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Supporting Information

An Orbital-Overlap Complement to Atomic Partial Charge

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Supporting Information

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1. Atomic Overlap Distance D_A

The atomic overlap distance D_A is constructed from the electron delocalization range function EDR(**r**;d). Formally, EDR(**r**;d)=$\int d^3\mathbf{r}'\gamma(\mathbf{r},\mathbf{r}')\chi_d(\mathbf{r}-\mathbf{r}')$. Test function $\chi_d(\mathbf{r}-\mathbf{r}')=C_d \exp(-|\mathbf{r}-\mathbf{r}'|^2/d^2)$ is a single normalized orbital lobe decaying over length scale d. Reduced density matrix $\gamma(\mathbf{r},\mathbf{r}')=\Sigma_i n_i\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')$ is computed from all molecular orbitals ψ_i with nonzero occupancies n_i in the (potentially multireference) wavefunction. EDR(**r**;d) is readily obtained from standard quantum chemistry calculations, requiring only overlap integrals between the atomic orbital basis functions and s-type Gaussian functions χ_d centered at **r**.[1] D(**r**), the distance d maximizing EDR(**r**;d), provides a chemically intuitive picture of the *size of orbital lobes* at **r**: the two lobes of the H_2^+ σ* antibonding orbital each have smaller D(**r**) than the one lobe of the σ bonding orbital,[1b] and the N and P lone pair regions of an aminophosphine ligand respectively have small and large D(**r**)[1c]. Topological analysis of D(**r**) following the principles of QTAIM gives additional insights[1e]. D(**r**) extends Fukui's frontier orbital studies[2] by considering all occupied orbitals, treating reactive and nonreactive regions on an equal theoretical footing (see also Ref.[3]). D(**r**) is related to the many other interpretive tools based on the electronic kinetic energy density[4], and its projection onto χ_d recalls the DFT+U method's projection onto predefined atomic states[5]. D_A is simply defined as the atomic average of D(**r**). Of the many choices of atomic averaging, we choose the Hirshfeld scheme.[1c, 1e] We emphasize following Ref 19 that D_C measures the size of *orbital lobes*, which is distinct from the delocalization of charge or spin over multiple centers. Figure S2 below illustrates how benzene's delocalized pi orbitals are combinations of tightly bound, compact atomic orbital lobes. The EDR and D(**r**) are currently implemented in the NCIplot program package and the Gaussian 16 package.

2. Computational Methods

Calculations use the development version of the Gaussian suite of programs.[6] D_A for spin polarized systems is evaluated from the spin-dependent atomic delocalization lengths $\{D_{A\uparrow}, D_{A\downarrow}\}$ and Hirshfeld populations $\{N_{A\uparrow}, N_{A\downarrow}\}$ as $D_A = (D_{A\uparrow}N_{A\uparrow} + D_{A\downarrow}N_{A\downarrow})/(N_{A\uparrow}+N_{A\downarrow})$. Unless noted otherwise, all calculations use spin-unrestricted density functional theory (DFT) Calculations on organic molecules use the 6-31+G(d,p) atom-centered basis set and the long-range-corrected Becke-Lee-Yang-Parr (LC-BLYP) functional appropriate for anions.[7] Calculations on alkenyl anions in Figure 3 use a continuum model[8] for 2-propanol solvent. The table in Figure 3 approximates $K_{eq}=\exp(-\Delta E/RT)$ at T=298 K, using ΔE taken directly from DFT calculations. No zero-point, thermal, or entropic corrections are included. Calculations on gold clusters in Figure 4 use the Perdew-Wang 1991 (PW91)[9] GGA, the def2-TZVP relativistic effective core potential and associated basis sets,

and geometries optimized with PW91 and the LANL2DZ relativistic effective core potential and associated basis sets.[10] Calculations on the clusters in point (f) use PW91/LANL2DZ DFT with geometries constrained to icosahedral symmstry and atom-atom distances Cu=2.56, Ag=2.89, Au=2.88 Angstrom taken from the bulk metals. Large molecules **197**-**199** are simulated with the 6-31G basis set. The former two are modeled as the central carbon of finite, hydrogen-terminated clusters $C_{35}H_{36}$ and $C_{54}H_{18}$. The partial charges of molecules **193**-**194** are obtained using natural bond order charges, following Refs. [11]

3. Method and Basis Dependence

Table S3 shows the method dependence of D_C and Q_C for small organic molecules methane, ethylene, benzene, and buta-1,3-diene. Results are shown for Hartree-Fock theory, CCSD (evaluated using response density matrices with the Z-vector method, Gaussian keyword "Density=Current"), and DFT with various functionals. For these "normal" molecules, atomic charge and overlap distance are both relatively invariant to the level of theory. QC varies by up to around 0.05e in methane, and is rather more stable in other molecules. DC varies by around 0.02 bohr. Table S4 shows the basis set dependence of LC-BLYP DC and QC for the moelcules in Table S3. Again, for these "normal" organic molecules, both quantities are quite stable with respect to basis set. DC in particular changes by <0.01 bohr between 6-31+G(d,p) and aug-cc-pVQZ basis sets.

4. Additional Studies of Alkynyl Benzamide Cyclization

Figure 2 shows how the atomic overlap distance D_H of the $R=CH_3$ group changes upon Z-E tautomerization. Additional evidence for interaction between the $R=CH_3$ group and the alkenyl anion comes from analyzing the computed geometries and bond orders. The LC-BLYP/6-31+G(d,p)/(2-propanal continuum solvent) R=CH3 C-H bonds closest to the anion slightly lenghen from 1.091 Angstrom in the Z form to 1.092 Angstrom in the E form, and hinting at a tiny amount of charge transfer to the $R=CH_3$. This effect is much larger for the more polarized $R=CHF_2$ group shown in Figure 2: Z→E tautomerization increases the $R=CHF_2$ group's D_H from 1.83 bohr to 1.90 bohr, increases the CF_2-H bond length from 1.086 Angstrom to 1.090 Angstrom, and decreases the CF_2-H Wiberg bond order from 0.89 to 0.87. Similar effects are seen for the $R=C^{\alpha}H_2C^{\beta}H_2NMe_2$ seen experimentally to increase E-5-exo yields: Z→E tautomerization increases the Cα-H bond length from 1.088 to 1.090 Angstrom. It is worth noting that the Z-5-exo form has a CH-pi interaction between the pendant aryl and the R group. Removing this interaction would further increase Z→E tautomerization.

5. Figures and Tables

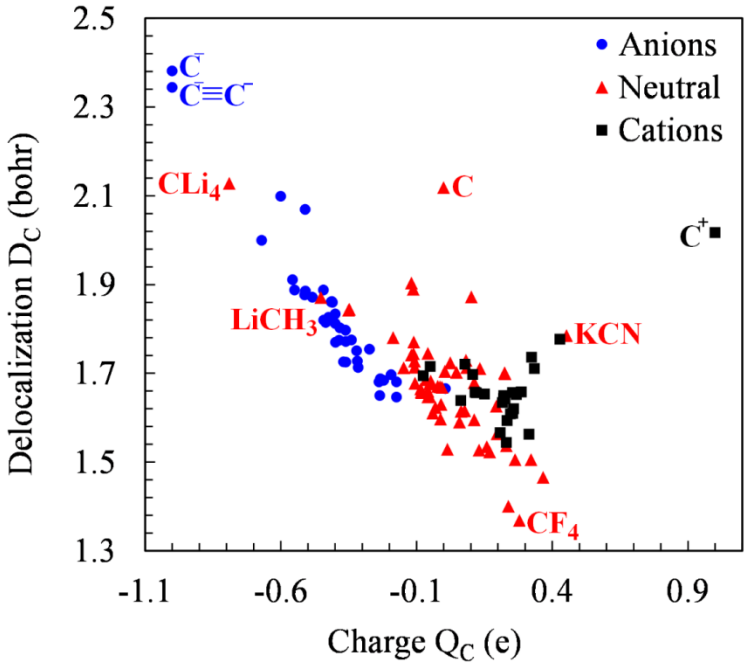

Figure S1. Relation between D_C and Q_C for the organic molecules in Table S1. Chemically interesting outliers are labeled.

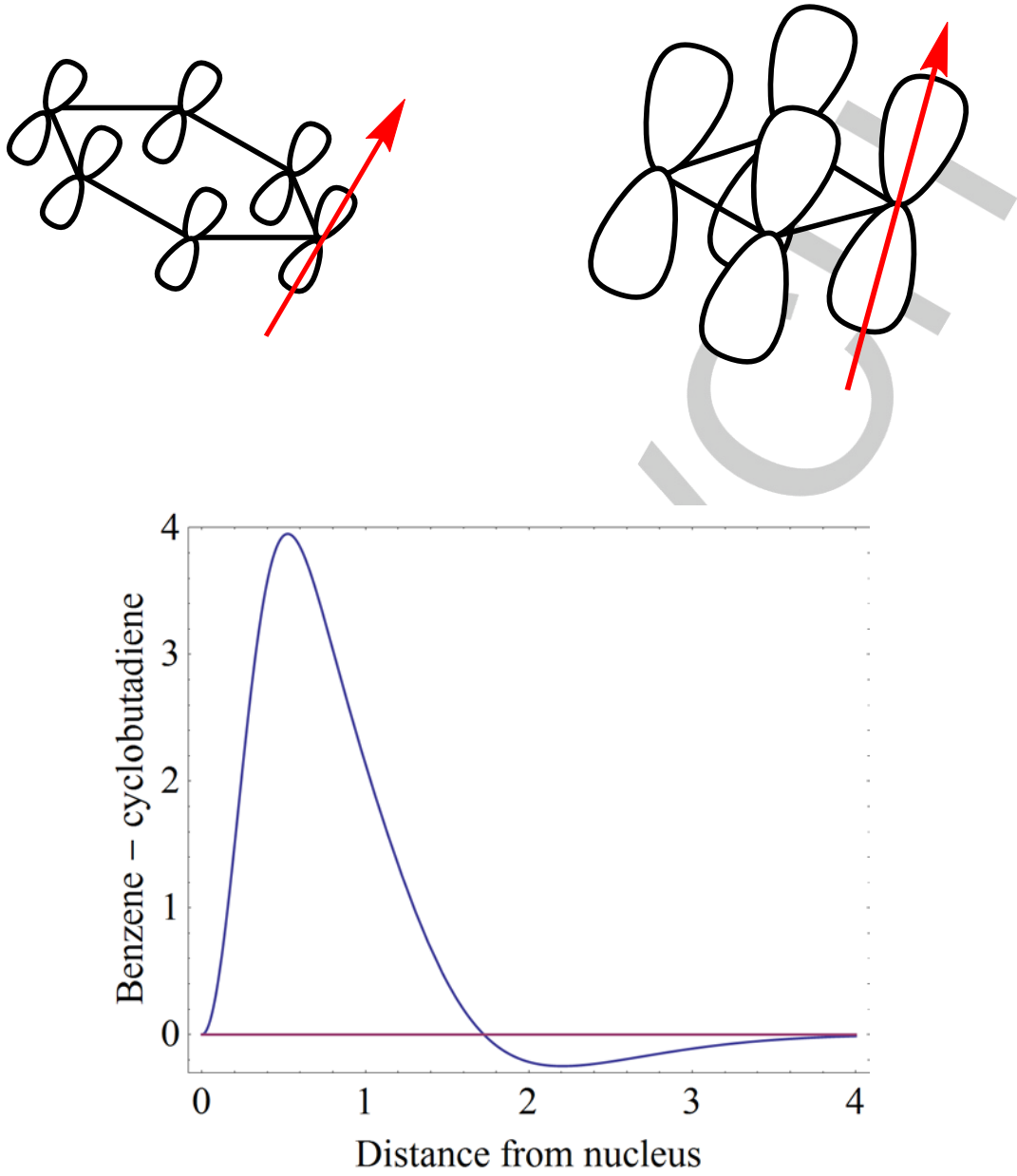

Figure S2. (Top) Exaggerated cartoon of pi orbital lobe size in aromatic benzene vs. anti-aromatic cyclobutadiene. Benzene's delocalized pi orbitals are linear combinations of tight, compact orbital lobes; while cyclobutadiene's pi orbitals are linear combinations of diffuse, weakly bound orbital lobes. (Bottom) Difference between the computed pi-electron densities of benzene and cyclobutadiene, plotted along the z axis (red arrows) in the top figure. Benzene's pi electrons are held closer to the nucleus, consistent with smaller orbital lobes and with the smaller D_C in Figure 1. Calculations plot $\Sigma_{\mu\nu}P_{\mu\nu}\chi_\mu(z)\chi_\nu(z)/\Sigma_{\mu\nu}P_{\mu\nu}S_{\mu\nu}$, where S is the atomic orbital overlap and functions μ,ν are p_z-type Gaussian atomic orbitals centered on carbon atom 1. This corrects for the slightly different normalizations of the partial trace over a single atom's p_z atomic orbitals.

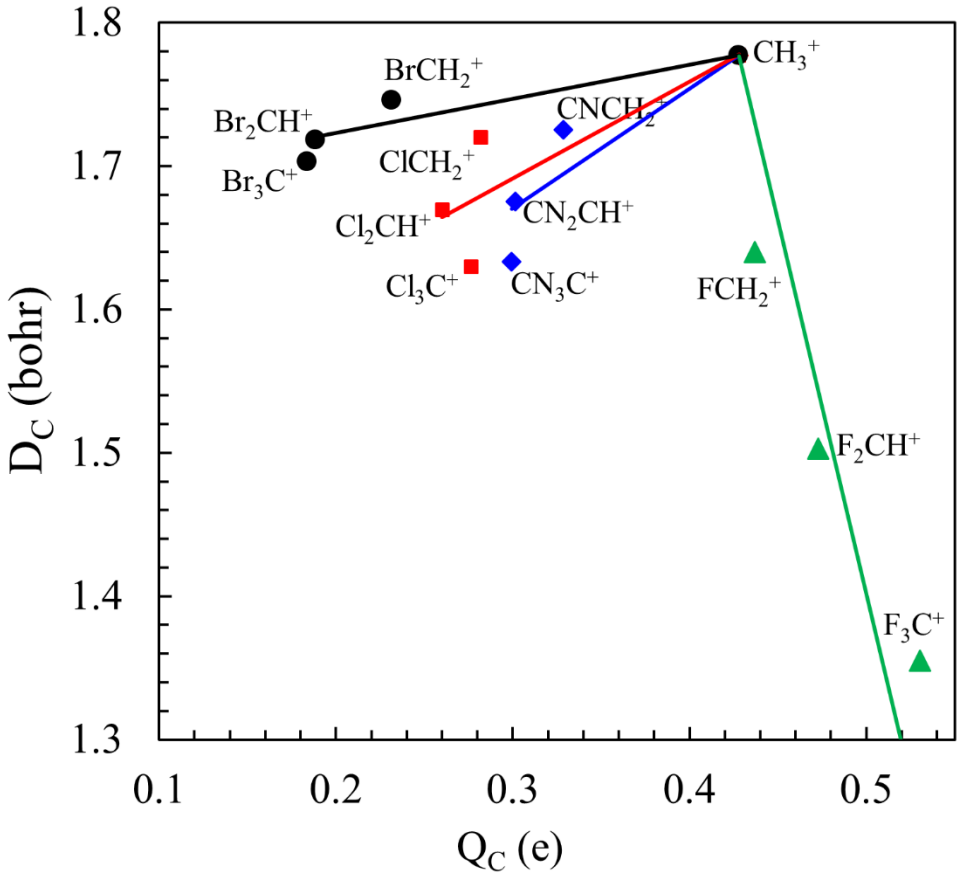

Figure S3. Charge vs. overlap distance of the central carbon in $[CH_nR_{3-n}]^+$, R=Cl, F, Br, CN.

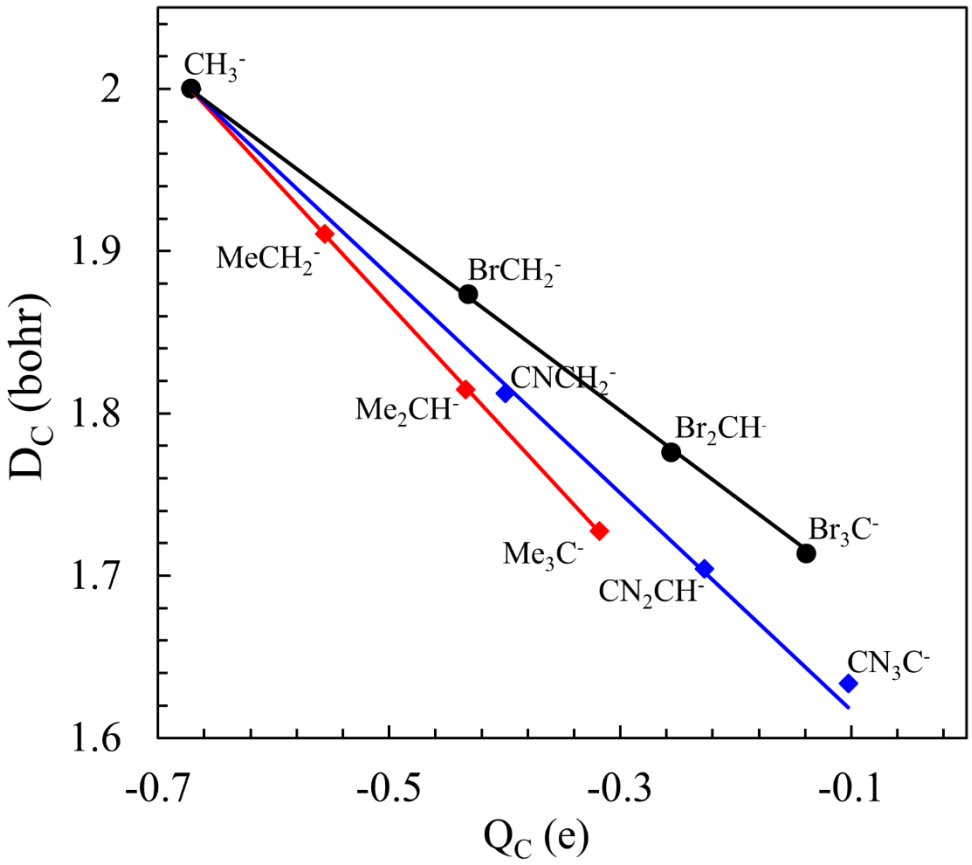

Figure S4. Charge vs. overlap distance of the central carbon in $[CH_nR_{3-n}]^-$, R=Me, Br, CN.

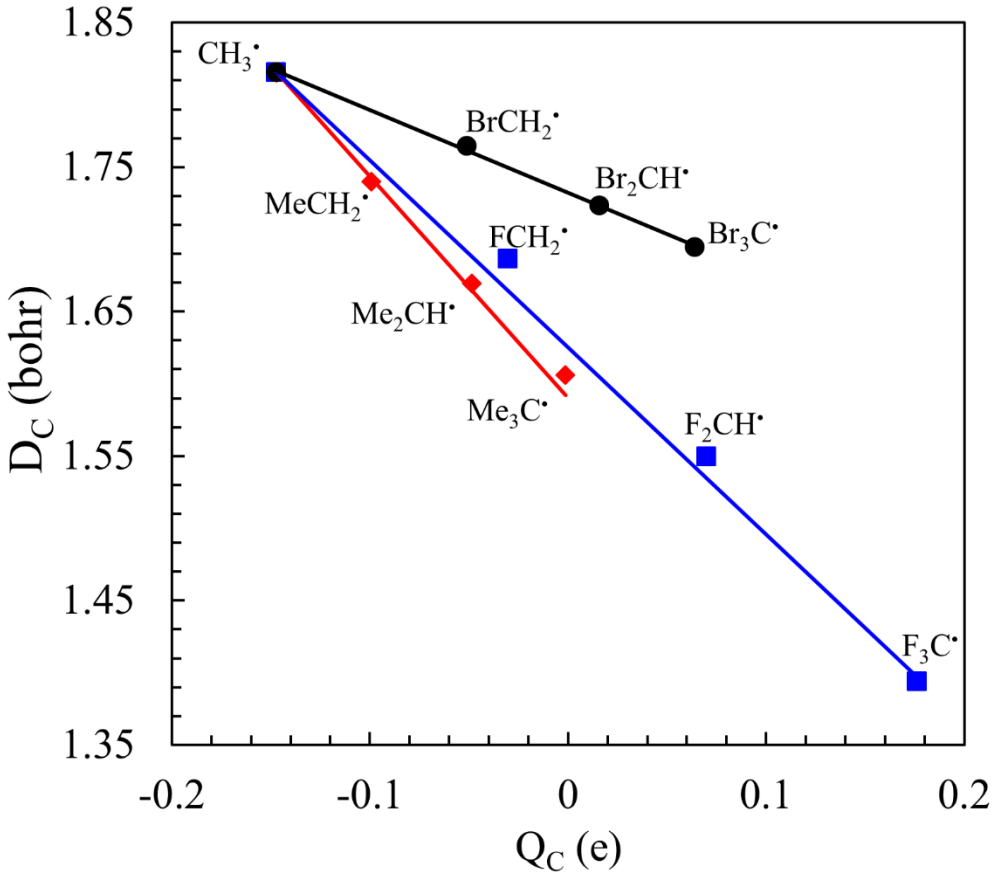

Figure S5. Charge vs. overlap distance of the central carbon in $[CH_nR_{3-n}]^{\bullet}$, R=Me, Br, F.

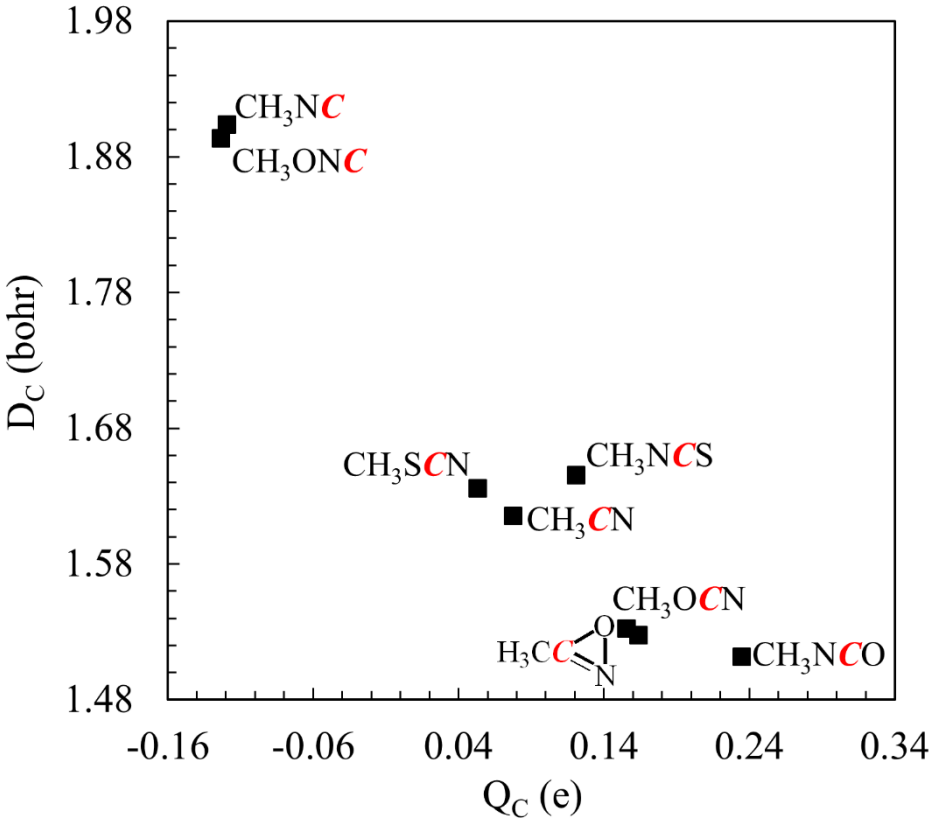

Figure S6. Trend in atomic overlap distance and charge on carbon atom in different positional isomers highlighting their relative stability and reactivity.

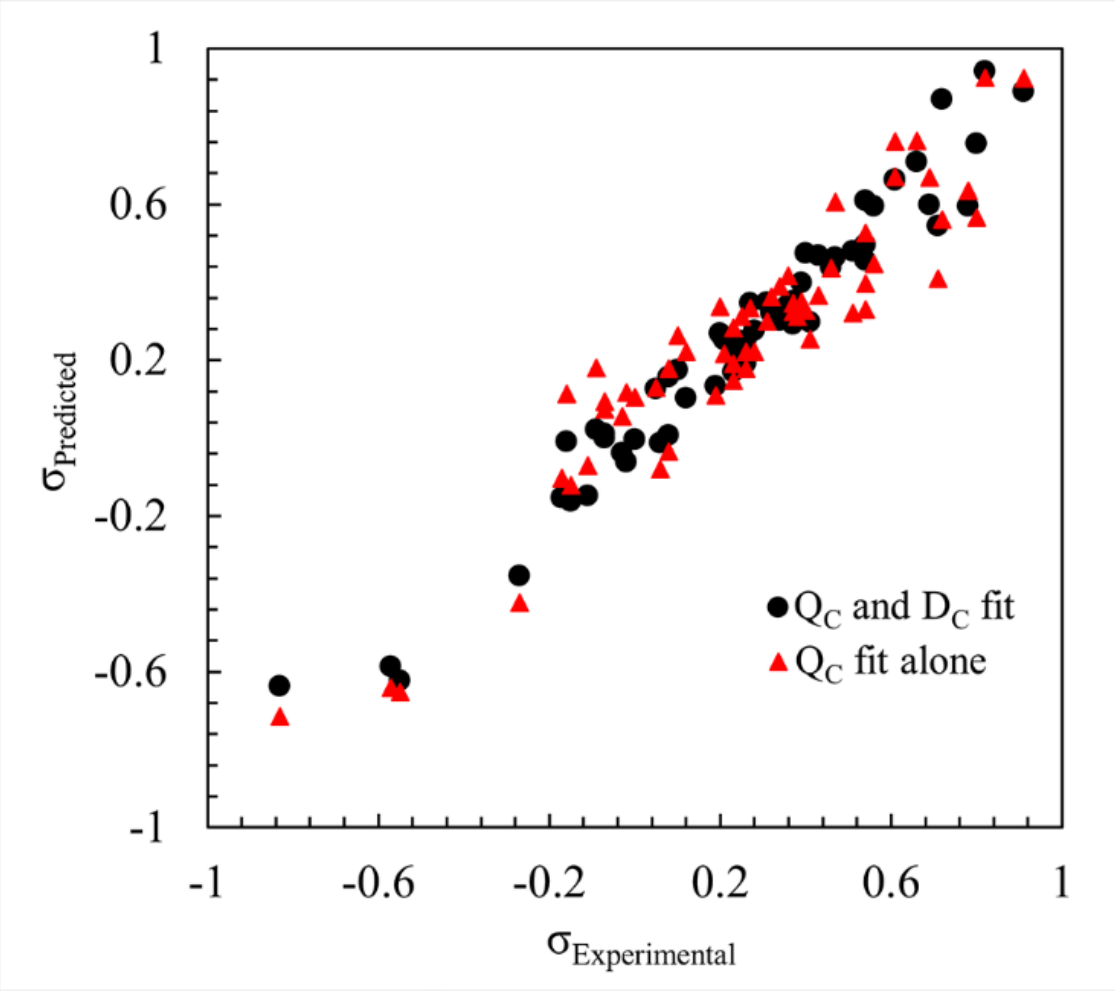

Figure S7. Correlation between experimental Hammett substituent effects at meta and para positions of 30 monosubstituted benzenes, and values fit to Eq. 1 (black circles). Fitting to Q_C alone (red triangles) reduces the agreement with experiment.

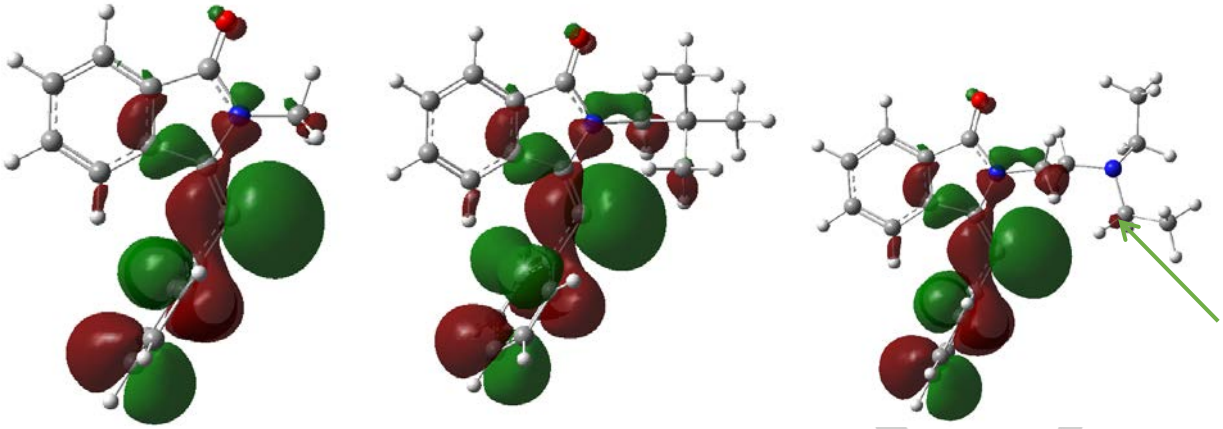

Figure S8. Predicted geometries and HOMO for E-5-exo anions of Figure 3, with substituents X=H (left), X=tBu (center), X=CH_2NEt_2 (right). The CH_2NEt_2 nitrogen lone pair faces away from the carbanion, and the electronegative nitrogen polarizes the adjacent CH bonds enhancing their interaction with the carbanion (arrow).

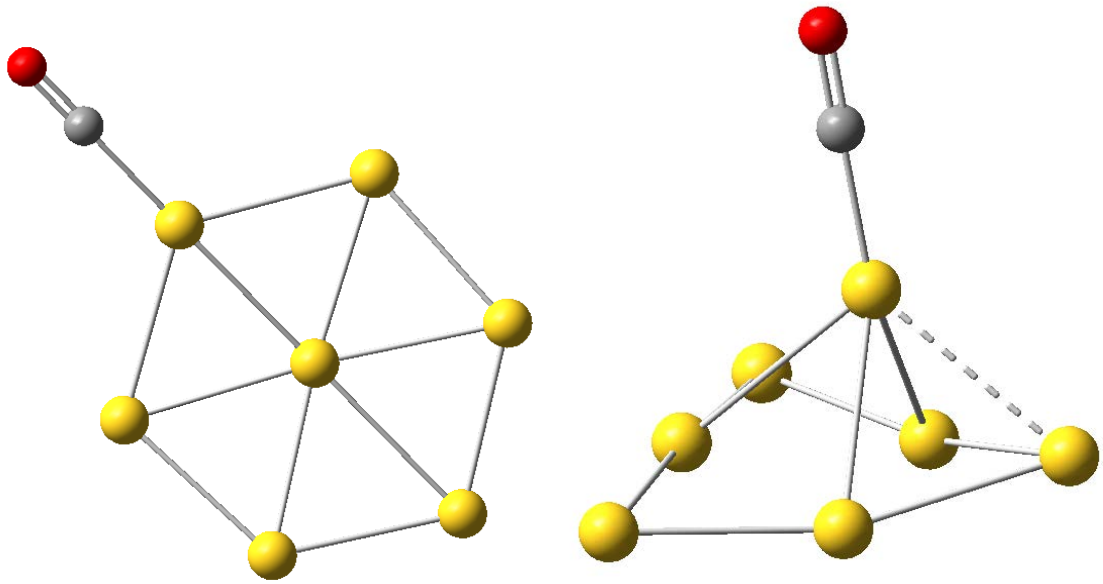

Figure S9 Predicted geometries for CO chemisorption to edge (left) and central (right) atoms of Au_7^+. Chemisorption to the unstable central atom (Figure 4) leads to significant structural rearrangement and a structure 10 kcal/mol more stable than edge chemisorption.

Table S1: Studied chemical system with Charge Q_C and overlap distance D_C.

Sr. #	Structure	Name	Q_C (e)	D_c (bohr)
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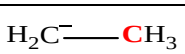
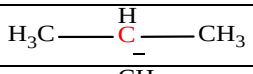
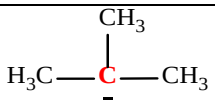
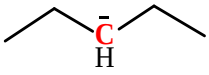
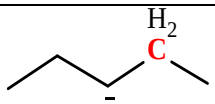
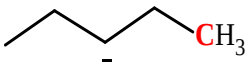
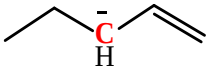
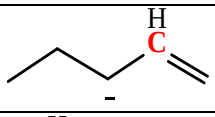
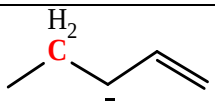
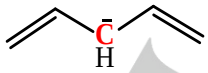
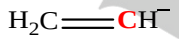
2		Methanide	-0.671	2.000
3		Ethanide	-0.556	1.911
			-0.205	1.766
4		Propan-2-ide	-0.434	1.815
5		2-methylpropan-2-ide	-0.318	1.727
6		pentan-3-ide	-0.385	1.774
			-0.124	1.688
			-0.160	1.736
7		pent-1-en-3-ide	-0.233	1.687
			-0.120	1.699
			-0.106	1.680
8		penta-1,4-dien-3-ide	0.006	1.666
9		ethenide	-0.509	1.885
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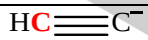
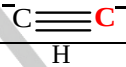
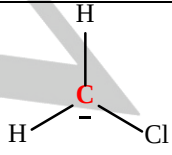
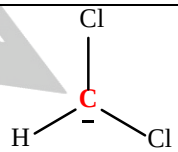
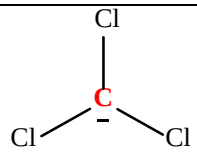
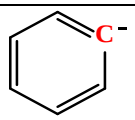
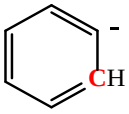
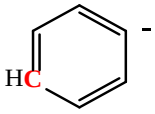
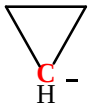
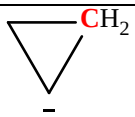
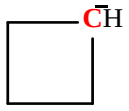
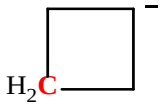
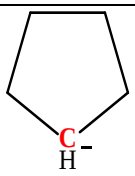
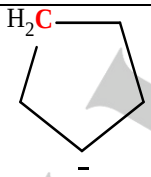
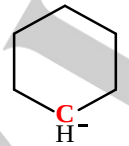
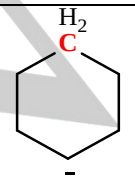
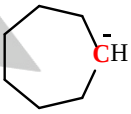
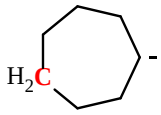
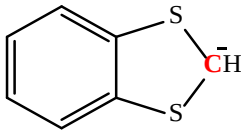
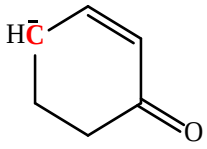
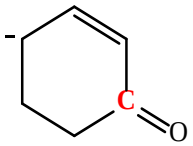
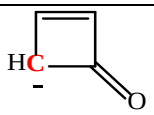
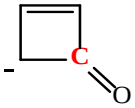
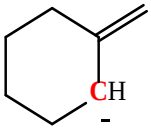
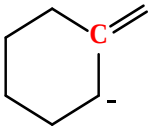
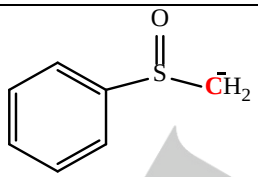
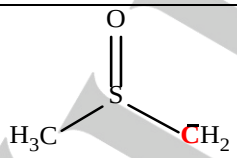
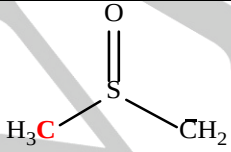
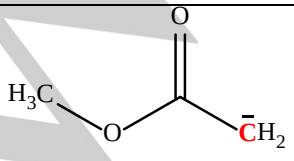
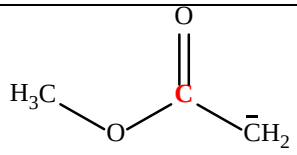
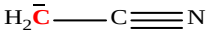
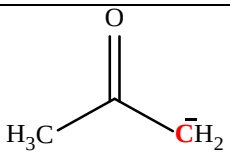
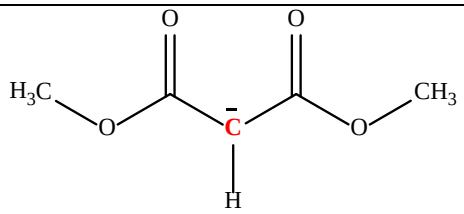
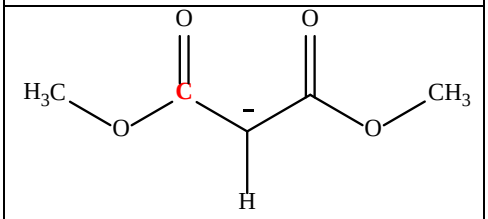
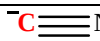
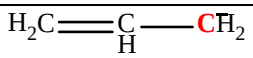
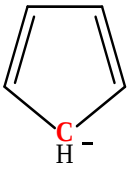
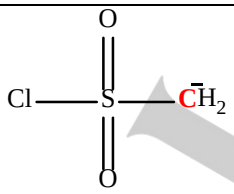
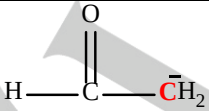
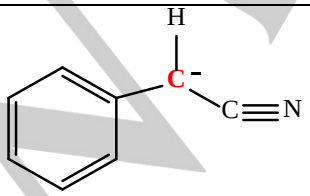
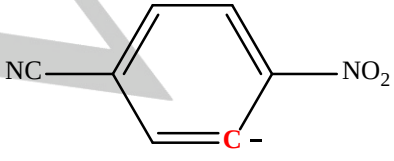
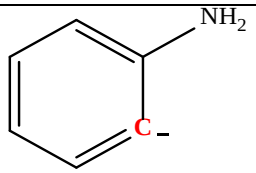
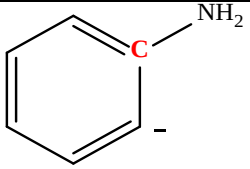
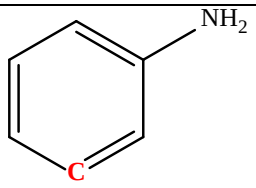
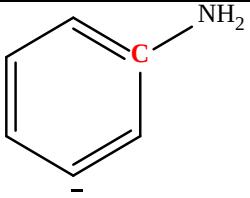
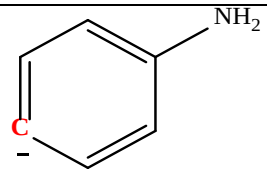
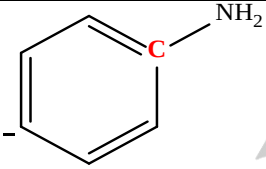
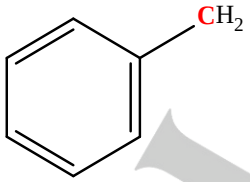
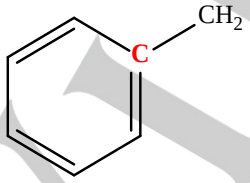
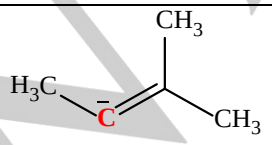
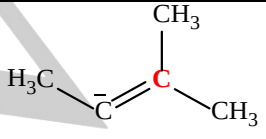
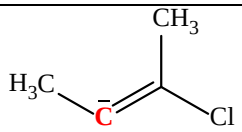
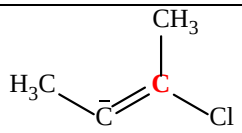
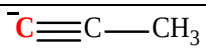
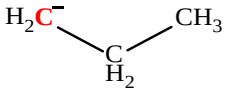
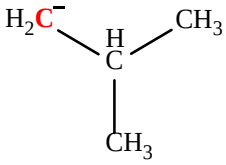
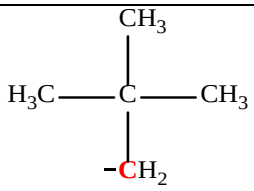
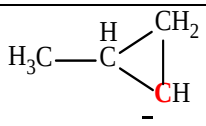
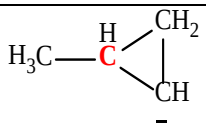
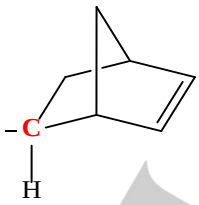
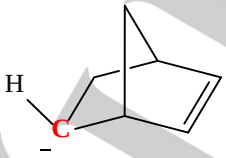
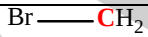
			-0.405	1.857
11		ethyne-1,2-diide	-1.000	2.344
12		chloromethanide	-0.484	1.871
13		dichloromethanide	-0.321	1.750

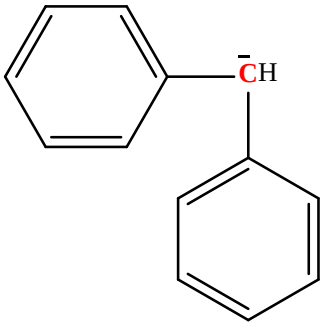
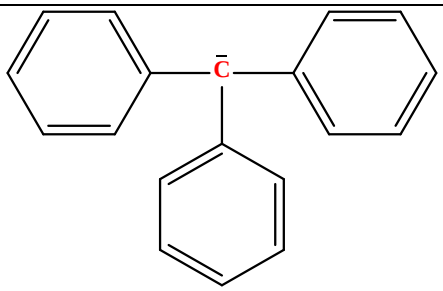
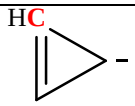
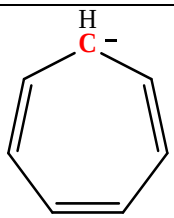
14		Chloroform (anion)	-0.174	1.646
15		benzen-1-ide	-0.411	1.861
			-0.138	1.697
			-0.127	1.675
16		cyclopropanide	-0.512	1.877
			-0.192	1.716
17		cyclobutanide	-0.442	1.820
			-0.123	1.684
18		cyclopentanide	-0.369	1.726
			-0.104	1.669
19		cyclohexanide	-0.360	1.725
			-0.092	1.667
20		cycloheptanide	-0.398	1.770

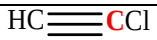
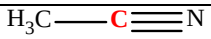
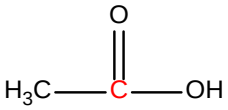
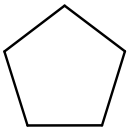
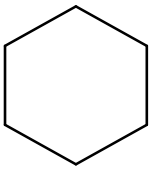
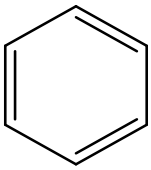
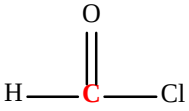
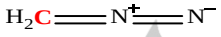
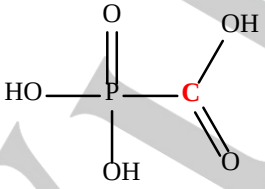
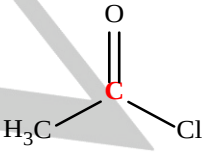
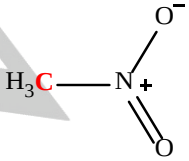
			-0.091	1.667
21		benzo[d][1,3]dithiol-2-ide	-0.443	1.888
22		4-oxocyclohex-2-en-1-ide	-0.174	1.681
			0.060	1.571
23		4-oxocyclobut-2-en-1-ide	-0.315	1.713
			0.072	1.588
24		2-methylenecyclohexan-1-ide	-0.238	1.680
			-0.057	1.630
25		(phenylsulfinyl)methanide	-0.383	1.802
26		(methylsulfinyl)methanide	-0.424	1.826
			-0.158	1.739
27		2-methoxy-2-oxoethan-1-ide	-0.361	1.771

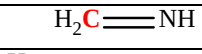
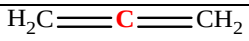
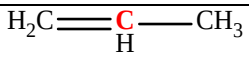
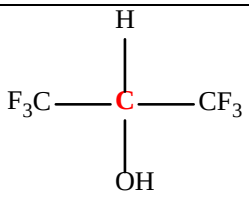
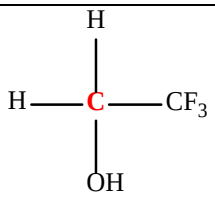
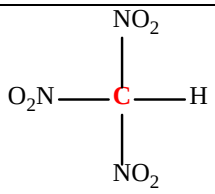
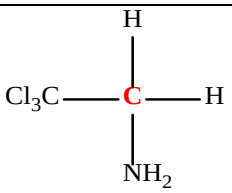
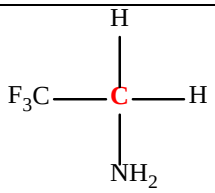
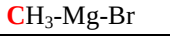
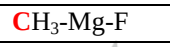
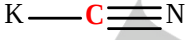
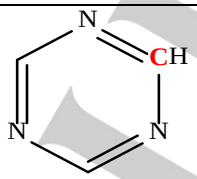
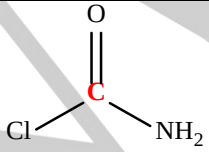
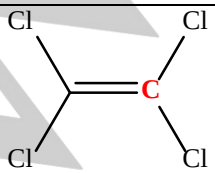
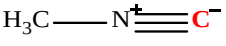
			0.091	1.550
28		cyanomethanide	-0.400	1.812
29		2-oxopropan-1-ide	-0.340	1.775
30		1,3-dimethoxy-1,3-dioxopropan-2-ide	-0.235	1.650
			0.154	1.526
31		cyanide	-0.510	2.069
32		prop-2-en-1-ide	-0.362	1.797
33		cyclopenta-2,4-dien-1-ide	-0.193	1.697
34		(chlorosulfonyl)methanide	-0.273	1.754
35		2-oxoethan-1-ide	-0.550	1.888
36		cyano(phenyl)methanide	-0.221	1.684
37		5-cyano-2-nitrobenzen-1-ide	-0.339	1.813

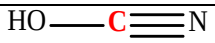
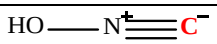
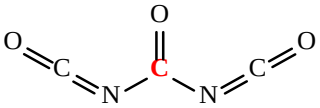
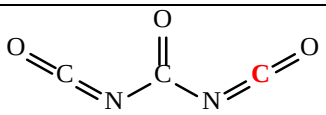
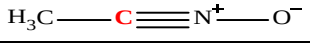
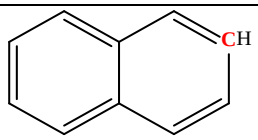
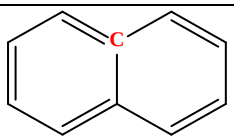
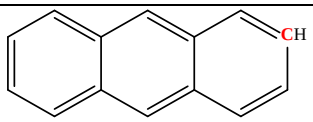
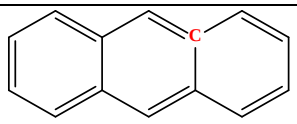
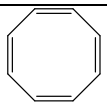
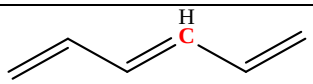
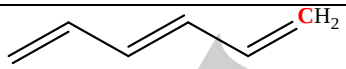
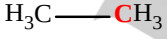
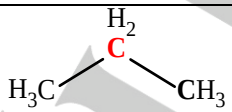
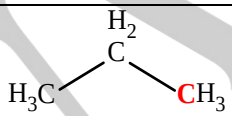
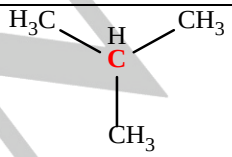
38		2-aminobenzen-1-ide	-0.399	1.834
			-0.015	1.603
39		3-aminobenzen-1-ide	-0.410	1.860
			-0.005	1.585
40		4-aminobenzen-1-ide	-0.415	1.861
			-0.018	1.5824
41		phenylmethanide	-0.474	1.831
			-0.016	1.634
42		3-methylbut-2-en-2-ide	-0.412	1.851
			-0.124	1.638

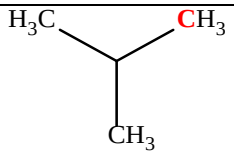
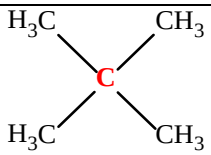
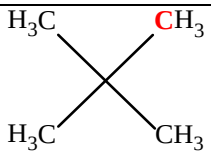
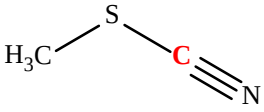
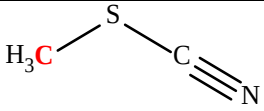
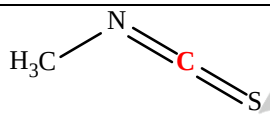
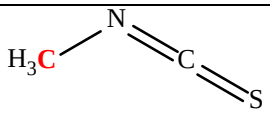
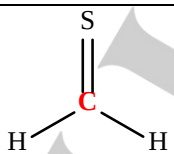
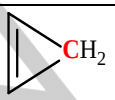
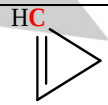
43		(E)-3-chlorobut-2-en-2-ide	-0.362	1.802
		(E)-3-chlorobut-2-en-2-ide	-0.064	1.659
44		prop-1-yn-1-ide	-0.629	2.081
45		propan-1-ide	-0.528	1.892
46		2-methylpropan-1-ide	-0.510	1.879
47		2,2-dimethylpropan-1-ide	-0.491	1.865
48		2-methylcyclopropan-1-ide	-0.481	1.860
			-0.118	1.646
49		endo-5H-norborborneide	-0.410	1.799
50		exo-5H-norborborneide	-0.436	1.817
51		bromomethanide	-0.431	1.873
52		floromethanide	-0.535	1.875

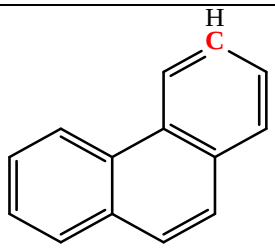
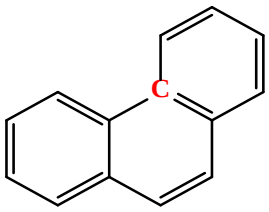
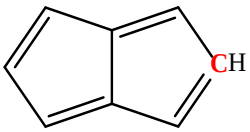
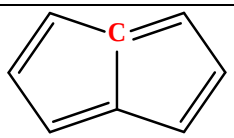
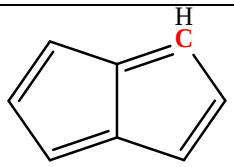
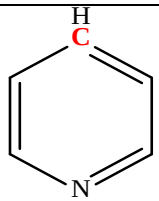
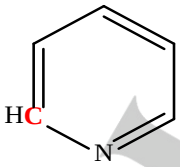
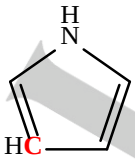
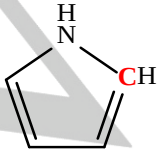
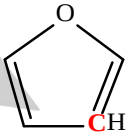
53		Diphenylmethanide	-0.200	1.662
54		Triphenylmethanide	-0.132	1.596
55		cycloprop-2-en-1-ide	-0.562	1.943
			-0.191	1.741
56		Cycloheptariene-1-ide	-0.261	1.733
57	C	Carbon	0.000	2.118
58	CLi_4	CLi4	-0.790	2.128
59	CH_4	methane	-0.186	1.780
60	CH_3Br	bromomethane	-0.058	1.745
61	CH_2Br_2	dibromomethane	0.025	1.723
62	$CHBr_3$	bromoform	0.085	1.713
63	CBr_4	carbontetrabromide	0.133	1.711
64	CF_4	carbontetrafloride	0.280	1.369
65	CO_2	carbon dioxide	0.367	1.465
66	CH_3OH	methanol	-0.048	1.682
67	$LiCH_3$	methyllithium	-0.452	1.871
68	CS_2	Carbondisulfide	0.082	1.729
69	HCN	hydrogen cyanide	0.047	1.702
70	H_3C-SH	methanethiol	-0.119	1.742
71	$H_2C=CH_2$	ethene	-0.111	1.744
72	$H_2C=\underset{H}{C}-Cl$	chloroethene	-0.108	1.728
73	$Cl-\underset{H}{C}=\underset{H}{C}-Cl$	1,2-dichloroethene	-0.013	1.670
74	$H_2C=CCl_2$	1,1-dichloroethene	-0.106	1.714
75	$HC\equiv CH$	ethyne	-0.110	1.771

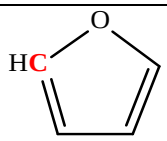
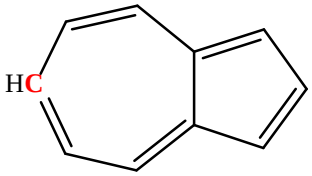
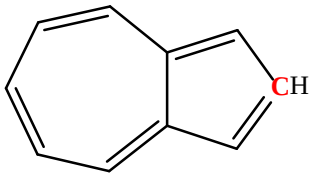
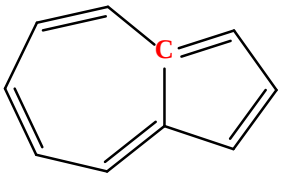
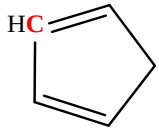
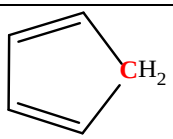
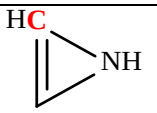
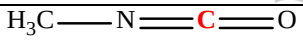
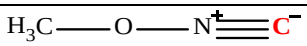
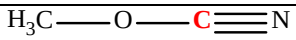
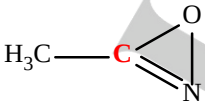
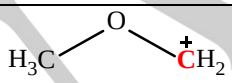
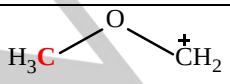
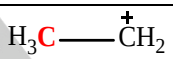
76		chloroethyne	-0.022	1.671
77		acetonitrile	0.078	1.615
78		acetic acid	0.226	1.699
79		cyclopropane	-0.106	1.677
80		cyclobutane	-0.085	1.665
81		cyclopentane	-0.083	1.658
82		cyclohexane	-0.081	1.657
83		benzene	-0.058	1.660
84		cyclobuta-1,3-diene	-0.064	1.686
85	CO	carbon monoxide	0.102	1.872
86	HCOOH	Formic acid	0.197	1.564
87	HCOH	formaldehyde	0.113	1.679
88		formyl chloride	0.194	1.626
89		diazomethane	-0.147	1.712
90		trifluoro(nitroso)methane	0.238	1.400
91		phosphonoformic acid	0.170	1.523
92		acetyl chloride	0.224	1.701
93		nitromethane	-0.045	1.678

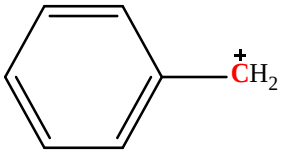
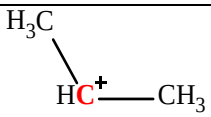
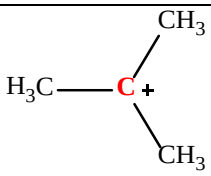
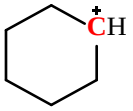
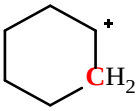
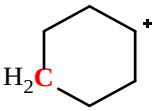
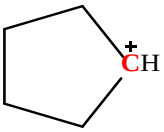
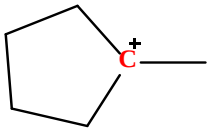
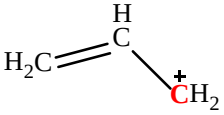
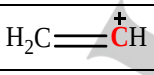
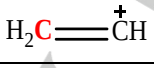
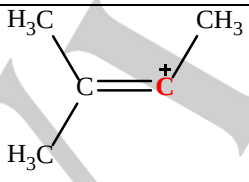
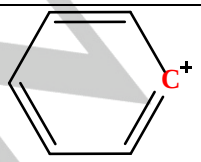
94		methanimine	0.004	1.704
95		propa-1,2-diene	-0.006	1.669
96		prop-1-ene	-0.053	1.676
97		1,1,1,3,3,3-hexafluoropropan-2-ol	0.014	1.528
98		2,2,2-trifluoroethan-1-ol	-0.012	1.597
99		trinitromethane	0.131	1.527
100		2,2,2-trichloroethan-1-amine	-0.030	1.623
101		2,2,2-trifluoroethan-1-amine	-0.040	1.610
102		methylmagnesium bromide	-0.350	1.842
103		methylmagnesium fluoride	-0.347	1.844
104		cyanopotassium	0.453	1.785
105		1,3,5-triazine	0.113	1.595
106		carbamic chloride	0.231	1.537
107		perchloroethene	0.064	1.614
108		isocyanomethane	-0.119	1.903

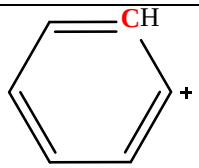
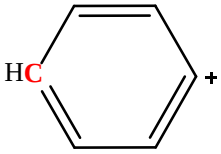
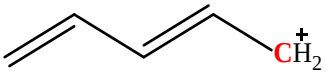
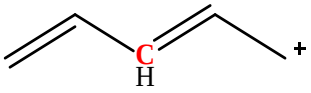
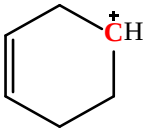
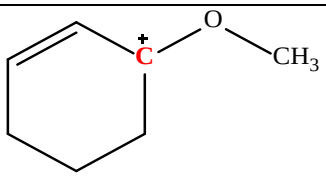
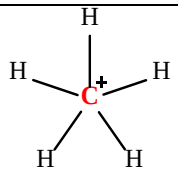
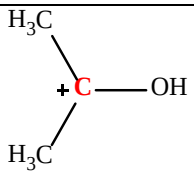
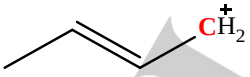
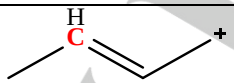
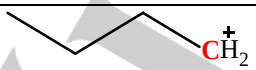
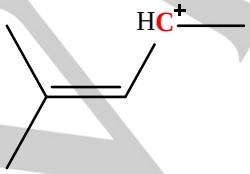
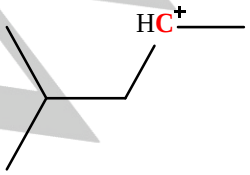
109		cyanic acid	0.159	1.534
110		fulminic acid	-0.112	1.889
111		carbonyl diisocyanate	0.264	1.505
112		carbonyl diisocyanate	0.322	1.505
113	o-carborane	o-carborane	-0.009	1.630
114	m-carborane	m-carborane	-0.058	1.647
115	p-carborane	p-carborane	-0.053	1.649
116		Acetonitrile oxide	0.058	1.590
117		Naphthalene	-0.059	1.660
			-0.004	1.587
118		Anthracene	-0.060	1.660
			-0.005	1.587
119		Cyclooctatetraene	-0.051	1.673
120		1,3,5-hexatriene	-0.055	1.671
			-0.115	1.736
121		Ethane	-0.129	1.719
122		Propane	-0.078	1.664
			-0.129	1.714
123		Isobutane	-0.034	1.615

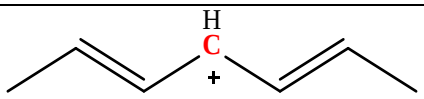
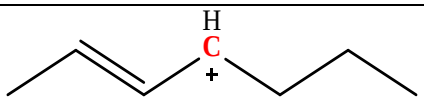
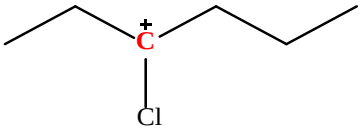
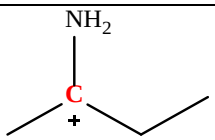
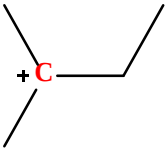
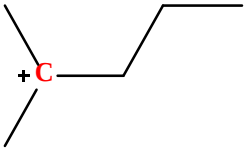
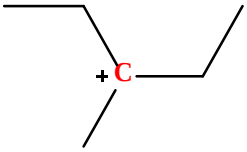
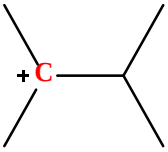
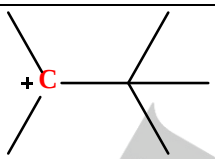
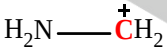
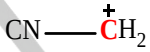
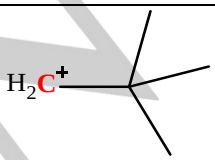
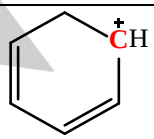
			-0.129	1.709
124		Neopentane	0.006	1.573
			-0.128	1.704
125	CH_3-Ph	Toulene	-0.122	1.712
126	CH_2-Ph_2	Diphenylmethane	-0.069	1.652
127	CH-Ph_3	Triphenylmethane	-0.021	1.602
128	CHCl-Ph_2	(chloromethylene)dibenzene	0.035	1.622
129	CH_3F	Floromethane	-0.028	1.670
130	CH_2F_2	Diflouromethane	0.095	1.568
131	CHF_3	Triflouromethane	0.192	1.469
132		thiocyanatomethane	0.054	1.635
			-0.099	1.733
133		isothiocyanatomethane	0.121	1.645
			-0.024	1.694
134		methanethial	-0.024	1.771
135		methanamine	-0.079	1.698
136		Cyclopropene	-0.111	1.697
			-0.065	1.685

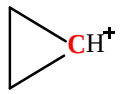
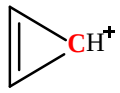
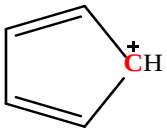
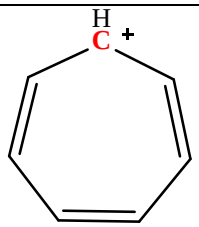
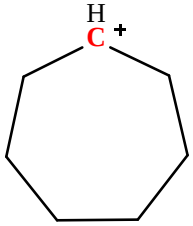
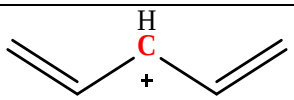
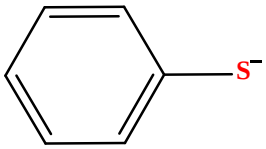
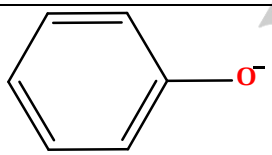
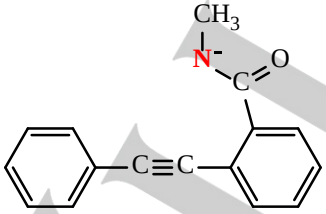
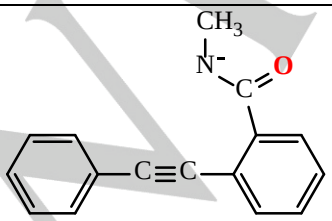
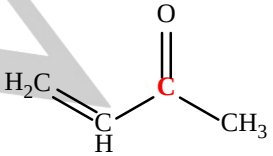
137		Phenanthrene	0.000	1.659
			-0.006	1.587
138		pentalene	-0.065	1.670
			-0.029	1.582
			-0.035	1.669
139		pyridine	-0.035	1.658
			0.016	1.628
140		pyrrole	-0.110	1.665
			-0.044	1.636
141		furan	-0.097	1.660

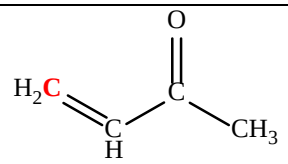
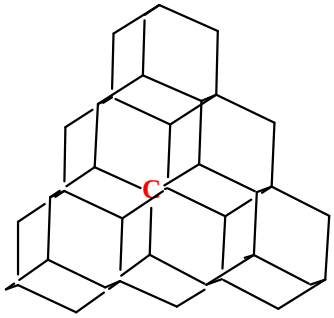
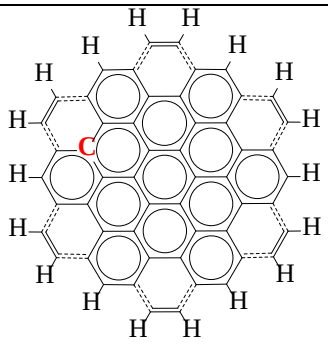
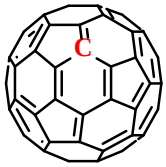
			0.004	1.618
142		Azulene	-0.029	1.660
			-0.061	1.667
			-0.010	1.591
143		Cyclopentadiene	-0.072	1.667
			-0.078	1.659
144		1H-azirine	-0.02	1.670
145		isocyanatomethane	0.235	1.511
146		(isocyanooxy)methane	-0.123	1.893
147		cyanatomethane	0.156	1.532
148		3-methyl-1,2-oxazirene	0.164	1.527
149	C+	Carbon-cation	1.000	2.017
150	CH3	methylium	0.428	1.777
151		methoxymethylium	0.286	1.658
			0.06	1.687
152		ethylium	0.106	1.697
			0.105	1.697

153		phenylmethylium	0.335	1.711
154		propan-2-ylium	0.254	1.657
155		2-methylpropan-2-ylium	0.254	1.610
156		cyclohexylium	0.227	1.644
			-0.033	1.636
			-0.068	1.647
157		cyclopentylium	0.227	1.645
158		methylcyclopentan-1-ylium	0.234	1.594
159		allylium	0.268	1.652
160		ethylium	0.324	1.736
			0.324	1.736
161		3-methylbut-2-en-2-ylium	0.217	1.634
162		benzene-1-ylium	0.257	1.620

			0.021	1.653
			-0.006	1.653
163		(E)-penta-2,4-dien-1-ylium	0.079	1.721
			0.135	1.658
164		cyclohex-3-en-1-ylium	0.221	1.643
165		1-methoxycyclohex-2-en-1-ylium	0.231	1.545
166		carbonium	-0.050	1.716
167		2-hydroxypropan-2-ylium	0.314	1.563
168		(E)-but-2-en-1-ylium	-0.076	1.695
			0.181	1.658
169		butan-1-ylium	0.221	1.650
170		4-methylpent-3-en-2-ylium	0.120	1.656
171		4-methylpentan-2-ylium	0.063	1.639

172		(2E,5E)-hepta-2,5-dien-4-ylium	0.115	1.657
173		(E)-hept-2-en-4-ylium	0.150	1.654
174		3-chlorohexan-3-ylium	0.247	1.609
175		butan-2-iminium	0.209	1.567
176		2-methylbutan-2-ylium	0.242	1.603
177		2-methylpentan-2-ylium	0.241	1.604
178		3-methylpentan-3-ylium	0.234	1.598
179		2,3-dimethylbutan-2-ylium	0.236	1.601
180		2,3,3-trimethylbutan-2-ylium	0.233	1.595
181		methaniminium	0.210	1.673
182		hydroxymethylium	0.338	1.661
183		flouromethylium	0.437	1.640
184		isocyanomethylium	0.328	1.725
185		2,2-dimethylpropan-1-ylium	0.330	1.725
186		cyclohexa-2,4-dien-1-ylium	0.111	1.654

187		cyclopropylium	0.000	1.650
188		cycloprop-2-en-1-ylium	0.156	1.659
189		cyclopenta-2,4-dien-1-ylium	0.230	1.662
190		cyclohepta-2,4,6-trien-1-ylium	-0.011	1.598
191		cycloheptylium	0.148	1.631
192		penta-1,4-dien-3-ylium	0.149	1.656
193		PhS^-	-0.561	2.028
194		PhO^-	-0.817	1.364
195		Deprotonated o-alkynylbenzamide	-0.364	1.198
			-0.478	1.108
196		Butenone	0.173	1.179

			-0.071	1.303
197		Diamond cluster model*	-0.003	1.54
198		Graphene cluster model*	-0.002	1.587
199		C_{60}*	0.00	1.597

* 6-31G basis

Table S2. Calculated D_C, Q_C and experimental Hammett parameters for selected benzene derivatives

Substituent	Position	Q_C	D_C	Hammett constants (σ)
Br	Meta	-0.0495	1.6572	0.39
	Para	-0.0550	1.6581	0.23
Cl	Meta	-0.0496	1.6577	0.37
	Para	-0.0565	1.6582	0.23
F	Meta	-0.0481	1.6588	0.34
	Para	-0.0644	1.6584	0.06
SO_2F	Meta	-0.0420	1.6547	0.8
	Para	-0.0296	1.6563	0.91
SiF_3	Meta	-0.0502	1.6563	0.54
	Para	-0.0384	1.6576	0.69
NO_2	Meta	-0.0474	1.6559	0.71
	Para	-0.0396	1.6573	0.78
N_3	Meta	-0.0504	1.6583	0.37
	Para	-0.0628	1.6586	0.08
H	Meta	-0.0580	1.6600	0
	Para	-0.0580	1.6600	0
$NHNH_2$	Meta	-0.0575	1.6608	-0.02
	Para	-0.0842	1.6609	-0.55
SiH_3	Meta	-0.0571	1.6586	0.05
	Para	-0.0525	1.6592	0.1
COCl	Meta	-0.0505	1.6559	0.51
	Para	-0.0352	1.6576	0.61
CCl_3	Meta	-0.0503	1.6560	0.4
	Para	-0.0465	1.6575	0.46
CF_3	Meta	-0.0489	1.6565	0.43
	Para	-0.0434	1.6576	0.54
CN	Meta	-0.0461	1.6556	0.56
	Para	-0.0351	1.6571	0.66
NCO	Meta	-0.0501	1.6577	0.27
	Para	-0.0578	1.6583	0.19
$C(NO_2)_3$	Meta	-0.0422	1.6532	0.72
	Para	-0.0295	1.6556	0.82
$CHCl_2$	Meta	-0.0512	1.6574	0.31
	Para	-0.0491	1.6583	0.32
OCHCl2	Meta	-0.0508	1.6578	0.38
	Para	-0.0554	1.6582	0.26
CHO	Meta	-0.0528	1.6576	0.41
	Para	-0.0406	1.6587	0.47
OCH_2Cl	Meta	-0.0508	1.6587	0.25
	Para	-0.0554	1.6586	0.08
$CONH_2$	Meta	-0.0539	1.6575	0.28
	Para	-0.0471	1.6585	0.36
Me	Meta	-0.0584	1.6597	-0.07
	Para	-0.0652	1.6600	-0.17
OMe	Meta	-0.0539	1.6597	0.12
	Para	-0.0763	1.6596	-0.27
CH_2NH_2	Meta	-0.0597	1.6600	-0.03

	Para	-0.0641	1.6602	-0.11
CF_2CF_3	Meta	-0.0494	1.6641	0.47
	Para	-0.0438	1.6648	0.52
CCH	Meta	-0.0541	1.6578	0.21
	Para	-0.0518	1.6590	0.23
CH_2CF_3	Meta	-0.0534	1.6657	0.12
	Para	-0.0538	1.6660	0.09
$CMe(NO_2)_2$	Meta	-0.0479	1.6550	0.54
	Para	-0.0384	1.6568	0.61
$SCHCH_2$	Meta	-0.0539	1.6579	0.26
	Para	-0.0499	1.6587	0.2
Et	Meta	-0.0591	1.6597	-0.07
	Para	-0.0658	1.6599	-0.15
$N(Me)_2$	Meta	-0.0577	1.6602	-0.16
	Para	-0.0864	1.6605	-0.83
$CH(CN)_2$	Meta	-0.0456	1.6640	0.53
	Para	-0.0458	1.6642	0.52
NH_2	Meta	-0.0554	1.6604	-0.09
	Para	-0.0838	1.6605	-0.57

Table S3. Calculated D_C, Q_C of some selected molecules using different methods with 6-31+G(d,p) basis set

Method	**Methane**		**Ethylene**		**Benzene**		**buta-1,3-diene**	
	Q_C	**D_C**	**Q_C**	**D_C**	**Q_C**	**D_C**	**Q_C**	**D_C**
HF	-0.147	1.781	-0.094	1.753	-0.050	1.672	-0.099	1.746
LSDA	-0.205	1.787	-0.122	1.752	-0.064	1.666	-0.120	1.744
B3LYP	-0.170	1.777	-0.103	1.746	-0.053	1.666	-0.105	1.739
LC-BLYP	-0.186	1.780	-0.111	1.744	-0.058	1.660	-0.114	1.736
B3PW91	-0.180	1.774	-0.109	1.743	-0.057	1.663	-0.110	1.736
ωB97X-D	-0.178	1.775	-0.108	1.743	-0.057	1.663	-0.110	1.736
CCSD	-0.153	1.766	-0.092	1.737	-0.048	1.660	-0.095	1.730

Table S4. Calculated D_C, Q_C of some selected molecules using different basis sets at LC-BYLP level of theory

Basis set	**Methane**		**Ethylene**		**Benzene**		**buta-1,3-diene**	
	Q_C	**D_C**	**Q_C**	**D_C**	**Q_C**	**D_C**	**Q_C**	**D_C**
6-31+G(d,p)	-0.186	1.780	-0.111	1.744	-0.058	1.660	-0.114	1.736
6-31++G(d,p)	-0.186	1.781	-0.111	1.744	-0.058	1.660	-0.114	1.736
6-311++G(d,p)	-0.185	1.781	-0.109	1.745	-0.058	1.660	-0.113	1.736
aug-cc-pVDZ	-0.185	1.784	-0.110	1.748	-0.057	1.663	-0.112	1.739
aug-cc-pVTZ	-0.185	1.778	-0.108	1.741	-0.057	1.663	-0.111	1.733
aug-cc-pVQZ	-0.186	1.777	-0.109	1.740	-0.057	1.663	-0.111	1.733

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Author Contributions

Arshad Mehmood performed the calculations, data collection, data analysis, wrote the original draft, and co-wrote the article. Benjamin G. Janesko designed and administrated the project, acquired the funding, developed the EDR and atomic overlap distance D_A, performed some of the calculations, and co-wrote the article.

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Computed geometries (Cartesian coordinates in Angstrom), total energies (Hartree), Hirshfeld population QA(e) and atomic overlap distances DA(bohr) of all systems given in Table SI-1, Table SI-2, Alkenyl anions (Fig. 3) and Au clusters (Fig. 5).
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Table SI-1
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Molecule 01-Carbon
Energy: -37.7131454546
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.0000	2.2238	2.6173	2.3812

Molecule 02-Methanide
Energy: -39.6946868929
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	1	0.000000	1.084453	0.000000
3	1	-0.939164	-0.542227	0.000000
4	1	0.939164	-0.542227	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.3294	1.9996	1.9996	1.9996
2	-0.1098	2.2233	2.2233	2.2233
3	-0.1098	2.2233	2.2233	2.2233
4	-0.1098	2.2233	2.2233	2.2233

Molecule 03-Ethanide
Energy: -78.8800820105
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.055661	-0.685026	0.000000
2	1	0.929949	-1.209105	0.000000
3	1	-0.593487	-1.081389	0.873333
4	1	-0.593487	-1.081389	-0.873333
5	6	-0.055661	0.836766	0.000000
6	1	0.462480	1.230721	0.889869
7	1	0.462480	1.230721	-0.889869

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.7947	1.7665	1.7665	1.7665
2	-0.0354	2.0198	2.0198	2.0198
3	-0.0104	2.0097	2.0097	2.0097
4	-0.0104	2.0097	2.0097	2.0097
5	1.4437	1.9106	1.9106	1.9106
6	-0.0910	2.1256	2.1256	2.1256
7	-0.0910	2.1256	2.1256	2.1256

Molecule 04-Propan-2-ide
Energy: -118.072779850
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.034676	-0.207765	1.230993
2	1	0.752715	-1.012052	1.235593
3	1	0.106325	0.373677	2.151596
4	1	-0.986802	-0.747434	1.353481
5	6	-0.034676	0.664006	0.000000
6	1	0.879687	1.280763	0.000000
7	6	-0.034676	-0.207765	-1.230993
8	1	-0.986802	-0.747434	-1.353481
9	1	0.106325	0.373677	-2.151596
10	1	0.752715	-1.012052	-1.235593

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	1.8034	1.7577	1.7577	1.7577
2	-0.0375	2.0619	2.0619	2.0619
3	-0.0068	2.0227	2.0227	2.0227
4	-0.0080	2.0080	2.0080	2.0080
5	1.5656	1.8147	1.8147	1.8147
6	-0.0678	2.0672	2.0672	2.0672
7	1.8034	1.7577	1.7577	1.7577
8	-0.0080	2.0080	2.0080	2.0080
9	-0.0068	2.0227	2.0227	2.0227
10	-0.0375	2.0619	2.0619	2.0619

Molecule 05-2-methylpropan-2-ide
Energy: -157.273519345
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.471842
2	6	0.000000	1.407019	0.050599
3	1	-0.882677	1.975555	-0.270043
4	1	0.000000	1.438303	1.180177
5	1	0.882677	1.975555	-0.270043
6	6	-1.218514	-0.703510	0.050599
7	1	-2.152220	-0.223357	-0.270043
8	1	-1.269543	-1.752199	-0.270043
9	1	-1.245607	-0.719152	1.180177
10	6	1.218514	-0.703510	0.050599
11	1	1.269543	-1.752199	-0.270043
12	1	2.152220	-0.223357	-0.270043
13	1	1.245607	-0.719152	1.180177

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6820	1.7273	1.7273	1.7273
2	1.8129	1.7486	1.7486	1.7486
3	-0.0012	2.0131	2.0131	2.0131
4	-0.0378	2.1116	2.1116	2.1116
5	-0.0012	2.0131	2.0131	2.0131
6	1.8130	1.7487	1.7487	1.7487
7	-0.0012	2.0130	2.0130	2.0130
8	-0.0012	2.0130	2.0130	2.0130
9	-0.0378	2.1116	2.1116	2.1116
10	1.8130	1.7487	1.7487	1.7487
11	-0.0012	2.0130	2.0130	2.0130
12	-0.0012	2.0130	2.0130	2.0130
13	-0.0378	2.1116	2.1116	2.1116

Molecule 06-pentan-3-ide
Energy: -196.461569845
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.015490	-0.322435	-2.529667
2	1	-0.036809	0.313537	-3.424012
3	1	0.915984	-0.941273	-2.580307
4	1	-0.843535	-1.002891	-2.551473
5	6	0.015490	0.479528	-1.238003
6	1	0.885238	1.155868	-1.253856
7	1	-0.869129	1.171033	-1.278425
8	6	0.058918	-0.373700	0.000000
9	1	-0.828759	-1.035465	0.000000
10	6	0.015490	0.479528	1.238003
11	1	-0.869129	1.171033	1.278425
12	1	0.885238	1.155868	1.253856
13	6	0.015490	-0.322435	2.529667
14	1	0.915984	-0.941273	2.580307
15	1	-0.036809	0.313537	3.424012
16	1	-0.843535	-1.002891	2.551473

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8396	1.7364	1.7364	1.7364

2	0.0037	1.9968	1.9968	1.9968
3	0.0059	2.0361	2.0361	2.0361
4	0.0177	1.9895	1.9895	1.9895
5	1.8754	1.6885	1.6885	1.6885
6	0.0022	1.9663	1.9663	1.9663
7	-0.0261	2.0178	2.0178	2.0178
8	1.6150	1.7743	1.7743	1.7743
9	-0.0518	2.0402	2.0402	2.0402
10	1.8754	1.6885	1.6885	1.6885
11	-0.0261	2.0178	2.0178	2.0178
12	0.0022	1.9663	1.9663	1.9663
13	1.8396	1.7364	1.7364	1.7364
14	0.0059	2.0361	2.0361	2.0361
15	0.0037	1.9968	1.9968	1.9968
16	0.0177	1.9895	1.9895	1.9895

Molecule 07-pent-1-en-3-ide
Energy: -195.274785005
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.264737	0.272932	-0.459177
2	1	3.235031	-0.244515	-0.433735
3	1	1.920728	0.325966	-1.496318
4	1	2.421231	1.301952	-0.119102
5	6	1.212934	-0.418228	0.411227
6	1	1.653739	-0.532386	1.418622
7	1	1.077860	-1.442820	0.036639
8	6	-0.119839	0.254470	0.451257
9	1	-0.175899	1.218564	0.960271
10	6	-1.259935	-0.285030	-0.107065
11	1	-1.097138	-1.265787	-0.574602
12	6	-2.569790	0.166205	-0.187008
13	1	-2.869586	1.126210	0.227390
14	1	-3.334606	-0.429274	-0.674573

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8447	1.7304	1.7304	1.7304
2	0.0072	2.0005	2.0005	2.0005
3	0.0224	1.9843	1.9843	1.9843
4	0.0206	1.9852	1.9852	1.9852
5	1.8939	1.6804	1.6804	1.6804
6	0.0007	1.9658	1.9658	1.9658
7	0.0185	1.9528	1.9528	1.9528
8	1.7666	1.6874	1.6874	1.6874
9	-0.0132	2.0280	2.0280	2.0280
10	1.8797	1.6991	1.6991	1.6991
11	0.0095	1.9965	1.9965	1.9965
12	1.6308	1.8001	1.8001	1.8001
13	-0.0347	2.0848	2.0848	2.0848
14	-0.0464	2.0896	2.0896	2.0896

Molecule 08-penta-1-4-dien-3-ide
Energy: -195.128745334
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.139705	-0.835687	1.723666
2	1	-0.716956	-1.480184	1.069684
3	1	0.855408	-1.242177	1.915463
4	6	-0.139705	0.626279	1.304214
5	1	-1.147701	1.050465	1.248459
6	1	0.448342	1.234049	2.001238
7	6	0.486047	0.509605	0.000000
8	1	1.558458	0.330962	0.000000
9	6	-0.139705	0.626279	-1.304214
10	1	0.448342	1.234049	-2.001238
11	1	-1.147701	1.050465	-1.248459

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12      6       -0.139705       -0.835687       -1.723666
13      1       0.855408        -1.242177       -1.915463
14      1       -0.716956       -1.480184       -1.069684
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.6108      1.8330      1.8330      1.8330
    2     -0.0208      2.0286      2.0286      2.0286
    3     -0.0355      2.0615      2.0615      2.0615
    4      1.8785      1.6800      1.6800      1.6800
    5      0.0239      1.9628      1.9628      1.9628
    6      0.0228      1.9564      1.9564      1.9564
    7      2.0062      1.6657      1.6657      1.6657
    8      0.0343      1.9528      1.9528      1.9528
    9      1.8785      1.6800      1.6800      1.6800
   10      0.0228      1.9564      1.9564      1.9564
   11      0.0239      1.9628      1.9628      1.9628
   12      1.6108      1.8330      1.8330      1.8330
   13     -0.0355      2.0615      2.0615      2.0615
   14     -0.0208      2.0286      2.0286      2.0286

Molecule 09-ethenide
Energy: -77.6224320722
Geometry:
Atom  Atomic No.   x               y               z
1       6       0.000000        -0.596229       0.000000
2       1       0.000000        -1.241693       0.911586
3       1       0.000000        -1.241693       -0.911586
4       6       0.000000        0.713678        0.000000
5       1       0.000003        1.778695        0.000000
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.7040      1.8246      1.8246      1.8246
    2     -0.0611      2.0837      2.0837      2.0837
    3     -0.0611      2.0837      2.0837      2.0837
    4      1.4908      1.8852      1.8852      1.8852
    5     -0.0730      2.2593      2.2593      2.2593
Molecule 10-ethynide
Energy: -76.4734042801
Geometry:
Atom  Atomic No.   x               y               z
1       6       0.000000        0.000000        -0.487008
2       1       0.000000        0.000000        -1.557183
3       6       0.000000        0.000000        0.746539
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.5947      1.8573      1.8573      1.8573
    2      0.0053      2.1807      2.1807      2.1807
    3      1.4000      2.0987      2.0987      2.0987

Molecule 11-ethyne-1-2-diide
Energy: -75.6587320756
Geometry:
Atom  Atomic No.   x               y               z
1       6       0.000000        0.000000        0.632188
2       6       0.000000        0.000000        -0.632188
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.0000      2.3438      2.3438      2.3438
    2      1.0000      2.3438      2.3438      2.3438

Molecule 12-chloromethanide
Energy: -499.039648969
Geometry:
Atom  Atomic No.   x               y               z
1       6       0.000000        0.000000        -1.175290
2       1       0.000000        -0.969315       -1.642643
3       1       0.000000        0.969315        -1.642643
4       17      0.000000        0.000000        0.608060
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
```

1	1.5161	1.8713	1.8713	1.8713
2	-0.0702	2.1317	2.1317	2.1317
3	-0.0702	2.1317	2.1317	2.1317
4	9.6243	1.7837	1.7837	1.7837

Molecule 13-dichloromethanide
Energy: -958.379520052
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.731518
2	1	0.000000	0.000000	1.803470
3	17	0.000000	1.486306	-0.182135
4	17	0.000000	-1.486306	-0.182135

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6788	1.7505	1.7505	1.7505
2	-0.0409	2.0684	2.0684	2.0684
3	9.6810	1.7695	1.7695	1.7695
4	9.6810	1.7695	1.7695	1.7695

Molecule 14-Chloroform_anion
Energy: -1417.71371191
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	17	0.000000	1.723968	0.000000
3	17	1.493000	-0.861984	0.000000
4	17	-1.493000	-0.861984	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8260	1.6464	1.6464	1.6464
2	9.7246	1.7581	1.7581	1.7581
3	9.7247	1.7581	1.7581	1.7581
4	9.7247	1.7581	1.7581	1.7581

Molecule 15-benzen-1-ide
Energy: -230.873611122
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.188252	0.643388	0.000005
2	6	0.000029	1.358418	0.000000
3	6	-1.188203	0.643477	-0.000007
4	6	-1.166779	-0.747494	0.000023
5	6	-0.000058	-1.534945	0.000000
6	6	1.166749	-0.747540	-0.000024
7	1	2.139495	1.177158	0.000024
8	1	0.000089	2.446583	0.000006
9	1	-2.139439	1.177259	-0.000024
10	1	-2.140633	-1.246337	-0.000029
11	1	2.140544	-1.246489	0.000039

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8888	1.6766	1.6766	1.6766
2	1.8724	1.6752	1.6752	1.6752
3	1.8888	1.6766	1.6766	1.6766
4	1.8621	1.6977	1.6977	1.6977
5	1.5887	1.8614	1.8614	1.8614
6	1.8621	1.6977	1.6977	1.6977
7	0.0161	2.0025	2.0025	2.0025
8	0.0164	2.0030	2.0030	2.0030
9	0.0161	2.0025	2.0025	2.0025
10	-0.0057	2.0214	2.0214	2.0214
11	-0.0057	2.0214	2.0214	2.0214

Molecule 16-cyclopropanide
Energy: -116.847455899
Geometry:

Atom	Atomic No.	x	y	z

1	6	0.000247	-0.932239	-0.211652
2	6	-0.751111	0.357598	0.019280
3	6	0.750717	0.358096	0.019050
4	1	0.001380	-1.536035	0.707504
5	1	-1.226370	0.593575	0.979118
6	1	-1.281924	0.823347	-0.814711
7	1	1.283959	0.825739	-0.812420
8	1	1.223840	0.592645	0.980436

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.4875	1.8768	1.8768	1.8768
2	1.8077	1.7167	1.7167	1.7167
3	1.8077	1.7167	1.7167	1.7167
4	-0.0557	2.0610	2.0610	2.0610
5	-0.0127	2.0038	2.0038	2.0038
6	-0.0108	2.0035	2.0035	2.0035
7	-0.0108	2.0037	2.0037	2.0037
8	-0.0129	2.0036	2.0036	2.0036

Molecule 17-cyclobutanide
Energy: -156.038566203
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.134397	1.120219	0.000000
2	6	0.134397	0.011224	1.057506
3	6	-0.505397	-0.896914	0.000000
4	6	0.134397	0.011224	-1.057506
5	1	1.007600	1.792373	0.000000
6	1	-0.411966	0.147044	2.004162
7	1	1.135857	-0.404987	1.319539
8	1	-1.593344	-0.784507	0.000000
9	1	-0.248807	-1.966504	0.000000
10	1	-0.411966	0.147044	-2.004162
11	1	1.135857	-0.404987	-1.319539

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5577	1.8196	1.8196	1.8196
2	1.8534	1.6993	1.6993	1.6993
3	1.8762	1.6845	1.6845	1.6845
4	1.8534	1.6993	1.6993	1.6993
5	-0.0698	2.0887	2.0887	2.0887
6	-0.0144	2.0048	2.0048	2.0048
7	-0.0226	2.0069	2.0069	2.0069
8	0.0095	1.9810	1.9810	1.9810
9	-0.0064	1.9971	1.9971	1.9971
10	-0.0144	2.0048	2.0048	2.0048
11	-0.0226	2.0069	2.0069	2.0069

Molecule 18-cyclopentanide
Energy: -195.250810492
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	1.274227
2	6	0.000000	1.237400	0.427481
3	6	-0.326518	0.687444	-0.962528
4	6	0.326518	-0.687444	-0.962528
5	6	0.000000	-1.237400	0.427481
6	1	0.000000	0.000000	2.359318
7	1	0.965854	1.801214	0.352746
8	1	-0.741811	2.011711	0.702383
9	1	-1.413004	0.564568	-1.059156
10	1	0.016944	1.327488	-1.788030
11	1	-0.016944	-1.327488	-1.788030
12	1	1.413004	-0.564568	-1.059156
13	1	-0.965854	-1.801214	0.352746
14	1	0.741811	-2.011711	0.702383

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	1.6307	1.7258	1.7258	1.7258
2	1.8619	1.6914	1.6914	1.6914
3	1.8955	1.6691	1.6691	1.6691
4	1.8955	1.6691	1.6691	1.6691
5	1.8619	1.6914	1.6914	1.6914
6	-0.0809	2.1148	2.1148	2.1148
7	-0.0359	1.9933	1.9933	1.9933
8	-0.0163	1.9797	1.9797	1.9797
9	0.0164	1.9495	1.9495	1.9495
10	0.0036	1.9742	1.9742	1.9742
11	0.0036	1.9742	1.9742	1.9742
12	0.0164	1.9495	1.9495	1.9495
13	-0.0359	1.9933	1.9933	1.9933
14	-0.0163	1.9797	1.9797	1.9797

Molecule 19-cyclohexanide
Energy: -234.442775732
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	1.500682
2	6	0.000000	1.272984	0.715858
3	6	-0.716904	1.059302	-0.616030
4	6	0.000000	0.000000	-1.463236
5	6	0.716904	-1.059302	-0.616030
6	6	0.000000	-1.272984	0.715858
7	1	0.000000	0.000000	2.585381
8	1	-0.493106	2.090573	1.262872
9	1	-1.733911	0.718837	-0.390725
10	1	-0.729023	-0.488117	-2.123386
11	1	0.800518	-1.992412	-1.193845
12	1	0.493106	-2.090573	1.262872
13	1	1.733911	-0.718837	-0.390725
14	1	-0.800518	1.992412	-1.193845
15	1	1.004279	1.697150	0.441088
16	1	-1.004279	-1.697150	0.441088
17	1	0.729023	0.488117	-2.123386

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6396	1.7250	1.7250	1.7250
2	1.8674	1.6869	1.6869	1.6869
3	1.8989	1.6666	1.6666	1.6666
4	1.9074	1.6678	1.6678	1.6678
5	1.8989	1.6666	1.6666	1.6666
6	1.8674	1.6869	1.6869	1.6869
7	-0.0814	2.1102	2.1102	2.1102
8	-0.0005	1.9679	1.9679	1.9679
9	0.0155	1.9504	1.9504	1.9504
10	0.0144	1.9500	1.9500	1.9500
11	0.0048	1.9695	1.9695	1.9695
12	-0.0005	1.9679	1.9679	1.9679
13	0.0155	1.9504	1.9504	1.9504
14	0.0048	1.9695	1.9695	1.9695
15	-0.0334	1.9922	1.9922	1.9922
16	-0.0334	1.9922	1.9922	1.9922
17	0.0144	1.9500	1.9500	1.9500

Molecule 20-cycloheptanide
Energy: -273.644871733
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.174353	-1.626556	0.391240
2	6	-1.428606	-0.942568	-0.090113
3	6	-1.607243	0.574281	0.111425
4	6	1.062206	-1.197873	-0.354775
5	6	-0.459331	1.434621	-0.400514
6	6	1.749386	0.148986	-0.015700

7	6	0.824210	1.283319	0.410301
8	1	-1.525519	-1.120248	-1.176922
9	1	-1.726513	0.776876	1.185454
10	1	-0.263624	1.198781	-1.455663
11	1	0.802228	-1.168458	-1.426030
12	1	2.346839	0.477818	-0.882117
13	1	-0.056304	-1.569746	1.486050
14	1	-2.317347	-1.417152	0.355443
15	1	-2.543705	0.901215	-0.372440
16	1	1.858907	-1.957143	-0.284966
17	1	-0.772158	2.487274	-0.375830
18	1	2.468760	-0.011543	0.799275
19	1	1.393127	2.222990	0.379786
20	1	0.537699	1.134072	1.456773

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6019	1.7700	1.7700	1.7700
2	1.8689	1.6853	1.6853	1.6853
3	1.8958	1.6669	1.6669	1.6669
4	1.8702	1.6847	1.6847	1.6847
5	1.9110	1.6630	1.6630	1.6630
6	1.8963	1.6698	1.6698	1.6698
7	1.9089	1.6614	1.6614	1.6614
8	-0.0018	1.9733	1.9733	1.9733
9	0.0146	1.9551	1.9551	1.9551
10	0.0285	1.9454	1.9454	1.9454
11	0.0030	1.9594	1.9594	1.9594
12	0.0050	1.9674	1.9674	1.9674
13	-0.0600	2.0695	2.0695	2.0695
14	-0.0053	1.9847	1.9847	1.9847
15	0.0037	1.9724	1.9724	1.9724
16	-0.0094	1.9849	1.9849	1.9849
17	0.0158	1.9416	1.9416	1.9416
18	0.0132	1.9550	1.9550	1.9550
19	0.0136	1.9448	1.9448	1.9448
20	0.0261	1.9358	1.9358	1.9358

Molecule 21-benzo-d-1-3-dithiol-2-ide
Energy: -1064.12069548
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.187956	-0.698504	0.000081
2	6	-0.187956	0.698505	-0.000040
3	6	-1.389634	1.385162	0.000034
4	6	-2.592491	0.691608	0.000226
5	6	-2.592491	-0.691608	0.000343
6	6	-1.389634	-1.385161	0.000271
7	6	2.462907	-0.000006	-0.000261
8	1	-1.386544	2.471441	-0.000059
9	1	-3.530987	1.238471	0.000283
10	1	-3.530987	-1.238470	0.000493
11	1	-1.386544	-2.471440	0.000363
12	16	1.409333	1.422422	-0.000281
13	16	1.409329	-1.422421	-0.000031

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9738	1.6175	1.6147	1.6161
2	1.9738	1.6175	1.6147	1.6161
3	1.9144	1.6568	1.6630	1.6598
4	1.9060	1.6665	1.6678	1.6671
5	1.9060	1.6665	1.6678	1.6671
6	1.9144	1.6568	1.6630	1.6598
7	1.5570	1.7971	2.0123	1.8878
8	0.0440	1.9754	1.9782	1.9768
9	0.0362	1.9813	1.9809	1.9811
10	0.0362	1.9813	1.9809	1.9811
11	0.0440	1.9754	1.9782	1.9768

12	9.8470	1.8804	1.9083	1.8941
13	9.8470	1.8804	1.9083	1.8941

Molecule 22-4-oxocyclohex-2-en-1-ide
Energy: -307.231471582
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.114156	-1.162699	-0.278916
2	6	-1.814951	0.118082	0.060470
3	6	-1.067926	1.240464	0.085062
4	6	0.349684	1.263107	-0.091214
5	6	1.094012	0.086055	-0.009029
6	6	0.293340	-1.177265	0.295134
7	1	-1.036936	-1.257883	-1.376588
8	1	-1.570378	2.196765	0.240489
9	1	0.881358	2.205831	-0.173395
10	1	0.872667	-2.032350	-0.063316
11	8	2.342812	-0.021344	-0.079015
12	1	0.240084	-1.254198	1.390873
13	1	-1.674575	-2.038743	0.069474
14	1	-2.894732	0.144864	0.175541

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8998	1.6698	1.6698	1.6698
2	1.8263	1.6807	1.6807	1.6807
3	1.9032	1.6798	1.6798	1.6798
4	1.7778	1.6747	1.6747	1.6747
5	2.0603	1.5718	1.5718	1.5718
6	1.8986	1.6571	1.6571	1.6571
7	0.0187	1.9552	1.9552	1.9552
8	0.0218	1.9945	1.9945	1.9945
9	-0.0016	2.0231	2.0231	2.0231
10	0.0240	1.9485	1.9485	1.9485
11	1.5254	1.3602	1.3602	1.3602
12	0.0274	1.9536	1.9536	1.9536
13	0.0181	1.9520	1.9520	1.9520
14	0.0001	2.0183	2.0183	2.0183

Molecule 23-4-oxocyclobut-2-en-1-ide
Energy: -228.752217439
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.409534	1.070394	0.000106
2	6	-0.579730	0.028560	0.000146
3	6	0.563096	-1.036537	0.000473
4	6	1.413638	0.022043	-0.000138
5	1	0.405265	2.149543	-0.000061
6	1	0.640413	-2.113944	-0.001100
7	1	2.502402	0.067778	-0.000859
8	8	-1.798413	-0.076267	-0.000188

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6851	1.7131	1.7131	1.7131
2	2.0719	1.5884	1.5884	1.5884
3	1.7544	1.7111	1.7111	1.7111
4	1.9083	1.7020	1.7020	1.7020
5	-0.0256	2.1069	2.1069	2.1069
6	-0.0058	2.0875	2.0875	2.0875
7	0.0261	2.0364	2.0364	2.0364
8	1.5853	1.3553	1.3553	1.3553

Molecule 24-2-methylenecyclohexan-1-ide
Energy: -272.471035592
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.189787	-1.242810	-0.120389
2	6	-0.301493	-1.260721	0.041442
3	6	-1.108097	-0.137214	0.028811

4	6	-0.418893	1.209758	0.170746
5	6	1.010153	1.221677	-0.339587
6	6	1.799743	0.087951	0.285760
7	1	1.663097	-2.044748	0.465942
8	1	-1.014016	1.970603	-0.344796
9	1	1.010437	1.092675	-1.430543
10	1	1.756742	0.190327	1.378160
11	1	-0.414107	1.483101	1.234345
12	1	1.482338	2.191181	-0.131569
13	1	2.857089	0.138173	-0.007902
14	1	1.506427	-1.434732	-1.168201
15	1	-0.786368	-2.231766	-0.059029
16	6	-2.495516	-0.083482	-0.048929
17	1	-3.020624	0.864122	0.029585
18	1	-3.095120	-0.989882	-0.073116

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8911	1.6741	1.6741	1.6741
2	1.7622	1.6805	1.6805	1.6805
3	1.9423	1.6301	1.6301	1.6301
4	1.9085	1.6612	1.6612	1.6612
5	1.9091	1.6602	1.6602	1.6602
6	1.9053	1.6613	1.6613	1.6613
7	0.0085	1.9508	1.9508	1.9508
8	0.0209	1.9538	1.9538	1.9538
9	0.0281	1.9431	1.9431	1.9431
10	0.0233	1.9443	1.9443	1.9443
11	0.0218	1.9468	1.9468	1.9468
12	0.0177	1.9469	1.9469	1.9469
13	0.0145	1.9523	1.9523	1.9523
14	-0.0021	1.9625	1.9625	1.9625
15	-0.0137	2.0159	2.0159	2.0159
16	1.6373	1.7876	1.7876	1.7876
17	-0.0416	2.0789	2.0789	2.0789
18	-0.0329	2.0790	2.0790	2.0790

Molecule 25-phenylsulfinyl-methanide
Energy: -743.080982008
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.116875	-1.181478	0.173892
2	6	0.736706	-1.165177	0.048762
3	6	0.071748	0.033222	-0.137887
4	6	0.789751	1.216680	-0.200412
5	6	2.167601	1.197793	-0.082530
6	6	2.837750	-0.002221	0.103521
7	1	2.633457	-2.124724	0.330667
8	1	0.128678	-2.062519	0.113669
9	1	0.234046	2.142223	-0.309711
10	1	2.724972	2.129762	-0.125678
11	1	3.919922	-0.015023	0.200396
12	16	-1.714342	-0.002924	-0.370638
13	8	-2.039866	-1.425616	0.124699
14	6	-2.176602	1.316572	0.560580
15	1	-1.979342	1.235780	1.630877
16	1	-3.176301	1.653870	0.296844

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9213	1.6654	1.6654	1.6654
2	1.9343	1.6504	1.6504	1.6504
3	1.9828	1.6117	1.6117	1.6117
4	1.9352	1.6563	1.6563	1.6563
5	1.9195	1.6655	1.6655	1.6655
6	1.9127	1.6664	1.6664	1.6664
7	0.0404	1.9758	1.9758	1.9758
8	0.0438	1.9480	1.9480	1.9480
9	0.0381	2.0002	2.0002	2.0002

10	0.0399	1.9767	1.9767	1.9767
11	0.0373	1.9798	1.9798	1.9798
12	10.1205	1.7628	1.7628	1.7628
13	1.4871	1.3708	1.3708	1.3708
14	1.6175	1.8022	1.8022	1.8022
15	-0.0122	2.0541	2.0541	2.0541
16	-0.0182	2.0502	2.0502	2.0502

Molecule 26-methylsulfinyl-methanide
Energy: -551.921372194
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.237385	-0.911319	0.117931
2	1	2.181117	-0.409074	-0.100449
3	1	1.145356	-1.056214	1.197776
4	1	1.168280	-1.869598	-0.395657
5	16	-0.110643	0.163116	-0.399808
6	6	-1.419153	-0.723526	0.198622
7	1	-2.358381	-0.367769	-0.223307
8	1	-1.430649	-0.809296	1.289406
9	8	0.269397	1.463896	0.341230

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8412	1.7394	1.7394	1.7394
2	0.0296	1.9724	1.9724	1.9724
3	0.0354	1.9889	1.9889	1.9889
4	0.0262	1.9996	1.9996	1.9996
5	10.0978	1.7771	1.7771	1.7771
6	1.5763	1.8261	1.8261	1.8261
7	-0.0258	2.0640	2.0640	2.0640
8	-0.0239	2.0717	2.0717	2.0717
9	1.4431	1.3804	1.3804	1.3804

Molecule 27-2-methoxy-2-oxoethan-1-ide
Energy: -267.151946756
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.775440	-0.118679	-0.000127
2	1	-2.527991	-0.913408	0.000758
3	1	-1.912088	0.516678	-0.882176
4	1	-1.911669	0.518355	0.880752
5	6	0.581832	0.119518	0.000046
6	6	1.781957	-0.542100	-0.000099
7	1	1.816051	-1.623968	-0.000146
8	1	2.699100	0.032120	-0.000220
9	8	-0.532430	-0.752132	0.000212
10	8	0.320743	1.341856	0.000051

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9260	1.6834	1.6834	1.6834
2	0.0219	1.9464	1.9464	1.9464
3	0.0254	1.9376	1.9376	1.9376
4	0.0254	1.9375	1.9375	1.9375
5	2.0911	1.5508	1.5508	1.5508
6	1.6391	1.7715	1.7715	1.7715
7	-0.0241	2.0639	2.0639	2.0639
8	-0.0199	2.0661	2.0661	2.0661
9	1.7857	1.2995	1.2995	1.2995
10	1.5295	1.3505	1.3505	1.3505

Molecule 28-cyanomethanide
Energy: -131.775834693
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.191825
2	1	0.000000	0.934714	-1.737039
3	1	0.000000	-0.934714	-1.737039

```
4       6       0.000000        0.000000        0.184404
5       7       0.000000        0.000000        1.359801
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.6003      1.8123      1.8123      1.8123
    2     -0.0298      2.0863      2.0863      2.0863
    3     -0.0298      2.0863      2.0863      2.0863
    4      1.9357      1.6740      1.6740      1.6740
    5      1.5237      1.6187      1.6187      1.6187

Molecule 29-2-oxopropan-1-ide
Energy: -192.052090669
Geometry:
Atom  Atomic No.   x               y               z
1       6       1.272181        -0.496129       0.000022
2       1       1.812312        -0.134109       0.880263
3       1       1.272747        -1.590377       0.000463
4       1       1.811930        -0.134961       -0.880786
5       6       -0.129914       0.106255        0.000069
6       6       -1.193001       -0.763508       -0.000095
7       1       -1.043418       -1.838561       -0.000014
8       1       -2.209035       -0.380461       0.000376
9       8       -0.167517       1.374846        -0.000035
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.8347      1.7273      1.7273      1.7273
    2      0.0206      1.9816      1.9816      1.9816
    3      0.0144      1.9898      1.9898      1.9898
    4      0.0206      1.9816      1.9816      1.9816
    5      2.0214      1.5943      1.5943      1.5943
    6      1.6604      1.7751      1.7751      1.7751
    7     -0.0277      2.0619      2.0619      2.0619
    8     -0.0226      2.0751      2.0751      2.0751
    9      1.4782      1.3671      1.3671      1.3671

Molecule 30-1-3-dimethoxy-1-3-dioxopropan-2-ide
Energy: -494.571119024
Geometry:
Atom  Atomic No.   x               y               z
1       6       0.253997        0.000045        -3.569432
2       1       -0.372008       0.882648        -3.732708
3       1       1.088598        -0.000099       -4.274321
4       1       -0.372153       -0.882479       -3.732561
5       6       -0.100085       -0.000033       -1.240847
6       6       0.555766        -0.000070       0.000000
7       1       1.636186        -0.000022       0.000000
8       6       -0.100085       -0.000033       1.240847
9       6       0.253997        0.000045        3.569432
10      1       -0.372153       -0.882479       3.732561
11      1       1.088598        -0.000099       4.274321
12      1       -0.372008       0.882648        3.732708
13      8       0.820590        0.000011        -2.288725
14      8       0.820590        0.000011        2.288725
15      8       -1.289752       -0.000002       1.530879
16      8       -1.289752       -0.000002       -1.530879
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9350      1.6805      1.6805      1.6805
    2      0.0341      1.9302      1.9302      1.9302
    3      0.0315      1.9380      1.9380      1.9380
    4      0.0341      1.9302      1.9302      1.9302
    5      2.1545      1.5263      1.5263      1.5263
    6      1.7649      1.6500      1.6500      1.6500
    7      0.0078      1.9803      1.9803      1.9803
    8      2.1545      1.5263      1.5263      1.5263
    9      1.9350      1.6805      1.6805      1.6805
   10      0.0341      1.9302      1.9302      1.9302
   11      0.0315      1.9380      1.9380      1.9380
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12	0.0341	1.9302	1.9302	1.9302
13	1.8070	1.2950	1.2950	1.2950
14	1.8070	1.2950	1.2950	1.2950
15	1.6173	1.3361	1.3361	1.3361
16	1.6173	1.3361	1.3361	1.3361

Molecule 31-cyanide
Energy: -92.6136090288
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.629574
2	7	0.000000	0.000000	0.539635

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.4898	2.0689	2.0689	2.0689
2	1.5102	1.6503	1.6503	1.6503

Molecule 32-prop-2-en-1-ide
Energy: -116.893456681
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.265045	-0.179093	0.000509
2	1	-1.409250	-1.257626	-0.000435
3	1	-2.153920	0.444027	-0.001814
4	6	-0.000004	0.382710	-0.000012
5	1	-0.000229	1.479651	0.000066
6	6	1.265048	-0.179041	-0.000159
7	1	2.153995	0.444032	0.000446
8	1	1.409413	-1.257542	-0.000292

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6382	1.7972	1.7972	1.7972
2	-0.0325	2.0813	2.0813	2.0813
3	-0.0438	2.0848	2.0848	2.0848
4	1.8705	1.7137	1.7137	1.7137
5	0.0055	2.0043	2.0043	2.0043
6	1.6383	1.7972	1.7972	1.7972
7	-0.0438	2.0849	2.0849	2.0849
8	-0.0325	2.0813	2.0813	2.0813

Molecule 33-cyclopenta-2-4-dien-1-ide
Energy: -192.925719144
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000111	-1.193483	0.000000
2	1	-0.000728	-2.279962	0.000000
3	6	0.000077	-0.368826	1.135155
4	1	-0.000218	-0.704609	2.168440
5	6	0.000077	0.965564	0.701481
6	1	-0.000011	1.844615	1.339997
7	6	0.000077	-0.368826	-1.135155
8	1	-0.000218	-0.704609	-2.168440
9	6	0.000077	0.965564	-0.701481
10	1	-0.000011	1.844615	-1.339997

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8066	1.6966	1.6966	1.6966
2	-0.0066	2.0511	2.0511	2.0511
3	1.8065	1.6966	1.6966	1.6966
4	-0.0066	2.0511	2.0511	2.0511
5	1.8066	1.6966	1.6966	1.6966
6	-0.0066	2.0511	2.0511	2.0511
7	1.8065	1.6966	1.6966	1.6966
8	-0.0066	2.0511	2.0511	2.0511
9	1.8066	1.6966	1.6966	1.6966
10	-0.0066	2.0511	2.0511	2.0511

Molecule 34-chlorosulfonyl-methanide

Energy: -1047.19665434
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.863443	1.626860	0.000000
2	1	-0.704702	2.134771	0.939751
3	1	-0.704702	2.134771	-0.939751
4	17	1.742391	-0.281656	0.000000
5	16	-0.575968	0.047297	0.000000
6	8	-0.863443	-0.624956	-1.256362
7	8	-0.863443	-0.624956	1.256362

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.7270	1.7539	1.7539	1.7539
2	0.0364	2.0031	2.0031	2.0031
3	0.0364	2.0031	2.0031	2.0031
4	9.5146	1.7990	1.7990	1.7990
5	10.4195	1.6325	1.6325	1.6325
6	1.6331	1.3430	1.3430	1.3430
7	1.6331	1.3430	1.3430	1.3430

Molecule 35-2-oxoethan-1-ide.log
Energy: -152.794943576
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.419050	0.000000
2	1	-0.182695	1.523198	0.000000
3	6	-1.189839	-0.449708	0.000000
4	1	-1.095497	-1.112607	0.876196
5	1	-1.095497	-1.112607	-0.876196
6	8	1.189091	0.110745	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0559	1.6665	1.6665	1.6665
2	-0.0165	2.0319	2.0319	2.0319
3	1.4504	1.8876	1.8876	1.8876
4	-0.0471	2.1042	2.1042	2.1042
5	-0.0471	2.1042	2.1042	2.1042
6	1.6044	1.3567	1.3567	1.3567

Molecule 36-cyano-phenyl-methanide
Energy: -362.153299888
Geometry:

Atom	Atomic No.	x	y	z
1	6	-2.238701	0.824711	-0.000308
2	6	-0.942621	1.287896	0.000008
3	6	0.170389	0.413968	0.000261
4	6	-0.142872	-0.966100	0.000282
5	6	-1.444519	-1.415235	0.000136
6	6	-2.521801	-0.536440	-0.000169
7	1	-3.054791	1.544656	-0.000526
8	1	-0.755277	2.358986	0.000048
9	1	0.675236	-1.680406	0.000432
10	1	-1.626964	-2.487967	0.000174
11	1	-3.544753	-0.898846	-0.000340
12	6	1.493243	0.909731	0.000243
13	1	1.666008	1.979292	0.000419
14	6	2.607613	0.077480	0.000148
15	7	3.536594	-0.627398	-0.000545

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9106	1.6702	1.6702	1.6702
2	1.8910	1.6614	1.6614	1.6614
3	1.9902	1.6117	1.6117	1.6117
4	1.8961	1.6587	1.6587	1.6587
5	1.9153	1.6694	1.6694	1.6694
6	1.8596	1.6731	1.6731	1.6731
7	0.0316	1.9837	1.9837	1.9837
8	0.0288	1.9825	1.9825	1.9825
9	0.0342	1.9746	1.9746	1.9746

10	0.0341	1.9808	1.9808	1.9808
11	0.0202	1.9991	1.9991	1.9991
12	1.7792	1.6842	1.6842	1.6842
13	0.0104	2.0041	2.0041	2.0041
14	1.9992	1.6401	1.6401	1.6401
15	1.5992	1.6072	1.6072	1.6072

Molecule 37-5-cyano-2-nitrobenzen-1-ide
Energy: -527.049030694
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.749369	-0.107321	0.000006
2	6	1.122533	-1.359056	0.000044
3	6	-0.284026	-1.240065	0.000029
4	6	-0.935920	-0.025559	-0.000020
5	6	-0.266140	1.191615	-0.000048
6	6	1.103711	1.138153	-0.000033
7	1	-0.903478	-2.132276	0.000061
8	1	-0.814205	2.123919	-0.000079
9	1	1.684077	2.056983	-0.000059
10	6	3.194361	-0.057278	0.000007
11	7	4.343321	0.027167	0.000005
12	7	-2.396854	0.009520	-0.000028
13	8	-2.951377	1.096815	0.000112
14	8	-3.010498	-1.040361	-0.000070

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9608	1.6274	1.6274	1.6274
2	1.6651	1.8133	1.8133	1.8133
3	1.9107	1.6675	1.6675	1.6675
4	2.0050	1.5679	1.5679	1.5679
5	1.9079	1.6479	1.6479	1.6479
6	1.9288	1.6577	1.6577	1.6577
7	0.0280	1.9552	1.9552	1.9552
8	0.0431	1.9509	1.9509	1.9509
9	0.0458	1.9695	1.9695	1.9695
10	2.0597	1.6323	1.6323	1.6323
11	1.6947	1.5927	1.5927	1.5927
12	2.2471	1.3537	1.3537	1.3537
13	1.7447	1.3148	1.3148	1.3148
14	1.7586	1.3132	1.3132	1.3132

Molecule 38-2-aminobenzen-1-ide
Energy: -286.115442635
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.113881	-1.219692	-0.006097
2	6	-0.278453	-1.306498	0.016317
3	6	-0.907242	-0.051251	0.030213
4	6	-0.229792	1.161345	0.033209
5	6	1.159561	1.178177	-0.005358
6	6	1.838869	-0.024106	-0.024972
7	1	1.699477	-2.143622	-0.018889
8	1	-0.784752	2.099261	0.074993
9	1	1.695923	2.124809	-0.011430
10	1	2.927982	-0.037761	-0.054232
11	7	-2.332135	-0.019934	0.065131
12	1	-2.735401	0.632706	-0.596183
13	1	-2.659224	-0.963703	-0.110050

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8649	1.6969	1.6969	1.6969
2	1.6005	1.8336	1.8336	1.8336
3	1.9843	1.6027	1.6027	1.6027
4	1.8747	1.6644	1.6644	1.6644
5	1.8792	1.6750	1.6750	1.6750
6	1.8732	1.6772	1.6772	1.6772

7	-0.0034	2.0185	2.0185	2.0185
8	0.0159	2.0012	2.0012	2.0012
9	0.0182	2.0011	2.0011	2.0011
10	0.0134	2.0066	2.0066	2.0066
11	1.7228	1.5172	1.5172	1.5172
12	0.0868	1.8479	1.8479	1.8479
13	0.0695	1.9447	1.9447	1.9447

Molecule 39-3-aminobenzen-1-ide
Energy: -286.103419538
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.151962	-1.388411	0.000029
2	6	-0.237621	-1.190544	0.000110
3	6	-0.873267	0.048866	-0.000394
4	6	-0.117663	1.206414	0.000065
5	6	1.265659	1.085150	0.000061
6	6	1.859499	-0.169703	-0.000116
7	1	-0.616498	2.171573	0.000194
8	1	1.881909	1.985058	0.000075
9	1	2.953124	-0.191606	0.000243
10	7	-2.315600	0.164784	0.000120
11	1	-2.699057	-0.303006	-0.814312
12	1	-2.698739	-0.303553	0.814414
13	1	-0.902953	-2.062592	0.000011

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5904	1.8597	1.8597	1.8597
2	1.8511	1.6853	1.6853	1.6853
3	1.9952	1.5856	1.5856	1.5856
4	1.8738	1.6633	1.6633	1.6633
5	1.8905	1.6761	1.6761	1.6761
6	1.8605	1.6972	1.6972	1.6972
7	0.0183	2.0072	2.0072	2.0072
8	0.0172	2.0019	2.0019	2.0019
9	-0.0048	2.0211	2.0211	2.0211
10	1.7227	1.5210	1.5210	1.5210
11	0.0970	1.8264	1.8264	1.8264
12	0.0970	1.8265	1.8265	1.8265
13	-0.0090	2.0205	2.0205	2.0205

Molecule 40-4-aminobenzen-1-ide
Energy: -286.101171100
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.193835	1.189411	0.000091
2	6	0.196715	1.165976	0.000231
3	6	0.879126	-0.041943	-0.000464
4	6	0.126948	-1.202052	0.000160
5	6	-1.264708	-1.137653	0.000087
6	6	-2.018551	0.048665	-0.000268
7	1	0.652156	-2.156135	0.000208
8	1	-1.789173	-2.097725	0.000072
9	7	2.321486	-0.118246	-0.000169
10	1	2.711526	0.336182	-0.818245
11	1	2.711302	0.333719	0.819408
12	1	0.767827	2.097125	0.000449
13	1	-1.658205	2.180130	0.000269

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8633	1.6978	1.6978	1.6978
2	1.8798	1.6643	1.6643	1.6643
3	1.9817	1.5824	1.5824	1.5824
4	1.8893	1.6647	1.6647	1.6647
5	1.8635	1.6974	1.6974	1.6974
6	1.5851	1.8609	1.8609	1.8609
7	0.0183	2.0058	2.0058	2.0058

8	-0.0043	2.0202	2.0202	2.0202
9	1.7247	1.5198	1.5198	1.5198
10	0.0953	1.8259	1.8259	1.8259
11	0.0953	1.8259	1.8259	1.8259
12	0.0127	2.0051	2.0051	2.0051
13	-0.0047	2.0211	2.0211	2.0211

Molecule 41-phenylmethanide
Energy: -270.049770906
Geometry:

Atom	Atomic No.	x	y	z
1	6	-2.472430	-0.000002	0.000000
2	1	-3.017344	-0.001704	-0.937531
3	1	-3.017344	0.001715	0.937530
4	6	-0.997997	-0.000001	0.000000
5	6	-0.235917	1.180600	-0.000078
6	6	-0.235916	-1.180601	0.000078
7	6	1.150098	1.190095	-0.000064
8	1	-0.789050	2.114672	-0.000156
9	6	1.150100	-1.190094	0.000064
10	1	-0.789047	-2.114674	0.000156
11	6	1.858919	0.000001	0.000000
12	1	1.682847	2.138910	-0.000125
13	1	1.682850	-2.138908	0.000125
14	1	2.945954	0.000002	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5261	1.8309	1.8309	1.8309
2	-0.0720	2.1371	2.1371	2.1371
3	-0.0720	2.1371	2.1371	2.1371
4	1.9834	1.6341	1.6341	1.6341
5	1.9103	1.6660	1.6660	1.6660
6	1.9103	1.6660	1.6660	1.6660
7	1.9043	1.6700	1.6700	1.6700
8	0.0138	2.0312	2.0312	2.0312
9	1.9043	1.6700	1.6700	1.6700
10	0.0138	2.0312	2.0312	2.0312
11	1.8920	1.6705	1.6705	1.6705
12	0.0294	1.9874	1.9874	1.9874
13	0.0294	1.9874	1.9874	1.9874
14	0.0272	1.9915	1.9915	1.9915

Molecule 42-3-methylbut-2-en-2-ide.
Energy: -195.244989339
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.398367	-0.100544	-0.000002
2	6	0.680608	-0.891597	0.000000
3	6	-1.796911	-0.698166	0.000001
4	1	-2.580591	0.073438	0.000011
5	1	-1.957837	-1.331855	-0.879105
6	1	-1.957828	-1.331869	0.879098
7	6	-0.421526	1.417673	0.000000
8	1	-0.950656	1.817650	-0.878755
9	1	-0.950628	1.817648	0.878773
10	1	0.582432	1.849171	-0.000016
11	6	2.033338	-0.203492	0.000000
12	1	2.863076	-0.918932	0.000007
13	1	2.184592	0.440748	-0.884353
14	1	2.184587	0.440758	0.884347

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8756	1.6380	1.6380	1.6380
2	1.5876	1.8509	1.8509	1.8509
3	1.8301	1.7406	1.7406	1.7406
4	0.0033	1.9910	1.9910	1.9910
5	0.0071	2.0223	2.0223	2.0223

6	0.0071	2.0223	2.0223	2.0223
7	1.8412	1.7287	1.7287	1.7287
8	0.0095	1.9849	1.9849	1.9849
9	0.0095	1.9849	1.9849	1.9849
10	0.0211	1.9665	1.9665	1.9665
11	1.8128	1.7547	1.7547	1.7547
12	-0.0076	2.0133	2.0133	2.0133
13	0.0012	2.0129	2.0129	2.0129
14	0.0012	2.0129	2.0129	2.0129

Molecule 43-E-3-chlorobut-2-en-2-ide
Energy: -615.417323595
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.057947	0.081533	0.000261
2	6	0.983247	-0.840165	0.000207
3	6	0.041092	1.578759	0.000172
4	1	1.066349	1.960686	0.000208
5	1	-0.472720	1.979629	-0.880845
6	1	-0.472827	1.979729	0.881078
7	6	2.419805	-0.398855	0.000080
8	1	2.940791	-0.814875	-0.870491
9	1	2.617782	0.692289	0.000012
10	1	2.940880	-0.814782	0.870639
11	17	-1.743106	-0.441783	-0.000290

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9359	1.6595	1.6595	1.6595
2	1.6378	1.8029	1.8029	1.8029
3	1.8495	1.7226	1.7226	1.7226
4	0.0276	1.9645	1.9645	1.9645
5	0.0219	1.9705	1.9705	1.9705
6	0.0219	1.9705	1.9705	1.9705
7	1.8313	1.7463	1.7463	1.7463
8	0.0124	1.9947	1.9947	1.9947
9	-0.0030	1.9949	1.9949	1.9949
10	0.0124	1.9947	1.9947	1.9947
11	9.6525	1.7824	1.7824	1.7824

Molecule 44-prop-1-yn-1-ide
Energy: -115.665905802
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.335473	0.000023	-0.000069
2	6	1.566630	-0.000010	0.000035
3	6	-1.129945	-0.000003	0.000015
4	1	-1.544346	-0.492545	-0.889269
5	1	-1.544252	-0.523924	0.871227
6	1	-1.544358	1.016411	0.018153

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.7168	1.7315	1.7315	1.7315
2	1.3712	2.0810	2.0810	2.0810
3	1.8523	1.7489	1.7489	1.7489
4	0.0198	1.9773	1.9773	1.9773
5	0.0198	1.9773	1.9773	1.9773
6	0.0198	1.9773	1.9773	1.9773

Molecule 45-propan-1-ide
Energy: -118.076458151
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.404265	0.018743	0.000000
2	1	-1.599568	-0.591254	0.896872
3	1	-1.599568	-0.591254	-0.896872
4	6	0.000000	0.567027	0.000000
5	1	0.146644	1.223218	0.873288

6	1	0.146644	1.223218	-0.873288
7	6	1.163335	-0.440750	0.000000
8	1	2.153846	0.045852	0.000000
9	1	1.098789	-1.089948	0.880302
10	1	1.098789	-1.089948	-0.880302

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.4721	1.8921	1.8921	1.8921
2	-0.0805	2.1227	2.1227	2.1227
3	-0.0805	2.1227	2.1227	2.1227
4	1.8626	1.7022	1.7022	1.7022
5	-0.0063	1.9852	1.9852	1.9852
6	-0.0063	1.9852	1.9852	1.9852
7	1.8296	1.7396	1.7396	1.7396
8	-0.0045	2.0221	2.0221	2.0221
9	0.0069	2.0114	2.0114	2.0114
10	0.0069	2.0114	2.0114	2.0114

Molecule 46-2-methylpropan-1-ide
Energy: -157.271861356
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.032273	0.078547	-0.367498
2	1	0.034411	0.029029	-1.469406
3	6	-1.421305	-0.031985	0.077061
4	1	-1.476954	0.054645	1.169756
5	1	-2.002707	0.791805	-0.342409
6	1	-1.882549	-0.988413	-0.207880
7	6	0.775988	-1.180357	0.113133
8	1	0.325411	-2.116406	-0.258607
9	1	1.820777	-1.149861	-0.209312
10	1	0.776796	-1.211718	1.209793
11	6	0.630110	1.402476	0.052953
12	1	1.669973	1.493730	-0.300878
13	1	0.632440	1.485096	1.155051

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9246	1.6432	1.6432	1.6432
2	0.0023	1.9498	1.9498	1.9498
3	1.8422	1.7286	1.7286	1.7286
4	0.0181	1.9912	1.9912	1.9912
5	0.0072	2.0319	2.0319	2.0319
6	0.0052	1.9876	1.9876	1.9876
7	1.8369	1.7304	1.7304	1.7304
8	0.0001	2.0063	2.0063	2.0063
9	0.0116	1.9976	1.9976	1.9976
10	0.0106	2.0051	2.0051	2.0051
11	1.4901	1.8793	1.8793	1.8793
12	-0.0757	2.1140	2.1140	2.1140
13	-0.0731	2.1107	2.1107	2.1107

Molecule 47-2-2-dimethylpropan-1-ide
Energy: -196.468356349
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.039205	0.070796	0.000000
2	6	-0.552359	1.499401	0.000000
3	1	-0.179129	2.033328	0.891452
4	1	-0.179129	2.033328	-0.891452
5	6	-0.552359	-0.662220	1.236748
6	1	-1.645066	-0.653189	1.241085
7	1	-0.197459	-1.702676	1.280871
8	1	-0.216400	-0.148778	2.144652
9	6	-0.552359	-0.662220	-1.236748
10	1	-0.216400	-0.148778	-2.144652
11	1	-0.197459	-1.702676	-1.280871
12	1	-1.645066	-0.653189	-1.241085

13	6	1.497448	-0.053754	0.000000
14	1	1.911804	0.445500	0.881825
15	1	1.845505	-1.100378	0.000000
16	1	1.911804	0.445500	-0.881825

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9772	1.5933	1.5933	1.5933
2	1.5093	1.8651	1.8651	1.8651
3	-0.0684	2.0983	2.0983	2.0983
4	-0.0684	2.0983	2.0983	2.0983
5	1.8481	1.7213	1.7213	1.7213
6	0.0118	2.0209	2.0209	2.0209
7	0.0072	1.9874	1.9874	1.9874
8	0.0204	1.9858	1.9858	1.9858
9	1.8481	1.7213	1.7213	1.7213
10	0.0204	1.9858	1.9858	1.9858
11	0.0072	1.9874	1.9874	1.9874
12	0.0118	2.0209	2.0209	2.0209
13	1.8433	1.7222	1.7222	1.7222
14	0.0146	1.9903	1.9903	1.9903
15	0.0029	1.9971	1.9971	1.9971
16	0.0146	1.9903	1.9903	1.9903

Molecule 48-2-methylcyclopropan-1-ide
Energy: -156.045517722
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.934613	0.783150	-0.388610
2	6	-0.136091	0.145114	0.443244
3	6	0.998096	-0.695659	-0.055090
4	1	1.638510	1.346159	0.240837
5	1	-0.154548	0.291993	1.531474
6	1	1.678432	-1.097139	0.704603
7	1	0.794998	-1.428153	-0.841810
8	6	-1.519300	-0.043592	-0.127050
9	1	-2.057456	-0.889554	0.327403
10	1	-2.128039	0.860676	0.006019
11	1	-1.435805	-0.218058	-1.203495

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5187	1.8599	1.8599	1.8599
2	1.8815	1.6466	1.6466	1.6466
3	1.8109	1.7108	1.7108	1.7108
4	-0.0528	2.0622	2.0622	2.0622
5	-0.0063	1.9781	1.9781	1.9781
6	-0.0106	2.0051	2.0051	2.0051
7	-0.0072	2.0014	2.0014	2.0014
8	1.8388	1.7375	1.7375	1.7375
9	0.0018	2.0040	2.0040	2.0040
10	0.0090	2.0141	2.0141	2.0141
11	0.0161	2.0223	2.0223	2.0223

Molecule 49-endo-5H-norborborneide
Energy: -271.217049633
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.011890	-1.064210	-0.522186
2	6	0.282882	-1.103371	0.327776
3	6	-0.190917	1.081247	0.329194
4	6	-1.328853	0.437669	-0.529857
5	1	-0.801244	-1.433573	-1.536504
6	1	-1.351283	0.893618	-1.534009
7	1	-2.288491	0.688425	-0.055359
8	6	-0.004472	-0.026250	1.370299
9	1	0.837750	0.174087	2.043709
10	1	-0.912482	-0.243038	1.939885
11	6	1.327619	-0.391794	-0.496234

12	1	2.036029	-0.892806	-1.152990
13	6	1.064802	0.921794	-0.477603
14	1	1.481179	1.680960	-1.133834
15	1	0.569367	-2.085459	0.715326
16	1	-0.405858	2.087276	0.705447

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5900	1.7993	1.7993	1.7993
2	1.9178	1.6330	1.6330	1.6330
3	1.9370	1.6224	1.6224	1.6224
4	1.8711	1.6860	1.6860	1.6860
5	-0.0582	2.0573	2.0573	2.0573
6	-0.0027	1.9867	1.9867	1.9867
7	-0.0064	1.9822	1.9822	1.9822
8	1.8958	1.6599	1.6599	1.6599
9	0.0081	1.9711	1.9711	1.9711
10	0.0201	1.9721	1.9721	1.9721
11	1.9043	1.6718	1.6718	1.6718
12	0.0234	2.0211	2.0211	2.0211
13	1.8644	1.6752	1.6752	1.6752
14	0.0156	2.0276	2.0276	2.0276
15	0.0069	1.9789	1.9789	1.9789
16	0.0129	1.9633	1.9633	1.9633

Molecule 50-exo-5H-norborborneide
Energy: -271.211806057
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.125341	0.789999	-0.747201
2	6	-0.070659	1.155596	0.159615
3	6	0.004772	-1.053494	0.437712
4	6	1.174529	-0.745354	-0.540065
5	1	1.037494	-1.336377	-1.458599
6	1	2.124905	-1.081388	-0.095794
7	6	0.048154	0.175329	1.343494
8	1	-0.789375	0.197782	2.054673
9	1	0.998845	0.288743	1.875491
10	6	-1.281220	0.570940	-0.526466
11	1	-1.935392	1.122337	-1.195147
12	6	-1.249546	-0.747542	-0.354164
13	1	-1.867861	-1.488177	-0.853510
14	1	-0.141834	2.218314	0.410058
15	1	0.039926	-2.034918	0.924017
16	1	2.025068	1.240844	-0.298740

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5638	1.8165	1.8165	1.8165
2	1.9170	1.6347	1.6347	1.6347
3	1.9382	1.6216	1.6216	1.6216
4	1.8706	1.6862	1.6862	1.6862
5	-0.0093	1.9854	1.9854	1.9854
6	0.0009	1.9743	1.9743	1.9743
7	1.8878	1.6610	1.6610	1.6610
8	0.0031	1.9803	1.9803	1.9803
9	0.0177	1.9590	1.9590	1.9590
10	1.9127	1.6775	1.6775	1.6775
11	0.0264	2.0401	2.0401	2.0401
12	1.8870	1.6709	1.6709	1.6709
13	0.0235	2.0191	2.0191	2.0191
14	0.0100	1.9810	1.9810	1.9810
15	0.0123	1.9647	1.9647	1.9647
16	-0.0618	2.0644	2.0644	2.0644

Molecule 51-bromomethanide
Energy: -2610.43215980
Geometry:

Atom	Atomic No.	x	y	z

1	6	0.000000	0.000000	-1.538806
2	1	0.000000	-0.970238	-2.003159
3	1	0.000000	0.970238	-2.003159
4	35	0.000000	0.000000	0.378262

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5689	1.8729	1.8729	1.8729
2	-0.0459	2.1139	2.1139	2.1139
3	-0.0459	2.1139	2.1139	2.1139
4	27.5228	1.9915	1.9915	1.9915

Molecule 52-Floromomethanide
Energy: -138.784558465
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.706099
2	1	0.000000	0.981200	-1.148729
3	1	0.000000	-0.981200	-1.148729
4	9	0.000000	0.000000	0.726006

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.4650	1.8746	1.8746	1.8746
2	-0.0920	2.1810	2.1810	2.1810
3	-0.0920	2.1810	2.1810	2.1810
4	1.7189	1.1728	1.1728	1.1728

Molecule 53-Diphenylmethanide
Energy: -500.466362080
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000012	-0.987929	-0.000304
2	1	0.000112	-2.076212	-0.000437
3	6	-1.289213	-0.409180	-0.006909
4	6	-1.614196	0.956378	-0.211121
5	6	-2.419631	-1.257639	0.163387
6	6	-2.919452	1.408706	-0.213909
7	1	-0.829313	1.669922	-0.417436
8	6	-3.711006	-0.795587	0.160055
9	1	-2.234776	-2.319132	0.309770
10	6	-3.995554	0.557296	-0.021335
11	1	-3.098526	2.468792	-0.383505
12	1	-4.524500	-1.503991	0.303999
13	1	-5.016263	0.925750	-0.019935
14	6	1.289149	-0.408931	0.006547
15	6	2.419585	-1.257549	-0.163380
16	6	1.614162	0.956484	0.210629
17	6	3.710974	-0.795713	-0.159620
18	1	2.234615	-2.319007	-0.309881
19	6	2.919571	1.408697	0.213968
20	1	0.829442	1.670250	0.416790
21	6	3.995568	0.557218	0.021899
22	1	4.524465	-1.504183	-0.303148
23	1	3.098578	2.468799	0.383460
24	1	5.016349	0.925511	0.020885

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.7997	1.6625	1.6625	1.6625
2	0.0034	1.9743	1.9743	1.9743
3	1.9863	1.6138	1.6138	1.6138
4	1.8915	1.6593	1.6593	1.6593
5	1.8972	1.6601	1.6601	1.6601
6	1.9129	1.6694	1.6694	1.6694
7	0.0313	1.9509	1.9509	1.9509
8	1.9084	1.6699	1.6699	1.6699
9	0.0293	1.9783	1.9783	1.9783
10	1.8587	1.6735	1.6735	1.6735
11	0.0322	1.9814	1.9814	1.9814
12	0.0311	1.9842	1.9842	1.9842

13	0.0194	2.0006	2.0006	2.0006
14	1.9863	1.6138	1.6138	1.6138
15	1.8973	1.6601	1.6601	1.6601
16	1.8915	1.6593	1.6593	1.6593
17	1.9084	1.6699	1.6699	1.6699
18	0.0293	1.9783	1.9783	1.9783
19	1.9129	1.6694	1.6694	1.6694
20	0.0313	1.9509	1.9509	1.9509
21	1.8587	1.6734	1.6734	1.6734
22	0.0311	1.9842	1.9842	1.9842
23	0.0322	1.9814	1.9814	1.9814
24	0.0194	2.0006	2.0006	2.0006

Molecule 54-Triphenylmethanide
Energy: -730.818552012
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000068	0.000184	-0.000131
2	6	0.239781	-1.427388	-0.000123
3	6	1.373934	-2.007392	-0.605202
4	6	-0.642594	-2.346088	0.605054
5	6	1.602979	-3.367168	-0.602011
6	1	2.082460	-1.356804	-1.106593
7	6	-0.414737	-3.706060	0.602000
8	1	-1.524763	-1.962696	1.106479
9	6	0.713114	-4.245109	0.000013
10	1	2.492974	-3.752083	-1.094788
11	1	-1.130093	-4.360612	1.094853
12	1	0.892948	-5.315606	0.000064
13	6	1.116353	0.921494	-0.000048
14	6	2.353580	0.615892	0.603961
15	6	1.051452	2.194315	-0.603915
16	6	3.417572	1.493009	0.601068
17	1	2.462912	-0.340325	1.104300
18	6	2.114696	3.072353	-0.600517
19	1	0.133618	2.483308	-1.104602
20	6	3.320266	2.739948	0.000457
21	1	4.342391	1.200096	1.092987
22	1	2.002881	4.036071	-1.092279
23	1	4.157507	3.430841	0.000697
24	6	-1.356237	0.506150	-0.000069
25	6	-2.425913	-0.187012	-0.603628
26	6	-1.710568	1.730524	0.603519
27	6	-3.718055	0.294434	-0.600577
28	1	-2.216961	-1.126593	-1.103789
29	6	-3.002301	2.213075	0.600269
30	1	-0.937423	2.303610	1.103958
31	6	-4.033294	1.504927	-0.000235
32	1	-4.496556	-0.284676	-1.092157
33	1	-3.211349	3.160557	1.091855
34	1	-5.050310	1.884375	-0.000297

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8682	1.5961	1.5961	1.5961
2	1.9962	1.6014	1.6014	1.6014
3	1.9134	1.6515	1.6515	1.6515
4	1.9134	1.6515	1.6515	1.6515
5	1.9151	1.6668	1.6668	1.6668
6	0.0394	1.9496	1.9496	1.9496
7	1.9151	1.6667	1.6667	1.6667
8	0.0394	1.9496	1.9496	1.9496
9	1.8795	1.6704	1.6704	1.6704
10	0.0360	1.9784	1.9784	1.9784
11	0.0360	1.9784	1.9784	1.9784
12	0.0271	1.9926	1.9926	1.9926
13	1.9962	1.6014	1.6014	1.6014

14	1.9133	1.6514	1.6514	1.6514
15	1.9133	1.6515	1.6515	1.6515
16	1.9151	1.6667	1.6667	1.6667
17	0.0394	1.9496	1.9496	1.9496
18	1.9151	1.6666	1.6666	1.6666
19	0.0394	1.9496	1.9496	1.9496
20	1.8795	1.6703	1.6703	1.6703
21	0.0360	1.9784	1.9784	1.9784
22	0.0360	1.9784	1.9784	1.9784
23	0.0271	1.9926	1.9926	1.9926
24	1.9962	1.6014	1.6014	1.6014
25	1.9133	1.6514	1.6514	1.6514
26	1.9133	1.6514	1.6514	1.6514
27	1.9151	1.6667	1.6667	1.6667
28	0.0394	1.9496	1.9496	1.9496
29	1.9151	1.6667	1.6667	1.6667
30	0.0394	1.9496	1.9496	1.9496
31	1.8795	1.6703	1.6703	1.6703
32	0.0360	1.9784	1.9784	1.9784
33	0.0360	1.9784	1.9784	1.9784
34	0.0271	1.9926	1.9926	1.9926

Molecule 55-cycloprop-2-en-1-ide
Energy: -115.563569539
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.026693	-0.430467	-0.645170
2	6	-0.026693	-0.430467	0.645170
3	6	-0.026693	0.973069	0.000000
4	1	-0.267768	-1.016139	-1.524638
5	1	-0.267768	-1.016139	1.524638
6	1	1.016007	1.359472	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8086	1.7410	1.7410	1.7410
2	1.8086	1.7410	1.7410	1.7410
3	1.4382	1.9431	1.9431	1.9431
4	0.0132	2.0819	2.0819	2.0819
5	0.0132	2.0819	2.0819	2.0819
6	-0.0817	2.0622	2.0622	2.0622

Molecule 56-cycloheptateiene-1-ide
Energy: -269.941665062
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.262950	-0.724675	0.229361
2	6	-1.780430	-0.667270	0.023716
3	6	-1.780123	0.667413	-0.023601
4	6	1.090035	-1.164176	-0.253319
5	6	-0.263062	0.724247	-0.229557
6	6	1.836615	0.000137	0.000171
7	6	1.089790	1.164260	0.253116
8	1	-0.184502	-0.661605	1.333891
9	1	-2.575861	-1.408355	0.046193
10	1	-2.575480	1.408607	-0.045898
11	1	-0.184524	0.661278	-1.334088
12	1	1.507248	-2.160715	-0.125108
13	1	2.927179	0.000228	0.000382
14	1	1.506697	2.160948	0.125298

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9197	1.6208	1.6208	1.6208
2	1.8990	1.6938	1.6938	1.6938
3	1.8990	1.6937	1.6937	1.6937
4	1.7390	1.7326	1.7326	1.7326
5	1.9197	1.6207	1.6207	1.6207
6	1.8737	1.6921	1.6921	1.6921

7	1.7391	1.7325	1.7325	1.7325
8	-0.0014	1.9471	1.9471	1.9471
9	0.0256	2.0331	2.0331	2.0331
10	0.0256	2.0331	2.0331	2.0331
11	-0.0014	1.9471	1.9471	1.9471
12	-0.0238	2.0639	2.0639	2.0639
13	0.0097	2.0296	2.0296	2.0296
14	-0.0238	2.0639	2.0639	2.0639

Molecule 57-Carbon
Energy: -37.6564888109
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0000	2.1181	2.1181	2.1181

Molecule 58-CLi4
Energy: -67.6804569044
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	3	1.062842	1.062842	1.062842
3	3	-1.062842	-1.062842	1.062842
4	3	-1.062842	1.062842	-1.062842
5	3	1.062842	-1.062842	-1.062842

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.2100	2.1278	2.1278	2.1278
2	2.1974	3.1521	3.1521	3.1521
3	2.1974	3.1521	3.1521	3.1521
4	2.1974	3.1521	3.1521	3.1521
5	2.1974	3.1521	3.1521	3.1521

Molecule 59-methane
Energy: -40.3776582100
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	1	0.629669	0.629669	0.629669
3	1	-0.629669	-0.629669	0.629669
4	1	-0.629669	0.629669	-0.629669
5	1	0.629669	-0.629669	-0.629669

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8143	1.7803	1.7803	1.7803
2	0.0464	1.9773	1.9773	1.9773
3	0.0464	1.9773	1.9773	1.9773
4	0.0464	1.9773	1.9773	1.9773
5	0.0464	1.9773	1.9773	1.9773

Molecule 60-bromomethane.log
Energy: -2611.09148638
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.500224
2	1	0.000000	1.030030	-1.847617
3	1	0.892032	-0.515015	-1.847617
4	1	-0.892032	-0.515015	-1.847617
5	35	0.000000	0.000000	0.415548

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9420	1.7448	1.7448	1.7448
2	0.0784	1.9251	1.9251	1.9251
3	0.0784	1.9251	1.9251	1.9251
4	0.0784	1.9251	1.9251	1.9251
5	27.8228	1.9369	1.9369	1.9369

Molecule 61-dibromomethane
Energy: -5181.80611677
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.928337
2	1	0.895357	0.000000	1.541051
3	1	-0.895357	0.000000	1.541051
4	35	0.000000	-1.586725	-0.123602
5	35	0.000000	1.586725	-0.123602

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0247	1.7232	1.7232	1.7232
2	0.1013	1.8874	1.8874	1.8874
3	0.1013	1.8874	1.8874	1.8874
4	27.8864	1.9275	1.9275	1.9275
5	27.8864	1.9275	1.9275	1.9275

Molecule 62-bromoform
Energy: -7752.52102089
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.546365
2	1	0.000000	0.000000	1.629742
3	35	0.000000	1.808429	-0.046742
4	35	-1.566146	-0.904215	-0.046742
5	35	1.566146	-0.904215	-0.046742

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0847	1.7130	1.7130	1.7130
2	0.1176	1.8602	1.8602	1.8602
3	27.9325	1.9190	1.9190	1.9190
4	27.9326	1.9191	1.9191	1.9191
5	27.9326	1.9191	1.9191	1.9191

Molecule 63-carbontetrabromide
Energy: -10323.2340146
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	35	1.101512	1.101512	1.101512
3	35	-1.101512	-1.101512	1.101512
4	35	-1.101512	1.101512	-1.101512
5	35	1.101512	-1.101512	-1.101512

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1334	1.7108	1.7108	1.7108
2	27.9667	1.9115	1.9115	1.9115
3	27.9667	1.9115	1.9115	1.9115
4	27.9667	1.9115	1.9115	1.9115
5	27.9667	1.9115	1.9115	1.9115

Molecule 64-carbontetrafloride
Energy: -436.818075299
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	9	0.761146	0.761146	0.761146
3	9	-0.761146	-0.761146	0.761146
4	9	-0.761146	0.761146	-0.761146
5	9	0.761146	-0.761146	-0.761146

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2797	1.3688	1.3688	1.3688
2	1.9301	1.1292	1.1292	1.1292
3	1.9301	1.1292	1.1292	1.1292
4	1.9301	1.1292	1.1292	1.1292
5	1.9301	1.1292	1.1292	1.1292

Molecule 65-carbondioxide

Energy: -188.195078490
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	1.158704
3	8	0.000000	0.000000	-1.158704

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.3668	1.4654	1.4654	1.4654
2	1.8166	1.3169	1.3169	1.3169
3	1.8166	1.3169	1.3169	1.3169

Molecule 66-methanol
Energy: -115.454787609
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.046218	0.658810	0.000000
2	1	1.089050	0.976820	0.000000
3	1	-0.439304	1.069447	0.892627
4	1	-0.439304	1.069447	-0.892627
5	8	0.046218	-0.748560	0.000000
6	1	-0.857498	-1.080091	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9523	1.6825	1.6825	1.6825
2	0.0573	1.9157	1.9157	1.9157
3	0.0438	1.9261	1.9261	1.9261
4	0.0438	1.9261	1.9261	1.9261
5	1.7288	1.3213	1.3213	1.3213
6	0.1740	1.6916	1.6916	1.6916

Molecule 67-methyllithium
Energy: -47.1959345769
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.384481
2	1	0.000000	1.015141	0.801989
3	1	0.879138	-0.507571	0.801989
4	1	-0.879138	-0.507571	0.801989
5	3	0.000000	0.000000	-1.570950

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.5477	1.8707	1.8707	1.8707
2	-0.0071	2.0356	2.0356	2.0356
3	-0.0071	2.0355	2.0355	2.0355
4	-0.0071	2.0355	2.0355	2.0355
5	2.4735	2.8684	2.8684	2.8684

Molecule 68-carbondisulfide
Energy: -833.817633525
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	16	0.000000	0.000000	1.541115
3	16	0.000000	0.000000	-1.541115

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0822	1.7290	1.7290	1.7290
2	9.9589	1.9317	1.9317	1.9317
3	9.9589	1.9317	1.9317	1.9317

Molecule 69-hydrogencyanide
Energy: -93.1721699611
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.495715
2	1	0.000000	0.000000	-1.567217
3	7	0.000000	0.000000	0.648786

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0473	1.7017	1.7017	1.7017
2	0.1476	2.0537	2.0537	2.0537
3	1.8051	1.5841	1.5841	1.5841

Molecule 70-methanethiol
Energy: -438.295649623
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.047681	1.141840	0.000000
2	1	-1.091464	1.455703	0.000000
3	1	0.430614	1.545869	0.891832
4	1	0.430614	1.545869	-0.891832
5	16	-0.047681	-0.660194	0.000000
6	1	1.279215	-0.835369	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8812	1.7417	1.7417	1.7417
2	0.0621	1.9382	1.9382	1.9382
3	0.0541	1.9361	1.9361	1.9361
4	0.0541	1.9361	1.9361	1.9361
5	9.8720	1.9232	1.9232	1.9232
6	0.0765	2.0531	2.0531	2.0531

Molecule 71-ethene
Energy: -78.3314830328
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.660018
2	1	0.000000	0.924204	1.229691
3	1	0.000000	-0.924204	1.229691
4	6	0.000000	0.000000	-0.660018
5	1	0.000000	-0.924204	-1.229691
6	1	0.000000	0.924204	-1.229691

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8888	1.7443	1.7443	1.7443
2	0.0556	1.9817	1.9817	1.9817
3	0.0556	1.9817	1.9817	1.9817
4	1.8888	1.7443	1.7443	1.7443
5	0.0556	1.9817	1.9817	1.9817
6	0.0556	1.9817	1.9817	1.9817

Molecule 72-chloroethene
Energy: -537.665358678
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.285965	1.029657	0.000000
2	1	1.611341	2.063587	0.000000
3	6	0.000000	0.754019	0.000000
4	1	-0.776731	1.509427	0.000000
5	17	-0.622972	-0.854461	0.000000
6	1	2.040129	0.250773	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8924	1.7275	1.7275	1.7275
2	0.0676	1.9761	1.9761	1.9761
3	1.9920	1.6840	1.6840	1.6840
4	0.0749	1.9416	1.9416	1.9416
5	9.9045	1.7342	1.7342	1.7342
6	0.0685	1.9793	1.9793	1.9793

Molecule 73-1-2-dichloroethene
Energy: -996.994936915
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	-0.659009	0.954362
2	1	0.000000	-1.207719	1.887705

3	6	0.000000	0.659009	0.954362
4	1	0.000000	1.207719	1.887705
5	17	0.000000	-1.638108	-0.447875
6	17	0.000000	1.638108	-0.447875

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9868	1.6697	1.6697	1.6697
2	0.0813	1.9357	1.9357	1.9357
3	1.9868	1.6697	1.6697	1.6697
4	0.0813	1.9357	1.9357	1.9357
5	9.9319	1.7293	1.7293	1.7293
6	9.9319	1.7293	1.7293	1.7293

Molecule 74-1-1-dichloroethene
Energy: -996.992094444
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	1.733435
2	1	0.000000	0.934190	2.280461
3	6	0.000000	0.000000	0.417900
4	17	0.000000	-1.444448	-0.513792
5	1	0.000000	-0.934190	2.280461
6	17	0.000000	1.444448	-0.513792

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8937	1.7135	1.7135	1.7135
2	0.0751	1.9683	1.9683	1.9683
3	2.0757	1.6356	1.6356	1.6356
4	9.9401	1.7252	1.7252	1.7252
5	0.0751	1.9683	1.9683	1.9683
6	9.9401	1.7252	1.7252	1.7252

Molecule 75-ethyne
Energy: -77.0810509471
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.597689
2	1	0.000000	0.000000	1.665829
3	6	0.000000	0.000000	-0.597689
4	1	0.000000	0.000000	-1.665829

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8898	1.7705	1.7705	1.7705
2	0.1102	2.0597	2.0597	2.0597
3	1.8898	1.7705	1.7705	1.7705
4	0.1102	2.0597	2.0597	2.0597

Molecule 76-chloroethyne
Energy: -536.403384969
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.615110
2	6	0.000000	0.000000	-1.808920
3	1	0.000000	0.000000	-2.876483
4	17	0.000000	0.000000	1.024745

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9780	1.6707	1.6707	1.6707
2	1.8852	1.7546	1.7546	1.7546
3	0.1136	2.0533	2.0533	2.0533
4	10.0231	1.7264	1.7264	1.7264

Molecule 77-acetonitrile
Energy: -132.380096558
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.172979	-0.000009	0.000023
2	1	1.545729	-0.887176	0.513115
3	1	1.545776	0.887992	0.511638

4	1	1.545805	-0.000872	-1.024821
5	6	-0.280354	0.000039	-0.000016
6	7	-1.427580	-0.000017	0.000003

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9209	1.7178	1.7178	1.7178
2	0.0807	1.9332	1.9332	1.9332
3	0.0807	1.9332	1.9332	1.9332
4	0.0807	1.9332	1.9332	1.9332
5	2.0777	1.6153	1.6153	1.6153
6	1.7592	1.5819	1.5819	1.5819

Molecule 78-acetic-acid
Energy: -228.578990913
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.385280	-0.120255	-0.000016
2	1	1.909207	0.832653	-0.001387
3	1	1.661301	-0.701948	0.881304
4	1	1.661475	-0.705197	-0.879089
5	6	-0.084974	0.119919	-0.000189
6	8	-0.786141	-1.023214	-0.000037
7	1	-1.728296	-0.788189	0.000584
8	8	-0.627049	1.193801	0.000014

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8815	1.6992	1.6992	1.6992
2	0.0668	1.9347	1.9347	1.9347
3	0.0692	1.9392	1.9392	1.9392
4	0.0692	1.9393	1.9393	1.9393
5	2.2264	1.5099	1.5099	1.5099
6	1.7965	1.3058	1.3058	1.3058
7	0.1985	1.7053	1.7053	1.7053
8	1.6919	1.3272	1.3272	1.3272

Molecule 79-cyclopropane
Energy: -117.523890422
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.746405	0.430945	0.000000
2	6	0.000000	-0.861792	0.000000
3	6	-0.746370	0.430892	0.000000
4	1	1.257328	0.725866	0.909985
5	1	1.257328	0.725866	-0.909985
6	1	-0.000064	-1.451760	0.909975
7	1	-0.000064	-1.451760	-0.909975
8	1	-1.257369	0.725761	-0.909970
9	1	-1.257369	0.725761	0.909970

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8945	1.6774	1.6774	1.6774
2	1.8945	1.6775	1.6775	1.6775
3	1.8945	1.6774	1.6774	1.6774
4	0.0528	1.9410	1.9410	1.9410
5	0.0528	1.9410	1.9410	1.9410
6	0.0528	1.9410	1.9410	1.9410
7	0.0528	1.9410	1.9410	1.9410
8	0.0528	1.9410	1.9410	1.9410
9	0.0528	1.9410	1.9410	1.9410

Molecule 80-cyclobutane
Energy: -156.716633006
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.086416	1.085716	-0.000171
2	6	1.085718	-0.086418	-0.000038
3	6	-0.086418	-1.085717	-0.000088
4	6	-1.085716	0.086417	0.000287

5	1	0.137545	1.726201	0.882457
6	1	0.137259	1.725619	-0.883237
7	1	1.725801	-0.137371	0.882891
8	1	1.726018	-0.137428	-0.882808
9	1	-0.137290	-1.726095	0.882633
10	1	-0.137512	-1.725717	-0.883068
11	1	-1.725489	0.137392	0.883442
12	1	-1.726334	0.137408	-0.882253

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9154	1.6650	1.6650	1.6650
2	1.9154	1.6650	1.6650	1.6650
3	1.9154	1.6650	1.6650	1.6650
4	1.9154	1.6650	1.6650	1.6650
5	0.0423	1.9312	1.9312	1.9312
6	0.0423	1.9312	1.9312	1.9312
7	0.0423	1.9312	1.9312	1.9312
8	0.0423	1.9312	1.9312	1.9312
9	0.0423	1.9312	1.9312	1.9312
10	0.0423	1.9312	1.9312	1.9312
11	0.0423	1.9312	1.9312	1.9312
12	0.0423	1.9312	1.9312	1.9312

Molecule 81-cyclopentane
Energy: -195.941403551
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	-1.228792	0.365966
2	6	-0.334393	-0.682738	-1.017903
3	6	0.334393	0.682738	-1.017903
4	6	0.000000	1.228792	0.365966
5	6	0.000000	0.000000	1.292750
6	1	-0.694266	-2.005632	0.694755
7	1	0.995605	-1.682328	0.343858
8	1	-1.418268	-0.559626	-1.124338
9	1	0.001733	-1.334851	-1.828054
10	1	1.418268	0.559626	-1.124338
11	1	-0.001733	1.334851	-1.828054
12	1	0.694266	2.005632	0.694755
13	1	-0.995605	1.682328	0.343858
14	1	0.874996	-0.005866	1.947155
15	1	-0.874996	0.005866	1.947155

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9175	1.6580	1.6580	1.6580
2	1.9164	1.6559	1.6559	1.6559
3	1.9164	1.6559	1.6559	1.6559
4	1.9175	1.6580	1.6580	1.6580
5	1.9180	1.6602	1.6602	1.6602
6	0.0422	1.9296	1.9296	1.9296
7	0.0399	1.9184	1.9184	1.9184
8	0.0408	1.9227	1.9227	1.9227
9	0.0432	1.9337	1.9337	1.9337
10	0.0408	1.9227	1.9227	1.9227
11	0.0432	1.9337	1.9337	1.9337
12	0.0422	1.9296	1.9296	1.9296
13	0.0399	1.9184	1.9184	1.9184
14	0.0407	1.9218	1.9218	1.9218
15	0.0407	1.9218	1.9218	1.9218

Molecule 82-cyclohexane
Energy: -235.133106254
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.510709
2	6	-0.386799	1.208543	-0.653581
3	6	0.386799	1.208543	0.653581

4	6	0.000000	0.000000	1.510709
5	6	-0.386799	-1.208543	0.653581
6	6	0.386799	-1.208543	-0.653581
7	1	-0.835129	-0.262814	-2.167682
8	1	-0.217084	2.135543	-1.208236
9	1	1.458889	1.180787	0.427843
10	1	0.835129	-0.262814	2.167682
11	1	-0.217084	-2.135543	1.208236
12	1	0.217084	-2.135543	-1.208236
13	1	0.217084	2.135543	1.208236
14	1	-1.458889	1.180787	-0.427843
15	1	0.835129	0.262814	-2.167682
16	1	1.458889	-1.180787	-0.427843
17	1	-1.458889	-1.180787	0.427843
18	1	-0.835129	0.262814	2.167682

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9195	1.6569	1.6569	1.6569
2	1.9187	1.6539	1.6539	1.6539
3	1.9187	1.6539	1.6539	1.6539
4	1.9195	1.6569	1.6569	1.6569
5	1.9187	1.6539	1.6539	1.6539
6	1.9187	1.6539	1.6539	1.6539
7	0.0401	1.9207	1.9207	1.9207
8	0.0425	1.9221	1.9221	1.9221
9	0.0391	1.9153	1.9153	1.9153
10	0.0401	1.9207	1.9207	1.9207
11	0.0425	1.9221	1.9221	1.9221
12	0.0425	1.9221	1.9221	1.9221
13	0.0425	1.9221	1.9221	1.9221
14	0.0391	1.9153	1.9153	1.9153
15	0.0401	1.9207	1.9207	1.9207
16	0.0391	1.9153	1.9153	1.9153
17	0.0391	1.9153	1.9153	1.9153
18	0.0401	1.9207	1.9207	1.9207

Molecule 83-benzene
Energy: -231.525068136
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.395399	-1.326485	0.000000
2	6	0.951148	-1.005619	0.000022
3	6	1.346516	0.320828	-0.000006
4	6	0.395334	1.326504	0.000005
5	6	-0.951099	1.005665	0.000008
6	6	-1.346500	-0.320893	-0.000014
7	1	-0.705277	-2.366516	-0.000010
8	1	1.696767	-1.794123	-0.000022
9	1	2.402147	0.572468	-0.000044
10	1	0.705345	2.366496	-0.000019
11	1	-1.696816	1.794076	0.000018
12	1	-2.402163	-0.572401	-0.000011

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9418	1.6597	1.6597	1.6597
2	1.9418	1.6597	1.6597	1.6597
3	1.9418	1.6597	1.6597	1.6597
4	1.9418	1.6597	1.6597	1.6597
5	1.9418	1.6597	1.6597	1.6597
6	1.9418	1.6597	1.6597	1.6597
7	0.0581	1.9596	1.9596	1.9596
8	0.0581	1.9595	1.9595	1.9595
9	0.0582	1.9595	1.9595	1.9595
10	0.0581	1.9596	1.9596	1.9596
11	0.0581	1.9595	1.9595	1.9595
12	0.0582	1.9595	1.9595	1.9595

Molecule 84-cyclobuta-1-3-diene
Energy: -154.193688394
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.778307	-0.661872	0.000001
2	6	0.778307	-0.661872	0.000000
3	6	0.778307	0.661872	0.000001
4	6	-0.778307	0.661872	0.000000
5	1	-1.543310	-1.427562	0.000001
6	1	1.543310	-1.427562	-0.000001
7	1	1.543310	1.427563	0.000001
8	1	-1.543310	1.427563	-0.000001

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9356	1.6856	1.6856	1.6856
2	1.9356	1.6856	1.6856	1.6856
3	1.9356	1.6856	1.6856	1.6856
4	1.9356	1.6856	1.6856	1.6856
5	0.0644	2.0019	2.0019	2.0019
6	0.0644	2.0019	2.0019	2.0019
7	0.0644	2.0019	2.0019	2.0019
8	0.0644	2.0019	2.0019	2.0019

Molecule 85-carbon-monoxide
Energy: -113.059681128
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.644061
2	8	0.000000	0.000000	0.483046

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1021	1.8719	1.8719	1.8719
2	1.8979	1.3247	1.3247	1.3247

Molecule 86-Formic-acid
Energy: -189.373345383
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.130553	0.402804	0.000003
2	1	0.112664	1.499591	0.000038
3	8	-1.105156	-0.090568	-0.000012
4	1	-1.044886	-1.061355	0.000076
5	8	1.123769	-0.266314	-0.000004

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1970	1.5641	1.5641	1.5641
2	0.0872	1.9367	1.9367	1.9367
3	1.8045	1.3078	1.3078	1.3078
4	0.2045	1.7073	1.7073	1.7073
5	1.7068	1.3286	1.3286	1.3286

Molecule 87-formaldehyde
Energy: -114.238740514
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.527858
2	1	0.000000	0.941200	-1.106024
3	1	0.000000	-0.941200	-1.106024
4	8	0.000000	0.000000	0.672400

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1128	1.6785	1.6785	1.6785
2	0.0659	1.9521	1.9521	1.9521
3	0.0659	1.9521	1.9521	1.9521
4	1.7553	1.3318	1.3318	1.3318

Molecule 88-formyl-chloride
Energy: -573.588506206
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.658254	0.423656	0.000000
2	1	-0.742992	1.517985	-0.000001
3	17	1.011714	-0.081001	0.000000
4	8	-1.563328	-0.335362	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1941	1.6259	1.6259	1.6259
2	0.0957	1.9333	1.9333	1.9333
3	9.9217	1.7329	1.7329	1.7329
4	1.7884	1.3221	1.3221	1.3221

Molecule 89-diazomethane
Energy: -148.351527624
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.132107	-0.000033	0.000000
2	1	-1.635085	-0.953960	0.000000
3	1	-1.633799	0.954788	0.000000
4	7	0.153347	-0.000089	0.000000
5	7	1.284014	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8530	1.7122	1.7122	1.7122
2	0.0689	1.9785	1.9785	1.9785
3	0.0688	1.9785	1.9785	1.9785
4	2.1121	1.4085	1.4085	1.4085
5	1.8973	1.5403	1.5403	1.5403

Molecule 90-trifluoro-nitroso-methane
Energy: -466.724135006
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.343690	-0.000573	-0.000010
2	9	0.991765	0.396931	-1.081386
3	9	0.226963	-1.309772	-0.004375
4	9	0.994563	0.389127	1.082556
5	7	-0.977654	0.714758	0.004058
6	8	-1.892272	-0.035806	0.000064

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2381	1.4002	1.4002	1.4002
2	1.9333	1.1320	1.1320	1.1320
3	1.9326	1.1310	1.1310	1.1310
4	1.9333	1.1320	1.1320	1.1320
5	2.0381	1.4523	1.4523	1.4523
6	1.9247	1.3039	1.3039	1.3039

Molecule 91-phosphonoformic-acid
Energy: -756.433858217
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.174202	0.040393	0.006974
2	8	0.979370	1.489578	-0.220716
3	1	0.211537	2.077327	-0.110687
4	15	0.666285	-0.019562	0.116688
5	8	1.153813	-0.599025	1.368803
6	8	1.140240	-0.771451	-1.199009
7	1	1.531932	-1.638660	-1.018488
8	8	-1.753511	1.097048	0.005515
9	8	-1.765128	-1.137917	-0.031425
10	1	-2.730797	-1.013456	-0.048345

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1698	1.5231	1.5231	1.5231
2	1.7477	1.3097	1.3097	1.3097
3	0.2027	1.7060	1.7060	1.7060
4	10.5061	1.6765	1.6765	1.6765
5	1.5924	1.3453	1.3453	1.3453

6	1.7455	1.3118	1.3118	1.3118
7	0.2235	1.6923	1.6923	1.6923
8	1.7458	1.3198	1.3198	1.3198
9	1.8474	1.2993	1.2993	1.2993
10	0.2190	1.6993	1.6993	1.6993

Molecule 92-acetyl-chloride
Energy: -612.795371279
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.323882	-0.973924	-0.000015
2	1	1.107907	-1.581460	-0.880475
3	1	1.108858	-1.580728	0.881187
4	1	2.366604	-0.660269	-0.000606
5	6	0.452614	0.234130	-0.000012
6	8	0.804806	1.364310	0.000002
7	17	-1.275340	-0.156074	0.000003

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8897	1.7008	1.7008	1.7008
2	0.0739	1.9393	1.9393	1.9393
3	0.0740	1.9393	1.9393	1.9393
4	0.0717	1.9338	1.9338	1.9338
5	2.2244	1.5728	1.5728	1.5728
6	1.7729	1.3205	1.3205	1.3205
7	9.8934	1.7325	1.7325	1.7325

Molecule 93-nitromethane
Energy: -244.488683688
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.308847	0.000798	-0.003088
2	1	1.647055	-0.901364	-0.505202
3	1	1.616345	-0.007570	1.042390
4	1	1.646476	0.910781	-0.491233
5	7	-0.167011	0.000010	-0.010141
6	8	-0.723811	-1.075933	0.002725
7	8	-0.725423	1.075095	0.002720

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9547	1.6777	1.6777	1.6777
2	0.0790	1.9153	1.9153	1.9153
3	0.0867	1.9174	1.9174	1.9174
4	0.0789	1.9153	1.9153	1.9153
5	2.2492	1.3511	1.3511	1.3511
6	1.7756	1.3117	1.3117	1.3117
7	1.7758	1.3117	1.3117	1.3117

Molecule 94-methanimine
Energy: -94.3697583293
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.056377	0.581272	0.000000
2	1	0.848782	1.197554	0.000000
3	1	-1.010229	1.110305	0.000000
4	1	0.894342	-1.050223	0.000000
5	7	-0.056377	-0.677895	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0045	1.7045	1.7045	1.7045
2	0.0595	1.9666	1.9666	1.9666
3	0.0639	1.9575	1.9575	1.9575
4	0.1212	1.8203	1.8203	1.8203
5	1.7510	1.5439	1.5439	1.5439

Molecule 95-propa-1-2-diene
Energy: -116.283638430
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	-1.297593	0.000004
2	1	-0.657731	-1.856056	-0.657895
3	1	0.657763	-1.856024	0.657899
4	6	0.000000	0.000000	-0.000010
5	6	0.000000	1.297593	0.000004
6	1	0.657731	1.856056	-0.657895
7	1	-0.657763	1.856024	0.657899

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8680	1.7423	1.7423	1.7423
2	0.0675	1.9864	1.9864	1.9864
3	0.0675	1.9864	1.9864	1.9864
4	1.9939	1.6686	1.6686	1.6686
5	1.8680	1.7423	1.7423	1.7423
6	0.0675	1.9864	1.9864	1.9864
7	0.0675	1.9864	1.9864	1.9864

Molecule 96-prop-1-ene
Energy: -117.524877843
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.269810	-0.225040	0.000046
2	1	-2.233361	0.272923	0.000242
3	1	-1.277954	-1.312384	-0.000124
4	6	-0.138460	0.458473	-0.000183
5	1	-0.189587	1.545483	0.000156
6	6	1.229612	-0.156390	0.000010
7	1	2.013027	0.602711	-0.009183
8	1	1.383133	-0.777980	0.885866
9	1	1.376692	-0.793007	-0.876192

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8699	1.7353	1.7353	1.7353
2	0.0513	1.9849	1.9849	1.9849
3	0.0512	1.9886	1.9886	1.9886
4	1.9474	1.6761	1.6761	1.6761
5	0.0522	1.9556	1.9556	1.9556
6	1.8750	1.7172	1.7172	1.7172
7	0.0488	1.9457	1.9457	1.9457
8	0.0521	1.9497	1.9497	1.9497
9	0.0521	1.9497	1.9497	1.9497

Molecule 97-hexafluoropropan-2-ol
Energy: -788.506328801
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.277972	-0.134587	-0.031574
2	6	-0.003167	0.550716	-0.491959
3	1	-0.001412	0.504792	-1.587923
4	6	1.260166	-0.160554	-0.025532
5	9	-2.328924	0.434332	-0.621805
6	9	-1.264460	-1.425481	-0.374767
7	9	-1.448488	-0.054841	1.281133
8	9	1.284339	-0.381554	1.282012
9	9	2.310623	0.620576	-0.328008
10	9	1.429506	-1.322378	-0.653359
11	8	-0.047581	1.843577	-0.001091
12	1	0.664543	2.377258	-0.375808

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2120	1.4170	1.4170	1.4170
2	2.0142	1.5284	1.5284	1.5284
3	0.0734	1.8480	1.8480	1.8480
4	2.2070	1.4173	1.4173	1.4173
5	1.9211	1.1336	1.1336	1.1336
6	1.9182	1.1334	1.1334	1.1334
7	1.9273	1.1323	1.1323	1.1323

8	1.9280	1.1322	1.1322	1.1322
9	1.9149	1.1339	1.1339	1.1339
10	1.9212	1.1333	1.1333	1.1333
11	1.7709	1.3050	1.3050	1.3050
12	0.1918	1.6799	1.6799	1.6799

Molecule 98-trifluoroethan-1-ol
Energy: -451.984902507
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.364027	0.196179	0.000000
2	6	1.138269	0.243724	0.000000
3	1	1.440292	0.800474	-0.893904
4	1	1.440292	0.800474	0.893904
5	9	-0.848676	1.448282	0.000000
6	9	-0.848676	-0.423182	1.076920
7	9	-0.848676	-0.423182	-1.076920
8	8	1.602847	-1.070745	0.000000
9	1	2.565441	-1.091676	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2100	1.4238	1.4238	1.4238
2	1.9879	1.5973	1.5973	1.5973
3	0.0625	1.8853	1.8853	1.8853
4	0.0625	1.8853	1.8853	1.8853
5	1.9051	1.1360	1.1360	1.1360
6	1.9139	1.1346	1.1346	1.1346
7	1.9139	1.1346	1.1346	1.1346
8	1.7544	1.3119	1.3119	1.3119
9	0.1897	1.6856	1.6856	1.6856

Molecule 99-trinitromethane
Energy: -652.662950501
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000157	0.000072	-0.542505
2	1	-0.000243	0.000143	-1.629856
3	8	0.407230	2.223185	-0.636090
4	8	1.461967	1.086859	0.877629
5	8	-2.129437	-0.757873	-0.637141
6	8	-1.671891	0.720711	0.879317
7	8	0.211695	-1.808107	0.879371
8	8	1.720707	-1.464923	-0.637449
9	7	0.701747	-1.216529	-0.043804
10	7	0.702873	1.216087	-0.043873
11	7	-1.404762	0.000529	-0.043779

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1307	1.5267	1.5267	1.5267
2	0.1137	1.8403	1.8403	1.8403
3	1.8251	1.3043	1.3043	1.3043
4	1.8413	1.3010	1.3010	1.3010
5	1.8251	1.3043	1.3043	1.3043
6	1.8412	1.3010	1.3010	1.3010
7	1.8411	1.3011	1.3011	1.3011
8	1.8251	1.3043	1.3043	1.3043
9	2.2522	1.3388	1.3388	1.3388
10	2.2522	1.3388	1.3388	1.3388
11	2.2522	1.3388	1.3388	1.3388

Molecule 100-trichloroethan-1-amine
Energy: -1512.76995791
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.128203	0.000128	0.066669
2	6	0.894461	0.000262	1.209461
3	1	0.672577	0.880715	1.818186

4	1	0.672458	-0.879955	1.818509
5	1	2.771582	0.840469	0.900279
6	1	2.770357	-0.841176	0.896131
7	17	-1.746572	-0.000130	0.779078
8	17	0.074725	-1.441161	-0.926938
9	17	0.074265	1.440975	-0.927318
10	7	2.239198	0.000425	0.741163

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1530	1.6161	1.6161	1.6161
2	1.9696	1.6234	1.6234	1.6234
3	0.0573	1.9006	1.9006	1.9006
4	0.0572	1.9006	1.9006	1.9006
5	0.1251	1.8009	1.8009	1.8009
6	0.1251	1.8009	1.8009	1.8009
7	9.9197	1.7227	1.7227	1.7227
8	9.9185	1.7212	1.7212	1.7212
9	9.9185	1.7212	1.7212	1.7212
10	1.7558	1.4958	1.4958	1.4958

Molecule 101-trifluoroethan-1-amine
Energy: -432.131565923
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.356733	0.233112	0.000000
2	6	-1.149561	0.240187	0.000000
3	1	-1.465848	0.804080	0.880679
4	1	-1.465848	0.804080	-0.880679
5	1	-1.536498	-1.599287	0.829517
6	1	-1.536498	-1.599287	-0.829517
7	9	0.852253	1.476867	0.000000
8	9	0.852253	-0.395758	-1.077226
9	9	0.852253	-0.395758	1.077226
10	7	-1.749880	-1.059649	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2044	1.4272	1.4272	1.4272
2	1.9601	1.6102	1.6102	1.6102
3	0.0684	1.8925	1.8925	1.8925
4	0.0684	1.8925	1.8925	1.8925
5	0.1214	1.7943	1.7943	1.7943
6	0.1214	1.7943	1.7943	1.7943
7	1.9068	1.1359	1.1359	1.1359
8	1.9010	1.1363	1.1363	1.1363
9	1.9010	1.1363	1.1363	1.1363
10	1.7472	1.5035	1.5035	1.5035

Molecule 102-methylmagnesium-bromide
Energy: -2811.04422200
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-3.139567
2	1	0.000000	1.017067	-3.541247
3	1	-0.880806	-0.508534	-3.541247
4	1	0.880806	-0.508534	-3.541247
5	12	0.000000	0.000000	-1.096964
6	35	0.000000	0.000000	1.217849

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6502	1.8425	1.8425	1.8425
2	0.0321	2.0006	2.0006	2.0006
3	0.0321	2.0007	2.0007	2.0007
4	0.0321	2.0007	2.0007	2.0007
5	10.6545	2.6074	2.6074	2.6074
6	27.5990	2.0181	2.0181	2.0181

Molecule 103-methylmagnesium-flouride
Energy: -339.416906497

Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.923448
2	1	0.000000	1.017479	-2.323399
3	1	-0.881163	-0.508739	-2.323399
4	1	0.881163	-0.508739	-2.323399
5	12	0.000000	0.000000	0.125897
6	9	0.000000	0.000000	1.888902

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.6530	1.8441	1.8441	1.8441
2	0.0318	2.0006	2.0006	2.0006
3	0.0318	2.0006	2.0006	2.0006
4	0.0318	2.0006	2.0006	2.0006
5	10.6683	2.3615	2.3615	2.3615
6	1.5832	1.1776	1.1776	1.1776

Molecule 104-cyanopotassium
Energy: -692.223159935
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.297912
2	19	0.000000	0.000000	1.315854
3	7	0.000000	0.000000	-2.459108

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.4528	1.7851	1.7851	1.7851
2	16.6982	1.5051	1.5051	1.5051
3	2.8490	1.4625	1.4625	1.4625

Molecule 105-1-3-5-triazine
Energy: -279.632036935
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.991818	0.819079	-0.000069
2	6	-1.205267	0.449393	0.000076
3	6	0.213437	-1.268476	0.000054
4	1	1.830097	1.511408	0.000078
5	1	-2.223974	0.829208	-0.000049
6	1	0.393873	-2.340603	-0.000210
7	7	-0.225308	1.337059	-0.000019
8	7	-1.045279	-0.863654	-0.000047
9	7	1.270599	-0.473403	0.000039

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1127	1.5951	1.5951	1.5951
2	2.1127	1.5953	1.5953	1.5953
3	2.1127	1.5953	1.5953	1.5953
4	0.0807	1.9262	1.9262	1.9262
5	0.0807	1.9262	1.9262	1.9262
6	0.0807	1.9263	1.9263	1.9263
7	1.8066	1.4820	1.4820	1.4820
8	1.8067	1.4820	1.4820	1.4820
9	1.8067	1.4820	1.4820	1.4820

Molecule 106-carbamic-chloride
Energy: -628.852887515
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.487176	0.160624	0.000314
2	1	0.641787	-1.893274	-0.000873
3	1	2.144798	-0.994505	0.001139
4	8	0.980277	1.245747	-0.000179
5	17	-1.264699	-0.054905	0.000014
6	7	1.135433	-1.015508	-0.000137

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2313	1.5367	1.5367	1.5367
2	0.1551	1.8037	1.8037	1.8037

3	0.1626	1.7970	1.7970	1.7970
4	1.7133	1.3235	1.3235	1.3235
5	9.9023	1.7295	1.7295	1.7295
6	1.8354	1.4726	1.4726	1.4726

Molecule 107-perchloroethene
Energy: -1915.63983812
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.664524
2	6	0.000000	0.000000	-0.664524
3	17	0.000000	1.440903	-1.579696
4	17	0.000000	-1.440903	-1.579696
5	17	0.000000	-1.440903	1.579696
6	17	0.000000	1.440903	1.579696

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0643	1.6144	1.6144	1.6144
2	2.0643	1.6144	1.6144	1.6144
3	9.9678	1.7189	1.7189	1.7189
4	9.9678	1.7189	1.7189	1.7189
5	9.9678	1.7189	1.7189	1.7189
6	9.9678	1.7189	1.7189	1.7189

Molecule 108-isocyanomethane
Energy: -132.346207989
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.102337	0.000002	-0.000013
2	1	-1.470401	0.886664	-0.517053
3	1	-1.470413	-0.891157	-0.509255
4	1	-1.470442	0.004507	1.026377
5	7	0.312047	-0.000008	-0.000005
6	6	1.473491	0.000005	0.000007

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9736	1.6963	1.6963	1.6963
2	0.0754	1.9190	1.9190	1.9190
3	0.0754	1.9190	1.9190	1.9190
4	0.0754	1.9189	1.9189	1.9189
5	1.9193	1.4505	1.4505	1.4505
6	1.8810	1.9033	1.9033	1.9033

Molecule 109-cyanic-acid
Energy: -168.256241524
Geometry:

Atom	Atomic No.	x	y	z
1	8	0.163674	-1.100523	0.000000
2	1	-0.682651	-1.573171	0.000000
3	6	0.000000	0.181009	0.000000
4	7	-0.089534	1.327328	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8601	1.3024	1.3024	1.3024
2	0.2382	1.6702	1.6702	1.6702
3	2.1586	1.5342	1.5342	1.5342
4	1.7431	1.5758	1.5758	1.5758

Molecule 110-fulminic_acid
Energy: -168.164795342
Geometry:

Atom	Atomic No.	x	y	z
1	8	0.069477	-1.079153	0.000000
2	1	-0.845386	-1.406717	0.000000
3	7	0.000000	0.235837	0.000000
4	6	0.048261	1.398180	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8927	1.3003	1.3003	1.3003

2	0.2267	1.6606	1.6606	1.6606
3	1.9929	1.4061	1.4061	1.4061
4	1.8877	1.8893	1.8893	1.8893

Molecule 111-carbonyl_diisocynate
Energy: -448.495182412
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000051	0.194950	0.000194
2	6	2.310088	-0.257242	0.000125
3	8	0.000196	1.395452	0.000116
4	8	3.447435	-0.065182	-0.000391
5	7	-1.141021	-0.585852	0.000185
6	7	1.140947	-0.586134	0.000202
7	6	-2.310170	-0.257112	0.000085
8	8	-3.447543	-0.065230	-0.000366

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2636	1.5053	1.5053	1.5053
2	2.3217	1.5054	1.5054	1.5054
3	1.7192	1.3204	1.3204	1.3204
4	1.8471	1.3156	1.3156	1.3156
5	1.8398	1.4478	1.4478	1.4478
6	1.8397	1.4478	1.4478	1.4478
7	2.3217	1.5054	1.5054	1.5054
8	1.8471	1.3156	1.3156	1.3156

Molecule 113-o-carborane
Energy: -330.803135195
Geometry:

Atom	Atomic No.	x	y	z
1	1	-1.483594	2.419901	0.136911
2	6	0.005960	-0.795719	1.258272
3	5	1.431990	0.008764	-0.899006
4	1	2.458399	0.015139	-1.486950
5	5	0.888011	-1.413677	-0.023699
6	1	1.483661	-2.419426	0.143690
7	5	1.431149	0.011357	0.842344
8	1	2.310619	0.019098	1.627437
9	5	0.867846	1.425892	-0.028061
10	1	1.448697	2.440720	0.136551
11	5	0.005983	-0.880352	-1.441708
12	1	0.009983	-1.524804	-2.434142
13	5	-1.430756	-0.008828	0.842930
14	1	-2.310062	-0.013628	1.628226
15	5	-0.867900	-1.426018	-0.023326
16	1	-1.448667	-2.440313	0.144821
17	5	-0.006437	0.875901	-1.444374
18	1	-0.010991	1.517038	-2.438951
19	5	-1.432284	-0.011592	-0.898449
20	1	-2.458775	-0.019608	-1.486226
21	1	-0.008631	1.283536	2.223273
22	1	0.009406	-1.276316	2.227372
23	6	-0.005525	0.799734	1.255792
24	5	-0.888133	1.413467	-0.027929

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	-0.0224	2.1244	2.1244	2.1244
2	1.9905	1.6303	1.6303	1.6303
3	1.9686	1.9014	1.9014	1.9014
4	-0.0232	2.1375	2.1375	2.1375
5	2.0100	1.8818	1.8818	1.8818
6	-0.0224	2.1243	2.1243	2.1243
7	2.0452	1.8665	1.8665	1.8665
8	-0.0248	2.1141	2.1141	2.1141
9	2.0099	1.8817	1.8817	1.8817
10	-0.0225	2.1242	2.1242	2.1242

11	1.9724	1.9037	1.9037	1.9037
12	-0.0249	2.1360	2.1360	2.1360
13	2.0452	1.8665	1.8665	1.8665
14	-0.0248	2.1140	2.1140	2.1140
15	2.0100	1.8817	1.8817	1.8817
16	-0.0225	2.1243	2.1243	2.1243
17	1.9724	1.9037	1.9037	1.9037
18	-0.0249	2.1360	2.1360	2.1360
19	1.9686	1.9014	1.9014	1.9014
20	-0.0232	2.1375	2.1375	2.1375
21	0.1210	1.8986	1.8986	1.8986
22	0.1210	1.8986	1.8986	1.8986
23	1.9905	1.6303	1.6303	1.6303
24	2.0100	1.8818	1.8818	1.8818

Molecule 114-m-carborane
Energy: -330.831441496
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.014447	-0.768533	-1.298573
2	1	0.024967	-1.337185	-2.219447
3	6	-0.000906	-0.810358	1.273058
4	5	-0.895279	1.433123	0.017907
5	1	-1.539901	2.424686	0.030149
6	5	-0.016069	0.868748	1.424150
7	1	-0.026783	1.349215	2.502986
8	5	-1.428713	-0.009788	0.865486
9	1	-2.381795	-0.126923	1.552300
10	5	-1.418345	0.018442	-0.882144
11	1	-2.362988	-0.076342	-1.583909
12	5	0.870864	1.447750	0.028731
13	1	1.498320	2.450154	0.048512
14	5	0.891921	-1.380392	-0.017068
15	1	1.434258	-2.426129	-0.030945
16	5	1.418195	0.013962	0.882771
17	1	2.364393	-0.086825	1.581590
18	5	0.000594	0.914380	-1.395440
19	1	0.002578	1.429222	-2.458363
20	5	1.428532	0.042454	-0.865103
21	1	2.383249	-0.035863	-1.555135
22	5	-0.868409	-1.395116	-0.027708
23	1	-1.392577	-2.449971	-0.047656
24	1	-0.001427	-1.408506	2.175101

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9420	1.6466	1.6466	1.6466
2	0.1204	1.9082	1.9082	1.9082
3	1.9420	1.6466	1.6466	1.6466
4	1.9694	1.9011	1.9011	1.9011
5	-0.0232	2.1380	2.1380	2.1380
6	2.0124	1.8833	1.8833	1.8833
7	-0.0245	2.1231	2.1231	2.1231
8	2.0096	1.8806	1.8806	1.8806
9	-0.0227	2.1252	2.1252	2.1252
10	2.0096	1.8806	1.8806	1.8806
11	-0.0227	2.1252	2.1252	2.1252
12	1.9693	1.9011	1.9011	1.9011
13	-0.0232	2.1380	2.1380	2.1380
14	2.0495	1.8565	1.8565	1.8565
15	-0.0204	2.1149	2.1149	2.1149
16	2.0097	1.8807	1.8807	1.8807
17	-0.0227	2.1252	2.1252	2.1252
18	2.0125	1.8833	1.8833	1.8833
19	-0.0245	2.1232	2.1232	2.1232
20	2.0097	1.8807	1.8807	1.8807
21	-0.0227	2.1252	2.1252	2.1252

22	2.0495	1.8564	1.8564	1.8564
23	-0.0204	2.1149	2.1149	2.1149
24	0.1204	1.9081	1.9081	1.9081

Molecule 115-p-carborane
Energy: -330.835730544
Geometry:

Atom	Atomic No.	x	y	z
1	1	-2.448742	0.567941	-1.332531
2	6	0.013640	-0.027174	1.506066
3	5	1.365484	0.607786	-0.741265
4	1	2.278276	1.016974	-1.367482
5	5	1.466240	-0.339319	0.720283
6	1	2.448715	-0.568410	1.332689
7	5	0.767882	1.273752	0.755799
8	1	1.283183	2.123471	1.392366
9	5	-0.147904	1.502166	-0.711111
10	1	-0.248075	2.509375	-1.317981
11	5	0.982522	-1.108060	-0.768630
12	1	1.638742	-1.846723	-1.414013
13	5	-1.365404	-0.607812	0.741136
14	1	-2.278265	-1.016615	1.367510
15	5	0.147605	-1.501914	0.711375
16	1	0.247182	-2.509179	1.318257
17	1	-0.023180	0.047170	-2.588468
18	5	-0.767532	-1.273972	-0.755856
19	1	-1.283008	-2.123408	-1.392653
20	1	-1.638363	1.846357	1.414105
21	1	0.023215	-0.046735	2.588381
22	5	-1.466390	0.339198	-0.720330
23	6	-0.013814	0.027517	-1.506061
24	5	-0.982230	1.107719	0.768558

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	-0.0222	2.1251	2.1251	2.1251
2	1.9472	1.6485	1.6485	1.6485
3	2.0090	1.8795	1.8795	1.8795
4	-0.0222	2.1254	2.1254	2.1254
5	2.0090	1.8795	1.8795	1.8795
6	-0.0222	2.1253	2.1253	2.1253
7	2.0090	1.8794	1.8794	1.8794
8	-0.0222	2.1253	2.1253	2.1253
9	2.0090	1.8794	1.8794	1.8794
10	-0.0222	2.1254	2.1254	2.1254
11	2.0090	1.8796	1.8796	1.8796
12	-0.0222	2.1254	2.1254	2.1254
13	2.0089	1.8794	1.8794	1.8794
14	-0.0222	2.1253	2.1253	2.1253
15	2.0090	1.8794	1.8794	1.8794
16	-0.0222	2.1253	2.1253	2.1253
17	0.1190	1.9061	1.9061	1.9061
18	2.0090	1.8795	1.8795	1.8795
19	-0.0222	2.1253	2.1253	2.1253
20	-0.0222	2.1253	2.1253	2.1253
21	0.1191	1.9060	1.9060	1.9060
22	2.0091	1.8794	1.8794	1.8794
23	1.9472	1.6486	1.6486	1.6486
24	2.0088	1.8793	1.8793	1.8793

Molecule 116-acetonitrile_oxide
Energy: -207.385937606
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.878898	-0.000322	-0.000117
2	1	2.258766	0.531468	0.873682
3	1	2.257976	0.490433	-0.897946

4	1	2.257066	-1.023563	0.023403
5	6	0.423519	0.000844	0.000376
6	8	-1.939851	-0.000290	-0.000118
7	7	-0.724214	0.000122	0.000036

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9184	1.7195	1.7195	1.7195
2	0.0772	1.9305	1.9305	1.9305
3	0.0772	1.9305	1.9305	1.9305
4	0.0772	1.9304	1.9304	1.9304
5	2.0580	1.5899	1.5899	1.5899
6	1.7079	1.3283	1.3283	1.3283
7	2.0841	1.3893	1.3893	1.3893

Molecule 117-Naphthalene
Energy: -384.700360753
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.411639	-0.705352	0.000000
2	6	1.236895	-1.389235	0.000012
3	6	-0.000018	-0.703614	-0.000004
4	6	0.000056	0.703647	0.000002
5	6	1.236943	1.389231	0.000000
6	6	2.411673	0.705304	-0.000009
7	1	-1.230963	-2.475119	-0.000003
8	1	3.355127	-1.240977	0.000007
9	1	1.230956	-2.475132	0.000018
10	6	-1.236956	-1.389224	-0.000010
11	6	-1.236930	1.389234	0.000006
12	1	1.231016	2.475125	-0.000010
13	1	3.355171	1.240909	-0.000007
14	6	-2.411635	0.705364	0.000009
15	6	-2.411668	-0.705358	-0.000007
16	1	-1.231010	2.475136	-0.000007
17	1	-3.355115	1.240999	0.000002
18	1	-3.355183	-1.240929	-0.000006

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9405	1.6597	1.6597	1.6597
2	1.9448	1.6532	1.6532	1.6532
3	1.9955	1.5872	1.5872	1.5872
4	1.9955	1.5872	1.5872	1.5872
5	1.9448	1.6532	1.6532	1.6532
6	1.9405	1.6597	1.6597	1.6597
7	0.0582	1.9599	1.9599	1.9599
8	0.0587	1.9586	1.9586	1.9586
9	0.0582	1.9599	1.9599	1.9599
10	1.9448	1.6532	1.6532	1.6532
11	1.9448	1.6532	1.6532	1.6532
12	0.0582	1.9599	1.9599	1.9599
13	0.0587	1.9586	1.9586	1.9586
14	1.9405	1.6597	1.6597	1.6597
15	1.9405	1.6597	1.6597	1.6597
16	0.0582	1.9599	1.9599	1.9599
17	0.0587	1.9586	1.9586	1.9586
18	0.0587	1.9586	1.9586	1.9586

Molecule 118-Anthracene
Energy: -537.867678143
Geometry:

Atom	Atomic No.	x	y	z
1	6	3.626955	0.712279	0.000032
2	6	2.462582	1.395490	-0.000014
3	6	1.210040	0.710495	-0.000028
4	6	1.210040	-0.710491	-0.000029
5	6	2.462580	-1.395490	0.000009
6	6	3.626955	-0.712284	0.000049

7	6	0.000001	1.387722	-0.000032
8	6	0.000001	-1.387719	-0.000040
9	6	-1.210043	-0.710490	-0.000026
10	6	-1.210043	0.710494	-0.000019
11	6	-2.462580	1.395488	0.000011
12	1	-2.457096	2.481457	0.000012
13	6	-3.626956	0.712277	0.000042
14	6	-3.626956	-0.712281	0.000029
15	6	-2.462578	-1.395489	-0.000005
16	1	0.000002	2.474678	-0.000046
17	1	4.572685	1.244104	0.000053
18	1	2.457097	2.481459	-0.000049
19	1	2.457086	-2.481460	-0.000003
20	1	4.572688	-1.244104	0.000099
21	1	0.000002	-2.474675	-0.000052
22	1	-4.572685	1.244104	0.000084
23	1	-4.572686	-1.244107	0.000044
24	1	-2.457086	-2.481458	-0.000023

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9403	1.6603	1.6603	1.6603
2	1.9454	1.6537	1.6537	1.6537
3	1.9944	1.5874	1.5874	1.5874
4	1.9944	1.5874	1.5874	1.5874
5	1.9454	1.6537	1.6537	1.6537
6	1.9403	1.6603	1.6603	1.6603
7	1.9468	1.6451	1.6451	1.6451
8	1.9468	1.6451	1.6451	1.6451
9	1.9944	1.5874	1.5874	1.5874
10	1.9944	1.5874	1.5874	1.5874
11	1.9454	1.6537	1.6537	1.6537
12	0.0587	1.9598	1.9598	1.9598
13	1.9403	1.6603	1.6603	1.6603
14	1.9403	1.6603	1.6603	1.6603
15	1.9454	1.6537	1.6537	1.6537
16	0.0577	1.9600	1.9600	1.9600
17	0.0588	1.9583	1.9583	1.9583
18	0.0587	1.9598	1.9598	1.9598
19	0.0587	1.9598	1.9598	1.9598
20	0.0588	1.9583	1.9583	1.9583
21	0.0577	1.9600	1.9600	1.9600
22	0.0588	1.9583	1.9583	1.9583
23	0.0588	1.9583	1.9583	1.9583
24	0.0587	1.9598	1.9598	1.9598

Molecule 119-Cyclooctatetraene
Energy: -308.534890882
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.820396	-0.671268	-0.085696
2	6	1.821148	0.670048	-0.085706
3	6	-1.821095	-0.669947	0.085985
4	6	0.543591	1.279551	0.382289
5	6	-1.820290	0.671295	0.085560
6	6	-0.542144	1.279377	-0.382743
7	1	2.715397	1.237744	-0.327432
8	1	0.396956	1.255432	1.462840
9	1	-2.715429	-1.237497	0.327723
10	1	2.714046	-1.239895	-0.327387
11	1	-2.713948	1.239887	0.327307
12	1	-0.395378	1.253988	-1.463250
13	6	0.542180	-1.279365	0.382539
14	1	0.395474	-1.253703	1.463067
15	6	-0.543756	-1.279756	-0.382236
16	1	-0.397290	-1.255568	-1.462822

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	1.9493	1.6733	1.6733	1.6733
2	1.9493	1.6733	1.6733	1.6733
3	1.9493	1.6733	1.6733	1.6733
4	1.9388	1.6635	1.6635	1.6635
5	1.9493	1.6733	1.6733	1.6733
6	1.9388	1.6635	1.6635	1.6635
7	0.0599	1.9749	1.9749	1.9749
8	0.0521	1.9466	1.9466	1.9466
9	0.0599	1.9749	1.9749	1.9749
10	0.0600	1.9749	1.9749	1.9749
11	0.0600	1.9749	1.9749	1.9749
12	0.0521	1.9466	1.9466	1.9466
13	1.9388	1.6635	1.6635	1.6635
14	0.0520	1.9466	1.9466	1.9466
15	1.9387	1.6635	1.6635	1.6635
16	0.0520	1.9467	1.9467	1.9467

Molecule 120-1-3-5-hexatriene
Energy: -232.657100673
Geometry:

Atom	Atomic No.	x	y	z
1	6	-3.048698	0.169913	-0.000001
2	1	-3.141386	1.252342	-0.000002
3	1	-3.968173	-0.404253	-0.000001
4	6	-1.860794	-0.419832	0.000001
5	1	-1.800089	-1.506720	0.000002
6	6	-0.595505	0.297114	0.000001
7	1	-0.649676	1.385195	0.000001
8	6	0.595505	-0.297114	0.000000
9	1	0.649676	-1.385195	0.000000
10	6	1.860794	0.419832	0.000000
11	1	1.800089	1.506720	0.000001
12	6	3.048698	-0.169913	-0.000001
13	1	3.141386	-1.252342	-0.000001
14	1	3.968173	0.404253	-0.000001

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8844	1.7366	1.7366	1.7366
2	0.0541	1.9859	1.9859	1.9859
3	0.0552	1.9817	1.9817	1.9817
4	1.9451	1.6712	1.6712	1.6712
5	0.0582	1.9600	1.9600	1.9600
6	1.9451	1.6629	1.6629	1.6629
7	0.0577	1.9629	1.9629	1.9629
8	1.9451	1.6629	1.6629	1.6629
9	0.0577	1.9629	1.9629	1.9629
10	1.9451	1.6712	1.6712	1.6712
11	0.0582	1.9600	1.9600	1.9600
12	1.8844	1.7366	1.7366	1.7366
13	0.0541	1.9859	1.9859	1.9859
14	0.0552	1.9817	1.9817	1.9817

Molecule 121-Ethane
Energy: -79.5659975310
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.758670
2	1	0.000000	1.017627	1.157078
3	1	-0.881291	-0.508814	1.157078
4	1	0.881291	-0.508814	1.157078
5	6	0.000000	0.000000	-0.758670
6	1	0.000000	-1.017627	-1.157078
7	1	-0.881291	0.508814	-1.157078
8	1	0.881291	0.508814	-1.157078

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8713	1.7193	1.7193	1.7193

2	0.0429	1.9466	1.9466	1.9466
3	0.0429	1.9466	1.9466	1.9466
4	0.0429	1.9466	1.9466	1.9466
5	1.8713	1.7193	1.7193	1.7193
6	0.0429	1.9466	1.9466	1.9466
7	0.0429	1.9466	1.9466	1.9466
8	0.0429	1.9466	1.9466	1.9466

Molecule 122-Propane
Energy: -118.757357156
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.585196	0.000000
2	1	0.000001	1.243481	-0.875227
3	1	-0.000001	1.243527	0.875193
4	6	-1.261310	-0.258295	0.000001
5	1	-1.300305	-0.904402	0.882070
6	1	-2.162687	0.359626	-0.000089
7	1	-1.300229	-0.904546	-0.881968
8	6	1.261310	-0.258295	0.000001
9	1	2.162687	0.359626	-0.000098
10	1	1.300309	-0.904395	0.882075
11	1	1.300226	-0.904553	-0.881963

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9215	1.6643	1.6643	1.6643
2	0.0413	1.9196	1.9196	1.9196
3	0.0413	1.9196	1.9196	1.9196
4	1.8705	1.7144	1.7144	1.7144
5	0.0419	1.9510	1.9510	1.9510
6	0.0435	1.9503	1.9503	1.9503
7	0.0419	1.9510	1.9510	1.9510
8	1.8705	1.7144	1.7144	1.7144
9	0.0435	1.9503	1.9503	1.9503
10	0.0419	1.9510	1.9510	1.9510
11	0.0419	1.9510	1.9510	1.9510

Molecule 123-Isobutane
Energy: -157.950681514
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.374698
2	1	0.000000	0.000000	1.472063
3	6	0.000000	1.444544	-0.095285
4	1	-0.884173	1.980529	0.260557
5	1	0.884173	1.980529	0.260557
6	1	0.000000	1.492525	-1.189488
7	6	-1.251012	-0.722272	-0.095285
8	1	-1.273102	-1.755981	0.260557
9	1	-2.157275	-0.224548	0.260557
10	1	-1.292565	-0.746263	-1.189488
11	6	1.251012	-0.722272	-0.095285
12	1	2.157275	-0.224548	0.260557
13	1	1.273102	-1.755981	0.260557
14	1	1.292565	-0.746263	-1.189488

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9660	1.6154	1.6154	1.6154
2	0.0410	1.8958	1.8958	1.8958
3	1.8709	1.7093	1.7093	1.7093
4	0.0427	1.9513	1.9513	1.9513
5	0.0427	1.9513	1.9513	1.9513
6	0.0413	1.9553	1.9553	1.9553
7	1.8709	1.7093	1.7093	1.7093
8	0.0427	1.9512	1.9512	1.9512
9	0.0427	1.9512	1.9512	1.9512
10	0.0413	1.9553	1.9553	1.9553

11	1.8709	1.7093	1.7093	1.7093
12	0.0427	1.9512	1.9512	1.9512
13	0.0427	1.9512	1.9512	1.9512
14	0.0413	1.9553	1.9553	1.9553

Molecule 124-Neopentane
Energy: -197.144801411
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.000000
2	6	0.879372	0.879372	0.879372
3	1	1.523075	0.272037	1.523075
4	1	1.523075	1.523075	0.272037
5	1	0.272037	1.523075	1.523075
6	6	-0.879372	-0.879372	0.879372
7	1	-1.523075	-1.523075	0.272037
8	1	-0.272037	-1.523075	1.523075
9	1	-1.523075	-0.272037	1.523075
10	6	-0.879372	0.879372	-0.879372
11	1	-0.272037	1.523075	-1.523075
12	1	-1.523075	0.272037	-1.523075
13	1	-1.523075	1.523075	-0.272037
14	6	0.879372	-0.879372	-0.879372
15	1	1.523075	-0.272037	-1.523075
16	1	1.523075	-1.523075	-0.272037
17	1	0.272037	-1.523075	-1.523075

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0062	1.5732	1.5732	1.5732
2	1.8721	1.7046	1.7046	1.7046
3	0.0421	1.9524	1.9524	1.9524
4	0.0421	1.9524	1.9524	1.9524
5	0.0421	1.9524	1.9524	1.9524
6	1.8721	1.7046	1.7046	1.7046
7	0.0421	1.9524	1.9524	1.9524
8	0.0421	1.9524	1.9524	1.9524
9	0.0421	1.9524	1.9524	1.9524
10	1.8721	1.7046	1.7046	1.7046
11	0.0421	1.9524	1.9524	1.9524
12	0.0421	1.9524	1.9524	1.9524
13	0.0421	1.9524	1.9524	1.9524
14	1.8721	1.7046	1.7046	1.7046
15	0.0421	1.9524	1.9524	1.9524
16	0.0421	1.9524	1.9524	1.9524
17	0.0421	1.9524	1.9524	1.9524

Molecule 125-Toulene
Energy: -270.719994604
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.028465	-2.403600	0.000000
2	1	0.465422	-2.812721	0.883653
3	1	-1.059121	-2.770388	0.000000
4	1	0.465422	-2.812721	-0.883653
5	6	0.004000	-0.905050	0.000000
6	6	0.007500	-0.193242	-1.191111
7	6	0.007500	-0.193242	1.191111
8	6	0.007500	1.189995	-1.194377
9	1	0.012355	-0.733688	-2.133713
10	6	0.007500	1.189995	1.194377
11	1	0.012355	-0.733688	2.133713
12	6	0.006406	1.887967	0.000000
13	1	0.011506	1.726624	-2.137879
14	1	0.011506	1.726624	2.137879
15	1	0.008915	2.973018	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	1.8779	1.7116	1.7116	1.7116
2	0.0504	1.9476	1.9476	1.9476
3	0.0523	1.9463	1.9463	1.9463
4	0.0504	1.9476	1.9476	1.9476
5	1.9986	1.5998	1.5998	1.5998
6	1.9358	1.6515	1.6515	1.6515
7	1.9358	1.6515	1.6515	1.6515
8	1.9416	1.6597	1.6597	1.6597
9	0.0547	1.9594	1.9594	1.9594
10	1.9416	1.6597	1.6597	1.6597
11	0.0547	1.9594	1.9594	1.9594
12	1.9348	1.6600	1.6600	1.6600
13	0.0574	1.9603	1.9603	1.9603
14	0.0574	1.9603	1.9603	1.9603
15	0.0564	1.9622	1.9622	1.9622

Molecule 126-Diphenylmethaneg
Energy: -501.063824919
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.003798	-1.432768	-0.107461
2	1	-0.034617	-2.022274	-1.028903
3	1	0.048265	-2.155304	0.713371
4	6	1.265671	-0.610095	-0.099421
5	6	2.313459	-0.922986	0.750639
6	6	1.412533	0.467187	-0.963892
7	6	3.485331	-0.183859	0.738655
8	1	2.212781	-1.760557	1.435332
9	6	2.579045	1.206148	-0.981106
10	1	0.594202	0.732894	-1.627052
11	6	3.621960	0.882890	-0.128151
12	1	4.293882	-0.444914	1.413991
13	1	2.675757	2.044153	-1.664076
14	1	4.537677	1.464883	-0.139732
15	6	-1.263683	-0.628217	0.008222
16	6	-1.444224	0.254584	1.065542
17	6	-2.280682	-0.761742	-0.922210
18	6	-2.613285	0.978595	1.190722
19	1	-0.649872	0.379085	1.796173
20	6	-3.455307	-0.036358	-0.802445
21	1	-2.153677	-1.445825	-1.756661
22	6	-3.625387	0.835624	0.254997
23	1	-2.736659	1.662710	2.024278
24	1	-4.239717	-0.154827	-1.543153
25	1	-4.543387	1.405952	0.351891

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9313	1.6517	1.6517	1.6517
2	0.0530	1.9174	1.9174	1.9174
3	0.0529	1.9175	1.9175	1.9175
4	1.9980	1.5943	1.5943	1.5943
5	1.9364	1.6516	1.6516	1.6516
6	1.9406	1.6493	1.6493	1.6493
7	1.9412	1.6597	1.6597	1.6597
8	0.0542	1.9586	1.9586	1.9586
9	1.9435	1.6592	1.6592	1.6592
10	0.0562	1.9551	1.9551	1.9551
11	1.9371	1.6598	1.6598	1.6598
12	0.0577	1.9602	1.9602	1.9602
13	0.0583	1.9592	1.9592	1.9592
14	0.0571	1.9614	1.9614	1.9614
15	1.9982	1.5941	1.5941	1.5941
16	1.9409	1.6494	1.6494	1.6494
17	1.9366	1.6516	1.6516	1.6516
18	1.9435	1.6592	1.6592	1.6592
19	0.0567	1.9556	1.9556	1.9556

20	1.9413	1.6596	1.6596	1.6596
21	0.0543	1.9585	1.9585	1.9585
22	1.9373	1.6598	1.6598	1.6598
23	0.0584	1.9591	1.9591	1.9591
24	0.0578	1.9601	1.9601	1.9601
25	0.0572	1.9614	1.9614	1.9614

Molecule 127-Triphenylmethane
Energy: -731.406677553
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000081	-0.001597	-0.756448
2	1	0.000677	-0.002585	-1.851616
3	6	0.020047	1.454761	-0.336096
4	6	0.797773	2.350755	-1.057911
5	6	-0.683736	1.924911	0.760277
6	6	0.875605	3.680564	-0.693642
7	1	1.357332	1.993481	-1.918409
8	6	-0.606632	3.257546	1.131487
9	1	-1.307598	1.244597	1.330416
10	6	0.172238	4.139632	0.407601
11	1	1.487815	4.363920	-1.273406
12	1	-1.166110	3.606752	1.993494
13	1	0.229091	5.184068	0.696276
14	6	-1.271483	-0.711219	-0.335049
15	6	-1.329368	-1.549895	0.765631
16	6	-2.434312	-0.490156	-1.061455
17	6	-2.522887	-2.147982	1.136574
18	1	-0.429442	-1.746321	1.338912
19	6	-3.625660	-1.086086	-0.697415
20	1	-2.402520	0.168138	-1.925636
21	6	-3.674272	-1.918898	0.408106
22	1	-2.547747	-2.802532	2.002000
23	1	-4.522042	-0.901190	-1.280699
24	1	-4.607785	-2.390706	0.696849
25	6	1.250834	-0.746689	-0.334086
26	6	2.007509	-0.373111	0.764164
27	6	1.641460	-1.865581	-1.058157
28	6	3.124366	-1.104451	1.134947
29	1	1.727709	0.505640	1.335592
30	6	2.755456	-2.596130	-0.694279
31	1	1.054536	-2.170277	-1.920641
32	6	3.502511	-2.217225	0.408686
33	1	3.704957	-0.795078	1.998202
34	1	3.044132	-3.465793	-1.275876
35	1	4.379816	-2.787015	0.696927

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9791	1.6017	1.6017	1.6017
2	0.0525	1.8831	1.8831	1.8831
3	1.9988	1.5889	1.5889	1.5889
4	1.9409	1.6491	1.6491	1.6491
5	1.9408	1.6474	1.6474	1.6474
6	1.9427	1.6592	1.6592	1.6592
7	0.0568	1.9557	1.9557	1.9557
8	1.9431	1.6590	1.6590	1.6590
9	0.0535	1.9454	1.9454	1.9454
10	1.9383	1.6597	1.6597	1.6597
11	0.0585	1.9594	1.9594	1.9594
12	0.0583	1.9585	1.9585	1.9585
13	0.0576	1.9610	1.9610	1.9610
14	1.9989	1.5889	1.5889	1.5889
15	1.9408	1.6475	1.6475	1.6475
16	1.9409	1.6490	1.6490	1.6490
17	1.9431	1.6590	1.6590	1.6590
18	0.0536	1.9457	1.9457	1.9457

19	1.9427	1.6593	1.6593	1.6593
20	0.0568	1.9556	1.9556	1.9556
21	1.9383	1.6598	1.6598	1.6598
22	0.0583	1.9585	1.9585	1.9585
23	0.0585	1.9594	1.9594	1.9594
24	0.0576	1.9610	1.9610	1.9610
25	1.9988	1.5889	1.5889	1.5889
26	1.9408	1.6474	1.6474	1.6474
27	1.9409	1.6491	1.6491	1.6491
28	1.9431	1.6589	1.6589	1.6589
29	0.0536	1.9455	1.9455	1.9455
30	1.9427	1.6592	1.6592	1.6592
31	0.0568	1.9557	1.9557	1.9557
32	1.9383	1.6597	1.6597	1.6597
33	0.0583	1.9585	1.9585	1.9585
34	0.0585	1.9594	1.9594	1.9594
35	0.0576	1.9611	1.9611	1.9611

Molecule 128-chloromethylene-dibenzene
Energy: -960.393401452
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.035693	0.905350	0.586956
2	1	-0.086712	1.126464	1.653217
3	6	-1.247120	0.092249	0.212972
4	6	-2.372195	0.141225	1.020029
5	6	-1.271418	-0.688450	-0.932024
6	6	-3.507486	-0.576640	0.690875
7	1	-2.361471	0.755276	1.916280
8	6	-2.405984	-1.403252	-1.265567
9	1	-0.391931	-0.742399	-1.565211
10	6	-3.526710	-1.350191	-0.455057
11	1	-4.380692	-0.530567	1.333320
12	1	-2.413494	-2.011037	-2.164449
13	1	-4.415348	-1.915344	-0.716410
14	6	1.272665	0.208794	0.311930
15	6	1.688386	-0.751328	1.224207
16	6	2.046263	0.446216	-0.810089
17	6	2.851640	-1.465761	1.016843
18	1	1.087169	-0.945089	2.108448
19	6	3.213180	-0.269602	-1.019922
20	1	1.742734	1.205521	-1.521710
21	6	3.619236	-1.226890	-0.110336
22	1	3.162992	-2.210841	1.741644
23	1	3.810932	-0.070363	-1.903445
24	1	4.535858	-1.783642	-0.274780
25	17	-0.131684	2.514806	-0.201871

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0350	1.6227	1.6227	1.6227
2	0.0628	1.8727	1.8727	1.8727
3	1.9898	1.5880	1.5880	1.5880
4	1.9439	1.6500	1.6500	1.6500
5	1.9469	1.6479	1.6479	1.6479
6	1.9447	1.6584	1.6584	1.6584
7	0.0584	1.9558	1.9558	1.9558
8	1.9467	1.6580	1.6580	1.6580
9	0.0569	1.9490	1.9490	1.9490
10	1.9454	1.6590	1.6590	1.6590
11	0.0605	1.9578	1.9578	1.9578
12	0.0608	1.9566	1.9566	1.9566
13	0.0602	1.9585	1.9585	1.9585
14	1.9938	1.5875	1.5875	1.5875
15	1.9435	1.6485	1.6485	1.6485
16	1.9423	1.6470	1.6470	1.6470
17	1.9457	1.6584	1.6584	1.6584

18	0.0588	1.9545	1.9545	1.9545
19	1.9463	1.6580	1.6580	1.6580
20	0.0550	1.9455	1.9455	1.9455
21	1.9428	1.6588	1.6588	1.6588
22	0.0606	1.9576	1.9576	1.9576
23	0.0606	1.9564	1.9564	1.9564
24	0.0599	1.9590	1.9590	1.9590
25	9.8786	1.7323	1.7323	1.7323

Molecule 129-Flouromethane
Energy: -139.469356998
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.633360
2	1	0.000000	1.034541	-0.981588
3	1	0.895939	-0.517270	-0.981588
4	1	-0.895939	-0.517270	-0.981588
5	9	0.000000	0.000000	0.749436

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9723	1.6704	1.6704	1.6704
2	0.0602	1.9148	1.9148	1.9148
3	0.0602	1.9148	1.9148	1.9148
4	0.0602	1.9148	1.9148	1.9148
5	1.8470	1.1495	1.1495	1.1495

Molecule 130-Diflouromethane
Energy: -238.580572851
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.503968
2	1	-0.915142	0.000000	1.099920
3	1	0.915142	0.000000	1.099920
4	9	0.000000	1.097376	-0.290203
5	9	0.000000	-1.097376	-0.290203

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0949	1.5678	1.5678	1.5678
2	0.0720	1.8682	1.8682	1.8682
3	0.0720	1.8682	1.8682	1.8682
4	1.8806	1.1427	1.1427	1.1427
5	1.8806	1.1427	1.1427	1.1427

Molecule 131-Triflouromethane
Energy: -337.701775708
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	0.341363
2	1	0.000000	0.000000	1.432994
3	9	0.000000	1.246995	-0.128932
4	9	-1.079929	-0.623497	-0.128932
5	9	1.079929	-0.623497	-0.128932

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1919	1.4692	1.4692	1.4692
2	0.0860	1.8423	1.8423	1.8423
3	1.9074	1.1361	1.1361	1.1361
4	1.9074	1.1360	1.1360	1.1360
5	1.9074	1.1360	1.1360	1.1360

Molecule 132-thiocyanatomethane
Energy: -530.289144564
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.457996	0.809566	-0.000002
2	1	2.499874	0.488723	-0.000126
3	1	1.265477	1.399958	0.894315
4	1	1.265338	1.400140	-0.894163

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5       16      0.472660        -0.699830       -0.000038
6       6       -1.071818       -0.008767       0.000247
7       7       -2.130045       0.443381        -0.000127
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9002      1.7335      1.7335      1.7335
    2      0.0724      1.9343      1.9343      1.9343
    3      0.0684      1.9287      1.9287      1.9287
    4      0.0684      1.9287      1.9287      1.9287
    5     10.0576      1.8650      1.8650      1.8650
    6      2.0537      1.6351      1.6351      1.6351
    7      1.7794      1.5802      1.5802      1.5802

Molecule 133-isothiocyanatomethane
Energy: -530.302191341
Geometry:
Atom  Atomic No.   x               y               z
 1      6       -2.390255       0.000099        -0.000133
2       1       -2.763873       -0.412612       -0.939240
3       1       -2.763876       1.019746        0.111900
4       1       -2.764201       -0.606782       0.826739
5       7       -0.981002       -0.000143       0.000083
6       6       0.186365        -0.000118       0.000439
7       16      1.773894        0.000048        -0.000113
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9753      1.6942      1.6942      1.6942
    2      0.0741      1.9171      1.9171      1.9171
    3      0.0741      1.9171      1.9171      1.9171
    4      0.0741      1.9171      1.9171      1.9171
    5      1.9145      1.4370      1.4370      1.4370
    6      2.1212      1.6448      1.6448      1.6448
    7      9.7666      1.9593      1.9593      1.9593

Molecule 134-methanethial
Energy: -437.060567926
Geometry:
Atom  Atomic No.   x               y               z
 1      6       0.000000        0.000000        -1.014162
2       1       0.000000        0.923810        -1.591936
3       1       0.000000        -0.923810       -1.591936
4       16      0.000000        0.000000        0.579303
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9756      1.7708      1.7708      1.7708
    2      0.0698      1.9591      1.9591      1.9591
    3      0.0698      1.9591      1.9591      1.9591
    4      9.8848      1.9502      1.9502      1.9502

Molecule 135-methanamine
Energy: -95.5946640863
Geometry:
Atom  Atomic No.   x               y               z
 1      6       0.044909        0.701354        0.000000
2       1       0.584573        1.064412        0.877450
3       1       -0.951645       1.163741        0.000000
4       1       0.584573        1.064412        -0.877450
5       7       0.044909        -0.747302       0.000000
6       1       -0.400658       -1.134789       0.822331
7       1       -0.400658       -1.134789       -0.822331
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9209      1.6977      1.6977      1.6977
    2      0.0487      1.9322      1.9322      1.9322
    3      0.0310      1.9405      1.9405      1.9405
    4      0.0487      1.9322      1.9322      1.9322
    5      1.7280      1.5147      1.5147      1.5147
    6      0.1113      1.8047      1.8047      1.8047
    7      0.1113      1.8047      1.8047      1.8047
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Molecule 136-cyclopropene
Energy: -116.251618962
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	-0.641556	-0.496213
2	6	0.000000	0.641556	-0.496213
3	6	0.000000	0.000000	0.853338
4	1	-0.000274	-1.574769	-1.034633
5	1	0.000274	1.574769	-1.034633
6	1	0.912605	-0.000043	1.451897
7	1	-0.912605	0.000043	1.451897

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9351	1.6850	1.6850	1.6850
2	1.9351	1.6850	1.6850	1.6850
3	1.8887	1.6972	1.6972	1.6972
4	0.0850	2.0157	2.0157	2.0157
5	0.0850	2.0157	2.0157	2.0157
6	0.0356	1.9481	1.9481	1.9481
7	0.0356	1.9481	1.9481	1.9481

Molecule 137-phenanthrene
Energy: -537.879682597
Geometry:

Atom	Atomic No.	x	y	z
1	6	3.529762	-0.294301	0.000030
2	6	2.812521	0.868252	0.000105
3	6	1.409205	0.852526	0.000046
4	6	0.726467	-0.371629	-0.000014
5	6	1.486804	-1.552303	-0.000107
6	6	2.854467	-1.518315	-0.000097
7	6	0.670284	2.080779	0.000037
8	6	-0.726468	-0.371626	0.000002
9	6	-1.409204	0.852526	-0.000060
10	6	-0.670284	2.080779	-0.000053
11	6	-2.812523	0.868252	-0.000080
12	1	-3.321514	1.827739	-0.000143
13	6	-3.529762	-0.294299	-0.000013
14	6	-2.854465	-1.518317	0.000096
15	6	-1.486805	-1.552305	0.000101
16	1	1.224752	3.014384	0.000095
17	1	4.614426	-0.270281	0.000061
18	1	3.321513	1.827739	0.000169
19	1	0.991585	-2.515364	-0.000242
20	1	3.416439	-2.446535	-0.000190
21	1	-1.224750	3.014385	-0.000099
22	1	-4.614426	-0.270285	-0.000029
23	1	-3.416444	-2.446532	0.000190
24	1	-0.991578	-2.515361	0.000224

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9409	1.6588	1.6588	1.6588
2	1.9447	1.6514	1.6514	1.6514
3	1.9942	1.5873	1.5873	1.5873
4	1.9988	1.5877	1.5877	1.5877
5	1.9447	1.6485	1.6485	1.6485
6	1.9418	1.6584	1.6584	1.6584
7	1.9433	1.6524	1.6524	1.6524
8	1.9988	1.5877	1.5877	1.5877
9	1.9942	1.5873	1.5873	1.5873
10	1.9433	1.6524	1.6524	1.6524
11	1.9447	1.6514	1.6514	1.6514
12	0.0579	1.9584	1.9584	1.9584
13	1.9409	1.6588	1.6588	1.6588
14	1.9418	1.6584	1.6584	1.6584
15	1.9447	1.6485	1.6485	1.6485

16	0.0590	1.9583	1.9583	1.9583
17	0.0594	1.9596	1.9596	1.9596
18	0.0579	1.9584	1.9584	1.9584
19	0.0564	1.9407	1.9407	1.9407
20	0.0587	1.9578	1.9578	1.9578
21	0.0590	1.9583	1.9583	1.9583
22	0.0594	1.9596	1.9596	1.9596
23	0.0587	1.9578	1.9578	1.9578
24	0.0564	1.9407	1.9407	1.9407

Molecule 138-pentalene
Energy: -307.418739918
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.434890	1.769155	0.000000
2	6	1.695419	1.321291	0.000001
3	6	1.703479	-0.170660	0.000000
4	6	0.434890	-0.584012	-0.000001
5	6	-0.434890	0.584012	-0.000001
6	6	-0.434890	-1.769155	0.000000
7	6	-1.695419	-1.321291	0.000001
8	6	-1.703479	0.170660	0.000000
9	1	0.114406	2.802454	0.000000
10	1	2.590521	1.931004	0.000002
11	1	2.602746	-0.775919	0.000001
12	1	-0.114406	-2.802454	0.000000
13	1	-2.590521	-1.931004	0.000002
14	1	-2.602746	0.775919	0.000001

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9408	1.6695	1.6695	1.6695
2	1.9342	1.6700	1.6700	1.6700
3	1.9647	1.6699	1.6699	1.6699
4	1.9704	1.5821	1.5821	1.5821
5	1.9704	1.5821	1.5821	1.5821
6	1.9408	1.6695	1.6695	1.6695
7	1.9342	1.6700	1.6700	1.6700
8	1.9647	1.6699	1.6699	1.6699
9	0.0645	1.9834	1.9834	1.9834
10	0.0593	1.9803	1.9803	1.9803
11	0.0661	1.9788	1.9788	1.9788
12	0.0645	1.9834	1.9834	1.9834
13	0.0593	1.9803	1.9803	1.9803
14	0.0661	1.9788	1.9788	1.9788

Molecule 139-pyridine
Energy: -247.557623308
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.134353	-0.715968	-0.000220
2	6	-1.188127	0.665885	-0.000126
3	6	0.000102	1.370617	0.000136
4	6	1.188226	0.665720	0.000221
5	6	1.134248	-0.716124	0.000098
6	7	-0.000103	-1.402475	-0.000095
7	1	0.000153	2.455839	0.000122
8	1	-2.049301	-1.302658	-0.000383
9	1	-2.146055	1.173326	-0.000248
10	1	2.146247	1.172987	0.000348
11	1	2.049106	-1.302950	0.000167

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0166	1.6289	1.6289	1.6289
2	1.9383	1.6535	1.6535	1.6535
3	1.9646	1.6579	1.6579	1.6579
4	1.9383	1.6535	1.6535	1.6535
5	2.0166	1.6289	1.6289	1.6289

6	1.8052	1.4903	1.4903	1.4903
7	0.0675	1.9545	1.9545	1.9545
8	0.0623	1.9437	1.9437	1.9437
9	0.0641	1.9590	1.9590	1.9590
10	0.0641	1.9590	1.9590	1.9590
11	0.0623	1.9437	1.9437	1.9437

Molecule 140-pyrrole
Energy: -209.567305103
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.327525	-1.114298	-0.000039
2	6	-0.974286	-0.708555	-0.000098
3	6	-0.974022	0.708915	0.000039
4	6	0.327939	1.114178	0.000046
5	7	1.113845	-0.000206	0.000036
6	1	2.121137	-0.000399	0.000151
7	1	0.757492	-2.105057	-0.000080
8	1	-1.838642	-1.357029	-0.000180
9	1	-1.838131	1.357718	0.000068
10	1	0.758298	2.104768	0.000101

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9556	1.6362	1.6362	1.6362
2	1.8904	1.6654	1.6654	1.6654
3	1.8904	1.6654	1.6654	1.6654
4	1.9556	1.6362	1.6362	1.6362
5	1.9110	1.4431	1.4431	1.4431
6	0.1586	1.7943	1.7943	1.7943
7	0.0636	1.9779	1.9779	1.9779
8	0.0556	1.9912	1.9912	1.9912
9	0.0556	1.9912	1.9912	1.9912
10	0.0636	1.9779	1.9779	1.9779

Molecule 141-furan
Energy: -229.414093201
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.084787	-0.345373	0.000154
2	6	0.713957	0.949034	0.000028
3	6	-0.713967	0.949026	0.000115
4	6	-1.084784	-0.345385	-0.000010
5	8	0.000007	-1.146305	-0.000265
6	1	2.042682	-0.841976	0.000213
7	1	1.372164	1.805307	0.000062
8	1	-1.372182	1.805293	0.000202
9	1	-2.042676	-0.841992	-0.000072

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0041	1.6186	1.6186	1.6186
2	1.9031	1.6597	1.6597	1.6597
3	1.9031	1.6597	1.6597	1.6597
4	2.0041	1.6186	1.6186	1.6186
5	1.8977	1.2898	1.2898	1.2898
6	0.0766	1.9596	1.9596	1.9596
7	0.0673	1.9857	1.9857	1.9857
8	0.0673	1.9857	1.9857	1.9857
9	0.0766	1.9596	1.9596	1.9596

Molecule 142-azulene
Energy: -384.632236614
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.479319	-0.001720	0.000003
2	6	1.893314	-1.256158	0.000011
3	6	0.546178	-1.579153	-0.000003
4	6	1.893995	1.255370	-0.000011

5	6	-0.549794	-0.740058	-0.000016
6	6	0.549306	1.579516	0.000003
7	6	-0.549428	0.740630	0.000013
8	1	3.566524	-0.002101	0.000004
9	1	2.580096	-2.097184	0.000026
10	1	0.313887	-2.642326	-0.000003
11	1	2.582444	2.095019	-0.000029
12	1	0.317433	2.642782	0.000007
13	6	-1.886254	-1.138819	-0.000013
14	1	-2.230788	-2.164991	-0.000005
15	6	-2.682556	0.000336	0.000013
16	1	-3.766305	0.001283	0.000014
17	6	-1.883419	1.140205	-0.000001
18	1	-2.227253	2.166625	-0.000011

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9710	1.6604	1.6604	1.6604
2	1.9351	1.6594	1.6594	1.6594
3	1.9856	1.6569	1.6569	1.6569
4	1.9350	1.6594	1.6594	1.6594
5	1.9897	1.5914	1.5914	1.5914
6	1.9853	1.6569	1.6569	1.6569
7	1.9893	1.5914	1.5914	1.5914
8	0.0620	1.9347	1.9347	1.9347
9	0.0556	1.9406	1.9406	1.9406
10	0.0656	1.9396	1.9396	1.9396
11	0.0556	1.9407	1.9407	1.9407
12	0.0656	1.9397	1.9397	1.9397
13	1.9002	1.6585	1.6585	1.6585
14	0.0532	1.9881	1.9881	1.9881
15	1.9386	1.6668	1.6668	1.6668
16	0.0594	1.9800	1.9800	1.9800
17	1.9002	1.6585	1.6585	1.6585
18	0.0532	1.9880	1.9880	1.9880

Molecule 143-cyclopentadiene
Energy: -193.498372707
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000095	0.982325	0.731714
2	6	-0.000095	0.982325	-0.731714
3	6	-0.000095	-0.278874	-1.168414
4	6	0.000186	-1.208120	0.000000
5	6	-0.000095	-0.278874	1.168414
6	1	-0.000023	1.873247	1.348620
7	1	-0.000023	1.873247	-1.348620
8	1	0.000066	-0.604694	-2.201321
9	1	-0.877775	-1.865364	0.000000
10	1	0.878855	-1.864428	0.000000
11	1	0.000066	-0.604694	2.201321

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9280	1.6668	1.6668	1.6668
2	1.9280	1.6668	1.6668	1.6668
3	1.9329	1.6629	1.6629	1.6629
4	1.9215	1.6598	1.6598	1.6598
5	1.9329	1.6629	1.6629	1.6629
6	0.0586	1.9825	1.9825	1.9825
7	0.0586	1.9825	1.9825	1.9825
8	0.0571	1.9809	1.9809	1.9809
9	0.0627	1.9452	1.9452	1.9452
10	0.0627	1.9451	1.9451	1.9451
11	0.0571	1.9809	1.9809	1.9809

Molecule 144-1H-azirine
Energy: -132.250154475
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.033856	-0.468888	0.633252
2	6	-0.033856	-0.468888	-0.633252
3	1	-0.138340	-0.885237	1.619407
4	1	-0.138340	-0.885237	-1.619407
5	7	-0.033856	0.878726	0.000000
6	1	0.919951	1.246054	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9802	1.6700	1.6700	1.6700
2	1.9802	1.6700	1.6700	1.6700
3	0.1004	2.0072	2.0072	2.0072
4	0.1004	2.0072	2.0072	2.0072
5	1.7377	1.5262	1.5262	1.5262
6	0.1011	1.7828	1.7828	1.7828

Molecule 145-isocyanatomethane
Energy: -207.481137780
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.812162	0.000046	0.000201
2	1	2.189771	0.844347	0.579987
3	1	2.190646	0.079941	-1.020569
4	1	2.190049	-0.924022	0.441684
5	7	0.400354	-0.000106	-0.000467
6	6	-0.772402	-0.000030	-0.000092
7	8	-1.951438	0.000047	0.000189

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9680	1.6971	1.6971	1.6971
2	0.0673	1.9180	1.9180	1.9180
3	0.0673	1.9180	1.9180	1.9180
4	0.0673	1.9179	1.9179	1.9179
5	1.8649	1.4364	1.4364	1.4364
6	2.2348	1.5106	1.5106	1.5106
7	1.7302	1.3291	1.3291	1.3291

Molecule 146-isocyanooxy-methane
Energy: -207.347905726
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.422194	-0.356565	0.000005
2	1	2.355984	0.201750	0.000031
3	1	1.340322	-0.971025	-0.898670
4	1	1.340295	-0.971105	0.898638
5	8	0.400992	0.643489	0.000105
6	7	-0.789513	0.095805	-0.000264
7	6	-1.875185	-0.323130	0.000164

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9810	1.6758	1.6758	1.6758
2	0.0763	1.9098	1.9098	1.9098
3	0.0658	1.9183	1.9183	1.9183
4	0.0658	1.9183	1.9183	1.9183
5	1.9359	1.2853	1.2853	1.2853
6	1.9978	1.4042	1.4042	1.4042
7	1.8775	1.8933	1.8933	1.8933

Molecule 147-cyanatomethane
Energy: -207.435583187
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.484641	-0.340482	0.000000
2	1	2.403089	0.241011	-0.000035
3	1	1.424528	-0.958234	-0.897193
4	1	1.424574	-0.958199	0.897221
5	8	0.418284	0.619398	-0.000002
6	6	-0.768555	0.129270	0.000008

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7       7       -1.842139       -0.287499       -0.000004
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9927      1.6782      1.6782      1.6782
    2      0.0775      1.9040      1.9040      1.9040
    3      0.0709      1.9133      1.9133      1.9133
    4      0.0709      1.9133      1.9133      1.9133
    5      1.8995      1.2871      1.2871      1.2871
    6      2.1556      1.5320      1.5320      1.5320
    7      1.7329      1.5784      1.5784      1.5784

Molecule 148-3-methyl-1-2-oxazirene
Energy: -207.360305893
Geometry:
Atom  Atomic No.   x               y               z
 1      6       -1.467341       -0.013904       -0.000045
2       1       -1.924574       0.974781        -0.000586
3       1       -1.780305       -0.571920       -0.884567
4       1       -1.780086       -0.570587       0.885476
5       6       -0.010627       0.091931        0.000009
6       7       0.957974        0.867429        -0.000016
7       8       0.955869        -0.796555       0.000001
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      1.9110      1.7045      1.7045      1.7045
    2      0.0789      1.9396      1.9396      1.9396
    3      0.0848      1.9360      1.9360      1.9360
    4      0.0848      1.9360      1.9360      1.9360
    5      2.1638      1.5267      1.5267      1.5267
    6      1.8642      1.5351      1.5351      1.5351
    7      1.8127      1.3222      1.3222      1.3222

Molecule 149-carbon
Energy: -37.3004699187
Geometry:
Atom  Atomic No.   x               y               z
 1      6       0.000000        0.000000        0.000000
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      3.0000      1.8352      2.3811      2.0172

Molecule 150-methylium
Energy: -39.3393104647
Geometry:
Atom  Atomic No.   x               y               z
 1      6       0.000000        0.000000        0.000000
2       1       0.000000        1.095880        0.000000
3       1       0.949060        -0.547940       0.000000
4       1       -0.949060       -0.547940       0.000000
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
    1      2.4282      1.7769      1.7769      1.7769
    2      0.1906      1.9048      1.9048      1.9048
    3      0.1906      1.9049      1.9049      1.9049
    4      0.1906      1.9049      1.9049      1.9049

Molecule 151-methoxymethylium
Energy: -153.685979361
Geometry:
Atom  Atomic No.   x               y               z
 1      6       0.100882        -1.329532       0.000000
2       1       1.171096        -1.528868       0.000000
3       1       -0.381306       -1.675666       0.910945
4       1       -0.381306       -1.675666       -0.910945
5       6       -0.114598       1.341797        0.000000
6       1       -0.163095       1.879276        -0.954938
7       1       -0.163095       1.879276        0.954938
8       8       0.000000        0.131007        0.000000
   Atom      QA       DA(alpha)   DA(beta)    DA(total)
```

1	2.0683	1.6869	1.6869	1.6869
2	0.1184	1.8865	1.8865	1.8865
3	0.1113	1.8846	1.8846	1.8846
4	0.1113	1.8846	1.8846	1.8846
5	2.2857	1.6579	1.6579	1.6579
6	0.1413	1.8958	1.8958	1.8958
7	0.1413	1.8958	1.8958	1.8958
8	2.0224	1.2599	1.2599	1.2599

Molecule 152-ethylium
Energy: -78.5971214449
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.061684	-0.684749	0.000000
2	1	-0.077033	-1.242340	0.936475
3	1	-0.077033	-1.242340	-0.936475
4	1	1.050329	0.001677	0.000000
5	6	-0.061684	0.684747	0.000000
6	1	-0.078030	1.241508	-0.936900
7	1	-0.078030	1.241508	0.936900

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1064	1.6972	1.6972	1.6972
2	0.1458	1.9100	1.9100	1.9100
3	0.1458	1.9100	1.9100	1.9100
4	0.2048	1.9245	1.9245	1.9245
5	2.1055	1.6971	1.6971	1.6971
6	0.1458	1.9100	1.9100	1.9100
7	0.1458	1.9100	1.9100	1.9100

Molecule 153-phenylmethylium
Energy: -269.725475894
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	1.117788	1.197422
2	6	0.000000	-0.262657	1.220033
3	6	0.000000	-0.942609	0.000000
4	6	0.000000	-0.262657	-1.220033
5	6	0.000000	1.117788	-1.197422
6	6	0.000000	1.807361	0.000000
7	1	0.000000	1.655024	2.139806
8	1	0.000000	-0.792857	2.165867
9	1	0.000000	-0.792857	-2.165867
10	1	0.000000	1.655024	-2.139806
11	1	0.000000	2.891776	0.000000
12	6	0.000000	-2.364208	0.000000
13	1	-0.934196	-2.940480	0.000000
14	1	0.934196	-2.940480	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9876	1.6497	1.6497	1.6497
2	1.9735	1.6521	1.6521	1.6521
3	1.9867	1.5848	1.5848	1.5848
4	1.9735	1.6521	1.6521	1.6521
5	1.9876	1.6497	1.6497	1.6497
6	1.9923	1.6501	1.6501	1.6501
7	0.0928	1.9335	1.9335	1.9335
8	0.0847	1.9351	1.9351	1.9351
9	0.0847	1.9351	1.9351	1.9351
10	0.0928	1.9335	1.9335	1.9335
11	0.0920	1.9332	1.9332	1.9332
12	2.3346	1.7108	1.7108	1.7108
13	0.1586	1.9015	1.9015	1.9015
14	0.1586	1.9015	1.9015	1.9015

Molecule 154-propan-2-ylium
Energy: -117.820223895

Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000089	-0.200716	1.276335
2	1	-0.001021	-1.288366	1.250000
3	1	0.855055	0.193830	1.852242
4	1	-0.853349	0.195520	1.853768
5	6	-0.000089	0.444585	0.000000
6	1	0.000236	1.539119	0.000000
7	6	-0.000089	-0.200716	-1.276335
8	1	-0.853349	0.195520	-1.853768
9	1	0.855055	0.193830	-1.852242
10	1	-0.001021	-1.288366	-1.250000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9373	1.6898	1.6898	1.6898
2	0.1018	1.9214	1.9214	1.9214
3	0.1333	1.9375	1.9375	1.9375
4	0.1332	1.9374	1.9374	1.9374
5	2.2536	1.6567	1.6567	1.6567
6	0.1353	1.8869	1.8869	1.8869
7	1.9373	1.6898	1.6898	1.6898
8	0.1332	1.9374	1.9374	1.9374
9	0.1333	1.9375	1.9375	1.9375
10	0.1018	1.9214	1.9214	1.9214

Molecule 155-2-methylpropan-2-ylium
Energy: -157.038811417
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	1.453590	-0.013944
2	1	-0.904365	1.898303	-0.429819
3	1	0.000000	1.700505	1.062880
4	1	0.904365	1.898303	-0.429819
5	6	0.000000	0.000000	-0.059789
6	6	-1.258845	-0.726795	-0.013944
7	1	-1.191796	-1.732354	-0.429819
8	1	-1.472680	-0.850252	1.062880
9	1	-2.096161	-0.165949	-0.429819
10	6	1.258845	-0.726795	-0.013944
11	1	1.191796	-1.732354	-0.429819
12	1	2.096161	-0.165949	-0.429819
13	1	1.472680	-0.850252	1.062880

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9238	1.6876	1.6876	1.6876
2	0.1006	1.9218	1.9218	1.9218
3	0.1236	1.9360	1.9360	1.9360
4	0.1006	1.9218	1.9218	1.9218
5	2.2544	1.6097	1.6097	1.6097
6	1.9238	1.6875	1.6875	1.6875
7	0.1006	1.9218	1.9218	1.9218
8	0.1236	1.9360	1.9360	1.9360
9	0.1006	1.9218	1.9218	1.9218
10	1.9238	1.6875	1.6875	1.6875
11	0.1006	1.9218	1.9218	1.9218
12	0.1006	1.9218	1.9218	1.9218
13	0.1236	1.9360	1.9360	1.9360

Molecule 156-cyclohexylium
Energy: -234.216873230
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.252315	0.733918	0.229831
2	6	1.266440	-0.763452	-0.026375
3	6	0.000712	-1.434028	0.007040
4	6	-1.265614	-0.764837	-0.026146
5	6	-1.253123	0.732716	0.229509

6	6	-0.000659	1.379271	-0.339301
7	1	1.304383	0.906272	1.309010
8	1	1.561996	-1.003993	-1.076080
9	1	0.001407	-2.526322	-0.043132
10	1	-1.561268	-1.005886	-1.075731
11	1	-2.153776	1.175843	-0.198391
12	1	-0.001409	2.446364	-0.111103
13	1	-2.013772	-1.340586	0.535643
14	1	2.015817	-1.338586	0.534379
15	1	2.152801	1.178325	-0.197114
16	1	-0.000444	1.301414	-1.433359
17	1	-1.306153	0.905628	1.308537

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9387	1.6469	1.6469	1.6469
2	1.9671	1.6366	1.6366	1.6366
3	2.2266	1.6442	1.6442	1.6442
4	1.9671	1.6366	1.6366	1.6366
5	1.9387	1.6469	1.6469	1.6469
6	1.9319	1.6469	1.6469	1.6469
7	0.0682	1.8990	1.8990	1.8990
8	0.1277	1.9197	1.9197	1.9197
9	0.1297	1.8936	1.8936	1.8936
10	0.1278	1.9198	1.9198	1.9198
11	0.0761	1.8971	1.8971	1.8971
12	0.0763	1.8982	1.8982	1.8982
13	0.1119	1.9108	1.9108	1.9108
14	0.1119	1.9107	1.9107	1.9107
15	0.0761	1.8972	1.8972	1.8972
16	0.0561	1.9091	1.9091	1.9091
17	0.0682	1.8990	1.8990	1.8990

Molecule 157-cyclopentylium
Energy: -195.016637973
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.002050	1.240274	0.000009
2	6	1.179445	0.437117	-0.097546
3	6	0.737479	-0.994581	0.204721
4	6	-0.734094	-0.996924	-0.204805
5	6	-1.181018	0.433263	0.097809
6	1	2.085677	0.844826	0.357744
7	1	1.340244	0.562206	-1.199255
8	1	1.335014	-1.736147	-0.324162
9	1	-1.329368	-1.740630	0.323592
10	1	-1.342415	0.557103	1.199463
11	1	-2.088382	0.837992	-0.357910
12	1	-0.003689	2.332281	-0.000384
13	1	-0.845015	-1.187405	-1.276245
14	1	0.849358	-1.185116	1.276029

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2266	1.6450	1.6450	1.6450
2	1.9705	1.6385	1.6385	1.6385
3	1.9459	1.6492	1.6492	1.6492
4	1.9459	1.6492	1.6492	1.6492
5	1.9705	1.6385	1.6385	1.6385
6	0.1110	1.9186	1.9186	1.9186
7	0.1339	1.9251	1.9251	1.9251
8	0.0827	1.9024	1.9024	1.9024
9	0.0827	1.9025	1.9025	1.9025
10	0.1338	1.9250	1.9250	1.9250
11	0.1110	1.9186	1.9186	1.9186
12	0.1408	1.9134	1.9134	1.9134
13	0.0724	1.9010	1.9010	1.9010
14	0.0724	1.9010	1.9010	1.9010

Molecule 158-methylcyclopentan-1-ylium
Energy: -234.237284535
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.497804	0.719452	-0.203358
2	6	1.472431	-0.740156	0.239108
3	6	0.058600	-1.179031	-0.132810
4	6	-0.769044	0.009465	-0.026901
5	6	0.074114	1.189895	0.087947
6	1	1.699078	0.797422	-1.275705
7	1	1.612010	-0.823710	1.320895
8	1	2.237819	-1.351230	-0.238234
9	1	0.003736	-1.366032	-1.226686
10	1	-0.031277	1.437525	1.164158
11	1	-0.307414	2.066228	-0.443126
12	1	2.248206	1.315988	0.314375
13	6	-2.218949	0.006549	0.005861
14	1	-2.664155	0.949854	-0.310754
15	1	-2.645681	-0.847785	-0.523715
16	1	-2.479563	-0.140581	1.067582
17	1	-0.362496	-2.074710	0.332127

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9412	1.6489	1.6489	1.6489
2	1.9415	1.6490	1.6490	1.6490
3	1.9583	1.6365	1.6365	1.6365
4	2.2340	1.5936	1.5936	1.5936
5	1.9576	1.6371	1.6371	1.6371
6	0.0680	1.9022	1.9022	1.9022
7	0.0678	1.9031	1.9031	1.9031
8	0.0793	1.9048	1.9048	1.9048
9	0.1174	1.9155	1.9155	1.9155
10	0.1156	1.9163	1.9163	1.9163
11	0.1002	1.9181	1.9181	1.9181
12	0.0789	1.9049	1.9049	1.9049
13	1.9221	1.6914	1.6914	1.6914
14	0.0970	1.9250	1.9250	1.9250
15	0.1011	1.9273	1.9273	1.9273
16	0.1204	1.9359	1.9359	1.9359
17	0.0996	1.9203	1.9203	1.9203

Molecule 159-allylium
Energy: -116.570495402
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.370224	0.004207	-0.000516
2	1	1.939500	-0.931298	-0.002095
3	1	1.917115	0.951643	-0.000379
4	6	0.109194	-0.028294	0.002536
5	1	-1.517912	1.071712	-0.017386
6	6	-1.293750	-0.016625	0.000204
7	1	-1.729723	-0.412859	0.921692
8	1	-1.722986	-0.434926	-0.915178

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0101	1.7068	1.7068	1.7068
2	0.1716	1.9721	1.9721	1.9721
3	0.1706	1.9725	1.9725	1.9725
4	2.2683	1.6522	1.6522	1.6522
5	0.1558	1.9400	1.9400	1.9400
6	1.9648	1.6983	1.6983	1.6983
7	0.1291	1.9206	1.9206	1.9206
8	0.1298	1.9210	1.9210	1.9210

Molecule 160-ethylium
Energy: -77.3273306222
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000036	-0.580994	0.000000
2	1	0.944805	-1.147106	0.000000
3	1	-0.944858	-1.147140	0.000000
4	6	-0.000036	0.670363	0.000000
5	1	0.000482	1.758033	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0601	1.7078	1.7078	1.7078
2	0.1992	1.9811	1.9811	1.9811
3	0.1992	1.9811	1.9811	1.9811
4	2.3240	1.7360	1.7360	1.7360
5	0.2175	1.9907	1.9907	1.9907

Molecule 161-3-methylbut-2-en-2-ylium
Energy: -194.978674931
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.179999	-1.320513	0.000058
2	1	1.811664	-1.360874	0.889512
3	1	0.511445	-2.180827	0.000096
4	1	1.811743	-1.361027	-0.889336
5	6	0.457129	0.009962	-0.000085
6	6	1.261644	1.283359	0.000019
7	1	0.645445	2.181118	-0.000333
8	1	1.897805	1.285949	0.887255
9	1	1.898342	1.285694	-0.886837
10	6	-0.812164	-0.005770	-0.000266
11	6	-2.221819	0.007340	-0.000148
12	1	-2.661931	-0.397995	0.914599
13	1	-2.440357	1.094490	0.004171
14	1	-2.662890	-0.392796	-0.916591

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9332	1.7064	1.7064	1.7064
2	0.0920	1.9205	1.9205	1.9205
3	0.0828	1.9236	1.9236	1.9236
4	0.0920	1.9205	1.9205	1.9205
5	2.0586	1.6014	1.6014	1.6014
6	1.9300	1.7063	1.7063	1.7063
7	0.0813	1.9243	1.9243	1.9243
8	0.0916	1.9213	1.9213	1.9213
9	0.0916	1.9213	1.9213	1.9213
10	2.2170	1.6344	1.6344	1.6344
11	1.9518	1.7013	1.7013	1.7013
12	0.1171	1.9223	1.9223	1.9223
13	0.1440	1.9427	1.9427	1.9427
14	0.1169	1.9222	1.9222	1.9222

Molecule 162-benzene-1-ylium
Energy: -230.527355047
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.205328	0.602228	-0.000013
2	6	-1.265862	-0.810771	0.000014
3	6	-0.000042	-1.168764	-0.000005
4	6	1.265802	-0.810830	-0.000011
5	6	1.205382	0.602161	0.000013
6	6	0.000042	1.282739	0.000000
7	1	-2.158138	1.124146	-0.000018
8	1	-2.177127	-1.397635	0.000026
9	1	2.177011	-1.397784	-0.000012
10	1	2.158220	1.124026	0.000021
11	1	0.000067	2.366669	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0305	1.6531	1.6531	1.6531
2	2.0211	1.6526	1.6526	1.6526

3	2.2574	1.6202	1.6202	1.6202
4	2.0211	1.6526	1.6526	1.6526
5	2.0305	1.6531	1.6531	1.6531
6	1.9935	1.6456	1.6456	1.6456
7	0.1170	1.9239	1.9239	1.9239
8	0.1523	1.9581	1.9581	1.9581
9	0.1523	1.9581	1.9581	1.9581
10	0.1170	1.9239	1.9239	1.9239
11	0.1075	1.9268	1.9268	1.9268

Molecule 163-E-penta-2-4-dien-1-ylium
Energy: -193.780107524
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.370605	-0.290177	-0.000279
2	1	2.340029	-1.377390	-0.000301
3	1	3.352848	0.174405	-0.000712
4	6	1.242628	0.446446	0.000081
5	1	1.278619	1.531710	0.000007
6	6	-0.000036	-0.206009	0.000458
7	1	-0.000040	-1.296888	0.001025
8	6	-1.242673	0.446590	0.000242
9	1	-1.278775	1.531819	-0.000077
10	6	-2.370525	-0.290265	-0.000289
11	1	-3.352776	0.174295	-0.001171
12	1	-2.339895	-1.377465	-0.000046

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0788	1.7208	1.7208	1.7208
2	0.1079	1.9407	1.9407	1.9407
3	0.1189	1.9333	1.9333	1.9333
4	1.9746	1.6510	1.6510	1.6510
5	0.0981	1.9348	1.9348	1.9348
6	2.1356	1.6585	1.6585	1.6585
7	0.1078	1.9209	1.9209	1.9209
8	1.9746	1.6510	1.6510	1.6510
9	0.0981	1.9348	1.9348	1.9348
10	2.0788	1.7208	1.7208	1.7208
11	0.1189	1.9333	1.9333	1.9333
12	0.1079	1.9407	1.9407	1.9407

Molecule 164-cyclohex-3-en-1-ylium
Energy: -232.987458135
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.458370	0.100875	-0.191846
2	6	-0.737533	-1.190915	0.142120
3	6	0.672453	-1.224883	-0.017635
4	6	1.466641	-0.030212	-0.112495
5	6	0.719188	1.247890	0.101192
6	6	-0.600686	1.302092	0.064807
7	1	-1.761982	0.076620	-1.244157
8	1	-0.618973	-1.291448	1.265101
9	1	2.384210	-0.134594	0.481985
10	1	1.314843	2.137237	0.273530
11	1	-1.104381	2.253222	0.203259
12	1	1.863684	-0.115811	-1.150402
13	1	1.181955	-2.191591	0.005121
14	1	-1.246006	-2.117364	-0.135839
15	1	-2.383504	0.154641	0.384540

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9490	1.6496	1.6496	1.6496
2	1.9814	1.6353	1.6353	1.6353
3	2.2207	1.6430	1.6430	1.6430
4	1.9674	1.6400	1.6400	1.6400
5	1.9455	1.6521	1.6521	1.6521

6	1.9706	1.6514	1.6514	1.6514
7	0.0809	1.9006	1.9006	1.9006
8	0.1428	1.9229	1.9229	1.9229
9	0.1115	1.9076	1.9076	1.9076
10	0.0857	1.9353	1.9353	1.9353
11	0.0886	1.9315	1.9315	1.9315
12	0.1294	1.9239	1.9239	1.9239
13	0.1341	1.8959	1.8959	1.8959
14	0.1099	1.9049	1.9049	1.9049
15	0.0826	1.8938	1.8938	1.8938

Molecule 165-1-methoxycyclohex-2-en-1-ylium
Energy: -347.335651648
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.242040	0.418668	-0.114992
2	6	1.797027	-0.951973	0.358277
3	6	0.450475	-1.318755	-0.238457
4	6	-0.544625	-0.240322	-0.050854
5	6	-0.154838	1.120339	0.040099
6	6	1.157705	1.420686	-0.034482
7	1	3.108026	0.778103	0.446930
8	1	2.535355	-1.709270	0.092190
9	1	0.531771	-1.462270	-1.325973
10	1	-0.899041	1.902814	0.111192
11	1	1.441460	2.471330	-0.053287
12	8	-1.758151	-0.624518	-0.037393
13	6	-2.872857	0.282826	0.082055
14	1	-3.754518	-0.351833	0.074980
15	1	-2.802584	0.825004	1.024921
16	1	-2.884971	0.959378	-0.772548
17	1	0.043145	-2.247637	0.165372
18	1	1.724455	-0.953062	1.450122
19	1	2.572547	0.394784	-1.164634

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9455	1.6445	1.6445	1.6445
2	1.9408	1.6464	1.6464	1.6464
3	1.9446	1.6344	1.6344	1.6344
4	2.2308	1.5445	1.5445	1.5445
5	1.9294	1.6362	1.6362	1.6362
6	2.0862	1.6513	1.6513	1.6513
7	0.0864	1.9001	1.9001	1.9001
8	0.0779	1.8971	1.8971	1.8971
9	0.0911	1.9049	1.9049	1.9049
10	0.0835	1.9286	1.9286	1.9286
11	0.1068	1.9136	1.9136	1.9136
12	1.9615	1.2758	1.2758	1.2758
13	2.0072	1.6732	1.6732	1.6732
14	0.0981	1.8893	1.8893	1.8893
15	0.0854	1.9036	1.9036	1.9036
16	0.0852	1.9039	1.9039	1.9039
17	0.0881	1.8963	1.8963	1.8963
18	0.0645	1.8996	1.8996	1.8996
19	0.0869	1.9142	1.9142	1.9142

Molecule 166-carbonium
Energy: -40.5716330548
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000005	0.000000
2	1	0.783574	0.784473	0.000000
3	1	0.287564	-1.070836	0.000000
4	1	0.000009	-0.000025	1.115287
5	1	-1.071155	0.286384	0.000000
6	1	0.000009	-0.000025	-1.115287

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9499	1.7156	1.7156	1.7156
2	0.1801	1.9207	1.9207	1.9207
3	0.1801	1.9208	1.9208	1.9208
4	0.2548	1.9665	1.9665	1.9665
5	0.1801	1.9207	1.9207	1.9207
6	0.2548	1.9665	1.9665	1.9665

Molecule 167-2-hydroxypropan-2-ylium
Energy: -192.935705962
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.040009	-0.651053	-1.282875
2	1	-1.021276	-0.819568	-1.528557
3	1	0.448375	-0.025547	-2.078303
4	1	0.519469	-1.627811	-1.230776
5	6	0.040009	0.039928	0.000000
6	6	0.040009	-0.651053	1.282875
7	1	0.448375	-0.025547	2.078303
8	1	-1.021276	-0.819568	1.528557
9	1	0.519469	-1.627811	1.230776
10	8	-0.134734	1.306060	0.000000
11	1	0.464566	2.070438	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9177	1.6851	1.6851	1.6851
2	0.1246	1.9292	1.9292	1.9292
3	0.1024	1.9228	1.9228	1.9228
4	0.1017	1.9215	1.9215	1.9215
5	2.3140	1.5630	1.5630	1.5630
6	1.9177	1.6851	1.6851	1.6851
7	0.1024	1.9228	1.9228	1.9228
8	0.1246	1.9292	1.9292	1.9292
9	0.1017	1.9215	1.9215	1.9215
10	1.9008	1.2797	1.2797	1.2797
11	0.2922	1.6997	1.6997	1.6997

Molecule 168-E-but-2-en-1-ylium
Energy: -155.803007145
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.830596	0.083265	-0.000165
2	1	-1.944275	1.165890	-0.000259
3	1	-2.346070	-0.360138	0.864299
4	1	-2.345936	-0.360315	-0.864580
5	6	-0.456902	-0.370559	0.000154
6	1	-0.289350	-1.449742	0.000418
7	6	0.663079	0.452621	0.000238
8	1	0.547944	1.532412	0.000284
9	6	1.887113	-0.128702	-0.000131
10	1	2.001738	-1.211070	-0.000141
11	1	2.799787	0.463219	-0.000594

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9245	1.6947	1.6947	1.6947
2	0.0923	1.9252	1.9252	1.9252
3	0.1160	1.9352	1.9352	1.9352
4	0.1160	1.9352	1.9352	1.9352
5	2.1815	1.6588	1.6588	1.6588
6	0.1175	1.9058	1.9058	1.9058
7	1.9813	1.6470	1.6470	1.6470
8	0.1042	1.9312	1.9312	1.9312
9	2.1199	1.7194	1.7194	1.7194
10	0.1178	1.9334	1.9334	1.9334
11	0.1289	1.9267	1.9267	1.9267

Molecule 169-butan-1-ylium

Energy: -157.016779847
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.928610	-0.144026	0.124740
2	1	-2.048514	-1.109283	-0.370926
3	1	-2.094501	-0.279112	1.194724
4	1	-2.699721	0.528807	-0.248980
5	6	-0.557130	0.448916	-0.113399
6	1	-0.398961	0.596866	-1.229717
7	1	-0.384088	1.443594	0.306586
8	6	0.588456	-0.383007	-0.104363
9	1	2.199039	-0.359766	1.089451
10	1	0.433524	-1.444901	-0.322544
11	6	1.943812	0.061363	0.097483
12	1	2.065279	1.143380	0.141983
13	1	2.648777	-0.419055	-0.587345

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9042	1.7040	1.7040	1.7040
2	0.0723	1.9302	1.9302	1.9302
3	0.0789	1.9217	1.9217	1.9217
4	0.0834	1.9183	1.9183	1.9183
5	1.9841	1.6407	1.6407	1.6407
6	0.1469	1.9190	1.9190	1.9190
7	0.1039	1.9063	1.9063	1.9063
8	2.2213	1.6496	1.6496	1.6496
9	0.1317	1.9402	1.9402	1.9402
10	0.1304	1.8993	1.8993	1.8993
11	1.9310	1.6915	1.6915	1.6915
12	0.0990	1.9250	1.9250	1.9250
13	0.1128	1.9250	1.9250	1.9250

Molecule 170-4-methylpent-3-en-2-ylium
Energy: -234.225295309
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.377170	1.377745	-0.001886
2	1	-2.203639	1.531140	0.697585
3	1	-0.580505	2.083482	0.216532
4	1	-1.785889	1.607846	-0.994212
5	6	-0.990044	-0.041659	-0.008207
6	6	-2.090253	-1.017310	-0.000156
7	1	-1.801267	-1.989821	-0.397991
8	1	-2.371573	-1.162960	1.053387
9	1	-2.979956	-0.638697	-0.506408
10	6	0.322168	-0.516045	-0.012769
11	1	0.472071	-1.591405	-0.044066
12	6	1.413045	0.297310	0.014332
13	1	1.274385	1.376058	0.045821
14	6	2.797635	-0.173384	-0.000748
15	1	3.323066	0.220867	0.877157
16	1	2.884753	-1.258693	-0.027928
17	1	3.316265	0.262240	-0.863274

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9101	1.6921	1.6921	1.6921
2	0.0951	1.9248	1.9248	1.9248
3	0.0764	1.9196	1.9196	1.9196
4	0.1021	1.9290	1.9290	1.9290
5	2.1812	1.6109	1.6109	1.6109
6	1.9115	1.6923	1.6923	1.6923
7	0.0862	1.9264	1.9264	1.9264
8	0.1048	1.9354	1.9354	1.9354
9	0.0893	1.9271	1.9271	1.9271
10	1.9484	1.6372	1.6372	1.6372
11	0.0850	1.9299	1.9299	1.9299
12	2.1203	1.6561	1.6561	1.6561

13	0.0984	1.9067	1.9067	1.9067
14	1.9125	1.6991	1.6991	1.6991
15	0.0984	1.9346	1.9346	1.9346
16	0.0815	1.9296	1.9296	1.9296
17	0.0987	1.9349	1.9349	1.9349

Molecule 171-4-methylpentan-2-ylium
Energy: -235.405991750
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.356111	1.393935	0.048547
2	1	-1.170255	1.520837	1.119920
3	1	-0.762609	2.125819	-0.503636
4	1	-2.404978	1.639905	-0.120032
5	6	-1.096030	-0.031066	-0.398814
6	1	-1.258838	-0.100876	-1.486778
7	6	-2.023852	-1.040061	0.271141
8	1	-1.844677	-2.060733	-0.074349
9	1	-1.908664	-1.016768	1.358648
10	1	-3.061829	-0.792869	0.047011
11	6	0.317154	-0.472385	-0.285164
12	1	0.526595	-1.514655	-0.539324
13	1	0.772397	-0.338127	1.000720
14	6	1.398400	0.293039	0.115378
15	1	1.204699	1.339024	0.353183
16	6	2.817799	-0.154498	0.049449
17	1	3.367823	0.135176	0.945513
18	1	2.911825	-1.229677	-0.108018
19	1	3.284349	0.359156	-0.796077

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8865	1.6991	1.6991	1.6991
2	0.0583	1.9376	1.9376	1.9376
3	0.0615	1.9278	1.9278	1.9278
4	0.0779	1.9217	1.9217	1.9217
5	1.9875	1.6052	1.6052	1.6052
6	0.0922	1.8782	1.8782	1.8782
7	1.8903	1.7019	1.7019	1.7019
8	0.0634	1.9332	1.9332	1.9332
9	0.0593	1.9375	1.9375	1.9375
10	0.0759	1.9227	1.9227	1.9227
11	2.1106	1.6320	1.6320	1.6320
12	0.1150	1.9041	1.9041	1.9041
13	0.1717	1.8994	1.8994	1.8994
14	2.0634	1.6389	1.6389	1.6389
15	0.1106	1.9011	1.9011	1.9011
16	1.9118	1.6999	1.6999	1.6999
17	0.0883	1.9207	1.9207	1.9207
18	0.0801	1.9280	1.9280	1.9280
19	0.0957	1.9232	1.9232	1.9232

Molecule 172-2E-5E-hepta-2-5-dien-4-ylium
Energy: -272.188022322
Geometry:

Atom	Atomic No.	x	y	z
1	6	-2.805242	-1.027999	-0.026756
2	1	-3.300994	-1.183080	-0.991326
3	1	-2.618908	-2.031276	0.372046
4	1	-3.475090	-0.491671	0.644589
5	6	-1.525804	-0.336525	-0.233560
6	1	-0.808437	-0.822198	-0.892927
7	6	-1.225278	0.894041	0.254156
8	1	-2.003363	1.469811	0.748664
9	6	-0.000002	1.524613	-0.000003
10	1	-0.000006	2.614815	-0.000015
11	6	1.225249	0.894039	-0.254160

12	1	2.003363	1.469773	-0.748665
13	6	1.525812	-0.336526	0.233592
14	1	0.808487	-0.822164	0.893034
15	6	2.805257	-1.027969	0.026742
16	1	3.301064	-1.183126	0.991263
17	1	2.618869	-2.031253	-0.372060
18	1	3.475060	-0.491673	-0.644672

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9058	1.7016	1.7016	1.7016
2	0.0919	1.9339	1.9339	1.9339
3	0.0894	1.9372	1.9372	1.9372
4	0.0781	1.9307	1.9307	1.9307
5	2.0835	1.6582	1.6582	1.6582
6	0.0844	1.9143	1.9143	1.9143
7	1.9597	1.6448	1.6448	1.6448
8	0.0926	1.9327	1.9327	1.9327
9	2.1155	1.6571	1.6571	1.6571
10	0.1134	1.9092	1.9092	1.9092
11	1.9597	1.6448	1.6448	1.6448
12	0.0926	1.9327	1.9327	1.9327
13	2.0835	1.6583	1.6583	1.6583
14	0.0844	1.9143	1.9143	1.9143
15	1.9058	1.7016	1.7016	1.7016
16	0.0919	1.9339	1.9339	1.9339
17	0.0895	1.9372	1.9372	1.9372
18	0.0781	1.9307	1.9307	1.9307

Molecule 173-E-hept-2-en-4-ylium
Energy: -273.399071726
Geometry:

Atom	Atomic No.	x	y	z
1	6	3.396967	-0.687278	-0.133979
2	1	3.500053	-1.459998	-0.906498
3	1	3.989266	0.187606	-0.397740
4	1	3.795884	-1.151433	0.777232
5	6	1.982640	-0.397396	0.063493
6	1	1.346053	-1.240486	0.327231
7	6	1.415935	0.844432	-0.063433
8	1	2.044403	1.686401	-0.337135
9	6	0.068480	1.059832	0.139871
10	1	-0.277598	2.084378	-0.010311
11	6	-0.982478	0.120792	0.520720
12	1	-1.365268	0.479415	1.488430
13	1	-0.630537	-0.900777	0.668703
14	6	-2.150856	0.157992	-0.478141
15	1	-1.795486	-0.162098	-1.461890
16	1	-2.503931	1.187890	-0.587472
17	6	-3.288004	-0.734561	-0.021357
18	1	-3.685967	-0.410526	0.943371
19	1	-4.105705	-0.708610	-0.743009
20	1	-2.967273	-1.774639	0.076044

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9163	1.6977	1.6977	1.6977
2	0.1036	1.9352	1.9352	1.9352
3	0.0851	1.9279	1.9279	1.9279
4	0.1041	1.9353	1.9353	1.9353
5	2.1431	1.6568	1.6568	1.6568
6	0.1031	1.9060	1.9060	1.9060
7	1.9587	1.6432	1.6432	1.6432
8	0.0921	1.9288	1.9288	1.9288
9	2.1504	1.6535	1.6535	1.6535
10	0.1120	1.9013	1.9013	1.9013
11	1.9444	1.6456	1.6456	1.6456
12	0.0952	1.9087	1.9087	1.9087
13	0.0662	1.9040	1.9040	1.9040

14	1.9420	1.6589	1.6589	1.6589
15	0.0570	1.9057	1.9057	1.9057
16	0.0604	1.9045	1.9045	1.9045
17	1.8860	1.7071	1.7071	1.7071
18	0.0572	1.9366	1.9366	1.9366
19	0.0678	1.9308	1.9308	1.9308
20	0.0552	1.9382	1.9382	1.9382

Molecule 174-3-chlorohexan-3-ylium
Energy: -694.746819983
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.970451	-0.645375	-0.072406
2	1	3.103075	-0.310941	-1.103087
3	1	3.658440	-1.473142	0.099236
4	1	3.256571	0.166610	0.596894
5	6	1.555385	-1.119738	0.176995
6	1	1.303295	-2.033183	-0.375433
7	1	1.421954	-1.418269	1.234886
8	6	0.452930	-0.180619	-0.009352
9	6	-0.914356	-0.656399	-0.186163
10	1	-0.944412	-0.878071	-1.271495
11	1	-0.993645	-1.643600	0.284483
12	6	-2.070111	0.259761	0.184643
13	1	-2.025097	1.176581	-0.407579
14	1	-1.974054	0.552419	1.234673
15	6	-3.399980	-0.434807	-0.040601
16	1	-3.489207	-1.339764	0.565357
17	1	-4.223687	0.225383	0.232710
18	1	-3.535179	-0.712846	-1.088883
19	17	0.757413	1.432464	-0.018850

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8910	1.7025	1.7025	1.7025
2	0.0672	1.9289	1.9289	1.9289
3	0.0809	1.9202	1.9202	1.9202
4	0.0651	1.9247	1.9247	1.9247
5	1.9581	1.6399	1.6399	1.6399
6	0.0982	1.8992	1.8992	1.8992
7	0.1141	1.9045	1.9045	1.9045
8	2.2466	1.6085	1.6085	1.6085
9	1.9533	1.6352	1.6352	1.6352
10	0.1118	1.9093	1.9093	1.9093
11	0.0916	1.9030	1.9030	1.9030
12	1.9329	1.6545	1.6545	1.6545
13	0.0579	1.8982	1.8982	1.8982
14	0.0598	1.9041	1.9041	1.9041
15	1.8870	1.7064	1.7064	1.7064
16	0.0575	1.9357	1.9357	1.9357
17	0.0705	1.9283	1.9283	1.9283
18	0.0576	1.9363	1.9363	1.9363
19	10.1990	1.6932	1.6932	1.6932

Molecule 175-butan-2-iminium
Energy: -212.338093418
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.856090	-0.591498	-0.000189
2	1	-1.944946	-1.236929	-0.878288
3	1	-1.944322	-1.239651	0.875935
4	1	-2.676612	0.125964	0.001146
5	6	-0.526640	0.050948	0.000130
6	6	0.698540	-0.782176	0.000351
7	1	0.615842	-1.447576	0.867947
8	1	0.615550	-1.448649	-0.866383
9	6	2.020295	-0.043200	-0.000291

10	1	2.149646	0.574982	0.892405
11	1	2.838940	-0.762894	-0.000153
12	1	2.149200	0.574197	-0.893592
13	7	-0.433684	1.333338	0.000113
14	1	-1.258080	1.928897	0.000035
15	1	0.473948	1.793847	0.000147

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9144	1.6911	1.6911	1.6911
2	0.0992	1.9246	1.9246	1.9246
3	0.0992	1.9246	1.9246	1.9246
4	0.0847	1.9231	1.9231	1.9231
5	2.2087	1.5665	1.5665	1.5665
6	1.9522	1.6416	1.6416	1.6416
7	0.0928	1.8985	1.8985	1.8985
8	0.0928	1.8985	1.8985	1.8985
9	1.8893	1.7014	1.7014	1.7014
10	0.0628	1.9260	1.9260	1.9260
11	0.0840	1.9189	1.9189	1.9189
12	0.0628	1.9260	1.9260	1.9260
13	1.9644	1.4620	1.4620	1.4620
14	0.2024	1.7735	1.7735	1.7735
15	0.1904	1.7839	1.7839	1.7839

Molecule 176-2-methylbutan-2-ylium
Energy: -196.236139392
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.526267	-0.000864	-0.012002
2	6	0.508063	1.450831	-0.014507
3	1	0.093369	1.761442	-0.986724
4	1	-0.218717	1.824845	0.714932
5	1	1.486574	1.907578	0.122771
6	6	1.798964	-0.702741	0.038595
7	1	2.182281	-0.543081	1.059956
8	1	1.726769	-1.774143	-0.144892
9	1	2.539156	-0.227273	-0.612503
10	6	-0.707758	-0.766978	-0.078744
11	1	-0.619688	-1.264970	-1.063974
12	1	-0.602709	-1.619480	0.607976
13	6	-2.031261	-0.051233	0.065497
14	1	-2.846259	-0.765199	-0.053553
15	1	-2.139489	0.401762	1.053361
16	1	-2.166931	0.724437	-0.690389

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2418	1.6032	1.6032	1.6032
2	1.9211	1.6870	1.6870	1.6870
3	0.1175	1.9357	1.9357	1.9357
4	0.1062	1.9287	1.9287	1.9287
5	0.0920	1.9212	1.9212	1.9212
6	1.9215	1.6883	1.6883	1.6883
7	0.1191	1.9348	1.9348	1.9348
8	0.0919	1.9235	1.9235	1.9235
9	0.1059	1.9281	1.9281	1.9281
10	1.9600	1.6390	1.6390	1.6390
11	0.1139	1.9085	1.9085	1.9085
12	0.1032	1.9055	1.9055	1.9055
13	1.8924	1.7024	1.7024	1.7024
14	0.0806	1.9201	1.9201	1.9201
15	0.0678	1.9274	1.9274	1.9274
16	0.0652	1.9268	1.9268	1.9268

Molecule 177-2-methylpentan-2-ylium
Energy: -235.428600860
Geometry:

Atom	Atomic No.	x	y	z

Atom	Atomic No.	x	y	z
1	6	1.088041	-0.041252	-0.014042
2	6	1.380705	1.381578	-0.032785
3	1	1.047103	1.760637	-1.011787
4	1	0.750708	1.912687	0.688567
5	1	2.434644	1.618168	0.102662
6	6	2.183870	-0.996180	0.037439
7	1	2.576518	-0.929074	1.065870
8	1	1.887345	-2.026953	-0.153529
9	1	3.016353	-0.684944	-0.600526
10	6	-0.279636	-0.527429	-0.065749
11	1	-0.316513	-0.999380	-1.068811
12	1	-0.353906	-1.405771	0.592389
13	6	-1.431994	0.439311	0.119384
14	1	-1.367902	0.896524	1.112099
15	1	-1.362489	1.251227	-0.610427
16	6	-2.767564	-0.265833	-0.029893
17	1	-3.590353	0.434573	0.116175
18	1	-2.880307	-0.703397	-1.025077
19	1	-2.881727	-1.065462	0.706268

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2415	1.6036	1.6036	1.6036
2	1.9206	1.6872	1.6872	1.6872
3	0.1172	1.9357	1.9357	1.9357
4	0.1051	1.9288	1.9288	1.9288
5	0.0913	1.9214	1.9214	1.9214
6	1.9213	1.6885	1.6885	1.6885
7	0.1191	1.9354	1.9354	1.9354
8	0.0919	1.9240	1.9240	1.9240
9	0.1045	1.9281	1.9281	1.9281
10	1.9560	1.6341	1.6341	1.6341
11	0.1117	1.9146	1.9146	1.9146
12	0.0983	1.9108	1.9108	1.9108
13	1.9329	1.6539	1.6539	1.6539
14	0.0604	1.9022	1.9022	1.9022
15	0.0580	1.9009	1.9009	1.9009
16	1.8864	1.7067	1.7067	1.7067
17	0.0693	1.9289	1.9289	1.9289
18	0.0569	1.9367	1.9367	1.9367
19	0.0577	1.9361	1.9361	1.9361

Molecule 178-3-methylpentan-3-ylium
Energy: -235.430465314
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.001540	0.433678	0.000011
2	6	-0.688487	-0.846118	0.000214
3	1	-0.258426	-1.403132	-0.849201
4	1	-0.258823	-1.402102	0.850550
5	6	-0.754273	1.678522	-0.000083
6	1	-1.431363	1.680645	0.864165
7	1	-0.133132	2.572640	0.000051
8	1	-1.430666	1.680534	-0.864930
9	6	1.455447	0.495726	0.000177
10	1	1.711882	1.144920	-0.853502
11	1	1.711416	1.144198	0.854560
12	6	2.258358	-0.784660	-0.000214
13	1	2.065191	-1.393108	0.885716
14	1	2.065748	-1.392078	-0.886975
15	6	-2.199678	-0.875282	-0.000119
16	1	-2.543818	-1.909531	0.000160
17	1	-2.619543	-0.394590	0.885694
18	1	-2.619039	-0.395177	-0.886489
19	1	3.321610	-0.544416	0.000284

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2338	1.5983	1.5983	1.5983

2	1.9580	1.6375	1.6375	1.6375
3	0.1052	1.9070	1.9070	1.9070
4	0.1052	1.9070	1.9070	1.9070
5	1.9185	1.6870	1.6870	1.6870
6	0.1086	1.9316	1.9316	1.9316
7	0.0888	1.9223	1.9223	1.9223
8	0.1086	1.9316	1.9316	1.9316
9	1.9579	1.6391	1.6391	1.6391
10	0.1059	1.9065	1.9065	1.9065
11	0.1059	1.9065	1.9065	1.9065
12	1.8914	1.7024	1.7024	1.7024
13	0.0653	1.9275	1.9275	1.9275
14	0.0653	1.9275	1.9275	1.9275
15	1.8916	1.7025	1.7025	1.7025
16	0.0791	1.9205	1.9205	1.9205
17	0.0655	1.9274	1.9274	1.9274
18	0.0655	1.9274	1.9274	1.9274
19	0.0797	1.9201	1.9201	1.9201

Molecule 179-2-3-dimethylbutan-2-ylium
Energy: -235.427383403
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.063093	0.746985	0.000000
2	6	-0.072998	1.473247	1.254720
3	1	-1.080731	1.224887	1.628656
4	1	0.604960	1.102524	2.026520
5	6	-0.072998	1.473247	-1.254720
6	1	0.604960	1.102524	-2.026520
7	1	-1.080731	1.224887	-1.628656
8	1	0.001271	2.553021	-1.145151
9	6	0.325464	-0.689704	0.000000
10	1	1.439134	-0.599787	0.000000
11	6	-0.072998	-1.439143	1.264902
12	1	0.347987	-1.016616	2.176528
13	1	-1.160931	-1.472027	1.365903
14	1	0.278185	-2.468364	1.194936
15	1	0.001271	2.553021	1.145151
16	6	-0.072998	-1.439143	-1.264902
17	1	-1.160931	-1.472027	-1.365903
18	1	0.347987	-1.016616	-2.176528
19	1	0.278185	-2.468364	-1.194936

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2359	1.6005	1.6005	1.6005
2	1.9196	1.6865	1.6865	1.6865
3	0.1161	1.9383	1.9383	1.9383
4	0.1010	1.9225	1.9225	1.9225
5	1.9196	1.6865	1.6865	1.6865
6	0.1010	1.9225	1.9225	1.9225
7	0.1161	1.9383	1.9383	1.9383
8	0.0910	1.9179	1.9179	1.9179
9	1.9947	1.5989	1.5989	1.5989
10	0.1127	1.8856	1.8856	1.8856
11	1.8933	1.6983	1.6983	1.6983
12	0.0638	1.9206	1.9206	1.9206
13	0.0668	1.9313	1.9313	1.9313
14	0.0768	1.9175	1.9175	1.9175
15	0.0910	1.9179	1.9179	1.9179
16	1.8933	1.6983	1.6983	1.6983
17	0.0668	1.9313	1.9313	1.9313
18	0.0638	1.9206	1.9206	1.9206
19	0.0768	1.9175	1.9175	1.9175

Molecule 180-2-3-3-trimethylbutan-2-ylium
Energy: -274.622144161

Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.218034	0.823558	0.000000
2	6	-0.382658	1.555978	1.249926
3	1	-1.437361	1.390183	1.529541
4	1	0.199240	1.145094	2.074328
5	6	-0.382658	1.555978	-1.249926
6	1	0.199240	1.145094	-2.074328
7	1	-1.437361	1.390183	-1.529541
8	1	-0.230955	2.629007	-1.147248
9	6	0.080876	-0.609241	0.000000
10	6	-0.382658	-1.345897	1.251707
11	1	0.045454	-0.949552	2.172475
12	1	-1.471869	-1.335708	1.339819
13	1	-0.071764	-2.388846	1.179065
14	1	-0.230955	2.629007	1.147248
15	6	-0.382658	-1.345897	-1.251707
16	1	-1.471869	-1.335708	-1.339819
17	1	0.045454	-0.949552	-2.172475
18	1	-0.071764	-2.388846	-1.179065
19	6	1.643915	-0.525021	0.000000
20	1	1.990570	-1.560584	0.000000
21	1	2.043596	-0.038257	-0.890964
22	1	2.043596	-0.038257	0.890964

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2328	1.5947	1.5947	1.5947
2	1.9178	1.6862	1.6862	1.6862
3	0.1156	1.9379	1.9379	1.9379
4	0.0940	1.9209	1.9209	1.9209
5	1.9178	1.6862	1.6862	1.6862
6	0.0940	1.9209	1.9209	1.9209
7	0.1156	1.9379	1.9379	1.9379
8	0.0907	1.9194	1.9194	1.9194
9	2.0196	1.5654	1.5654	1.5654
10	1.8903	1.6941	1.6941	1.6941
11	0.0611	1.9221	1.9221	1.9221
12	0.0640	1.9323	1.9323	1.9323
13	0.0732	1.9213	1.9213	1.9213
14	0.0907	1.9194	1.9194	1.9194
15	1.8903	1.6941	1.6941	1.6941
16	0.0640	1.9323	1.9323	1.9323
17	0.0611	1.9221	1.9221	1.9221
18	0.0732	1.9213	1.9213	1.9213
19	1.9134	1.7000	1.7000	1.7000
20	0.0861	1.9206	1.9206	1.9206
21	0.0675	1.9255	1.9255	1.9255
22	0.0675	1.9255	1.9255	1.9255

Molecule 181-methaniminium
Energy: -94.7116165910
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000083	0.670841	0.000000
2	1	-0.000533	1.212176	0.944474
3	1	-0.000533	1.212176	-0.944474
4	7	-0.000083	-0.597209	0.000000
5	1	0.001073	-1.134468	0.869405
6	1	0.001073	-1.134468	-0.869405

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.2103	1.6725	1.6725	1.6725
2	0.1521	1.9058	1.9058	1.9058
3	0.1521	1.9058	1.9058	1.9058
4	2.0241	1.4664	1.4664	1.4664
5	0.2307	1.7543	1.7543	1.7543
6	0.2307	1.7543	1.7543	1.7543

Molecule 182-hydroxymethylium
Energy: -114.485780776
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000100	0.641773	0.000000
2	1	-0.000042	1.172642	0.959736
3	1	-0.000042	1.172642	-0.959736
4	8	0.000100	-0.580045	0.000000
5	1	-0.001316	-1.555559	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.3375	1.6613	1.6613	1.6613
2	0.1585	1.8872	1.8872	1.8872
3	0.1585	1.8872	1.8872	1.8872
4	2.0027	1.2677	1.2677	1.2677
5	0.3427	1.7035	1.7035	1.7035

Molecule 183-flouromethylium
Energy: -138.463794139
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-0.593259
2	1	0.000000	0.981066	-1.089043
3	1	0.000000	-0.981066	-1.089043
4	9	0.000000	0.000000	0.637515

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.4375	1.6405	1.6405	1.6405
2	0.1935	1.8797	1.8797	1.8797
3	0.1935	1.8797	1.8797	1.8797
4	2.1755	1.1182	1.1182	1.1182

Molecule 184-isocyanomethylium
Energy: -131.331615992
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	0.000000	-1.180050
2	1	0.000000	0.951208	-1.725331
3	1	0.000000	-0.951208	-1.725331
4	6	0.000000	0.000000	0.183191
5	7	0.000000	0.000000	1.347402

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.3285	1.7252	1.7252	1.7252
2	0.1908	1.9064	1.9064	1.9064
3	0.1908	1.9064	1.9064	1.9064
4	2.1826	1.5763	1.5763	1.5763
5	2.1074	1.5541	1.5541	1.5541

Molecule 185-2-2-dimethylpropan-1-ylium
Energy: -196.231150330
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.887626	0.752393	0.000000
2	1	-1.494144	0.866487	-0.897983
3	1	-1.494144	0.866487	0.897983
4	6	-0.100881	-0.457588	0.000000
5	6	0.289252	-1.069412	1.264142
6	1	-0.503473	-1.812299	1.458125
7	1	1.231088	-1.615917	1.215115
8	1	0.263480	-0.370591	2.101301
9	6	0.289252	1.792772	0.000000
10	1	1.288248	1.344117	0.000000
11	1	0.221178	2.414001	-0.891390
12	1	0.221178	2.414001	0.891390
13	6	0.289252	-1.069412	-1.264142
14	1	0.263480	-0.370591	-2.101301

15	1	1.231088	-1.615917	-1.215115
16	1	-0.503473	-1.812299	-1.458125

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9552	1.6452	1.6452	1.6452
2	0.0907	1.8957	1.8957	1.8957
3	0.0907	1.8957	1.8957	1.8957
4	2.2311	1.6012	1.6012	1.6012
5	1.9202	1.6889	1.6889	1.6889
6	0.1192	1.9354	1.9354	1.9354
7	0.0956	1.9236	1.9236	1.9236
8	0.0964	1.9244	1.9244	1.9244
9	1.9258	1.7084	1.7084	1.7084
10	0.0709	1.9217	1.9217	1.9217
11	0.0865	1.9144	1.9144	1.9144
12	0.0865	1.9144	1.9144	1.9144
13	1.9202	1.6889	1.6889	1.6889
14	0.0964	1.9244	1.9244	1.9244
15	0.0956	1.9236	1.9236	1.9236
16	0.1192	1.9354	1.9354	1.9354

Molecule 186-cyclohexadienylium
Energy: -231.816069787
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.019638	-1.385388	0.000122
2	6	-1.250706	-0.604322	0.000112
3	6	-1.222787	0.751507	-0.000060
4	6	0.019823	1.398765	0.000284
5	6	1.243610	0.716718	-0.000101
6	6	1.233031	-0.639427	-0.000161
7	1	-0.029460	-2.089190	0.851799
8	1	-2.196379	-1.140319	-0.000832
9	1	-2.136712	1.334264	-0.000895
10	1	0.035095	2.486822	0.000277
11	1	2.173738	1.273241	-0.000340
12	1	2.163195	-1.201938	-0.000307
13	1	-0.029474	-2.089999	-0.850870

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9664	1.6359	1.6359	1.6359
2	2.0803	1.6473	1.6473	1.6473
3	1.9806	1.6438	1.6438	1.6438
4	2.1107	1.6538	1.6538	1.6538
5	1.9806	1.6438	1.6438	1.6438
6	2.0803	1.6474	1.6474	1.6474
7	0.1289	1.9214	1.9214	1.9214
8	0.1121	1.9158	1.9158	1.9158
9	0.1012	1.9281	1.9281	1.9281
10	0.1169	1.9104	1.9104	1.9104
11	0.1012	1.9281	1.9281	1.9281
12	0.1121	1.9158	1.9158	1.9158
13	0.1289	1.9213	1.9213	1.9213

Molecule 187-cyclopropylium
Energy: -116.581690135
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000164	-0.498783	0.000288
2	6	-1.170853	0.211724	0.000016
3	6	1.170876	0.211804	-0.000036
4	1	-0.000053	-1.584381	-0.000012
5	1	-2.141108	-0.283716	-0.001200
6	1	-1.170077	1.301244	0.000476
7	1	1.168674	1.301334	-0.000213
8	1	2.141448	-0.282954	-0.000655

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	2.0002	1.6496	1.6496	1.6496
2	2.1722	1.7188	1.7188	1.7188
3	2.1721	1.7188	1.7188	1.7188
4	0.1151	1.9229	1.9229	1.9229
5	0.1404	1.9194	1.9194	1.9194
6	0.1298	1.9255	1.9255	1.9255
7	0.1297	1.9255	1.9255	1.9255
8	0.1404	1.9195	1.9195	1.9195

Molecule 188-cycloprop-2-en-1-ylium.log
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000095	0.780885	0.000000
2	6	0.000095	-0.390326	0.676610
3	6	0.000095	-0.390326	-0.676610
4	1	0.000935	1.865794	0.000000
5	1	-0.001319	-0.933596	1.615680
6	1	-0.001319	-0.933596	-1.615680

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.1563	1.6591	1.6591	1.6591
2	2.1565	1.6592	1.6592	1.6592
3	2.1565	1.6592	1.6592	1.6592
4	0.1769	1.9708	1.9708	1.9708
5	0.1769	1.9708	1.9708	1.9708
6	0.1769	1.9708	1.9708	1.9708

Molecule 189-cyclopenta-2-4-dien-1-ylium
Energy: -192.537748903
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.000096	-0.344963	1.192051
2	6	-0.000096	0.922632	0.775553
3	6	-0.000096	0.922632	-0.775553
4	6	-0.000096	-0.344963	-1.192051
5	6	0.000290	-1.149056	0.000000
6	1	-0.000282	1.823888	1.380094
7	1	0.000011	-0.722795	-2.205105
8	1	0.001098	-2.239876	0.000000
9	1	0.000011	-0.722795	2.205105
10	1	-0.000282	1.823888	-1.380094

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9679	1.6435	1.6435	1.6435
2	2.1045	1.6603	1.6603	1.6603
3	2.1045	1.6603	1.6603	1.6603
4	1.9679	1.6435	1.6435	1.6435
5	2.2299	1.6621	1.6621	1.6621
6	0.1274	1.9332	1.9332	1.9332
7	0.1136	1.9481	1.9481	1.9481
8	0.1430	1.9152	1.9152	1.9152
9	0.1136	1.9481	1.9481	1.9481
10	0.1274	1.9332	1.9332	1.9332

Molecule 190-cyclohept-2-4-6-trien-1-ylium.log
Energy: -269.743073754
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.310511	0.765284	0.583020
2	6	0.965239	1.117270	-0.027884
3	6	1.710979	-0.000393	-0.341303
4	6	-1.502778	0.657879	-0.387321
5	6	0.964531	-1.117677	-0.028198
6	6	-1.503451	-0.657396	-0.386681
7	6	-0.310974	-0.764951	0.583212
8	1	-0.533101	1.294559	1.514925
9	1	1.266790	2.138192	-0.254608

10	1	2.678132	-0.000558	-0.829179
11	1	1.264935	-2.138701	-0.255967
12	1	-2.110404	1.436690	-0.830641
13	1	-2.112015	-1.436000	-0.829080
14	1	-0.532554	-1.294286	1.515477

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9892	1.5981	1.5981	1.5981
2	2.1376	1.6492	1.6492	1.6492
3	1.9871	1.6443	1.6443	1.6443
4	1.9889	1.6622	1.6622	1.6622
5	2.1376	1.6492	1.6492	1.6492
6	1.9889	1.6622	1.6622	1.6622
7	1.9892	1.5981	1.5981	1.5981
8	0.1067	1.9151	1.9151	1.9151
9	0.1253	1.9265	1.9265	1.9265
10	0.1086	1.9436	1.9436	1.9436
11	0.1253	1.9266	1.9266	1.9266
12	0.1046	1.9665	1.9665	1.9665
13	0.1046	1.9665	1.9665	1.9665
14	0.1067	1.9152	1.9152	1.9152

Molecule 191-cycloheptylium
Energy: -273.409505424
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.589341	0.497922	-0.151356
2	6	0.488374	1.534650	0.036415
3	6	-0.883110	1.052432	-0.398932
4	6	1.266376	-0.864885	0.440349
5	6	-1.573117	0.071097	0.692244
6	6	0.126807	-1.553192	-0.297324
7	6	-1.172978	-0.854100	-0.276958
8	1	1.801587	0.380528	-1.220671
9	1	0.441166	1.861992	1.078441
10	1	-0.817177	0.649902	-1.427686
11	1	-1.009560	0.132841	1.617478
12	1	1.047830	-0.784460	1.510141
13	1	-0.110994	-2.527844	0.157288
14	1	2.507201	0.882904	0.297094
15	1	0.724225	2.423146	-0.554894
16	1	-1.644339	1.826102	-0.511915
17	1	2.142320	-1.511769	0.364838
18	1	-2.635033	0.270871	0.793810
19	1	0.404492	-1.777341	-1.331343
20	1	-1.901879	-1.130416	-1.039202

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9308	1.6474	1.6474	1.6474
2	1.9382	1.6461	1.6461	1.6461
3	2.0029	1.6452	1.6452	1.6452
4	1.9352	1.6473	1.6473	1.6473
5	1.9804	1.6468	1.6468	1.6468
6	1.9507	1.6405	1.6405	1.6405
7	2.1478	1.6305	1.6305	1.6305
8	0.0563	1.9061	1.9061	1.9061
9	0.0647	1.8978	1.8978	1.8978
10	0.0989	1.8763	1.8763	1.8763
11	0.0993	1.8995	1.8995	1.8995
12	0.0588	1.9043	1.9043	1.9043
13	0.1011	1.9066	1.9066	1.9066
14	0.0727	1.8974	1.8974	1.8974
15	0.0764	1.8950	1.8950	1.8950
16	0.1070	1.8834	1.8834	1.8834
17	0.0760	1.8935	1.8935	1.8935
18	0.1037	1.8942	1.8942	1.8942
19	0.0810	1.8975	1.8975	1.8975

20	0.1181	1.8799	1.8799	1.8799

Molecule 192-penta-1-4-dien-3-ylium
Energy: -193.768486711
Geometry:

Atom	Atomic No.	x	y	z
1	6	-1.224488	-0.396919	0.249449
2	1	-2.001334	-0.953516	0.767109
3	6	0.000001	-1.043388	-0.000001
4	1	0.000001	-2.134266	-0.000002
5	6	1.224489	-0.396919	-0.249448
6	1	2.001338	-0.953515	-0.767105
7	6	-1.499851	0.818991	-0.265075
8	1	-2.460432	1.294255	-0.085540
9	1	-0.818620	1.324113	-0.943082
10	6	1.499849	0.818993	0.265075
11	1	2.460430	1.294259	0.085540
12	1	0.818614	1.324117	0.943077

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9830	1.6493	1.6493	1.6493
2	0.1055	1.9256	1.9256	1.9256
3	2.1491	1.6567	1.6567	1.6567
4	0.1245	1.9056	1.9056	1.9056
5	1.9830	1.6493	1.6493	1.6493
6	0.1055	1.9256	1.9256	1.9256
7	2.0614	1.7189	1.7189	1.7189
8	0.1167	1.9328	1.9328	1.9328
9	0.0966	1.9372	1.9372	1.9372
10	2.0614	1.7189	1.7189	1.7189
11	0.1167	1.9328	1.9328	1.9328
12	0.0966	1.9372	1.9372	1.9372

Molecule 193-PhS-
Energy: -628.904511804
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.588604	-0.000007	-0.000179
2	6	0.160966	-1.188643	-0.000019
3	6	1.542124	-1.189170	0.000023
4	6	2.257005	0.000002	0.000005
5	6	1.542113	1.189178	0.000034
6	6	0.160963	1.188640	-0.000026
7	1	-0.383759	-2.127724	0.000034
8	1	2.072819	-2.139025	0.000080
9	1	3.343098	0.000010	0.000043
10	1	2.072811	2.139031	0.000083
11	1	-0.383780	2.127711	0.000017
12	16	-2.323037	0.000000	0.000044

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0014	1.6505	1.6505	1.6505
2	1.9119	1.6615	1.6615	1.6615
3	1.9214	1.6688	1.6688	1.6688
4	1.8892	1.6712	1.6712	1.6712
5	1.9214	1.6688	1.6688	1.6688
6	1.9119	1.6615	1.6615	1.6615
7	0.0147	1.9931	1.9931	1.9931
8	0.0216	1.9834	1.9834	1.9834
9	0.0137	1.9940	1.9940	1.9940
10	0.0216	1.9834	1.9834	1.9834
11	0.0147	1.9931	1.9931	1.9931
12	9.3563	2.0289	2.0289	2.0289

Molecule 194-PhO-
Energy: -306.056350601
Geometry:

Atom	Atomic No.	x	y	z
1	6	1.063829	0.000017	-0.000042
2	6	0.286233	-1.201822	0.000006
3	6	-1.090099	-1.189461	-0.000005
4	6	-1.814768	0.000001	0.000001
5	6	-1.090113	1.189445	0.000020
6	6	0.286237	1.201827	-0.000009
7	1	0.835147	-2.140085	0.000017
8	1	-1.624487	-2.139132	0.000017
9	1	-2.900475	-0.000016	-0.000025
10	1	-1.624487	2.139124	0.000020
11	1	0.835099	2.140121	-0.000015
12	8	2.328911	-0.000007	0.000020

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0531	1.5721	1.5721	1.5721
2	1.8724	1.6652	1.6652	1.6652
3	1.9141	1.6749	1.6749	1.6749
4	1.8499	1.6769	1.6769	1.6769
5	1.9141	1.6749	1.6749	1.6749
6	1.8724	1.6652	1.6652	1.6652
7	0.0045	2.0013	2.0013	2.0013
8	0.0129	1.9918	1.9918	1.9918
9	-0.0020	2.0086	2.0086	2.0086
10	0.0129	1.9918	1.9918	1.9918
11	0.0045	2.0013	2.0013	2.0013
12	1.4913	1.3641	1.3641	1.3641

Molecule 195-Deprotonated o-alkynylbenzamide
Energy: -744.731399060
Geometry:

Atomic No.	x	y	z
6	1.968492	-2.363577	-0.142083
6	1.490989	-1.039392	-0.020998
6	2.413203	0.033503	0.079052
6	3.782958	-0.260038	0.051915
6	4.248002	-1.572758	-0.064083
6	3.335682	-2.630000	-0.160470
1	1.252211	-3.175638	-0.223942
1	4.493945	0.558769	0.122600
1	5.316278	-1.769825	-0.081425
1	3.686894	-3.653512	-0.252310
6	1.952686	1.468389	0.277104
8	1.643103	1.796127	1.476804
6	0.080885	-0.808233	-0.016915
6	-1.126733	-0.641583	-0.016784
7	1.950025	2.210875	-0.806628
6	1.527118	3.593334	-0.602886
1	1.553045	4.125741	-1.560621
1	0.503079	3.673700	-0.202037
1	2.176864	4.138666	0.101645
6	-2.538417	-0.428325	-0.013485
6	-3.432507	-1.520592	-0.040548
6	-3.064990	0.881411	0.017844
6	-4.810485	-1.304662	-0.036220
1	-3.036886	-2.531106	-0.064213
6	-4.444353	1.087243	0.021669
1	-2.384561	1.726721	0.038245
6	-5.322396	-0.002393	-0.005209
1	-5.486146	-2.154760	-0.056862
1	-4.834746	2.100429	0.045570
1	-6.395789	0.161727	-0.002115

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	-0.0580	1.2605	1.2605	1.2605
2	-0.0006	1.2234	1.2234	1.2234
3	0.0234	1.2152	1.2152	1.2152

4	-0.0545	1.2588	1.2588	1.2588
5	-0.0643	1.2655	1.2655	1.2655
6	-0.0824	1.2660	1.2660	1.2660
7	0.0413	1.9617	1.9617	1.9617
8	0.0478	1.9598	1.9598	1.9598
9	0.0390	1.9664	1.9664	1.9664
10	0.0349	1.9698	1.9698	1.9698
11	0.0999	1.1709	1.1709	1.1709
12	-0.4785	1.1082	1.1082	1.1082
13	-0.0314	1.2597	1.2597	1.2597
14	-0.0732	1.2598	1.2598	1.2598
15	-0.3641	1.1985	1.1985	1.1985
16	-0.0958	1.2961	1.2961	1.2961
17	0.0050	1.9615	1.9615	1.9615
18	0.0109	1.9641	1.9641	1.9641
19	0.0103	1.9649	1.9649	1.9649
20	0.0152	1.2253	1.2253	1.2253
21	-0.0516	1.2588	1.2588	1.2588
22	-0.0362	1.2561	1.2561	1.2561
23	-0.0641	1.2637	1.2637	1.2637
24	0.0504	1.9558	1.9558	1.9558
25	-0.0572	1.2625	1.2625	1.2625
26	0.0671	1.9468	1.9468	1.9468
27	-0.0679	1.2649	1.2649	1.2649
28	0.0437	1.9609	1.9609	1.9609
29	0.0485	1.9571	1.9571	1.9571
30	0.0419	1.9633	1.9633	1.9633

Molecule 196-Butenone
Energy: -230.611543095
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.539293	-0.184478	-0.000023
2	8	-1.424518	-1.011999	0.000033
3	6	0.873066	-0.635505	-0.000038
4	6	1.919309	0.173713	0.000026
5	1	0.988914	-1.715602	-0.000089
6	1	2.931449	-0.216448	0.000030
7	1	1.813980	1.254146	0.000078
8	6	-0.847454	1.283762	-0.000021
9	1	-0.422054	1.767431	0.882584
10	1	-0.421562	1.767645	-0.882261
11	1	-1.928344	1.413880	-0.000275

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	0.1733	1.1793	1.1793	1.1793
2	-0.2837	1.0795	1.0795	1.0795
3	-0.0547	1.2555	1.2555	1.2555
4	-0.0715	1.3037	1.3037	1.3037
5	0.0610	1.9428	1.9428	1.9428
6	0.0618	1.9623	1.9623	1.9623
7	0.0567	1.9587	1.9587	1.9587
8	-0.1104	1.2884	1.2884	1.2884
9	0.0552	1.9389	1.9389	1.9389
10	0.0552	1.9389	1.9389	1.9389
11	0.0570	1.9312	1.9312	1.9312

Molecule 197-diamond
Energy: -1351.11148437
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.892850	0.892850	0.892850
2	6	-0.013099	1.769252	1.769252
3	1	0.626132	2.401996	2.401996
4	6	0.000000	0.000000	0.000000
5	6	-0.892850	-0.892850	0.892850

6	6	-0.878955	0.878955	2.661651
7	1	-1.515566	1.515566	3.289520
8	6	-1.769252	0.013099	1.769252
9	1	-2.401996	-0.626132	2.401996
10	6	-2.661651	0.878955	0.878955
11	1	-3.289520	1.515566	1.515566
12	6	-0.878955	2.661651	0.878955
13	1	-1.515566	3.289520	1.515566
14	6	-0.892850	0.892850	-0.892850
15	6	-1.769252	1.769252	0.013099
16	1	-2.401996	2.401996	-0.626132
17	6	0.013099	-1.769252	1.769252
18	1	-0.626132	-2.401996	2.401996
19	6	-1.769252	-1.769252	-0.013099
20	1	-2.401996	-2.401996	0.626132
21	6	0.892850	-0.892850	-0.892850
22	6	1.769252	0.013099	-1.769252
23	1	2.401996	-0.626132	-2.401996
24	6	1.769252	1.769252	-0.013099
25	1	2.401996	2.401996	0.626132
26	6	2.661651	0.878955	-0.878955
27	1	3.289520	1.515566	-1.515566
28	6	0.013099	1.769252	-1.769252
29	1	-0.626132	2.401996	-2.401996
30	6	0.878955	2.661651	-0.878955
31	1	1.515566	3.289520	-1.515566
32	6	0.878955	0.878955	-2.661651
33	1	1.515566	1.515566	-3.289520
34	6	0.000000	3.541767	0.000000
35	1	0.623813	4.192204	0.623813
36	1	-0.623813	4.192204	-0.623813
37	6	1.769252	-1.769252	0.013099
38	1	2.401996	-2.401996	-0.626132
39	6	0.878955	-2.661651	0.878955
40	1	1.515566	-3.289520	1.515566
41	6	-0.878955	-2.661651	-0.878955
42	1	-1.515566	-3.289520	-1.515566
43	6	-0.013099	-1.769252	-1.769252
44	1	0.626132	-2.401996	-2.401996
45	6	0.000000	-3.541767	0.000000
46	1	-0.623813	-4.192204	0.623813
47	1	0.623813	-4.192204	-0.623813
48	6	1.769252	-0.013099	1.769252
49	1	2.401996	0.626132	2.401996
50	6	2.661651	-0.878955	0.878955
51	1	3.289520	-1.515566	1.515566
52	6	0.878955	-0.878955	2.661651
53	1	1.515566	-1.515566	3.289520
54	6	0.000000	0.000000	3.541767
55	1	-0.623813	-0.623813	4.192204
56	1	0.623813	0.623813	4.192204
57	6	-1.769252	-0.013099	-1.769252
58	1	-2.401996	0.626132	-2.401996
59	6	-0.878955	-0.878955	-2.661651
60	1	-1.515566	-1.515566	-3.289520
61	6	-2.661651	-0.878955	-0.878955
62	1	-3.289520	-1.515566	-1.515566
63	6	-3.541767	0.000000	0.000000
64	1	-4.192204	-0.623813	0.623813
65	1	-4.192204	0.623813	-0.623813
66	6	3.541767	0.000000	0.000000
67	1	4.192204	0.623813	0.623813
68	1	4.192204	-0.623813	-0.623813
69	6	0.000000	0.000000	-3.541767
70	1	0.623813	-0.623813	-4.192204

71 1 -0.623813 0.623813 -4.192204

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9969	1.5405	1.5405	1.5405
2	1.9599	1.5883	1.5883	1.5883
3	0.0384	1.7758	1.7758	1.7758
4	1.9967	1.5174	1.5174	1.5174
5	1.9969	1.5405	1.5405	1.5405
6	1.9602	1.5981	1.5981	1.5981
7	0.0403	1.7741	1.7741	1.7741
8	1.9599	1.5883	1.5883	1.5883
9	0.0384	1.7758	1.7758	1.7758
10	1.9602	1.5981	1.5981	1.5981
11	0.0403	1.7741	1.7741	1.7741
12	1.9602	1.5981	1.5981	1.5981
13	0.0403	1.7741	1.7741	1.7741
14	1.9969	1.5405	1.5405	1.5405
15	1.9599	1.5883	1.5883	1.5883
16	0.0384	1.7758	1.7758	1.7758
17	1.9599	1.5883	1.5883	1.5883
18	0.0384	1.7758	1.7758	1.7758
19	1.9599	1.5883	1.5883	1.5883
20	0.0384	1.7758	1.7758	1.7758
21	1.9969	1.5405	1.5405	1.5405
22	1.9599	1.5883	1.5883	1.5883
23	0.0384	1.7758	1.7758	1.7758
24	1.9599	1.5883	1.5883	1.5883
25	0.0384	1.7758	1.7758	1.7758
26	1.9602	1.5981	1.5981	1.5981
27	0.0403	1.7741	1.7741	1.7741
28	1.9599	1.5883	1.5883	1.5883
29	0.0384	1.7758	1.7758	1.7758
30	1.9602	1.5981	1.5981	1.5981
31	0.0403	1.7741	1.7741	1.7741
32	1.9602	1.5981	1.5981	1.5981
33	0.0403	1.7741	1.7741	1.7741
34	1.9173	1.6536	1.6536	1.6536
35	0.0409	1.7949	1.7949	1.7949
36	0.0409	1.7949	1.7949	1.7949
37	1.9599	1.5883	1.5883	1.5883
38	0.0384	1.7758	1.7758	1.7758
39	1.9602	1.5981	1.5981	1.5981
40	0.0403	1.7741	1.7741	1.7741
41	1.9602	1.5981	1.5981	1.5981
42	0.0403	1.7741	1.7741	1.7741
43	1.9599	1.5883	1.5883	1.5883
44	0.0384	1.7758	1.7758	1.7758
45	1.9173	1.6536	1.6536	1.6536
46	0.0409	1.7949	1.7949	1.7949
47	0.0409	1.7949	1.7949	1.7949
48	1.9599	1.5883	1.5883	1.5883
49	0.0384	1.7758	1.7758	1.7758
50	1.9602	1.5981	1.5981	1.5981
51	0.0403	1.7741	1.7741	1.7741
52	1.9602	1.5981	1.5981	1.5981
53	0.0403	1.7741	1.7741	1.7741
54	1.9173	1.6536	1.6536	1.6536
55	0.0409	1.7949	1.7949	1.7949
56	0.0409	1.7949	1.7949	1.7949
57	1.9599	1.5883	1.5883	1.5883
58	0.0384	1.7758	1.7758	1.7758
59	1.9602	1.5981	1.5981	1.5981
60	0.0403	1.7741	1.7741	1.7741
61	1.9602	1.5981	1.5981	1.5981
62	0.0403	1.7741	1.7741	1.7741
63	1.9173	1.6536	1.6536	1.6536

64	0.0409	1.7949	1.7949	1.7949
65	0.0409	1.7949	1.7949	1.7949
66	1.9173	1.6536	1.6536	1.6536
67	0.0409	1.7949	1.7949	1.7949
68	0.0409	1.7949	1.7949	1.7949
69	1.9173	1.6536	1.6536	1.6536
70	0.0409	1.7949	1.7949	1.7949
71	0.0409	1.7949	1.7949	1.7949

Molecule 198-Graphene
Energy: -2062.10351850
Geometry:

Atom	Atomic No.	x	y	z
1	6	-3.533535	1.203125	0.000000
2	6	-2.828511	-0.009811	0.000000
3	6	-3.525131	-1.227588	0.000000
4	6	-4.935790	-1.228456	0.000000
5	6	-5.616731	-0.019487	0.000000
6	6	-4.944248	1.194080	0.000000
7	6	-2.808779	-2.458416	0.000000
8	6	-5.618703	-2.492222	0.000000
9	6	-4.942531	-3.653944	0.000000
10	6	-3.506310	-3.684456	0.000000
11	6	-2.791415	-4.873728	0.000000
12	6	-1.404035	-4.888506	0.000000
13	6	-0.650872	-6.111876	0.000000
14	6	0.693265	-6.107240	0.000000
15	6	-2.825801	2.438820	0.000000
16	6	-3.531824	3.660026	0.000000
17	6	-1.422756	2.444501	0.000000
18	6	-2.825281	4.854192	0.000000
19	6	-0.724840	3.661532	0.000000
20	6	-0.705322	1.211788	0.000000
21	6	-1.437965	4.878660	0.000000
22	1	-3.371176	5.792045	0.000000
23	6	0.699333	3.666496	0.000000
24	6	0.696862	1.216652	0.000000
25	6	-0.693292	6.107179	0.000000
26	6	1.405707	2.454347	0.000000
27	6	1.404037	4.888534	0.000000
28	6	1.402174	0.004883	0.000000
29	6	0.650907	6.111860	0.000000
30	1	-1.248252	7.038502	0.000000
31	6	2.808774	2.458448	0.000000
32	6	2.791454	4.873747	0.000000
33	6	2.828542	0.009816	0.000000
34	6	0.705301	-1.211833	0.000000
35	1	1.199466	7.046985	0.000000
36	6	3.506307	3.684484	0.000000
37	6	3.525122	1.227638	0.000000
38	1	3.330878	5.815347	0.000000
39	6	3.533561	-1.203111	0.000000
40	6	1.422741	-2.444591	0.000000
41	6	4.942537	3.653995	0.000000
42	6	4.935792	1.228508	0.000000
43	6	2.825798	-2.438883	0.000000
44	6	4.944270	-1.194076	0.000000
45	6	0.724807	-3.661549	0.000000
46	6	5.618696	2.492289	0.000000
47	1	5.471699	4.600215	0.000000
48	6	5.616741	0.019546	0.000000
49	6	3.531813	-3.660083	0.000000
50	6	5.635890	-2.453163	0.000000
51	6	1.437932	-4.878669	0.000000
52	1	6.702801	2.484856	0.000000

53	1	6.701895	0.023324	0.000000
54	6	2.825235	-4.854252	0.000000
55	6	4.967816	-3.619588	0.000000
56	1	6.719927	-2.438289	0.000000
57	1	5.503478	-4.562158	0.000000
58	6	-0.699361	-3.666473	0.000000
59	6	-1.402120	-0.004846	0.000000
60	6	-0.696803	-1.216651	0.000000
61	6	-1.405686	-2.454380	0.000000
62	6	-5.635911	2.453167	0.000000
63	6	-4.967847	3.619531	0.000000
64	1	-6.719952	2.438296	0.000000
65	1	-5.503515	4.562102	0.000000
66	1	3.371144	-5.792096	0.000000
67	1	1.248227	-7.038557	0.000000
68	1	-1.199422	-7.046995	0.000000
69	1	-3.330908	-5.815283	0.000000
70	1	-5.471696	-4.600158	0.000000
71	1	-6.702815	-2.484749	0.000000
72	1	-6.701889	-0.023207	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9979	1.5877	1.5877	1.5877
2	1.9991	1.5868	1.5868	1.5868
3	1.9979	1.5876	1.5876	1.5876
4	1.9940	1.6034	1.6034	1.6034
5	1.9439	1.6610	1.6610	1.6610
6	1.9940	1.6035	1.6035	1.6035
7	1.9979	1.5886	1.5886	1.5886
8	1.9447	1.6690	1.6690	1.6690
9	1.9448	1.6686	1.6686	1.6686
10	1.9940	1.6038	1.6038	1.6038
11	1.9439	1.6605	1.6605	1.6605
12	1.9940	1.6049	1.6049	1.6049
13	1.9448	1.6683	1.6683	1.6683
14	1.9447	1.6683	1.6683	1.6683
15	1.9979	1.5891	1.5891	1.5891
16	1.9940	1.6038	1.6038	1.6038
17	1.9991	1.5878	1.5878	1.5878
18	1.9439	1.6605	1.6605	1.6605
19	1.9979	1.5882	1.5882	1.5882
20	1.9987	1.5874	1.5874	1.5874
21	1.9940	1.6049	1.6049	1.6049
22	0.0602	1.8271	1.8271	1.8271
23	1.9979	1.5882	1.5882	1.5882
24	1.9987	1.5874	1.5874	1.5874
25	1.9448	1.6683	1.6683	1.6683
26	1.9991	1.5879	1.5879	1.5879
27	1.9940	1.6049	1.6049	1.6049
28	1.9987	1.5864	1.5864	1.5864
29	1.9448	1.6683	1.6683	1.6683
30	0.0623	1.8238	1.8238	1.8238
31	1.9979	1.5886	1.5886	1.5886
32	1.9439	1.6605	1.6605	1.6605
33	1.9991	1.5868	1.5868	1.5868
34	1.9987	1.5874	1.5874	1.5874
35	0.0623	1.8238	1.8238	1.8238
36	1.9940	1.6038	1.6038	1.6038
37	1.9979	1.5877	1.5877	1.5877
38	0.0602	1.8271	1.8271	1.8271
39	1.9979	1.5877	1.5877	1.5877
40	1.9991	1.5878	1.5878	1.5878
41	1.9448	1.6686	1.6686	1.6686
42	1.9940	1.6035	1.6035	1.6035
43	1.9979	1.5891	1.5891	1.5891
44	1.9940	1.6035	1.6035	1.6035

45	1.9979	1.5882	1.5882	1.5882
46	1.9447	1.6690	1.6690	1.6690
47	0.0623	1.8239	1.8239	1.8239
48	1.9439	1.6610	1.6610	1.6610
49	1.9940	1.6038	1.6038	1.6038
50	1.9447	1.6690	1.6690	1.6690
51	1.9940	1.6049	1.6049	1.6049
52	0.0623	1.8239	1.8239	1.8239
53	0.0602	1.8273	1.8273	1.8273
54	1.9439	1.6605	1.6605	1.6605
55	1.9448	1.6686	1.6686	1.6686
56	0.0623	1.8239	1.8239	1.8239
57	0.0623	1.8239	1.8239	1.8239
58	1.9979	1.5882	1.5882	1.5882
59	1.9987	1.5864	1.5864	1.5864
60	1.9987	1.5874	1.5874	1.5874
61	1.9991	1.5879	1.5879	1.5879
62	1.9447	1.6690	1.6690	1.6690
63	1.9447	1.6685	1.6685	1.6685
64	0.0623	1.8239	1.8239	1.8239
65	0.0623	1.8239	1.8239	1.8239
66	0.0602	1.8271	1.8271	1.8271
67	0.0623	1.8238	1.8238	1.8238
68	0.0623	1.8238	1.8238	1.8238
69	0.0602	1.8271	1.8271	1.8271
70	0.0623	1.8239	1.8239	1.8239
71	0.0623	1.8239	1.8239	1.8239
72	0.0602	1.8273	1.8273	1.8273

Molecule 199-C60
Energy: -2278.68902042
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.908736	0.918995	3.275573
2	6	0.123431	-0.274518	3.508528
3	6	0.609000	-1.501653	3.126341
4	6	1.905863	-1.601062	2.490932
5	6	2.651271	-0.468223	2.269966
6	6	2.139600	0.824670	2.672520
7	6	0.002408	1.986113	2.907790
8	6	-1.343020	1.452051	2.913419
9	6	-1.268246	0.054919	3.284664
10	6	-2.103654	-0.859586	2.690074
11	6	-0.271096	-2.465108	2.499800
12	6	1.827179	-2.625981	1.471711
13	6	2.497839	-2.465926	0.283284
14	6	3.283100	-1.272405	0.050461
15	6	3.357768	-0.299601	1.017807
16	6	3.282899	1.097546	0.646557
17	6	2.530060	1.792382	1.669212
18	6	1.669803	2.805200	1.320134
19	6	0.372976	2.904593	1.955543
20	6	-2.249408	1.863609	1.966469
21	6	-1.859013	2.831369	0.963233
22	6	-0.582029	3.338331	0.957918
23	6	0.124596	3.506915	-0.294170
24	6	1.516360	3.177528	-0.070284
25	6	2.230891	2.517969	-1.040944
26	6	3.137231	1.450868	-0.673157
27	6	3.058612	0.425934	-1.692356
28	6	3.129617	-0.900170	-1.340005
29	6	0.481765	-3.160004	1.477249
30	6	-0.002412	-1.986113	-2.907791
31	6	-0.372980	-2.904591	-1.955546
32	6	-1.669802	-2.805199	-1.320136

33	6	-2.530062	-1.792382	-1.669216
34	6	-2.139601	-0.824671	-2.672518
35	6	-0.123431	0.274520	-3.508529
36	6	1.268248	-0.054922	-3.284663
37	6	1.343023	-1.452045	-2.913419
38	6	2.249410	-1.863604	-1.966469
39	6	1.859014	-2.831371	-0.963226
40	6	0.582031	-3.338331	-0.957913
41	6	-1.516361	-3.177525	0.070284
42	6	-2.230889	-2.517969	1.040942
43	6	-3.137231	-1.450863	0.673158
44	6	-3.282904	-1.097544	-0.646559
45	6	-3.357768	0.299597	-1.017807
46	6	-2.651276	0.468223	-2.269966
47	6	-1.905863	1.601060	-2.490931
48	6	-0.608999	1.501651	-3.126340
49	6	2.103659	0.859586	-2.690075
50	6	1.591988	2.152505	-2.287387
51	6	0.271096	2.465108	-2.499796
52	6	-0.481761	3.160003	-1.477249
53	6	-1.827182	2.625978	-1.471709
54	6	-2.497840	2.465923	-0.283287
55	6	-3.283100	1.272404	-0.050457
56	6	-3.129620	0.900168	1.340001
57	6	-3.058614	-0.425936	1.692351
58	6	-0.124592	-3.506913	0.294167
59	6	-1.591986	-2.152505	2.287388
60	6	-0.908734	-0.918997	-3.275570

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0000	1.5971	1.5971	1.5971
2	2.0000	1.5971	1.5971	1.5971
3	2.0000	1.5969	1.5969	1.5969
4	2.0000	1.5972	1.5972	1.5972
5	2.0000	1.5972	1.5972	1.5972
6	2.0000	1.5972	1.5972	1.5972
7	2.0001	1.5969	1.5969	1.5969
8	2.0000	1.5974	1.5974	1.5974
9	2.0000	1.5971	1.5971	1.5971
10	2.0000	1.5971	1.5971	1.5971
11	2.0000	1.5978	1.5978	1.5978
12	2.0000	1.5971	1.5971	1.5971
13	2.0000	1.5976	1.5976	1.5976
14	2.0000	1.5971	1.5971	1.5971
15	2.0001	1.5979	1.5979	1.5979
16	2.0000	1.5971	1.5971	1.5971
17	2.0000	1.5974	1.5974	1.5974
18	2.0000	1.5973	1.5973	1.5973
19	2.0000	1.5968	1.5968	1.5968
20	2.0000	1.5973	1.5973	1.5973
21	2.0000	1.5971	1.5971	1.5971
22	1.9999	1.5973	1.5973	1.5973
23	1.9999	1.5971	1.5971	1.5971
24	1.9999	1.5974	1.5974	1.5974
25	1.9999	1.5975	1.5975	1.5975
26	1.9999	1.5974	1.5974	1.5974
27	2.0000	1.5974	1.5974	1.5974
28	2.0000	1.5972	1.5972	1.5972
29	1.9999	1.5971	1.5971	1.5971
30	2.0001	1.5969	1.5969	1.5969
31	2.0000	1.5968	1.5968	1.5968
32	2.0000	1.5973	1.5973	1.5973
33	2.0000	1.5974	1.5974	1.5974
34	2.0000	1.5972	1.5972	1.5972
35	2.0000	1.5971	1.5971	1.5971
36	2.0000	1.5971	1.5971	1.5971

37	2.0000	1.5974	1.5974	1.5974
38	2.0000	1.5973	1.5973	1.5973
39	2.0000	1.5971	1.5971	1.5971
40	1.9999	1.5973	1.5973	1.5973
41	1.9999	1.5974	1.5974	1.5974
42	1.9999	1.5975	1.5975	1.5975
43	1.9999	1.5974	1.5974	1.5974
44	2.0000	1.5971	1.5971	1.5971
45	2.0001	1.5979	1.5979	1.5979
46	2.0000	1.5972	1.5972	1.5972
47	2.0000	1.5972	1.5972	1.5972
48	2.0000	1.5969	1.5969	1.5969
49	2.0000	1.5971	1.5971	1.5971
50	2.0000	1.5973	1.5973	1.5973
51	2.0000	1.5978	1.5978	1.5978
52	1.9999	1.5971	1.5971	1.5971
53	2.0000	1.5971	1.5971	1.5971
54	2.0000	1.5976	1.5976	1.5976
55	2.0000	1.5971	1.5971	1.5971
56	2.0000	1.5972	1.5972	1.5972
57	2.0000	1.5974	1.5974	1.5974
58	1.9999	1.5971	1.5971	1.5971
59	2.0000	1.5973	1.5973	1.5973
60	2.0000	1.5971	1.5971	1.5971

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Table SI-2
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Molecule Ph-Br
Energy: -2802.25408950
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.086681	0.000000	-0.000001
2	6	-0.767524	1.201392	0.000000
3	6	-2.150280	1.195139	0.000000
4	6	-2.846484	0.000000	0.000000
5	6	-2.150280	-1.195139	0.000000
6	6	-0.767524	-1.201392	0.000000
7	1	-0.218363	2.135941	0.000000
8	1	-2.686771	2.138260	0.000000
9	1	-3.931145	0.000000	0.000000
10	1	-2.686771	-2.138260	0.000000
11	1	-0.218363	-2.135941	0.000000
12	35	1.781544	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0298	1.6270	1.6270	1.6270
2	1.9615	1.6475	1.6475	1.6475
3	1.9505	1.6572	1.6572	1.6572
4	1.9450	1.6581	1.6581	1.6581
5	1.9505	1.6572	1.6572	1.6572
6	1.9615	1.6475	1.6475	1.6475
7	0.0727	1.9504	1.9504	1.9504
8	0.0637	1.9547	1.9547	1.9547
9	0.0624	1.9570	1.9570	1.9570
10	0.0637	1.9547	1.9547	1.9547
11	0.0727	1.9504	1.9504	1.9504
12	27.8660	1.9287	1.9287	1.9287

Molecule Ph-Cl
Energy: -690.858082024
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.000000	-0.173706	1.203317
2	6	0.000000	-1.556975	1.196687

3	6	0.000000	-2.251173	0.000000
4	6	0.000000	-1.556975	-1.196687
5	6	0.000000	-0.173706	-1.203317
6	6	0.000000	0.504192	0.000000
7	1	0.000000	0.379761	2.135759
8	1	0.000000	-2.095204	2.138931
9	1	0.000000	-3.336167	0.000000
10	1	0.000000	-2.095204	-2.138931
11	1	0.000000	0.379761	-2.135759
12	17	0.000000	2.236300	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9438	1.6483	1.6483	1.6483
2	1.9504	1.6577	1.6577	1.6577
3	1.9435	1.6582	1.6582	1.6582
4	1.9504	1.6577	1.6577	1.6577
5	1.9438	1.6483	1.6483	1.6483
6	2.0373	1.6091	1.6091	1.6091
7	0.0669	1.9547	1.9547	1.9547
8	0.0639	1.9550	1.9550	1.9550
9	0.0619	1.9574	1.9574	1.9574
10	0.0639	1.9550	1.9550	1.9550
11	0.0669	1.9547	1.9547	1.9547
12	9.9073	1.7313	1.7313	1.7313

Molecule Ph-F
Energy: -330.630228282
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.258778	1.207675	0.000000
2	6	-1.124789	1.198116	0.000000
3	6	-1.818492	0.000000	0.000000
4	6	-1.124789	-1.198116	0.000000
5	6	0.258778	-1.207675	0.000000
6	6	0.917363	0.000000	0.000000
7	1	0.829170	2.129364	0.000000
8	1	-1.664606	2.139301	0.000000
9	1	-2.902949	0.000000	0.000000
10	1	-1.664606	-2.139301	0.000000
11	1	0.829170	-2.129364	0.000000
12	9	2.263636	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9319	1.6446	1.6446	1.6446
2	1.9519	1.6588	1.6588	1.6588
3	1.9356	1.6584	1.6584	1.6584
4	1.9519	1.6588	1.6588	1.6588
5	1.9319	1.6446	1.6446	1.6446
6	2.0715	1.5422	1.5422	1.5422
7	0.0698	1.9576	1.9576	1.9576
8	0.0639	1.9548	1.9548	1.9548
9	0.0603	1.9581	1.9581	1.9581
10	0.0639	1.9548	1.9548	1.9548
11	0.0698	1.9576	1.9576	1.9576
12	1.8976	1.1436	1.1436	1.1436

Molecule Ph-SO2F
Energy: -878.686789177
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.294351	-0.000150	0.078017
2	6	0.959685	-1.211467	0.052713
3	6	2.339481	-1.203021	-0.004952
4	6	3.023885	0.000133	-0.035838
5	6	2.339283	1.203135	-0.005049
6	6	0.959457	1.211280	0.052922
7	1	0.399143	-2.139167	0.088934

8	1	2.883389	-2.140935	-0.022374
9	1	4.108057	0.000173	-0.079589
10	1	2.882916	2.141206	-0.022567
11	1	0.398951	2.138989	0.089379
12	16	-1.453413	-0.000118	0.134308
13	8	-1.941513	1.255519	0.618341
14	8	-1.941536	-1.256367	0.616737
15	9	-1.761145	0.000994	-1.434469

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9766	1.5886	1.5886	1.5886
2	1.9684	1.6451	1.6451	1.6451
3	1.9580	1.6547	1.6547	1.6547
4	1.9704	1.6563	1.6563	1.6563
5	1.9580	1.6547	1.6547	1.6547
6	1.9684	1.6451	1.6451	1.6451
7	0.0755	1.9323	1.9323	1.9323
8	0.0706	1.9491	1.9491	1.9491
9	0.0710	1.9480	1.9480	1.9480
10	0.0706	1.9491	1.9491	1.9491
11	0.0755	1.9323	1.9323	1.9323
12	10.5148	1.5441	1.5441	1.5441
13	1.7136	1.3267	1.3267	1.3267
14	1.7136	1.3267	1.3267	1.3267
15	1.8949	1.1449	1.1449	1.1449

Molecule Ph-SiF3.log
Energy: -819.511149724
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.377764	-0.007557	0.000147
2	6	1.086789	-1.206520	0.000039
3	6	2.467537	-1.205237	-0.000182
4	6	3.156556	-0.004085	-0.000179
5	6	2.465764	1.193372	0.000010
6	6	1.082612	1.191713	0.000216
7	1	0.558616	-2.156006	0.000122
8	1	3.010016	-2.144652	-0.000357
9	1	4.241841	-0.003283	-0.000416
10	1	3.005331	2.134484	-0.000013
11	1	0.546083	2.135749	0.000350
12	9	-2.063036	-0.732224	-1.267592
13	14	-1.441395	0.001294	0.000016
14	9	-2.062596	-0.736284	1.265463
15	9	-1.985978	1.495783	0.002105

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8887	1.6376	1.6376	1.6376
2	1.9660	1.6540	1.6540	1.6540
3	1.9501	1.6563	1.6563	1.6563
4	1.9616	1.6576	1.6576	1.6576
5	1.9496	1.6563	1.6563	1.6563
6	1.9652	1.6531	1.6531	1.6531
7	0.0684	1.9423	1.9423	1.9423
8	0.0650	1.9536	1.9536	1.9536
9	0.0662	1.9526	1.9526	1.9526
10	0.0648	1.9537	1.9537	1.9537
11	0.0659	1.9343	1.9343	1.9343
12	1.8337	1.1505	1.1505	1.1505
13	10.4821	1.7250	1.7250	1.7250
14	1.8337	1.1505	1.1505	1.1505
15	1.8390	1.1500	1.1500	1.1500

Molecule Ph-NO2
Energy: -435.643365715
Geometry:

Atom	Atomic No.	x	y	z

1	6	2.490884	-0.000002	0.000028
2	6	1.803256	1.201865	-0.000006
3	6	0.421766	1.210483	-0.000035
4	6	-0.238557	0.000002	-0.000044
5	6	0.421763	-1.210484	-0.000016
6	6	1.803254	-1.201865	0.000025
7	1	3.576035	0.000005	0.000063
8	1	2.345815	2.140977	-0.000002
9	1	-0.148430	2.131014	-0.000050
10	1	-0.148431	-2.131016	-0.000023
11	1	2.345806	-2.140981	0.000045
12	7	-1.701345	0.000000	-0.000081
13	8	-2.267223	-1.072980	0.000021
14	8	-2.267224	1.072980	0.000082

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9648	1.6570	1.6570	1.6570
2	1.9539	1.6557	1.6557	1.6557
3	1.9611	1.6416	1.6416	1.6416
4	2.0291	1.5600	1.5600	1.5600
5	1.9611	1.6416	1.6416	1.6416
6	1.9539	1.6557	1.6557	1.6557
7	0.0689	1.9502	1.9502	1.9502
8	0.0684	1.9506	1.9506	1.9506
9	0.0697	1.9305	1.9305	1.9305
10	0.0697	1.9305	1.9305	1.9305
11	0.0684	1.9506	1.9506	1.9506
12	2.2547	1.3490	1.3490	1.3490
13	1.7880	1.3082	1.3082	1.3082
14	1.7880	1.3082	1.3082	1.3082

Molecule Ph-N3
Energy: -394.735198309
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.150062	-0.377864	0.000000
2	6	-0.884054	-1.300077	0.000000
3	6	-2.192140	-0.861665	0.000000
4	6	-2.478256	0.493902	0.000000
5	6	-1.441522	1.408349	0.000000
6	6	-0.126173	0.980352	0.000000
7	1	-0.641704	-2.356782	0.000000
8	1	-2.998506	-1.587569	0.000000
9	1	-3.507394	0.835808	0.000000
10	1	-1.654361	2.472273	0.000000
11	1	0.678895	1.708849	0.000000
12	7	1.460158	-0.907394	0.000000
13	7	2.384175	-0.100164	0.000000
14	7	3.292176	0.560336	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0394	1.5731	1.5731	1.5731
2	1.9396	1.6475	1.6475	1.6475
3	1.9502	1.6583	1.6583	1.6583
4	1.9372	1.6586	1.6586	1.6586
5	1.9490	1.6583	1.6583	1.6583
6	1.9217	1.6477	1.6477	1.6477
7	0.0637	1.9613	1.9613	1.9613
8	0.0632	1.9552	1.9552	1.9552
9	0.0602	1.9587	1.9587	1.9587
10	0.0630	1.9551	1.9551	1.9551
11	0.0512	1.9568	1.9568	1.9568
12	1.8506	1.4614	1.4614	1.4614
13	2.1936	1.3669	1.3669	1.3669
14	1.9171	1.5351	1.5351	1.5351

Molecule Ph-H

Energy: -231.525068136
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.395399	-1.326485	0.000000
2	6	0.951148	-1.005619	0.000022
3	6	1.346516	0.320828	-0.000006
4	6	0.395334	1.326504	0.000005
5	6	-0.951099	1.005665	0.000008
6	6	-1.346500	-0.320893	-0.000014
7	1	-0.705277	-2.366516	-0.000010
8	1	1.696767	-1.794123	-0.000022
9	1	2.402147	0.572468	-0.000044
10	1	0.705345	2.366496	-0.000019
11	1	-1.696816	1.794076	0.000018
12	1	-2.402163	-0.572401	-0.000011

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9418	1.6597	1.6597	1.6597
2	1.9418	1.6597	1.6597	1.6597
3	1.9418	1.6597	1.6597	1.6597
4	1.9418	1.6597	1.6597	1.6597
5	1.9418	1.6597	1.6597	1.6597
6	1.9418	1.6597	1.6597	1.6597
7	0.0581	1.9596	1.9596	1.9596
8	0.0581	1.9595	1.9595	1.9595
9	0.0582	1.9595	1.9595	1.9595
10	0.0581	1.9596	1.9596	1.9596
11	0.0581	1.9595	1.9595	1.9595
12	0.0582	1.9595	1.9595	1.9595

Molecule Ph-NHNH2
Energy: -341.951483233
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.441598	-0.250789	0.061219
2	6	0.492461	-1.281029	0.006070
3	6	1.841719	-0.997166	-0.043613
4	6	2.287680	0.314166	-0.040586
5	6	1.355960	1.334842	0.012446
6	6	0.000277	1.064878	0.061819
7	1	0.153153	-2.313527	0.009420
8	1	2.555239	-1.814189	-0.085971
9	1	3.348444	0.535696	-0.080427
10	1	1.687059	2.368847	0.014666
11	1	-0.731337	1.861750	0.102377
12	7	-1.793315	-0.572571	0.147928
13	1	-2.031661	-1.505479	-0.161917
14	7	-2.727372	0.420217	-0.100272
15	1	-3.077194	0.422182	-1.052630
16	1	-3.477878	0.401790	0.576757

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0439	1.5667	1.5667	1.5667
2	1.9137	1.6497	1.6497	1.6497
3	1.9414	1.6608	1.6608	1.6608
4	1.9158	1.6609	1.6609	1.6609
5	1.9435	1.6609	1.6609	1.6609
6	1.9160	1.6479	1.6479	1.6479
7	0.0499	1.9649	1.9649	1.9649
8	0.0566	1.9609	1.9609	1.9609
9	0.0516	1.9671	1.9671	1.9671
10	0.0564	1.9599	1.9599	1.9599
11	0.0462	1.9546	1.9546	1.9546
12	1.8808	1.4376	1.4376	1.4376
13	0.1238	1.7787	1.7787	1.7787
14	1.8179	1.4844	1.4844	1.4844
15	0.1196	1.7917	1.7917	1.7917

16	0.1228	1.7851	1.7851	1.7851

Molecule Ph-SiH3
Energy: -521.965288527
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.463811	0.000000	-0.013570
2	6	-0.253172	-1.192741	-0.010348
3	6	-1.636444	-1.196599	0.003052
4	6	-2.330390	0.000000	0.011129
5	6	-1.636444	1.196599	0.003052
6	6	-0.253172	1.192741	-0.010348
7	1	0.275477	-2.142354	-0.023505
8	1	-2.175625	-2.138512	0.004325
9	1	-3.415710	0.000000	0.019542
10	1	-2.175625	2.138512	0.004325
11	1	0.275477	2.142354	-0.023505
12	14	2.326955	0.000000	0.006092
13	1	2.847758	0.000000	1.392112
14	1	2.832870	-1.210111	-0.678191
15	1	2.832870	1.210111	-0.678191

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8969	1.6583	1.6583	1.6583
2	1.9517	1.6579	1.6579	1.6579
3	1.9429	1.6586	1.6586	1.6586
4	1.9475	1.6592	1.6592	1.6592
5	1.9429	1.6586	1.6586	1.6586
6	1.9517	1.6579	1.6579	1.6579
7	0.0584	1.9596	1.9596	1.9596
8	0.0593	1.9587	1.9587	1.9587
9	0.0600	1.9585	1.9585	1.9585
10	0.0593	1.9587	1.9587	1.9587
11	0.0584	1.9596	1.9596	1.9596
12	10.2432	2.2844	2.2844	2.2844
13	-0.0584	2.2944	2.2944	2.2944
14	-0.0569	2.2926	2.2926	2.2926
15	-0.0569	2.2926	2.2926	2.2926

Molecule Ph-COCl
Energy: -803.948716434
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.129753	0.186290	0.000013
2	6	-0.573183	-1.127055	0.000008
3	6	-1.929268	-1.392222	-0.000003
4	6	-2.840056	-0.351223	-0.000008
5	6	-2.398149	0.961452	-0.000003
6	6	-1.045736	1.231197	0.000006
7	1	0.139981	-1.941962	0.000012
8	1	-2.276011	-2.419830	-0.000007
9	1	-3.904195	-0.564020	-0.000015
10	1	-3.112167	1.777845	-0.000007
11	1	-0.676766	2.250765	0.000009
12	6	1.300301	0.565811	0.000021
13	17	2.463066	-0.765026	-0.000005
14	8	1.706515	1.682142	-0.000013

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9786	1.5879	1.5879	1.5879
2	1.9597	1.6477	1.6477	1.6477
3	1.9488	1.6559	1.6559	1.6559
4	1.9648	1.6576	1.6576	1.6576
5	1.9502	1.6559	1.6559	1.6559
6	1.9667	1.6447	1.6447	1.6447
7	0.0617	1.9404	1.9404	1.9404
8	0.0652	1.9527	1.9527	1.9527

9	0.0672	1.9519	1.9519	1.9519
10	0.0659	1.9528	1.9528	1.9528
11	0.0672	1.9327	1.9327	1.9327
12	2.2189	1.5707	1.5707	1.5707
13	9.9104	1.7281	1.7281	1.7281
14	1.7747	1.3184	1.3184	1.3184

Molecule Ph-CCl3
Energy: -1648.69025523
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.070336	1.302164	-1.195726
2	6	0.070336	2.683856	-1.193987
3	6	0.072868	3.379990	0.000000
4	6	0.070336	2.683856	1.193987
5	6	0.070336	1.302164	1.195726
6	6	0.079202	0.601571	0.000000
7	1	0.065759	0.770840	-2.139259
8	1	0.069469	3.218064	-2.138065
9	1	0.076215	4.464897	0.000000
10	1	0.069469	3.218064	2.138065
11	1	0.065759	0.770840	2.139259
12	6	-0.004583	-0.911784	0.000000
13	17	0.771394	-1.617412	1.425928
14	17	-1.714533	-1.394211	0.000000
15	17	0.771394	-1.617412	-1.425928

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9477	1.6450	1.6450	1.6450
2	1.9497	1.6560	1.6560	1.6560
3	1.9535	1.6575	1.6575	1.6575
4	1.9497	1.6560	1.6560	1.6560
5	1.9477	1.6450	1.6450	1.6450
6	1.9797	1.5848	1.5848	1.5848
7	0.0581	1.9384	1.9384	1.9384
8	0.0642	1.9535	1.9535	1.9535
9	0.0645	1.9553	1.9553	1.9553
10	0.0642	1.9535	1.9535	1.9535
11	0.0581	1.9384	1.9384	1.9384
12	2.1657	1.6241	1.6241	1.6241
13	9.9375	1.7170	1.7170	1.7170
14	9.9219	1.7223	1.7223	1.7223
15	9.9375	1.7170	1.7170	1.7170

Molecule Ph-CF3
Energy: -568.054278356
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.738035	-1.202247	-0.019193
2	6	-2.119839	-1.199258	0.001788
3	6	-2.809948	0.000000	0.012879
4	6	-2.119839	1.199258	0.001788
5	6	-0.738035	1.202247	-0.019193
6	6	-0.054430	0.000000	-0.029391
7	1	-0.188358	-2.136927	-0.034214
8	1	-2.660646	-2.139453	0.006774
9	1	-3.894889	0.000000	0.027491
10	1	-2.660646	2.139453	0.006774
11	1	-0.188358	2.136927	-0.034214
12	6	1.438469	0.000000	-0.003102
13	9	1.955692	1.078781	-0.606891
14	9	1.915599	0.000000	1.253109
15	9	1.955692	-1.078781	-0.606891

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9529	1.6457	1.6457	1.6457
2	1.9511	1.6565	1.6565	1.6565

3	1.9566	1.6576	1.6576	1.6576
4	1.9511	1.6565	1.6565	1.6565
5	1.9529	1.6457	1.6457	1.6457
6	1.9654	1.5689	1.5689	1.5689
7	0.0649	1.9345	1.9345	1.9345
8	0.0651	1.9532	1.9532	1.9532
9	0.0653	1.9534	1.9534	1.9534
10	0.0651	1.9532	1.9532	1.9532
11	0.0649	1.9345	1.9345	1.9345
12	2.2181	1.4328	1.4328	1.4328
13	1.9128	1.1353	1.1353	1.1353
14	1.9012	1.1368	1.1368	1.1368
15	1.9128	1.1353	1.1353	1.1353

Molecule Ph-CN
Energy: -323.530828437
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.091009	1.205217	0.000000
2	6	-1.471744	1.200196	0.000000
3	6	-2.161062	0.000000	0.000000
4	6	-1.471744	-1.200196	0.000000
5	6	-0.091009	-1.205217	0.000000
6	6	0.598125	0.000000	0.000000
7	1	0.460107	2.139077	0.000000
8	1	-2.013480	2.139809	0.000000
9	1	-3.246080	0.000000	0.000000
10	1	-2.013480	-2.139809	0.000000
11	1	0.460107	-2.139077	0.000000
12	6	2.034038	0.000000	0.000000
13	7	3.182751	0.000000	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9645	1.6501	1.6501	1.6501
2	1.9526	1.6559	1.6559	1.6559
3	1.9604	1.6573	1.6573	1.6573
4	1.9526	1.6559	1.6559	1.6559
5	1.9645	1.6501	1.6501	1.6501
6	2.0090	1.6041	1.6041	1.6041
7	0.0723	1.9471	1.9471	1.9471
8	0.0670	1.9522	1.9522	1.9522
9	0.0669	1.9519	1.9519	1.9519
10	0.0670	1.9522	1.9522	1.9522
11	0.0723	1.9471	1.9471	1.9471
12	2.0794	1.6087	1.6087	1.6087
13	1.7715	1.5814	1.5814	1.5814

Molecule Ph-NCO
Energy: -398.640435542
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.078156	-0.207196	0.000000
2	6	-0.808393	-1.270447	0.000000
3	6	-2.167960	-1.025436	0.000000
4	6	-2.645602	0.273215	0.000000
5	6	-1.753456	1.331115	0.000000
6	6	-0.392013	1.097346	0.000000
7	1	-0.418442	-2.281849	0.000000
8	1	-2.861141	-1.859986	0.000000
9	1	-3.713752	0.461358	0.000000
10	1	-2.119374	2.352462	0.000000
11	1	0.311962	1.922851	0.000000
12	7	1.441403	-0.474926	0.000000
13	8	3.686814	0.243534	0.000000
14	6	2.558670	-0.068368	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)

1	2.0586	1.5776	1.5776	1.5776
2	1.9438	1.6467	1.6467	1.6467
3	1.9501	1.6577	1.6577	1.6577
4	1.9422	1.6583	1.6583	1.6583
5	1.9497	1.6577	1.6577	1.6577
6	1.9397	1.6467	1.6467	1.6467
7	0.0654	1.9547	1.9547	1.9547
8	0.0639	1.9545	1.9545	1.9545
9	0.0617	1.9571	1.9571	1.9571
10	0.0641	1.9547	1.9547	1.9547
11	0.0636	1.9511	1.9511	1.9511
12	1.8635	1.4415	1.4415	1.4415
13	1.7699	1.3246	1.3246	1.3246
14	2.2637	1.5096	1.5096	1.5096

Molecule Ph-CNO2_3
Energy: -883.009332097
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.894206	0.071385	0.040497
2	6	1.605559	1.258977	0.051263
3	6	2.988563	1.227063	0.051932
4	6	3.658891	0.021143	0.040675
5	6	2.945982	-1.166077	0.021637
6	6	1.569629	-1.143574	0.017558
7	1	1.101239	2.215768	0.067873
8	1	3.540345	2.160347	0.059773
9	1	4.743608	0.002439	0.041195
10	1	3.465473	-2.117586	0.005679
11	1	1.021017	-2.078850	0.000667
12	6	-0.599507	0.024687	0.006680
13	7	-1.074837	-0.870250	-1.129425
14	8	-1.917135	-1.690414	-0.866049
15	8	-0.548304	-0.674051	-2.189950
16	7	-1.245741	-0.547192	1.267232
17	8	-0.618225	-1.389144	1.851855
18	8	-2.339077	-0.128086	1.538246
19	7	-1.259940	1.363878	-0.188943
20	8	-1.933272	1.522544	-1.170884
21	8	-1.042486	2.163051	0.686946

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9642	1.5761	1.5761	1.5761
2	1.9556	1.6425	1.6425	1.6425
3	1.9567	1.6534	1.6534	1.6534
4	1.9705	1.6556	1.6556	1.6556
5	1.9589	1.6530	1.6530	1.6530
6	1.9550	1.6389	1.6389	1.6389
7	0.0581	1.9129	1.9129	1.9129
8	0.0707	1.9476	1.9476	1.9476
9	0.0719	1.9485	1.9485	1.9485
10	0.0716	1.9475	1.9475	1.9475
11	0.0623	1.9208	1.9208	1.9208
12	2.1611	1.5046	1.5046	1.5046
13	2.2469	1.3400	1.3400	1.3400
14	1.8278	1.3016	1.3016	1.3016
15	1.8330	1.3025	1.3025	1.3025
16	2.2458	1.3402	1.3402	1.3402
17	1.8351	1.3017	1.3017	1.3017
18	1.8301	1.3004	1.3004	1.3004
19	2.2520	1.3386	1.3386	1.3386
20	1.8388	1.3006	1.3006	1.3006
21	1.8337	1.3003	1.3003	1.3003

Molecule Ph-CHCl2
Energy: -1189.37503598

Geometry:

Atom	Atomic No.	x	y	z
1	6	0.355859	-0.000040	-0.230550
2	6	0.823181	0.000410	1.075303
3	6	2.179524	0.000473	1.322529
4	6	3.080317	0.000084	0.268122
5	6	2.617524	-0.000360	-1.032333
6	6	1.254683	-0.000426	-1.280599
7	1	0.116259	0.000724	1.899014
8	1	2.540672	0.000828	2.345515
9	1	4.147146	0.000132	0.465868
10	1	3.316777	-0.000654	-1.861704
11	1	0.891594	-0.000769	-2.304229
12	6	-1.110444	-0.000139	-0.527809
13	1	-1.279289	-0.000450	-1.601453
14	17	-1.909950	1.451586	0.102220
15	17	-1.909874	-1.451576	0.103016

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9842	1.5848	1.5848	1.5848
2	1.9506	1.6475	1.6475	1.6475
3	1.9504	1.6571	1.6571	1.6571
4	1.9509	1.6583	1.6583	1.6583
5	1.9471	1.6576	1.6576	1.6576
6	1.9475	1.6496	1.6496	1.6496
7	0.0624	1.9531	1.9531	1.9531
8	0.0637	1.9545	1.9545	1.9545
9	0.0629	1.9559	1.9559	1.9559
10	0.0628	1.9560	1.9560	1.9560
11	0.0613	1.9528	1.9528	1.9528
12	2.0817	1.6409	1.6409	1.6409
13	0.0740	1.8643	1.8643	1.8643
14	9.9001	1.7293	1.7293	1.7293
15	9.9001	1.7293	1.7293	1.7293

Molecule Ph-OCHCl2
Energy: -1264.45563124
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.424970	0.819932	0.000000
2	6	-0.014544	1.354072	-1.204042
3	6	0.850587	2.432696	-1.197962
4	6	1.287814	2.969740	0.000000
5	6	0.850587	2.432696	1.197962
6	6	-0.014544	1.354072	1.204042
7	1	-0.378273	0.925840	-2.130207
8	1	1.181101	2.858972	-2.139131
9	1	1.965367	3.816849	0.000000
10	1	1.181101	2.858972	2.139131
11	1	-0.378273	0.925840	2.130207
12	8	-1.348376	-0.217057	0.000000
13	6	-0.942705	-1.514449	0.000000
14	1	-1.842870	-2.121256	0.000000
15	17	-0.014544	-1.959451	1.447644
16	17	-0.014544	-1.959451	-1.447644

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0626	1.5547	1.5547	1.5547
2	1.9394	1.6441	1.6441	1.6441
3	1.9492	1.6578	1.6578	1.6578
4	1.9446	1.6582	1.6582	1.6582
5	1.9492	1.6578	1.6578	1.6578
6	1.9394	1.6441	1.6441	1.6441
7	0.0640	1.9514	1.9514	1.9514
8	0.0634	1.9549	1.9549	1.9549
9	0.0617	1.9568	1.9568	1.9568
10	0.0634	1.9549	1.9549	1.9549

11	0.0640	1.9514	1.9514	1.9514
12	1.8582	1.2816	1.2816	1.2816
13	2.1537	1.6064	1.6064	1.6064
14	0.0832	1.8412	1.8412	1.8412
15	9.9022	1.7244	1.7244	1.7244
16	9.9022	1.7244	1.7244	1.7244

Molecule Ph-CHO
Energy: -344.603230301
Geometry:

Atom	Atomic No.	x	y	z
1	6	2.195978	-0.247928	0.000156
2	6	1.314337	-1.318921	-0.000009
3	6	-0.045877	-1.090847	-0.000207
4	6	-0.525206	0.211717	-0.000240
5	6	0.356462	1.279775	-0.000074
6	6	1.720240	1.051219	0.000124
7	1	3.265930	-0.430196	0.000312
8	1	1.695041	-2.334907	0.000017
9	1	-0.760290	-1.907688	-0.000341
10	1	-0.029845	2.295757	-0.000102
11	1	2.413058	1.885943	0.000253
12	6	-1.976426	0.467667	-0.000462
13	1	-2.270328	1.536244	0.000573
14	8	-2.818827	-0.395155	0.000444

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9594	1.6587	1.6587	1.6587
2	1.9492	1.6574	1.6574	1.6574
3	1.9649	1.6478	1.6478	1.6478
4	1.9751	1.5876	1.5876	1.5876
5	1.9557	1.6523	1.6523	1.6523
6	1.9452	1.6578	1.6578	1.6578
7	0.0644	1.9538	1.9538	1.9538
8	0.0638	1.9547	1.9547	1.9547
9	0.0664	1.9429	1.9429	1.9429
10	0.0620	1.9603	1.9603	1.9603
11	0.0627	1.9561	1.9561	1.9561
12	2.1340	1.6110	1.6110	1.6110
13	0.0579	1.9508	1.9508	1.9508
14	1.7393	1.3294	1.3294	1.3294

Molecule Ph-OCH2Cl
Energy: -805.127032655
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.476866	-0.199685	0.000090
2	6	1.334781	-1.290610	0.000078
3	6	2.695844	-1.087454	-0.000099
4	6	3.217648	0.199513	-0.000145
5	6	2.356576	1.275426	-0.000064
6	6	0.980643	1.088248	0.000082
7	1	0.905008	-2.285958	0.000156
8	1	3.362500	-1.943662	-0.000135
9	1	4.290643	0.355775	-0.000192
10	1	2.749702	2.286883	-0.000027
11	1	0.327614	1.952153	0.000236
12	8	-0.851871	-0.497909	0.000232
13	6	-1.753972	0.557084	0.000103
14	1	-1.644837	1.171237	-0.897475
15	1	-1.645108	1.170986	0.897876
16	17	-3.375345	-0.116428	-0.000151

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0758	1.5533	1.5533	1.5533
2	1.9321	1.6442	1.6442	1.6442
3	1.9516	1.6587	1.6587	1.6587

4	1.9297	1.6586	1.6586	1.6586
5	1.9480	1.6588	1.6588	1.6588
6	1.9162	1.6463	1.6463	1.6463
7	0.0667	1.9554	1.9554	1.9554
8	0.0630	1.9554	1.9554	1.9554
9	0.0584	1.9606	1.9606	1.9606
10	0.0615	1.9556	1.9556	1.9556
11	0.0562	1.9444	1.9444	1.9444
12	1.8574	1.2844	1.2844	1.2844
13	2.0646	1.6343	1.6343	1.6343
14	0.0645	1.8836	1.8836	1.8836
15	0.0645	1.8836	1.8836	1.8836
16	9.8897	1.7308	1.7308	1.7308

Molecule Ph-CONH2
Energy: -399.866594975
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.213841	0.021314	-0.017938
2	6	-0.509243	1.195694	0.116430
3	6	-1.889509	1.162257	0.143130
4	6	-2.555639	-0.045465	0.022916
5	6	-1.838316	-1.218513	-0.128263
6	6	-0.455985	-1.185871	-0.147227
7	1	0.037442	2.129120	0.193803
8	1	-2.450382	2.084185	0.255118
9	1	-3.640373	-0.071919	0.039944
10	1	-2.357714	-2.164465	-0.239682
11	1	0.092877	-2.110093	-0.297392
12	6	1.702846	0.131009	-0.034797
13	8	2.260350	1.181571	-0.289487
14	7	2.405811	-0.995957	0.242490
15	1	3.410145	-0.903921	0.284187
16	1	1.976552	-1.806327	0.656984

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9817	1.5863	1.5863	1.5863
2	1.9606	1.6457	1.6457	1.6457
3	1.9487	1.6574	1.6574	1.6574
4	1.9529	1.6585	1.6585	1.6585
5	1.9435	1.6577	1.6577	1.6577
6	1.9446	1.6500	1.6500	1.6500
7	0.0644	1.9374	1.9374	1.9374
8	0.0629	1.9552	1.9552	1.9552
9	0.0626	1.9560	1.9560	1.9560
10	0.0609	1.9568	1.9568	1.9568
11	0.0567	1.9435	1.9435	1.9435
12	2.1834	1.5258	1.5258	1.5258
13	1.6735	1.3299	1.3299	1.3299
14	1.8169	1.4770	1.4770	1.4770
15	0.1482	1.8073	1.8073	1.8073
16	0.1386	1.8110	1.8110	1.8110

Molecule Ph-Me
Energy: -270.719994604
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.028465	-2.403600	0.000000
2	1	0.465422	-2.812721	0.883653
3	1	-1.059121	-2.770388	0.000000
4	1	0.465422	-2.812721	-0.883653
5	6	0.004000	-0.905050	0.000000
6	6	0.007500	-0.193242	-1.191111
7	6	0.007500	-0.193242	1.191111
8	6	0.007500	1.189995	-1.194377
9	1	0.012355	-0.733688	-2.133713

10	6	0.007500	1.189995	1.194377
11	1	0.012355	-0.733688	2.133713
12	6	0.006406	1.887967	0.000000
13	1	0.011506	1.726624	-2.137879
14	1	0.011506	1.726624	2.137879
15	1	0.008915	2.973018	0.000000

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.8779	1.7116	1.7116	1.7116
2	0.0504	1.9476	1.9476	1.9476
3	0.0523	1.9463	1.9463	1.9463
4	0.0504	1.9476	1.9476	1.9476
5	1.9986	1.5998	1.5998	1.5998
6	1.9358	1.6515	1.6515	1.6515
7	1.9358	1.6515	1.6515	1.6515
8	1.9416	1.6597	1.6597	1.6597
9	0.0547	1.9594	1.9594	1.9594
10	1.9416	1.6597	1.6597	1.6597
11	0.0547	1.9594	1.9594	1.9594
12	1.9348	1.6600	1.6600	1.6600
13	0.0574	1.9603	1.9603	1.9603
14	0.0574	1.9603	1.9603	1.9603
15	0.0564	1.9622	1.9622	1.9622

Molecule Ph-OMe
Energy: -345.797622017
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.448025	-0.272640	0.000151
2	6	0.495027	-1.293572	-0.000036
3	6	1.837049	-0.988937	-0.000134
4	6	2.261188	0.333534	-0.000083
5	6	1.319368	1.340106	0.000021
6	6	-0.038288	1.049494	0.000162
7	1	0.143283	-2.319285	-0.000166
8	1	2.566206	-1.792845	-0.000303
9	1	3.319325	0.570668	-0.000051
10	1	1.634821	2.378656	0.000076
11	1	-0.757388	1.858508	0.000225
12	8	-1.744062	-0.665114	0.000428
13	6	-2.742598	0.320494	-0.000365
14	1	-2.680428	0.950577	-0.894191
15	1	-3.694850	-0.207655	-0.000275
16	1	-2.680798	0.951411	0.892964

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0750	1.5525	1.5525	1.5525
2	1.9266	1.6454	1.6454	1.6454
3	1.9473	1.6597	1.6597	1.6597
4	1.9237	1.6596	1.6596	1.6596
5	1.9449	1.6597	1.6597	1.6597
6	1.9138	1.6469	1.6469	1.6469
7	0.0620	1.9586	1.9586	1.9586
8	0.0600	1.9579	1.9579	1.9579
9	0.0553	1.9634	1.9634	1.9634
10	0.0587	1.9579	1.9579	1.9579
11	0.0540	1.9468	1.9468	1.9468
12	1.8473	1.2886	1.2886	1.2886
13	1.9655	1.6749	1.6749	1.6749
14	0.0513	1.9240	1.9240	1.9240
15	0.0628	1.9118	1.9118	1.9118
16	0.0513	1.9240	1.9240	1.9240

Molecule Ph-CH2NH2
Energy: -325.942701231
Geometry:

Atom	Atomic No.	x	y	z

1	6	-0.423644	0.253232	0.126846
2	6	0.496363	1.279265	-0.022776
3	6	1.849746	1.008794	-0.123756
4	6	2.298887	-0.298613	-0.083926
5	6	1.385628	-1.329261	0.057148
6	6	0.033976	-1.055630	0.161738
7	1	0.147896	2.307932	-0.063903
8	1	2.556069	1.824493	-0.241301
9	1	3.359006	-0.514955	-0.167575
10	1	1.729803	-2.358393	0.085812
11	1	-0.689950	-1.856743	0.265924
12	6	-1.888657	0.563849	0.281268
13	1	-2.077281	1.567196	-0.126054
14	1	-2.124884	0.613691	1.349658
15	7	-2.726297	-0.465269	-0.300439
16	1	-3.704161	-0.341118	-0.070771
17	1	-2.626215	-0.515034	-1.307971

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9930	1.5916	1.5916	1.5916
2	1.9342	1.6521	1.6521	1.6521
3	1.9393	1.6600	1.6600	1.6600
4	1.9359	1.6602	1.6602	1.6602
5	1.9414	1.6599	1.6599	1.6599
6	1.9386	1.6489	1.6489	1.6489
7	0.0530	1.9615	1.9615	1.9615
8	0.0567	1.9611	1.9611	1.9611
9	0.0561	1.9623	1.9623	1.9623
10	0.0569	1.9602	1.9602	1.9602
11	0.0519	1.9534	1.9534	1.9534
12	1.9741	1.6377	1.6377	1.6377
13	0.0357	1.9126	1.9126	1.9126
14	0.0545	1.9036	1.9036	1.9036
15	1.7485	1.5068	1.5068	1.5068
16	0.1147	1.8029	1.8029	1.8029
17	0.1154	1.8039	1.8039	1.8039

Molecule Ph-CF2CF3
Energy: -805.455870177
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.717171	0.011838	0.320566
2	6	-1.386878	1.206931	0.126541
3	6	-2.726915	1.190153	-0.210979
4	6	-3.389702	-0.015330	-0.355740
5	6	-2.714562	-1.207782	-0.162693
6	6	-1.375105	-1.197320	0.174912
7	1	-0.860185	2.147125	0.246653
8	1	-3.256272	2.125109	-0.359480
9	1	-4.442175	-0.026158	-0.619546
10	1	-3.234941	-2.152942	-0.273546
11	1	-0.838639	-2.126450	0.332669
12	6	0.735734	0.024543	0.669505
13	6	1.676247	-0.017648	-0.541248
14	9	1.463664	-1.123846	-1.250745
15	9	1.464453	1.035697	-1.326942
16	9	2.945249	-0.004285	-0.153902
17	9	1.064887	-1.041467	1.434007
18	9	1.064226	1.140679	1.358479

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9636	1.5694	1.5694	1.5694
2	1.9522	1.6446	1.6446	1.6446
3	1.9513	1.6562	1.6562	1.6562
4	1.9579	1.6574	1.6574	1.6574
5	1.9513	1.6562	1.6562	1.6562
6	1.9521	1.6445	1.6445	1.6445

7	0.0637	1.9304	1.9304	1.9304
8	0.0656	1.9528	1.9528	1.9528
9	0.0658	1.9529	1.9529	1.9529
10	0.0656	1.9528	1.9528	1.9528
11	0.0636	1.9304	1.9304	1.9304
12	2.1421	1.4587	1.4587	1.4587
13	2.2016	1.4086	1.4086	1.4086
14	1.9240	1.1337	1.1337	1.1337
15	1.9239	1.1337	1.1337	1.1337
16	1.9242	1.1322	1.1322	1.1322
17	1.9157	1.1369	1.1369	1.1369
18	1.9162	1.1369	1.1369	1.1369

Molecule Ph-CCH
Energy: -307.437816282
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.580988	-0.000045	-0.000001
2	6	0.119566	1.200741	-0.000001
3	6	1.500945	1.197838	0.000001
4	6	2.194215	0.000062	0.000001
5	6	1.501038	-1.197768	0.000000
6	6	0.119659	-1.200777	0.000000
7	1	-0.429710	2.135974	-0.000001
8	1	2.040857	2.138985	0.000001
9	1	3.279328	0.000104	0.000002
10	1	2.041022	-2.138873	0.000001
11	1	-0.429545	-2.136052	-0.000001
12	6	-3.211226	-0.000111	-0.000002
13	6	-2.013689	-0.000102	-0.000003
14	1	-4.279078	0.000823	0.000025

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0054	1.6071	1.6071	1.6071
2	1.9546	1.6519	1.6519	1.6519
3	1.9459	1.6578	1.6578	1.6578
4	1.9482	1.6590	1.6590	1.6590
5	1.9459	1.6578	1.6578	1.6578
6	1.9546	1.6519	1.6519	1.6519
7	0.0643	1.9542	1.9542	1.9542
8	0.0616	1.9566	1.9566	1.9566
9	0.0612	1.9573	1.9573	1.9573
10	0.0616	1.9566	1.9566	1.9566
11	0.0643	1.9542	1.9542	1.9542
12	1.8744	1.7613	1.7613	1.7613
13	1.9524	1.6685	1.6685	1.6685
14	0.1056	2.0579	2.0579	2.0579

Molecule Ph-CH2CF3
Energy: -607.251265851
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.543862	0.000577	-0.554971
2	6	-1.207387	-1.194415	-0.324484
3	6	-2.512832	-1.196729	0.130779
4	6	-3.168941	-0.000542	0.359388
5	6	-2.513706	1.196164	0.131253
6	6	-1.208215	1.194958	-0.324008
7	1	-0.693892	-2.135081	-0.500292
8	1	-3.020843	-2.139181	0.306693
9	1	-4.194220	-0.000992	0.714448
10	1	-3.022360	2.138203	0.307523
11	1	-0.695429	2.136084	-0.499436
12	6	0.877949	0.001129	-1.035587
13	6	1.877171	0.000036	0.084437
14	9	1.758163	1.076691	0.872872

15	9	1.758645	-1.078633	0.870274
16	9	3.132444	0.000873	-0.392470
17	1	1.091152	0.883843	-1.642026
18	1	1.091265	-0.880319	-1.643828

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9883	1.5901	1.5901	1.5901
2	1.9435	1.6487	1.6487	1.6487
3	1.9466	1.6580	1.6580	1.6580
4	1.9462	1.6586	1.6586	1.6586
5	1.9466	1.6580	1.6580	1.6580
6	1.9435	1.6487	1.6487	1.6487
7	0.0590	1.9504	1.9504	1.9504
8	0.0616	1.9566	1.9566	1.9566
9	0.0611	1.9575	1.9575	1.9575
10	0.0616	1.9566	1.9566	1.9566
11	0.0590	1.9505	1.9505	1.9505
12	1.9166	1.6265	1.6265	1.6265
13	2.2129	1.4313	1.4313	1.4313
14	1.9084	1.1362	1.1362	1.1362
15	1.9084	1.1362	1.1362	1.1362
16	1.9019	1.1363	1.1363	1.1363
17	0.0675	1.9027	1.9027	1.9027
18	0.0675	1.9027	1.9027	1.9027

Molecule Ph-CCH3NO2_2
Energy: -718.128467010
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.714691	-0.117055	0.156605
2	6	-1.212354	0.695303	-0.855034
3	6	-2.572996	0.819529	-1.037479
4	6	-3.452517	0.137268	-0.213803
5	6	-2.963115	-0.669872	0.793044
6	6	-1.597631	-0.797671	0.977128
7	1	-0.532446	1.238915	-1.500487
8	1	-2.950017	1.458464	-1.828530
9	1	-4.523001	0.237603	-0.359387
10	1	-3.643848	-1.208922	1.442872
11	1	-1.235536	-1.438401	1.771121
12	6	0.772196	-0.265360	0.349965
13	6	1.222366	-1.162874	1.472580
14	1	2.309691	-1.215394	1.484169
15	1	0.872163	-0.755588	2.422021
16	1	0.823973	-2.164563	1.331016
17	7	1.456140	1.077414	0.580171
18	8	2.664057	1.055934	0.552899
19	8	0.769103	2.033559	0.834606
20	7	1.364404	-0.754038	-0.959515
21	8	1.532942	0.068631	-1.827318
22	8	1.564856	-1.939543	-1.055865

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9729	1.5789	1.5789	1.5789
2	1.9507	1.6395	1.6395	1.6395
3	1.9550	1.6544	1.6544	1.6544
4	1.9616	1.6568	1.6568	1.6568
5	1.9493	1.6555	1.6555	1.6555
6	1.9529	1.6451	1.6451	1.6451
7	0.0565	1.9182	1.9182	1.9182
8	0.0679	1.9500	1.9500	1.9500
9	0.0676	1.9522	1.9522	1.9522
10	0.0653	1.9527	1.9527	1.9527
11	0.0625	1.9313	1.9313	1.9313
12	2.1173	1.5283	1.5283	1.5283
13	1.8756	1.6822	1.6822	1.6822
14	0.0610	1.9089	1.9089	1.9089

15	0.0660	1.9259	1.9259	1.9259
16	0.0642	1.9142	1.9142	1.9142
17	2.2479	1.3429	1.3429	1.3429
18	1.8033	1.3047	1.3047	1.3047
19	1.8192	1.3053	1.3053	1.3053
20	2.2524	1.3424	1.3424	1.3424
21	1.8147	1.3027	1.3027	1.3027
22	1.8161	1.3053	1.3053	1.3053

Molecule Ph-SCHCH2
Energy: -706.600493793
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.081751	0.006450	-0.467209
2	6	-0.746176	1.202805	-0.245599
3	6	-2.064216	1.195867	0.173402
4	6	-2.723392	-0.005199	0.367554
5	6	-2.063648	-1.200412	0.141708
6	6	-0.745629	-1.195665	-0.277351
7	1	-0.222064	2.139777	-0.402158
8	1	-2.579838	2.134843	0.345895
9	1	-3.758365	-0.009762	0.693730
10	1	-2.578837	-2.143856	0.289316
11	1	-0.221078	-2.127919	-0.458642
12	16	1.595730	0.014312	-1.031606
13	6	2.493655	-0.006416	0.474492
14	1	3.564048	-0.003712	0.285346
15	6	2.027937	-0.023537	1.711404
16	1	0.966517	-0.026708	1.933953
17	1	2.717262	-0.035012	2.547833

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9898	1.6178	1.6178	1.6178
2	1.9505	1.6510	1.6510	1.6510
3	1.9461	1.6579	1.6579	1.6579
4	1.9501	1.6587	1.6587	1.6587
5	1.9461	1.6579	1.6579	1.6579
6	1.9505	1.6510	1.6510	1.6510
7	0.0634	1.9566	1.9566	1.9566
8	0.0621	1.9566	1.9566	1.9566
9	0.0620	1.9566	1.9566	1.9566
10	0.0621	1.9566	1.9566	1.9566
11	0.0634	1.9566	1.9566	1.9566
12	9.9720	1.8616	1.8616	1.8616
13	1.9411	1.6954	1.6954	1.6954
14	0.0671	1.9518	1.9518	1.9518
15	1.8658	1.7321	1.7321	1.7321
16	0.0514	1.9749	1.9749	1.9749
17	0.0566	1.9804	1.9804	1.9804

Molecule Ph-ethylbenzene
Energy: -309.909813786
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.011610	1.031208	-0.000049
2	6	1.360966	1.352034	-0.000035
3	6	2.315529	0.355374	0.000020
4	6	1.911217	-0.970414	0.000077
5	6	0.567451	-1.283443	0.000009
6	6	-0.405773	-0.289328	-0.000051
7	1	-0.719892	1.831511	-0.000100
8	1	1.663384	2.394541	-0.000051
9	1	3.371164	0.606250	0.000050
10	1	2.650647	-1.765039	0.000133
11	1	0.258210	-2.325694	0.000034
12	6	-1.858726	-0.690215	-0.000132

13	1	-2.037591	-1.327695	-0.872669
14	1	-2.037580	-1.328094	0.872113
15	6	-2.862335	0.445402	0.000138
16	1	-2.753629	1.079637	-0.883383
17	1	-3.880770	0.051626	0.000082
18	1	-2.753575	1.079250	0.883932

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9349	1.6499	1.6499	1.6499
2	1.9409	1.6596	1.6596	1.6596
3	1.9342	1.6599	1.6599	1.6599
4	1.9410	1.6598	1.6598	1.6598
5	1.9361	1.6505	1.6505	1.6505
6	1.9984	1.5959	1.5959	1.5959
7	0.0532	1.9453	1.9453	1.9453
8	0.0566	1.9601	1.9601	1.9601
9	0.0561	1.9626	1.9626	1.9626
10	0.0571	1.9605	1.9605	1.9605
11	0.0548	1.9601	1.9601	1.9601
12	1.9275	1.6576	1.6576	1.6576
13	0.0491	1.9158	1.9158	1.9158
14	0.0491	1.9158	1.9158	1.9158
15	1.8736	1.7111	1.7111	1.7111
16	0.0449	1.9431	1.9431	1.9431
17	0.0473	1.9441	1.9441	1.9441
18	0.0449	1.9431	1.9431	1.9431

Molecule Ph-NMe2
Energy: -365.122585508
Geometry:

Atom	Atomic No.	x	y	z
1	6	0.180576	-0.000039	-0.070353
2	6	-0.543796	-1.196338	-0.033069
3	6	-1.923869	-1.187185	0.016036
4	6	-2.632335	0.000041	0.038966
5	6	-1.923797	1.187239	0.016391
6	6	-0.543733	1.196300	-0.032708
7	1	-0.029682	-2.148170	-0.044346
8	1	-2.452926	-2.134981	0.040474
9	1	-3.715766	0.000061	0.079489
10	1	-2.452789	2.135061	0.041180
11	1	-0.029516	2.148085	-0.043587
12	7	1.559692	-0.000035	-0.145167
13	6	2.270020	-1.234787	0.058873
14	1	3.339609	-1.052394	-0.037093
15	1	2.083621	-1.673156	1.049771
16	1	1.998846	-1.977037	-0.696899
17	6	2.270038	1.234789	0.058213
18	1	3.339567	1.052497	-0.038652
19	1	1.998215	1.976861	-0.697474
20	1	2.084355	1.673298	1.049202

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	2.0493	1.5657	1.5657	1.5657
2	1.9131	1.6481	1.6481	1.6481
3	1.9423	1.6602	1.6602	1.6602
4	1.9136	1.6605	1.6605	1.6605
5	1.9423	1.6602	1.6602	1.6602
6	1.9131	1.6481	1.6481	1.6481
7	0.0482	1.9420	1.9420	1.9420
8	0.0563	1.9596	1.9596	1.9596
9	0.0516	1.9677	1.9677	1.9677
10	0.0563	1.9596	1.9596	1.9596
11	0.0482	1.9420	1.9420	1.9420
12	1.8978	1.4167	1.4167	1.4167
13	1.9346	1.6821	1.6821	1.6821
14	0.0556	1.9233	1.9233	1.9233

15	0.0430	1.9418	1.9418	1.9418
16	0.0508	1.9213	1.9213	1.9213
17	1.9346	1.6821	1.6821	1.6821
18	0.0556	1.9233	1.9233	1.9233
19	0.0508	1.9213	1.9213	1.9213
20	0.0430	1.9418	1.9418	1.9418

Molecule Ph-CHCN2
Energy: -454.708481463
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.209571	-0.022546	-0.248442
2	6	-1.043577	-1.066560	-0.617553
3	6	-2.400754	-0.982173	-0.385480
4	6	-2.932217	0.147211	0.215804
5	6	-2.100629	1.186516	0.581893
6	6	-0.737103	1.104183	0.351379
7	1	-0.628051	-1.955778	-1.083330
8	1	-3.048381	-1.802193	-0.675775
9	1	-3.999290	0.214312	0.398069
10	1	-2.510298	2.073675	1.052353
11	1	-0.089973	1.926324	0.638162
12	6	1.280960	-0.169800	-0.515913
13	1	1.422677	-0.468361	-1.561083
14	6	1.867041	-1.232475	0.309358
15	7	2.303537	-2.090911	0.930491
16	6	2.028806	1.074789	-0.331351
17	7	2.601546	2.059077	-0.205714

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9955	1.5904	1.5904	1.5904
2	1.9466	1.6471	1.6471	1.6471
3	1.9539	1.6563	1.6563	1.6563
4	1.9542	1.6569	1.6569	1.6569
5	1.9549	1.6561	1.6561	1.6561
6	1.9477	1.6466	1.6466	1.6466
7	0.0644	1.9510	1.9510	1.9510
8	0.0666	1.9522	1.9522	1.9522
9	0.0660	1.9531	1.9531	1.9531
10	0.0672	1.9513	1.9513	1.9513
11	0.0630	1.9434	1.9434	1.9434
12	2.0396	1.6236	1.6236	1.6236
13	0.0999	1.8750	1.8750	1.8750
14	2.0873	1.5993	1.5993	1.5993
15	1.7976	1.5767	1.5767	1.5767
16	2.0942	1.5969	1.5969	1.5969
17	1.8016	1.5758	1.5758	1.5758

Molecule Ph-NH2
Energy: -286.760404274
Geometry:

Atom	Atomic No.	x	y	z
1	6	-0.219307	-1.196463	-0.007004
2	6	1.161752	-1.191183	0.003678
3	6	1.866341	-0.000058	0.009352
4	6	1.161710	1.191217	0.003479
5	6	-0.219218	1.196503	-0.006869
6	6	-0.928256	-0.000017	-0.011011
7	1	-0.760675	-2.138154	-0.018157
8	1	1.694962	-2.136791	0.007327
9	1	2.950551	0.000001	0.017828
10	1	1.695059	2.136740	0.006947
11	1	-0.760713	2.138158	-0.017168
12	7	-2.313317	-0.000063	-0.057624
13	1	-2.782242	-0.845417	0.229005
14	1	-2.781860	0.845906	0.227842

Atom	QA	DA(alpha)	DA(beta)	DA(total)
1	1.9157	1.6493	1.6493	1.6493
2	1.9446	1.6604	1.6604	1.6604
3	1.9162	1.6605	1.6605	1.6605
4	1.9446	1.6604	1.6604	1.6604
5	1.9158	1.6493	1.6493	1.6493
6	2.0481	1.5729	1.5729	1.5729
7	0.0520	1.9626	1.9626	1.9626
8	0.0579	1.9595	1.9595	1.9595
9	0.0526	1.9664	1.9664	1.9664
10	0.0579	1.9595	1.9595	1.9595
11	0.0520	1.9626	1.9626	1.9626
12	1.7826	1.4921	1.4921	1.4921
13	0.1300	1.8085	1.8085	1.8085
14	0.1300	1.8085	1.8085	1.8085

==========
Alkenyl anions
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Computed geometries (Cartesian coordinates in Angstrom) and
total energies (Hartree) from LC-BLYP/6-31+G(d,p) calculations
on all alkenyl anions in Figure 3. Calculations use a continuum solvent,
Gaussian keyword scrf=(cpcm,solvent=2-propanol)

"B1m" and "B2m" denote the Z and E alkenyl anion intermediates, "P1" and "P2"
denote the corresponding products. Results are shown from only the most stable
confirmations found of each species.

Molecule CH2CH2NEt2 B1 file B1mNEt2-g
Energy: -996.017487264
Geometry:

Atomic No.	x	y	z
6	-4.007255	-1.412404	0.471397
6	-2.961331	-0.578218	0.103859
6	-3.223060	0.743159	-0.213167
6	-4.499350	1.276141	-0.180363
6	-5.538055	0.443572	0.184272
6	-5.285607	-0.891604	0.506632
1	-3.814406	-2.449978	0.722379
1	-4.670654	2.317431	-0.435149
1	-6.554019	0.822686	0.222049
1	-6.115015	-1.532220	0.791068
6	-1.948797	1.383795	-0.564139
8	-1.764944	2.555460	-0.914725
6	-1.521969	-0.846089	-0.020532
6	-0.919411	-2.003204	0.218935
7	-0.992384	0.441249	-0.443702
6	0.378334	0.745091	-0.766297
1	0.861453	-0.165883	-1.113521
1	0.377169	1.466646	-1.586313
6	0.482787	-2.317012	0.129176
6	1.304045	-2.314218	1.268581
6	1.070049	-2.775532	-1.062597
6	2.622315	-2.722765	1.214133
1	0.881783	-1.990495	2.215779
6	2.389743	-3.181068	-1.111108
1	0.464525	-2.813403	-1.963988
6	3.185103	-3.162077	0.025633
1	3.222699	-2.696500	2.119611
1	2.804637	-3.521979	-2.055915
1	4.219741	-3.486298	-0.014026
6	1.122371	1.354871	0.408208
1	0.560090	2.232684	0.731697
1	1.131309	0.645952	1.252888
7	2.467870	1.762004	0.048112

6	3.382013	0.629315	0.032606
1	3.711085	0.391108	1.058895
1	2.838563	-0.251240	-0.314245
6	2.954151	2.829480	0.907719
1	2.755246	2.587360	1.966652
1	4.040128	2.878359	0.804951
6	2.379255	4.188196	0.567178
1	2.647000	4.470469	-0.453813
1	1.289983	4.206917	0.646378
1	2.771966	4.947672	1.247928
6	4.583011	0.843445	-0.863897
1	4.262923	1.003316	-1.896378
1	5.179200	1.706767	-0.558964
1	5.235692	-0.033067	-0.838396

Molecule CH2CH2NEt2 B2 file B2mNEt2-f
Energy: -996.021110135
Geometry:

Atomic No.	x	y	z
6	2.987570	1.278483	0.232745
6	1.630221	1.278087	-0.067621
6	0.959837	2.490527	-0.156186
6	1.586087	3.705883	0.041717
6	2.934715	3.699954	0.339487
6	3.621796	2.490943	0.432416
1	3.542353	0.351394	0.309701
1	1.026533	4.632886	-0.036743
1	3.462906	4.633706	0.501952
1	4.681814	2.501352	0.667465
6	-0.449184	2.217992	-0.479894
8	-1.359578	3.042446	-0.637327
6	0.679934	0.184290	-0.333822
6	0.793959	-1.138041	-0.376376
7	-0.564099	0.885172	-0.576998
6	-1.808677	0.237240	-0.884117
1	-2.362319	0.862088	-1.588540
1	-1.566608	-0.710899	-1.364356
6	2.077611	-1.759435	-0.126558
6	2.971872	-2.044170	-1.167815
6	2.457647	-2.168470	1.159258
6	4.188743	-2.654946	-0.929867
1	2.700245	-1.765217	-2.182156
6	3.675091	-2.779051	1.394198
1	1.778461	-1.988417	1.987969
6	4.558619	-3.026286	0.354170
1	4.860326	-2.845109	-1.762715
1	3.938451	-3.067969	2.408102
1	5.512828	-3.508464	0.539355
6	-2.651422	0.019807	0.359854
1	-2.054187	-0.516341	1.116181
1	-2.887757	0.999845	0.778457
7	-3.886505	-0.685410	0.072056
6	-4.927047	-0.363311	1.035886
1	-5.702671	-1.128524	0.966523
1	-4.526851	-0.421402	2.063381
6	-3.664458	-2.121017	-0.017071
1	-2.688523	-2.285408	-0.478543
1	-3.603000	-2.560103	0.994232
6	-4.713065	-2.842566	-0.836797
1	-5.716381	-2.723870	-0.421590
1	-4.724380	-2.460601	-1.860353
1	-4.496309	-3.913147	-0.871709
6	-5.565822	0.988973	0.800459
1	-4.839542	1.803066	0.854600
1	-6.034737	1.021666	-0.185800

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1       -6.333967       1.182249        1.553410

Molecule CH2CH2NEt2 P1  file P1mNEt2-h
Energy: -996.553742885
Geometry:
Atomic No.   x            y               z
6       -3.809007       -1.422999       -0.789740
6       -2.865561       -0.596860       -0.209068
6       -3.241056       0.620827        0.321548
6       -4.544976       1.068389        0.294090
6       -5.490449       0.247303        -0.292057
6       -5.120914       -0.983219       -0.827384
1       -3.543348       -2.388354       -1.207216
1       -4.811603       2.030657        0.718555
1       -6.528048       0.560201        -0.336324
1       -5.878662       -1.612412       -1.282776
6       -2.033879       1.273263        0.853827
8       -1.936156       2.382134        1.353680
6       -1.416774       -0.772189       0.006488
6       -0.732034       -1.850519       -0.365816
7       -0.993688       0.399744        0.664216
6       0.366361        0.845633        0.878187
1       0.321423        1.639795        1.623273
1       0.959457        0.034442        1.292657
6       0.669420        -2.235213       -0.119246
6       1.167986        -2.377126       1.170561
6       1.492756        -2.561044       -1.191617
6       2.467289        -2.804357       1.382437
1       0.524226        -2.162943       2.018268
6       2.791776        -2.985523       -0.981920
1       1.108198        -2.474186       -2.203513
6       3.284617        -3.105422       0.306782
1       2.840265        -2.907609       2.396291
1       3.423500        -3.225218       -1.831135
1       4.303278        -3.440528       0.472589
6       0.985561        1.394006        -0.395986
1       0.938517        0.637479        -1.197034
1       0.375809        2.238084        -0.724964
7       2.346442        1.842692        -0.177828
6       2.713048        2.916826        -1.088599
1       3.801399        2.999936        -1.091063
1       2.420589        2.658506        -2.121259
6       3.286745        0.733053        -0.248154
1       2.809260        -0.150121       0.180442
1       3.499918        0.481897        -1.301677
6       4.577571        0.990605        0.499186
1       5.119152        1.853953        0.106379
1       4.375044        1.172141        1.557424
1       5.238523        0.123814        0.419628
6       2.130494        4.259083        -0.700602
1       1.038476        4.244335        -0.675664
1       2.485663        4.557227        0.288590
1       2.432155        5.024762        -1.419504
1       -1.307059       -2.577094       -0.933622

Molecule CH2CH2NEt2 P2 file P2mNEt2-i
Energy: -996.555196533
Geometry:
Atomic No.   x            y               z
6       -3.004490       1.321383        -0.421378
6       -1.665415       1.383340        -0.079052
6       -1.017311       2.607881        -0.072431
6       -1.657282       3.789614        -0.372942
6       -3.000210       3.728014        -0.699013
6       -3.657850       2.504345        -0.726844
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1	-3.540017	0.381636	-0.454584
1	-1.116900	4.730388	-0.358633
1	-3.542776	4.635268	-0.942054
1	-4.708561	2.472065	-0.995966
6	0.400477	2.384261	0.261790
8	1.292756	3.212262	0.368079
6	-0.670789	0.345338	0.261062
6	-0.779000	-0.974920	0.373372
7	0.544999	1.041475	0.432443
6	1.808512	0.441419	0.780277
1	2.402159	1.218047	1.264054
1	1.644409	-0.351718	1.513044
6	-2.021003	-1.766040	0.295549
6	-3.071378	-1.551421	1.179110
6	-2.129351	-2.794306	-0.633776
6	-4.215579	-2.326787	1.117013
1	-2.987592	-0.767716	1.925671
6	-3.273709	-3.568352	-0.699764
1	-1.307167	-2.983799	-1.317557
6	-4.322090	-3.335063	0.174549
1	-5.027468	-2.144203	1.813652
1	-3.345785	-4.361163	-1.437340
1	-5.218987	-3.943900	0.125752
6	2.535704	-0.110624	-0.434136
1	1.923431	-0.894914	-0.882811
1	2.630934	0.683399	-1.193608
7	3.828181	-0.659957	-0.078493
6	4.840657	0.383101	0.011242
1	5.194402	0.656760	-0.997739
1	4.371219	1.279977	0.421789
6	4.231526	-1.726290	-0.983039
1	4.083121	-1.415251	-2.031559
1	5.304378	-1.884853	-0.860136
6	3.520361	-3.036400	-0.719713
1	3.727545	-3.384841	0.294736
1	2.436957	-2.949950	-0.831681
1	3.861746	-3.800228	-1.422591
6	6.012633	0.009239	0.893348
1	5.674058	-0.189925	1.912778
1	6.534847	-0.878972	0.531327
1	6.737294	0.826435	0.925070
1	0.127972	-1.547643	0.544765

Molecule CH3 B1 file B1mH
Energy: -744.848439487
Geometry:

Atomic No.	x	y	z
6	-2.345854	-1.934829	-0.000148
6	-1.736569	-0.688681	-0.000069
6	-2.519621	0.452769	0.000072
6	-3.901786	0.404936	0.000144
6	-4.505674	-0.836626	0.000062
6	-3.725760	-1.994629	-0.000084
1	-1.744584	-2.837569	-0.000258
1	-4.486435	1.319683	0.000256
1	-5.587715	-0.917365	0.000111
1	-4.217439	-2.962865	-0.000148
6	-1.624166	1.618700	0.000106
8	-1.949375	2.812375	0.000256
6	-0.316982	-0.313640	-0.000089
6	0.723782	-1.138641	-0.000187
7	-0.365838	1.137333	0.000078
6	0.779355	2.006219	0.000073
1	1.396859	1.839648	-0.884134
1	0.416454	3.033479	0.000184

6	2.112139	-0.743666	-0.000122
6	2.834844	-0.595541	1.193513
6	2.834929	-0.595396	-1.193686
6	4.179294	-0.276864	1.191226
1	2.317012	-0.730579	2.139056
6	4.179378	-0.276714	-1.191264
1	2.317166	-0.730321	-2.139284
6	4.869980	-0.109578	0.000016
1	4.698478	-0.158813	2.138585
1	4.698629	-0.158545	-2.138572
1	5.926701	0.136506	0.000068
1	1.396991	1.839499	0.884158

Atom	Type	D(alpha)	D(beta)	D(total)
1	6	1.660916	1.660916	1.660916
2	6	1.580776	1.580776	1.580776
3	6	1.570236	1.570236	1.570236
4	6	1.657681	1.657681	1.657681
5	6	1.663081	1.663081	1.663081
6	6	1.663029	1.663029	1.663029
7	1	2.007750	2.007750	2.007750
8	1	1.964990	1.964990	1.964990
9	1	1.961704	1.961704	1.961704
10	1	1.957562	1.957562	1.957562
11	6	1.513686	1.513686	1.513686
12	8	1.344541	1.344541	1.344541
13	6	1.590594	1.590594	1.590594
14	6	1.744420	1.744420	1.744420
15	7	1.405636	1.405636	1.405636
16	6	1.681866	1.681866	1.681866
17	1	1.932305	1.932305	1.932305
18	1	1.923987	1.923987	1.923987
19	6	1.612602	1.612602	1.612602
20	6	1.658659	1.658659	1.658659
21	6	1.658653	1.658653	1.658653
22	6	1.664266	1.664266	1.664266
23	1	1.976118	1.976118	1.976118
24	6	1.664266	1.664266	1.664266
25	1	1.976112	1.976112	1.976112
26	6	1.666583	1.666583	1.666583
27	1	1.964891	1.964891	1.964891
28	1	1.964893	1.964893	1.964893
29	1	1.975573	1.975573	1.975573
30	1	1.932302	1.932302	1.932302

Molecule CH3 B2 file B2mH
Energy: -744.852090272
Geometry:

Atomic No.	x	y	z
6	0.006097	1.644756	0.000184
6	0.800646	0.504705	0.000099
6	2.181453	0.644996	-0.000095
6	2.805939	1.876828	-0.000215
6	2.011407	3.007083	-0.000125
6	0.623650	2.882453	0.000073
1	-1.074647	1.571819	0.000328
1	3.889365	1.945224	-0.000365
1	2.463824	3.993271	-0.000207
1	0.011608	3.779344	0.000140
6	2.784800	-0.697828	-0.000133
8	3.991108	-0.975647	-0.000319
6	0.467813	-0.930649	0.000158
6	-0.675589	-1.606842	0.000263

7	1.763203	-1.568770	-0.000048
6	1.944245	-2.990276	-0.000093
1	1.484555	-3.438083	-0.883659
1	3.014204	-3.194641	-0.000326
6	-1.936408	-0.894857	0.000151
6	-2.594139	-0.565066	1.193398
6	-2.594348	-0.565758	-1.193175
6	-3.809183	0.093791	1.191794
1	-2.126995	-0.827973	2.138432
6	-3.809401	0.093084	-1.191746
1	-2.127366	-0.829207	-2.138138
6	-4.430962	0.435091	-0.000021
1	-4.279933	0.344110	2.138661
1	-4.280317	0.342852	-2.138676
1	-5.386646	0.948878	-0.000086
1	1.484941	-3.438089	0.883673

Atom	Type	D(alpha)	D(beta)	D(total)
1	6	1.656132	1.656132	1.656132
2	6	1.582386	1.582386	1.582386
3	6	1.570499	1.570499	1.570499
4	6	1.656855	1.656855	1.656855
5	6	1.662462	1.662462	1.662462
6	6	1.661904	1.661904	1.661904
7	1	1.954917	1.954917	1.954917
8	1	1.964412	1.964412	1.964412
9	1	1.961074	1.961074	1.961074
10	1	1.956484	1.956484	1.956484
11	6	1.513383	1.513383	1.513383
12	8	1.345487	1.345487	1.345487
13	6	1.587503	1.587503	1.587503
14	6	1.753073	1.753073	1.753073
15	7	1.403065	1.403065	1.403065
16	6	1.690229	1.690229	1.690229
17	1	1.964506	1.964506	1.964506
18	1	1.928719	1.928719	1.928719
19	6	1.611433	1.611433	1.611433
20	6	1.659132	1.659132	1.659132
21	6	1.659136	1.659136	1.659136
22	6	1.664108	1.664108	1.664108
23	1	1.979051	1.979051	1.979051
24	6	1.664109	1.664109	1.664109
25	1	1.979066	1.979066	1.979066
26	6	1.666127	1.666127	1.666127
27	1	1.964946	1.964946	1.964946
28	1	1.964947	1.964947	1.964947
29	1	1.974377	1.974377	1.974377
30	1	1.964543	1.964543	1.964543

Molecule CH3 P1 file P1mH
Energy: -745.384136179
Geometry:

Atomic No.	x	y	z
6	2.326278	-1.927637	-0.000106
6	1.751516	-0.671806	0.000011
6	2.545191	0.458137	0.000056
6	3.921882	0.391599	-0.000034
6	4.501656	-0.864347	-0.000144
6	3.708680	-2.007638	-0.000176
1	1.724425	-2.830229	-0.000154
1	4.522376	1.295269	0.000006
1	5.581870	-0.962617	-0.000202
1	4.184102	-2.983030	-0.000269

6	1.659828	1.636877	0.000245
8	1.977891	2.815821	0.000192
6	0.340368	-0.244134	0.000054
6	-0.711531	-1.054299	0.000008
7	0.378388	1.161672	0.000114
6	-0.758278	2.048607	0.000217
1	-1.373138	1.897330	0.888184
1	-0.372173	3.066653	0.000386
6	-2.150392	-0.703397	-0.000031
6	-2.842518	-0.564592	-1.195806
6	-2.842776	-0.565430	1.195692
6	-4.194625	-0.269385	-1.196833
1	-2.311871	-0.680744	-2.135859
6	-4.194883	-0.270223	1.196634
1	-2.312333	-0.682238	2.135779
6	-4.874185	-0.118892	-0.000120
1	-4.720006	-0.155752	-2.139656
1	-4.720466	-0.157246	2.139423
1	-5.934159	0.113538	-0.000153
1	-1.373103	1.897614	-0.887820
1	-0.484627	-2.117461	-0.000010

Molecule CH3 P2 file P2mH
Energy: -745.386649398
Geometry:

Atomic No.	x	y	z
6	0.057513	1.677358	-0.000032
6	0.839390	0.537064	-0.000045
6	2.220213	0.646152	0.000036
6	2.866166	1.861807	0.000189
6	2.084381	3.004179	0.000215
6	0.698586	2.906500	0.000095
1	-1.024078	1.624797	-0.000098
1	3.949932	1.913831	0.000242
1	2.553172	3.982353	0.000314
1	0.102378	3.813139	0.000112
6	2.796217	-0.713009	-0.000165
8	3.975409	-1.031976	0.000079
6	0.503765	-0.899657	-0.000148
6	-0.672313	-1.514563	-0.000223
7	1.739801	-1.571768	-0.000149
6	1.880702	-3.001434	-0.000094
1	1.421036	-3.437478	-0.890399
1	2.944761	-3.231507	-0.000113
6	-1.981158	-0.823180	-0.000093
6	-2.610906	-0.504589	1.195905
6	-2.611782	-0.505827	-1.195959
6	-3.837737	0.136125	1.197073
1	-2.127429	-0.753505	2.135588
6	-3.838610	0.134894	-1.196888
1	-2.128997	-0.755712	-2.135740
6	-4.453752	0.459679	0.000150
1	-4.314302	0.385231	2.139761
1	-4.315861	0.383036	-2.139483
1	-5.414822	0.963560	0.000242
1	1.421074	-3.437420	0.890260
1	-0.692792	-2.601134	-0.000387

Molecule CH2tBu B1 file B1mtBu
Energy: -901.614168095
Geometry:

Atomic No.	x	y	z
6	-2.734205	-2.150264	0.731193
6	-2.052128	-1.056993	0.216153
6	-2.765648	-0.010332	-0.339087

6	-4.147324	-0.006064	-0.408075
6	-4.823658	-1.092059	0.110050
6	-4.114014	-2.153161	0.676366
1	-2.187376	-2.979932	1.166104
1	-4.675802	0.830032	-0.855638
1	-5.907781	-1.125686	0.079759
1	-4.661967	-2.998991	1.080830
6	-1.804204	1.002111	-0.797269
8	-2.060611	2.055585	-1.389149
6	-0.611503	-0.791867	0.100697
6	0.351220	-1.670621	0.350878
7	-0.575245	0.557582	-0.456331
6	0.611990	1.346431	-0.686314
1	1.442606	0.656533	-0.821578
1	0.473204	1.890274	-1.625787
6	1.760196	-1.570847	0.073574
6	2.715033	-1.450920	1.096021
6	2.261292	-1.725962	-1.231023
6	4.069852	-1.433327	0.826573
1	2.373077	-1.376272	2.124139
6	3.617326	-1.722730	-1.493857
1	1.557082	-1.847269	-2.049513
6	4.541565	-1.567835	-0.470939
1	4.772332	-1.324010	1.648532
1	3.959091	-1.838984	-2.518879
1	5.606363	-1.564129	-0.678970
6	0.976818	2.352675	0.416516
6	0.000414	3.520253	0.453846
6	0.998185	1.681224	1.781117
6	2.368019	2.878984	0.086248
1	-0.038240	4.035295	-0.509739
1	-1.012228	3.188960	0.690361
1	0.311151	4.241002	1.216553
1	1.714149	0.858053	1.807075
1	1.280699	2.405395	2.551240
1	0.014123	1.280540	2.037372
1	2.679649	3.629486	0.818220
1	3.107369	2.072300	0.094237
1	2.388747	3.347478	-0.902799

Molecule CH2tBu B2 file B2mtBu-b
Energy: -901.619392966
Geometry:

Atomic No.	x	y	z
6	-1.743067	1.775231	0.342603
6	-0.482121	1.292145	0.010198
6	0.572464	2.185860	-0.101033
6	0.424769	3.544772	0.099762
6	-0.829012	4.019028	0.432118
6	-1.898739	3.133223	0.550855
1	-2.589471	1.106391	0.438691
1	1.275527	4.211480	-0.001921
1	-0.985868	5.079209	0.601586
1	-2.879056	3.519443	0.813355
6	1.782002	1.432641	-0.466224
8	2.898290	1.900481	-0.720637
6	0.005722	-0.063627	-0.290951
6	-0.608938	-1.228481	-0.451720
7	1.432918	0.133975	-0.491064
6	2.338693	-0.911536	-0.892363
1	1.724580	-1.684448	-1.359038
1	3.015476	-0.493995	-1.644469
6	-2.037225	-1.334092	-0.258936
6	-2.590168	-1.646528	0.992076
6	-2.936320	-1.204298	-1.327769

6	-3.954613	-1.775978	1.169077
1	-1.923892	-1.778836	1.840090
6	-4.300347	-1.331932	-1.146615
1	-2.544193	-0.988576	-2.317841
6	-4.828807	-1.615738	0.104119
1	-4.342988	-2.006148	2.157597
1	-4.963447	-1.209365	-1.998820
1	-5.899676	-1.720212	0.244031
6	3.177553	-1.548278	0.223215
6	4.106666	-0.528243	0.865709
6	2.288057	-2.155720	1.297489
6	4.011862	-2.646833	-0.423076
1	4.769841	-0.073716	0.125867
1	3.543157	0.277734	1.340709
1	4.721019	-1.011988	1.631393
1	1.637951	-2.929482	0.883687
1	2.902683	-2.602257	2.085359
1	1.646883	-1.396001	1.750730
1	4.639133	-3.143059	0.322969
1	3.374814	-3.406981	-0.885417
1	4.670200	-2.240556	-1.197236

Molecule CH2tBu P1 file P1mtBu-b
Energy: -902.152132094
Geometry:

Atomic No.	x	y	z
6	-2.595402	-2.214329	0.685660
6	-1.990679	-1.087654	0.160829
6	-2.758038	-0.080618	-0.387921
6	-4.134609	-0.144103	-0.439143
6	-4.743377	-1.265312	0.093641
6	-3.977224	-2.285242	0.650635
1	-2.017438	-3.024284	1.117786
1	-4.711825	0.661526	-0.880852
1	-5.824259	-1.354616	0.079246
1	-4.474446	-3.156170	1.065020
6	-1.848859	0.980925	-0.849809
8	-2.141560	2.029017	-1.400214
6	-0.568804	-0.724330	0.004949
6	0.432298	-1.561027	0.271342
7	-0.574586	0.579558	-0.534216
6	0.535063	1.504429	-0.669938
1	1.432331	0.945193	-0.923443
1	0.293749	2.145441	-1.520917
6	1.874316	-1.477835	-0.011073
6	2.790023	-1.764251	0.996196
6	2.352993	-1.214053	-1.288912
6	4.148667	-1.745842	0.743370
1	2.428233	-1.994952	1.993914
6	3.712985	-1.199819	-1.545642
1	1.649548	-1.031782	-2.095658
6	4.615407	-1.458737	-0.529220
1	4.848579	-1.960456	1.544492
1	4.067891	-0.990956	-2.549719
1	5.681714	-1.447636	-0.729918
6	0.821404	2.387686	0.551746
6	-0.373623	3.265832	0.894701
6	1.189696	1.547580	1.766346
6	2.003357	3.271849	0.173852
1	-0.674579	3.881467	0.043989
1	-1.237442	2.668718	1.197899
1	-0.120617	3.927144	1.728283
1	2.058357	0.915340	1.566587
1	1.432872	2.198609	2.610822
1	0.363179	0.901310	2.072074

1	2.267256	3.931846	1.004455
1	2.885019	2.671902	-0.071165
1	1.768651	3.899043	-0.691330
1	0.124241	-2.486614	0.750007

Molecule CH2tBu P2 file P2mtBu
Energy: -902.155652856
Geometry:

Atomic No.	x	y	z
6	-1.639081	1.917294	0.447241
6	-0.418060	1.403058	0.047169
6	0.670302	2.247642	-0.081757
6	0.591297	3.603955	0.145318
6	-0.633011	4.119739	0.529760
6	-1.729311	3.279214	0.683463
1	-2.507709	1.284970	0.576916
1	1.465973	4.235855	0.031890
1	-0.739606	5.182110	0.720993
1	-2.679685	3.698288	0.997587
6	1.843127	1.440286	-0.458384
8	2.968156	1.832561	-0.723925
6	0.037128	0.031188	-0.255899
6	-0.646914	-1.105075	-0.333250
7	1.432269	0.137801	-0.468160
6	2.308160	-0.925129	-0.912790
1	1.718775	-1.632356	-1.501860
1	3.032459	-0.463480	-1.588652
6	-2.110917	-1.252197	-0.219424
6	-2.651381	-2.058372	0.775487
6	-2.969431	-0.648695	-1.129726
6	-4.020054	-2.232208	0.877245
1	-1.988910	-2.548594	1.482759
6	-4.338323	-0.823829	-1.031861
1	-2.556587	-0.033504	-1.923241
6	-4.868288	-1.612960	-0.025340
1	-4.426419	-2.857435	1.665755
1	-4.994923	-0.342862	-1.749780
1	-5.941864	-1.750745	0.051920
6	3.074159	-1.669089	0.187292
6	3.938775	-0.700513	0.981620
6	2.129841	-2.391331	1.138064
6	3.964594	-2.689438	-0.509762
1	4.633044	-0.163501	0.331281
1	3.328445	0.040815	1.503654
1	4.518517	-1.245556	1.731752
1	1.535181	-3.147113	0.616930
1	2.703481	-2.902229	1.916242
1	1.445856	-1.695480	1.630173
1	4.536781	-3.261701	0.225259
1	3.372626	-3.397074	-1.098087
1	4.675981	-2.200820	-1.182015
1	-0.098209	-2.025926	-0.497760

Molecule CHF2 B1 file B1mF2
Energy: -943.068880926
Geometry:

Atomic No.	x	y	z
6	2.465799	-2.183563	0.000072
6	1.836242	-0.946074	-0.000005
6	2.602389	0.205305	-0.000055
6	3.987197	0.179776	-0.000033
6	4.608502	-1.050226	0.000039
6	3.844424	-2.220785	0.000090
1	1.876370	-3.093651	0.000115
1	4.556393	1.103963	-0.000074

1	5.691369	-1.115350	0.000056
1	4.351051	-3.181145	0.000146
6	1.706140	1.363042	-0.000140
8	2.003485	2.549880	-0.000199
6	0.407589	-0.620604	-0.000024
6	-0.604183	-1.473040	0.000093
7	0.430731	0.855026	-0.000136
6	-0.694958	1.677227	-0.000359
1	-1.614487	1.100168	-0.000430
6	-2.008708	-1.146647	0.000190
6	-2.733884	-1.023503	-1.194914
6	-2.733600	-1.023009	1.195416
6	-4.090106	-0.758215	-1.191145
1	-2.210593	-1.136197	-2.140107
6	-4.089825	-0.757732	1.191860
1	-2.210083	-1.135305	2.140532
6	-4.785741	-0.619546	0.000412
1	-4.613684	-0.659521	-2.138025
1	-4.613180	-0.658651	2.138823
1	-5.851041	-0.414565	0.000496
9	-0.705899	2.510542	-1.085564
9	-0.706187	2.510746	1.084679

Molecule CHF2 B2 file B2mF2
Energy: -943.074692702
Geometry:

Atomic No.	x	y	z
6	0.787605	1.900551	-0.000331
6	-0.268283	0.994971	-0.000257
6	-1.569559	1.477266	-0.000267
6	-1.865816	2.828331	-0.000308
6	-0.814704	3.720825	-0.000387
6	0.498993	3.250986	-0.000403
1	1.814994	1.557743	-0.000317
1	-2.897428	3.165753	-0.000315
1	-1.004384	4.788917	-0.000442
1	1.315656	3.966372	-0.000461
6	-2.500744	0.343142	-0.000286
8	-3.725930	0.367234	-0.000032
6	-0.282748	-0.473363	-0.000118
6	0.643219	-1.418921	0.000000
7	-1.716854	-0.772408	0.000064
6	-2.188698	-2.079103	0.000338
1	-1.341451	-2.764750	0.000548
6	2.046213	-1.055516	0.000082
6	2.762571	-0.902840	-1.193428
6	2.762329	-0.902380	1.193683
6	4.104918	-0.572478	-1.191812
1	2.243559	-1.039160	-2.137994
6	4.104679	-0.572037	1.192216
1	2.243119	-1.038321	2.138194
6	4.791488	-0.398755	0.000238
1	4.623872	-0.449526	-2.138424
1	4.623443	-0.448730	2.138886
1	5.845809	-0.142421	0.000296
9	-2.983842	-2.331971	-1.084293
9	-2.983997	-2.331470	1.084968

Molecule CHF2 P1 file P1mF2
Energy: -943.598241617
Geometry:

Atomic No.	x	y	z
6	2.385560	-2.212557	0.083616
6	1.810668	-0.955574	0.037145
6	2.601513	0.162835	-0.140562

6	3.973399	0.085714	-0.272856
6	4.550378	-1.167453	-0.216552
6	3.759998	-2.300646	-0.038215
1	1.788080	-3.108076	0.215030
1	4.568587	0.981676	-0.413882
1	5.625282	-1.274689	-0.312149
1	4.234287	-3.275560	0.004271
6	1.740145	1.350929	-0.141156
8	2.047145	2.517605	-0.236981
6	0.402002	-0.539584	0.097148
6	-0.645048	-1.356235	0.129836
7	0.437499	0.879756	0.023502
6	-0.592789	1.736296	0.455040
1	-1.476738	1.182406	0.759106
6	-2.077566	-1.053949	-0.018987
6	-2.541599	-0.239912	-1.046856
6	-2.999886	-1.645174	0.837229
6	-3.895329	0.000118	-1.196676
1	-1.835450	0.202573	-1.743153
6	-4.352739	-1.401513	0.690252
1	-2.649348	-2.298481	1.630571
6	-4.804224	-0.575581	-0.325678
1	-4.241725	0.637201	-2.003822
1	-5.059989	-1.862793	1.371738
1	-5.866210	-0.387056	-0.443439
9	-0.935187	2.613875	-0.523610
1	-0.401945	-2.407582	0.254398
9	-0.177190	2.495564	1.503200

Molecule CHF2 P2 file P2mF2-b
Energy: -943.603424561
Geometry:

Atomic No.	x	y	z
6	0.290781	2.102635	-0.162394
6	-0.597428	1.045531	-0.059992
6	-1.959342	1.301357	-0.033958
6	-2.481458	2.576408	-0.084534
6	-1.591935	3.629447	-0.171749
6	-0.223389	3.386541	-0.215529
1	1.360198	1.943792	-0.201693
1	-3.554355	2.735323	-0.062332
1	-1.958600	4.649188	-0.213691
1	0.461240	4.224534	-0.294971
6	-2.683586	0.027236	0.020713
8	-3.878394	-0.179772	0.064309
6	-0.392437	-0.414026	-0.019009
6	0.705461	-1.158497	-0.038984
7	-1.708828	-0.954710	0.008276
6	-2.052776	-2.306964	0.080373
1	-3.136166	-2.417097	0.112514
6	2.093018	-0.660386	0.008431
6	2.974344	-0.971415	-1.020002
6	2.559745	0.065470	1.096631
6	4.286942	-0.537620	-0.976336
1	2.623766	-1.554047	-1.866613
6	3.874127	0.494787	1.144262
1	1.884319	0.293475	1.915441
6	4.739888	0.198776	0.105538
1	4.961363	-0.779387	-1.791374
1	4.224025	1.062090	2.000636
1	5.770586	0.536068	0.142119
9	-1.500367	-2.895258	1.176909
1	0.592195	-2.236890	-0.091144
9	-1.554226	-2.994918	-0.983804

Molecule CH2F B1 file B1mF-b
Energy: -843.958667266
Geometry:

Atomic No.	x	y	z
6	2.444476	-2.008311	-0.233340
6	1.812265	-0.785199	-0.052391
6	2.578175	0.355003	0.120957
6	3.962830	0.330646	0.118813
6	4.585942	-0.885319	-0.063371
6	3.823427	-2.043586	-0.237958
1	1.858106	-2.910576	-0.367886
1	4.531638	1.244813	0.256693
1	5.668927	-0.948592	-0.072066
1	4.331382	-2.992681	-0.380334
6	1.673085	1.494603	0.284493
8	1.960303	2.678339	0.443356
6	0.384611	-0.454589	0.001693
6	-0.635604	-1.293382	-0.112507
7	0.405103	0.990941	0.227280
6	-0.702746	1.847009	0.278221
1	-1.572909	1.346221	0.692123
1	-0.440468	2.749853	0.828060
6	-2.032310	-0.937570	-0.025178
6	-2.784508	-0.611201	-1.162935
6	-2.726209	-0.999250	1.193169
6	-4.134249	-0.327846	-1.079022
1	-2.287070	-0.574668	-2.127762
6	-4.076095	-0.714099	1.271694
1	-2.182466	-1.274755	2.092525
6	-4.797977	-0.372212	0.137987
1	-4.678919	-0.068088	-1.982681
1	-4.573769	-0.762507	2.236390
1	-5.858645	-0.152664	0.200269
9	-1.062737	2.268018	-1.017231

Molecule CH2F B2 file B2mF
Energy: -843.962726464
Geometry:

Atomic No.	x	y	z
6	0.328394	1.826983	-0.099324
6	-0.591947	0.791402	0.025290
6	-1.946905	1.094753	0.042294
6	-2.425453	2.387978	-0.061043
6	-1.507171	3.409866	-0.185239
6	-0.142508	3.121478	-0.203078
1	1.392782	1.627156	-0.115282
1	-3.493224	2.582565	-0.044121
1	-1.841375	4.438521	-0.269384
1	0.568234	3.936346	-0.301489
6	-2.705583	-0.153588	0.180731
8	-3.925315	-0.302096	0.229150
6	-0.412372	-0.662052	0.155025
6	0.639711	-1.467074	0.198944
7	-1.781759	-1.145842	0.251912
6	-2.129938	-2.492098	0.383866
1	-1.325186	-3.030674	0.879859
1	-3.090250	-2.586924	0.888522
6	1.975524	-0.914159	0.107345
6	2.625182	-0.766709	-1.125202
6	2.703774	-0.563249	1.251728
6	3.907473	-0.257493	-1.209662
1	2.099678	-1.052830	-2.031992
6	3.986001	-0.054420	1.164160
1	2.240667	-0.687997	2.226564
6	4.602546	0.109272	-0.067134

1	4.372545	-0.145942	-2.185322
1	4.513356	0.218705	2.074086
1	5.610255	0.505857	-0.134382
9	-2.290335	-3.092495	-0.881760

Molecule CH2F P1 file P1mF-b
Energy: -844.491098086
Geometry:

Atomic No.	x	y	z
6	-2.384454	-2.027320	0.256188
6	-1.816432	-0.783677	0.051521
6	-2.619817	0.331797	-0.084974
6	-3.996803	0.263298	-0.028105
6	-4.566555	-0.979075	0.172483
6	-3.764177	-2.108647	0.311959
1	-1.777804	-2.919037	0.371284
1	-4.602418	1.156688	-0.137953
1	-5.645220	-1.079480	0.223347
1	-4.232395	-3.074716	0.469449
6	-1.752985	1.498046	-0.293203
8	-2.060206	2.658901	-0.477672
6	-0.406258	-0.370608	-0.044230
6	0.638346	-1.184354	0.050719
7	-0.452379	1.027498	-0.263551
6	0.619719	1.898432	-0.544213
1	1.448742	1.366991	-1.004723
1	0.259313	2.713603	-1.169725
6	2.081694	-0.876901	0.043201
6	2.655915	-0.072586	1.018744
6	2.902293	-1.458947	-0.916910
6	4.018837	0.167656	1.017839
1	2.028525	0.371985	1.783572
6	4.263216	-1.215779	-0.920653
1	2.464516	-2.104039	-1.672808
6	4.825394	-0.398791	0.046652
1	4.452779	0.800528	1.785239
1	4.889560	-1.669504	-1.681866
1	5.893875	-0.209501	0.046496
9	1.099072	2.480583	0.631497
1	0.389590	-2.237725	0.148332

Molecule CH2F P2 file P2mF
Energy: -844.492541894
Geometry:

Atomic No.	x	y	z
6	0.031896	1.954294	-0.225035
6	-0.751422	0.831970	-0.017878
6	-2.132002	0.957985	-0.001974
6	-2.772197	2.167668	-0.163479
6	-1.986887	3.288761	-0.354032
6	-0.601857	3.174338	-0.388660
1	1.111687	1.894797	-0.260287
1	-3.855420	2.225909	-0.146607
1	-2.449290	4.261084	-0.484495
1	-0.000083	4.062798	-0.549426
6	-2.728623	-0.373328	0.175470
8	-3.901847	-0.683338	0.245993
6	-0.418367	-0.595959	0.142820
6	0.736094	-1.252472	0.123997
7	-1.670451	-1.249767	0.260316
6	-1.848558	-2.626064	0.479838
1	-1.126277	-3.012170	1.199420
1	-2.873830	-2.800903	0.801963
6	2.085563	-0.661583	0.097188
6	2.984598	-1.043536	-0.892140

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6       2.508277        0.224960        1.079571
6       4.266111        -0.524622       -0.918165
1       2.671310        -1.751536       -1.653616
6       3.791651        0.741449        1.057629
1       1.823622        0.507661        1.873220
6       4.672657        0.372057        0.055929
1       4.953124        -0.825371       -1.702504
1       4.106129        1.433582        1.832065
1       5.679418        0.776512        0.038713
9       -1.650649       -3.337115       -0.707308
1       0.701778        -2.338774       0.120691

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    Au Clusters
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Summary table of QAu and DAu from PW91/LANL2DZ calculations on all cationic Au cluster
s

# Filename TotalCharge AtomIndex   QAu   DAu  KEAu
    Au10p-a.log   1    1    0.1197  1.0831  0.4389
    Au10p-a.log   1    2    0.0716  1.0936  0.4410
    Au10p-a.log   1    3    0.1055  1.0806  0.4391
    Au10p-a.log   1    4    0.1052  1.0807  0.4391
    Au10p-a.log   1    5    0.0839  1.1092  0.4425
    Au10p-a.log   1    6    0.0715  1.0935  0.4410
    Au10p-a.log   1    7    0.1199  1.0830  0.4389
    Au10p-a.log   1    8    0.0951  1.0801  0.4396
    Au10p-a.log   1    9    0.1323  1.0682  0.4376
    Au10p-a.log   1   10    0.0953  1.0800  0.4396
    Au10p-b.log   1    1    0.0652  1.0915  0.4411
    Au10p-b.log   1    2    0.1238  1.0745  0.4380
    Au10p-b.log   1    3    0.0652  1.0915  0.4411
    Au10p-b.log   1    4    0.0941  1.1004  0.4409
    Au10p-b.log   1    5    0.0941  1.1004  0.4409
    Au10p-b.log   1    6    0.0931  1.0827  0.4394
    Au10p-b.log   1    7    0.1237  1.0745  0.4380
    Au10p-b.log   1    8    0.1239  1.0745  0.4380
    Au10p-b.log   1    9    0.1237  1.0745  0.4380
    Au10p-b.log   1   10    0.0931  1.0827  0.4394
    Au10p-c.log   1    1    0.0676  1.0936  0.4414
    Au10p-c.log   1    2    0.0736  1.0888  0.4405
    Au10p-c.log   1    3    0.0896  1.0883  0.4401
    Au10p-c.log   1    4    0.0726  1.1009  0.4413
    Au10p-c.log   1    5    0.0758  1.0961  0.4408
    Au10p-c.log   1    6    0.0990  1.0869  0.4395
    Au10p-c.log   1    7    0.1063  1.0826  0.4396
    Au10p-c.log   1    8    0.1404  1.0732  0.4377
    Au10p-c.log   1    9    0.1385  1.0710  0.4376
    Au10p-c.log   1   10    0.1365  1.0707  0.4375
    Au10p-d.log   1    1    0.0894  1.0861  0.4392
    Au10p-d.log   1    2    0.0860  1.0851  0.4395
    Au10p-d.log   1    3    0.0890  1.0861  0.4392
    Au10p-d.log   1    4    0.0840  1.0859  0.4396
    Au10p-d.log   1    5    0.1429  1.0753  0.4379
    Au10p-d.log   1    6    0.0812  1.0879  0.4397
    Au10p-d.log   1    7    0.0723  1.0914  0.4400
    Au10p-d.log   1    8    0.1310  1.0784  0.4387
    Au10p-d.log   1    9    0.1433  1.0752  0.4379
    Au10p-d.log   1   10    0.0810  1.0880  0.4397
    Au11p-a.log   1    1    0.0606  1.0954  0.4416
    Au11p-a.log   1    2    0.0767  1.0870  0.4402
    Au11p-a.log   1    3    0.0514  1.1045  0.4425
    Au11p-a.log   1    4    0.0806  1.0975  0.4409
    Au11p-a.log   1    5    0.0839  1.1025  0.4415
    Au11p-a.log   1    6    0.0958  1.0768  0.4388
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Au11p-a.log	1	7	0.1035	1.0791	0.4390
Au11p-a.log	1	8	0.0655	1.0972	0.4414
Au11p-a.log	1	9	0.1473	1.0653	0.4367
Au11p-a.log	1	10	0.0850	1.0887	0.4404
Au11p-a.log	1	11	0.1495	1.0674	0.4371
Au11p-b.log	1	1	0.0700	1.0910	0.4411
Au11p-b.log	1	2	0.1012	1.0757	0.4390
Au11p-b.log	1	3	0.0703	1.1027	0.4419
Au11p-b.log	1	4	0.0575	1.1054	0.4426
Au11p-b.log	1	5	0.0702	1.1028	0.4419
Au11p-b.log	1	6	0.1461	1.0734	0.4376
Au11p-b.log	1	7	0.0699	1.0910	0.4411
Au11p-b.log	1	8	0.1179	1.0785	0.4385
Au11p-b.log	1	9	0.1179	1.0784	0.4385
Au11p-b.log	1	10	0.1010	1.0757	0.4390
Au11p-b.log	1	11	0.0780	1.0858	0.4405
Au11p-c.log	1	1	0.0759	1.0901	0.4408
Au11p-c.log	1	2	0.0759	1.0901	0.4408
Au11p-c.log	1	3	0.0758	1.0901	0.4408
Au11p-c.log	1	4	0.0658	1.1044	0.4418
Au11p-c.log	1	5	0.0315	1.0970	0.4418
Au11p-c.log	1	6	0.0659	1.1044	0.4418
Au11p-c.log	1	7	0.0760	1.0901	0.4408
Au11p-c.log	1	8	0.1333	1.0712	0.4376
Au11p-c.log	1	9	0.1332	1.0712	0.4376
Au11p-c.log	1	10	0.1333	1.0712	0.4376
Au11p-c.log	1	11	0.1333	1.0712	0.4376
Au12p-a.log	1	1	0.0611	1.0918	0.4402
Au12p-a.log	1	2	0.0711	1.0941	0.4404
Au12p-a.log	1	3	0.1025	1.0831	0.4395
Au12p-a.log	1	4	0.0719	1.0947	0.4405
Au12p-a.log	1	5	0.0849	1.0886	0.4405
Au12p-a.log	1	6	0.1017	1.0834	0.4395
Au12p-a.log	1	7	0.0724	1.0938	0.4404
Au12p-a.log	1	8	0.0726	1.0947	0.4405
Au12p-a.log	1	9	0.0632	1.0916	0.4402
Au12p-a.log	1	10	0.0837	1.0891	0.4406
Au12p-a.log	1	11	0.1079	1.0818	0.4392
Au12p-a.log	1	12	0.1068	1.0820	0.4392
Au12p-b.log	1	1	0.0857	1.0873	0.4407
Au12p-b.log	1	2	0.0857	1.0873	0.4407
Au12p-b.log	1	3	0.0555	1.0994	0.4417
Au12p-b.log	1	4	0.0735	1.0882	0.4402
Au12p-b.log	1	5	0.0735	1.0882	0.4402
Au12p-b.log	1	6	0.0555	1.0994	0.4417
Au12p-b.log	1	7	0.0735	1.0882	0.4402
Au12p-b.log	1	8	0.0735	1.0882	0.4402
Au12p-b.log	1	9	0.0728	1.0892	0.4408
Au12p-b.log	1	10	0.1409	1.0751	0.4382
Au12p-b.log	1	11	0.1409	1.0751	0.4382
Au12p-b.log	1	12	0.0686	1.0882	0.4400
Au12p-c.log	1	1	0.0902	1.0823	0.4391
Au12p-c.log	1	2	0.0851	1.0872	0.4406
Au12p-c.log	1	3	0.0851	1.0872	0.4406
Au12p-c.log	1	4	0.0743	1.0904	0.4404
Au12p-c.log	1	5	0.0743	1.0904	0.4404
Au12p-c.log	1	6	0.0721	1.0901	0.4402
Au12p-c.log	1	7	0.0721	1.0901	0.4402
Au12p-c.log	1	8	0.1220	1.0785	0.4392
Au12p-c.log	1	9	0.0653	1.0927	0.4404
Au12p-c.log	1	10	0.0653	1.0927	0.4404
Au12p-c.log	1	11	0.0551	1.0927	0.4412
Au12p-c.log	1	12	0.1387	1.0737	0.4381
Au12p-d.log	1	1	0.0619	1.0922	0.4407
Au12p-d.log	1	2	0.1558	1.0697	0.4374

Au12p-d.log	1	3	0.0600	1.0968	0.4407
Au12p-d.log	1	4	0.0986	1.0845	0.4392
Au12p-d.log	1	5	0.0859	1.0841	0.4393
Au12p-d.log	1	6	0.0625	1.0939	0.4410
Au12p-d.log	1	7	0.0604	1.0924	0.4413
Au12p-d.log	1	8	0.1030	1.0839	0.4400
Au12p-d.log	1	9	0.0859	1.0841	0.4393
Au12p-d.log	1	10	0.0625	1.0939	0.4410
Au12p-d.log	1	11	0.0604	1.0924	0.4413
Au12p-d.log	1	12	0.1030	1.0839	0.4400
Au12p-e.log	1	1	0.0714	1.0936	0.4405
Au12p-e.log	1	2	0.0714	1.0936	0.4405
Au12p-e.log	1	3	0.0714	1.0936	0.4405
Au12p-e.log	1	4	0.0714	1.0936	0.4405
Au12p-e.log	1	5	0.0730	1.0898	0.4405
Au12p-e.log	1	6	0.0730	1.0898	0.4405
Au12p-e.log	1	7	0.1055	1.0805	0.4396
Au12p-e.log	1	8	0.1055	1.0805	0.4396
Au12p-e.log	1	9	0.0730	1.0898	0.4405
Au12p-e.log	1	10	0.0730	1.0898	0.4405
Au12p-e.log	1	11	0.1055	1.0805	0.4396
Au12p-e.log	1	12	0.1055	1.0805	0.4396
Au12p-f.log	1	1	0.0742	1.0885	0.4398
Au12p-f.log	1	2	0.0742	1.0885	0.4398
Au12p-f.log	1	3	0.0742	1.0885	0.4398
Au12p-f.log	1	4	0.0742	1.0885	0.4398
Au12p-f.log	1	5	0.0733	1.0961	0.4408
Au12p-f.log	1	6	0.0779	1.0888	0.4401
Au12p-f.log	1	7	0.1215	1.0803	0.4387
Au12p-f.log	1	8	0.1062	1.0830	0.4399
Au12p-f.log	1	9	0.1215	1.0803	0.4387
Au12p-f.log	1	10	0.1062	1.0830	0.4399
Au12p-f.log	1	11	0.0484	1.0953	0.4416
Au12p-f.log	1	12	0.0484	1.0953	0.4416
Au12p-h.log	1	1	0.0940	1.0779	0.4389
Au12p-h.log	1	2	0.0980	1.0747	0.4383
Au12p-h.log	1	3	0.0976	1.0786	0.4390
Au12p-h.log	1	4	0.0194	1.1018	0.4429
Au12p-h.log	1	5	0.0999	1.0748	0.4383
Au12p-h.log	1	6	0.0877	1.0970	0.4408
Au12p-h.log	1	7	0.0207	1.0998	0.4427
Au12p-h.log	1	8	0.0989	1.0772	0.4388
Au12p-h.log	1	9	0.0894	1.0968	0.4408
Au12p-h.log	1	10	0.1003	1.0751	0.4384
Au12p-h.log	1	11	0.0972	1.0783	0.4390
Au12p-h.log	1	12	0.0969	1.0765	0.4386
Au13p-a.log	1	1	0.0808	1.0860	0.4397
Au13p-a.log	1	2	0.0833	1.0868	0.4406
Au13p-a.log	1	3	0.0833	1.0868	0.4406
Au13p-a.log	1	4	0.0786	1.0892	0.4400
Au13p-a.log	1	5	0.0786	1.0892	0.4400
Au13p-a.log	1	6	0.0654	1.0919	0.4404
Au13p-a.log	1	7	0.0654	1.0919	0.4404
Au13p-a.log	1	8	0.0539	1.0918	0.4414
Au13p-a.log	1	9	0.1130	1.0797	0.4394
Au13p-a.log	1	10	0.0654	1.0919	0.4404
Au13p-a.log	1	11	0.0654	1.0919	0.4404
Au13p-a.log	1	12	0.0539	1.0918	0.4414
Au13p-a.log	1	13	0.1130	1.0797	0.4394
Au13p-b.log	1	1	0.1042	1.0817	0.4397
Au13p-b.log	1	2	0.0790	1.0871	0.4397
Au13p-b.log	1	3	0.0643	1.0915	0.4404
Au13p-b.log	1	4	0.1042	1.0817	0.4397
Au13p-b.log	1	5	0.1232	1.0770	0.4390
Au13p-b.log	1	6	0.0790	1.0871	0.4397

Au13p-b.log	1	7	0.0849	1.0878	0.4397
Au13p-b.log	1	8	0.0647	1.0907	0.4412
Au13p-b.log	1	9	0.0574	1.0953	0.4408
Au13p-b.log	1	10	0.0647	1.0907	0.4412
Au13p-b.log	1	11	0.0627	1.0940	0.4407
Au13p-b.log	1	12	0.0491	1.0924	0.4415
Au13p-b.log	1	13	0.0627	1.0940	0.4407
Au13p-c.log	1	1	0.1572	1.0672	0.4372
Au13p-c.log	1	2	0.1572	1.0672	0.4372
Au13p-c.log	1	3	0.0630	1.0937	0.4408
Au13p-c.log	1	4	0.0630	1.0937	0.4408
Au13p-c.log	1	5	0.0582	1.0964	0.4413
Au13p-c.log	1	6	0.0630	1.0937	0.4408
Au13p-c.log	1	7	0.0582	1.0964	0.4413
Au13p-c.log	1	8	0.0630	1.0937	0.4408
Au13p-c.log	1	9	0.0363	1.1008	0.4424
Au13p-c.log	1	10	0.0709	1.0898	0.4413
Au13p-c.log	1	11	0.1024	1.0811	0.4394
Au13p-c.log	1	12	0.0709	1.0898	0.4413
Au13p-c.log	1	13	0.0363	1.1008	0.4424
Au13p-d.log	1	1	0.0451	1.1006	0.4421
Au13p-d.log	1	2	0.0338	1.1028	0.4424
Au13p-d.log	1	3	0.0451	1.1006	0.4421
Au13p-d.log	1	4	0.1493	1.0677	0.4374
Au13p-d.log	1	5	0.1493	1.0677	0.4374
Au13p-d.log	1	6	0.0451	1.1006	0.4421
Au13p-d.log	1	7	0.0451	1.1006	0.4421
Au13p-d.log	1	8	0.0338	1.1028	0.4424
Au13p-d.log	1	9	0.0603	1.0945	0.4412
Au13p-d.log	1	10	0.0983	1.0807	0.4394
Au13p-d.log	1	11	0.0983	1.0807	0.4394
Au13p-d.log	1	12	0.0983	1.0807	0.4394
Au13p-d.log	1	13	0.0983	1.0807	0.4394
Au13p-e.log	1	1	0.0976	1.0843	0.4402
Au13p-e.log	1	2	0.0976	1.0843	0.4402
Au13p-e.log	1	3	0.0728	1.0923	0.4400
Au13p-e.log	1	4	0.0699	1.0898	0.4403
Au13p-e.log	1	5	0.0603	1.0915	0.4410
Au13p-e.log	1	6	0.0728	1.0923	0.4400
Au13p-e.log	1	7	0.0603	1.0915	0.4410
Au13p-e.log	1	8	0.0699	1.0898	0.4403
Au13p-e.log	1	9	0.0917	1.0839	0.4400
Au13p-e.log	1	10	0.1187	1.0800	0.4394
Au13p-e.log	1	11	0.0516	1.0940	0.4419
Au13p-e.log	1	12	0.0602	1.0913	0.4407
Au13p-e.log	1	13	0.0768	1.0853	0.4397
Au13p-f.log	1	1	0.0855	1.0843	0.4394
Au13p-f.log	1	2	0.0597	1.0940	0.4410
Au13p-f.log	1	3	0.0847	1.0912	0.4397
Au13p-f.log	1	4	0.0808	1.0900	0.4398
Au13p-f.log	1	5	0.0852	1.0856	0.4400
Au13p-f.log	1	6	0.0884	1.0850	0.4401
Au13p-f.log	1	7	0.0718	1.0891	0.4404
Au13p-f.log	1	8	0.0884	1.0850	0.4401
Au13p-f.log	1	9	0.0852	1.0856	0.4400
Au13p-f.log	1	10	0.0718	1.0891	0.4404
Au13p-f.log	1	11	0.0599	1.0935	0.4405
Au13p-f.log	1	12	0.0599	1.0935	0.4405
Au13p-f.log	1	13	0.0786	1.0871	0.4403
Au13p-g.log	1	1	0.0606	1.0944	0.4419
Au13p-g.log	1	2	0.0606	1.0944	0.4419
Au13p-g.log	1	3	0.0575	1.0938	0.4411
Au13p-g.log	1	4	0.0672	1.0933	0.4405
Au13p-g.log	1	5	0.0672	1.0933	0.4405
Au13p-g.log	1	6	0.0575	1.0938	0.4411

Au13p-g.log	1	7	0.0672	1.0933	0.4405
Au13p-g.log	1	8	0.0672	1.0933	0.4405
Au13p-g.log	1	9	0.0636	1.0875	0.4408
Au13p-g.log	1	10	0.1042	1.0817	0.4396
Au13p-g.log	1	11	0.1042	1.0817	0.4396
Au13p-g.log	1	12	0.1116	1.0765	0.4381
Au13p-g.log	1	13	0.1116	1.0765	0.4381
Au13p-h.log	1	1	0.1443	1.0702	0.4377
Au13p-h.log	1	2	0.1443	1.0702	0.4377
Au13p-h.log	1	3	0.0626	1.0942	0.4409
Au13p-h.log	1	4	0.0485	1.0999	0.4415
Au13p-h.log	1	5	0.0485	1.0999	0.4415
Au13p-h.log	1	6	0.0626	1.0942	0.4409
Au13p-h.log	1	7	0.0485	1.0999	0.4415
Au13p-h.log	1	8	0.0485	1.0999	0.4415
Au13p-h.log	1	9	0.1598	1.0676	0.4363
Au13p-h.log	1	10	0.0833	1.0855	0.4402
Au13p-h.log	1	11	0.0833	1.0855	0.4402
Au13p-h.log	1	12	0.0327	1.1006	0.4421
Au13p-h.log	1	13	0.0327	1.1006	0.4421
Au13p-i.log	1	1	0.0535	1.0977	0.4414
Au13p-i.log	1	2	0.0785	1.0899	0.4410
Au13p-i.log	1	3	0.0785	1.0899	0.4410
Au13p-i.log	1	4	0.0533	1.0978	0.4414
Au13p-i.log	1	5	0.0533	1.0978	0.4414
Au13p-i.log	1	6	0.0798	1.0869	0.4397
Au13p-i.log	1	7	0.0798	1.0869	0.4397
Au13p-i.log	1	8	0.0535	1.0977	0.4414
Au13p-i.log	1	9	0.0785	1.0899	0.4410
Au13p-i.log	1	10	0.0785	1.0899	0.4410
Au13p-i.log	1	11	0.1528	1.0731	0.4383
Au13p-i.log	1	12	0.0798	1.0869	0.4397
Au13p-i.log	1	13	0.0798	1.0869	0.4397
Au13p-j.log	1	1	0.1257	1.0761	0.4387
Au13p-j.log	1	2	0.1257	1.0761	0.4387
Au13p-j.log	1	3	0.0568	1.0958	0.4410
Au13p-j.log	1	4	0.0485	1.1020	0.4419
Au13p-j.log	1	5	0.0485	1.1020	0.4419
Au13p-j.log	1	6	0.0568	1.0958	0.4410
Au13p-j.log	1	7	0.0485	1.1020	0.4419
Au13p-j.log	1	8	0.0485	1.1020	0.4419
Au13p-j.log	1	9	0.0988	1.0824	0.4396
Au13p-j.log	1	10	0.0772	1.0873	0.4404
Au13p-j.log	1	11	0.0772	1.0873	0.4404
Au13p-j.log	1	12	0.0937	1.0834	0.4390
Au13p-j.log	1	13	0.0937	1.0834	0.4390
Au13p-k.log	1	1	0.0529	1.0948	0.4421
Au13p-k.log	1	2	0.0529	1.0948	0.4421
Au13p-k.log	1	3	0.0669	1.0961	0.4408
Au13p-k.log	1	4	0.0669	1.0961	0.4408
Au13p-k.log	1	5	0.0447	1.0991	0.4420
Au13p-k.log	1	6	0.0669	1.0961	0.4408
Au13p-k.log	1	7	0.0447	1.0991	0.4420
Au13p-k.log	1	8	0.0669	1.0961	0.4408
Au13p-k.log	1	9	0.1642	1.0664	0.4363
Au13p-k.log	1	10	0.1067	1.0783	0.4390
Au13p-k.log	1	11	0.1642	1.0664	0.4363
Au13p-k.log	1	12	0.1067	1.0783	0.4390
Au13p-k.log	1	13	-0.0049	1.1047	0.4438
Au13p-l.log	1	1	0.0498	1.1043	0.4420
Au13p-l.log	1	2	0.1155	1.0815	0.4396
Au13p-l.log	1	3	0.0730	1.0872	0.4399
Au13p-l.log	1	4	0.1155	1.0815	0.4396
Au13p-l.log	1	5	0.0058	1.1060	0.4427
Au13p-l.log	1	6	0.0592	1.0891	0.4400

Au13p-l.log	1	7	0.0058	1.1060	0.4427
Au13p-l.log	1	8	0.0770	1.0891	0.4397
Au13p-l.log	1	9	0.1337	1.0783	0.4378
Au13p-l.log	1	10	0.0770	1.0891	0.4397
Au13p-l.log	1	11	0.0770	1.0891	0.4397
Au13p-l.log	1	12	0.1337	1.0783	0.4378
Au13p-l.log	1	13	0.0770	1.0891	0.4397
Au13p-m.log	1	1	0.0917	1.0894	0.4388
Au13p-m.log	1	2	0.0877	1.0855	0.4396
Au13p-m.log	1	3	0.0552	1.0930	0.4410
Au13p-m.log	1	4	0.0877	1.0855	0.4396
Au13p-m.log	1	5	0.0552	1.0930	0.4410
Au13p-m.log	1	6	0.0528	1.0954	0.4413
Au13p-m.log	1	7	0.1028	1.0820	0.4388
Au13p-m.log	1	8	0.0528	1.0954	0.4413
Au13p-m.log	1	9	0.1028	1.0820	0.4388
Au13p-m.log	1	10	0.1028	1.0820	0.4388
Au13p-m.log	1	11	0.0528	1.0954	0.4413
Au13p-m.log	1	12	0.1028	1.0820	0.4388
Au13p-m.log	1	13	0.0528	1.0954	0.4413
Au13p-n.log	1	1	0.1184	1.0803	0.4376
Au13p-n.log	1	2	0.1407	1.0733	0.4370
Au13p-n.log	1	3	0.0398	1.0962	0.4420
Au13p-n.log	1	4	0.0398	1.0962	0.4420
Au13p-n.log	1	5	0.0398	1.0962	0.4420
Au13p-n.log	1	6	0.1407	1.0733	0.4370
Au13p-n.log	1	7	0.0398	1.0962	0.4420
Au13p-n.log	1	8	0.0398	1.0962	0.4420
Au13p-n.log	1	9	0.1407	1.0733	0.4370
Au13p-n.log	1	10	0.0398	1.0962	0.4420
Au13p-n.log	1	11	0.0398	1.0962	0.4420
Au13p-n.log	1	12	0.0398	1.0962	0.4420
Au13p-n.log	1	13	0.1407	1.0733	0.4370
Au13p-o.log	1	1	0.1049	1.0775	0.4377
Au13p-o.log	1	2	0.0746	1.0891	0.4401
Au13p-o.log	1	3	0.0746	1.0891	0.4401
Au13p-o.log	1	4	0.0746	1.0891	0.4401
Au13p-o.log	1	5	0.0746	1.0891	0.4401
Au13p-o.log	1	6	0.0746	1.0891	0.4401
Au13p-o.log	1	7	0.0746	1.0891	0.4401
Au13p-o.log	1	8	0.0746	1.0891	0.4401
Au13p-o.log	1	9	0.0746	1.0891	0.4401
Au13p-o.log	1	10	0.0746	1.0891	0.4401
Au13p-o.log	1	11	0.0746	1.0891	0.4401
Au13p-o.log	1	12	0.0746	1.0891	0.4401
Au13p-o.log	1	13	0.0746	1.0891	0.4401
Au19p-a.log	1	1	0.0366	1.1001	0.4425
Au19p-a.log	1	2	0.0367	1.1001	0.4425
Au19p-a.log	1	3	0.0365	1.1001	0.4425
Au19p-a.log	1	4	0.0365	1.1001	0.4425
Au19p-a.log	1	5	0.0478	1.0910	0.4407
Au19p-a.log	1	6	0.0364	1.1002	0.4425
Au19p-a.log	1	7	0.0366	1.1001	0.4425
Au19p-a.log	1	8	0.0870	1.0886	0.4409
Au19p-a.log	1	9	0.0869	1.0886	0.4408
Au19p-a.log	1	10	0.0868	1.0887	0.4409
Au19p-a.log	1	11	0.0503	1.0963	0.4411
Au19p-a.log	1	12	0.0462	1.0960	0.4415
Au19p-a.log	1	13	0.0456	1.0961	0.4415
Au19p-a.log	1	14	0.0503	1.0963	0.4411
Au19p-a.log	1	15	0.0502	1.0963	0.4411
Au19p-a.log	1	16	0.0458	1.0961	0.4415
Au19p-a.log	1	17	0.0615	1.0911	0.4412
Au19p-a.log	1	18	0.0612	1.0912	0.4413
Au19p-a.log	1	19	0.0612	1.0912	0.4412

Au20p-a.log	1	1	0.0295	1.1005	0.4426
Au20p-a.log	1	2	0.0294	1.1005	0.4426
Au20p-a.log	1	3	0.0401	1.1017	0.4426
Au20p-a.log	1	4	0.0394	1.1018	0.4426
Au20p-a.log	1	5	0.0502	1.0961	0.4411
Au20p-a.log	1	6	0.0393	1.1018	0.4426
Au20p-a.log	1	7	0.0398	1.1018	0.4426
Au20p-a.log	1	8	0.0904	1.0862	0.4405
Au20p-a.log	1	9	0.0907	1.0861	0.4405
Au20p-a.log	1	10	0.0905	1.0862	0.4405
Au20p-a.log	1	11	0.0507	1.0962	0.4411
Au20p-a.log	1	12	0.0302	1.1003	0.4426
Au20p-a.log	1	13	0.0394	1.1018	0.4426
Au20p-a.log	1	14	0.0502	1.0960	0.4411
Au20p-a.log	1	15	0.0507	1.0961	0.4411
Au20p-a.log	1	16	0.0392	1.1018	0.4426
Au20p-a.log	1	17	0.0304	1.1002	0.4426
Au20p-a.log	1	18	0.0403	1.1017	0.4425
Au20p-a.log	1	19	0.0397	1.1018	0.4426
Au20p-a.log	1	20	0.0902	1.0863	0.4405
Au2p.log	1	1	0.5000	1.0037	0.4216
Au2p.log	1	2	0.5000	1.0037	0.4216
Au3p-l.log	1	1	0.3333	1.0288	0.4286
Au3p-l.log	1	2	0.3333	1.0289	0.4286
Au3p-l.log	1	3	0.3334	1.0288	0.4286
Au4p-l.log	1	1	0.2645	1.0482	0.4318
Au4p-l.log	1	2	0.2355	1.0544	0.4334
Au4p-l.log	1	3	0.2645	1.0482	0.4318
Au4p-l.log	1	4	0.2355	1.0544	0.4334
Au4p-t.log	1	1	0.2963	1.0399	0.4304
Au4p-t.log	1	2	0.2727	1.0402	0.4312
Au4p-t.log	1	3	0.1286	1.0811	0.4383
Au4p-t.log	1	4	0.3024	1.0436	0.4299
Au5p-b.log	1	1	0.2312	1.0496	0.4330
Au5p-b.log	1	2	0.0752	1.0929	0.4408
Au5p-b.log	1	3	0.2312	1.0495	0.4330
Au5p-b.log	1	4	0.2312	1.0496	0.4330
Au5p-b.log	1	5	0.2312	1.0495	0.4330
Au5p-h.log	1	1	0.2080	1.0564	0.4346
Au5p-h.log	1	2	0.1622	1.0734	0.4368
Au5p-h.log	1	3	0.2110	1.0535	0.4336
Au5p-h.log	1	4	0.2110	1.0534	0.4336
Au5p-h.log	1	5	0.2077	1.0564	0.4346
Au6p-e.log	1	1	0.1344	1.0767	0.4376
Au6p-e.log	1	2	0.1343	1.0768	0.4376
Au6p-e.log	1	3	0.2131	1.0555	0.4333
Au6p-e.log	1	4	0.1536	1.0736	0.4374
Au6p-e.log	1	5	0.2112	1.0560	0.4334
Au6p-e.log	1	6	0.1535	1.0736	0.4374
Au6p-h.log	1	1	0.1966	1.0596	0.4349
Au6p-h.log	1	2	0.1730	1.0679	0.4361
Au6p-h.log	1	3	0.1048	1.0970	0.4402
Au6p-h.log	1	4	0.1560	1.0678	0.4363
Au6p-h.log	1	5	0.1731	1.0679	0.4361
Au6p-h.log	1	6	0.1966	1.0596	0.4349
Au6p-p.log	1	1	0.1544	1.0703	0.4369
Au6p-p.log	1	2	0.1109	1.0865	0.4390
Au6p-p.log	1	3	0.1566	1.0725	0.4373
Au6p-p.log	1	4	0.1287	1.0805	0.4381
Au6p-p.log	1	5	0.2240	1.0514	0.4330
Au6p-p.log	1	6	0.2255	1.0511	0.4329
Au6p-s.log	1	1	0.1781	1.0692	0.4366
Au6p-s.log	1	2	0.1273	1.0865	0.4387
Au6p-s.log	1	3	0.1809	1.0857	0.4375
Au6p-s.log	1	4	0.2086	1.0584	0.4350

Au6p-s.log	1	5	0.1268	1.0865	0.4387
Au6p-s.log	1	6	0.1783	1.0691	0.4366
Au7p-b.log	1	1	0.1726	1.0685	0.4364
Au7p-b.log	1	2	0.0877	1.1006	0.4410
Au7p-b.log	1	3	0.0687	1.0855	0.4400
Au7p-b.log	1	4	0.1123	1.0867	0.4392
Au7p-b.log	1	5	0.1388	1.0770	0.4380
Au7p-b.log	1	6	0.1879	1.0595	0.4355
Au7p-b.log	1	7	0.2320	1.0464	0.4327
Au7p-c.log	1	1	0.1250	1.0778	0.4381
Au7p-c.log	1	2	0.1249	1.0777	0.4381
Au7p-c.log	1	3	0.1877	1.0585	0.4341
Au7p-c.log	1	4	0.1250	1.0778	0.4381
Au7p-c.log	1	5	0.1875	1.0585	0.4341
Au7p-c.log	1	6	0.1249	1.0777	0.4381
Au7p-c.log	1	7	0.1250	1.0777	0.4380
Au7p-d.log	1	1	0.1260	1.0751	0.4383
Au7p-d.log	1	2	0.1416	1.0742	0.4375
Au7p-d.log	1	3	0.1417	1.0742	0.4375
Au7p-d.log	1	4	0.1863	1.0582	0.4346
Au7p-d.log	1	5	0.1261	1.0751	0.4383
Au7p-d.log	1	6	0.0920	1.0878	0.4404
Au7p-d.log	1	7	0.1862	1.0582	0.4346
Au7p-h.log	1	1	0.1465	1.0668	0.4367
Au7p-h.log	1	2	0.1466	1.0669	0.4367
Au7p-h.log	1	3	0.1468	1.0668	0.4367
Au7p-h.log	1	4	0.1465	1.0668	0.4367
Au7p-h.log	1	5	0.1468	1.0668	0.4367
Au7p-h.log	1	6	0.1466	1.0669	0.4367
Au7p-h.log	1	7	0.1202	1.0986	0.4401
Au7p-t.log	1	1	0.0532	1.1060	0.4428
Au7p-t.log	1	2	0.1128	1.0840	0.4387
Au7p-t.log	1	3	0.1129	1.0840	0.4387
Au7p-t.log	1	4	0.1299	1.0837	0.4385
Au7p-t.log	1	5	0.1666	1.0654	0.4364
Au7p-t.log	1	6	0.1666	1.0654	0.4364
Au7p-t.log	1	7	0.2581	1.0334	0.4309
Au7p-tt.log	1	1	0.1450	1.0768	0.4380
Au7p-tt.log	1	2	0.0771	1.0962	0.4408
Au7p-tt.log	1	3	0.0771	1.0961	0.4408
Au7p-tt.log	1	4	0.1304	1.0712	0.4374
Au7p-tt.log	1	5	0.1304	1.0712	0.4374
Au7p-tt.log	1	6	0.2200	1.0496	0.4335
Au7p-tt.log	1	7	0.2200	1.0496	0.4335
Au8p-a.log	1	1	0.1627	1.0671	0.4367
Au8p-a.log	1	2	0.0765	1.1008	0.4412
Au8p-a.log	1	3	0.0981	1.0902	0.4401
Au8p-a.log	1	4	0.1627	1.0671	0.4367
Au8p-a.log	1	5	0.0981	1.0902	0.4401
Au8p-a.log	1	6	0.0765	1.1008	0.4412
Au8p-a.log	1	7	0.1627	1.0672	0.4367
Au8p-a.log	1	8	0.1627	1.0672	0.4367
Au8p-d.log	1	1	0.1573	1.0717	0.4373
Au8p-d.log	1	2	0.1210	1.0779	0.4377
Au8p-d.log	1	3	0.1210	1.0779	0.4377
Au8p-d.log	1	4	0.1573	1.0717	0.4373
Au8p-d.log	1	5	0.1211	1.0778	0.4377
Au8p-d.log	1	6	0.1206	1.0779	0.4378
Au8p-d.log	1	7	0.1209	1.0806	0.4385
Au8p-d.log	1	8	0.0808	1.0895	0.4398
Au8p-g.log	1	1	0.1200	1.0792	0.4380
Au8p-g.log	1	2	0.1427	1.0726	0.4372
Au8p-g.log	1	3	0.1201	1.0792	0.4380
Au8p-g.log	1	4	0.1065	1.0839	0.4384
Au8p-g.log	1	5	0.1308	1.0764	0.4378

Au8p-g.log	1	6	0.1065	1.0839	0.4384
Au8p-g.log	1	7	0.1426	1.0727	0.4373
Au8p-g.log	1	8	0.1308	1.0764	0.4378
Au8p-i.log	1	1	0.0838	1.0887	0.4398
Au8p-i.log	1	2	0.1111	1.0815	0.4384
Au8p-i.log	1	3	0.1247	1.0771	0.4377
Au8p-i.log	1	4	0.0822	1.0894	0.4399
Au8p-i.log	1	5	0.1226	1.0774	0.4377
Au8p-i.log	1	6	0.1677	1.0683	0.4369
Au8p-i.log	1	7	0.1401	1.0754	0.4379
Au8p-i.log	1	8	0.1677	1.0684	0.4369
Au9p-b.log	1	1	0.0965	1.0816	0.4388
Au9p-b.log	1	2	0.1413	1.0720	0.4372
Au9p-b.log	1	3	0.0894	1.0845	0.4390
Au9p-b.log	1	4	0.1413	1.0720	0.4372
Au9p-b.log	1	5	0.0626	1.0985	0.4409
Au9p-b.log	1	6	0.0966	1.0816	0.4388
Au9p-b.log	1	7	0.1413	1.0720	0.4372
Au9p-b.log	1	8	0.0894	1.0845	0.4390
Au9p-b.log	1	9	0.1415	1.0720	0.4372
Au9p-c.log	1	1	0.1658	1.0689	0.4372
Au9p-c.log	1	2	0.0779	1.0884	0.4399
Au9p-c.log	1	3	0.0776	1.0884	0.4400
Au9p-c.log	1	4	0.1659	1.0688	0.4372
Au9p-c.log	1	5	0.0776	1.0884	0.4399
Au9p-c.log	1	6	0.0778	1.0883	0.4399
Au9p-c.log	1	7	0.1011	1.0784	0.4384
Au9p-c.log	1	8	0.1282	1.0770	0.4384
Au9p-c.log	1	9	0.1282	1.0771	0.4384
Au9p-d.log	1	1	0.1416	1.0741	0.4376
Au9p-d.log	1	2	0.0972	1.0837	0.4387
Au9p-d.log	1	3	0.1108	1.0784	0.4382
Au9p-d.log	1	4	0.1418	1.0740	0.4376
Au9p-d.log	1	5	0.0972	1.0837	0.4387
Au9p-d.log	1	6	0.1107	1.0783	0.4382
Au9p-d.log	1	7	0.1085	1.0803	0.4388
Au9p-d.log	1	8	0.0661	1.0944	0.4404
Au9p-d.log	1	9	0.1262	1.0747	0.4376
Au9p-e.log	1	1	0.0924	1.0859	0.4401
Au9p-e.log	1	2	0.1831	1.0582	0.4349
Au9p-e.log	1	3	0.0779	1.0966	0.4409
Au9p-e.log	1	4	0.0884	1.0904	0.4403
Au9p-e.log	1	5	0.1037	1.0934	0.4397
Au9p-e.log	1	6	0.0925	1.0859	0.4401
Au9p-e.log	1	7	0.1368	1.0720	0.4379
Au9p-e.log	1	8	0.0884	1.0904	0.4404
Au9p-e.log	1	9	0.1367	1.0720	0.4379
Au9p-f.log	1	1	0.1787	1.0632	0.4358
Au9p-f.log	1	2	0.0666	1.0885	0.4402
Au9p-f.log	1	3	0.0662	1.0885	0.4402
Au9p-f.log	1	4	0.1785	1.0633	0.4358
Au9p-f.log	1	5	0.0911	1.1023	0.4413
Au9p-f.log	1	6	0.0848	1.0949	0.4409
Au9p-f.log	1	7	0.0844	1.0950	0.4410
Au9p-f.log	1	8	0.1252	1.0731	0.4383
Au9p-f.log	1	9	0.1244	1.0734	0.4383
Au9p-g.log	1	1	0.0844	1.0853	0.4393
Au9p-g.log	1	2	0.1589	1.0716	0.4374
Au9p-g.log	1	3	0.0901	1.0829	0.4391
Au9p-g.log	1	4	0.1588	1.0716	0.4374
Au9p-g.log	1	5	0.0843	1.0853	0.4393
Au9p-g.log	1	6	0.0902	1.0829	0.4391
Au9p-g.log	1	7	0.0844	1.0853	0.4393
Au9p-g.log	1	8	0.1588	1.0716	0.4374
Au9p-g.log	1	9	0.0901	1.0829	0.4391

Au9p-h.log	1	1	0.0951	1.0833	0.4386
Au9p-h.log	1	2	0.0850	1.0887	0.4395
Au9p-h.log	1	3	0.1046	1.0793	0.4386
Au9p-h.log	1	4	0.1046	1.0793	0.4386
Au9p-h.log	1	5	0.0851	1.0887	0.4394
Au9p-h.log	1	6	0.0952	1.0832	0.4386
Au9p-h.log	1	7	0.1698	1.0657	0.4362
Au9p-h.log	1	8	0.1303	1.0759	0.4381
Au9p-h.log	1	9	0.1303	1.0759	0.4381
Aup.log	1	1	1.0000	0.8961	0.3990
ZnAu5p-a.log	1	1	0.1670	1.0689	0.4368
ZnAu5p-a.log	1	2	0.0601	1.1004	0.4412
ZnAu5p-a.log	1	3	0.0601	1.1003	0.4412
ZnAu5p-a.log	1	4	0.0996	1.0940	0.4401
ZnAu5p-a.log	1	5	0.0996	1.0940	0.4401
ZnAu5p-a.log	1	6	10.5136	0.8753	0.1013

==========

Computed geometries (Cartesian coordinates in Angstrom)
and total energies (Hartree) from PW91/def2-TZVP//PW91/LANL2DZ calculations on all cationic Au clusters.

Molecule Au10p-a.log
Energy: -1358.50099444
Geometry:
79 -1.931996 -0.844546 2.975175
79 -1.396457 -3.141500 4.339031
79 1.537690 1.476373 5.345123
79 -0.483769 1.481069 3.454877
79 0.083594 -0.870451 4.869598
79 0.704065 -3.144627 6.310865
79 2.107179 -0.851695 6.756711
79 3.495000 1.468545 7.182262
79 -0.763577 -5.348842 5.766971
79 -2.447605 1.479946 1.624837

Molecule Au10p-b.log
Energy: -1358.53090699
Geometry:
79 -1.615261 -0.122833 3.338501
79 -1.690129 -2.802972 4.043864
79 2.168996 0.406933 6.337217
79 0.348377 1.479863 4.512911
79 0.205854 -1.196069 5.162451
79 0.061981 -3.937659 5.830695
79 1.960599 -2.289578 6.938836
79 2.245900 3.086753 5.630203
79 -1.406133 2.573041 2.735485
79 0.497387 4.218699 3.838530

Molecule Au10p-c.log
Energy: -1358.53037787
Geometry:
79 -1.517839 -0.141343 3.217705
79 -1.786199 -2.760241 3.957694
79 2.163623 0.348834 6.222916
79 0.470572 1.555734 4.319288
79 0.214901 -1.216585 5.097020
79 0.045951 -3.820058 5.922285
79 2.016199 -2.277786 7.011905
79 2.446285 2.903824 5.554795
79 -1.870730 -5.321724 4.848786
79 -1.278640 2.433618 2.473054

Molecule Au10p-d.log
Energy: -1358.52178499
Geometry:
79 1.283026 3.353244 -4.257779
79 -0.976066 1.770212 -4.778775
79 -1.006299 3.490823 -2.564469
79 1.177104 5.156180 -2.151491
79 3.606729 2.042833 -3.200193
79 1.481955 0.485654 -3.774138
79 1.486947 2.369783 -1.495679
79 -0.740613 -1.031266 -4.237484
79 -0.787443 2.310284 0.035877
79 -0.819524 0.615632 -2.060684

Molecule Au11p-a.log
Energy: -1494.43203891
Geometry:
79 -1.269127 -0.576529 3.134753
79 -1.834155 -3.003288 4.219038
79 1.980635 0.421017 6.679203
79 0.655302 1.219063 4.329732
79 0.069628 -1.260397 5.412176
79 -0.494500 -3.726781 6.491920
79 1.359097 -2.031419 7.682623
79 2.437326 3.012850 5.342717
79 -0.655847 1.877281 2.098814
79 1.173343 3.761834 3.094345
79 3.704807 2.324517 7.545192

Molecule Au11p-b.log
Energy: -1494.41193312
Geometry:
79 -1.071322 -0.487954 3.315275
79 -1.305908 -2.929080 4.355114
79 2.330413 0.585016 6.579954
79 0.744269 1.329522 4.386715
79 0.513634 -1.234290 5.501513
79 2.060751 -1.879600 7.587266
79 2.557790 3.144413 5.464960
79 -0.818922 2.053662 2.220588
79 0.983452 3.858218 3.288827
79 4.076618 2.461690 7.543652
79 -0.559950 4.534011 1.171713

Molecule Au11p-c.log
Energy: -1494.42653836
Geometry:
79 -1.309503 0.237363 3.288852
79 -2.228287 -2.161369 4.370141
79 2.536781 0.057041 6.153146
79 1.089983 1.386785 4.159486
79 0.155010 -1.052056 5.261131
79 -0.779893 -3.489229 6.362813
79 1.619672 -2.342489 7.234122
79 3.387902 2.390825 5.067521
79 -0.372603 2.568465 2.268314
79 0.681359 -4.674642 8.252402
79 -3.077980 -4.495228 5.458040

Molecule Au12p-a.log
Energy: -1630.30413769
Geometry:
79 0.803190 -0.638400 -1.806357
79 -1.916446 0.241093 -0.904879

79 -1.778121 2.818760 0.393590
79 0.656471 1.958181 -0.375341
79 3.104224 1.095520 -1.148188
79 1.761927 -2.821032 -0.407085
79 1.927003 -0.244200 0.899066
79 -0.652425 -1.962308 0.414648
79 -0.805611 0.646179 1.807274
79 -3.114119 -1.088624 1.127707
79 0.601459 -1.456689 2.924563
79 -0.587551 1.451519 -2.924998

Molecule Au12p-b.log
Energy: -1630.33034452
Geometry:
79 -0.000002 3.632772 0.411418
79 0.000002 -3.632773 0.411416
79 0.000012 1.391276 2.022410
79 1.422242 1.396844 -0.422914
79 -1.422236 1.396830 -0.422905
79 -0.000012 -1.391273 2.022407
79 -1.422241 -1.396845 -0.422913
79 1.422235 -1.396832 -0.422904
79 0.000000 0.000001 4.310907
79 2.709450 -0.000003 -2.438715
79 -2.709450 -0.000003 -2.438715
79 0.000000 0.000006 -2.609491

Molecule Au12p-c.log
Energy: -1630.31822787
Geometry:
79 -1.781733 1.423424 0.000004
79 0.226479 -0.512856 -3.617023
79 0.226476 -0.512857 3.617024
79 1.405582 -1.686620 1.355553
79 1.405579 -1.686621 -1.355550
79 -1.324203 -1.049130 1.418153
79 -1.324205 -1.049134 -1.418155
79 -3.648292 -0.598610 -0.000002
79 0.795608 1.076972 1.416865
79 0.795607 1.076973 -1.416865
79 3.126120 0.151701 -0.000002
79 0.096982 3.366759 -0.000001

Molecule Au12p-d.log
Energy: -1630.31744404
Geometry:
79 -1.239408 -1.767227 -0.000001
79 3.367920 -0.123433 0.000001
79 1.016354 1.337526 0.000001
79 -1.662898 2.063636 0.000001
79 1.291422 -1.166577 -1.446993
79 -1.170307 0.192565 -1.980730
79 -0.103184 2.696348 -2.241958
79 -0.758916 -2.477588 -2.659593
79 1.291423 -1.166582 1.446992
79 -1.170302 0.192566 1.980731
79 -0.103184 2.696352 2.241958
79 -0.758920 -2.477587 2.659592

Molecule Au12p-e.log
Energy: -1630.31627525
Geometry:
79 1.432112 1.432089 0.000014
79 1.432112 -1.432089 0.000014
79 -1.432112 -1.432089 0.000015

79 -1.432112 1.432089 0.000014
79 0.000000 -1.338048 2.428309
79 -0.000001 1.338048 2.428309
79 0.000000 -3.637089 0.754001
79 0.000000 3.637089 0.754001
79 1.338044 -0.000001 -2.428296
79 -1.338043 0.000001 -2.428295
79 3.637111 0.000000 -0.754043
79 -3.637111 0.000000 -0.754043

Molecule Au12p-f.log
Energy: -1630.30824485
Geometry:
79 -1.424553 1.526656 -0.329681
79 -1.424556 -1.526657 -0.329686
79 1.424556 -1.526656 -0.329685
79 1.424559 1.526658 -0.329690
79 -0.000003 0.000000 1.837988
79 -0.000002 0.000000 -2.369392
79 -2.805027 -0.000002 1.460671
79 0.000001 -2.715625 -2.402159
79 2.805021 0.000002 1.460676
79 -0.000002 2.715625 -2.402159
79 0.000000 -2.701906 1.866558
79 0.000006 2.701906 1.866558

Molecule Au12p-h.log
Energy: -1630.30558539
Geometry:
79 1.412705 -3.441917 1.514674
79 1.576051 -4.315700 3.943661
79 1.836102 0.061526 5.397379
79 1.179290 1.085958 2.871686
79 2.137062 -2.597585 5.877632
79 1.577686 -1.581817 3.403511
79 1.126894 -0.897868 0.781336
79 -0.062401 -0.133408 -1.543015
79 0.253628 1.637784 0.347601
79 -0.977120 2.304280 -2.009030
79 0.596528 3.589787 2.116370
79 -0.440492 4.286993 -0.236756

Molecule Au13p-a.log
Energy: -1766.23141189
Geometry:
79 0.000000 -0.000006 -2.374015
79 0.000000 -3.598429 0.266122
79 0.000000 3.598435 0.266119
79 0.000000 1.387128 1.983836
79 0.000000 -1.387119 1.983826
79 -1.563579 1.409561 -0.347094
79 -1.563589 -1.409564 -0.347101
79 -2.442851 -0.000002 2.080720
79 -2.711856 0.000000 -2.449469
79 1.563579 1.409561 -0.347094
79 1.563589 -1.409564 -0.347101
79 2.442851 -0.000002 2.080720
79 2.711856 0.000000 -2.449469

Molecule Au13p-b.log
Energy: -1766.23087382
Geometry:
79 0.172540 2.507142 -2.663571
79 1.734587 0.651238 -1.451619
79 -0.486805 2.071533 -0.000001

79 0.172536 2.507143 2.663569
79 3.582096 -0.752164 0.000001
79 1.734589 0.651242 1.451618
79 -1.837530 -1.752555 0.000000
79 -0.448744 -2.565640 -2.284457
79 0.966053 -1.706194 -0.000001
79 -0.448745 -2.565643 2.284456
79 -1.032838 0.093703 1.928257
79 -3.074896 0.766489 0.000002
79 -1.032842 0.093705 -1.928254

Molecule Au13p-c.log
Energy: -1766.22880942
Geometry:
79 0.000000 3.606775 0.467296
79 0.000000 -3.606775 0.467295
79 1.418978 1.435860 -0.408608
79 -1.418978 1.435861 -0.408607
79 -0.000001 1.403609 2.091408
79 1.418978 -1.435860 -0.408608
79 0.000000 -1.403609 2.091408
79 -1.418978 -1.435860 -0.408608
79 1.322179 -0.000001 -2.840444
79 -3.636067 0.000001 -1.079847
79 0.000000 0.000000 4.357606
79 3.636067 0.000001 -1.079847
79 -1.322179 -0.000001 -2.840444

Molecule Au13p-d.log
Energy: -1766.22617853
Geometry:
79 -1.426513 2.016713 -0.325311
79 -2.786555 0.000000 1.084365
79 -1.426513 -2.016713 -0.325311
79 0.000000 2.593412 -2.595172
79 0.000000 -2.593412 -2.595172
79 1.426512 -2.016712 -0.325310
79 1.426512 2.016712 -0.325310
79 2.786557 0.000000 1.084366
79 0.000001 0.000000 -1.745464
79 3.239742 -2.595890 1.517080
79 -3.239743 -2.595890 1.517080
79 3.239742 2.595890 1.517080
79 -3.239743 2.595890 1.517080

Molecule Au13p-e.log
Energy: -1766.21954019
Geometry:
79 -0.132974 -0.723518 3.619779
79 -0.132975 -0.723517 -3.619779
79 0.878500 0.646529 1.426490
79 -1.778953 -0.461672 1.464701
79 0.469373 -2.258274 1.352276
79 0.878500 0.646529 -1.426489
79 0.469374 -2.258275 -1.352277
79 -1.778953 -0.461673 -1.464700
79 0.778070 3.072407 0.000000
79 -3.937369 0.336637 0.000000
79 3.264587 1.431401 0.000000
79 -1.644602 1.974384 -0.000001
79 2.667422 -1.220957 0.000000

Molecule Au13p-f.log
Energy: -1766.21378586
Geometry:

79 -3.298944 -0.925812 0.000000
79 1.596992 -1.672995 0.000000
79 1.414863 1.213316 0.000000
79 -1.458213 1.213329 0.000000
79 -0.041426 1.203917 -2.429450
79 -2.769341 0.400775 -2.380480
79 2.418885 -0.072306 -2.278022
79 -2.769341 0.400775 2.380480
79 -0.041426 1.203917 2.429451
79 2.418885 -0.072306 2.278022
79 -0.740188 -1.386023 -1.402624
79 -0.740188 -1.386023 1.402624
79 4.009440 -0.120564 0.000000

Molecule Au13p-g.log
Energy: -1766.21410489
Geometry:
79 -0.000004 3.621035 0.186568
79 0.000004 -3.621035 0.186568
79 0.000003 1.391066 1.863854
79 1.397758 1.413841 -0.754552
79 -1.397761 1.413843 -0.754558
79 -0.000003 -1.391068 1.863855
79 -1.397758 -1.413841 -0.754550
79 1.397761 -1.413842 -0.754556
79 0.000000 -0.000001 -2.820546
79 3.830815 0.000003 -0.719597
79 -3.830815 0.000001 -0.719597
79 -2.418906 0.000006 1.588555
79 2.418906 -0.000008 1.588555

Molecule Au13p-h.log
Energy: -1766.21263731
Geometry:
79 -0.000048 3.605489 -0.393054
79 0.000048 -3.605489 -0.393054
79 0.000092 1.473161 1.296971
79 1.495075 1.400768 -1.085162
79 -1.495142 1.400693 -1.085011
79 -0.000092 -1.473161 1.296971
79 -1.495075 -1.400768 -1.085162
79 1.495142 -1.400693 -1.085011
79 0.000000 0.000000 3.604311
79 3.253872 0.000010 -2.523819
79 -3.253872 -0.000010 -2.523819
79 -2.312962 0.000112 1.987920
79 2.312962 -0.000112 1.987920

Molecule Au13p-i.log
Energy: -1766.20393484
Geometry:
79 1.325456 1.913262 0.000000
79 0.723881 2.687931 -2.688417
79 0.723881 2.687931 2.688417
79 1.326417 0.000246 1.908150
79 1.326417 0.000246 -1.908150
79 -1.247739 1.424811 1.425179
79 -1.247739 1.424811 -1.425179
79 1.325975 -1.912752 0.000000
79 0.724628 -2.687439 -2.688603
79 0.724628 -2.687439 2.688603
79 -3.210636 -0.000451 0.000000
79 -1.247585 -1.425578 1.425128
79 -1.247585 -1.425578 -1.425128

Molecule Au13p-j.log
Energy: -1766.20580269
Geometry:
79 -0.000001 3.577504 0.243423
79 0.000001 -3.577504 0.243423
79 0.000001 1.411821 1.973937
79 1.482892 1.396059 -0.487036
79 -1.482892 1.396059 -0.487039
79 -0.000001 -1.411821 1.973937
79 -1.482892 -1.396059 -0.487036
79 1.482892 -1.396059 -0.487039
79 0.000000 0.000000 4.234855
79 3.764502 0.000000 -0.448651
79 -3.764502 0.000000 -0.448652
79 -0.000002 -1.317827 -2.912060
79 0.000002 1.317827 -2.912060

Molecule Au13p-k.log
Energy: -1766.19853447
Geometry:
79 -0.000001 3.660870 0.661009
79 0.000000 -3.660870 0.661009
79 1.418005 1.428544 -0.087330
79 -1.418005 1.428543 -0.087331
79 0.000001 1.321940 2.348778
79 1.418007 -1.428544 -0.087329
79 -0.000002 -1.321938 2.348776
79 -1.418006 -1.428545 -0.087331
79 2.740445 0.000000 -2.103854
79 -3.787487 -0.000001 0.427236
79 -2.740446 0.000001 -2.103855
79 3.787488 0.000000 0.427236
79 0.000000 0.000000 -2.317014

Molecule Au13p-l.log
Energy: -1766.18982486
Geometry:
79 0.000001 -0.000002 -1.169286
79 0.000000 -2.708124 2.903665
79 -0.000001 0.000006 2.903077
79 0.000000 2.708132 2.903637
79 -0.000001 2.370707 -2.487451
79 0.000000 0.000017 -3.905725
79 -0.000001 -2.370689 -2.487494
79 -1.422015 -1.515535 0.827053
79 -2.782478 -0.000019 -0.984297
79 -1.422018 1.515529 0.827033
79 1.422016 -1.515534 0.827053
79 2.782480 -0.000019 -0.984297
79 1.422020 1.515528 0.827033

Molecule Au13p-m.log
Energy: -1766.16463564
Geometry:
79 0.000000 0.000000 0.000000
79 2.330724 -1.380352 0.000000
79 0.000000 0.000000 3.071326
79 -2.330724 1.380352 0.000000
79 0.000000 0.000000 -3.071326
79 0.237722 -2.486551 2.029919
79 -2.104402 -1.097420 -1.409393
79 -0.237722 2.486551 -2.029919
79 2.104402 1.097420 1.409393
79 -2.104402 -1.097420 1.409393
79 0.237722 -2.486551 -2.029919

79 2.104402 1.097420 -1.409393
79 -0.237722 2.486551 2.029919

Molecule Au13p-n.log
Energy: -1766.16086201
Geometry:
79 0.000001 -0.000005 0.000001
79 0.000122 1.909195 1.908244
79 2.154151 2.034894 -0.000061
79 -2.154151 2.034895 0.000065
79 -2.153823 0.000065 2.035445
79 -0.000119 -1.909202 1.908243
79 2.153824 -0.000065 2.035444
79 2.153836 0.000061 -2.035450
79 -0.000125 1.909196 -1.908244
79 -2.153838 -0.000066 -2.035450
79 -2.154150 -2.034885 -0.000062
79 2.154150 -2.034886 0.000073
79 0.000121 -1.909197 -1.908248

Molecule Au13p-o.log
Energy: -1766.12993641
Geometry:
79 0.000000 -0.000007 0.000012
79 0.000001 1.352917 2.506513
79 1.352910 2.506504 -0.000015
79 -1.352910 2.506504 -0.000012
79 -2.506532 0.000007 1.352903
79 0.000000 -1.352942 2.506472
79 2.506530 0.000007 1.352904
79 2.506539 -0.000015 -1.352897
79 0.000000 1.352915 -2.506500
79 -2.506537 -0.000014 -1.352898
79 -1.352906 -2.506494 0.000015
79 1.352907 -2.506492 0.000012
79 -0.000001 -1.352890 -2.506508

Molecule Au19p-a.log
Energy: -2581.64702609
Geometry:
79 2.939629 -2.176667 3.791230
79 0.292342 -2.504967 3.295750
79 2.005640 0.780234 7.697590
79 3.844578 -0.441571 6.121501
79 1.061347 -0.818144 5.496854
79 -1.765512 -1.139710 5.066667
79 -0.957018 0.413465 7.137731
79 0.015053 1.938319 9.230266
79 -2.438036 -2.769442 2.934744
79 5.597135 -1.767115 4.441749
79 -0.719865 -2.411644 7.387432
79 0.296247 -0.768071 9.534241
79 -1.420350 -4.065072 5.119893
79 1.429815 -3.844881 5.534721
79 2.371932 -2.029305 7.967633
79 4.204668 -3.365105 6.173966
79 0.618002 -3.478580 9.628364
79 -0.276818 -5.191661 7.328851
79 2.651916 -4.830132 7.876608

Molecule Au20p-a.log
Energy: -2717.54538622
Geometry:
79 3.127258 -2.338316 4.006903
79 0.537853 -2.002072 3.199934

```
79 2.365995 0.304799 8.094894
79 4.081631 -1.087550 6.502338
79 1.405501 -0.685392 5.597032
79 -1.323305 -0.390309 4.815755
79 -0.530459 0.676820 7.193105
79 0.471929 1.671228 9.564823
79 -2.109236 -1.671935 2.503051
79 5.700873 -2.680134 4.934771
79 -0.893233 -2.147045 7.022386
79 0.145815 -1.064136 9.468960
79 -1.645992 -3.422378 4.585427
79 1.071585 -3.817592 5.355902
79 2.094560 -2.529837 7.953260
79 3.758993 -4.117825 6.267239
79 -0.136816 -3.774360 9.262951
79 -1.124423 -4.977853 6.760360
79 1.769489 -5.347594 7.663469
79 -0.386640 -6.501432 8.941023

Molecule Au2p.log
Energy: -271.350311251
Geometry:
79 0.000000 0.000000 0.015761
79 0.000000 0.000000 2.674239

Molecule Au3p-l.log
Energy: -407.283856502
Geometry:
79 -1.173326 0.000000 1.411755
79 1.212026 0.000000 2.617387
79 -1.024929 0.000000 4.081876

Molecule Au4p-l.log
Energy: -543.153169400
Geometry:
79 0.362080 -0.000048 4.266762
79 0.194350 0.000048 1.557693
79 -2.090511 -0.000048 3.025143
79 -1.922781 0.000048 5.734212

Molecule Au4p-t.log
Energy: -543.144936308
Geometry:
79 -1.297162 0.000000 1.656139
79 1.229049 0.000000 2.442376
79 -0.766663 0.000000 4.294142
79 -2.622086 0.000000 6.191153

Molecule Au5p-b.log
Energy: -679.064550918
Geometry:
79 -1.397166 0.000000 1.177728
79 -0.073874 0.000000 3.553642
79 -2.789676 0.000000 3.397886
79 1.249419 0.000000 5.929556
79 2.641929 0.000000 3.709397

Molecule Au5p-h.log
Energy: -679.058265869
Geometry:
79 -1.932750 0.000000 1.371788
79 0.380708 0.000000 2.770656
79 -2.077041 0.000000 4.023751
79 0.514180 0.000000 5.522045
79 2.745537 0.000000 4.079963
```

Molecule Au6p-e.log
Energy: -814.925053051
Geometry:
79 -0.621244 -0.231499 2.167341
79 -1.002233 1.356605 4.427350
79 -1.713951 2.454081 1.815011
79 -0.655713 4.030224 3.884445
79 0.921145 2.250066 2.399651
79 0.004071 1.259312 -0.058547

Molecule Au6p-h.log
Energy: -814.945531612
Geometry:
79 -0.681589 -0.000007 1.289453
79 1.150545 0.000004 3.242229
79 -1.554795 0.000010 3.832798
79 0.363754 -0.000003 5.898878
79 -2.343290 -0.000005 6.487828
79 -4.155380 0.000002 4.515770

Molecule Au6p-p.log
Energy: -814.930504316
Geometry:
79 0.954668 -1.997198 2.238083
79 -0.152225 0.222760 3.209815
79 -1.561856 2.180438 4.456313
79 -1.032734 -2.330228 4.059985
79 -1.161233 -0.194908 5.948988
79 -2.962562 -0.226380 3.950703

Molecule Au6p-s.log
Energy: -814.950261906
Geometry:
79 -0.129043 -0.000618 1.308042
79 0.469012 0.000470 3.898966
79 -2.178951 -0.000448 3.019900
79 0.718172 0.000836 6.557198
79 -1.838940 0.000216 5.790302
79 -4.261006 -0.000457 4.692549

Molecule Au7p-b.log
Energy: -950.854731085
Geometry:
79 -2.550788 -0.000381 1.915124
79 0.170928 0.000615 2.674431
79 -1.901595 -0.000322 4.572704
79 0.913168 0.000993 5.302576
79 2.751432 -0.000967 3.361132
79 -1.111995 -0.000206 7.098687
79 -0.549413 0.000268 0.106795

Molecule Au7p-c.log
Energy: -950.830768670
Geometry:
79 0.621425 -1.713719 2.387259
79 -0.863826 0.751829 2.214554
79 -1.284958 -1.038864 4.358326
79 1.131888 -2.252231 5.173238
79 1.114013 0.397242 4.197969
79 -0.039795 -0.120465 6.722545
79 -1.273016 1.734995 4.893317

Molecule Au7p-d.log
Energy: -950.819712929

Geometry:
79 -3.808030 0.866584 0.679589
79 0.356474 0.051788 4.159837
79 -1.773264 0.457008 2.443433
79 0.041180 -0.746750 6.730489
79 2.514737 -0.320294 5.778095
79 -2.235565 -0.367398 5.049381
79 -4.350769 0.059061 3.181626

Molecule Au7p-h.log
Energy: -950.861962258
Geometry:
79 -1.669744 -0.000519 1.825037
79 1.086796 0.000343 1.879052
79 -3.095854 0.000672 4.185072
79 0.992990 0.000720 6.652708
79 2.418941 -0.000538 4.292537
79 -1.763815 -0.000774 6.598929
79 -0.338509 0.000096 4.238947

Molecule Au7p-t.log
Energy: -950.825918020
Geometry:
79 -1.239513 0.000016 1.590755
79 1.101984 0.000029 2.880393
79 -1.781607 0.000030 4.208385
79 0.619753 0.000085 5.628912
79 3.108811 -0.000064 4.629433
79 -1.757530 -0.000065 6.870585
79 -2.330159 -0.000031 -0.777014

Molecule Au7p-tt.log
Energy: -950.843432810
Geometry:
79 -2.631506 -0.000001 2.132184
79 -0.024277 0.000001 2.609899
79 -1.935190 0.000001 4.689079
79 0.098162 0.000000 6.530696
79 1.982135 0.000000 4.480929
79 -2.441460 -0.000001 7.347988
79 2.582943 -0.000001 1.881508

Molecule Au8p-a.log
Energy: -1086.74674201
Geometry:
79 -3.090174 -1.265495 1.479248
79 -0.714793 -0.382554 2.322397
79 -2.463064 -1.712672 4.052070
79 2.361229 -0.001702 5.958801
79 1.737038 0.439731 3.384267
79 -0.024704 -0.861662 5.121741
79 -1.821469 -2.144992 6.623904
79 1.091749 0.880591 0.814819

Molecule Au8p-d.log
Energy: -1086.73071867
Geometry:
79 -3.167105 -1.419191 2.820832
79 -0.637561 -0.374765 2.212690
79 -2.123130 0.646272 4.401269
79 0.911867 -2.616761 6.156109
79 1.477020 -1.002743 3.935063
79 -0.009949 0.027417 6.122948
79 0.476807 1.661062 3.851251
79 -1.171692 -2.129113 4.502098

Molecule Au8p-g.log
Energy: -1086.72205204
Geometry:
79 0.825838 0.335632 3.135738
79 -1.704065 0.359904 4.174605
79 0.743503 4.328923 2.664195
79 -0.031396 2.537145 4.771526
79 2.621816 2.462167 3.667106
79 -1.115468 2.200309 2.134756
79 -1.791621 4.438739 3.688958
79 1.552294 2.132177 1.066834

Molecule Au8p-i.log
Energy: -1086.73869621
Geometry:
79 0.644667 1.000604 1.642861
79 -1.882393 2.201909 2.501668
79 -0.412976 4.611421 3.144212
79 0.465131 2.128530 4.235792
79 -0.160809 3.542636 0.619130
79 -1.937624 3.207328 5.033108
79 2.527237 0.606079 3.493505
79 -1.546399 1.181953 -0.003856

Molecule Au9p-b.log
Energy: -1222.62694111
Geometry:
79 -2.777021 -1.598922 2.464437
79 -1.310328 0.743530 1.661422
79 -2.508849 0.510295 4.319064
79 0.720886 -2.595042 5.322458
79 0.101336 -0.951518 3.249255
79 -0.426582 -0.079305 6.129564
79 0.138060 1.680940 3.919875
79 -2.153803 -2.096330 5.169982
79 -0.727972 -3.532906 3.065368

Molecule Au9p-c.log
Energy: -1222.66231880
Geometry:
79 -2.832519 0.089123 2.630678
79 -0.200991 -0.404292 2.028756
79 -1.577067 -1.852486 4.108734
79 1.021878 1.589144 6.229256
79 1.795102 0.365949 3.897805
79 0.414356 -1.074475 5.978759
79 -0.988243 0.970115 4.464549
79 -0.484565 -3.582047 5.822362
79 2.403813 -0.550056 1.466817

Molecule Au9p-d.log
Energy: -1222.63550575
Geometry:
79 -2.294040 -2.575381 3.838787
79 -1.327609 -0.129506 2.679221
79 -1.918342 -0.367128 5.436775
79 2.782891 -1.145594 5.063451
79 1.328705 0.614414 3.317127
79 0.725526 0.375778 6.072632
79 -0.863931 2.073986 4.451235
79 0.306494 -1.950260 4.297294
79 0.812071 -1.345333 1.471194

Molecule Au9p-e.log

Energy: -1222.64294191
Geometry:
79 -1.702827 -1.120234 2.327776
79 -1.701704 -2.728715 4.588879
79 2.171774 1.229129 4.461151
79 0.222072 0.789367 2.367822
79 0.143244 -0.841746 4.529464
79 -0.024828 -2.619740 6.796832
79 2.013119 2.710874 2.197256
79 1.843101 -0.659423 6.630525
79 3.730753 1.174744 6.678340

Molecule Au9p-f.log
Energy: -1222.62164990
Geometry:
79 -1.819414 0.034032 3.454534
79 -1.429748 -2.679832 3.847231
79 1.905754 1.494780 5.904790
79 0.433212 1.615622 3.562814
79 0.312868 -0.710193 4.993765
79 0.422410 -3.168964 6.066860
79 2.175426 -1.274810 6.841738
79 3.886414 0.819370 7.492729
79 -1.468268 -4.976651 5.122584

Molecule Au9p-g.log
Energy: -1222.65209624
Geometry:
79 0.148476 0.325041 3.236553
79 -2.385696 0.270012 4.219014
79 -0.585950 4.177141 2.052994
79 0.391391 4.921261 4.620719
79 1.624990 2.799627 3.450416
79 0.569637 1.974200 0.817909
79 -1.050786 2.618577 4.522944
79 2.647535 0.610293 2.203988
79 -2.004471 1.799084 1.847666

Molecule Au9p-h.log
Energy: -1222.63658415
Geometry:
79 0.439618 0.508914 1.997623
79 -1.647651 2.411437 2.718921
79 -0.394751 4.986475 2.916931
79 -0.498419 0.628189 4.656192
79 1.205489 2.740076 3.717429
79 0.513184 3.206593 0.923457
79 -1.013804 3.390531 5.213521
79 2.882870 1.919561 1.779722
79 -1.564012 1.418688 0.219182

Molecule Aup.log
Energy: -135.454747110
Geometry:
79 0.000000 0.000000 0.000000

Molecule ZnAu5p-a.log
Energy: -2458.71811419
Geometry:
79 -1.262031 -0.001268 1.542600
79 0.980656 -0.000718 2.979445
79 -1.627398 -0.000143 4.180737
79 2.994447 0.000259 4.746571
79 -1.593462 0.001481 6.859828
30 0.623115 0.000388 5.635702