制，用來設定額外的結構資訊，像是鍵結度和鍵角數值，以決定採用哪一種參數。可慮丙二烯分子（如下圖示）。碳原子都屬於原子類型 CM，但有兩個鍵結是形式上的雙鍵，一個是單鍵。預設的作法，Amber 對每一種定義的原子類型組合的拉長能量函數使用相同的力常數和平衡鍵長。但是，子結構可用來對不同的鍵結類型設定不同的餐數值。

子結構編號加到函數名稱後面，以連字元分隔：例如：HrmStr-1，HrmStr-2，等等。在這個範例中，編號代表鍵結度（見以下子結構定義）。有時，可用多重子結構字尾（例如，AmbTrs-1-2）。

丙二烯計算的輸入檔案在分子結構圖形之後：



Butadiene Molecule

```
# Amber=SoftFirst Geom=Connectivity

Butadiene

0 1
 C-CM -2.49 -0.07 0.00
 H-HA -1.96 -1.00 0.00
 H-HA -3.56 -0.07 0.00
 C-CM -1.82 1.09 0.00
 H-HA -2.35 2.02 0.00
 C-CM -0.28 1.09 0.00
 H-HA 0.24 0.16 0.00
 C-CM 0.39 2.26 -0.00
 H-HA -0.13 3.19 0.00
 H-HA 1.46 2.26 -0.00

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4 5 1.0 6 1.0
 5
 6 7 1.0 8 2.0
 7
 8 9 1.0 10 1.0
 9
 10

HrmBnd1 HA CM HA 40.0 120.0      這裡的參數值只是為了說明的目的!
HrmBnd1 CM CM CM 70.0 120.0
HrmStr1-1 CM CM 350.0 1.51       子結構: 和鍵結度有關的拉長項參數.
HrmStr1-2 CM CM 500.0 1.37
```

這個範例對雙鍵使用 HrmStr1 函數設定較大的力常數數值，較短的平衡鍵長。

注意，這裡使用的數值只是為了說明的目的。事實上，產出式計算還需要對單鍵或雙中心鍵定義扭轉能量的參數，使用類似的機制。

除了鍵結度，其它子結構的範例有是否這能量項在環狀結構上，有多少個氫原子和這原子鍵結，等等。注意，多重子結構字尾可和許多種函數合用，例如：HrmStr1-1-0-4。

不同函數的文義中子結構段落的含意大致上是一致的。第一個子結構字尾定意見節度或一角度範圍，第二個設定和當前原子鍵結的原子數目，第三個描述環狀結構環境（若有的話）。認一個子結構的位置的數值為零，當作萬用字元或指示佔

用位置，表示在這項目中忽略這個子結構。排在最後的子結構若不需要，可設為零或直接省略。

以下子結構適用於只和原子類型有關的能量函數：

第三子結構: 環狀結構 (第一和第二子結構必須是 0):

-0-0-1　　以下環狀結構定義都不適用

-0-0-3　　三元環上的原子

-0-0-4　　四元環上的原子

-0-0-5　　五元環上的原子

以下子結構適用於和鍵結拉長有關的能量函數:

第一子結構: 鍵結度

-0　　忽略這個子結構 (子結構 “萬用字元”)

-1　　單鍵: $0.00 \leq$ *鍵結度* < 1.50

-2　　雙鍵: $1.50 \leq$ *鍵結度* < 2.50

-3　　三鍵: *鍵結度* ≥ 2.50

第三子結構: 環狀結構 (若使用到，第二子結構必須是 0):

-*x*-0-1　　以下環狀結構定義都不適用

-*x*-0-3　　三元環上的鍵結

-*x*-0-4　　四元環上的鍵結

-*x*-0-5　　五元環上的鍵結

以下子結構適用於包含鍵角的能量函數（角度數值單位是度）:

第一子結構: angle　value　range

-1　　$0° \leq \theta \leq 45°$

-2　　$45° < \theta \leq 135°$

-3　　$135° < \theta \leq 180°$

S 第二子結構: 鍵結原子的數目

-*x*-0　　忽略這個子結構 (子結構 “萬用字元”)

-*x*-*n*　　*n* 是和中央原子鍵結的原子數目。

第三子結構: 環狀結構

-*x*-*y*-0　　忽略這個子結構 (子結構 “萬用字元”)

-*x*-*y*-1　　以下環狀結構定義都不適用

-x-y-3　三元環上的彎曲

-x-y-4　四元環上的彎曲

-x-y-5　五元環上的彎曲

第四子結構: 鍵結氫原子的數目

-x-y-z-n　和中心原子鍵結的氫原子數為 *n*+1 (構成鍵角的氫原子除外)

以下子結構適用於包含雙面角的能量函數。

第一子結構：鍵結度

-0　跳過這個子結構 (子結構 “萬用字元”)

-1　單中心鍵: 0.00 ≤ 鍵結度 < 1.50

-2　雙中心鍵: 1.50 ≤ 鍵結度 < 2.50

-3　三中心鍵: 鍵結度 ≥ 2.50

第二子結構：中心漸的鍵結類型

-x-0　跳過這個子結構 (子結構 “萬用字元”)

-x-1　共振中心鍵 (1.30 ≤ 鍵結度 ≤ 1.70)

-x-2　Amide 中心鍵 (較共振優先)

-x-3　其他中心鍵類型

第三子結構: 環狀結構

-x-y-1　不適用下列環狀結構定義

-x-y-4　雙面角在一四圓環上

-x-y-5　雙面角在一五圓環上

例如，HrmStr1-2-0-4 設定 HrmStr1 項只適用在四圓環上雙鍵的拉長（ 而 HrmStr1-2 適用到所有雙鍵）。子結構數值為零類似萬用字元的功能：HrnStr1-0-0-4 設定這項適用到任何鍵結度的拉長，但必須是四圓環上的鍵結。

注意，子結構不是一定需要。有些函數明確包含鍵結度，並在函數定義中包含類似的結構資訊。例如，UFF 力場的 HrmStr3 拉長項的第三個參數就是鍵結度。在對每一個鍵結做 UFF 計算時，這參數值設定為 -1.0 可被傳遞到這能量函數中，在輸入檔中藥做類似以下的設定 (以及 UFF 關鍵字的適當選項):

```
HrmStr3 * * -1.0 0.1332
```

定義新的原子類型

Gaussian 了解 Dreiding，UFF，和 Amber 力場定義的標準分子力學原子類型。但是，當所研究的分子系統不是這些力場做參數化的對象，就沒有適當的原子類

型可用。這時，使用者只能在分子系統設定段落內用新的原子類型標籤定義新的原子類型。很自然的，因為內建的能量函數表中沒有任何新原子類型，使用者必須在輸入檔內定義所有新原子類型所用的函數。

非鍵結作用主函數

前面已經看到，非鍵結作用項的設定會很冗長，需要許多項的 NBTerm。當在輸入檔案內設定非鍵結作用時（使用 MM 關鍵字的選項），可用 NonBon 函數做設定。這函數使用單一項目設定非鍵結作用，程式會自動將這設定展開程式當的 NBDir 和 NBTerm 項目。

這函數有以下一般形式：

NonBon *V-Type C-Type V-Cutoff C-Cutoff VScale1 VScale2 VScale3 CScale1 CScale2 CScale3*

V-Type 和 *C-Type* 是整數，分別指示採用哪一種凡得瓦和庫侖作用類型。其它的項有這兩種作用的門檻值，這兩種作用各有三個幅度因子，分別適用在相隔 1，2 和 3 或更多鍵結距離的原子對。當幅度因子的數值設為 -1.0 時，表示採用準 Amber 的幅度因子 1.0/1.2 。

例如，這個函數用來當作標準 Amber 力場:

```
NonBon 3 1 0 0 0.0 0.0 0.5 0.0 0.0 -1.0
```

這能量函數設定 Amber 算術式凡得瓦作用，1/R 庫侖作用，沒有門檻值。超過兩個鍵結距離的原子對的凡得瓦作用幅度調整 0.5，並且從鄰近原子對中排除。超過兩個鍵結距離的原子對的庫侖作用幅度調整 1.0/1.2，也從鄰近原子對中排除。

全域參數

在某些情況，位能函數所需的參數和特定的原子類型完全無關。介電常數就是一個例子。對於這種情況，程式使用全域參數：定義的數值考在位能函數裡作為參數使用。任何有定義的全域參數和在輸出檔案中的分子力學力場定義段落（以關鍵字 IOp(4/33=3 要求）內印出。 這裡是介電常數定義的範例：

```
Dielc 78.39
```

全域參數也可以向量或矩陣格式設定。以下來自 MM2 力場定義說明計算凡得瓦作用時，在函數中使用矩陣，這函數設定氫原子的漂移（即，原子間距離的幅度調整）：

```
VDWShf1 *       1    0.0          預設選項，使用 VDWShf2 的指標值 1
VDWShf1 MM5     2 -1.0          原子類型 MM5 使用指標值 2
VDWShf1 MM36 3 -1.0          原子類型 MM36 使用指標值 3
```

VDWShf2 1 2 0.915 *幅度因子: 矩陣元素 (1,2)*
VDWShf2 1 3 0.915 *幅度因子: 矩陣元素 (1,3)*

我們以相反的次序考慮這些能量函數。VDWShf2 對原子間距離建立調福音子的下三角矩陣。元素 (1,2) 和 (1,3) 都設為 0.915; 其它矩陣元素—(1,1), (2,2), (2,3) 和 (3,3)—保留預設值，表示在計算凡得瓦作用時這些距離維持不變。注意，這公式和原子類型無關。

VDWShf1 能量函數定義各種原子類型要使用哪些矩陣元素。第一個項目設定預設的指標值是 1 ，剩下兩個項目設定 MM5 原子類型用指標值 2 ，MM36 原子類型用指標值 3。這函數的第三個參數設定參與作用的第二個原子中心。在第一個項目，函數值為零的當作萬用字元，而其他兩個項目的數值，-1 告知程式要自動輸入適當的原子中心。

這些函數造成的結果是，只有涉及原子類型 MM5 (H) 或 MM36 (D) 與其他另種原子類型原子間的鍵結，有鍵長漂移的調整。當計算這些函數的時候，MM5-X 類型作用使用元素 (1,2)，MM36-X 類型作用使用元素 (1,3)。其他類型的作用使用 (1,1)，而 MM5-MM5，MM5-MM36 和 MM36-MM36 作用分別使用 (2,2)，(2,3) 和 (3,3)，—這些作用的計算都使用未調整的原子間距離。

利用這個機制，參數的設定變得更乾淨和精簡。沒有這個機制的話，每一對原子就需要一個項目才能達到相同的目的。

Step-down 表
萬用字元提供一種機制，用來設定廣義參數 / 預設值　這些參數和特定能量項中包含的每一種原子類型沒有明顯相關。 Step-down 表的目的相同，但是用途更精緻。考慮以下範例，來自 UFF 力場項目，UseTable 和 StepDown 項目不是位能函數，不包含參數，而是描述一個 step-down 機制，用來處理關聯到位能函數及所含參數的項目。

這個範例中，第一組 UFFBnd3 各行定義位能函數，而 UFFBnd2 各行和第二組 UFFBnd3 各行使用 step-down 機制：

```
UseTable UFFBnd2
#3
用來設定函數所設定 step-down 表
StepDown UFFBnd2 0 1
0                                                    設定函數
的相符規則
StepDown UFFBnd2 0 2 0
StepDown UFFBnd3 0 1 0 StepDown UFFBnd3 0 2 0 Table #3 C_R
Trig
 定義替代原子類型
Table #3 N_R Trig Table #3 H_ Lin Table #3 Li Lin UFFBnd3 0 C_3 0 109.471
-1.0 -1.0 0.1332              以明確原子類型定義的函數
```

UFFBnd3 0 N_3 0 106.700 -1.0 -1.0 0.1332
UFFBnd3 0 N_2 0 111.200 -1.0 -1.0 0.1332 UFFBnd3 0 O_3 0 104.510 -1.0 -1.0 0.1332 UFFBnd2-O-2 0 Lin 0 2 -1.0 -1.0 0.1332 *以 step-down*
UFFBnd2-O-3 0 Trig 0 3 -1.0 -1.0
0.1332

類型和子結構定義的函數
UFFBnd3-O-3 0 Lin 0 180.0 -1.0 -1.0 0.1332
UFFBnd3-O-4 0 Lin 0 180.0 -1.0 -1.0 0.1332
UFFBnd3-O-5 0 Lin 0 180.0 -1.0 -1.0 0.1332
UFFBnd3-O-6 0 Lin 0 180.0 -1.0 -1.0 0.1332
UFFBnd3-O-2 0 Trig 0 120.0 -1.0 -1.0 0.1332
UFFBnd3-O-4 0 Trig 0 120.0 -1.0 -1.0 0.1332
UFFBnd3-O-5 0 Trig 0 120.0 -1.0 -1.0 0.1332
UFFBnd3-O-6 0 Trig 0 120.0 -1.0 -1.0 0.1332

H_ 和 N_R 是 UFF 力場內的 UFF 原子類型。若在分子內有涉及鍵角 —H_－N_R－H_—程式需要決定要採用哪一種適當的位能函數和參數。首先，程式先決定一個可用彎曲能量函數的適當的 step-down 表。在這個範例中，兩個可用的彎曲函數: UFFBnd2 和 UFFBnd3 使用表#3。

表中的項目 對特定的原子類型定義替代類型。通常，這些項目將許多特定的原子類型映射到一個較廣泛的擬類型（例如，在這個範例中的 Lin 和 Trig）。這些替代類型接受較大範圍的預設數值，用來設定函數的參數，能夠有效的自動估計未定義參數的數值。

StepDown 項目設定相符規則，選出特定的函數項目。在這個範例中，兩個彎曲函數使用兩個相同的項目：0 1 0 和 0 2 0。要求程式應先尋找將原始原子類型設定為中心原子的項目（數值為零的函數當作萬用字元），若這樣的項目不存在，則採用第一個將替代原子類型設定為中心原子的項目。

在這範例中，程式會尋找將 N_R 設定為中央原子的彎曲能量函數，但是找不到，接著，會尋找以 Trig 為中心原子原子類型的彎曲能量函數，可以找到四種：UFFBnd2-O-3 和 UFFBnd3-O 和第二子結構 2，4 和 5。依照與中央氮原子鍵結的原子數目決定要選用哪一個。

注意，在實務上，step-down 表可對各種原子類型設定多種替代定義，也包含對列表的每一個替代定義對應許多原子類型。

使用 step-down 表時，在其它函數設定中用到的任何萬用字元都被忽略。換句話說，使用者選擇使用 step-down 表，在其它地方就不能使用萬用字元。

可用的力場函數

預先注意事項：

- 單位： 除非另外指明，距離的單位是埃，角度的單位是度，能量的單位是 kcal/mol 電荷的單位是原子單位。
- 方程式中，R 代表距離， θ 代表角度。數值和變數下標代表原子中心，“*eq*” 代表平衡：例如，R_{12} 和 R_{ij} 分別代表原子 1 和原子 2，及原子 i 與原子 j 的鍵長，R_i 是原子 i 的鍵長半徑， R_{eq} 和 θ_{eq} 分別是平衡狀態的鍵長和鍵角，R_{eq12} 是原子 1 和原子 2 之間的平衡鍵長（通常用在一角度項）。
- 任何函數定義都可使用萬用字母，以 0 或星號 （ * ）表示。
- 和標準力場中等同的函數以括號標示。

VDW: 凡得瓦參數，在 NBDir 和 NBTerm 中使用（見稍後 MMFF94 的 MMFF94-類型的凡得瓦參數）。

VDW *Atom-type Radius Well-depth*

VDW94: MMFF94 類型的凡得瓦參數（用在 NBDir 和 NBTerm）

VDW94 *原子類型 Atomic-pol NE Scale1 Scale2 DFlag*

Atomic-pol	原子極化度 Atomic polarizability (埃 ^{3})。
NE	價電子的 Slater-Kirkwood 有效數 (沒有單位)。
Scale1	調幅因子 (埃 $^{1/4}$)。
Scale2	調幅因子 (沒有單位)。
DFlag	1.0 供給氫原子類型原子， 2.0 接受氫原子類型原子，否則為 0.0.

Buf94: MMFF94 靜電緩衝

Buf94 *Atom-type Value*

NonBon: 非鍵結作用主函數。這函數計算分子力學能量之前，先展開成原子對的貢獻和一直接函數（NBDir 和 NBTerm）。

NonBon V-Type C-Type, V-Cutoff C-Cutoff VScale1 VScale2 VScale3 CScale1 CScale2 CScale3

V-Type 凡得瓦作用類型：

0	沒有凡得瓦
1	算術的 Arithmetic (Dreiding)
2	幾何的 Geometric (UFF)
3	算術的 Arithmetic (Amber)
4	MMFF94-類型的凡得瓦
5	MM2-類型的凡得瓦
6	OPLS-類型的凡得瓦

C-Type 庫侖作用類型：

0	沒有庫侖項
1	1/R
2	$1/R^2$
3	1/R 緩衝（buffered) (MMFF94)
10	雙極--雙極作用項，沒有門檻距離

V-Cutoff 和 *C-Cutoff* 分別是凡得瓦和庫侖作用門檻距離；

0	沒有門檻
>0	硬門檻
<0	軟門檻

Vscale1-3 是相隔 1- 到 3-鍵結原子對的 van der Waals 幅度因子。*CScale1-3* 是相隔 1- 到 3-鍵結原子對的庫侖作用幅度因子。若任何幅度因子 < 0.0，使用 1.0/1.2 幅度調整(和 Amber 一樣)。

NBDir: 庫倫和凡得瓦直接項（對所有成對原子做計算）

NBDir *V-Type* *C-Type* *V-Cutoff* *C-Cutoff*

V-Type, *C-Type*, *V-Cutoff*, 和 *C-Cutoff* 如前述。

NBTerm: 庫倫和凡得瓦位能單項門檻

NBTerm *Atom-type1* *Atom-type2* *V-Type* *C-Type* *V-Cutoff* *C-Cutoff* *V-Scale* *C-Scale*

V-Type, *C-Type*, *V-Cutoff*, *C-Cutoff*, *V-Scale*, 和 *C-Scale* 如前述。

AtRad: 原子單鍵半徑

AtRad *Atom-type* *Radius*

EffChg: 有效電荷 (UFF)

EffChg *Atom-type* *Charge*

EleNeg: GMP 陰電性 (Electronegativity) (UFF)

EleNeg *Atom-type* *Value*

Table: Step down 表

Table *Original-atom-type* *Stepping-down-type(s)*

HrmStr1: 諧和拉長能量函數 I (Amber 1): $ForceC*(R - R_{eq})^2$

HrmStr1 *Atom-type1* *Atom-type2* *ForceC* R_{eq}

ForceC 力常數

R_{eq} 平衡鍵長

HrmStr2: 諧和拉長能量函數 II (Dreiding 4a): $ForceC*[R - (R_i+R_j - Delta)]^2$

HrmStr2 *Atom-type1* *Atom-type2* *ForceC* *Delta*

ForceC	力常數
Delta	Delta

R_i 和 R_j 是原子鍵結半徑，由 AtRad 設定。

HrmStr3: 諧和拉長能量函數 III (UFF 1a): $k*(R-R_{ij})^2$

平衡鍵長 $R_{ij} = (1 - PropC*\ln BO)*(R_i + R_j) - R_{en}$
力常數: $k = 664.12*Z_i*Z_j/(R_{ij}^3)$
陰電性（Electronegativity）校正: $R_{en} = R_i*R_j*[SQRT(X_i) - SQRT(X_j)]^2/(X_i*R_i + X_j*R_j)$

HrmStr3 *Atom-type1* *Atom-type2* *BO* *PropC*

BO	鍵度（Bond order） (若 <0，由成是在計算時決定)
PropC	比例常數（Proportionality constant）

R_i 和 R_j 是原子鍵結半徑，由 AtRad 設定。X_i 和 X_j 是 GMP 陰電性（electronegativity），數值由 EleNeg 設定。 Z_i 和 Z_j 是有效原子電荷，由 EffChg 設定。

MrsStr1: Morse 拉長能量函數 I (Amber): $DLim*(e^{-a(R-Req)} - 1)^2$ ，這裡 $a = SQRT(ForceC/DLim)$

MrsStr1 *Atom-type1* *Atom-type2* *ForceC* R_{eq} *DLim*

ForceC	力常數
R_{eq}	平衡鍵長
DLim	解離極限距離

MrsStr2: Morse 拉長能量函數 II (Dreiding 5a): $DLim*(e^{-a(Ri+Rj-Delta)} - 1)^2$ ，這裡 $a = SQRT(ForceC/DLim)$

MrsStr2 *Atom-type1* *Atom-type2* *ForceC* *Delta* *DLim*

ForceC	力常數
Delta	Delta

DLim 解離極限距離

R_i 和 R_j 是原子鍵結半徑，由 AtRad 設定。

MrsStr3: Morse 拉長能量函數 III (UFF 1b): $BO*DLim*(e^{-a(R-Rij)}-1)^2$，這裡 a = SQRT(k/[$BO*DLim$])

平衡鍵長 R_{ij} = (1 - $PropC*\ln BO$)*(R_i + R_j) - R_{en}
力常數: k = 664.12*Z_i*Z_j/(R_{ij}^3)
陰電性校正: R_{en} = R_i*R_j*[SQRT(X_i) - SQRT(X_j)]^2/(X_i*R_i + X_j*R_j)

MrsStr3 *Atom-type1* *Atom-type2* *BO* *PropC* *DLim*

BO 鍵結度（Bond order） (若 <0，由成是在計算中決定)
PropC 比例常數
DLim 解離極限距離

R_i 和 R_j 是原子鍵結半徑，由 AtRad 設定。X_i 和 X_j 是 GMP 陰電性，數值由 EleNeg 設定。 Z_i 和 Z_j 是有效原子電荷，由 EffChg 設定。

QStr1: 四階拉長能量函數 I (MMFF94 2):
(R_{eq}/2)*(R - *ForceC*)^2*[1+*CStr**(R - *ForceC*+(7/12)*$CStr^2$*(R - *ForceC*)^2]

QStr1 *Atom-type1* *Atom-type2* *ForceC* R_{eq} *CStr*

ForceC 力常數 (md-埃$^{-1}$)
R_{eq} 平衡鍵長
CStr 三階拉長常數 (埃$^{-1}$)

UFFVOx: 氧族原子的原子扭轉能障 (UFF 16)

UFFVOx *Atom-type* *Barrier*

UFFsp3: 原子 SP3 扭轉障礙 (UFF 16)

UFFVsp3 *Atom-type* *Barrier*

UFFVsp2: 原子 SP2 扭轉障礙 (UFF 17)

UFFVsp2 *Atom-type* *Barrier*

HrmBnd1: 諧和彎曲能量函數 (Amber 1): $ForceC*(\theta - \theta_{eq})^2$

HrmBnd1 *Atom-type1* *Atom-type2* *Atom-type3* *ForceC* θ_{eq}

ForceC 力常數 (單位 kcal/(mol*rad^2))

θ_{eq} 平衡鍵角

HrmBdn2: 諧和彎曲能量函數 (Dreiding 10a):
$[ForceC/\sin(\theta_{eq}^2)]*(\cos(\theta) - \cos(\theta_{eq}))^2$

HrmBnd2 *Atom-type1* *Atom-type2* *Atom-type3* *ForceC* θ_{eq}

ForceC 力常數

θ_{eq} 平衡鍵角

LinBnd1: Dreiding 線性彎曲能量函數 (Dreiding 10c): $ForceC*(1+\cos(\theta))$

LinBnd1 *Atom-type1* *Atom-type2* *Atom-type3* *ForceC*

ForceC 力常數

UFFBnd3: UFF 三項彎曲能量函數 (UFF 11): $k*(C0 + C1*\cos(\theta)+C2*\cos(2\theta)$
where $C2=1/(4 * \sin(\theta_{eq}^2))$,
$C1 = -4*C2*\cos(\theta_{eq})$
$C0=C2*(2*\cos(\theta_{eq}^2)+1)$

力常數: $k = 664.12*Z_i*Z_k*(3*R_{ij}*R_{jk}*(1-\cos(\theta_{eq}^2)) - \cos(\theta_{eq})*R_{ik}^2)/R_{ik}^5$

UFFBnd3 Atom-type1 Atom-type2 Atom-type3 θ_{eq} BO_{12} BO_{23} PropC

θ_{eq} 平衡鍵角

BO_{12}	*Atom-type1–Atom-type2* 的鍵結度(若<0，由程式在計算中決定)
BO_{23}	*Atom-type2–Atom-type3* 的鍵結度(若<0，由程式在計算中決定)
PropC	比例常數

R_i ，R_j 和 R_k 是原子鍵結半徑，由 AtRad 設定 X_i，X_j 和 X_k 是 GMP 陰電性，數值由 EleNeg 設定。Z_i，Z_j 和 Z_k 是有效原子電荷，由 EffChg 設定。

UFFBnd2：UFF 兩項彎曲能量函數 (UFF 10)：$[k/(Per^2)]*[1-\cos(Per*\theta)]$

力常數：$k = 664.12*Z_i*Z_k*(3*R_{ij}*R_{jk}*(1-\cos(Per^2))-\cos(Per)*R_{ik}^2)/R_{ik}^5$

UFFBnd2 *Atom-type1* *Atom-type2* *Atom-type3* *Per* BO_{12} BO_{23} *PropC*

Per	週期性：2 是線性,3 是三角形，4 是平面正方形
BO_{12}	*Atom-type1–Atom-type2* 的鍵結度(若<0，由程式在計算中決定)
BO_{23}	*Atom-type2–Atom-type3* 的鍵結度(若<0，由程式在計算中決定)
PropC	比例常數

R_i ，R_j 和 R_k 是原子鍵結半徑，由 AtRad 設定 X_i，X_j 和 X_k 是 GMP 陰電性，數值由 EleNeg 設定。Z_i，Z_j 和 Z_k 是有效原子電荷，由 EffChg 設定。

ZeroBnd：零彎曲項：用在彎曲為零的稀有情況。程式需要這一項以避免遇到未定義的鍵角時產生的錯誤訊息。

ZeroBnd *Atom-type1* *Atom-type2* *Atom-type3*

CubBnd：三階彎曲能量函數 (MMFF94 3)：
$(ForceC/2)*(1+CBend*(\theta-\theta_{eq}))*(\theta-\theta_{eq})^2$

CubBnd
Atom-type1 *Atom-type2* *Atom-type3* *ForceC* θ_{eq} *CBend*

ForceC	力常數 (單位 md*Angstrom/rad^2)
θ_{eq}	平衡角度
CBend	三階彎曲常數 (單位 deg^{-1})

LinBnd2: MMFF94 線性彎曲能量函數 (MMFF94 4): $ForceC*(1+\cos(\theta))$

LinBnd2 *Atom-type1* *Atom-type2* *Atom-type3* *ForceC*

ForceC	力常數 (md)

AmbTrs: Amber 扭轉能量函數 (Amber 1): $\Sigma_{i=1,4}$ $(Mag_i*[1+\cos(i*\theta - I(i+4))])/NPaths$

AmbTrs Atom-type1 A-type2 A-type3 A-type4 PO1 PO2 PO3 PO4 Mag_1 Mag_2 Mag_3 Mag_4 NPaths

PO1–PO4	相位差
Mag_1–Mag_4	V/2 數值
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

DreiTrs: Dreiding 扭轉能量函數 (Dreiding 13):
$V*[1-\cos(Period*(\theta - PO))]/(2*NPaths)$

DreiTrs Atom-type1 Atom-type2 Atom-type3 Atom-type4 V PO Period NPaths

V	能障高度 V
PO	相位差
Period	週期性
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

UFFTorC: UFF 扭轉能量函數，固定能障 (UFF 15):
$[V/2]*[1-\cos(Period*PO)*\cos(V*\theta)]/NPaths$

UFFTorC Atom-type1 Atom-type2 Atom-type3 Atom-type4 Period PO V NPaths

Period	週期性
PO	相位差
V	能障高度 V
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

UFFTorB: UFF 扭轉能量函數，能障和鍵結度有關 (UFF 17):
$[V/2]*[1-\cos(Period*PO)*\cos(Period*\theta)]/NPaths$ where $V = 5*SQRT(U_j*U_k)*[1+4.18*Log(BO_{12})]$

UFFTorB Atom-type1 Atom-type2 Atom-type3 Atom-type4 Period PO BO_{12} NPaths

Period	週期性
PO	相位差
BO_{12}	*原子類型 1–原子類型 2* 的鍵結度(小於零，表示計算執行時再做決定)
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

U_j 和 U_k 是原子常數，由 UFFVsp2 定義。

UFFTor1: UFF 扭轉能量函數，能障和原子類型有關 (UFF 16):
$[V/2]*[1-\cos(Period*PO)*\cos(Period*\theta)]/NPaths$ where $V=SQRT(V_j*V_k)$

UFFTor1 Atom-type1 Atom-type2 Atom-type3 Atom-type4 Period PO NPaths

Period	週期性
PO	相位差
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

V_j 和 V_k 為原子常數，以 UFFVsp3 定義。

UFFTor2: UFF 扭轉能量函數,能障和原子類型有關 (UFF 16) (和 UFFTor1 的差異在所用的原子參數):
$[V/2]*[1-\cos(Period*PO)*\cos(Period*\theta)]/NPAths$ where $V=SQRT(V_j*V_k)$

UFFTor2 Atom-type1 Atom-type2 Atom-type3 Atom-type4 Period PO NPaths

Period	週期性
PO	相位差
NPaths	路徑數。零或是負值，表示計算執行時再做決定。

V_j 和 V_k 為原子常數，以 UFFVOx 定義。

VDWDreiTRS: Dreiding 特殊扭轉能量函數，和 Gaussian 98 程式碼相容。進行處理時，更換成 DreiTRS，代入以下參數：

- 若有三個原子和第三個原子中心鍵結，且第四個原子中心是氫原子，移除這氫原子。
- 若有三個原子和第三個原子中心鍵結，且其中至少有一個是氫原子，但第四個原子中心不是氫原子，則使用以下這些數值：*V*=4.0, *PO*=0.0, *Period*=3.0, 和 *NPaths*=－1.0。
- 除此之外，使用這些數值：*V*=1.0, *PO*=0.0, *Period*=6.0, 和 *NPaths*=－1.0。

OldTor Atom-type1 Atom-type2 Atom-type3 Atom-type4

ImpTrs: Improper 扭轉能量函數 (Amber 1): $Mag*[1+\cos(Period*(\theta - PO))]$

ImpTrs Atom-type1 Atom-type2 Atom-type3 Atom-type4 Mag PO Period

Mag	*V*/2 大小
PO	相位差
Period	週期性

Wilson: 三項 Wilson 角能量函數 (Dreiding 28c, UFF 19): $ForceC*(C1 + C2*\cos(\theta) + C3*\cos(2\theta))$ 對三個 Wilson 角 θ 平均

Wilson Atom-type1 Atom-type2 Atom-type3 Atom-type4 ForceC C1 C2 C3

ForceC	力常數
C1, C2, C3	係數

HrmWil1: 諧和 Wilson 角能量函數 I (MMFF94 6): $(ForceC/2)*(\theta^2)$ 對三個 Wilson 角 θ 求和

HrmWil1 Atom-type1 Atom-type2 Atom-type3 Atom-type4 ForceC

ForceC	力常數

MM2Wil: MM2 Wilson 六階彎曲能量函

數 (MM2): $\Sigma_{i=1,2,3}(ForceC_i/2)*(\theta_i^2)*[1+6Bend*(\theta_i^4)]$

MM2Wil

Atom-type1 *Atom-type2* *Atom-type3* *Atom-type4* *ForceC1* *ForceC2* *ForceC3* *6Bend*

ForceC1–ForceC3 力常數

6Bend 六階彎曲常數 (單位 deg^{-4})

StrBnd: 拉長--彎曲能量函數 (MMFF94 5):

$(ForceC1*(R_{12} - R_{eq12}) + ForceC2*(R_{23} - R_{eq23}))*(\theta - \theta_{eq})$

StrBnd

Atom-type1 *Atom-type2* *Atom-type3* *ForceC1* *ForceC2* R_{eq12} R_{eq23} θ_{eq}

ForceC1, *ForceC2* 力常數

R_{eq12}, R_{eq23} 平衡鍵長 (若 <0，從適當的拉長項中讀取)

θ_{eq} 平衡鍵角

CubStr1: 三階拉長能量函數 1 (MM2):

$(ForceC/2)*(1 - CStr*(R - R_{eq}))*(R - R_{eq})^2$

CubStr1 *Atom-type1* *Atom-type2* *ForceC* R_{eq} *CStr*

ForceC 力常數

R_{eq} 平衡鍵長

CStr 三階拉長常數 (埃 $^{-1}$)

SixBnd1: 六階彎曲能量函數 (MM2):

$(ForceC/2)*(\theta - \theta_{eq})^2(1+6Bend*(\theta - \theta_{eq})^4)$

SixBnd1

Atom-type1 Atom-type2 Atom-type3 ForceC θ_{eq} 6Bend

ForceC 力常數

θ_{eq} 平衡鍵角

6Bend 六階彎曲常數 (deg^{-4})

MM2Tors: MM2 扭角能量函數 (MM2):
En1/2(1+cos θ)+*En2*/2(1 - cos2 θ)+*En3*/2(1+cos3 θ)

MM2Tors
Atom-type1 Atom-type2 Atom-type3 Atom-type4 En1 En2 En3

En1–En3 能量

MM2VDW: MM2 凡得瓦函數的參數(MM2)

MM2VDW Par1 Par1 Par3 Par4 Par5

Par1–Par5 參數

VDWX: 凡得瓦參數矩陣 (MM2)。這些數值和原子類型無關，可當作原子參數的另種選擇，在 MM2 力場內會用到（見上面的討論)。

VDWX Index1 Index2 Radius Well-depth IsDef

IsDef 指示是否 (1.0) 或 (0.0) 尚未定義

VDWI: 原子標籤，用來標示 VDWXM (MM2)中的矩陣。

VDWI Atom-type Index

VDWShf2: 在凡得瓦計算中原子移動的參數矩陣 (MM2)

VDWShf2 *Index1* *Index2* *Shift*

VDWShf1: VDWShf2 矩陣的原子標籤(MM2)

VDWShf1 *Atom-type* *Index* *BondTo*

BondTo 形成鍵結的原子中心 (若 –1.0，則由程式決定)

SixBndI: 六階彎曲能量函數 (MM2)：
$(ForceC/2)*(\theta - \theta_{eq})^2(1+6Bend*(\theta - \theta_{eq})^4)$

SixBndI *Atom-type1* *Atom-type2* *Atom-type3* *ForceC* θ_{eq} *6Bend* *Flag*

ForceC	立場數
θ_{eq}	平衡鍵角
6Bend	六階彎曲常數 (單位 deg^{-4})
Flag	若 ≥0.0，即使中心原子在三角形中心，也不要投射到平面上。

若是三角形中心，這彎曲會投射到平面上。若中心不是三角形，則會計算一個正常的彎曲。

Dipole: 鍵雙極

Dipole *Atom-type1* *Atom-type2* *DMom* *DPos*

DMom	雙極矩 (單位 Debye)
DPos	在原子 1 -- 原子 2 鍵上的雙極位置

DielC: 介電常數。容許經由參數檔設定介電常數；預設值是 1。

DielC *DielConst*

DielConst	介電常數

QStr2: 四階拉長能量函數 2 (MM2/Tinker)：
$(ForceC/2)*(1+CStr*(R - R_{eq})+QStr*(R - R_{eq})^2)(R - R_{eq})^2)$

QStr2 *Atom-type1* *Atom-type2* *ForceC* R_{eq} *CStr* *QStr*

ForceC	力常數
R_{eq}	平衡位置鍵長
CStr	三階拉長常數(埃$^{-1}$)
QStr	四階拉長常數(埃$^{-2}$)

CubStr2：三階拉長能量函數 2（為了和舊版 MMVB 相容）：
$(ForceC/2)*(1 - CStr*(R - R_{eq}))*(R - R_{eq})^2$)

CubStr2 *Atom-type1* *Atom-type2* *ForceC* R_{eq} *CStr*

ForceC	力常數
R_{eq}	平衡位置鍵長
CStr	三階拉長常數 (埃$^{-1}$；當 R > 15 Å 時，設為零)

NBonds：形式鍵結數目，根據這原子中心的原子類型而定

NBonds Atom-type *NumBnd*

NumBnd	形式鍵結數目

StrUnit：拉長（stretching）函數中力常數的單位

StrUnit *Flag*

Flag	0 表示使用 kcal/(mol*Angstrom^2); 1 表示使用 md/Angstrom

BndUnit：彎曲（bending）函數中力常數的單位

BndUnit *Flag*

Flag	0 表示使用 kcal/(mol*rad^2); 1 表示使用 md*Angstrom/rad^2

TorUnit：扭轉函數中能量障礙的單位

TorUnit *Flag*

Flag	0 表示使用 kcal/mol; 1 表示使用 md*Angstrom

OOPUnit：脫離平面彎曲函數（out-of-plane bending）力常數的單位

OOPUnit *Flag*

Flag	0 表示使用 kcal/(mol*rad^2); 1 表示使用 md*Angstrom/rad^2

SBUnit: 拉長--彎曲函數中力常數的單位

SBUnit *Flag*

Flag 0 表示使用 kcal/(mol*Angstrom*rad); 1 表示使用單位 md/rad

StrFact: 拉長（stretching）函數的係數。

StrFact *Value*

BndFact: 彎曲（bending）函數的係數。

BndFact *Value*

TorFact: 扭轉函數的係數。

TorFact *Value*

OOPFact: 脫離平面（out-of-plane）函數的係數。

OOPFact *Value*

SBFact: 拉長-彎曲（ stretch-bend ）函數的係數。

SBFact *Value*

Last updated on: 2 September 2009

電子密度泛函數（DFT）方法

描述

Gaussian 09 提供多種電子密度泛函數理論 (DFT) [Hohenberg64, Kohn65, Parr89, Salahub89] 模型 (DFT 方法的討論和應用請參考 [Salahub89, Labanowski91, Andzelm92, Becke92, Gill92, Perdew92, Scuseria92, Becke92a, Perdew92a, Perdew93a, Sosa93a, Stephens94, Stephens94a, Ricca95])。所有 DFT 模型都可計算能量 [Pople92]，解析梯度，和真實解析頻率[Johnson93a, Johnson94, Stratmann97]。

自洽反應場方法 (SCRF) 可和 DFT 方法合用，計算溶液模型系統的能量，幾何優選和頻率。

純粹 DFT 計算將時常要利用電子密度適配的優點。參考基底函數 的說明。

以下章節概略說明 DFT 方法。接著是 *Gaussian 09* 程式內可用的泛函數種類。最後討論 DFT 計算準確度有關的話題。

由 freqmem 工具程式估算的最佳記憶體容量數值也適用於 DFT 頻率計算。

極化張量微分 (拉曼光譜強度) 和超極化張量在 DFT 頻率計算工作中不是預設的選項。要做這些計算需用選項 Freq=Raman 明確指定做此計算，而關鍵字 Polar 指定的計算自動包含極化張量微分和超級化張量的計算。

注意: 雙重混合泛函數的討論併入關鍵字 MP2 的章節中，因為兩者的計算成本相似。

背景說明

依據 Hartree-Fock 理論，分子系統具有以下能量形式：

$$E_{HF} = V + \langle hP \rangle + 1/2\langle PJ(P) \rangle - 1/2\langle PK(P) \rangle$$

各項的意義如下

V	原子核互斥能量
P	電子密度矩陣
<hP>	單電子能量（動能加位能）
1/2<PJ(P)>	電子的古典庫侖互斥能量
-1/2<PK(P)>	源自電子量子本性(fermion)的交換能量

在 Kohn-Sham 電子密度函數理論 的公式中[Kohn65]，單一行列式的正確交換能量 (HF) 以一較廣義的公式代替，即交換 - 相干泛函數，這泛函數可包含在 Hartree-Fock 理論中被省略的電子交換和電子相干能量，電子相干作用能量在 Hartree-Fock 理論中並未考慮：

$$E_{KS} = V + \langle hP \rangle + 1/2\langle PJ(P) \rangle + E_X[P] + E_C[P]$$

這裡 $E_X[P]$ 是交換能量泛函數， $E_C[P]$ 是相干作用能量泛函數。

在 Kohn-Sham 公式架構內，Hartree-Fock 理論可被視為密度泛含裡的一個特例，$E_X[P]$ 是交換作用積分 $-1/2\langle PK(P) \rangle$ 且 $E_C=0$。密度泛函理論中使用的泛函數，通常是某些密度的函數，也有可能是密度梯度的函數：

$$E_X[P] = \int f(\rho_\alpha(r),\rho_\beta(r),\nabla\rho_\alpha(r),\nabla\rho_\beta(r))dr$$

不同的電子密度理論模型對於 E_X 和 E_C 使用不同的函數 f。除了純粹的 DFT 方法之外，Gaussian 程式支援多種混合模型，其中的交換作用泛函數是 Hartree-Fock 交換作用項和一個上述形式的泛函數的線性組合。若提出的泛函數導致的積分沒有解析方法可做計算，會用數值積分方法進行。

DFT 方法的關鍵字

各種純粹 DFT 模型的名稱由交換作用和相干作用泛函數的名稱組合而成。在某些情況中，這領域使用的標準同義字也可用來作為關鍵字。

交換作用泛函數 *Gaussian 09* 程式可使用以下交換作用關鍵字。除非另外指明，這些交換作用泛函數必須和一個相干作用泛函數做組合，才能產生一個可用的方法。

- S: Slater 交換作用， $\rho^{4/3}$ 理論係數 2/3，也稱為局部自旋密度交換作用 [Hohenberg64, Kohn65, Slater74]。若單獨使用，表示是 HFS。
- XA: XAlpha 交換作用， $\rho^{4/3}$ 經驗係數 0.7，通常當作單獨使用的交換作用泛函數，沒有搭配的相干作用泛函數 [Hohenberg64, Kohn65, Slater74]。單獨使用的關鍵字：XAlpha。
- B: Becke 的 1988 泛函數，包含 Slater 交換作用泛函數，加上密度梯度的校正 [Becke88b]。若單獨使用，表示是 HFB。
- PW91: Perdew 和 Wang 1991 泛函數的交換作用項 [Perdew91, Perdew92, Perdew93a, Perdew96, Burke98]。
- mPW: Perdew-Wang 1991 交換作用泛函數的 Adamo 和 Barone 修正 [Adamo98]。
- G96: Gill1996 交換作用泛函數 [Gill96, Adamo98a]。
- PBE: Perdew, Burke 和 Ernzerhof 1996 提出的泛函數[Perdew96a, Perdew97]。
- O: Becke 交換作用泛函數的 Handy 的 OPTX 修正 [Handy01, Hoe01]。
- TPSS: Tao，Perdew，Staroverov，和 Scuseria 的交換作用泛函數[Tao03]。
- BRx: Becke 1989 交換作用泛函數 [Becke89a]。
- PKZB: Perdew，Kurth，Zupan 和 Blaha 泛函數的交換作用部份 [Perdew99]。

- wPBEh: Heyd，Scuseria 和 Ernzerhof 的根據遮蔽庫侖位能的泛函數的交換作用部份（也稱為 HSE） [Heyd03, Izmaylov06, Henderson09]。
- PBEh: 1998 修訂版的 PBE [Ernzerhof98]。

相干作用泛函數。 以下是可用的相干作用泛函數，以對應的關鍵字部份表，這些關鍵字都可和所要的交換作用關鍵字做組合：

- VWN: Vosko，Wilk，和 Nusair 1980 相干作用泛函數(III)，是配到均勻電子氣體的 RPA 解，通常稱為局部自旋密度(LSD)相干作用泛函數[Vosko80] (這篇論文中的泛函數 III)。
- VWN5: Functional V from 參考文獻 [Vosko80] 中的泛函數 V，適配到均勻電子氣體的 Ceperly-Alder 解。（這是 [Vosko80]論文中推薦的泛函數）。
- LYP: Lee，Yang，和 Parr 的相干作用泛函數，包含局部和非局部項 [Lee88, Miehlich89]。
- PL (Perdew Local): Perdew 泛函數的局部作用（無梯度校正）項 (1981) [Perdew81]。
- P86 (Perdew 86): Perdew 泛函數的梯度校正項，加上他的 1981 局部相干作用泛函數 [Perdew86]。
- PW91 (Perdew/Wang 91): Perdew 和 Wang 1991 梯度校正相干作用泛函數 [Perdew91, Perdew92, Perdew93a, Perdew96, Burke98]。
- B95 (Becke 95): Becke τ-相依梯度校正相干作用泛函數（Becke 單參數混合泛函數中的一部分 [Becke96])。
- PBE: Perdew，Burke 和 Ernzerhof 1996 梯度校正相干泛函數 [Perdew96a, Perdew97]。
- TPSS: Tao，Perdew，Staroverov， 和 Scuseria 的 τ-相依梯度校正相干作用泛函數 [Tao03]。
- KCIS: Krieger-Chen-Iafrate-Savin 相干作用泛函數 [Rey98, Krieger99, Krieger01, Toulouse02]。
- BRC: Becke-Roussel 相干作用泛函數 [Becke89a]。
- PKZB: Perdew，Kurth，Zupan 和 Blaha 泛函數的相干作用部份 [Perdew99]。

設定真實的泛函數。將一個交換作用泛函數部份關鍵字，和一個所要的相干作用泛函數組合起來，設定一個真實的泛函數。例如，Becke 交換作用泛函數 (B) 和 LYP 相干作用泛函數的組合，構成 BLYP 關鍵字。同樣的，SVWN 指定一個 Slater 交換作用泛函數 (S) 和 VWN 相干作用泛函數的組合，在文獻中視當作 LSDA (局部自旋密度近似 Local Spin Density Approximation)的同義字。. LSDA 是 SVWN 的同義字。某些其他有 DFT 計算功能了應用軟體做 LSDA 計算時，所用的是相當於 SVWN5 的計算方法。在做比較時，要仔細檢查所用軟體的使用手冊對所用泛函數名稱的定義。

相干作用泛函數的變形。以下相干作用泛函數結合來自不同相干作用函數的局部和非局部項：

- VP86: VWN5 局部和 P86 非局部相干作用泛函數。
- V5LYP: VWN5 局部和 LYP 非局部相干作用泛函數。

獨自使用的泛函數。 以下泛函數是完整的泛函數，不和其他任何泛函數關鍵字部份做組合：

- VSXC: van Voorhis 和 Scuseria 的 τ-相依梯度校正相干泛函數 [VanVoorhis98]。
- HCTH/*: Handy 的泛函數系列，包括梯度校正相干作用 [Hamprecht98, Boese00, Boese01]。 HCTH 代表 HCTH/407，HCTH93 代表 HCTH/93，HCTH147 代表 HCTH/147，且 HCTH407 代表 HCTH/407。注意相關的 HCTH/120 泛函數尚未實做到程式裡。
- tHCTH: τHCTH 系列泛函數的 τ-相依成員 [Boese02]。見以下的 tHCTHhyb。
- M06L: Truhlar 和 Zhao 的純粹泛函數[Zhao06a]。見以下的 M06 。
- B97D: Grimme 的泛函數，包含色散項 （dispersion） [Grimme06]。

混合型泛函數。 有計種混合型範函數，其中包含一個 Hartree-Fock 交換項和 DFT 交換--相干作用項的混合，可用以下關鍵字做指定：

- Becke 三參數混合泛函數，由 Becke 在 1993 年提出[Becke93a]：

  $A*E_X^{Slater}+(1-A)*E_X^{HF}+B*\Delta E_X^{Becke}+E_C^{VWN}+C*\Delta E_C^{non-local}$

  這裡常數 *A*，*B*，和 *C* 是由 Becke 經做適配到 G1 測試分子組後決定的。

  這混合泛函數有幾種變形。B3LYP 採用 LYP 方程式的非局部相干作用泛函數，和 VWN 泛函數 III 做為局部相干泛函數（非泛函數 V）。注意因為 LYP 包含局部和非局部項，實際上採用的相干作用泛函數是：

  $C*E_C^{LYP}+(1-C)*E_C^{VWN}$

  換句話說，VWN 提供所需過量的局部相干作用，因為 LYP 包含的局部項基本上和 VWN 相同。

- B3P86 指示採用 Perdew 86 提供的非局部相干作用相同的泛函數。B3PW91 指示採用 Perdew/Wang 91 非局部相干作用泛函數。
- Becke 單參數泛函數。關鍵字 B1B95 代表在原始論文中發表的 Becke 單參數泛函數[Becke96] 。.

  Adamo 和 Barone 實做過其它相似單參數混合泛函數 [Adamo97]。其中一種變形，B1LYP ，採用 LYP 相干泛函數（前述的 B3LYP ）。另一種版本， mPW1PW91， 採用 Adamo 和 Barone 修改過的 Perdew-Wang 交換泛函數和 Perdew-Wang 91 相干泛函數做組合 [Adamo98]。mPW1LYP，mPW1PBE 和 mPW3PBE 等變形組合也都可以使用。

- Becke B97 泛函數的 1998 修訂版 [Becke97, Schmider98]。關鍵字是 B98，是文獻 [Schmider98] 方程式 2c 的實做。
- Handy，Tozer 和同僚 B97 泛函數的修改版本：B971 [Hamprecht98]。
- Wilson，Bradley 和 Tozer 的 B97 泛函數的修訂版本：B972 [Wilson01a]。
- Perdew,Burke 和 Ernzerhof 1996 純粹泛函數[Perdew96a, Perdew97]， 由 Adamo 設計的份合泛函數 [Adamo99a]. 關鍵字是 PBE1PBE。這泛函數使用 25% 的交換作用項和 75% 的相干作用項權重，文獻中稱為 PBE0。
- HSEh1PBE：完整 Heyd-Scuseria-Ernzerhof 泛函數的推薦版本，文獻中稱為 HSE06 in the literature [Heyd04, Heyd04a, Heyd05, Heyd06, Izmaylov06, Krukau06, Henderson09]。也有兩種較早得版本可用：
  - HSE2PBE：這泛函數的第一型，文獻中稱為 HSE03。
  - HSE1PBE：此用修改前的泛函數版本，以支援三階微分計算。

- PBEh1PBE：使用 PBE 純粹泛函數 1998 修訂版的混合泛函數（交換作用和相干作用） [Ernzerhof98]。
- O3LYP：三參數泛函數，和 B3LYP 相似：

  $A*E_X^{LSD}+(1-A)*E_X^{HF}+B*\Delta E_X^{OPTX}+C*\Delta E_C^{LYP}+(1-C)E_C^{VWN}$

  這裡 A，B 和 C 由 Cohen 和 Handy 在文獻 [Cohen01]中定義。

- TPSSh：使用 TPSS 泛函數的混合泛函數 [Tao03]。
- BMK：Boese 和 Martin 的 τ-相依混合泛函數 [Boese04]。
- M06： Truhlar 和 Zhao 的混合泛函數 [Zhao08]。還有新關的變形 M06HF [Zhao06b, Zhao06c] 和 M062X [Zhao08] ，以及較早得版本 M05 [Zhao05] 和 M052X [Zhao06]。
- X3LYP：Xu 和 Goddard 的泛函數[Xu04]。
-
- 各佔一半(Half-and-half)泛函數，實做以下的泛函數。注意，這和 Becke [Becke93] 提出的各佔一半泛函數不相同。提供這泛函數是為了和舊版程式功能相容。
  - BHandH：$0.5*E_X^{HF} + 0.5*E_X^{LSDA} + E_C^{LYP}$
  - BHandHLYP：$0.5*E_X^{HF} + 0.5*E_X^{LSDA} + 0.5*\Delta E_X^{Becke88} + E_C^{LYP}$

長距離校正泛函數。交換作用泛函數的非庫侖項通成會遞減的很快，在長距離處變的很不準確，因此不適用於模擬電子激發到高階軌域這類型的過程。為了處理這類型的課題，發展了計種計算策略。Gaussian 09 程式提供以下包含長距離校正的泛函數：

- LC-wPBE：wPBE 的長距離校正版本 [Tawada04, Vydrov06, Vydrov06a, Vydrov07]。
- CAM-B3LYP： Handy 和同僚的 B3LYP 長距離校正版本，使用庫侖衰減（ Coulomb-attenuating）方法 [Yanai04]。
- wB97XD：Head-Gordon 和同僚最新的泛函數，包含經驗散射（empirical dispersion） [Chai08a]。 也有 wB97 和 wB97X [Chai08] 變形。這些泛函數也包含長距離校正。

此外，字首 LC- 可加到任一純粹泛函數關計字之前，表示加上 Hirao 和同僚的長距離校正 [Iikura01]：例如： LC-BLYP。

使用者自訂模型。Gaussian 09 可使用具有以下一般形式的任何模型：

$$P_2E_X^{HF} + P_1(P_4E_X^{Slater} + P_3\Delta E_x^{non\text{-}local}) + P_6E_C^{local} + P_5\Delta E_C^{non\text{-}local}$$

局部交換作用泛函數只有 *Slater* 可用 (S)，只考慮局部交換作用時使用。可和任何非局部交換作用校正泛函數關鍵字（已在前面列出）做組合。

其中的六個參數要以程式的非標準選項方式加以指定：

- IOp(3/76=*mmmmmnnnnn*) 設定 P_1 為 *mmmmm*/10000 和 P_2 為 *nnnnn*/10000。P_1 通常設為 1.0 或 0.0，依是否需要包含交換作用泛函數而定，所有幅度的調整是經由 P_3 和 P_4 參數來做。
- IOp(3/77=*mmmmmnnnnn*) 設定 P_3 為 *mmmmm*/10000 和 P_4 為 *nnnnn*/10000。
- IOp(3/78=*mmmmmnnnnn*) 設定 P_5 為 *mmmmm*/10000 和 P_6 為 *nnnnn*/10000。

例如， IOp(3/76=1000005000) 設定 P_1 為 1.0 和 P_2 為 0.5。這一這些數值必須用五位數表示，若有不足須以零補滿。

以下的範例在計算路徑段落內指定使用對應 B3LYP 關鍵字的泛函數：

```
#P BLYP IOp(3/76=1000002000) IOp(3/77=0720008000) IOp(3/78=0810010000)
```

輸出檔案中會印出所用的數值：

```
 IExCor= 402 DFT=T Ex=B+HF Corr=LYP ExCW=0 ScaHFX= 0.200000
 ScaDFX= 0.800000 0.720000 1.000000 0.810000
```

這裡 ScaHFX 的數值是 P_2， 所印出的 ScaDFX 一系列數值是 P_4, P_3, P_6 和 d P_5。

準確度的考量

DFT 計算在 Hartree-Fock 計算的每一主要階段加上一額外的步驟。這步驟是泛函數（或各種泛函數微分）的數值積分。因此在 Hartree-Fock 計算的數值誤差來源之外（積分的準確度，SCF 收斂條件，CPHF 的收斂條件等），DFT 計算的準確度和用來做數值積分的格點數有關。

Gaussian 09 的 “ fine ” 積分格點 (相當於 Integral=FineGrid) 為預設的積分格點。只花最少的額外成本，這格點能顯著增加積分的準確度。我們建議在做正式的 DFT 計算時，不要使用比 fine 更小的格點。若要做能量比較（如計算能量差，生成熱等）的所有計算需要使用相同的積分格點。

若有需要可使用較大的格點(例如對某類分子系統的做較準確的幾何優選計算)。在計算執行路徑中使用 Integral(Grid=*N*) 可選用不同的積分格點（參考關鍵字 Integral 章節的討論。

可用方法

能量，解析梯度和解析頻率。ADMP 計算。

三階分子性質，像是超極化張量和拉曼光譜強度，若泛函數的三階微分沒有實做到程式裡，就無法計算：這些泛函數包括，交換作用泛函數 Gill96，P (Perdew86)，BRx，PKZB，TPSS，wPBEh 和 PBEh；相干作用泛函數 PKZB 和 TPSS；以及混合泛函數 HSE1PBE 和 HSE2PBE。

相關的關鍵字

IOp, Int=Grid, Stable, TD, DenFit

使用範例

DFT 計算能量印出的形式和 Hartree-Fock 的情況相似。以下是一 B3LYP 計算的能量輸出：

SCF Done: E(RB+HF-LYP) = -75.3197099428 A.U. after 5 cycles

其中 E 後括號內的符號說明所使用的方法。由一 BLYP 計算所得的能量因出很類似的內容：

SCF Done: E(RB-LYP) = -75.2867073414 A.U. after 5 cycles

可用泛函數清單

組合形式		單獨泛函數		
交換作用	相干作用	只有交換作用	純粹	混合
S	VWN	HFS	VSXC	B3LYP
XA	VWN5	XAlpha	HCTH	B3P86
B	LYP	HFB	HCTH93	B3PW91
PW91	PL		HCTH147	B1B95
mPW	P86		HCTH407	mPW1PW91
G96	PW91		tHCTH	mPW1LYP
PBE	B95		M06L	mPW1PBE

O	PBE	B97D	mPW3PBE
TPSS	TPSS		B98
BRx	KCIS		B971
PKZB	BRC		B972
wPBEh	PKZB		PBE1PBE
PBEh	VP86		B1LYP
	V5LYP		O3LYP
			BHandH
			BHandHLYP
長距離校正			BMK
LC-			M06
			M06HF
			M062X
			tHCTHhyb
			HSEh1PBE
			HSE2PBE
			HSEhPBE
			PBEh1PBE
			wB97XD
			wB97
			wB97X
			TPSSh
			X3LYP
			LC-wPBE
			CAM-B3LYP

Last updated on: 5 Aug 2009

CBS-4M

CBS-QB3

CBS-APNO

描述

這方法關鍵字指示使用由 Petersson 和同僚的各種完全基底函數組（CBS）進行非常準確的能量計算[Nyden81, Petersson88, Petersson91, Petersson91a, Montgomery94, Ochterski96, Montgomery99, Montgomery00] 。這些關鍵字分別指定進行改進的版本 CBS-4 [Ochterski96, Montgomery00]，CBS-Q//B3 [Montgomery99, Montgomery00]和 CBS-APNO[Ochterski96] 方法。 使用這些關鍵字時不需再指定基底函數。RO 可當作字首，放在 CBS-QB3 之前，成為 ROCBS-QB3 方法 [Wood06]。

些方法是複雜的能量計算，涉及對指定的分子系統進行多次預先定義的計算。只需指定這些關鍵字中的一個，程式即自動進行這多步驟的計算工作，並將最後計算的能量印在輸出檔案中。

關鍵字 Opt=Maxcyc=***n*** 或 QCISD=Maxcyc=***n*** 或 CCSD=Maxcyc=***n*** 可和這些關鍵字合用，以分別指定優選計算或 QCISD 或 CCSD 迭代的最大次數。

選項

ReadIsotopes
這選項用來設定和預設溫度，壓力，頻率調幅因子和同位素質量不同的數值。預設的數值是 298.15 K，1 大氣壓，不調整幅度，以及最豐同位素質量。這選項用來從檢查檔讀取資料，但要用另一組參數重做熱化學分析計算。

注意，所有這些數值都可在計算路徑段落中設定（Temperature，Pressure 和 Scale 關鍵字，也可在分子設定段落中指定（Iso= 參數），例如：

#T *Method*/6-31G(d) *JobType* Temperature=300.0 …

…

0 1
C(Iso=13)
…

ReadIsotopes input has the following format:
temp pressure [*scale*] *數值必須是實數。*
原子 1 的同位素質量
原子 2 的同位素質量
…
原子 n 的同位素質量
這裡 *temp*，*pressure*，和 *scale* 是所要的溫度，壓力，和選項頻率數據的調幅因子（用來做熱化學分析時會用到，預設是不做幅度調整）。後面幾行是分子中所有原子的同位素質量，以分子設定段落中各原子出現的行數順序排列。若用整數設定同位素質量，程式會自動採用最接近的真實同位素質量的數值（例如，18 指定 ^{18}O，Gaussian 程式使用 17.99916）。

Restart
從稍早的 CBS 計算的檢查檔重新啟動一個計算工作。新計算工作將從前次（還未結束）最後一次成功的計算週期之後開始。

可用方法

只能計算能量。 CBS-4M and CBS-QB3 可用在第一列和第二列週期表的原子；CBS-APNO 只能用在第一列原子。ROCBS-QB3 [Wood06] 用在限定自旋狀態未填滿殼層系統。

CBS-4 模型化學已做更新，採用新的局部化程序和改善的經驗參數[Montgomery00]。建議新的研究採用新版本 CBS-4M, （M 標示使用最小分佈局部化 Minimal Population localization） ；

RO 可和 CBS-4M 及 CBS-QB3 共用。

使用範例

CBS 方法中每一步驟的計算結果都會印在輸出檔案中。檔案的最後段落包括整個計算的總結。

CBS 計算的總結部份。這是 CH_2（自旋三重態）的 CBS-QB3 計算的結果：

```
 Complete Basis Set (CBS) Extrapolation:
 M. R. Nyden and G. A. Petersson, JCP 75, 1843 (1981)
 G. A. Petersson and M. A. Al-Laham, JCP 94, 6081 (1991)
 G. A. Petersson, T. Tensfeldt, and J. A. Montgomery, JCP 94, 6091 (1991)
 J. A. Montgomery, J. W. Ochterski, and G. A. Petersson, JCP 101, 5900
(1994)

 Temperature= 298.150000 Pressure= 1.000000
 E(ZPE)= 0.016991 E(Thermal)= 0.019855
 E(SCF)= -38.936447 DE(MP2)= -0.114761
 DE(CBS)= -0.011936 DE(MP34)= -0.018720
 DE(CCSD)= -0.002759 DE(Int)= 0.004204
 DE(Empirical)= -0.006404
 CBS-QB3 (0 K)= -39.069832 CBS-QB3 Energy= -39.066969
 CBS-QB3 Enthalpy= -39.066025 CBS-QB3 Free Energy= -39.088192
```

先是溫度和壓力，然後是 CBS-QB3 能量的各個部份。倒數第二行為 CBS-QB3 能量值：在 0 K 和指定的溫度值（298.15K，這是預設溫度值）。最後一行是 CBS-QB3 的焓值（包括在指定溫度的校正）和由 CBS-QB3 方法計算的 Gibbs 自由能（即 CBS-QB3 能量包括頻率計算的自由能校正）。所有能量的單位都是 Hartree。

在另一溫度重新進行計算：這是一個兩階段計算工作，說明在另一個溫度執行第二個（很快的） CBS 計算。這工作計算在溫度為 298.15 K 和 300K 的 CBS-QB3 能量。

各能量標籤有以下含意（CBS-QB3 用來當作範例）：

CBS-QB3 (0 K)	零點校正的電子能量: $E_0 = E_{elec} + ZPE$
CBS-QB3 Energy	熱校正能量：$E = E_0 + E_{trans} + E_{rot} + E_{vib}$
CBS-QB3 Enthalpy	用 CBS-QB3 預測的能量所計算得焓： $H = E + RT$
CBS-QB3 Free Energy	利用 CBS-QB3 預測的能量計算 Gibbs 自由能：$G = H - TS$

```
%Chk=cbs
# CBS-QB3 Test

CBS-QB3 on formaldehyde

0 1
```
分子系統設定段落

```
--Link1--
%Chk=cbs
%NoSave
# CBS-QB3(Restart,ReadIso) Geom=AllCheck Test
300.0 1.0
```
同位素設定區

Last updated on: 2 September 2009

G1
G2
G2MP2
G3
G3MP2
G3B3

G3MP2B3
G4
G4MP2

描述

這些方法關鍵字指示使用 Gaussian-1 (簡稱 G1)[Pople89, Curtiss90] ，Gaussian-2 (簡稱 G2) [Curtiss91]，Gaussian-3 (G3) [Curtiss98] 和 Gaussian-4 (G4) [Curtiss07] 方法進行高度準確能量計算。G2MP2 指示使用 G2 的修改版本 G2(MP2)，其中使用 MP2 方法而非 MP4 方法處理基底函數組延伸校正[Curtiss93]，這方法幾乎和完全的 G2 方法有相同的準確程度，但計算成本卻顯著的低了許多。G3MP2 指示使用相似的修改版本 G3(MP2)[Curtiss99]。這 G3 的變形方法使用 B3LYP 結構和頻率 [Baboul99] ，可用關鍵字 G3B3 和 G3MP2B3 指定。G4 和 G4MP2 指示使用第四代方法 [Curtiss07, Curtiss07a]。

這些方法都是複雜的能量計算，其中包括對指定的分子系統進行幾次已預定的計算步驟。使用這些關鍵字時，所有這些預定的計算步驟都是自動執行的，最後計算的能量印在輸出檔案內。使用這些關鍵字時不需指定基底函數組。

通常使用者在採用這些方法之前，應先考慮使用其他高準確度計算方法，CBS-QB3 方法也有相同的準確度，但計算速度要快很多，而 W1U 方法會更準確，但會比較慢。

這些關鍵字可和關鍵字 Opt=Maxcyc=*n*，QCISD=Maxcyc=*n* 或 CCSD=Maxcyc=*n* 一起使用，分別以指定優選計算， QCISD 計算或 CCSD 計算階段中最大迭代次數。

選項

ReadIsotopes
這選項用來設定和預設溫度，壓力，頻率調幅因子和同位素質量不同的數值。預設的數值是 298.15 K，1 大氣壓，不調整幅度，以及最豐同位素質量。這選項用來從檢查檔讀取資料，但要用另一組參數重做熱化學分析計算。

注意，所有這些數值都可在計算路徑段落中設定（Temperature，Pressure 和 Scale 關鍵字，也可在分子設定段落中指定（Iso= 參數），例如：

#T *Method*/6-31G(d) *JobType* Temperature=300.0 …

…

0 1

C(Iso=13)
…

ReadIsotopes 輸入資料格式：
temp pressure [*scale*]　　*數值必須是實數。*
原子 1 的同位素質量
原子 2 的同位素質量
…
原子 n 的同位素質量

這裡 *temp*，*pressure*，和 *scale* 是
所要的溫度，壓力，和選項頻率數據的調幅因子（用來做熱化學分析時會用到，預設是不做幅度調整）。後面幾行是分子中所有原子的同位素質量，以分子設定段落
中各原子出現的行數順序排列。若用整數設定同位素質量，程式會自動採用最接近的真實同位素質量的數值(例如,18 指定 ^{18}O,Gaussian 程式使用 17.99916)。

Restart
指示由一檢查檔重新啟動未完成的計算工作。當和 ReadIso 選項合用時，可使用不同的熱化學參數和同位素質量進行快速計算。

使用範例

計算結果總結輸出。所有計算步驟的結果印出之後，*Gaussian* 印出這些方法的結果表格，以下是 G2 計算的輸出部份：

```
Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= .020511 E(Thermal)= .023346
E(QCISD(T))= -76.276078 E(Empiric)= -.024560
DE(Plus)= -.010827 DE(2DF)= -.037385
G1(0 K)= -76.328339 G1 Energy= -76.325503
G1 Enthalpy= -76.324559 G1 Free Energy= -76.303182
E(Delta-G2)= -.008275 E(G2-Empiric)= .004560
G2(0 K)= -76.332054 G2 Energy= -76.329219
G2 Enthalpy= -76.328274 G2 Free Energy= -76.306897
```

先出現溫度和壓力，然後是用來計算 G2 能量的各個分量。在 0 K 和指定溫度的 G2 能量（後者包含全部的熱力學校正，不只是零點能量校正）以及（最後一行）G2 理論預測的焓值和 Gibbs 自由能（兩者使用熱力學校正過的 G2 能量計算）。注意：在這輸出段落內也印出這相物理量的 G1 理論預測值。

這些能量標籤有以下的含意（以 G2 為例）：

G2 (0 K)　　零點校正電子能量: $E_0 = E_{elec} + ZPE$

G2 Energy　　熱校正能量: $E = E_0 + E_{trans} + E_{rot} + E_{vib}$

G2 Enthalpy　　用 G2 預測的能量計算焓: $H = E + RT$

G2 Free Energy　　用 G2 預測的能量計算的 Gibbs 自由能: $G = H - TS$

在另一溫度重新進行計算。以下是一個兩步驟算工作，第二階段在另一溫度進行一次的 G2 計算（這部分計算會非常快速）。這計算工作先計算在 298.15 K 計算 G2 能量，然後在 300 K 在計算一次 G2 能量：

```
%Chk=formald
# G2 Test

G2 on formaldehyde

0 1
分子系統設定段落
--Link1--
%Chk=formald
%NoSave
# G2(Restart,ReadIso) Geom=Check
300.0 1.0
同位素設定段落
```

Last updated on: 2 September 2009

Frozen Core 內層軌域凍結選項

描述

這些選項指定在後 SCF 計算中哪些內層軌域要被凍結。*Gaussian 09* 新增一些選項可做內層軌域凍結 [Austin02]。

選項

FC
指示做內層軌域凍結(frozen-core)計算，表示在做相干作用計算時排除內層原子子軌域的貢獻。這是預設的計算模式。注意，FC，Full，RW 和 Window 彼此是不相容的。在 6-31G 和 6-311G 基底函數組相當於 FreezeG2，其它所有基底函數組相當於 FreezeNobleGasCore ，除了第三列元素和後段鹼金屬及鹼土金屬原子的外層 s 和 p 的核心軌域之外（和 G2/G3/G4 的規定一致）。

FreezeNobleGasCore
在後-SCF 計算中最大的惰性氣體殼層軌域被凍結。同義字是 FrzNGC。 I

FreezeInnerNobleGasCore
在後-SCF 計算中次大的惰性氣體殼層軌域被凍結。最外圈的核心殼層還是納入計算。同義字是 FrzINGC 和 FC1 。

FreezeG2
根據 G2 的規定凍結內層軌域：主族元素的 d 軌域被凍結，但第三列元素和後段鹼金屬及鹼土金屬原子的核心的外圈 sp 軌域保留在價鍵軌域。

FreezeG3
根據 G3 的規定凍結內層軌域。

FreezeG4
根據 G4 的規定凍結內層軌域。

Full
指示在相干作用計算中使用全部的電子。

RW
這讀軌域範圍（read window）選項指示要從輸入檔內讀入設定資料，設定在後-SCF 計算中要包含哪些軌域。同義字是 ReadWindow。

所要求的輸入資料段落只有一行，這一行內有兩個數字標示開始和結束的軌域編號，然後以一行空白結束。數值 0 表示是第一個或最後一個軌域，和這數值所在為置有關。若第一個軌域的數值是負值(-*m*)，表示包含最高的 *m* 個軌域要納入計算；若最後一個軌域的數值是負值(-*n*)，表示凍結最高的 *n* 個軌域。若 *m* 是正值而 *n* 省略， *n* 的預設值為 0。若 *m* 是負值而 *n* 省略，則最高的 |*m*| 個填入軌域和最低的 |*m*| 個未填入軌域會包含在相干作用計算中。

以下是 C_4H_4 計算的一些範例：

0,0 相當於 **Full**.

5,0 將 4 個內層軌域凍結，保留所有未填入軌域在相干作用計算中 (若基底函數有單一 zeta 內層軌域，相當於 **FC**)。

5,-4 將 4 個內層軌域和最高的四個未填入軌域凍結。適用於具有雙 zeta 內層軌域基底函數的凍結內層軌域設定。

6,22 在後-SCF 計算中納入由第 6 到第 22 個軌域。例如， C_4H_4 有 28 個電子，若是填滿殼層計算，填入的軌域有 14 個，其中 5 個會被凍結，後-SCF 計算會用到 9 個填入軌域 (軌域 6-14) 和 8 個未填入軌域 (軌域 15-22)。

-6 將軌域 9 到軌域 20 納入相干作用計算。

Window=(*m*[,*n*])
和 ReadWindow 選項有相同作用，但從計算路徑段落的參數取得輸入資料。

ChkWindow
從檢查檔中讀取前次計算工作中的軌域範圍資料。

ListWindow
從輸入檔中的輸入資料段落讀取要凍結的軌域範圍資料，資料段落以空行結束。無自旋限制計算工作要讀取兩個軌域範圍清單。可指定軌域的範圍，例如：　2　　7-10　　14

Last updated on: 2 September 2009

MP2
MP3
MP4
MP5
B2PLYP
mPW2PLYP

描述

MP*n* 方法關鍵字指示在 Hartree-Fock 計算（單自旋態 RHF，高自旋態 UHF）後接著進行 Møller-Plesset 相干作用能量校正計算[Moller34]，只做到二階項校正的是 MP2 [Head-Gordon88a, Saebo89, Frisch90b, Frisch90c, Head-Gordon94]，做到三階項校正的是[Pople76, Pople77]，做到四階項校正的是 MP4 [Raghavachari78]，做到五階項校正的是 MP5 [Raghavachari90]。MP2[Pople79, Handy84, Frisch90b, Frisch90c]，MP3 和 MP4(SDQ)等方法有解析梯度 [Trucks88, Trucks88a]，MP2 方法有解析頻率[Head-Gordon94]。 ROMP2，ROMP3 和 ROMP4 有能量計算 [Knowles91, Lauderdale91, Lauderdale92]。

Gaussian 09 還有一些雙混合方法，在一 DFT 計算中結合完整的 HF 交換作用項和類似 MP2 的相干作用項。這些方法的計算成本和 MP2 類似(而不像 DFT 的計算成本）。Gaussian 09 包含 Grimme 的 B2PLYP [Grimme06a] 和 mPW2PLYP [Schwabe06] 方法（使用相同盟撐得關鍵字）：在關鍵字名稱後加上字母 D 表示加

上經驗散射（empirical dispersion）校正項: 例如, B2PLYPD 代表 B2PLYP 加上經驗散射 [Schwabe07]。可計算能量，梯度和頻率。

MP4 的其他形式

MP4(DQ) 指定只用到雙重和四重取代的軌域空間， MP4(SDQ) 指定用到單一，雙重和四取代的軌域空間， MP4(SDTQ) 指定完整的 MP4 加上單一，雙重，三重，和四重取代的軌域空間 [Raghavachari78, Raghavachari80]。只設定 MP4 相當於 MP4(SDTQ)。

MP5 的限制

MP5 方法的程式指示用於未填滿殼層的分子系統，因此設定 MP5 預設執行一個 UMP5 計算。這方法需要的磁碟空間和 O^3V^3 成比例，計算時間和 O^4V^4 成比例。

凍結內層軌域選項

FC
所有凍結內層的選項都可和這關鍵字合用。細節請見 FC 選項章節的討論。

MP2 和雙重混合 DFT 方法的計算方法選擇選項

The appropriate algorithm for MP2 will be selected automatically 根據 %Mem 和 MaxDisk. 的設定，程式會自動選擇適當的 MP2 計算方法。因此以下這些選項幾乎是不必要的。（細節請見 計算效能的考量 這一章節）。

FullDirect
指示使用完全直接計算方法，除了 SCF 所需要的磁碟空間外無額外的磁碟空間需求。主記憶體的最少需求是 $2OVN$ 個 64 位元計算機字（O 為填滿軌域數，V 為未填電子的軌域數，N 為基底函數數）。只適用於有很大的主記憶容量而磁碟空間卻很有限的計算機環境。

SemiDirect
指示使用半直接計算方法。

Direct
指示使用某種程度的直接方法。根據主記憶體的大小，磁碟空間限制和計算問題的大小決定選用 in-core，完全直接和半直接方法。

InCore
指示採用全部存放記憶體的計算方法。若能使用，這是非常快的方法，但需要 $N^4/4$ 個字的記憶體。通常和 SCF=InCore. 一起使用。 NoInCore 是反義字。

可用方法

MP2, B2PLYP[D], mPW2PLYP[D] : 能量，解析梯度和解析頻率。

MP3, MP4(DQ) 和 MP4(SDQ): 能量，解析梯度和數值頻率。

MP4(SDTQ) 和 MP5: 解析能量，數值梯度和數值頻率。

RO 可和 MP2, MP3 和 MP4 組合，只能計算能量。

相關的關鍵字

HF, SCF, Transformation, MaxDisk

使用範例

能量。The MP2 energy appears in the output as follows, labeled as EUMP2:

```
E2= -.3906492545D-01 EUMP2= -.75003727493390D+02
```

Energies for higher-order Møller-Plesset methods follow. Here is the output from an MP4(SDTQ) calculation:

```
Time for triples= .04 seconds.
MP4(T)= -.55601167D-04
E3= -.10847902D-01 EUMP3= -.75014575395D+02
E4(DQ)= -.32068082D-02 UMP4(DQ)= -.75017782203D+02
E4(SDQ)= -.33238377D-02 UMP4(SDQ)= -.75017899233D+02
E4(SDTQ)= -.33794389D-02 UMP4(SDTQ)= -.75017954834D+02
```

The energy labeled EUMP3 is the MP3 energy, and the various MP4-level corrections appear after it, with the MP4(SDTQ) output coming in the final line (labeled UMP4(SDTQ)).

B2PLYP 計算輸出範例。B2PLYP 能量在輸出檔內列印的標籤是 E(B2PLYP):

```
 E2(B2PLYP) = -0.3262340664D-01 E(B2PLYP) = -0.39113226645200D+02
```

Last updated on: 2 September 2009

半經驗方法

描述

Gaussian 09 程式裡有許多種半經驗方法可用。AM1 和 PM3 方法以重新實做 [Thiel92, Thiel96, Frisch09] ，採用標準積分程序架構（而非採用公眾版 MOPAC 內的程式碼）。除了提昇計算效率，也新增解析梯度和頻率的計算功能。PM6 和 PDDG 也用這種方式實做。其他的半經驗方法是模組 402 的 MOPAC 修改版本，稍候會有說明。

- AM1: 要求使用 AM1 能量函數進行半經驗方法計算 [Dewar77, Dewar78a, Davis81, Dewar85, Dewar86, Dewar88, Dewar88a, Dewar89, Dewar90, Dewar90a, Anders93]。
- PM3: 要求使用 PM3 能量函數進行半經驗方法計算 [Stewart89, Stewart89a]。 Li 的參數已經更新 [Anders93]。PM3MM 指示採用 PM3 模型，並包含 HCON 鍵結的分子力學校正
- PM6: 要求使用 PM6 能量函數進行半經驗方法計算 [Stewart07]。也有變形 PDDG 可用 [Repasky02, Tubert-Brohman04, Tubert-Brohman05, Sattelmeyer06, Tirado-Rives08]。

使用半經驗方法關鍵字時不可設定基底函數。

有支援的原子的編準參數由程式自動產生，除非 NoGenerate 選項另有設定。額外的或另一種參數可用多種方式讀進（見以下討論）若兩種都有指定，讀進的參數較內存的參數優先採用。

選項

Generate
對選定的半經驗方法產生標準參數，這是預設選項。NoGenerate 要求不產生任何參數，所有參數都要從輸入檔案中讀進。

Input
以 Gaussian 程式格式從輸入檔案中讀進參數。任何參數都可指定或覆蓋。參數輸入段落以一空行結束。Cards 是同義字 Input。

MOPACExternal
以 MOPAC 外部格式和單位，從輸入檔案中讀進參數。大部分但非全部的參數可以被改變。參數輸入段落以一空行結束。

Both
從輸入檔案中讀進參數，先是 Gaussian 程式格式的參數，再來更多的參數是 MOPAC 格式，這兩個參數輸入段落都以一空行結束。

Checkpoint
從檢查檔讀取參數。Chk 和 Read 是 Checkpoint 的同義字。

TCheckpoint
從檢查檔讀取參數，若參數不存在由程式計算產生。

RWF
從讀寫檔讀取參數。

Print
將目前計算工作中的元素所用的參數以 Gaussian 程式格式印出。若參數是從輸入檔中讀進，這是預設的選項。NoPrint 要求不要印出參數，若使用的是內存的標準參數，這是預設的選項。

PrintAll
將所有元素的參數印出（以 Gaussian 程式格式），包含在分子系統設定段落中沒有出現的原子。

Zero
印出所有參數，不論參數的值是否為零。預設的選項是 NonZero, 只印出非零的參數。

Old
使用舊版 MOPAC-程式碼。二階微分用數值方法計算。只適用於 AM1 和 PM3。預設的選項是 New，要求使用新的實做程式碼。

設定半經驗方法參數

半經驗方法參數可用兩種格式做設定，Gaussian 和 MOPAC，分別經由 Input 和 MOPACExternal 選項來完成。從原生 G09 半經驗方法參數格式開始，這格式適用性很廣。

這是 FeCH 的 Gaussian 格式參數範例：

全分子系統最初斷落
Method=40 CoreType=2 PM6R6=0.0000124488 PM6R12=0.0000007621
****
H *氫原子參數*
PQN=1 NValence=1 F0ss=0.5309794634 ZetaOverlap=1.2686410000
U=-0.4133181193
Beta=-0.3069665271 CoreKO=0.9416560046 KON=0,0,0,0.9416560046
EISol=-0.4133181193
EHeat=0.0830298228
GCore=0.0016794859,0.8557539899,3.3750716603
DCore=1,3,1.8737858033,2.2435870000

****
C　　*碳原子參數*
PQN=2,2 NValence=4 F0ss=0.4900713271 F0sp=0.4236511476
F0pp=0.3644399975 F2pp=0.1978513243
G1sp=0.0790832988
ZetaOverlap=2.0475580000,1.7028410000
U=-1.8775102825,-1.4676916178
Beta=-0.5653970441,-0.2745883502 DDN=0,1,0.7535642510
DDN=1,1,0.7192361890
CoreKO=1.0202596487 KON=0,0,0,1.0202596487 KON=1,0,1,1.2918442312
KON=0,1,1,1.0202596487
KON=2,1,1,0.7626764584 EISol=-4.2335803497 EHeat=0.2723305520
DipHyp=1.5070417957
GCore=0.0032154961,0.5881175739,2.5208171825
DCore=1,4,0.2878149911,0.2165060000
DCore=2,3,1.6101301385,3.2139710000
DCore=3,3,1.7155258339,16.1800020000
DCore=4,3,2.2293611369,25.0358790000
DCore=5,3,1.5446719761,1.8748590000
DCore=6,5,1.3831173494,0.8135100000,3.1644797074,9.2800000000
****
Fe　　*鐵原子參數*
PQN=4,4,3 NValence=8 F0ss=0.2931506917 F0sp=0.2861621092
F0pp=0.2797829041
F0sd=0.3417747898 F0pd=0.3378189937 F0dd=0.5580709105
F2pp=0.1567537881 F2pd=0.1236661383
F2dd=0.2945882511 F4dd=0.1921227725 G1sp=0.2072870321
G1pd=0.1102204721 G2sd=0.0588483485
G3pd=0.0671224585 Rsppd=0.1364112343 Rsdpp=0.1031169651
Rsddd=0.1510228569
ZetaOverlap=1.4791500000,6.0022460000,1.0807470000
Zeta1C=1.4591520000,1.3926140000,2.1619090000
U=-2.5913804076,-2.3138503107,-3.8083983722
Beta=0.2950096563,-0.0413709206,-0.1288993981 DDN=0,1,0.0896587028
DDN=1,1,0.3534210933
DDN=0,2,1.6776352014 DDN=1,2,0.0796789968 DDN=2,2,1.3085519205
CoreKO=1.2720920000
KON=0,0,0,1.7056074374 KON=1,0,1,0.2359511557 KON=0,1,1,1.7056074374
KON=2,1,1,0.4977547907
KON=2,0,2,1.6958541322 KON=1,1,2,0.2947417183 KON=0,2,2,0.8959434914
KON=2,2,2,1.2449263774
EISol=-15.6859079709 EHeat=0.1582446241 DipHyp=0.1793070893
DCore=1,3,0.4521755746,0.0251950000
DCore=6,3,2.1121277473,0.3668350000

DCore=7,3,1.3232002016,0.1553420000
DCore=8,3,0.9135254945,0.1364220000
DCore=9,3,2.2726610620,3.6573500000
DCore=15,3,1.3586804751,0.4312910000
DCore=16,3,0.5233514967,0.0334780000
DCore=17,3,0.6507784269,0.0194730000
DCore=19,3,1.0583544172,6.0000000000
DCore=26,3,1.4397774115,1.8468900000
****

輸入資料採用原子單位。參數段落以一行四個星號做區隔。

在全分子系統段落中設定以下各項：

Method	對應所要的半經驗方法的整數。這數值應對應在計算路徑段落裡設定的計算方法，作為檢查。AM1 的數值是 8， PM3 的數值是 9，PM33MM 的數值是 10， PM6 的數值是 40， PDDG 的數值是 41。
CoreType	內層核心互斥項的類型，1 代表 AM1，PM3，或 PDDG， 2 代表 PM6。
PeptideFC	胜肽鍵的力常數，只適用於 PM3MM。
RIJScale	AM1 方法中 O-H 和 N-H 鍵結的 R_{ij} 調幅因子。
PM6R6	PM6 內層核心互斥的 R6 參數。
PM6R12	PM6 內層核心互斥的 R12 參數。

以下各項設定一個原子的參數：

PQN	每一殼層主量子數（s，p，d)。決定在這元素使用哪些基底函數。
NValence	價電子數目。
ZetaOverlap	用來計算核心能量函數（core Hamiltonian）的重疊貢獻所用的基底函數的 Slater 指數。
Zeta1C	計算單原子中心雙電子積分（one-center two-electron integrals）所用的基底函數的 Slater 指數。
F0*, G*, Rs*	單原子中心雙電子積分的 Slater-Condon 參數。若其中任何一個參數沒有指定，這參數會從 Zeta1C 指數中計算。當印出內存參數時，會印出所有使用到的參數，不論是否從 Zeta1C 計算所得，或是一個特定的數值。這些參數完整清單是： F0ss，F0sp，F0pp，F0sd，F0pd，F0dd，F2pp，F2pd，F2dd，F4dd，G1sp，G1pd，G2sd，G3pd，Rsppd，Rsdpp 和 Rsddd。
U	對角核心能量函數矩陣元素（Diagonal core Hamiltonian matrix elements），每個角動量有一組數值。
Beta	非對角核心能量函數矩陣元素（Off-diagonal core

Hamiltonian parameters），每個角動量有一組數值。

DDN	雙原子中心雙電子積分多極近似的點電荷距離參數。每一筆資料的格式是 *L1*, *L2*, *Value* ，適用於涉及一個角動量為 *L1* 的基底函數與另一角動量為 *L2* 的基底函數間的電荷分佈。若所需要的參數沒有設定，會從 Zeta1C 指數計算。
KON	雙原子中心雙電子積分的 Klopman-Ohno 參數。要求的但未被設定的參數，利用將單原子中心積分的極限適配到由 Slater-Condon 參數和 Zeta1C 計算所得的單原子中心積分的方式計算，並使用設定的會預設的 DD 數值。每一筆資料的格式是 *LT*, *L1*, *L2*, *Value*，適用到角動量 *L1* 和 *L2* 函數的乘積的 *LT* 角動量分量。
CoreKO	Klopman-Ohno 參數，用在原子核吸引項，若未指定，則使用 0, 0, 0 (L=0 SS) 參數。
EHeat	孤立原子的生成熱。
EISol	孤立原子的能量。若沒有提供，則從其他參數以及這原子的標準電子組態計算。
DipHyp	雙極矩混成參數。
DCore	內層核心互斥作用參數。每一筆資料的格式是 *El*, *IType*, *Value1*, *Value2*。每一項設定目前這元素和元素 *El* 的內層核心互斥作用。*IType* 設定鍵結類型： 1 是一般 AM1，2 是 AM1 N-H 和 O-H，3 是一般 PM6，4 是 PM6 O-H，5 是 PM6 CC 三鍵，6 是 PM6 Si-O。和特定的函數形式有關，還有一個或兩個參數。

MOPAC-風格半經驗方法參數輸入。若使用 PM6=MOPACExternal 或 AM1=MOPACExternal，則要讀進一個參數輸入段落，其中的參數格式和 MOPAC 程式用關鍵字 External 所要求得參數格式相同。這格式的廣泛性不如原生的 Gaussian 格式，但包含最普遍的參數。有關細節請參考 MOPAC 文獻。這種格式採用的單位被程式 Gaussian 解讀，和被程式 MOPAC 解讀的形式相同，是原子單位和其他單位的混合。

這蛟單列出 MOPAC 外部參數標籤和原生 Gaussian 輸入參數資料格式間的對照關係：

MOPAC	**Gaussian**
USS,UPP,UDD	U
ZS,ZP,ZD	ZetaOverlap
ZSN,ZPN,ZDN	Zeta1C
BetaS,BetaP,BetaD	Beta
GSS,GPP,…,FODD,…	F0ss,F0pp, 等等†

DD2	DDN=0,1,*數值*
DD3	DDN=1,1,*數值*
DD4	DDN=0,2,*數值*
DD5	DDN=1,2,*數值*
DD6	DDN=2,2,*數值*
PO1	KON=0,0,0,*數值*
PO2	KON=1,0,1,*數值*
PO3	KON=2,1,1,*數值*
PO4	KON=2,0,2,*數值*
PO5	KON=1,1,2,*數值*
PO6	KON=2,2,2,*數值*
PO7	KON=0,1,1,*數值*
PO8	KON=0,2,2,*數值*
PO9	CoreKO
EHeat	EHeat
EISol	EISol
AlpB_NN,XFac_NN	DCore=*NN*,3,*Alpha*,*XFac*

†注意 MOPAC 的 GSP 和 GP2 是 F0sp 和 G1sp.的線性組合。Gaussian 使用標準的 Slater-Condon 命名和參數定義。

這是 Cr 的 MOPAC 外部資料格式參數，以預設的選項由程式 MOPAC 印出：

```
 PARAMETER VALUES USED IN THE CALCULATION

 NI TYPE VALUE UNIT
 24 USS -34.86433900 EV ONE-CENTER ENERGY FOR S
 24 UPP -26.97861500 EV ONE-CENTER ENERGY FOR P
 24 UDD -54.43103600 EV ONE-CENTER ENERGY FOR D
 24 ZS 3.28346000 AU ORBITAL EXPONENT FOR S
 24 ZP 1.02939400 AU ORBITAL EXPONENT FOR P
 24 ZD 1.62311900 AU ORBITAL EXPONENT FOR D
 24 BETAS -5.12261500 EV BETA PARAMETER FOR S
 24 BETAP 3.92671100 EV BETA PARAMETER FOR P
 24 BETAD -4.23055000 EV BETA PARAMETER FOR D
 24 GSS 8.85557242 EV ONE-CENTER INTEGRAL (SS,SS)
 24 GPP 5.05309383 EV ONE-CENTER INTEGRAL (PP,PP)
 24 GSP 5.58863066 EV ONE-CENTER INTEGRAL (SS,PP)
 24 GP2 4.42952965 EV ONE-CENTER INTEGRAL (PP*,PP*)
```

```
 24 HSP 0.64803936 EV ONE-CENTER INTEGRAL (SP,SP)
 24 ZSN 1.61985300 AU INTERNAL EXPONENT FOR S - (IJ,KL)
 24 ZPN 0.84826600 AU INTERNAL EXPONENT FOR P - (IJ,KL)
 24 ZDN 1.40501500 AU INTERNAL EXPONENT FOR D - (IJ,KL)
 24 F0DD 9.86923654 EV SLATER-CONDON PARAMETER F0DD
 24 F2DD 5.20966257 EV SLATER-CONDON PARAMETER F2DD
 24 F4DD 3.39760602 EV SLATER-CONDON PARAMETER F4DD
 24 F0SD 6.15013600 EV SLATER-CONDON PARAMETER F0SD
 24 G2SD 2.00030000 EV SLATER-CONDON PARAMETER G2SD
 24 F0PD 5.63536196 EV SLATER-CONDON PARAMETER F0PD
 24 F2PD 1.91648791 EV SLATER-CONDON PARAMETER F2PD
 24 G1PD 1.58022558 EV SLATER-CONDON PARAMETER G1PD
 24 G3PD 0.96233144 EV SLATER-CONDON PARAMETER G3PD
 24 DD2 0.28669123 BOHR CHARGE SEPARATION, SP, L=1
 24 DD3 2.91433601 BOHR CHARGE SEPARATION, PP, L=2
 24 DD4 1.12394737 BOHR CHARGE SEPARATION, SD, L=2
 24 DD5 0.81804068 BOHR CHARGE SEPARATION, PD, L=1
 24 DD6 1.23219554 BOHR CHARGE SEPARATION, DD, L=2
 24 PO1 1.53639890 BOHR KLOPMAN-OHNO TERM, SS, L=0
 24 PO2 0.72875078 BOHR KLOPMAN-OHNO TERM, SP, L=1
 24 PO3 1.96024483 BOHR KLOPMAN-OHNO TERM, PP, L=2
 24 PO4 0.94950312 BOHR KLOPMAN-OHNO TERM, SD, L=2
 24 PO5 1.66105265 BOHR KLOPMAN-OHNO TERM, PD, L=1
 24 PO6 1.08400979 BOHR KLOPMAN-OHNO TERM, DD, L=2
 24 PO7 1.53639890 BOHR KLOPMAN-OHNO TERM, PP, L=0
 24 PO8 1.37859617 BOHR KLOPMAN-OHNO TERM, DD, L=0
 24 PO9 1.53639890 BOHR KLOPMAN-OHNO TERM, CORE
 24 CORE 6.00000000 E CORE CHARGE
 24 EHEAT 95.00000000 KCAL/MOL HEAT OF FORMATION OF THE ATOM (EXP)
 24 EISOL -185.72482255 EV TOTAL ENERGY OF THE ATOM (CALC)
 24 ALPB_24 4.65541900 ALPB factor
 24 XFAC_24 10.31860700 XFAC factor
```

可用方法

能量，幾何優選和頻率。

程式內存以下元素的參數：

- AM1: H, Li-F, Mg-Cl, Cr, Zn, Ge, Br, Sn, I 和 Hg.
- PM3: H, Li-F, Na-Cl, K, Ca, Cr, Zn-Br, Rb, Sr, Cd-I, Cs, Ba 和 Hg-Bi.
- PM6: H-Ba 和 Lu-Bi.

相關的關鍵字

CNDO， INDO，MINDO，MINDO3

使用範例

這些計算的計算結果在輸出檔案中列印如下：

```
SCF Done: E(RAM1) = -0.185015348024 A.U. after 14 cycles          AM1
SCF Done: E(RPM3) = -0.185015348024 A.U. after 14 cycles          PM3
SCF Done: E(RPM3MM) = -0.185015348024 A.U. after 14 cycles        PM3MM
SCF Done: E(RPM6) = -0.185015348024 A.U. after 14 cycles          PM6
SCF Done: E(RPDDG) = -0.185015348024 A.U. after 14 cycles         PDDG
```

印出的能量是各半經驗方法模型計算的生成熱。

Last updated on: 2 September 2009