Quantum Chemistry Advisor

Quantum Chemistry packages comparison

Software packages availability

Information about the newest quantum chemistry software versions available on PL-Grid clusters. See also PL-Grid Infrastructure - scientific software availability.

HPC Centre	Gaussian	Turbomole	GAMESS	NWChem	ORCA	Terachem	ADF	CFOUR	CP2K	CPMD	Crystal09	Dalton	DFT-D3	Molcas
ACK CYFRONET AGH	09.D1	6.6	2013.R1	6.3		1.5	2013.01	1.0	2.5.1	3.17.1		2013.1	3.0.2	
ICM UW	09.D1		2012.R2					1.0						
PSNC	09.D1		2009.R3	6.0				1.0		3.13.2				
CI TASK	09.D1		2012.R2	6.1.1				1.0				2.0		
WCSS	09.D1	6.6	2013.R1	6.5	3.0.1?		2013.01	1.0	2.5.1	3.13.2	2.0.1	2013		7.8

Software packages capabilities

Legend

In all tables below symbols have meaning shown in legend:

Symbol	Meaning
energy	electronic energy calculations only
grad	analytic algorithm of computing gradients
num grad	numerical differentiation for computing gradients
freq	analytic algorithm of computing vibrational frequencies
num freq	numerical differentiation for computing vibrational frequencies
RI	Resolution of Identity/Density Fitting algorithm available

Self-consistent ab initio and DFT methods (in vacuum)

Method	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
RHF	freq	freq	grad	freq	freq	freq	grad	
UHF	freq	freq	grad	grad	freq	freq	grad	
ROHF	freq	freq	grad	freq	grad	freq	grad	
DFT	freq^{RI}	freq^{RI}	grad^{RI}	grad	freq	freq^{RI}	grad	freq

Post-HF methods (in vacuum)

Method	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
MP2	freq	freq^{RI}	grad^{RI}	grad	grad	num grad^{RI}		
MP3	freq	energy	num grad					
MP4+	num grad	energy	num grad					
CIS	freq		num grad	energy	energy	grad		
CI	grad		num grad	grad	energy	num grad^{RI}		
CC2		freq^{RI}						
CCSD	num freq	energy^{RI}	grad	energy	energy	num grad^{RI}		
CCSD+T(CCSD)					energy			
CCSD(T)		energy^{RI}	num grad	energy	energy	num grad^{RI}		

QCISD	num freq		grad			num grad^{RI}		
QCISD(T)	num grad		grad			num grad^{RI}		
CASSCF	freq		grad	energy	grad	num grad		

Methods of solvents or environment treatment

Method	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
PCM	x			x				
Onsager model	x							
EFP				x				
COSMO		x	x		x	x		x

Self-consistent ab initio and DFT methods (in solvents)

Method	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
RHF	freq	num freq	grad	grad	num grad	grad		
UHF	freq	num freq	grad	grad	num grad	grad		
ROHF	freq	num freq	grad	grad	num grad	grad		
DFT	freq	num freq^{RI}	grad^{RI}	grad	num grad	grad^{RI}		freq

Post-HF methods (in solvents)

Method	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
MP2	freq	num freq^{RI}		grad	energy			
MP3	freq	energy						
MP4+		energy						
CIS	freq							
CI								
CC2		num freq^{RI}						
CCSD	num freq	energy^{RI}		energy	energy			
CCSD+T(CCSD)					energy			
CCSD(T)		energy^{RI}			energy			
QCISD	num freq							
QCISD(T)								
CASSCF	freq			energy				

Available DFT functionals

Exchange Functionals

Could be used with correlation functionals from table below

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
S	x	x	x	x	x	x	x	x
Xa	x					x		x
B	x	x	x	x	x	x	x	x
BR			x					
PW86			x		x			x
PW91	x		x	x	x	x		x
mPW	x					x		x
G96	x		x	x	x	x		
PBE	x	x	x	x	x	x	x	x
PBE96					x		x	x
O	x			x	x	x		x

TPSS	x					x		x
RevTPSS	x			x				x
BRx	x							
PKZB	x							
PBEh	x							
LHF		x	x		x			
OEP		x						
CS1			x					
CS2			x					
HTBS								x
BEE								x

Correlation Functionals

Could be used with exchange functionals from table above

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
VWN	x	x	x	x	x	x	x	x
VWN5	x	x	x	x	x	x		x
LYP	x	x	x	x	x	x	x	x
PL	x							
P86	x	x		x	x			x
PW91	x		x	x	x	x		x
PW92			x					x
PZ81				x				
OP				x	x		x	
B88			x		x			
B95	x		x		x			x
PBE	x	x	x	x	x	x	x	x
TPSS	x	x		x	x	x		x
RevTPSS	x			x				x
KCIS	x							
BRC	x							
PKZB	x							

Exchange-Correlation Functionals

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
VSXC	x				x			
HCTH/*	x		x	x	x			
tHCTH	x							
M06L	x		x					
M08			x					
B97D	x							
BW			x					
SOGGA			x	x	x			
SOGGA11	x		x	x	x			
M11L	x			x				
MN12L	x							
N12	x							
THGFL			x					
THGFCO			x					
TH1			x					
TH2			x					
TH3			x					
TH4			x					

Hybrid Functionals

Functionals which include of Hartree-Fock exchange with DFT exchange-correlation

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
B3LYP	x	x		x	x	x	x	x
B3P86	x			x				
B3PW91	x			x				
B1LYP	x					x		x
B1B95	x					x		
B97			x	x	x	x	x	
B98	x			x	x			
B971	x							
B972	x							
PBE1PBE	x							
PBE0	x	x		x	x	x	x	x
HSEH1PBE (HSE06)	x							
PBEh1PBE	x							
O3LYP	x					x		
TPSSh	x	x		x		x		x
TPSS0						x		
BMK	x			x				
M05	x		x	x	x			
M052X	x			x	x			
M06	x		x	x	x			x
M06L			x	x	x			x
M06HF	x		x	x	x			x
M062X	x		x	x	x			x
M08			x	x	x			
X3LYP	x			x		x		x
BHandH	x				x			x
BHandHLYP	x				x	x		x
APFD	x							
HISSbPBE	x							
M11	x		x	x				
SOGGA11X	x			x	x			
N12SX	x							
MN12SX	x							

Functionals which include dispersion

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
APFD	x							
B97D	x	x		x		x		
B97D3	x					x		
wB97xD	x							
DFT-D2, DFT-D3 correcion	x	x		x	x		x	x
SSB-D								x
S12g								x

Long range corrected functionals

Functional	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
LC-wPBE	x			x	x			
CAM-B3LYP	x			x	x	x	x	x

wB97XD	x			x		x		
wB97X	x			x		x	x	
wB97	x			x		x	x	
LC-BLYP	x			x	x	x		
LC-PBE0	x				x			
LC-PBE					x			
BNL					x			
LC-wPBEh					x			
HSE03	x				x			
HSE06	x				x			

Basis sets

Types of basis sets

Basis set type	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem	ADF
GTO	x	x	x	x	x	x	x	
STO								x
PW					x			

In table below basis sets native for software package are listed. More could be obtained from EMSL Basis Set Exchange.

Basis set	Gaussian	Turbomole	Molpro	GAMESS	NWChem	ORCA	Terachem
STO-*n*G	H-Xe		H-Ne	H-Xe	H-I		H-Cd
3-21G	H-Xe (+)	H-Ar	H-Te	H-Xe	H-Xe	H-Xe	H-Cs
6-21G	H-Cl (*,**)			H-Ar	H-Zn	H-Cl	
4-31G	H-Ne (*,**)			H-Ne, P-Cl	H-Cl		H-Ar
6-31G	H-Kr (*,**,+,++)	H-Ar (*)		H-Kr	H-Ca		H-Zn
6-311G	H-Kr (*,**,+,++)	H-Ar, Ga-Kr (*, **)		H-Ne	H-I		H-Kr
D95	H-Cl (without Na and Mg;*,**,+, ++)			H-Al	H-Cl		H-Cl
D95V	H-Ne (*,**,+,++)			H,Li, Be-Ne, Al-Cl, K-Kr		H-Ne	
LanL2DZ	H, Li-La, Hf-Bi	K-Au			H, Li-La, Hf-Bi	H, Li-La, Hf-Bi	
(aug-)cc-pVDZ	(H-Ar, Sc-Kr), H-Ar, Ca-Kr	H-Hg	H-Kr	H-Li, Be-Ne, Na-Ar, K-Ca	H-Kr	H-Kr	H-Zn
(aug-)cc-pVTZ	(H-Ar, Sc-Kr), H-Ar, Ca-Kr	H-Hg	H-Kr	H-Li, Be-Ne, Na-Ar, K-Ca, Sc-Zn	H-Kr	H-Kr	H-Kr
(aug-)cc-pVQZ	(H-Ar, Sc-Kr), H-Ar, Ca-Kr	H-Hg	H-Kr	H-Li, Be-Ne, Na-Ar, K-Ca, Sc-Zn	H-Kr	H-Kr	H-Kr
(aug-)cc-pV5Z	(H-Na, Al-Ar Sc-Kr), H-Ar, Ca-Kr	H-Hg	H-Kr	H-Li, Be-Ne, Na-Ar, K-Ca	H-Kr	H-Kr	H-Kr
(aug-)cc-pV6Z	(H, B-O),H, B-Ne			H-Li, Be-Ne, Na-Ar, K-Ca	H-Ar	H-Ar	
(aug-)cc-pCVDZ		H-Kr	H-Kr	H-Ar	Li-Ar	H-Ar	H-Zn
(aug-)cc-pCVTZ		H-Kr	H-Kr	H-Ar	Li-Ar	H-Ar	H-Kr
(aug-)cc-pCVQZ		H-Kr	H-Kr	H-Ar	Li-Ar	H-Ar	H-Zn
(aug-)cc-pCV5Z		H-Kr	H-Kr	H-Ne	B-Ar	H-Ne	
(aug-)cc-pCV6Z			H-Ar		B-Ar		
SV and SVP	H-Kr	H-Kr	H-Kr		H-Kr	H-Ar	H-Ne
TZV and TZVP	H-Kr	H-Kr	H-Kr	H, Li, Be-Ne, Na-Ar, K-Ca, Sc-Zn	H-Kr	H-Ar	H-Ne
QZVP	H-La, Hf-Rn	H-Kr	H-Kr			H-Ar	
def2-SV/SVP	H-La, Hf-Rn	H-Rn	H-Rn		H-Rn		
def2-TZVP/TZVPP	H-La, Hf-Rn	H-Rn	H-Rn		H-Rn		
def2-QZVP/QZVPP	H-La, Hf-Rn	H-Rn	H-Rn		H-Rn		
EPR-II, EPR-III	H, B, C, N, O, F					H, B, C, N, O, F	
IGLO-II, IGLO-III						H,C,N,O,F, Al, Si, P, S, Cl	H,C,N,O,F, Al, Si, P, S, Cl

def2-SVPD		H-Rn	H-Rn		H-Rn		
def2-TZVPD /TZVPPD		H-Rn	H-Rn		H-Rn		
def2-QZVPD /QZVPPD		H-Rn	H-Rn		H-Rn		