QM Methods

Perturbation Methods	Reference Methods	Local Gradient Corrected Methods	Hybrid Methods	Meta GGA / Hybrid Meta GGA Methods
MP2	CCSD	HFS	B1LYP	TPSS
RI-MP2	CCSD(T)	LDA	B3LYP	TPSSh
SCS-MP2	CCSD-F12	VWN	O3LYP	TPSS0
RI-SCS-MP2	CCSD(T)-F12	VWN3	X3LYP	M06L
OO-RI-MP2	CCSD-F12/RI	PWLDA	B1P	M06
OO-RI-SCS-MP2	CCSD-F12D/RI	BP86	B3P	M062X
MP2-F12	CCSD(T)-F12/RI	BLYP	B3PW	PW6B95
MP2-F12-RI	CCSD(T)-F12D/RI	OLYP	PW1PW	B97M-V
MP2-F12D-RI	QCISD	GLYP	mPW1PW	B97M-D3BJ
-	QCISD(T)	XLYP	mPW1LYP	B97M-D4
-	QCISD-F12	PW91	PBE0	PBE0
-	QCISD(T)-F12	mPWPW	REVPBE0	SCANfunc
-	QCISD-F12/RI	mPWLYP	REVPBE38	-
-	QCISD(T)-F12/RI	PBE	BHANDHLYP	-
-	CPF/1	RPBE	-	-
-	NCPF/1	REVPBE	-	-
-	CEPA/1	RPW86PBE	-	-
-	NCEPA/1	PWP	-	-
-	RI-CEPA/1-F12	-	-	-
-	MP3	-	-	-
-	SCS-MP3	-	-	-

Pople Basis Sets	Pople Polarized Basis Sets	Pople Polarized Diffused Basis Sets	Correlation Consistent Basis Sets	DEF2 Basis Sets	DEF2 Diffused Basis Sets
STO-3G	6-31G(d)	6-31+G(d)	cc-pVDZ	def2-SVP	ma-def2-SVP
3-21G	6-31G(d,p)	6-31+G(d,p,)	cc-pVTZ	def2-SVP(P)	ma-def2-SV(P)
3-21GSP	6-31G(2d)	6-31+G(2d)	cc-pVQZ	def2-TZVP	ma-def2-TZVP
4-22GSP	6-31G(2df)	6-31+G(2df)	cc-pV5Z	def2-TZVP(-f)	ma-def2-TZVP(-f)
6-31G	6-31G(2d,p)	6-31+G(2d,p)	cc-pV6Z	def2-TZVPP	ma-def2-TZVPP
m6-31G	6-31G(2d,2p)	6-31+G(2d,2p)	aug-cc-pVDZ	def2-QZVP	ma-def2-QZVPP
6-311G	6-31G(2df,2p)	6-31+G(2df,2pd)	aug-cc-pVTZ	def2-QZVPP	def2-SVPD
-	6-31G(2df,2pd)	6-311+G(d)	aug-cc-pVDZ	SV	def2-TZVPD
-	6-311G(d)	6-311+G(d,p)	aug-cc-pV5Z	SV(P)	def2-TZVPPD
-	6-311G(d,p)	6-311+G(2d)	aug-cc-pV6Z	SVP	def2-QZVPD
-	6-311G(2d)	6-311+G(2df)	cc-pCVDZ	TZV	def2-QZVPPD
-	6-311G(2d,p)	6-311+G(2d,p)	cc-pCVTZ	TZV(P)	-
-	6-311G(2d,2p)	6-311+G(2d,2p)	cc-pCVQZ	TZVP	-
-	6-311G(2df,2pd)	6-311+G(2df,2p)	cc-pCV5Z	TZVPP	-
-	6-311G(3df)	6-311+G(2df.2pd)	cc-pCV6Z	QZVP	-
-	6-311G(3df,3pd)	6-311+G(3df)	aug-cc-pCVDZ	QZVPP	-
-	-	6-311+G(3df,3pd)	aug-cc-pCVTZ	-	-
-	-	6-31++G(d,p)	aug-cc-pCVQZ	-	-
-	-	6-31++G(2d,p)	aug-cc-pCV5Z	-	-
-	-	6-31++G(2d,2p)	aug-cc-pCV6Z	-	-
-	-	6-31++G(2df,2p)	cc-pwCVDZ	-	-
-	-	6-31++G(2df,2pd)	cc-pwCVTZ	-	-
-	-	6-311++G(d,p)	cc-pwCVQZ	-	-
-	-	6-311++G(2d,p)	cc-pwCV5Z	-	-
-	-	6-311++G(2d,2p)	aug-cc-pwCVDZ	-	-
-	-	6-311++G(2df,2p)	aug-cc-pwCVTZ	-	-
-	-	6-311++G(2df,2pd)	aug-cc-pwCVQZ	-	-
-	-	6-311++G(3df,3pd)	aug-cc-pwCV5Z	-	-
-	-	-	cc-pVD(+d)Z	-	-
-	-	-	cc-pVT(+d)Z	-	-
-	-	-	cc-pVQ(+d)Z	-	-
-	-	-	cc-pV5(+d)Z	-	-

Auxiliary Coulomb Fit Basis Sets	Auxiliary Coulomb Fit / Exchange Basis Sets	Auxiliary Correlation Consistent Basis Sets
Def2/J	Def2/JK	Def2-SVP/C
f2/JKsmall	Def2/JKsmall	Def2-TZVP/C
x2c/J	cc-pVTZ/JK	Def2-TZVPP/C
-	cc-pVQZ/JK	Def2-QZVPP/C
-	cc-pV5Z/JK	Def2-SVPD/C
-	aug-cc-pVTZ/JK	Def2-TZVPD/C
-	aug-cc-pV5Z/JK	Def2-TZVPPD/C
-	-	Def2-QZVPPD/C
-	-	cc-pVDZ/C
-	-	cc-pVTZ/C
-	-	cc-pVQZ/C
-	-	cc-pV5Z/C
-	-	cc-pV6Z/C
-	-	aug-cc-pVDZ/C
-	-	aug-cc-pVTZ/C
-	-	aug-cc-pVQZ/C
-	-	aug-cc-pV5Z/C
-	-	aug-cc-pV6Z/C
-	-	cc-pwCVDZ/C
-	-	cc-pwCVTZ/C
-	-	cc-pwCVQZ/C
-	-	cc-pwCV5Z/C
-	-	aug-cc-pwCVDZ/C
-	-	aug-cc-pwCVTZ/C
-	-	aug-cc-pwCVQZ/C
-	-	aug-cc-pwCV5Z/C
-	-	cc-pVDZ-PP/C
-	-	cc-pVTZ-PP/C
-	-	cc-pVQZ-PP/C
-	-	aug-cc-pVDZ-PP/C
-	-	aug-cc-pVTZ-PP/C
-	-	aug-cc-pVQZ-PP/C
-	-	cc-pVDZ-F12-MP2fit
-	-	cc-pVTZ-F12-MP2fit
-	-	cc-pVQZ-F12-MP2fit
-	-	cc-pCVDZ-F12-MP2fit
-	-	cc-pCVTZ-F12-MP2fit
-	-	cc-pCVQZ-F12-MP2fit
-	-	cc-pVDZ-PP-F12-MP2fit
-	-	cc-pVTZ-PP-F12-MP2fit
-	-	cc-pVQZ-PP-F12-MP2fit
-	-	aug-cc-pwCVDZ-PP/C
-	-	aug-cc-pwCVTZ-PP/C
-	-	aug-cc-pwCVQZ-PP/C
-	-	cc-pwCVDZ-PP/C
-	-	cc-pwCVTZ-PP/C
-	-	cc-pwCVQZ-PP/C

QM2 Methods

QM2 Semiempirical Methods		Tight Binding DFT Methods		Composite Methods	
	AM1		XTB		HF-3C
	PM3		XTB1		PBEH-3C
	-		-		R2SCAN-3C

QM/QM2 Charge Methods

QM / QM2 Charge Methods
HIRSHFELD
CHELPG
MULLIKEN
LOEWDIN