# 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 | | |