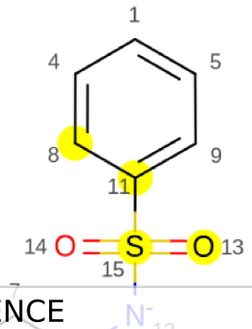
Charged molecule



Relative energies in kcal/mol

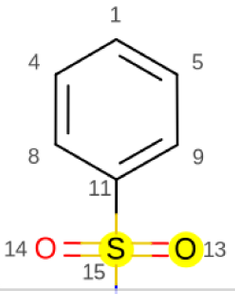
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

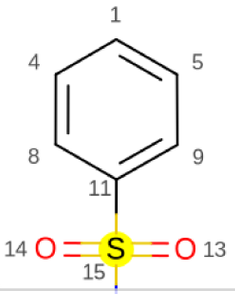


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

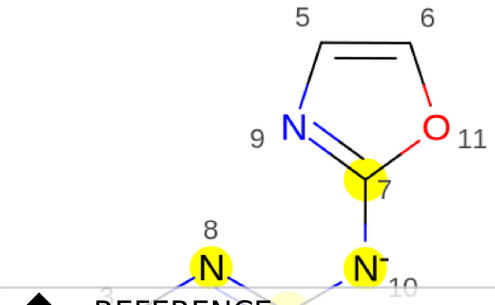


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

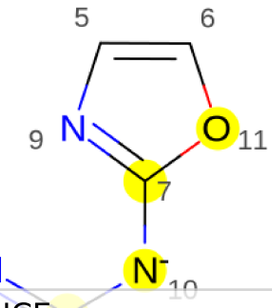


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

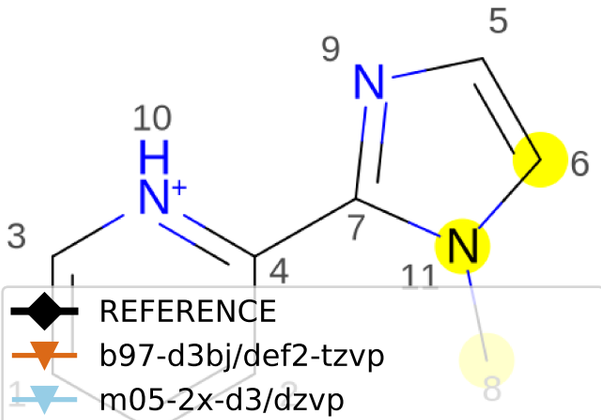


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

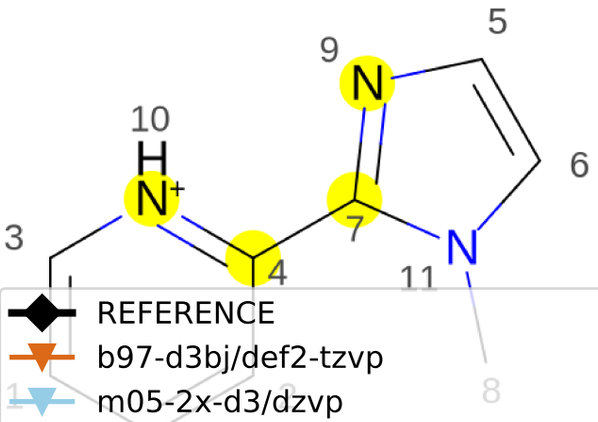


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

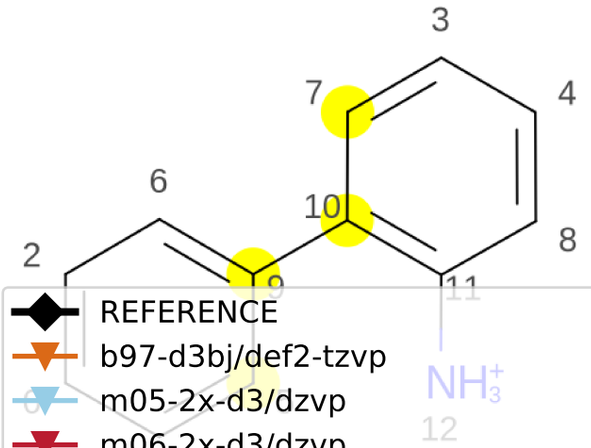


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

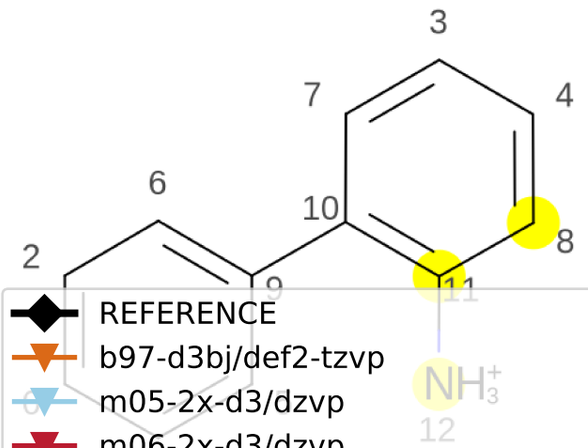


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

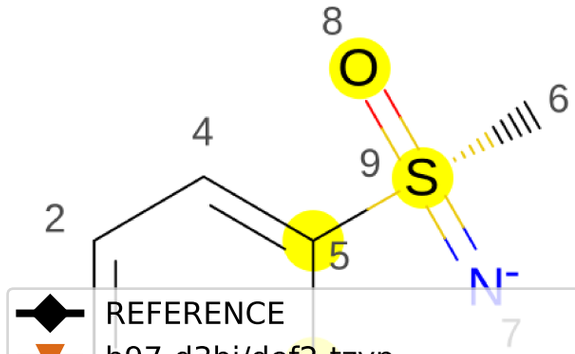


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

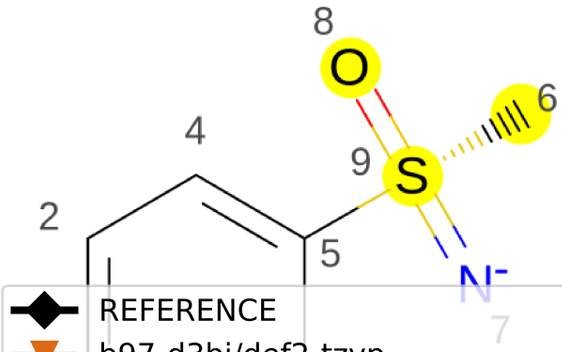


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule



Relative energies in kcal/mol

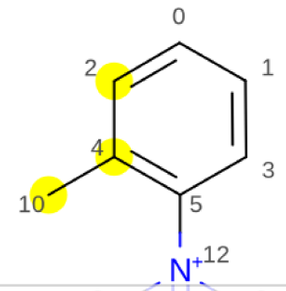
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule



Relative energies in kcal/mol

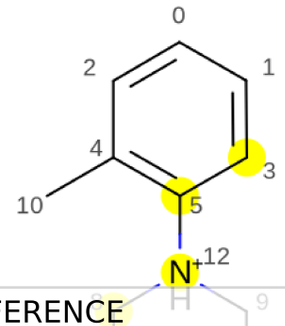
1.50
1.25
1.00
0.75
0.50
0.25
0.00

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

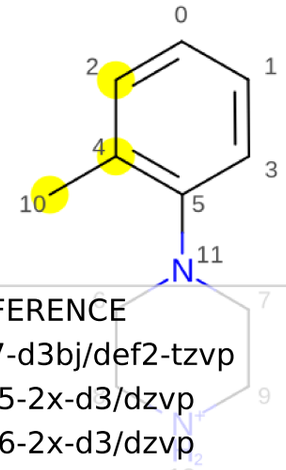


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

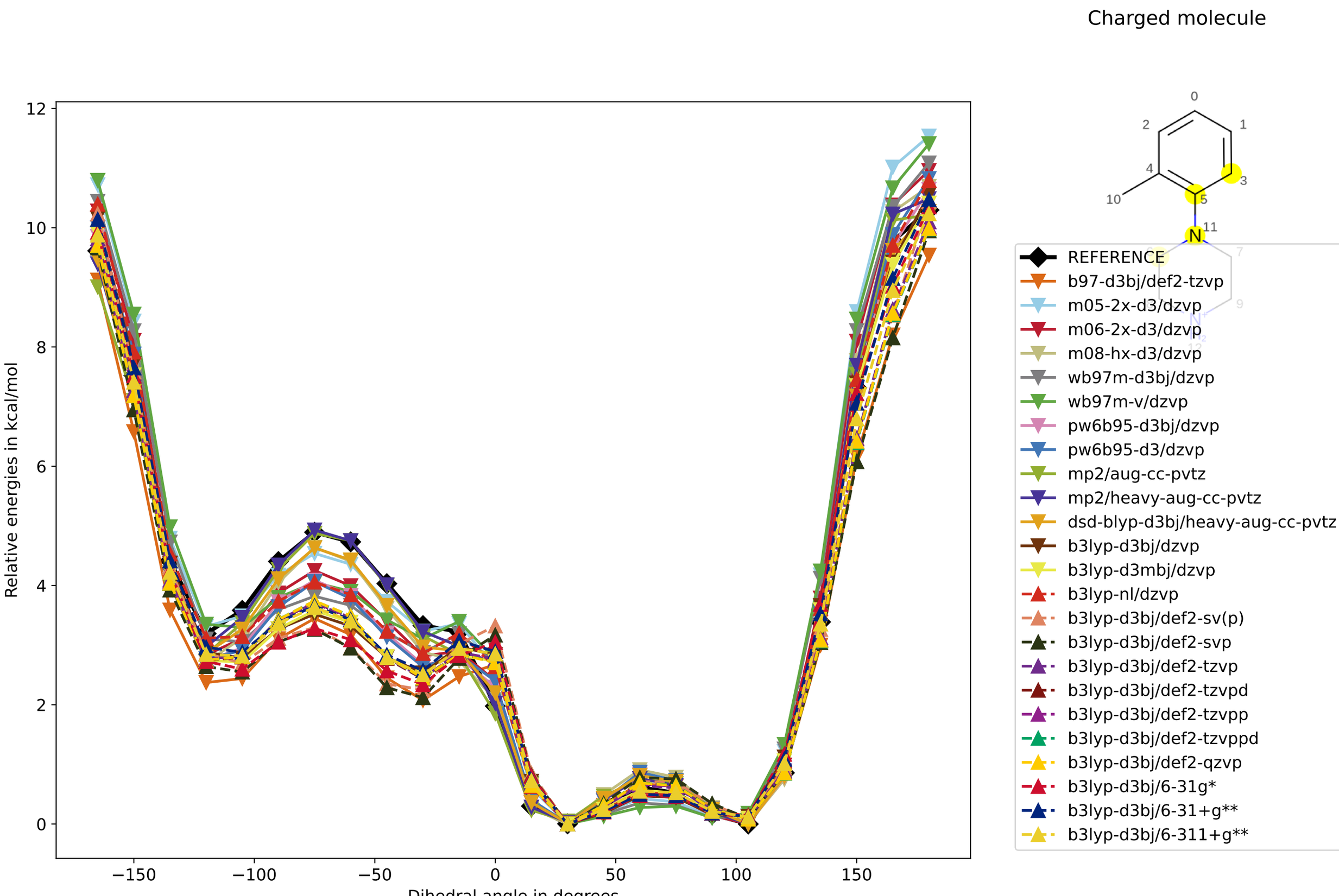
Charged molecule



Relative energies in kcal/mol

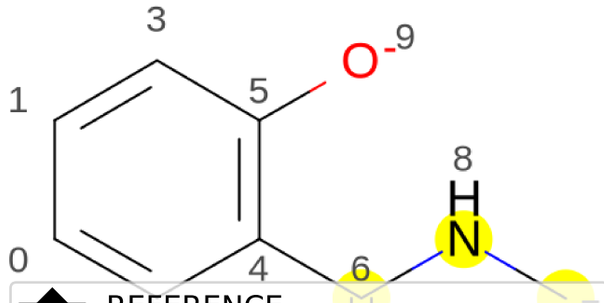
Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**



Charged molecule
Relative energies in kcal/mol
Dihedral angle in degrees
12
10
8
6
4
2
0
−150
−100
−50
0
50
100
150
0
1
2
3
4
5
10
11
N
REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

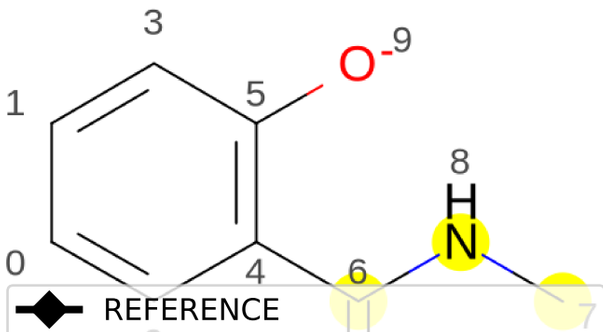


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule



Relative energies in kcal/mol

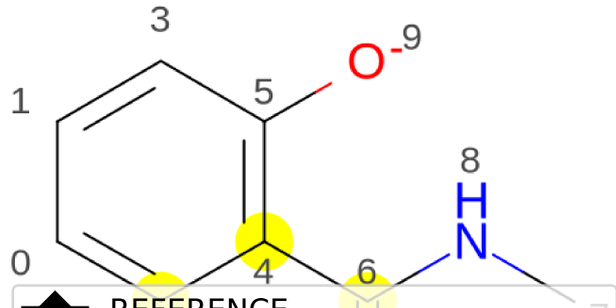
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

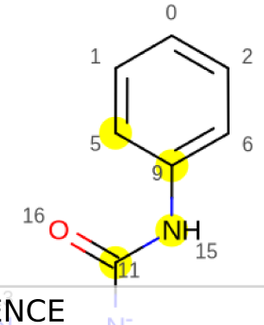


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule



REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
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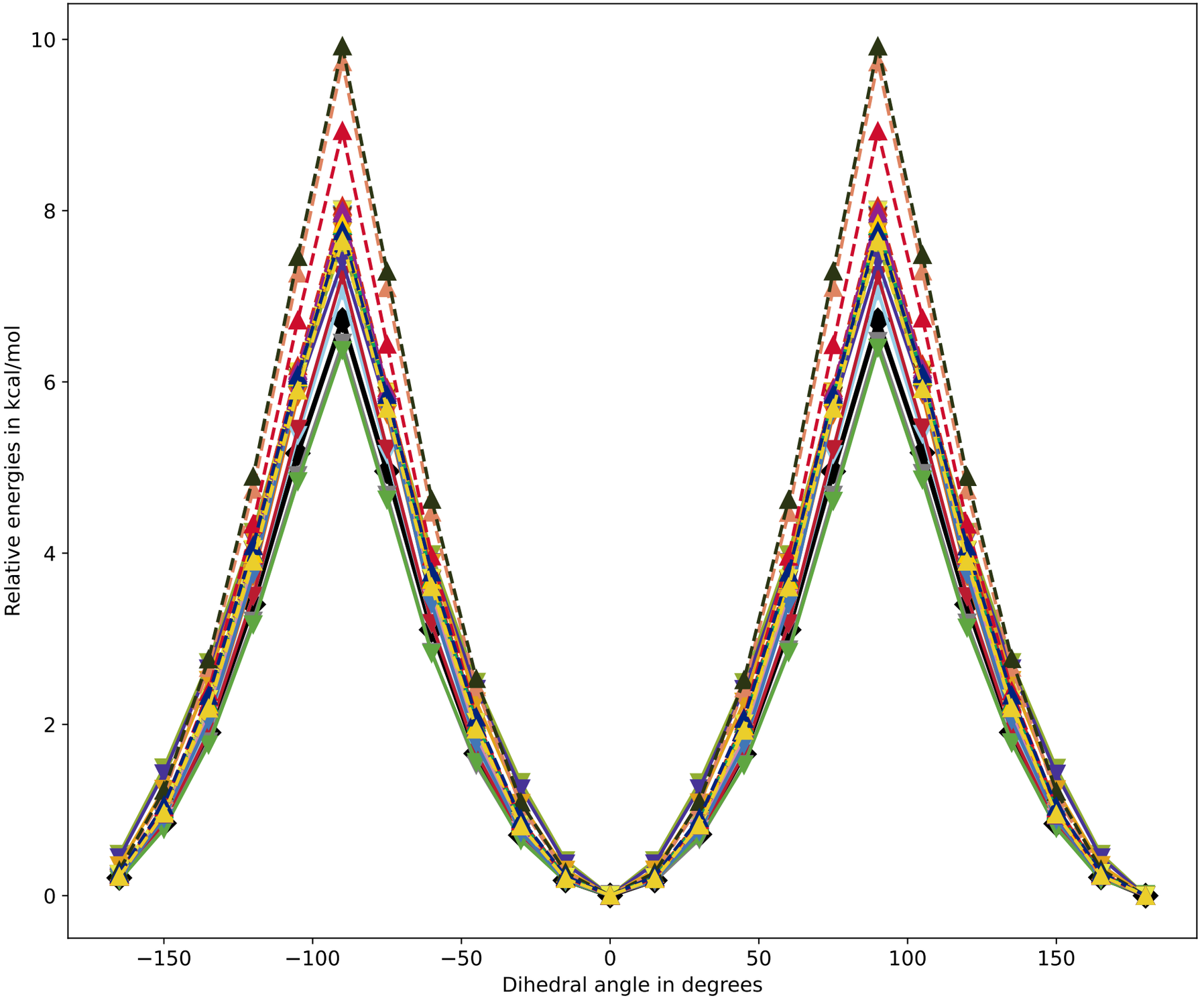
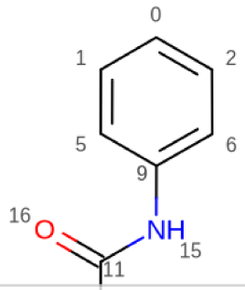
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**



Charged molecule



Relative energies in kcal/mol

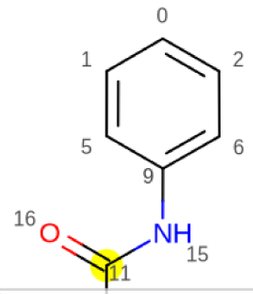
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-d3mbj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-sv(p)
- b3lyp-d3bj/def2-svp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31g*
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule

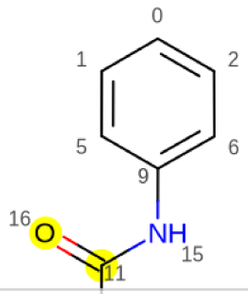


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

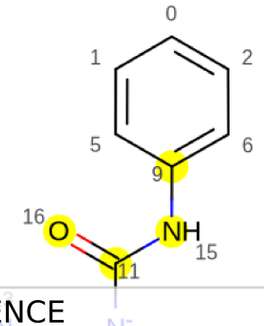


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

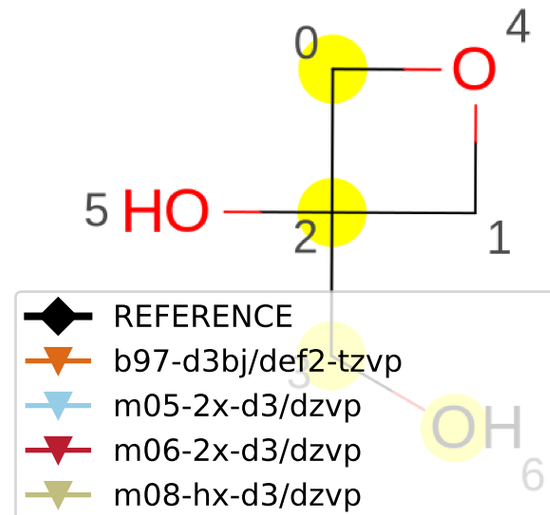


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

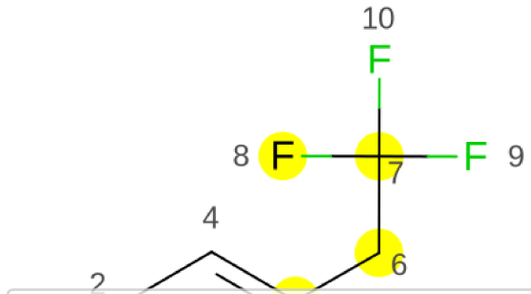


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule



Relative energies in kcal/mol

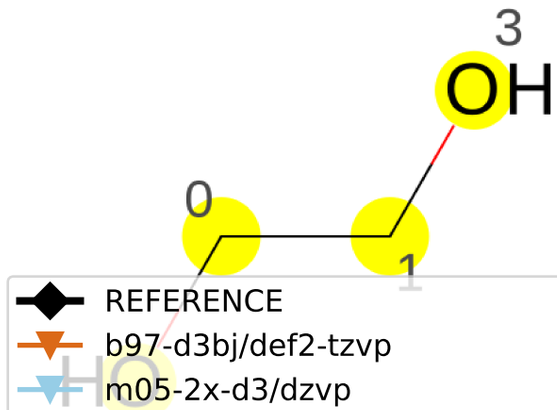
Dihedral angle in degrees

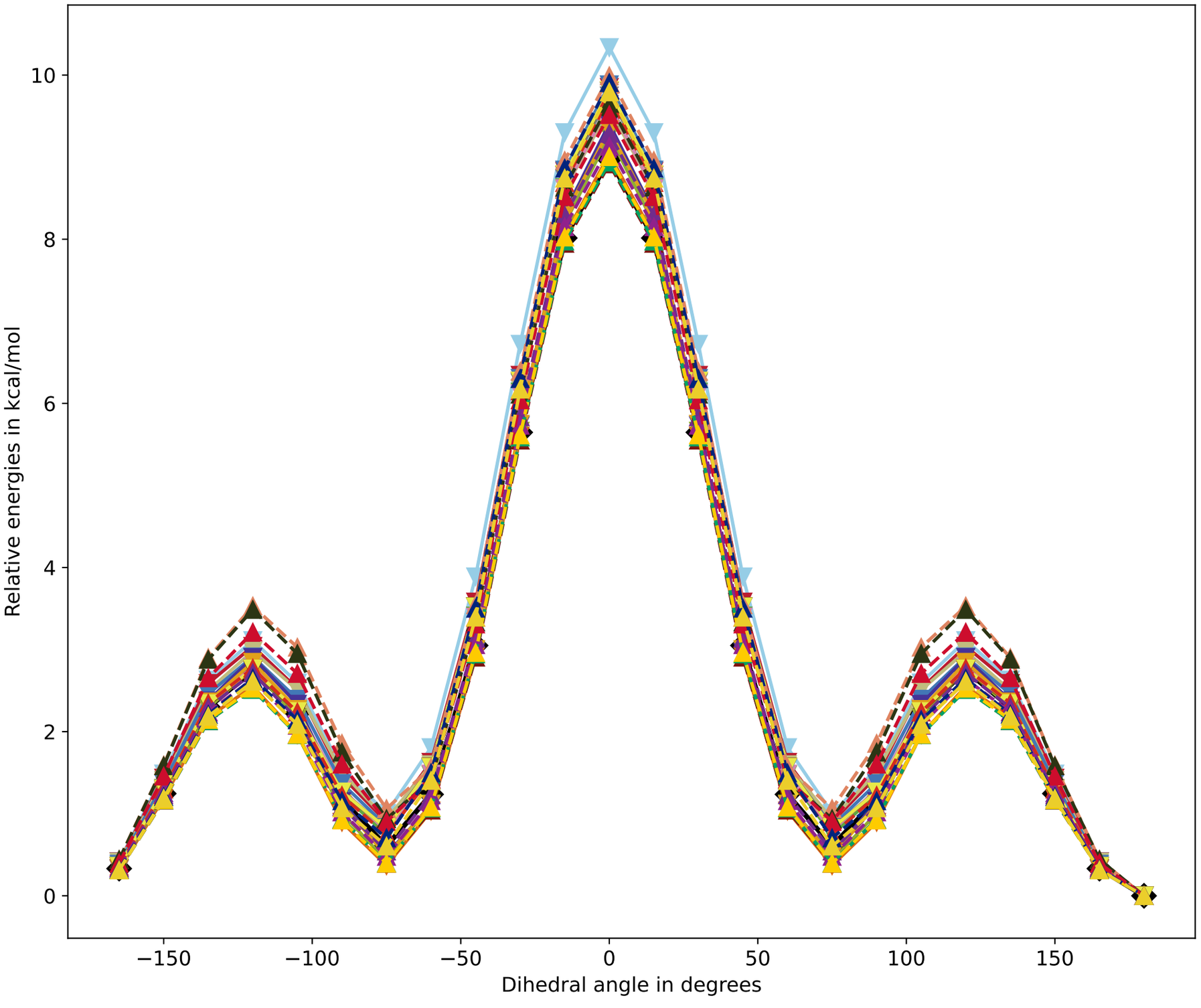
−150 −100 −50 0 50 100 150

0 1 2 3 4

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

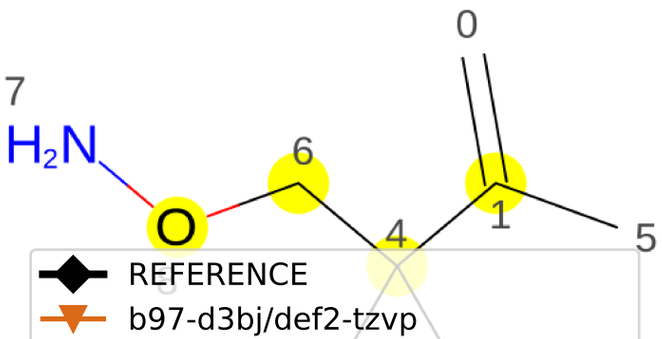
Neutral molecule





- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-d3mbj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-sv(p)
- b3lyp-d3bj/def2-svp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31g*
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule

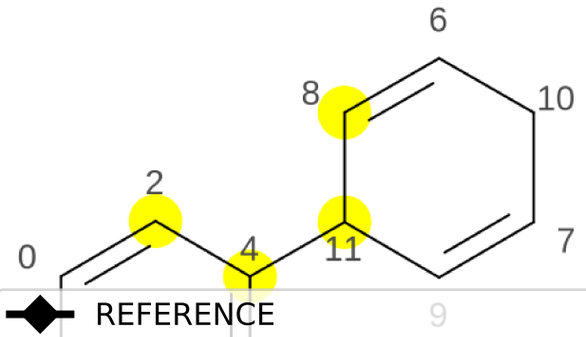


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

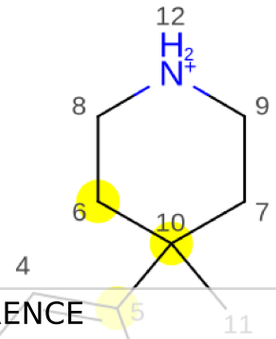


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

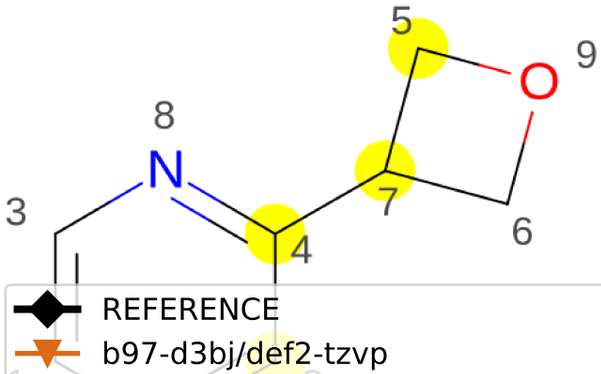


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule



Relative energies in kcal/mol

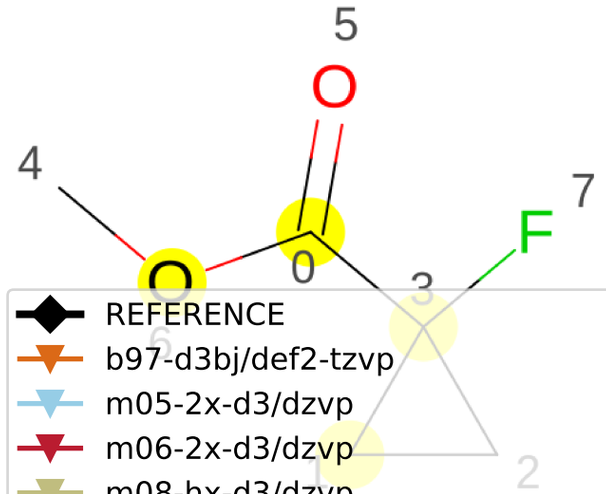
3.0
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

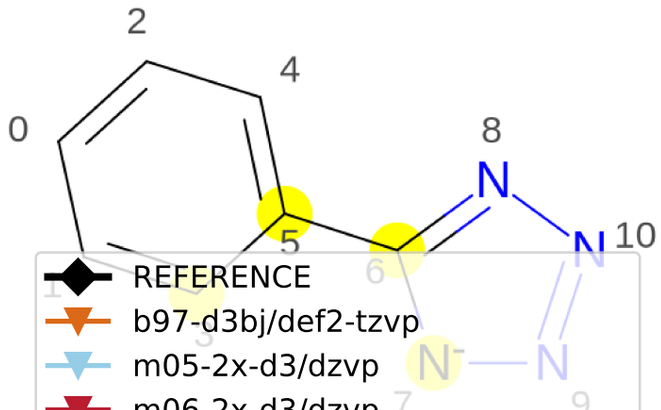


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

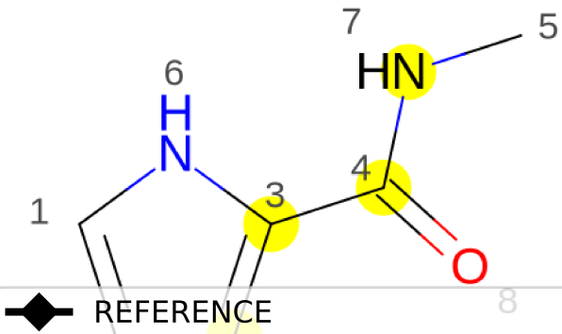


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

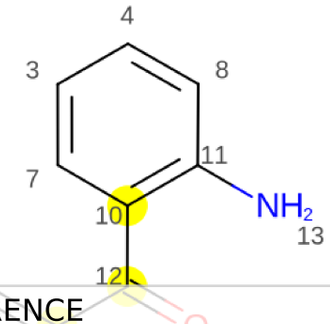


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

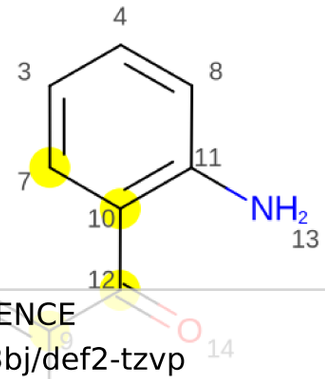


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

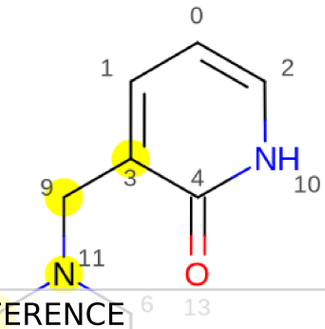


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

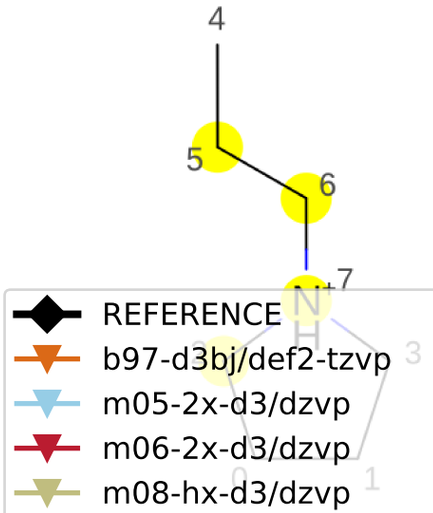


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule

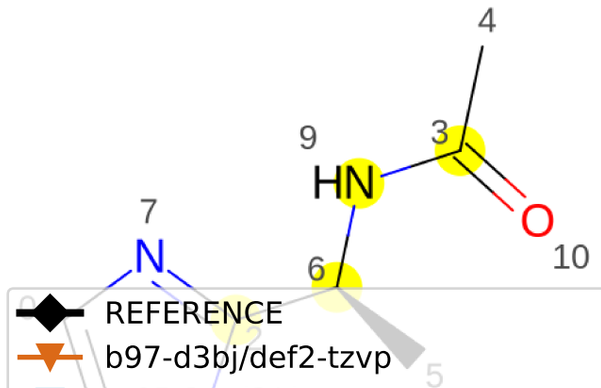


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

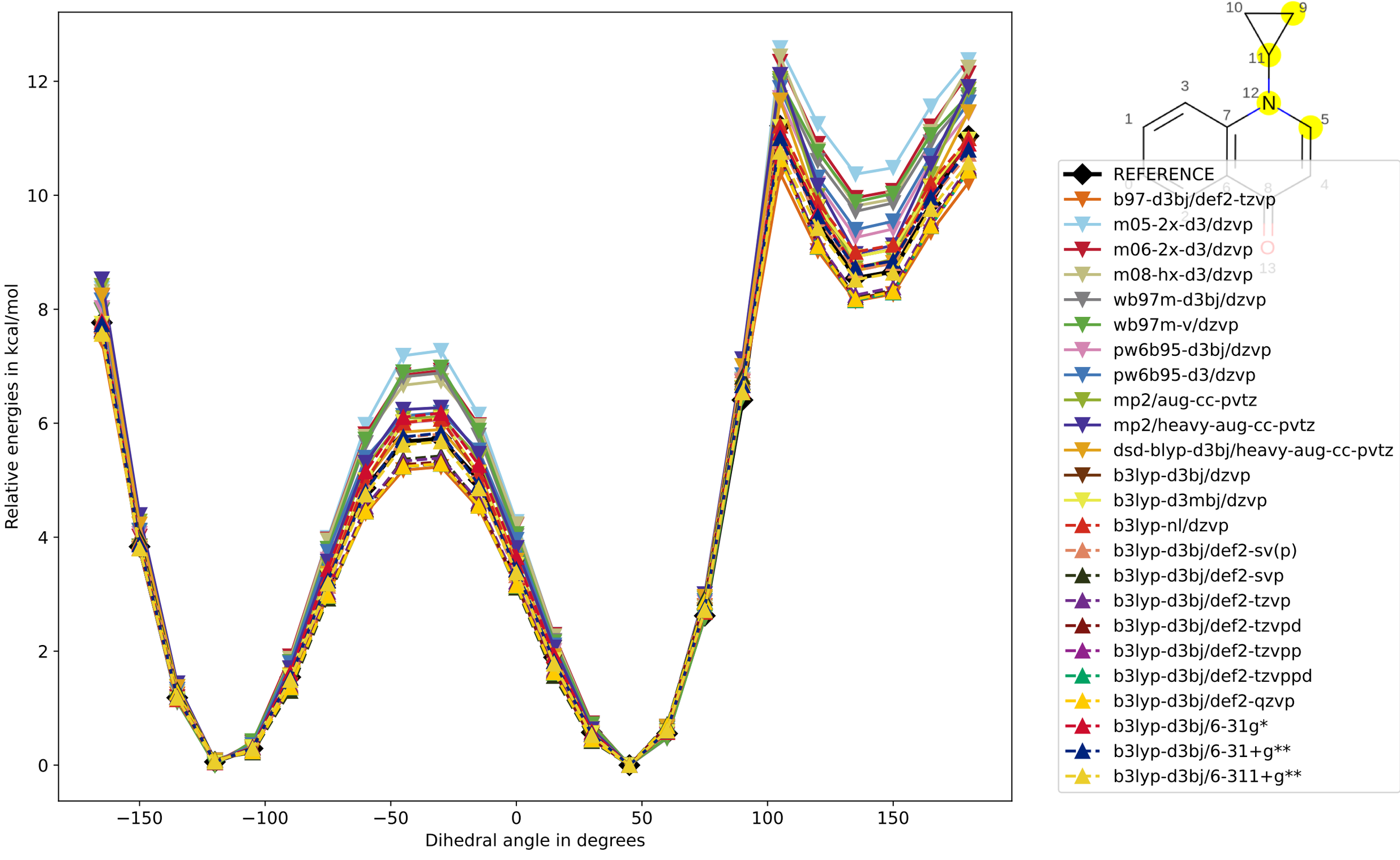


Relative energies in kcal/mol

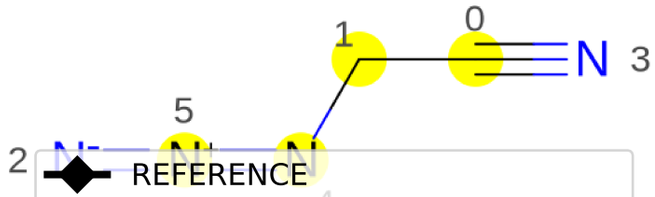
Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule



Charged molecule



Relative energies in kcal/mol

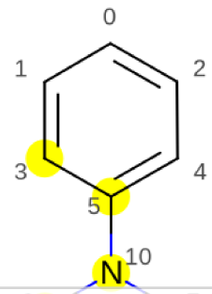
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Charged molecule



Relative energies in kcal/mol

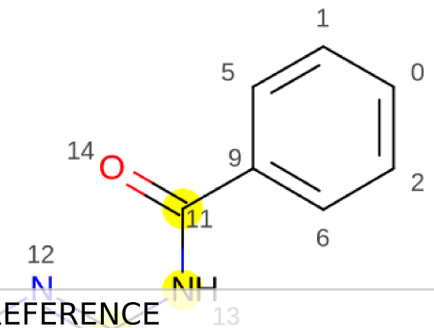
3.0
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

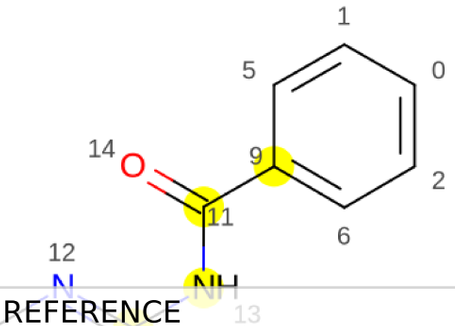


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

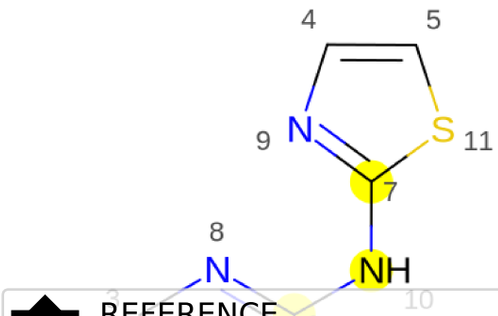


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

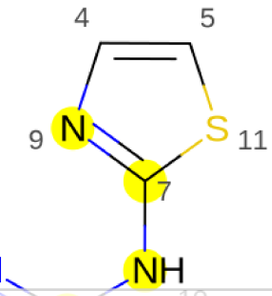


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

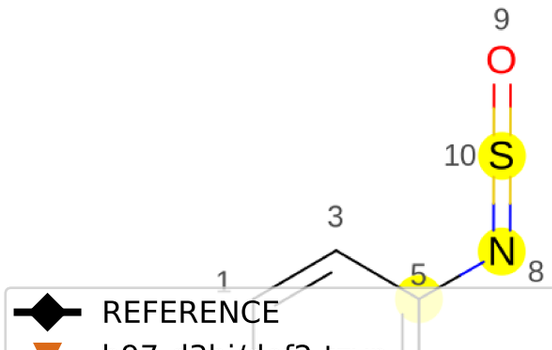


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule



Relative energies in kcal/mol

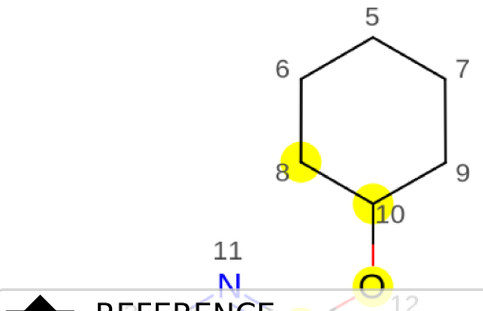
3.0
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

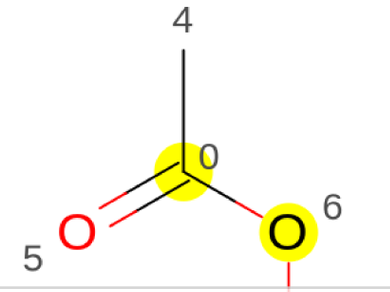


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

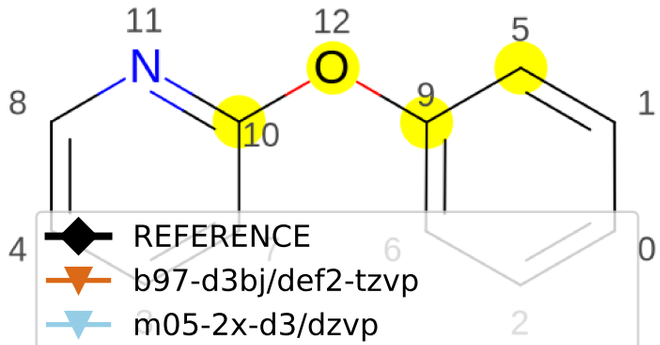


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule



Relative energies in kcal/mol

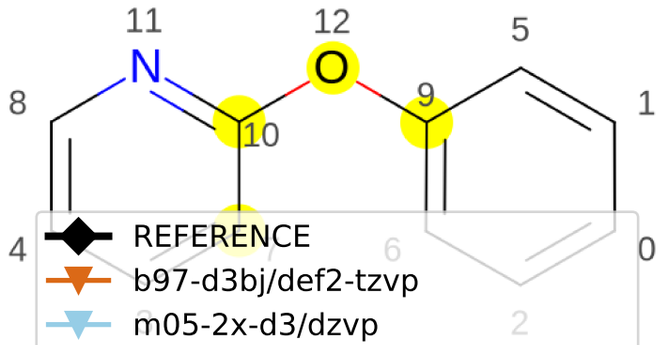
2.5
2.0
1.5
1.0
0.5
0.0

−150
−100
−50
0
50
100
150

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

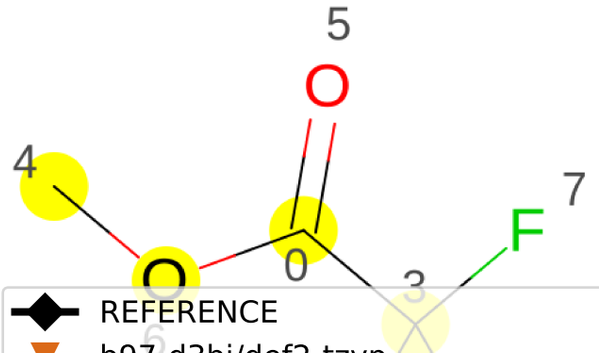


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

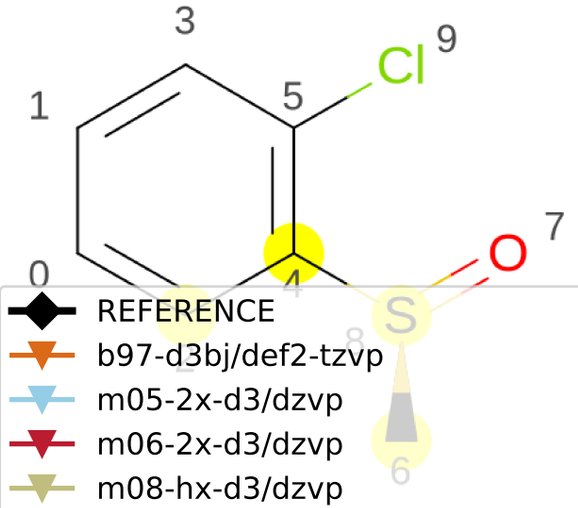


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

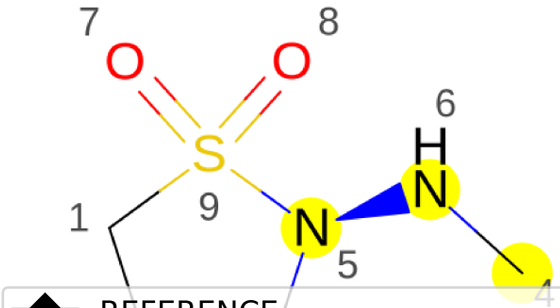


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

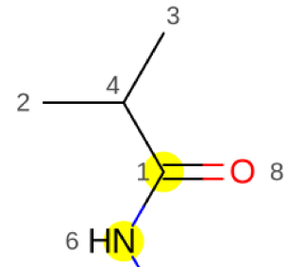


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

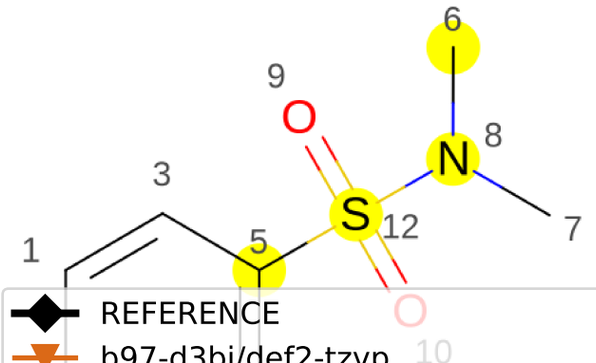


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

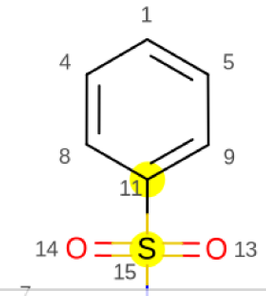


Relative energies in kcal/mol

Dihedral angle in degrees

- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-d3mbj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-sv(p)
- b3lyp-d3bj/def2-svp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31g*
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule

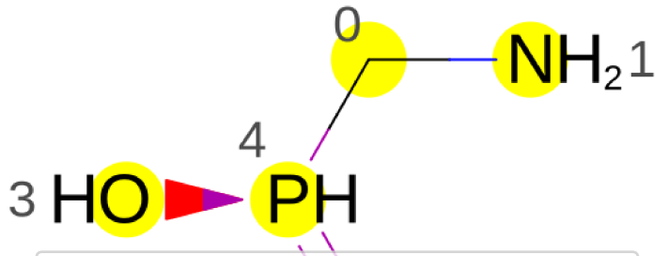


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

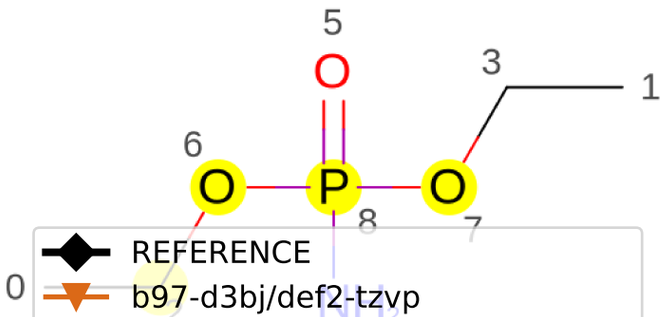


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

Neutral molecule

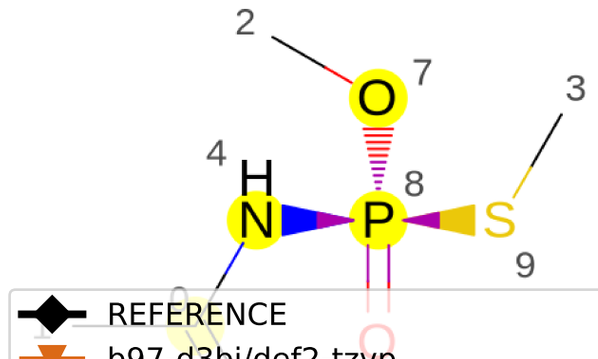


Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**

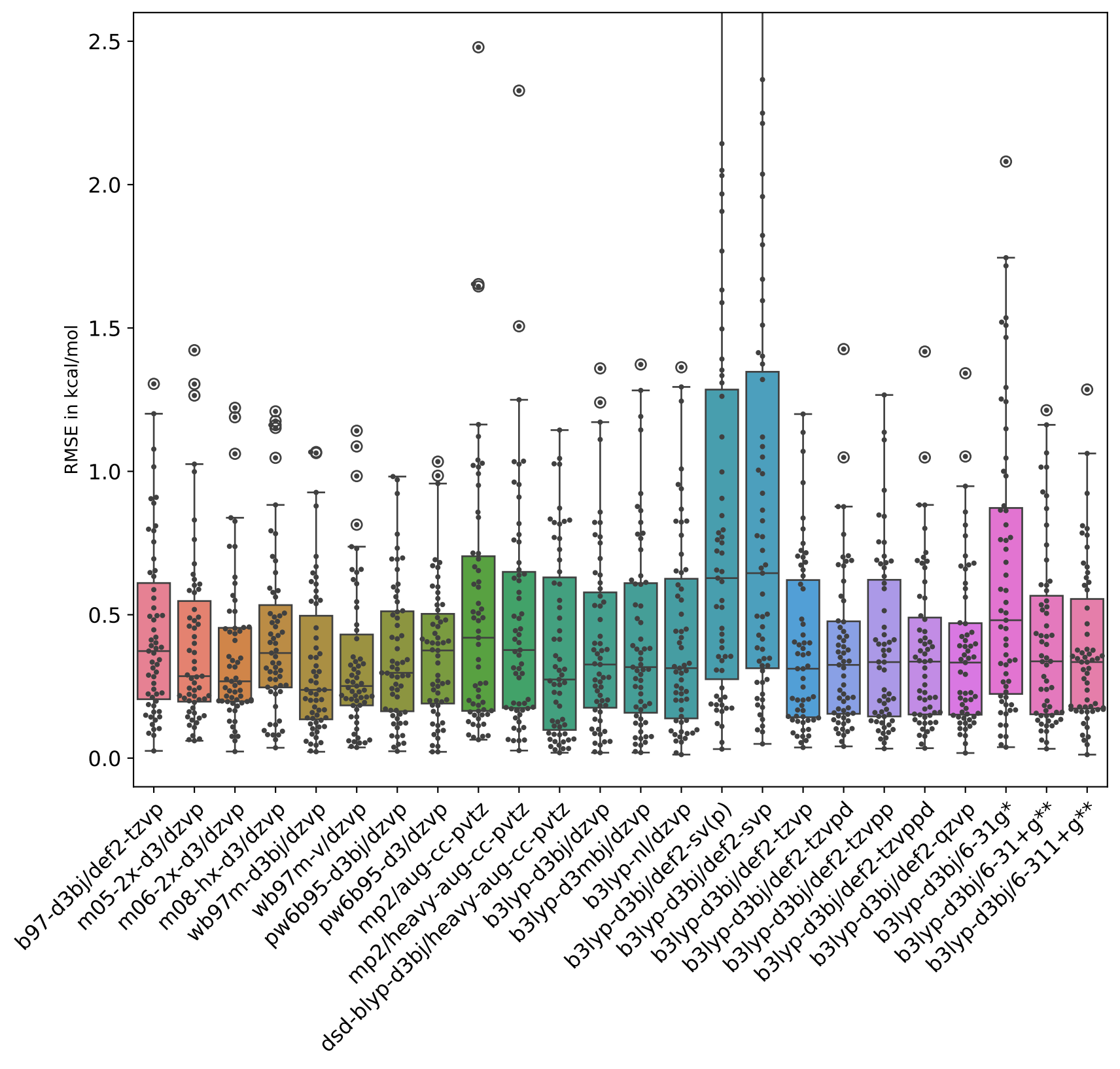
Neutral molecule



Relative energies in kcal/mol

Dihedral angle in degrees

REFERENCE
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
pw6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**


RMSE in kcal/mol
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1.0
1.5
2.0
2.5
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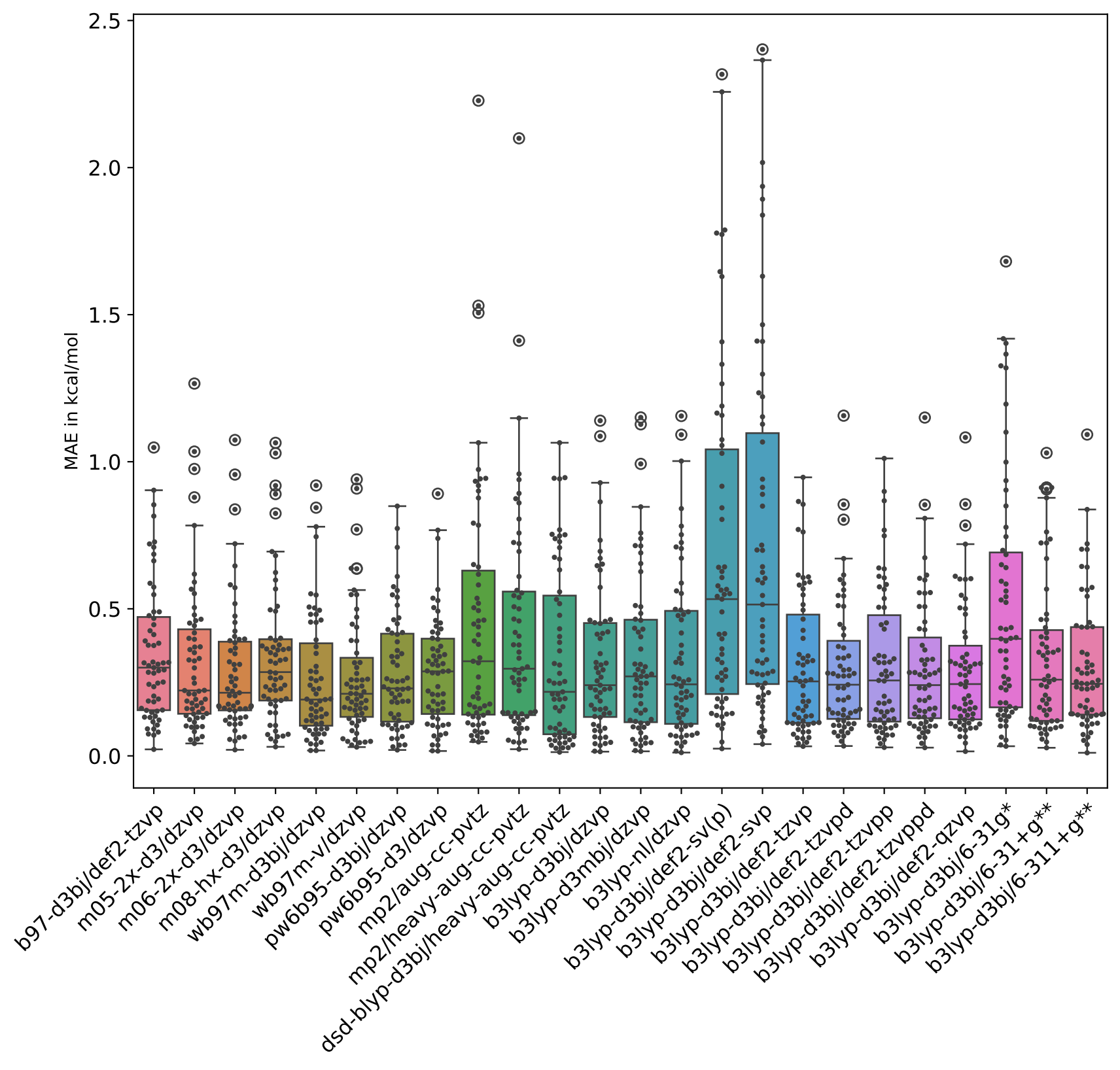
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
wb6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**


MAE in kcal/mol
2.5
2.0
1.5
1.0
0.5
0.0
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m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
wb6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
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b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
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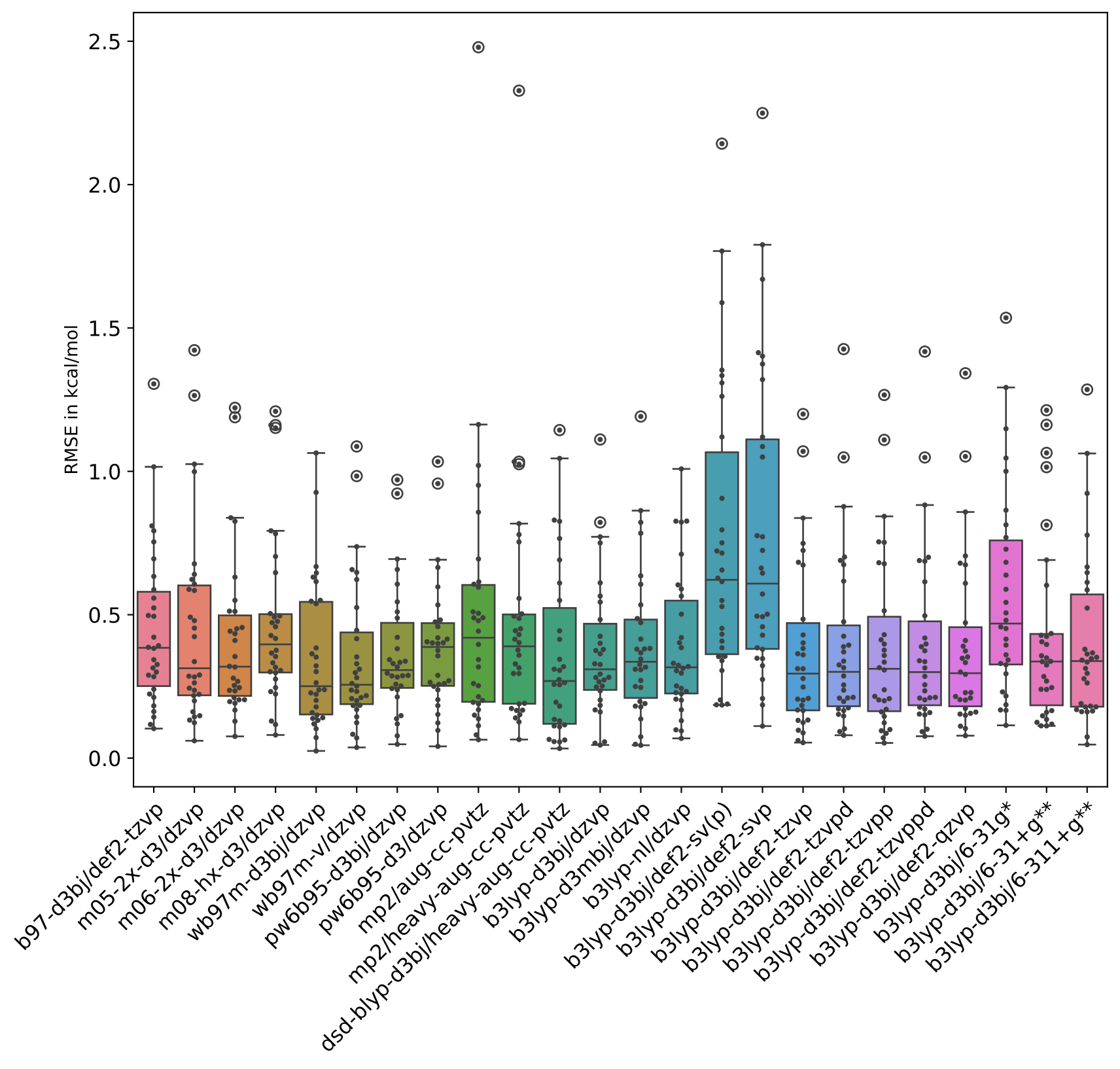
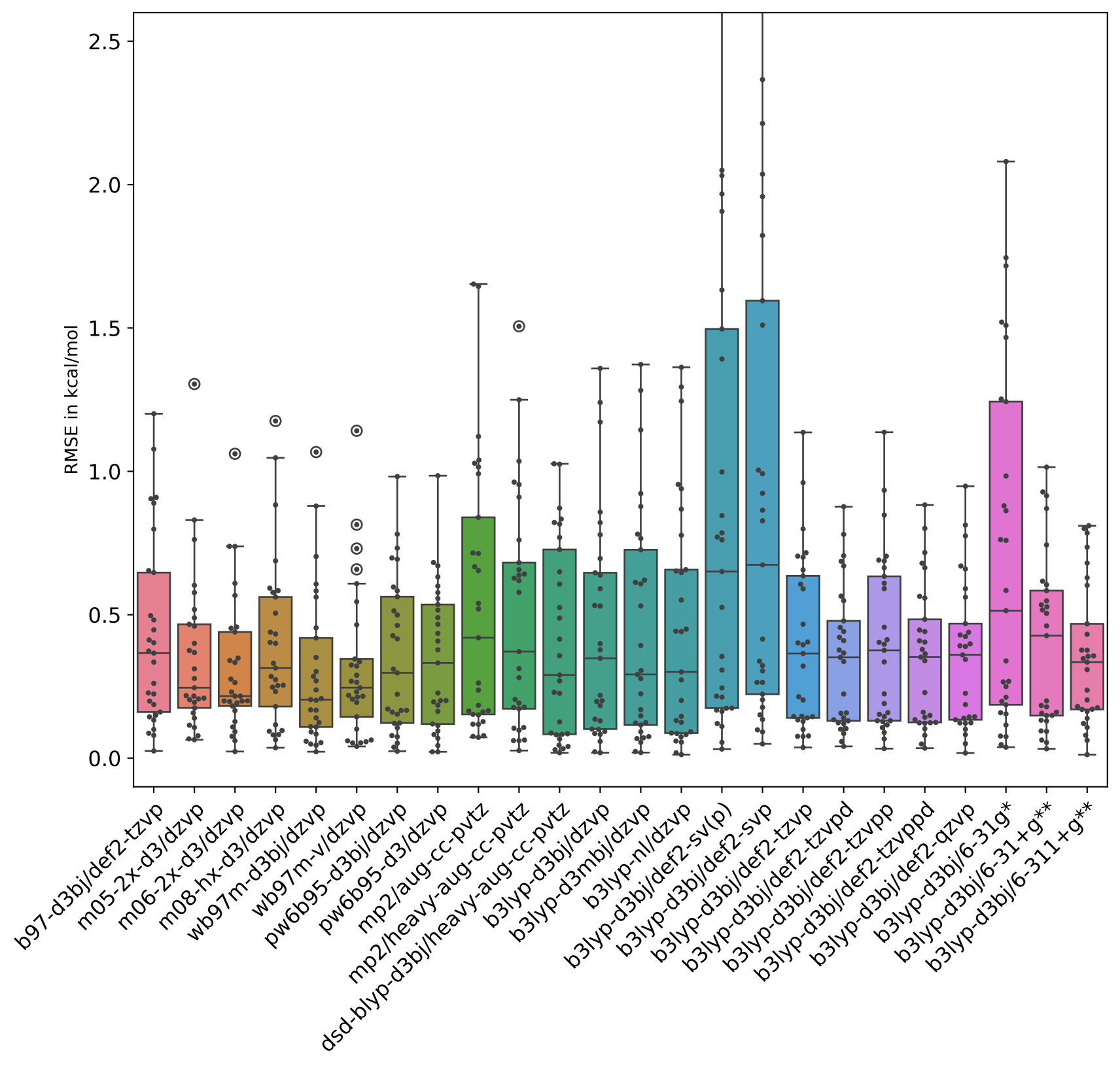
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**


RMSE in kcal/mol
0.0
0.5
1.0
1.5
2.0
2.5
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
wb6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**


RMSE in kcal/mol
0.0
0.5
1.0
1.5
2.0
2.5
b97-d3bj/def2-tzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
wb97m-d3bj/dzvp
wb97m-v/dzvp
wb6b95-d3bj/dzvp
pw6b95-d3/dzvp
mp2/aug-cc-pvtz
mp2/heavy-aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/dzvp
b3lyp-d3mbj/dzvp
b3lyp-nl/dzvp
b3lyp-d3bj/def2-sv(p)
b3lyp-d3bj/def2-svp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-d3bj/6-31g*
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**