

Evaluation of Quantum Chemistry Calculation Methods for Conformational Analysis of Organic Molecules Using A-Value Estimation as a Benchmark Test

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General

The calculations were performed using the Gaussian 09W program,¹ except for those with the ω B97X-V functional, for which the Spartan'18W program² was used. Conformational search were systematically performed by changing dihedral angles by 60° in initial geometries of axial and equatorial conformers. Geometry optimization was performed with the tight convergent criteria option. A larger grid (99,590) was applied to integral computation using the B3LYP, B3LYP-D3, ω B97X-D, M06-2X, and ω B97X-V functionals. For solvation correction with the Polarizable Continuum Model, the following parameters were used, except for *tert*-butylcyclohexane and cyclohexylethene (dichloromethane), 1-cyclohexylethanone and *N,N*-dimethylcyclohexanamine (toluene), and methylthiocyclohexane (chloroform), for which the solvent keywords are available:

methylcyclohexane, ethylcyclohexane, and isopropylcyclohexane (CFCl₃/CDCl₃ 9:1)

eps=2.58422, epsinf=1.930, vmol=92.0159, density=0.0065468

trifluoromethylcyclohexane (CFCl₃)

eps=2.38, epsinf=2.178576, vmol=93.1, density=0.006470565

cyclohexyltrimethylsilane (CDCl₃/CD₂Cl₂ 6:4)

eps=6.68416, epsinf=2.0655, vmol=72.8762, density=0.0082662

cyclohexylethyne, cyclohexanecarbonitrile, fluorocyclohexane, chlorocyclohexane, bromocyclohexane, iodocyclohexane, methoxycyclohexane, cyclohexyl acetate, nitrocyclohexane (CFCl₃/TMS 19:1)

eps=2.368, epsinf=1.909, vmol=94.95, density=0.0063

cyclohexylbenzene (propane)

eps=1.6, epsinf=1.796, vmol=75.9, density=0.00793689

Summary of the calculated A-value of each substituent

X = Me, *t*-Bu, CF₃, TMS, C≡CH, CN, F, Cl, Br, I in Figures 1 and 2^a

methods ^b	Me	<i>t</i> -Bu	CF ₃	TMS	C≡CH	CN	F	Cl	Br ^c	I ^c	RMSE ^d
experimental values	1.74	4.9	2.5	2.50	0.515	0.21	0.36	0.507	0.485	0.490	
B3LYP-D3//HF	2.10 (2.11)	5.39 (5.41)	2.39 (2.30)	2.60 (2.63)	0.87 (0.74)	0.54 (0.37)	0.46 (0.29)	0.62 (0.49)	0.55 (0.42)	0.51 (0.41)	0.26 (0.23)
B3LYP-D3//B3LYP	2.03 (2.03)	4.98 (5.00)	2.43 (2.34)	2.28 (2.31)	0.88 (0.75)	0.54 (0.37)	0.45 (0.27)	0.56 (0.43)	0.46 (0.33)	0.42 (0.32)	0.20 (0.17)
B3LYP-D3//B3LYP-D3	2.07 (2.08)	5.22 (5.24)	2.54 (2.44)	2.58 (2.61)	0.90 (0.76)	0.57 (0.38)	0.49 (0.30)	0.60 (0.47)	0.56 (0.43)	0.49 (0.39)	0.23 (0.19)
B3LYP-D3//ωB97X-D	2.08 (2.08)	6.27 (6.28)	2.30 (2.20)	2.63 (2.65)	0.88 (0.73)	0.59 (0.39)	0.39 (0.21)	0.64 (0.50)	0.51 (0.37)	0.49 (0.38)	<i>0.48</i> (0.48)
B3LYP-D3//M06-2X	2.07 (2.08)	5.61 (5.62)	2.60 (2.50)	3.40 (3.42)	1.05 (0.89)	0.70 (0.51)	0.67 (0.47)	0.66 (0.51)	0.61 (0.47)	0.58 (0.46)	<i>0.46</i> (0.42)
B3LYP-D3//ωB97X-V ^e	2.07 (2.08)	5.68 (5.72)	2.57 (2.39)	2.70 (2.76)	1.05 (0.84)	0.68 (0.44)	0.61 (0.36)	0.66 (0.47)	0.52 (0.38)	0.54 (0.40)	<i>0.37</i> (0.32)
B3LYP-D3//MP2	2.10 (2.10)	5.78 (5.80)	2.50 (2.40)	2.63 (2.65)	1.21 (1.11)	0.79 (0.58)	0.66 (0.47)	0.73 (0.58)	0.67 (0.51)	0.67 (0.50)	<i>0.44</i> (0.38)
ωB97X-D//HF	1.85 (1.85)	5.05 (5.06)	2.46 (2.38)	2.40 (2.42)	0.54 (0.42)	0.28 (0.13)	0.51 (0.36)	0.76 (0.64)	0.77 (0.66)	0.75 (0.66)	0.17 (0.12)
ωB97X-D//B3LYP	1.77 (1.77)	4.69 (4.70)	2.54 (2.45)	2.08 (2.10)	0.54 (0.41)	0.26 (0.10)	0.52 (0.36)	0.71 (0.60)	0.70 (0.59)	0.67 (0.59)	0.19 (0.16)
ωB97X-D//B3LYP-D3	1.80 (1.81)	4.85 (4.86)	2.68 (2.59)	2.30 (2.32)	0.55 (0.41)	0.27 (0.10)	0.58 (0.40)	0.78 (0.65)	0.83 (0.72)	0.77 (0.69)	0.20 (0.14)
ωB97X-D//ωB97X-D	1.80 (1.80)	5.82 (5.83)	2.43 (2.34)	2.24 (2.26)	0.52 (0.37)	0.29 (0.11)	0.47 (0.30)	0.80 (0.67)	0.77 (0.64)	0.74 (0.65)	<i>0.34</i> (0.33)
ωB97X-D//M06-2X	1.78 (1.79)	5.15 (5.16)	2.77 (2.68)	2.92 (2.94)	0.67 (0.51)	0.39 (0.21)	0.79 (0.60)	0.83 (0.70)	0.87 (0.73)	0.82 (0.72)	<i>0.30</i> (0.22)
ωB97X-D//ωB97X-V ^e	1.80 (1.82)	5.25 (5.28)	2.71 (2.54)	2.34 (2.38)	0.67 (0.47)	0.35 (0.15)	0.69 (0.48)	0.81 (0.65)	0.74 (0.65)	0.77 (0.65)	0.24 (0.16)
ωB97X-D//MP2	1.81 (1.81)	5.37 (5.39)	2.64 (2.55)	2.26 (2.28)	0.87 (0.71)	0.44 (0.24)	0.75 (0.55)	0.87 (0.73)	0.88 (0.74)	0.83 (0.72)	<i>0.32</i> (0.23)
M06-2X//HF	2.00 (2.00)	5.44 (5.45)	2.51 (2.43)	2.68 (2.69)	0.42 (0.30)	0.14 (-0.01)	0.27 (0.12)	0.51 (0.39)	0.49 (0.38)	0.50 (0.41)	0.20 (0.24)
M06-2X//B3LYP	1.90 (1.90)	5.14 (5.16)	2.52 (2.43)	2.44 (2.46)	0.38 (0.25)	0.09 (-0.07)	0.27 (0.11)	0.45 (0.33)	0.41 (0.29)	0.38 (0.30)	0.12 (0.20)
M06-2X//B3LYP-D3	1.92 (1.92)	5.21 (5.23)	2.62 (2.53)	2.53 (2.55)	0.37 (0.23)	0.08 (-0.10)	0.28 (0.11)	0.47 (0.35)	0.49 (0.37)	0.42 (0.34)	0.14 (0.21)
M06-2X//ωB97X-D	1.91 (1.91)	6.10 (6.11)	2.39 (2.30)	2.34 (2.35)	0.32 (0.18)	0.06 (-0.12)	0.23 (0.06)	0.50 (0.38)	0.43 (0.31)	0.41 (0.31)	<i>0.40</i> (0.44)
M06-2X//M06-2X	1.88 (1.88)	5.42 (5.43)	2.66 (2.56)	2.86 (2.87)	0.44 (0.29)	0.16 (-0.02)	0.42 (0.24)	0.47 (0.33)	0.46 (0.33)	0.40 (0.30)	0.22 (0.26)
M06-2X//ωB97X-V ^e	1.89 (1.91)	5.54 (5.57)	2.65 (2.48)	2.45 (2.49)	0.46 (0.26)	0.11 (-0.10)	0.37 (0.17)	0.48 (0.32)	0.40 (0.30)	0.37 (0.25)	0.22 (0.28)
M06-2X//MP2	1.92 (1.92)	5.69 (5.71)	2.58 (2.49)	2.37 (2.38)	0.63 (0.48)	0.15 (-0.04)	0.42 (0.22)	0.51 (0.37)	0.49 (0.35)	0.43 (0.32)	0.27 (0.29)
ωB97X-V//HF	1.96 (1.97)	5.48 (5.51)	2.45 (2.31)	2.36 (2.41)	0.53 (0.38)	0.19 (0.03)	0.25 (0.05)	0.56 (0.43)	0.57 (0.45)	0.54 (0.43)	0.21 (0.25)
ωB97X-V//B3LYP ^e	1.91 (1.93)	5.07 (5.09)	2.49 (2.36)	2.04 (2.08)	0.50 (0.34)	0.14 (-0.03)	0.19 (-0.01)	0.49 (0.33)	0.48 (0.34)	0.43 (0.32)	0.18 (0.24)
ωB97X-V//B3LYP-D3 ^e	1.96 (1.98)	5.43 (5.45)	2.67 (2.51)	1.88 (1.94)	0.52 (0.34)	0.16 (-0.03)	0.27 (0.05)	0.55 (0.41)	0.56 (0.40)	0.51 (0.38)	0.28 (0.30)
ωB97X-V//ωB97X-D ^e	2.03 (2.05)	6.26 (6.30)	2.48 (2.32)	2.77 (2.81)	0.50 (0.30)	0.15 (-0.04)	0.19 (0.00)	0.53 (0.38)	0.52 (0.39)	0.44 (0.34)	<i>0.45</i> (0.50)
ωB97X-V//M06-2X ^e	1.95 (1.97)	5.60 (5.64)	2.66 (2.49)	3.07 (3.10)	0.60 (0.39)	0.24 (0.02)	0.37 (0.15)	0.50 (0.34)	0.47 (0.32)	0.44 (0.33)	<i>0.30</i> (0.34)
ωB97X-V//ωB97X-V ^e	1.95 (1.97)	5.65 (5.68)	2.59 (2.43)	2.62 (2.66)	0.58 (0.38)	0.22 (0.02)	0.37 (0.16)	0.57 (0.41)	0.56 (0.42)	0.50 (0.39)	0.25 (0.28)

ω B97X-V//MP2 ^e	1.91 (1.93)	5.74 (5.78)	2.62 (2.45)	2.64 (2.69)	0.84 (0.63)	0.30 (0.08)	0.45 (0.22)	0.61 (0.44)	0.61 (0.45)	0.56 (0.43)	0.32 (0.30)
MP2//HF	2.03 (2.03)	5.53 (5.55)	2.68 (2.60)	2.76 (2.78)	0.25 (0.14)	0.09 (-0.06)	0.33 (0.17)	0.77 (0.64)	0.70 (0.57)	0.79 (0.80)	0.31 (0.31)
MP2//B3LYP	1.92 (1.92)	5.15 (5.18)	2.69 (2.60)	2.44 (2.47)	0.18 (0.06)	0.02 (-0.14)	0.34 (0.17)	0.72 (0.60)	0.62 (0.49)	0.78 (0.68)	0.21 (0.23)
MP2//B3LYP-D3	1.94 (1.94)	5.27 (5.30)	2.79 (2.69)	2.63 (2.65)	0.14 (0.01)	-0.01 (-0.18)	0.35 (0.17)	0.73 (0.60)	0.69 (0.55)	0.83 (0.72)	0.26 (0.28)
MP2// ω B97X-D	1.93 (1.93)	6.22 (6.24)	2.58 (2.49)	2.53 (2.55)	0.07 (-0.06)	-0.04 (-0.21)	0.30 (0.13)	0.75 (0.61)	0.60 (0.46)	0.75 (0.64)	0.47 (0.51)
MP2/M06-2X	1.89 (1.89)	5.53 (5.55)	2.84 (2.77)	3.13 (3.15)	0.15 (0.01)	0.05 (-0.12)	0.51 (0.31)	0.68 (0.54)	0.57 (0.43)	0.69 (0.57)	0.34 (0.36)
MP2// ω B97X-V ^{e,f}	1.95 (1.96)	5.68 (5.70)	2.78 (2.68)	2.84 (2.66)	0.15 (0.01)	-0.01 (-0.27)	0.40 (0.21)	0.65 (0.51)	0.51 (0.37)	0.65 (0.54)	0.31 (0.35)
MP2//MP2	1.93 (1.93)	5.80 (5.82)	2.79 (2.69)	2.53 (2.55)	0.31 (0.17)	0.01 (-0.18)	0.52 (0.31)	0.71 (0.56)	0.56 (0.41)	0.61 (0.56)	0.33 (0.35)
RMSE ^d	0.22 (0.22)	0.70 (0.72)	0.16 (0.13)	0.31 (0.31)	0.28 (0.30)	0.23 (0.25)	0.17 (0.19)	0.17 (0.12)	0.16 (0.13)	0.18 (0.16)	
solvation effect ^g	0.00	0.02	0.11	0.03	0.15	0.18	0.19	0.14	0.13	0.11	

^a The values are A-values (kcal/mol) calculated with solvation correction of the Polarizable Continuum Model, while those in parentheses were calculated without solvation correction. ^b Performed using Gaussian 09W program unless otherwise noted. Methods on the left and right of double slash are for energy calculation with 6-311+G(2df,2p) basis set and geometry optimization with 6-31G* basis set, respectively. ^c LANL2DZ and def2-TZVPD were used for geometry optimization and energy calculations in places of 6-31G* and 6-311+G(2df,2p), respectively, for bromine and iodine atoms unless otherwise noted. ^d Root means squared error from the experimental values in kcal/mol. The values in parentheses were those without solvation correction. ^e Performed using Spartan 18W program with 6-31G* basis set for geometry optimization and frequency calculations, except for an iodine atom, for which LANL2DZ basis set was used, and with 6-311+G(2df,2p) for energy calculations. ^f Energy calculation was performed using Gaussian 09W program. ^g Average absolute differences between A-values with and without solvation correction (kcal/mol).

X = Et, *i*-Pr, vinyl, Ph, Ac, MeO, AcO, Me₂N, NO₂, MeS in Figure 3-M-S^a

methods ^b	Et	<i>i</i> -Pr	vinyl	Ph	Ac	MeO	AcO	Me ₂ N	NO ₂	MeS	RMSE ^c
experimental values	1.79	2.21	1.68	2.7	1.21	0.75	0.785	1.35	1.13	1.00	
B3LYP-D3//HF	2.00 (2.01)	2.40 (2.41)	2.04 (1.99)	3.16 (3.14)	1.80 (1.60)	0.73 (0.52)	0.61 (0.56)	2.03 (1.86)	0.88 (0.64)	1.37 (1.16)	0.33 (0.30)
B3LYP-D3//B3LYP	2.00 (2.01)	2.29 (2.30)	1.99 (1.94)	3.11 (3.09)	1.76 (1.55)	0.68 (0.46)	0.61 (0.55)	1.88 (1.69)	0.78 (0.53)	1.31 (1.10)	0.28 (0.27)
B3LYP-D3//B3LYP-D3	2.00 (2.01)	2.07 (2.08)	2.03 (1.97)	2.95 (2.93)	1.87 (1.64)	0.72 (0.50)	0.64 (0.58)	1.99 (1.77)	1.13 (0.88)	1.36 (1.14)	0.30 (0.25)
ωB97X-D//HF	1.76 (1.77)	2.11 (2.11)	1.76 (1.71)	2.79 (2.77)	1.56 (1.36)	0.73 (0.52)	0.64 (0.58)	1.83 (1.65)	0.81 (0.60)	1.50 (1.31)	0.23 (0.21)
ωB97X-D//B3LYP	1.75 (1.76)	1.99 (2.00)	1.70 (1.65)	2.71 (2.69)	1.50 (1.29)	0.69 (0.48)	0.65 (0.59)	1.66 (1.45)	0.42 (0.48)	1.45 (1.26)	0.22 (0.23)
ωB97X-D//B3LYP-D3	1.73 (1.73)	1.74 (1.75)	1.73 (1.6=)	2.55 (2.52)	1.60 (1.37)	0.72 (0.49)	0.70 (0.64)	1.78 (1.55)	1.10 (0.87)	1.51 (1.31)	0.25 (0.22)
ωB97X-D//ωB97X-V ^d	1.71 (1.74)	2.01 (2.04)	1.74 (1.69)	2.95 (2.89)	1.80 (1.53)	0.97 (0.66)	0.84 (0.75)	2.01 (1.67)	2.17 (1.92)	1.55 (1.29)	0.38 (0.28)
M06-2X//HF	1.93 (1.94)	2.16 (2.17)	1.83 (1.78)	2.78 (2.76)	1.28 (1.08)	0.55 (0.35)	0.57 (0.51)	1.37 (1.19)	0.39 (0.16)	1.18 (1.00)	0.24 (0.29)
M06-2X//B3LYP	1.92 (1.92)	2.04 (2.05)	1.76 (1.70)	2.66 (2.63)	1.19 (0.99)	0.51 (0.30)	0.56 (0.49)	1.22 (1.02)	0.23 (0.01)	1.11 (0.93)	0.24 (0.31)
M06-2X//B3LYP-D3	1.85 (1.86)	1.78 (1.78)	1.76 (1.70)	2.48 (2.46)	1.21 (0.99)	0.43 (0.21)	0.57 (0.50)	1.30 (1.07)	0.52 (0.28)	1.16 (0.97)	0.22 (0.29)
M06-2X//M06-2X	1.97 (1.97)	2.06 (2.07)	1.80 (1.73)	2.60 (2.56)	1.37 (1.14)	0.61 (0.39)	0.64 (0.56)	1.46 (1.22)	1.71 (1.45)	0.89 (0.66)	0.22 (0.22)
M06-2X//ωB97X-V ^d	1.83 (1.85)	2.01 (2.04)	1.76 (1.70)	2.74 (2.69)	1.41 (1.14)	0.62 (0.33)	0.68 (0.59)	1.46 (1.12)	1.68 (1.41)	1.15 (0.90)	0.22 (0.21)
M06-2X//MP2	1.85 (1.85)	2.15 (2.15)	1.84 (1.76)	2.71 (2.67)	1.33 (1.09)	0.63 (0.40)	0.66 (0.58)	1.52 (1.27)	1.07 (0.81)	1.09 (0.87)	0.20 (0.23)
ωB97X-V//HF ^d	1.89 (1.92)	2.11 (2.14)	1.82 (1.79)	2.99 (2.96)	1.57 (1.34)	0.56 (0.60)	0.46 (0.39)	1.55 (1.32)	0.55 (0.38)	1.27 (1.06)	0.25 (0.27)
ωB97X-V//B3LYP ^d	1.84 (1.87)	2.07 (2.08)	1.47 (1.44)	2.90 (2.86)	1.44 (1.21)	0.56 (0.29)	0.49 (0.41)	1.36 (1.11)	0.37 (0.19)	1.16 (0.95)	0.24 (0.29)
ωB97X-V//B3LYP-D3 ^d	1.84 (1.87)	1.78 (1.82)	1.81 (1.78)	2.74 (2.69)	1.55 (1.31)	0.56 (0.27)	0.55 (0.47)	1.14 (0.81)	1.62 (1.38)	1.23 (1.00)	0.26 (0.29)
ωB97X-V//ωB97X-V ^d	1.88 (1.90)	2.13 (2.16)	1.82 (1.78)	3.00 (2.96)	1.69 (1.43)	0.73 (0.43)	0.62 (0.52)	1.69 (1.35)	1.87 (1.62)	1.24 (0.98)	0.30 (0.24)
MP2//B3LYP	1.87 (1.88)	1.89 (1.90)	1.76 (1.71)	2.80 (2.77)	1.46 (1.28)	0.39 (0.16)	0.40 (0.33)	0.83 (0.60)	0.79 (0.56)	1.22 (1.02)	0.26 (0.32)
MP2//B3LYP-D3	1.82 (1.82)	1.62 (1.63)	1.76 (1.71)	2.57 (2.54)	1.48 (1.28)	0.34 (0.11)	0.39 (0.32)	0.96 (0.69)	1.05 (0.82)	1.25 (1.03)	0.29 (0.33)
RMSE ^c	0.12 (0.12)	0.27 (0.25)	0.17 (0.14)	0.21 (0.20)	0.37 (0.21)	0.19 (0.40)	0.22 (0.28)	0.38 (0.36)	0.55 (0.63)	0.31 (0.17)	
solvation effect ^e	0.01	0.01	0.05	0.03	0.22	0.24	0.07	0.24	0.23	0.21	

^a The values are A-values (kcal/mol) calculated with solvation correction of the polarizable continuum model, while those in parentheses were calculated without solvation correction. ^b Performed using Gaussian 09W unless otherwise noted. Methods on the left and right of double slash are for energy calculation with 6-311+G(2df,2p) basis set and geometry optimization/frequency calculations with 6-31G*, respectively. ^c Root means squared error from the experimental values (kcal/mol) of the results in Tables 1 and 2. The values in parentheses are those without solvation correction. ^d Performed using Spartan 18W program. ^e Average absolute differences between A-values with and without solvation correction (kcal/mol).

X = Me, *t*-Bu, CF₃, TMS, C≡CH, CN, F, Cl, Br, I in Figure 3-T^a

theoretical levels	Me	<i>t</i> -Bu	CF ₃	TMS	C≡CH	CN	F	Cl	Br ^b	I ^b	RMSE ^c
experimental values	1.74	4.9	2.5	2.50	0.515	0.21	0.36	0.507	0.485	0.490	
HF//HF	2.56 (2.56)	6.71 (6.73)	3.33 (3.23)	3.88 (3.91)	1.38 (1.24)	1.00 (0.81)	0.55 (0.037)	1.29 (1.15)	1.41 (1.28)	1.61 (1.50)	1.03 (0.97)
HF//B3LYP	2.56 (2.56)	6.40 (6.42)	3.51 (3.40)	3.66 (3.70)	1.43 (1.29)	1.02 (0.83)	0.56 (0.37)	1.25 (1.12)	1.36 (1.23)	1.57 (1.47)	0.96 (0.90)
HF//B3LYP-D3	2.71 (2.71)	6.73 (6.76)	3.70 (3.59)	4.01 (4.03)	1.51 (1.34)	1.08 (0.86)	0.62 (0.42)	1.35 (1.21)	1.53 (1.39)	1.69 (1.59)	1.14 (1.08)
HF//ωB97X-D	2.73 (2.73)	7.79 (7.81)	3.41 (3.30)	4.13 (4.15)	1.52 (1.35)	1.14 (0.92)	0.48 (0.29)	1.36 (1.21)	1.45 (1.31)	1.66 (1.55)	1.33 (1.28)
HF//M06-2X	2.75 (2.76)	7.18 (7.20)	3.83 (3.71)	5.00 (5.02)	1.76 (1.58)	1.26 (1.04)	0.81 (0.59)	1.45 (1.29)	1.62 (1.46)	1.83 (1.71)	1.45 (1.38)
HF//ωB97X-V	2.78 (2.78)	7.20 (7.22)	3.67 (3.55)	4.22 (4.24)	1.67 (1.49)	1.25 (1.02)	0.69 (0.48)	1.37 (1.21)	1.51 (1.35)	1.75 (1.63)	1.29 (1.21)
HF//MP2	2.76 (2.76)	7.29 (7.31)	3.66 (3.54)	4.14 (4.16)	1.96 (1.78)	1.40 (1.16)	0.76 (0.53)	1.49 (1.31)	1.65 (1.48)	1.85 (1.72)	1.36 (1.28)
B3LYP//HF	2.46 (2.46)	6.00 (6.02)	2.89 (2.80)	3.45 (3.47)	1.24 (1.11)	0.89 (0.72)	0.62 (0.45)	1.15 (1.02)	1.26 (1.14)	1.33 (1.23)	0.75 (0.68)
B3LYP//B3LYP	2.46 (2.46)	5.57 (5.58)	3.00 (2.91)	3.12 (3.15)	1.27 (1.14)	0.91 (0.74)	0.63 (0.45)	1.11 (0.98)	1.21 (1.08)	1.27 (1.17)	0.65 (0.57)
B3LYP//B3LYP-D3	2.52 (2.52)	5.93 (5.95)	3.17 (3.07)	3.49 (3.52)	1.32 (1.13)	0.96 (0.76)	0.70 (0.51)	1.19 (1.05)	1.34 (1.20)	1.35 (1.25)	0.80 (0.72)
B3LYP//ωB97X-D	2.53 (2.53)	7.03 (7.04)	2.90 (2.80)	3.62 (3.64)	1.31 (1.16)	0.98 (0.79)	0.57 (0.39)	1.20 (1.06)	1.26 (1.12)	1.33 (1.22)	0.98 (0.93)
B3LYP//M06-2X	2.53 (2.53)	6.37 (6.39)	3.26 (3.15)	4.46 (4.48)	1.50 (1.34)	1.09 (0.90)	0.90 (0.70)	1.26 (1.11)	1.39 (1.25)	1.44 (1.32)	1.07 (1.00)
B3LYP//ωB97X-V	2.57 (2.57)	6.44 (6.46)	3.11 (3.01)	3.71 (3.73)	1.44 (1.28)	1.07 (0.87)	0.78 (0.58)	1.19 (1.04)	1.30 (1.15)	1.38 (1.27)	0.93 (0.85)
B3LYP//MP2	2.55 (2.55)	6.50 (6.52)	3.11 (3.00)	3.61 (3.63)	1.69 (1.54)	1.20 (0.98)	0.88 (0.66)	1.32 (1.17)	1.44 (1.29)	1.49 (1.36)	1.00 (0.92)
RMSE ^c	0.87 (0.87)	1.85 (1.87)	0.88 (0.78)	1.47 (1.49)	1.00 (0.85)	0.89 (0.69)	0.35 (0.17)	0.78 (0.64)	0.93 (0.79)	1.07 (0.96)	
solvation effect ^d	0.00	0.02	0.11	0.02	0.16	0.20	0.20	0.15	0.14	0.11	

^a The values are A-values (kcal/mol) calculated with solvation correction of the polarizable continuum model, while those in parentheses were calculated without solvation correction. The calculations were performed using Gaussian 09W program except for those with ωB97X-V, which was performed using Spartan 18W program. ^b Except for ωB97X-V, def2-TZVPD basis set was used for bromine and iodine atoms.

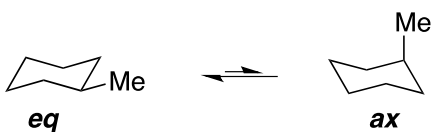
^c Root means squared error from the experimental values (kcal/mol). The values in parentheses are those without solvation correction. ^d Average absolute differences between A-values with and without solvation correction (kcal/mol).

X = Et, *i*-Pr, vinyl, Ph, Ac, MeO, AcO, Me₂N, NO₂, MeS in Figure 3-T^a

theoretical levels	Et	<i>i</i> -Pr	vinyl	Ph	Ac	MeO	AcO	Me ₂ N	NO ₂	MeS	RMSE ^b
experimental values	1.79	2.21	1.68	2.7	1.21	0.75	0.785	1.35	1.13	1.00	
HF//HF	2.71 (2.72)	3.27 (3.28)	2.66 (2.62)	4.55 (4.52)	2.71 (2.48)	1.11 (0.88)	1.05 (0.99)	3.09 (2.90)	2.09 (1.84)	2.13 (1.90)	1.11 (1.06)
HF//B3LYP	2.75 (2.76)	3.19 (3.20)	2.64 (2.61)	4.58 (4.55)	2.69 (2.45)	1.08 (0.84)	1.05 (0.98)	2.89 (2.68)	1.93 (1.69)	2.14 (1.91)	1.06 (1.00)
HF//B3LYP-D3	2.81 (2.82)	3.04 (3.06)	2.70 (2.67)	4.50 (4.58)	2.94 (2.68)	1.27 (1.02)	1.18 (1.12)	3.09 (2.85)	2.42 (2.17)	2.24 (2.00)	1.20 (1.13)
HF//ωB97X-D	2.83 (2.84)	3.41 (3.43)	2.78 (2.41)	4.69 (4.65)	3.07 (2.82)	1.48 (1.24)	1.14 (1.07)	2.89 (2.64)	2.79 (2.53)	2.16 (1.92)	1.34 (1.28)
HF//M06-2X	3.18 (3.19)	3.50 (3.52)	2.78 (2.75)	5.06 (5.02)	3.30 (3.03)	1.78 (1.53)	1.30 (1.23)	3.50 (3.24)	3.59 (3.30)	2.02 (1.75)	1.56 (1.49)
HF//ωB97X-V	2.89 (2.90)	3.40 (3.42)	2.75 (2.72)	5.14 (5.10)	3.15 (2.89)	1.50 (1.24)	1.30 (1.23)	3.31 (3.05)	3.45 (3.16)	2.27 (2.01)	1.44 (1.37)
HF//MP2	2.91 (2.92)	3.56 (3.57)	2.86 (2.72)	4.98 (4.94)	3.21 (2.92)	1.58 (1.32)	1.33 (1.24)	3.56 (3.29)	3.09 (2.81)	2.26 (1.99)	1.48 (1.40)
B3LYP//HF	2.49 (2.50)	2.98 (2.99)	2.49 (2.45)	3.87 (3.85)	2.52 (2.32)	1.13 (0.92)	1.09 (1.03)	2.66 (2.48)	1.55 (1.31)	1.86 (1.66)	0.81 (0.76)
B3LYP//B3LYP	2.50 (2.51)	2.87 (2.88)	2.46 (2.42)	3.85 (3.83)	2.49 (2.29)	1.09 (0.87)	1.08 (1.02)	2.49 (2.30)	1.44 (1.20)	1.84 (1.64)	0.74 (0.69)
B3LYP//B3LYP-D3	2.56 (2.56)	2.72 (2.73)	2.51 (2.47)	3.73 (3.71)	2.71 (2.49)	1.26 (1.04)	1.22 (1.15)	2.72 (2.50)	1.92 (1.66)	1.91 (1.69)	0.87 (0.80)
B3LYP//ωB97X-D	2.56 (2.57)	3.07 (3.08)	2.58 (2.54)	3.89 (3.87)	2.82 (2.62)	1.47 (1.26)	1.45 (1.39)	2.44 (2.22)	2.28 (2.02)	1.84 (1.62)	1.00 (0.94)
B3LYP//M06-2X	2.87 (2.87)	3.14 (3.15)	2.57 (2.53)	4.23 (4.20)	3.02 (2.79)	1.18 (0.92)	1.31 (1.25)	3.03 (2.80)	3.07 (2.80)	1.70 (1.45)	1.17 (1.10)
B3LYP//ωB97X-V	2.60 (2.61)	3.05 (3.07)	2.54 (2.50)	4.33 (4.30)	2.89 (2.67)	1.48 (1.25)	1.33 (1.26)	2.87 (2.64)	2.95 (2.68)	1.92 (1.69)	1.08 (1.01)
B3LYP//MP2	2.63 (2.64)	3.20 (3.21)	2.64 (2.59)	4.08 (4.05)	2.94 (2.70)	1.58 (1.34)	1.37 (1.29)	3.10 (2.85)	2.58 (2.31)	1.91 (1.67)	1.11 (1.03)
RMSE ^b	0.96 (0.97)	0.99 (1.00)	0.97 (0.93)	1.75 (1.72)	1.70 (1.46)	0.64 (0.42)	0.46 (0.40)	1.66 (1.43)	1.53 (1.29)	1.03 (0.80)	
solvation effect ^c	0.01	0.01	0.04	0.03	0.24	0.24	0.07	0.23	0.26	0.24	

^a The values are A-values (kcal/mol) calculated with solvation correction of the polarizable continuum model, while those in parentheses were calculated without solvation correction. The calculations were performed using Gaussian 09W program except for those with ωB97X-V, which was performed using Spartan 18W program. ^b Root means squared error from the experimental values (kcal/mol) of the results in Tables 3 and 4. The values in parentheses are those without solvation correction. ^c Average absolute differences between A-values with and without solvation correction (kcal/mol).

Methylcyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-273.243663	0.182015			
ax RHF/6-31G(d)	-273.239998	0.182435			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.302925	-275.120910	0	97.2	2.10
ax RB3LYP-D3/6-311+G(2df,2p)	-275.299992	-275.117556	2.1048	2.8	
eq R ω B97X-D/6-311+G(2df,2p)	-275.201489	-275.019474	0	95.8	1.85
ax R ω B97X-D/6-311+G(2df,2p)	-275.198962	-275.016527	1.850	4.2	
eq RM06-2X/6-311+G(2df,2p)	-275.138560	-274.956545	0	96.7	2.00
ax RM06-2X /6-311+G(2df,2p)	-275.135797	-274.953361	1.998	3.3	
eq RMP2(FC)/6-311+G(2df,2p)	-274.523347	-274.341332	0	96.9	2.03
ax RMP2(FC)/6-311+G(2df,2p)	-274.520535	-274.338099	2.028	3.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-273.243664	0.181801			
ax RHF/6-31G*	-273.239998	0.182184			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-275.208102	-275.026301	0	96.5	1.96
ax R ω B97X-V/6-311+G(2df,2p)	-275.205367	-275.023183	1.957	3.5	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-275.195637	0.168624			
ax RB3LYP/6-31G(d)	-275.192113	0.168938			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.302896	-275.134272	0	96.9	2.03
ax RB3LYP-D3/6-311+G(2df,2p)	-275.299978	-275.131039	2.029	3.1	
eq R ω B97X-D/6-311+G(2df,2p)	-275.201197	-275.032573	0	95.2	1.77
ax R ω B97X-D/6-311+G(2df,2p)	-275.198697	-275.029759	1.765	4.8	

eq RM06-2X/6-311+G(2df,2p)	-275.138200	-274.969576	0	96.1	
ax RM06-2X /6-311+G(2df,2p)	-275.135490	-274.966552	1.897	3.9	1.90
eq RMP2(FC)/6-311+G(2df,2p)	-274.522738	-274.354114	0	96.2	
ax RMP2(FC)/6-311+G(2df,2p)	-274.519998	-274.351060	1.916	3.7	1.92
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-275.195622	0.158471			
ax RB3LYP/6-31G*	-275.192127	0.158823			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-275.208495	-275.050024	0	96.2	
ax RωB97X-V/6-311+G(2df,2p)	-275.205801	-275.046978	1.911	3.8	1.91
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-275.212368	0.169314			
ax RB3LYP-D3/6-31G(d)	-275.209542	0.169709			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.302938	-275.133624	0	97.1	
ax RB3LYP-D3/6-311+G(2df,2p)	-275.300027	-275.130318	2.074	2.9	2.07
eq RωB97X-D/6-311+G(2df,2p)	-275.201274	-275.031960	0	95.5	
ax RωB97X-D/6-311+G(2df,2p)	-275.198795	-275.029085	1.804	4.5	1.80
eq RM06-2X/6-311+G(2df,2p)	-275.138333	-274.969019	0	96.3	
ax RM06-2X /6-311+G(2df,2p)	-275.135667	-274.965957	1.921	3.7	1.92
eq RMP2(FC)/6-311+G(2df,2p)	-274.522915	-274.353601	0	96.4	
ax RMP2(FC)/6-311+G(2df,2p)	-274.520219	-274.350510	1.940	3.6	1.94
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-275.212353	0.169052			
ax RB3LYP-D3/6-31G*	-275.209555	0.169505			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-275.208588	-275.039536	0	96.5	
ax RωB97X-V/6-311+G(2df,2p)	-275.205916	-275.036411	1.960	3.5	1.96
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RωB97X-D/6-31G(d)	-275.118975	0.170847			

ax RωB97X-D/6-31G(d) -275.116562 0.171237

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.303082	-275.132235	0	97.1	2.08
ax RB3LYP-D3/6-311+G(2df,2p)	-275.300158	-275.128921	2.079	2.9	
eq RωB97X-D/6-311+G(2df,2p)	-275.201621	-275.030773	0	95.5	1.80
ax RωB97X-D/6-311+G(2df,2p)	-275.199143	-275.027906	1.799	4.5	
eq RM06-2X/6-311+G(2df,2p)	-275.138699	-274.967851	0	96.2	1.91
ax RM06-2X /6-311+G(2df,2p)	-275.136043	-274.964806	1.911	3.8	
eq RMP2(FC)/6-311+G(2df,2p)	-274.523401	-274.352554	0	96.3	1.93
ax RMP2(FC)/6-311+G(2df,2p)	-274.520723	-274.349485	1.925	3.7	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RωB97X-D/6-31G*	-275.118965	0.158500
ax RωB97X-D/6-31G*	-275.116573	0.159060

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-275.208788	-275.050288	0	96.9	2.03
ax RωB97X-V/6-311+G(2df,2p)	-275.206120	-275.047060	2.026	3.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G(d)	-275.047823	0.170500
ax RM06-2X/6-31G(d)	-275.045200	0.170849

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.303052	-275.132553	0	97.1	2.07
ax RB3LYP-D3/6-311+G(2df,2p)	-275.300097	-275.129249	2.073	2.9	
eq RωB97X-D/6-311+G(2df,2p)	-275.201660	-275.031160	0	95.3	1.78
ax RωB97X-D/6-311+G(2df,2p)	-275.199168	-275.028320	1.782	4.7	
eq RM06-2X/6-311+G(2df,2p)	-275.138804	-274.968305	0	96.0	1.88
ax RM06-2X /6-311+G(2df,2p)	-275.136160	-274.965311	1.879	4.0	
eq RMP2(FC)/6-311+G(2df,2p)	-274.523579	-274.353079	0	96.1	1.89
ax RMP2(FC)/6-311+G(2df,2p)	-274.520920	-274.350071	1.887	3.9	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G*	-275.047827	0.170162

ax RM06-2X/6-31G* -275.045254 0.170594

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-275.208811	-275.038649	0	96.4	1.95
ax RωB97X-V/6-311+G(2df,2p)	-275.206135	-275.035541	1.950	3.6	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RωB97X-V/6-31G*	-275.124825	0.170593
ax RωB97X-V/6-31G*	-275.122289	0.171027

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.303254	-275.132661	0	97.1	2.07
ax RB3LYP-D3/6-311+G(2df,2p)	-275.300389	-275.129362	2.070	2.9	
eq RωB97X-D/6-311+G(2df,2p)	-275.201739	-275.031146	0	95.5	1.80
ax RωB97X-D/6-311+G(2df,2p)	-275.199308	-275.028281	1.798	4.5	
eq RM06-2X/6-311+G(2df,2p)	-275.138868	-274.968275	0	96.1	1.89
ax RM06-2X /6-311+G(2df,2p)	-275.136288	-274.965261	1.891	3.9	
eq RωB97X-V/6-311+G(2df,2p)	-275.208629	-275.038036	0	96.4	1.95
ax RωB97X-V/6-311+G(2df,2p)	-275.205961	-275.034934	1.947	3.5	
eq RMP2(FC)/6-311+G(2df,2p)	-274.523611	-274.353018	0	96.5	1.95
ax RMP2(FC)/6-311+G(2df,2p)	-274.520936	-274.349909	1.951	3.5	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RMP2(FC)/6-31G(d)	-274.161772	0.173212
ax RMP2(FC)/6-31G(d)	-274.158747	0.173611

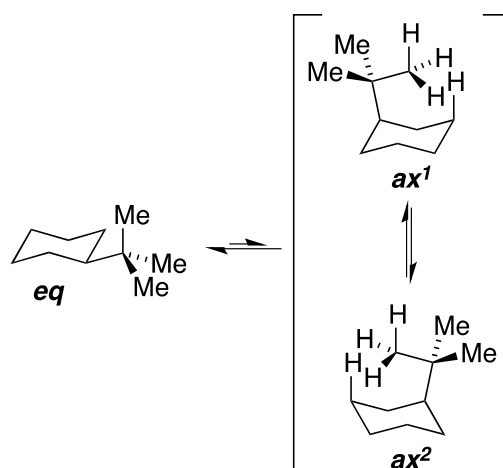
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-275.303029	-275.129817	0	97.2	2.10
ax RB3LYP-D3/6-311+G(2df,2p)	-275.300082	-275.126471	2.100	2.8	
eq RωB97X-D/6-311+G(2df,2p)	-275.201689	-275.028477	0	95.6	1.81
ax RωB97X-D/6-311+G(2df,2p)	-275.199201	-275.025590	1.812	4.4	
eq RM06-2X/6-311+G(2df,2p)	-275.138808	-274.956596	0	96.3	1.92
ax RM06-2X /6-311+G(2df,2p)	-275.136148	-274.962537	1.920	3.7	
eq RMP2(FC)/6-311+G(2df,2p)	-274.523611	-274.350399	0	96.3	1.93
ax RMP2(FC)/6-311+G(2df,2p)	-274.520936	-274.347325	1.929	3.7	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-274.161772	0.173008			
ax RMP2(FC)/6-31G*	-274.158747	0.173371			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-275.208800	-275.035792	0	96.2	1.91
ax R ω B97X-V/6-311+G(2df,2p)	-275.206123	-275.032752	1.908	3.8	

geometry method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-273.309789	-273.130797	0	98.8	2.62
ax RHF/6-311+G(d,p)	-273.306066	-273.126569	2.615	1.2	
eq RB3LYP/6-311+G(d,p)	-275.270822	-275.104498	0	98.4	2.43
ax RB3LYP/6-311+G(d,p)	-275.267357	-275.100628	2.428	1.6	
eq RB3LYP-D3/6-311+G(d,p)	-275.287551	-275.120523	0	97.0	2.05
ax RB3LYP-D3/6-311+G(d,p)	-275.284782	-275.117261	2.047	3.0	
eq R ω B97X-D/6-311+G(d,p)	-275.187083	-275.018650	0	95.3	1.78
ax R ω B97X-D/6-311+G(d,p)	-275.184754	-275.015812	1.781	4.7	
eq RM06-2X/6-311+G(d,p)	-275.123401	-274.954877	0	95.7	1.83
ax RM06-2X/6-311+G(d,p)	-275.120900	-274.951955	1.834	4.3	
eq R ω B97X-V/6-311+G**	-275.195371	-275.027542	0	96.1	1.89
ax R ω B97X-V/6-311+G**	-275.192862	-275.024538	1.885	3.9	
eq RMP2(FC)/6-311+G(d,p)	-274.370782	-274.201564	0	96.8	2.02
ax RMP2(FC)/6-311+G(d,p)	-274.368089	-274.198348	2.018	3.2	

tert-Butylcyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G(d)	-390.337398	0.267681
ax RHF/6-31G(d)	-390.327630	0.269276

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288454	-393.020773	0	100.0	100.0
ax RB3LYP-D3/6-311+G(2df,2p)	-393.280809	-393.011533	5.798	0.005	0.01
eq R ω B97X-D/6-311+G(2df,2p)	-393.144859	-392.877178	0	100.0	100.0
ax R ω B97X-D/6-311+G(2df,2p)	-393.137756	-392.868480	5.458	0.01	0.02
eq RM06-2X/6-311+G(2df,2p)	-393.055552	-392.787871	0	100.0	100.0
ax RM06-2X /6-311+G(2df,2p)	-393.047832	-392.778557	5.845	0.005	0.01
eq RMP2(FC)/6-311+G(2df,2p)	-392.179467	-391.911787	0	100.0	100.0
ax RMP2(FC)/6-311+G(2df,2p)	-392.171594	-391.902318	5.942	0.004	0.009

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G*	-390.337397	0.266888
ax RHF/6-31G*	-390.327630	0.268597

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-393.154454	-392.887566	0	100	100
ax R ω B97X-V/6-311+G(2df,2p)	-393.146782	-392.878185	5.887	0.004	0.009

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP/6-31G(d)	-393.129360	0.248472

ax RB3LYP/6-31G(d) -393.120845 0.249462

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288420	-393.039947	0	100	100
ax RB3LYP-D3/6-311+G(2df,2p)	-393.280827	-393.031365	5.385	0.01	0.02
eq R ω B97X-D/6-311+G(2df,2p)	-393.144553	-392.896081	0	100	100
ax R ω B97X-D/6-311+G(2df,2p)	-393.137418	-392.887956	5.098	0.02	0.04
eq RM06-2X/6-311+G(2df,2p)	-393.055145	-392.806673	0	100	100
ax RM06-2X /6-311+G(2df,2p)	-393.04729	-392.797829	5.550	0.008	0.02
eq RMP2(FC)/6-311+G(2df,2p)	-392.178722	-391.930249	0	100	100
ax RMP2(FC)/6-311+G(2df,2p)	-392.170849	-391.921388	5.560	0.008	0.02

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP/6-31G*	-393.129355	0.233298
ax RB3LYP/6-31G*	-393.120830	0.234352

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-393.155131	-392.921833	0	100	100
ax R ω B97X-V/6-311+G(2df,2p)	-393.147455	-392.913103	5.478	0.009	0.02

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP-D3/6-31G(d)	-393.159630	0.249510
ax RB3LYP-D3/6-31G(d)	-393.152150	0.250966

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288517	-393.039007	0	100	100
ax RB3LYP-D3/6-311+G(2df,2p)	-393.280995	-393.030029	5.633	0.007	0.01
eq R ω B97X-D/6-311+G(2df,2p)	-393.144724	-392.895214	0	100	100
ax R ω B97X-D/6-311+G(2df,2p)	-393.137802	-392.886836	5.257	0.01	0.03
eq RM06-2X/6-311+G(2df,2p)	-393.055397	-392.805887	0	100	100
ax RM06-2X /6-311+G(2df,2p)	-393.047896	-392.796931	5.620	0.007	0.02
eq RMP2(FC)/6-311+G(2df,2p)	-392.179049	-391.929539	0	100	100
ax RMP2(FC)/6-311+G(2df,2p)	-392.171446	-391.920480	5.684	0.007	0.01

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
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eq RB3LYP-D3/6-31G* -393.159626 0.273148

ax RB3LYP-D3/6-31G* -393.152136 0.250271

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-393.155315	-392.906814	0	100	100
ax R ω B97X-V/6-311+G(2df,2p)	-393.147787	-392.897516	5.834	0.005	0.01

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq R ω B97X-D/6-31G(d)	-393.027018	0.250520
ax R ω B97X-D/6-31G(d)	-393.020086	0.253542

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288662	-393.038141	0	100	100
ax RB3LYP-D3/6-311+G(2df,2p)	-393.281046	-393.027505	6.675	0.001	0.003
eq R ω B97X-D/6-311+G(2df,2p)	-393.145232	-392.894711	0	100	100
ax R ω B97X-D/6-311+G(2df,2p)	-393.138330	-392.884788	6.227	0.003	0.005
eq RM06-2X/6-311+G(2df,2p)	-393.055982	-392.805462	0	100	100
ax RM06-2X /6-311+G(2df,2p)	-393.048631	-392.795089	6.509	0.002	0.003
eq RMP2(FC)/6-311+G(2df,2p)	-392.179842	-391.929321	0	100	100
ax RMP2(FC)/6-311+G(2df,2p)	-392.172301	-391.918760	6.627	0.001	0.003

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq R ω B97X-D/6-31G*	-393.027013	0.232419
ax R ω B97X-D/6-31G*	-393.020079	0.235528

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-393.155653	-392.923234	0	100	100
ax R ω B97X-V/6-311+G(2df,2p)	-393.148137	-392.912609	6.667	0.001	0.003

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G(d)	-392.926148	0.251202
ax RM06-2X/6-31G(d)	-392.918707	0.253154

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288434	-393.037233	0	100	100
ax RB3LYP-D3/6-311+G(2df,2p)	-393.280801	-393.027647	6.015	0.004	0.008

eq R ω B97X-D/6-311+G(2df,2p)	-393.145224	-392.894023	0	100	100	5.15
ax R ω B97X-D/6-311+G(2df,2p)	-393.138325	-392.885171	5.555	0.008	0.02	
eq RM06-2X/6-311+G(2df,2p)	-393.056182	-392.804981	0	100	100	5.42
ax RM06-2X /6-311+G(2df,2p)	-393.048852	-392.795698	5.825	0.005	0.01	
eq RMP2(FC)/6-311+G(2df,2p)	-392.180108	-391.928906	0	100	100	5.53
ax RMP2(FC)/6-311+G(2df,2p)	-392.172588	-391.919434	5.944	0.004	0.009	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RM06-2X/6-31G*	-392.926196	0.250561				
ax RM06-2X/6-31G*	-392.918749	0.252620				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq R ω B97X-V/6-311+G(2df,2p)	-393.155638	-392.905077	0	100	100	5.60
ax R ω B97X-V/6-311+G(2df,2p)	-393.148122	-392.895502	6.008	0.004	0.008	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq R ω B97X-V/6-31G*	-393.035290	0.250599				
ax R ω B97X-V/6-31G*	-393.027828	0.252736				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RB3LYP-D3/6-311+G(2df,2p)	-393.289202	-393.038603	0	100	100	5.68
ax RB3LYP-D3/6-311+G(2df,2p)	-393.281636	-393.028900	6.089	0.003	0.007	
eq R ω B97X-D/6-311+G(2df,2p)	-393.145715	-392.895116	0	100	100	5.25
ax R ω B97X-D/6-311+G(2df,2p)	-393.138833	-392.886097	5.659	0.007	0.01	
eq RM06-2X/6-311+G(2df,2p)	-393.056570	-392.805971	0	100	100	5.54
ax RM06-2X /6-311+G(2df,2p)	-393.049227	-392.796491	5.949	0.004	0.008	
eq R ω B97X-V/6-311+G(2df,2p)	-393.155443	-392.904844	0	100	100	5.65
ax R ω B97X-V/6-311+G(2df,2p)	-393.147926	-392.895190	6.058	0.003	0.007	
eq RMP2(FC)/6-311+G(2df,2p)	-393.179286	-392.928687	0	100	100	5.68
ax RMP2(FC)/6-311+G(2df,2p)	-393.171724	-392.918988	6.086	0.003	0.007	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RMP2(FC)/6-31G(d)	-391.660148	0.254236				
ax RMP2(FC)/6-31G(d)	-391.651634	0.256531				

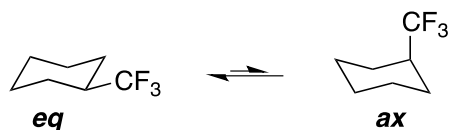
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %		A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-393.288534	-393.034295	0	100	100	5.78
ax RB3LYP-D3/6-311+G(2df,2p)	-393.280965	-393.024434	6.188	0.003	0.006	
eq R ω B97X-D/6-311+G(2df,2p)	-393.145334	-392.891095	0	100	100	5.37
ax R ω B97X-D/6-311+G(2df,2p)	-393.138411	-392.881880	5.783	0.006	0.01	
eq RM06-2X/6-311+G(2df,2p)	-393.056171	-392.801932	0	100	100	5.69
ax RM06-2X /6-311+G(2df,2p)	-393.048735	-392.792204	6.104	0.003	0.006	
eq RMP2(FC)/6-311+G(2df,2p)	-392.180245	-391.926006	0	100	100	5.80
ax RMP2(FC)/6-311+G(2df,2p)	-392.172647	-391.916116	6.206	0.003	0.005	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-391.660148	0.253693			
ax RMP2(FC)/6-31G*	-391.651634	0.255953			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %		A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-393.155688	-392.901995	0	100	100	5.74
ax R ω B97X-V/6-311+G(2df,2p)	-393.148155	-392.892202	6.145	0.003	0.006	

geometry method	E (au)	G (au)	rel G (kcal/mol)	Population %		A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-390.432176	-390.169126	0	100	100	6.71
ax RHF/6-311+G(d,p)	-390.422567	-390.157796	7.110	0.0006	0.001	
eq RB3LYP/6-311+G(d,p)	-393.236552	-392.991571	0	100	100	5.36
ax RB3LYP/6-311+G(d,p)	-393.228129	-392.982379	5.768	0.006	0.01	
eq RB3LYP-D3/6-311+G(d,p)	-393.266844	-393.020757	0	100	100	5.06
ax RB3LYP-D3/6-311+G(d,p)	-393.259425	-393.012045	5.467	0.01	0.02	
eq R ω B97X-D/6-311+G(d,p)	-393.124948	-392.877726	0	100	100	5.34
ax R ω B97X-D/6-311+G(d,p)	-393.118188	-392.868567	5.747	0.006	0.01	
eq RM06-2X/6-311+G(d,p)	-393.034582	-392.786236	0	100	100	5.32
ax RM06-2X/6-311+G(d,p)	-393.027344	-392.777100	5.733	0.006	0.01	
eq R ω B97X-V/6-311+G**	-393.136936	-392.890814	0	100	100	5.66
ax R ω B97X-V/6-311+G**	-393.129566	-392.881138	6.072	0.003	0.007	
eq RMP2(FC)/6-311+G(d,p)	-391.961753	-391.712592	0	100	100	5.31

Trifluoromethylcyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G(d)	-569.836362	0.155360
ax RHF/6-31G(d)	-569.832482	0.155887

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.148821	-572.993461	0	98.3	2.39
ax RB3LYP-D3/6-311+G(2df,2p)	-573.145541	-572.989654	2.389	1.7	
eq R ω B97X-D/6-311+G(2df,2p)	-572.968281	-572.812921	0	98.5	2.46
ax R ω B97X-D/6-311+G(2df,2p)	-572.964880	-572.808993	2.465	1.5	
eq RM06-2X/6-311+G(2df,2p)	-572.909062	-572.753701	0	98.6	2.51
ax RM06-2X /6-311+G(2df,2p)	-572.905590	-572.749703	2.509	1.4	
eq RMP2(FC)/6-311+G(2df,2p)	-571.933535	-571.778175	0	98.9	2.68
ax RMP2(FC)/6-311+G(2df,2p)	-571.929785	-571.773898	2.684	1.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G*	-569.836362	0.154665
ax RHF/6-31G*	-569.832482	0.155216

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-572.967560	-572.812895	0	98.4	2.45
ax R ω B97X-V/6-311+G(2df,2p)	-572.964213	-572.808997	2.446	1.6	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP/6-31G(d)	-572.922037	0.142311
ax RB3LYP/6-31G(d)	-572.919429	0.142956

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.150452	-573.008141	0	98.4	2.43

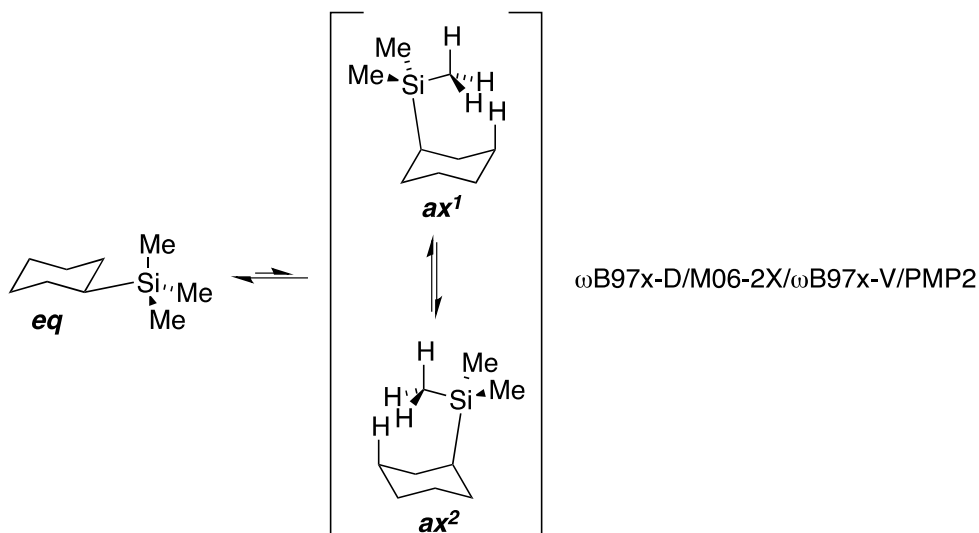
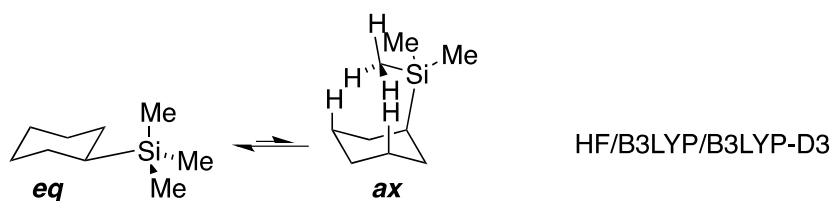
ax RB3LYP-D3/6-311+G(2df,2p)	-573.147224	-573.004267	2.431	1.6	
eq R ω B97X-D/6-311+G(2df,2p)	-572.968351	-572.826040	0	98.7	2.54
ax R ω B97X-D/6-311+G(2df,2p)	-572.964949	-572.821992	2.540	1.3	
eq RM06-2X/6-311+G(2df,2p)	-572.908715	-572.766404	0	98.6	2.52
ax RM06-2X /6-311+G(2df,2p)	-572.905342	-572.762386	2.521	1.4	
eq RMP2(FC)/6-311+G(2df,2p)	-571.933500	-571.791190	0	99.0	2.69
ax RMP2(FC)/6-311+G(2df,2p)	-571.929857	-571.786900	2.692	1.0	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-572.922041	0.132709			
ax RB3LYP/6-31G*	-572.919424	0.133387			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-572.969080	-572.836371	0	98.6	2.49
ax R ω B97X-V/6-311+G(2df,2p)	-572.965786	-572.832399	2.492	1.4	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-572.941382	0.142916			
ax RB3LYP-D3/6-31G(d)	-572.939725	0.143673			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.150453	-573.007537	0	98.7	2.54
ax RB3LYP-D3/6-311+G(2df,2p)	-573.147169	-573.003496	2.536	1.3	
eq R ω B97X-D/6-311+G(2df,2p)	-572.968354	-572.825438	0	98.9	2.68
ax R ω B97X-D/6-311+G(2df,2p)	-572.964842	-572.821169	2.679	1.1	
eq RM06-2X/6-311+G(2df,2p)	-572.908858	-572.765941	0	98.8	2.62
ax RM06-2X /6-311+G(2df,2p)	-572.905443	-572.761770	2.617	1.2	
eq RMP2(FC)/6-311+G(2df,2p)	-571.933674	-571.790757	0	99.1	2.79
ax RMP2(FC)/6-311+G(2df,2p)	-571.929992	-571.786319	2.785	0.9	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-572.941383	0.142215			
ax RB3LYP-D3/6-31G*	-572.939727	0.143061			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)

eq R ω B97X-V/6-311+G(2df,2p)	-572.969128	-572.826913	0	98.9	
ax R ω B97X-V/6-311+G(2df,2p)	-572.965725	-572.822664	2.666	1.1	2.67
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-D/6-31G(d)	-572.774116	0.144523			
ax R ω B97X-D/6-31G(d)	-572.771818	0.144947			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.150566	-573.006042	0	98.0	
ax RB3LYP-D3/6-311+G(2df,2p)	-573.147320	-573.002373	2.302	2.0	2.30
eq R ω B97X-D/6-311+G(2df,2p)	-572.969047	-572.824524	0	98.4	
ax R ω B97X-D/6-311+G(2df,2p)	-572.965595	-572.820648	2.432	1.6	2.43
eq RM06-2X/6-311+G(2df,2p)	-572.909610	-572.765087	0	98.3	
ax RM06-2X /6-311+G(2df,2p)	-572.906218	-572.761271	2.394	1.7	2.39
eq RMP2(FC)/6-311+G(2df,2p)	-571.934395	-571.789872	0	98.8	
ax RMP2(FC)/6-311+G(2df,2p)	-571.930703	-571.785757	2.582	1.2	2.58
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-D/6-31G*	-572.774126	0.132995			
ax R ω B97X-D/6-31G*	-572.771819	0.133583			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-572.969447	-572.836447	0	98.5	
ax R ω B97X-V/6-311+G(2df,2p)	-572.966090	-572.832507	2.475	1.5	2.48
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G(d)	-572.698196	0.144351			
ax RM06-2X/6-31G(d)	-572.696070	0.145150			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.150328	-573.005976	0	98.8	
ax RB3LYP-D3/6-311+G(2df,2p)	-573.146980	-573.001829	2.602	1.2	2.60
eq R ω B97X-D/6-311+G(2df,2p)	-572.968974	-572.824622	0	99.1	
ax R ω B97X-D/6-311+G(2df,2p)	-572.965352	-572.820202	2.774	0.9	2.77
eq RM06-2X/6-311+G(2df,2p)	-572.909785	-572.765433	0	98.9	
ax RM06-2X /6-311+G(2df,2p)	-572.906340	-572.761190	2.663	1.1	2.66

eq RMP2(FC)/6-311+G(2df,2p)	-571.934560	-571.790208	0	99.2	
ax RMP2(FC)/6-311+G(2df,2p)	-571.930789	-571.785638	2.868	0.8	2.87
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G*	-572.698274			0.143784	
ax RM06-2X/6-31G*	-572.696125			0.144516	
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-572.969342	-572.825558	0	98.9	
ax RωB97X-V/6-311+G(2df,2p)	-572.965839	-572.821322	2.657	1.1	2.66
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RωB97X-V/6-31G*	-572.767048			0.143931	
ax RωB97X-V/6-31G*	-572.765295			0.144637	
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.152413	-573.008482	0	98.7	
ax RB3LYP-D3/6-311+G(2df,2p)	-573.149018	-573.004381	2.573	1.3	2.57
eq RωB97X-D/6-311+G(2df,2p)	-572.970568	-572.826637	0	99.0	
ax RωB97X-D/6-311+G(2df,2p)	-572.966961	-572.822324	2.706	1.0	2.71
eq RM06-2X/6-311+G(2df,2p)	-572.911327	-572.767396	0	98.9	
ax RM06-2X /6-311+G(2df,2p)	-572.907815	-572.763178	2.647	1.1	2.65
eq RωB97X-V/6-311+G(2df,2p)	-572.969271	-572.825340	0	98.8	
ax RωB97X-V/6-311+G(2df,2p)	-572.965856	-572.821219	2.586	1.2	2.59
eq RMP2(FC)/6-311+G(2df,2p)	-571.933970	-571.790039	0	99.1	
ax RMP2(FC)/6-311+G(2df,2p)	-571.930247	-571.785610	2.779	0.9	2.78
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-571.255410			0.146312	
ax RMP2(FC)/6-31G(d)	-571.253042			0.146993	
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-573.150501	-573.004189	0	98.6	
ax RB3LYP-D3/6-311+G(2df,2p)	-573.147199	-573.000205	2.500	1.4	2.50
eq RωB97X-D/6-311+G(2df,2p)	-572.968611	-572.822299	0	98.9	
ax RωB97X-D/6-311+G(2df,2p)	-572.965079	-572.818085	2.644	1.1	2.64

eq RM06-2X/6-311+G(2df,2p)	-572.909173	-572.762861	0	98.8	
ax RM06-2X /6-311+G(2df,2p)	-572.905736	-572.758742	2.584	1.2	2.58
eq RMP2(FC)/6-311+G(2df,2p)	-571.934275	-571.787963	0	99.1	
ax RMP2(FC)/6-311+G(2df,2p)	-571.930517	-571.783523	2.786	0.9	2.79
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-571.255410	0.145618			
ax RMP2(FC)/6-31G*	-571.253042	0.146342			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-572.969323	-572.823705	0	98.8	
ax RωB97X-V/6-311+G(2df,2p)	-572.965879	-572.819537	2.615	1.2	2.62
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-569.990557	-569.837673	0	99.5	
ax RHF/6-311+G(d,p)	-569.986012	-569.832714	3.112	0.5	3.11
eq RB3LYP/6-311+G(d,p)	-573.101481	-572.961423	0	99.0	
ax RB3LYP/6-311+G(d,p)	-573.097585	-572.957141	2.687	1.0	2.69
eq RB3LYP-D3/6-311+G(d,p)	-573.120742	-572.980116	0	97.9	
ax RB3LYP-D3/6-311+G(d,p)	-573.117697	-572.976483	2.280	2.1	2.28
eq RωB97X-D/6-311+G(d,p)	-572.939952	-572.797702	0	97.1	
ax RωB97X-D/6-311+G(d,p)	-572.936749	-572.794381	2.084	2.9	2.08
eq RM06-2X/6-311+G(d,p)	-572.879748	-572.737122	0	97.9	
ax RM06-2X/6-311+G(d,p)	-572.876661	-572.733522	2.259	2.1	2.26
eq RωB97X-V/6-311+G**	-572.941066	-572.799990	0	97.9	
ax RωB97X-V/6-311+G**	-572.937955	-572.796360	2.278	2.1	2.28
eq RMP2(FC)/6-311+G(d,p)	-571.638222	-571.495220	0	98.9	
ax RMP2(FC)/6-311+G(d,p)	-571.634642	-571.490990	2.654	1.1	2.65

Cyclohexyltrimethylsilane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-641.418841	0.251244			
ax RHF/6-31G(d)	-641.413221	0.251875			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728475	-644.477231	0	98.8	2.60
ax RB3LYP-D3/6-311+G(2df,2p)	-644.724957	-644.473082	2.603	1.2	
eq R ω B97X-D/6-311+G(2df,2p)	-644.575553	-644.324309	0	98.3	2.40
ax R ω B97X-D/6-311+G(2df,2p)	-644.572361	-644.320486	2.399	1.7	
eq RM06-2X/6-311+G(2df,2p)	-644.472316	-644.221072	0	98.9	2.68
ax RM06-2X /6-311+G(2df,2p)	-644.468680	-644.216806	2.677	1.1	
eq RMP2(FC)/6-311+G(2df,2p)	-643.227856	-642.976612	0	99.1	2.76
ax RMP2(FC)/6-311+G(2df,2p)	-643.224090	-642.972215	2.759	0.9	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-641.418841	0.249507			
ax RHF/6-31G*	-641.413217	0.249664			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-644.538673	-644.289166	0	98.2	2.37
ax R ω B97X-V/6-311+G(2df,2p)	-644.535061	-644.285397	2.365	1.8	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-644.548524	0.233243			
ax RB3LYP/6-31G(d)	-644.543641	0.233418			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728429	-644.495187	0	97.9	2.28
ax RB3LYP-D3/6-311+G(2df,2p)	-644.724974	-644.491556	2.279	2.1	
eq R ω B97X-D/6-311+G(2df,2p)	-644.575247	-644.342005	0	97.1	2.08
ax R ω B97X-D/6-311+G(2df,2p)	-644.572115	-644.338697	2.076	2.9	
eq RM06-2X/6-311+G(2df,2p)	-644.471927	-644.238685	0	98.4	2.44
ax RM06-2X /6-311+G(2df,2p)	-644.468214	-644.234796	2.440	1.6	
eq RMP2(FC)/6-311+G(2df,2p)	-643.227213	-642.993971	0	98.4	2.44
ax RMP2(FC)/6-311+G(2df,2p)	-643.223507	-642.990088	2.436	1.6	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-644.548521	0.217541			
ax RB3LYP/6-31G*	-644.543631	0.217282			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-644.539851	-644.322310	0	96.9	2.04
ax R ω B97X-V/6-311+G(2df,2p)	-644.536344	-644.319062	2.038	3.1	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-644.574007	0.233781			
ax RB3LYP-D3/6-31G(d)	-644.570504	0.234460			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728665	-644.494880	0	98.8	2.58
ax RB3LYP-D3/6-311+G(2df,2p)	-644.725226	-644.490765	2.582	1.2	
eq R ω B97X-D/6-311+G(2df,2p)	-644.575672	-644.341887	0	98.0	2.30
ax R ω B97X-D/6-311+G(2df,2p)	-644.572682	-644.338222	2.300	2.0	

eq RM06-2X/6-311+G(2df,2p)	-644.472414	-644.238630	0	98.6		
ax RM06-2X /6-311+G(2df,2p)	-644.469056	-644.234596	2.531	1.4		2.53
eq RMP2(FC)/6-311+G(2df,2p)	-643.227699	-642.993915	0	98.8		
ax RMP2(FC)/6-311+G(2df,2p)	-643.224185	-642.989725	2.629	1.2		2.63
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RB3LYP-D3/6-31G*	-644.574005	0.231914				
ax RB3LYP-D3/6-31G*	-644.570479	0.231446				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RωB97X-V/6-311+G(2df,2p)	-644.540218	-644.308304	0	96.0		
ax RωB97X-V/6-311+G(2df,2p)	-644.536754	-644.305308	1.880	4.0	1.88	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RωB97X-D/6-31G(d)	-644.434423	0.236216				
ax RωB97X-D/6-31G(d)	-644.431404	0.237495				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728925	-644.492708	0	98.9	98.8	
ax RB3LYP-D3/6-311+G(2df,2p)	-644.725364	-644.487869	3.037	0.6	1.2	2.63
eq RωB97X-D/6-311+G(2df,2p)	-644.576329	-644.340112	0	97.9	97.9	
ax RωB97X-D/6-311+G(2df,2p)	-644.573377	-644.335882	2.654	1.1	2.2	2.24
eq RM06-2X/6-311+G(2df,2p)	-644.473111	-644.236895	0	98.2	98.2	
ax RM06-2X /6-311+G(2df,2p)	-644.470006	-644.232510	2.751	0.9	1.9	2.34
eq RMP2(FC)/6-311+G(2df,2p)	-643.228438	-642.992221	0	98.7	98.6	
ax RMP2(FC)/6-311+G(2df,2p)	-643.225031	-642.987536	2.940	0.7	1.4	2.53
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RωB97X-D/6-31G*	-644.434417	0.217347				
ax RωB97X-D/6-31G*	-644.431386	0.219032				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RωB97X-V/6-311+G(2df,2p)	-644.540621	-644.323274	0	99.2	99.1	
ax RωB97X-V/6-311+G(2df,2p)	-644.537241	-644.318209	3.178	0.5	0.9	2.77
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RM06-2X/6-31G(d)	-644.316900	0.235059				

ax RM06-2X/6-31G(d) -644.313768 0.237261

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728897	-644.493838	0	99.7	99.7
ax RB3LYP-D3/6-311+G(2df,2p)	-644.725022	-644.487760	3.814	0.2	0.3
eq RωB97X-D/6-311+G(2df,2p)	-644.576399	-644.341340	0	99.3	99.3
ax RωB97X-D/6-311+G(2df,2p)	-644.573289	-644.336028	3.333	0.4	0.7
eq RM06-2X/6-311+G(2df,2p)	-644.473257	-644.238198	0	99.2	99.2
ax RM06-2X /6-311+G(2df,2p)	-644.470245	-644.232984	3.272	0.4	0.8
eq RMP2(FC)/6-311+G(2df,2p)	-643.228624	-642.993565	0	99.5	99.5
ax RMP2(FC)/6-311+G(2df,2p)	-643.225193	-642.987932	3.535	0.3	0.5

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G*	-644.316954	0.233656
ax RM06-2X/6-31G*	-644.313814	0.235682

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-644.540652	-644.306996	0	99.4	99.4
ax RωB97X-V/6-311+G(2df,2p)	-644.537134	-644.301452	3.479	0.3	0.6

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RωB97X-V/6-31G*	-644.396591	0.234584
ax RωB97X-V/6-31G*	-644.393193	0.236031

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.729580	-644.494996	0	99.0	99.0
ax RB3LYP-D3/6-311+G(2df,2p)	-644.726070	-644.490039	3.111	0.5	1.0
eq RωB97X-D/6-311+G(2df,2p)	-644.576878	-644.342294	0	98.1	98.1
ax RωB97X-D/6-311+G(2df,2p)	-644.573942	-644.337911	2.750	0.9	1.9
eq RM06-2X/6-311+G(2df,2p)	-644.473778	-644.239194	0	98.5	98.5
ax RM06-2X /6-311+G(2df,2p)	-644.470663	-644.234632	2.863	0.8	1.5
eq RωB97X-V/6-311+G(2df,2p)	-644.540324	-644.305740	0	98.8	98.8
ax RωB97X-V/6-311+G(2df,2p)	-644.536947	-644.300916	3.027	0.6	1.2
eq RMP2(FC)/6-311+G(2df,2p)	-643.933970	-643.699386	0	99.2	99.2
ax RMP2(FC)/6-311+G(2df,2p)	-643.930247	-643.694216	3.244	0.4	0.8

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-642.684355	0.239687			
ax RMP2(FC)/6-31G(d)	-642.680360	0.240969			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-644.728888	-644.489202	0	98.8	98.8
ax RB3LYP-D3/6-311+G(2df,2p)	-644.725329	-644.484360	3.038	0.6	1.2
eq RωB97X-D/6-311+G(2df,2p)	-644.576294	-644.336608	0	97.9	97.9
ax RωB97X-D/6-311+G(2df,2p)	-644.573318	-644.332349	2.672	1.1	2.1
eq RM06-2X/6-311+G(2df,2p)	-644.473099	-644.233413	0	98.2	98.2
ax RM06-2X /6-311+G(2df,2p)	-644.469954	-644.228985	2.779	0.9	1.8
eq RMP2(FC)/6-311+G(2df,2p)	-643.228533	-642.988847	0	98.6	98.6
ax RMP2(FC)/6-311+G(2df,2p)	-643.225136	-642.984167	2.937	0.7	1.4

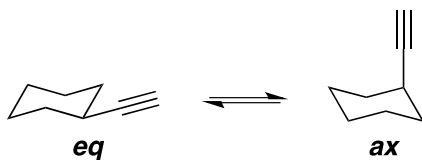
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-642.684355	0.238124			
ax RMP2(FC)/6-31G*	-642.680360	0.239596			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-644.540557	-644.302433	0	98.9	98.9
ax RωB97X-V/6-311+G(2df,2p)	-644.537166	-644.297570	3.052	0.6	1.1

geometry method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-641.531227	-641.284199	0	99.8	99.8
ax RHF/6-311+G(d,p)	-641.525824	-641.278297	3.704	0.2	3.70
eq RB3LYP/6-311+G(d,p)	-644.677491	-644.447696	0	99.2	99.2
ax RB3LYP/6-311+G(d,p)	-644.672793	-644.442544	3.233	0.4	0.8
eq RB3LYP-D3/6-311+G(d,p)	-644.703037	-644.472443	0	98.4	98.4
ax RB3LYP-D3/6-311+G(d,p)	-644.699689	-644.468575	2.427	1.6	2.43
eq RωB97X-D/6-311+G(d,p)	-644.551813	-644.318932	0	95.9	95.9
ax RωB97X-D/6-311+G(d,p)	-644.549060	-644.315306	2.275	2.0	4.1
eq RM06-2X/6-311+G(d,p)	-644.448033	-644.215768	0	99.0	99.0
ax RM06-2X/6-311+G(d,p)	-644.445231	-644.210795	3.121	0.5	1.0
eq RωB97X-V/6-311+G**	-644.517419	-644.287181	0	98.5	98.5

ax RωB97X-V/6-311+G**	-644.514251	-644.282596	2.877	0.8	1.5	
eq RMP2(FC)/6-311+G(d,p)	-643.005567	-642.772310	0	99.2	99.2	
ax RMP2(FC)/6-311+G(d,p)	-643.002175	-642.767157	3.234	0.4	0.8	2.82

Cyclohexylethyne



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G(d)	-309.879346	0.161516
ax RHF/6-31G(d)	-309.878268	0.161877

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.141316	-311.979801	0	81.3	
ax RB3LYP-D3/6-311+G(2df,2p)	-312.140294	-311.978416	0.869	18.7	0.87
eq RωB97X-D/6-311+G(2df,2p)	-312.021138	-311.859622	0	71.5	
ax RωB97X-D/6-311+G(2df,2p)	-312.020635	-311.858757	0.542	28.5	0.54
eq RM06-2X/6-311+G(2df,2p)	-311.974268	-311.812752	0	67.0	
ax RM06-2X /6-311+G(2df,2p)	-311.973964	-311.812086	0.418	33.0	0.42
eq RMP2(FC)/6-311+G(2df,2p)	-311.286638	-311.125124	0	60.6	
ax RMP2(FC)/6-311+G(2df,2p)	-311.286596	-311.124717	0.255	39.4	0.25

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RHF/6-31G*	-309.879346	0.161104
ax RHF/6-31G*	-309.878268	0.161470

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-312.036586	-311.875482	0	71.2	
ax RωB97X-V/6-311+G(2df,2p)	-312.036101	-311.874631	0.534	28.8	0.53

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP/6-31G(d)	-312.018542	0.148289
ax RB3LYP/6-31G(d)	-312.017591	0.148648

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.141648	-311.993359	0	81.6	0.88
ax RB3LYP-D3/6-311+G(2df,2p)	-312.140604	-311.991956	0.880	18.4	
eq R ω B97X-D/6-311+G(2df,2p)	-312.020986	-311.872696	0	71.3	0.54
ax R ω B97X-D/6-311+G(2df,2p)	-312.020489	-311.871841	0.537	28.7	
eq RM06-2X/6-311+G(2df,2p)	-311.974066	-311.825777	0	65.4	0.38
ax RM06-2X /6-311+G(2df,2p)	-311.973825	-311.825177	0.377	34.6	
eq RMP2(FC)/6-311+G(2df,2p)	-311.287623	-311.139333	0	57.4	0.18
ax RMP2(FC)/6-311+G(2df,2p)	-311.287698	-311.139050	0.177	42.6	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-312.018548	0.148817			
ax RB3LYP/6-31G*	-312.017590	0.139235			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-312.037165	-311.898275	0	70.0	0.50
ax R ω B97X-V/6-311+G(2df,2p)	-312.036712	-311.897477	0.501	30.0	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-312.034251	0.142916			
ax RB3LYP-D3/6-31G(d)	-312.033944	0.149157			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.141701	-311.992884	0	82.1	0.90
ax RB3LYP-D3/6-311+G(2df,2p)	-312.140607	-311.991449	0.901	17.9	
eq R ω B97X-D/6-311+G(2df,2p)	-312.021067	-311.872250	0	71.6	0.55
ax R ω B97X-D/6-311+G(2df,2p)	-312.020535	-311.871378	0.547	28.4	
eq RM06-2X/6-311+G(2df,2p)	-311.974211	-311.825394	0	65.0	0.37
ax RM06-2X /6-311+G(2df,2p)	-311.973968	-311.824811	0.366	35.0	
eq RMP2(FC)/6-311+G(2df,2p)	-311.287772	-311.138955	0	55.8	0.14
ax RMP2(FC)/6-311+G(2df,2p)	-311.287894	-311.138736	0.137	44.2	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-312.034251	0.148376			

ax RB3LYP-D3/6-31G* -312.033943 0.148738

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-312.037239	-311.888863	0	70.7	0.52
ax RωB97X-V/6-311+G(2df,2p)	-312.036774	-311.888036	0.519	29.3	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RωB97X-D/6-31G(d)	-311.922982	0.150487
ax RωB97X-D/6-31G(d)	-311.923058	0.150761

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.141875	-311.991389	0	81.6	0.88
ax RB3LYP-D3/6-311+G(2df,2p)	-312.140747	-311.989985	0.881	18.4	
eq RωB97X-D/6-311+G(2df,2p)	-312.021488	-311.871002	0	70.7	0.52
ax RωB97X-D/6-311+G(2df,2p)	-312.020936	-311.870174	0.519	29.3	
eq RM06-2X/6-311+G(2df,2p)	-311.974650	-311.824164	0	63.4	0.32
ax RM06-2X /6-311+G(2df,2p)	-311.974409	-311.823647	0.324	36.6	
eq RMP2(FC)/6-311+G(2df,2p)	-311.288138	-311.137651	0	53.2	0.07
ax RMP2(FC)/6-311+G(2df,2p)	-311.288293	-311.137532	0.074	46.8	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RωB97X-D/6-31G*	-311.922982	0.139098
ax RωB97X-D/6-31G*	-311.923057	0.139401

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-312.037530	-311.898432	0	69.8	0.50
ax RωB97X-V/6-311+G(2df,2p)	-312.037044	-311.897643	0.495	30.2	

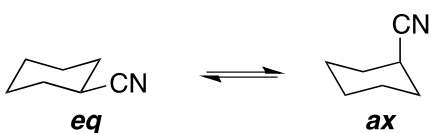
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G(d)	-311.866747	0.150444
ax RM06-2X/6-31G(d)	-311.867080	0.150871

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.141819	-311.991375	0	85.5	1.05
ax RB3LYP-D3/6-311+G(2df,2p)	-312.140575	-311.989704	1.049	14.5	
eq RωB97X-D/6-311+G(2df,2p)	-312.021499	-311.871055	0	75.6	0.67

ax RωB97X-D/6-311+G(2df,2p)	-312.020861	-311.869989	0.669	24.4	
eq RM06-2X/6-311+G(2df,2p)	-311.974727	-311.824283	0	67.8	
ax RM06-2X /6-311+G(2df,2p)	-311.974454	-311.823582	0.440	32.2	0.44
eq RMP2(FC)/6-311+G(2df,2p)	-311.288268	-311.137824	0	56.4	
ax RMP2(FC)/6-311+G(2df,2p)	-311.288454	-311.137582	0.152	43.6	0.15
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G*	-311.866782		0.150029		
ax RM06-2X/6-31G*	-311.867115		0.150436		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-312.037549	-311.887520	0	73.4	
ax RωB97X-V/6-311+G(2df,2p)	-312.037002	-311.886566	0.599	26.6	0.60
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RωB97X-V/6-31G*	-311.936606		0.150272		
ax RωB97X-V/6-31G*	-311.936903		0.150687		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.142966	-311.992694	0	85.6	
ax RB3LYP-D3/6-311+G(2df,2p)	-312.141700	-311.991013	1.055	14.4	1.05
eq RωB97X-D/6-311+G(2df,2p)	-312.022574	-311.872302	0	75.8	
ax RωB97X-D/6-311+G(2df,2p)	-312.021914	-311.871227	0.675	24.2	0.67
eq RM06-2X/6-311+G(2df,2p)	-311.975827	-311.825555	0	68.5	
ax RM06-2X /6-311+G(2df,2p)	-311.975509	-311.824822	0.460	31.5	0.46
eq RωB97X-V/6-311+G(2df,2p)	-312.037369	-311.887097	0	72.7	
ax RωB97X-V/6-311+G(2df,2p)	-312.036861	-311.886174	0.579	27.3	0.58
eq RMP2(FC)/6-311+G(2df,2p)	-311.287775	-311.137503	0	56.3	
ax RMP2(FC)/6-311+G(2df,2p)	-311.287953	-311.137266	0.149	43.7	0.15
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-310.909314		0.150855		
ax RMP2(FC)/6-31G(d)	-310.910043		0.151498		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-312.140987	-311.990131	0	89.5	1.27

ax RB3LYP-D3/6-311+G(2df,2p)	-312.139613	-311.988114	1.266	10.5	
eq RωB97X-D/6-311+G(2df,2p)	-312.020545	-311.869689	0	81.2	0.87
ax RωB97X-D/6-311+G(2df,2p)	-312.019809	-311.868310	0.865	18.8	
eq RM06-2X/6-311+G(2df,2p)	-311.973733	-311.822877	0	74.3	0.63
ax RM06-2X /6-311+G(2df,2p)	-311.973374	-311.821875	0.629	25.7	
eq RMP2(FC)/6-311+G(2df,2p)	-311.288450	-311.137594	0	63.0	0.31
ax RMP2(FC)/6-311+G(2df,2p)	-311.288593	-311.137095	0.313	37.0	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-310.909314	0.150390			
ax RMP2(FC)/6-31G*	-310.910044	0.151072			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-312.036725	-311.886335	0	80.6	0.84
ax RωB97X-V/6-311+G(2df,2p)	-312.036065	-311.884993	0.842	19.4	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-309.956999	-309.797797	0	89.0	1.23
ax RHF/6-311+G(d,p)	-309.955388	-309.795833	1.232	11.0	
eq RB3LYP/6-311+G(d,p)	-312.107997	-311.961179	0	86.2	1.08
ax RB3LYP/6-311+G(d,p)	-312.106500	-311.959458	1.080	13.8	
eq RB3LYP-D3/6-311+G(d,p)	-312.123714	-311.976376	0	76.8	0.71
ax RB3LYP-D3/6-311+G(d,p)	-312.122791	-311.975250	0.707	23.2	
eq RωB97X-D/6-311+G(d,p)	-312.004486	-311.855644	0	64.3	0.35
ax RωB97X-D/6-311+G(d,p)	-312.004147	-311.855090	0.348	35.7	
eq RM06-2X/6-311+G(d,p)	-311.955962	-311.806894	0	61.3	0.27
ax RM06-2X/6-311+G(d,p)	-311.955920	-311.806460	0.272	38.7	
eq RωB97X-V/6-311+G**	-312.021179	-311.872838	0	65.6	0.38
ax RωB97X-V/6-311+G**	-312.020902	-311.872231	0.381	34.4	
eq RMP2(FC)/6-311+G(d,p)	-311.117501	-310.968891	0	52.6	0.06
ax RMP2(FC)/6-311+G(d,p)	-311.117812	-310.968794	0.061	47.4	

Cyclohexanecarbonitrile



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-325.943512	0.150474			
ax RHF/6-31G(d)	-325.942800	0.150732			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-328.247522	-327.097047	0	71.2	0.54
ax RB3LYP-D3/6-311+G(2df,2p)	-328.246926	-327.096194	0.535	28.8	
eq R ω B97X-D/6-311+G(2df,2p)	-328.123690	-327.973215	0	61.5	0.28
ax R ω B97X-D/6-311+G(2df,2p)	-328.123504	-327.972772	0.278	38.5	
eq RM06-2X/6-311+G(2df,2p)	-328.079757	-327.929282	0	55.7	0.14
ax RM06-2X /6-311+G(2df,2p)	-328.079798	-327.929066	0.136	44.3	
eq RMP2(FC)/6-311+G(2df,2p)	-327.386884	-327.236409	0	54.0	0.09
ax RMP2(FC)/6-311+G(2df,2p)	-327.386991	-327.236259	0.094	46.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-325.943512	0.150072			
ax RHF/6-31G*	-325.942800	0.150321			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-328.141165	-327.991093	0	57.9	0.19
ax R ω B97X-V/6-311+G(2df,2p)	-328.141114	-327.990793	0.188	42.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-328.120624	0.138346			
ax RB3LYP/6-31G(d)	-328.119965	0.138588			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-328.247845	-328.109499	0	71.4	0.54
ax RB3LYP-D3/6-311+G(2df,2p)	-328.247226	-328.108638	0.540	28.6	
eq R ω B97X-D/6-311+G(2df,2p)	-328.123396	-327.985050	0	60.7	0.26
ax R ω B97X-D/6-311+G(2df,2p)	-328.123227	-327.984639	0.258	39.3	

eq RM06-2X/6-311+G(2df,2p)	-328.079251	-327.940905	0	53.7	
ax RM06-2X /6-311+G(2df,2p)	-328.079355	-327.940768	0.086	46.3	0.09
eq RMP2(FC)/6-311+G(2df,2p)	-327.388735	-327.250389	0	50.7	
ax RMP2(FC)/6-311+G(2df,2p)	-327.388951	-327.250364	0.016	49.3	0.02
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-328.120631	0.129469			
ax RB3LYP/6-31G*	-328.119966	0.129682			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-328.141627	-328.012158	0	55.7	
ax RωB97X-V/6-311+G(2df,2p)	-328.141624	-328.011942	0.136	44.3	0.14
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-328.136068	0.138875			
ax RB3LYP-D3/6-31G(d)	-328.136004	0.139106			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-328.247903	-328.109028	0	72.3	
ax RB3LYP-D3/6-311+G(2df,2p)	-328.247228	-328.108122	0.568	27.7	0.57
eq RωB97X-D/6-311+G(2df,2p)	-328.123480	-327.984605	0	61.4	
ax RωB97X-D/6-311+G(2df,2p)	-328.123273	-327.984167	0.274	38.6	0.27
eq RM06-2X/6-311+G(2df,2p)	-328.079400	-327.940525	0	53.2	
ax RM06-2X /6-311+G(2df,2p)	-328.079509	-327.940403	0.076	46.8	0.08
eq RMP2(FC)/6-311+G(2df,2p)	-327.388883	-327.250008	0.047	49.5	
ax RMP2(FC)/6-311+G(2df,2p)	-327.389131	-327.250025	0	50.5	-0.01
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-328.136067	0.138440			
ax RB3LYP-D3/6-31G*	-328.136005	0.138687			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-328.141714	-328.003274	0	56.8	
ax RωB97X-V/6-311+G(2df,2p)	-328.141705	-328.003018	0.161	43.2	0.16
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq R**w**B97X-D/6-31G(d) -328.020962 0.140316

ax R**w**B97X-D/6-31G(d) -328.021264 0.140556

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-328.248150	-328.107833	0	73.0	0.59
ax RB3LYP-D3/6-311+G(2df,2p)	-328.247452	-328.106896	0.588	27.0	
eq R w B97X-D/6-311+G(2df,2p)	-328.123978	-327.983662	0	61.9	0.29
ax R w B97X-D/6-311+G(2df,2p)	-328.123760	-327.983204	0.287	38.1	
eq RM06-2X/6-311+G(2df,2p)	-328.079922	-327.939606	0	52.5	0.06
ax RM06-2X /6-311+G(2df,2p)	-328.080070	-327.939513	0.058	47.5	
eq RMP2(FC)/6-311+G(2df,2p)	-327.389212	-327.248895	0.036	48.5	-004
ax RMP2(FC)/6-311+G(2df,2p)	-327.389509	-327.248953	0	51.5	

geometry method *E* (au) Thermal correction to Gibbs Free Energy (au/Particle)

eq R**w**B97X-D/6-31G* -328.020970 0.129537

ax R**w**B97X-D/6-31G* -328.021266 0.129759

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq R w B97X-V/6-311+G(2df,2p)	-328.142089	-328.012552	0	56.5	0.15
ax R w B97X-V/6-311+G(2df,2p)	-328.142064	-328.012305	0.155	43.5	

geometry method *E* (au) Thermal correction to Gibbs Free Energy (au/Particle)

eq RM06-2X/6-31G(d) -327.867782 0.137424

ax RM06-2X/6-31G(d) -327.868348 0.137835

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-328.247511	-328.110088	0	76.7	0.70
ax RB3LYP-D3/6-311+G(2df,2p)	-328.246800	-328.108966	0.704	23.3	
eq R w B97X-D/6-311+G(2df,2p)	-328.123505	-327.986081	0	66.0	0.39
ax R w B97X-D/6-311+G(2df,2p)	-328.123292	-327.985458	0.391	34.0	
eq RM06-2X/6-311+G(2df,2p)	-328.079467	-327.942043	0	56.6	0.16
ax RM06-2X /6-311+G(2df,2p)	-328.079627	-327.941792	0.157	43.4	
eq RMP2(FC)/6-311+G(2df,2p)	-327.389266	-327.251843	0	52.3	0.05
ax RMP2(FC)/6-311+G(2df,2p)	-327.389591	-327.251757	0.054	47.7	

geometry method *E* (au) Thermal correction to Gibbs Free Energy (au/Particle)

eq RM06-2X/6-31G* -327.967471 0.139751

ax RM06-2X/6-31G* -327.968108 0.140023

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RωB97X-V/6-311+G(2df,2p) -328.142172 -328.002421 0 59.9 0.24

ax RωB97X-V/6-311+G(2df,2p) -328.142066 -328.002043 0.237 40.1

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
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eq RωB97X-V/6-31G* -328.035963 0.139996

ax RωB97X-V/6-31G* -328.036512 0.140296

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RB3LYP-D3/6-311+G(2df,2p) -328.249681 -328.109685 0 75.9 0.68

ax RB3LYP-D3/6-311+G(2df,2p) -328.248900 -328.108604 0.678 24.1

eq RωB97X-D/6-311+G(2df,2p) -328.125410 -327.985414 0 64.5 0.35

ax RωB97X-D/6-311+G(2df,2p) -328.125146 -327.984850 0.354 35.5

eq RM06-2X/6-311+G(2df,2p) -328.081406 -327.941410 0 54.6 0.11

ax RM06-2X /6-311+G(2df,2p) -328.081533 -327.941237 0.109 45.4

eq RωB97X-V/6-311+G(2df,2p) -328.141896 -328.001900 0 59.2 0.22

ax RωB97X-V/6-311+G(2df,2p) -328.141846 -328.001550 0.220 40.8

eq RMP2(FC)/6-311+G(2df,2p) -327.388874 -327.248878 0.013 49.4 -0.01

ax RMP2(FC)/6-311+G(2df,2p) -327.389195 -327.248899 0 50.6

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
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eq RMP2(FC)/6-31G(d) -327.005224 0.141341

ax RMP2(FC)/6-31G(d) -327.006175 0.141681

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RB3LYP-D3/6-311+G(2df,2p) -328.246144 -328.104802 0 79.2 0.79

ax RB3LYP-D3/6-311+G(2df,2p) -328.246144 -328.103541 0.791 20.8

eq RωB97X-D/6-311+G(2df,2p) -328.121760 -327.980418 0 67.7 0.44

ax RωB97X-D/6-311+G(2df,2p) -328.121403 -327.979722 0.437 32.3

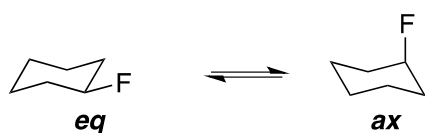
eq RM06-2X/6-311+G(2df,2p) -328.077577 -327.936236 0 56.4 0.15

ax RM06-2X /6-311+G(2df,2p) -328.077674 -327.935992 0.153 43.6

eq RMP2(FC)/6-311+G(2df,2p) -327.389420 -327.248078 0 50.5 0.01

ax RMP2(FC)/6-311+G(2df,2p)	-327.389742	-327.248060	0.011	49.5	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-327.005224		0.140915		
ax RMP2(FC)/6-31G*	-327.006175		0.141255		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-328.140046	-327.999131	0	62.4	0.30
ax RωB97X-V/6-311+G(2df,2p)	-328.139911	-327.998656	0.298	37.6	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-326.025853	-325.877513	0	80.5	0.84
ax RHF/6-311+G(d,p)	-326.024715	-325.876179	0.837	19.5	
eq RB3LYP/6-311+G(d,p)	-328.214465	-328.077674	0	77.7	0.74
ax RB3LYP/6-311+G(d,p)	-328.213418	-328.076499	0.737	22.3	
eq RB3LYP-D3/6-311+G(d,p)	-328.229921	-328.092690	0	67.5	0.43
ax RB3LYP-D3/6-311+G(d,p)	-328.229404	-328.092001	0.432	32.5	
eq RωB97X-D/6-311+G(d,p)	-328.106896	-327.968306	0	54.8	0.11
ax RωB97X-D/6-311+G(d,p)	-328.106871	-327.968125	0.114	45.2	
eq RM06-2X/6-311+G(d,p)	-328.061862	-327.923065	0.074	46.9	-0.07
ax RM06-2X/6-311+G(d,p)	-328.062196	-327.923183	0	53.1	
eq RωB97X-V/6-311+G**	-328.125546	-327.987441	0	51.7	0.04
ax RωB97X-V/6-311+G**	-328.125735	-327.987376	0.041	48.3	
eq RMP2(FC)/6-311+G(d,p)	-327.213261	-327.074782	0.099	45.8	-0.10
ax RMP2(FC)/6-311+G(d,p)	-327.213677	-327.074939	0	54.2	

Fluorocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-333.063777	0.144765			
ax RHF/6-31G(d)	-333.064194	0.144984			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-335.250627	-335.105861	0	68.5	0.46
ax RB3LYP-D3/6-311+G(2df,2p)	-335.250115	-335.105131	0.459	31.5	
eq R ω B97X-D/6-311+G(2df,2p)	-335.135742	-334.990977	0	70.4	0.51
ax R ω B97X-D/6-311+G(2df,2p)	-335.135150	-334.990161	0.512	29.6	
eq RM06-2X/6-311+G(2df,2p)	-335.082273	-334.937508	0	61.2	0.27
ax RM06-2X /6-311+G(2df,2p)	-335.082062	-334.937077	0.270	38.8	
eq RMP2(FC)/6-311+G(2df,2p)	-334.433731	-334.288966	0	63.7	0.33
ax RMP2(FC)/6-311+G(2df,2p)	-334.433419	-334.288435	0.333	36.3	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-333.063777	0.144570			
ax RHF/6-31G*	-333.064194	0.144745			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-335.139234	-334.994664	0	60.5	0.25
ax R ω B97X-V/6-311+G(2df,2p)	-335.139008	-334.994263	0.252	39.5	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-335.114886	0.133372			
ax RB3LYP/6-31G(d)	-335.115171	0.133570			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-335.251176	-335.117804	0	68.2	0.45
ax RB3LYP-D3/6-311+G(2df,2p)	-335.250654	-335.117084	0.452	31.8	
eq R ω B97X-D/6-311+G(2df,2p)	-335.135744	-335.002373	0	70.8	0.52
ax R ω B97X-D/6-311+G(2df,2p)	-335.135111	-335.001541	0.522	29.2	

eq RM06-2X/6-311+G(2df,2p)	-335.082090	-334.948718	0	61.1	
ax RM06-2X /6-311+G(2df,2p)	-335.081862	-334.948292	0.267	38.9	0.27
eq RMP2(FC)/6-311+G(2df,2p)	-334.433511	-334.300139	0	64.0	
ax RMP2(FC)/6-311+G(2df,2p)	-334.433167	-334.299597	0.341	36.0	0.34
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-335.114892	0.125099			
ax RB3LYP/6-31G*	-335.115156	0.125175			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-335.140002	-335.014903	0	58.0	
ax RωB97X-V/6-311+G(2df,2p)	-335.139774	-335.014599	0.191	42.0	0.19
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-335.128963	0.133776			
ax RB3LYP-D3/6-31G(d)	-335.129540	0.133927			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-335.251188	-335.117412	0	69.7	
ax RB3LYP-D3/6-311+G(2df,2p)	-335.250555	-335.116628	0.412	30.3	0.49
eq RωB97X-D/6-311+G(2df,2p)	-335.135777	-335.002001	0	72.6	
ax RωB97X-D/6-311+G(2df,2p)	-335.135011	-335.001084	0.575	27.4	0.58
eq RM06-2X/6-311+G(2df,2p)	-335.082179	-334.948403	0	61.6	
ax RM06-2X /6-311+G(2df,2p)	-335.081883	-334.947956	0.280	38.4	0.28
eq RMP2(FC)/6-311+G(2df,2p)	-334.433629	-334.299853	0	64.3	
ax RMP2(FC)/6-311+G(2df,2p)	-334.433226	-334.299298	0.348	35.7	0.35
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-335.128963	0.133580			
ax RB3LYP-D3/6-31G*	-335.129539	0.133687			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-335.140053	-335.006473	0	61.4	
ax RωB97X-V/6-311+G(2df,2p)	-335.139723	-335.006036	0.274	38.6	0.27
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq R**w**B97X-D/6-31G(d) -335.023149 0.135282

ax R**w**B97X-D/6-31G(d) -335.023266 0.135375

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-335.251200	-335.115919	0	66.1	0.39
ax RB3LYP-D3/6-311+G(2df,2p)	-335.25067	-335.115292	0.393	33.9	
eq R w B97X-D/6-311+G(2df,2p)	-335.136081	-335.000799	0	69.0	0.47
ax R w B97X-D/6-311+G(2df,2p)	-335.135420	-335.000046	0.473	31.0	
eq RM06-2X/6-311+G(2df,2p)	-335.082539	-334.947257	0	59.4	0.23
ax RM06-2X /6-311+G(2df,2p)	-335.082273	-334.946898	0.225	40.6	
eq RMP2(FC)/6-311+G(2df,2p)	-334.434020	-334.298739	0	62.5	0.30
ax RMP2(FC)/6-311+G(2df,2p)	-334.433632	-334.298257	0.302	37.5	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq R w B97X-D/6-31G*	-335.023150	0.125202
ax R w B97X-D/6-31G*	-335.023264	0.125236

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq R w B97X-V/6-311+G(2df,2p)	-335.140157	-335.014955	0	57.9	0.19
ax R w B97X-V/6-311+G(2df,2p)	-335.139890	-335.014654	0.189	42.1	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G(d)	-334.959863	0.135018
ax RM06-2X/6-31G(d)	-334.960517	0.135315

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-335.251060	-335.116042	0	75.6	0.67
ax RB3LYP-D3/6-311+G(2df,2p)	-335.250292	-335.114977	0.669	24.4	
eq R w B97X-D/6-311+G(2df,2p)	-335.136042	-335.001024	0	79.1	0.79
ax R w B97X-D/6-311+G(2df,2p)	-335.135087	-334.999772	0.786	20.9	
eq RM06-2X/6-311+G(2df,2p)	-335.082597	-334.947579	0	67.2	0.42
ax RM06-2X /6-311+G(2df,2p)	-335.082218	-334.946903	0.424	32.8	
eq RMP2(FC)/6-311+G(2df,2p)	-334.434090	-334.299071	0	70.2	0.51
ax RMP2(FC)/6-311+G(2df,2p)	-334.433580	-334.298264	0.507	29.8	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
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eq RM06-2X/6-31G* -334.959914 0.134883

ax RM06-2X/6-31G* -334.960530 0.134998

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RωB97X-V/6-311+G(2df,2p) -335.140082 -335.005199 0 65.3 0.37

ax RωB97X-V/6-311+G(2df,2p) -335.139603 -335.004605 0.373 34.7

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
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eq RωB97X-V/6-31G* -335.023246 0.135076

ax RωB97X-V/6-31G* -335.024098 0.135253

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RB3LYP-D3/6-311+G(2df,2p) -335.252175 -335.117099 0 73.7 0.61

ax RB3LYP-D3/6-311+G(2df,2p) -335.251381 -335.116128 0.609 26.3

eq RωB97X-D/6-311+G(2df,2p) -335.136924 -335.001848 0 76.4 0.69

ax RωB97X-D/6-311+G(2df,2p) -335.135996 -335.000743 0.693 23.6

eq RM06-2X/6-311+G(2df,2p) -335.083443 -334.948367 0 65.2 0.37

ax RM06-2X /6-311+G(2df,2p) -335.083027 -334.947774 0.372 34.8

eq RωB97X-V/6-311+G(2df,2p) -335.140065 -335.004989 0 65.2 0.37

ax RωB97X-V/6-311+G(2df,2p) -335.139651 -335.004398 0.371 34.8

eq RMP2(FC)/6-311+G(2df,2p) -334.433705 -334.298629 0 66.5 0.40

ax RMP2(FC)/6-311+G(2df,2p) -334.433237 -334.297984 0.405 33.5

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
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eq RMP2(FC)/6-31G(d) -334.014691 0.137063

ax RMP2(FC)/6-31G(d) -334.015810 0.137361

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
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eq RB3LYP-D3/6-311+G(2df,2p) -335.251354 -335.114291 0 75.3 0.66

ax RB3LYP-D3/6-311+G(2df,2p) -335.250601 -335.113240 0.659 24.7

eq RωB97X-D/6-311+G(2df,2p) -335.136111 -334.999048 0 78.1 0.75

ax RωB97X-D/6-311+G(2df,2p) -335.135211 -334.997850 0.751 21.9

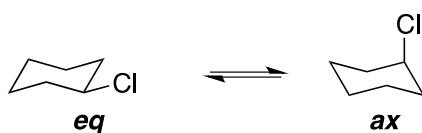
eq RM06-2X/6-311+G(2df,2p) -335.082537 -334.945474 0 67.0 0.42

ax RM06-2X /6-311+G(2df,2p) -335.082168 -334.944807 0.419 33.0

eq RMP2(FC)/6-311+G(2df,2p) -334.434231 -334.297169 0 70.6 0.52

ax RMP2(FC)/6-311+G(2df,2p)	-334.433703	-334.296343	0.518	29.4	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-334.014691		0.136872		
ax RMP2(FC)/6-31G*	-334.015810		0.137136		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-335.140300	-335.003428	0	68.3	0.45
ax RωB97X-V/6-311+G(2df,2p)	-335.139841	-335.002705	0.454	31.7	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-333.155283	-333.012730	0	63.2	0.32
ax RHF/6-311+G(d,p)	-333.154872	-333.012221	0.319	36.8	
eq RB3LYP/6-311+G(d,p)	-335.220229	-335.088647	0	66.1	0.39
ax RB3LYP/6-311+G(d,p)	-335.219647	-335.088018	0.395	33.9	
eq RB3LYP-D3/6-311+G(d,p)	-335.234271	-335.102318	0	59.1	0.22
ax RB3LYP-D3/6-311+G(d,p)	-335.233851	-335.101970	0.218	40.9	
eq RωB97X-D/6-311+G(d,p)	-335.119729	-334.986381	0	63.8	0.33
ax RωB97X-D/6-311+G(d,p)	-335.119275	-334.985849	0.334	36.2	
eq RM06-2X/6-311+G(d,p)	-335.065550	-334.932010	0	55.7	0.13
ax RM06-2X/6-311+G(d,p)	-335.065394	-334.931795	0.135	44.3	
eq RωB97X-V/6-311+G**	-335.124762	-334.991781	0	52.0	0.05
ax RωB97X-V/6-311+G**	-335.124646	-334.991706	0.047	48.0	
eq RMP2(FC)/6-311+G(d,p)	-334.256015	-334.121816	0	64.9	0.36
ax RMP2(FC)/6-311+G(d,p)	-334.255536	-334.121236	0.364	35.1	

Chlorocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-693.114672	0.142398			
ax RHF/6-31G(d)	-693.113065	0.142636			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.606827	-695.464429	0	74.1	0.62
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606077	-695.463441	0.620	25.9	
eq R ω B97X-D/6-311+G(2df,2p)	-695.502351	-695.359954	0	78.3	0.76
ax R ω B97X-D/6-311+G(2df,2p)	-695.501380	-695.358745	0.759	21.7	
eq RM06-2X/6-311+G(2df,2p)	-695.442203	-695.299805	0	70.2	0.51
ax RM06-2X /6-311+G(2df,2p)	-695.441633	-695.298997	0.507	29.8	
eq RMP2(FC)/6-311+G(2df,2p)	-694.416732	-694.274335	0	78.6	0.77
ax RMP2(FC)/6-311+G(2df,2p)	-694.415744	-694.273108	0.770	21.4	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-693.114672	0.142152			
ax RHF/6-31G*	-693.113065	0.142325			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-695.445731	-695.303579	0	72.0	0.56
ax R ω B97X-V/6-311+G(2df,2p)	-695.445016	-695.302691	0.557	28.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-695.480675	0.131082			
ax RB3LYP/6-31G(d)	-695.479313	0.131277			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.606969	-695.475888	0	72.1	0.56
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606273	-695.474996	0.560	27.9	
eq R ω B97X-D/6-311+G(2df,2p)	-695.501960	-695.370878	0	77.0	0.71
ax R ω B97X-D/6-311+G(2df,2p)	-695.501019	-695.369742	0.713	23.0	

eq RM06-2X/6-311+G(2df,2p)	-695.441682	-695.310601	0	68.1	
ax RM06-2X /6-311+G(2df,2p)	-695.441166	-695.309889	0.447	31.9	0.45
eq RMP2(FC)/6-311+G(2df,2p)	-694.415921	-694.284840	0	77.3	
ax RMP2(FC)/6-311+G(2df,2p)	-694.414966	-694.283689	0.722	22.7	0.72
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-695.480682	0.122784			
ax RB3LYP/6-31G*	-695.479304	0.122894			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-695.445792	-695.323008	0	69.5	
ax RωB97X-V/6-311+G(2df,2p)	-695.445127	-695.322233	0.486	30.5	0.49
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-695.496567	0.131615			
ax RB3LYP-D3/6-31G(d)	-695.496109	0.131887			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.6069972	-695.475382	0	73.5	
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606308	-695.474421	0.603	26.5	0.60
eq RωB97X-D/6-311+G(2df,2p)	-695.502015	-695.370400	0	78.9	
ax RωB97X-D/6-311+G(2df,2p)	-695.501048	-695.369161	0.777	21.1	0.78
eq RM06-2X/6-311+G(2df,2p)	-695.441801	-695.310186	0	69.0	
ax RM06-2X /6-311+G(2df,2p)	-695.441318	-695.309431	0.473	31.0	0.47
eq RMP2(FC)/6-311+G(2df,2p)	-694.416067	-694.284451	0	77.5	
ax RMP2(FC)/6-311+G(2df,2p)	-694.415176	-694.283289	0.729	22.5	0.73
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-695.496567	0.131378			
ax RB3LYP-D3/6-31G*	-695.496101	0.131577			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-695.445872	-695.314494	0	71.6	
ax RωB97X-V/6-311+G(2df,2p)	-695.445207	-695.313622	0.547	28.4	0.55
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq R ω B97X-D/6-31G(d)	-695.399602	0.133022
ax R ω B97X-D/6-31G(d)	-695.398763	0.133330

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.607021	-695.473999	0	74.7	0.64
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606312	-695.472982	0.638	25.3	
eq R ω B97X-D/6-311+G(2df,2p)	-695.502459	-695.369437	0	79.5	0.80
ax R ω B97X-D/6-311+G(2df,2p)	-695.501491	-695.368161	0.8001	20.5	
eq RM06-2X/6-311+G(2df,2p)	-695.442310	-695.309288	0	70.1	0.50
ax RM06-2X /6-311+G(2df,2p)	-695.441815	-695.308485	0.504	29.9	
eq RMP2(FC)/6-311+G(2df,2p)	-694.416778	-694.283756	0	78.1	0.75
ax RMP2(FC)/6-311+G(2df,2p)	-694.415889	-694.282560	0.751	21.9	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq R ω B97X-D/6-31G*	-695.399614	0.122973
ax R ω B97X-D/6-31G*	-695.398760	0.123132

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-695.446288	-695.323315	0	70.9	0.53
ax R ω B97X-V/6-311+G(2df,2p)	-695.445607	-695.322475	0.527	29.1	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RM06-2X/6-31G(d)	-695.327729	0.132734
ax RM06-2X/6-31G(d)	-695.327418	0.133021

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.606913	-695.474179	0	75.2	0.66
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606154	-695.473133	0.657	24.8	
eq R ω B97X-D/6-311+G(2df,2p)	-695.502474	-695.369740	0	80.4	0.83
ax R ω B97X-D/6-311+G(2df,2p)	-695.501434	-695.368413	0.833	19.6	
eq RM06-2X/6-311+G(2df,2p)	-695.442419	-695.309685	0	68.7	0.47
ax RM06-2X /6-311+G(2df,2p)	-695.441964	-695.308943	0.466	31.3	
eq RMP2(FC)/6-311+G(2df,2p)	-694.416977	-694.284243	0	76.0	0.68
ax RMP2(FC)/6-311+G(2df,2p)	-694.416181	-694.283160	0.680	24.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G*	-695.327790	0.132592			
ax RM06-2X/6-31G*	-695.327444	0.132699			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-695.446340	-695.313748	0	70.0	0.50
ax R ω B97X-V/6-311+G(2df,2p)	-695.445648	-695.312949	0.501	30.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-V/6-31G*	-695.341789	0.132915			
ax R ω B97X-V/6-31G*	-695.341364	0.133139			

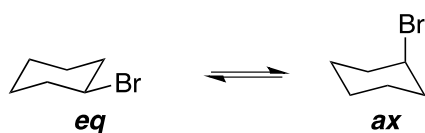
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.607714	-695.474796	0	75.2	0.66
ax RB3LYP-D3/6-311+G(2df,2p)	-695.606891	-695.473752	0.655	24.8	
eq R ω B97X-D/6-311+G(2df,2p)	-695.503207	-695.370289	0	79.7	0.81
ax R ω B97X-D/6-311+G(2df,2p)	-695.502140	-695.369001	0.808	20.3	
eq RM06-2X/6-311+G(2df,2p)	-695.443183	-695.310265	0	69.2	0.48
ax RM06-2X /6-311+G(2df,2p)	-695.442644	-695.309505	0.477	30.8	
eq R ω B97X-V/6-311+G(2df,2p)	-695.446170	-695.313252	0	72.3	0.57
ax R ω B97X-V/6-311+G(2df,2p)	-695.445490	-695.312351	0.565	27.7	
eq RMP2(FC)/6-311+G(2df,2p)	-694.416518	-694.283600	0	74.9	0.65
ax RMP2(FC)/6-311+G(2df,2p)	-694.415710	-694.282571	0.646	25.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-694.029071	0.134951			
ax RMP2(FC)/6-31G(d)	-694.027936	0.135269			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-695.606730	-695.471779	0	77.6	0.73
ax RB3LYP-D3/6-311+G(2df,2p)	-695.605878	-965.470609	0.734	22.4	
eq R ω B97X-D/6-311+G(2df,2p)	-695.502452	-695.367500	0	81.4	0.87
ax R ω B97X-D/6-311+G(2df,2p)	-695.501378	-695.366109	0.873	18.6	
eq RM06-2X/6-311+G(2df,2p)	-695.442396	-695.307445	0	70.4	0.51
ax RM06-2X /6-311+G(2df,2p)	-695.441898	-695.306629	0.512	29.6	

eq RMP2(FC)/6-311+G(2df,2p)	-694.417024	-694.282073	0	76.8	0.71
ax RMP2(FC)/6-311+G(2df,2p)	-694.416216	-694.280947	0.707	23.2	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-694.029071	0.134720			
ax RMP2(FC)/6-31G*	-694.027936	0.134981			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-695.446309	-695.311589	0	73.9	0.61
ax RωB97X-V/6-311+G(2df,2p)	-695.445591	-695.310610	0.614	26.1	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-693.198823	-693.058635	0	87.4	1.14
ax RHF/6-311+G(d,p)	-693.197198	-693.056811	1.145	12.6	
eq RB3LYP/6-311+G(d,p)	-695.575085	-695.445687	0	83.4	0.95
ax RB3LYP/6-311+G(d,p)	-695.573703	-695.444167	0.954	16.6	
eq RB3LYP-D3/6-311+G(d,p)	-695.590951	-695.461060	0	67.8	0.44
ax RB3LYP-D3/6-311+G(d,p)	-695.590461	-695.460357	0.441	32.2	
eq RωB97X-D/6-311+G(d,p)	-695.486786	-695.355559	0	74.4	0.63
ax RωB97X-D/6-311+G(d,p)	-695.486031	-695.354553	0.631	25.6	
eq RM06-2X/6-311+G(d,p)	-695.426225	-695.294905	0	64.1	0.34
ax RM06-2X/6-311+G(d,p)	-695.425951	-695.294360	0.342	35.9	
eq RωB97X-V/6-311+G**	-695.431435	-695.300539	0	66.3	0.40
ax RωB97X-V/6-311+G**	-695.430975	-695.299904	0.398	33.7	
eq RMP2(FC)/6-311+G(d,p)	-694.238102	-694.106074	0	79.8	0.81
ax RMP2(FC)/6-311+G(d,p)	-694.237123	-694.104782	0.811	20.2	

Bromocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-246.568190	0.140523			
ax RHF/6-31G(d)	-246.566599	0.140773			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298445	-652.157922	0	71.7	0.55
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297822	-652.157049	0.548	28.3	
eq Rwb97X-D/6-311+G(2df,2p)	-652.213238	-652.072716	0	78.6	0.77
ax Rwb97X-D/6-311+G(2df,2p)	-652.212264	-652.071491	0.769	21.4	
eq RM06-2X/6-311+G(2df,2p)	-652.272729	-652.132206	0	69.7	0.49
ax RM06-2X /6-311+G(2df,2p)	-652.272195	-652.131421	0.493	30.3	
eq RMP2(FC)/6-311+G(2df,2p)	-650.460800	-650.320278	0	76.5	0.70
ax RMP2(FC)/6-311+G(2df,2p)	-650.459940	-650.319166	0.698	23.5	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-2805.737677	0.140334			
ax RHF/6-31G*	-2805.735790	0.140491			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq Rwb97X-V/6-311+G(2df,2p)	-2809.181747	-2809.041410	0	72.3	0.57
ax Rwb97X-V/6-311+G(2df,2p)	-2809.180998	-2809.040508	0.566	27.7	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-248.450842	0.129329			
ax RB3LYP/6-31G(d)	-248.449423	0.129509			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298455	-652.169126	0	68.6	0.46
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297899	-652.168389	0.462	31.4	
eq Rwb97X-D/6-311+G(2df,2p)	-652.212644	-652.083315	0	76.7	0.70
ax Rwb97X-D/6-311+G(2df,2p)	-652.211705	-652.082195	0.703	23.3	

eq RM06-2X/6-311+G(2df,2p)	-652.272108	-652.142780	0	66.5	
ax RM06-2X /6-311+G(2df,2p)	-652.271643	-652.142134	0.405	33.5	0.41
eq RMP2(FC)/6-311+G(2df,2p)	-650.459756	-650.330427	0	74.0	
ax RMP2(FC)/6-311+G(2df,2p)	-650.458953	-650.329444	0.617	26.0	0.62
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-2809.166756	0.120960			
ax RB3LYP/6-31G*	-2809.165096	0.121036			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-2809.181746	-2809.060790	0	69.2	
ax RωB97X-V/6-311+G(2df,2p)	-2809.181062	-2809.060026	0.479	30.8	0.48
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-248.467442	0.129849			
ax RB3LYP-D3/6-31G(d)	-248.467234	0.130189			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298474	-652.168626	0	72.2	
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297917	-652.167728	0.563	27.8	0.56
eq RωB97X-D/6-311+G(2df,2p)	-652.212688	-652.082839	0	80.4	
ax RωB97X-D/6-311+G(2df,2p)	-652.211698	-652.081509	0.835	19.6	0.83
eq RM06-2X/6-311+G(2df,2p)	-652.272208	-652.142359	0	69.6	
ax RM06-2X /6-311+G(2df,2p)	-652.271768	-652.141579	0.490	30.4	0.49
eq RMP2(FC)/6-311+G(2df,2p)	-650.459905	-650.330056	0	76.1	
ax RMP2(FC)/6-311+G(2df,2p)	-650.459153	-650.328964	0.686	23.9	0.69
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-2809.183353	0.129570			
ax RB3LYP-D3/6-31G*	-2809.182883	0.129781			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-2809.181820	-2809.052247	0	71.9	
ax RωB97X-V/6-311+G(2df,2p)	-2809.181146	-2809.051363	0.555	28.1	0.55
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq R ω B97X-D/6-31G(d) -248.394062 0.131220

ax R ω B97X-D/6-31G(d) -248.393447 0.131452

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298547	-652.167326	0	70.3	0.51
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297970	-652.166517	0.508	29.7	
eq R ω B97X-D/6-311+G(2df,2p)	-652.213359	-652.082139	0	78.5	0.77
ax R ω B97X-D/6-311+G(2df,2p)	-652.212372	-652.080919	0.765	21.5	
eq RM06-2X/6-311+G(2df,2p)	-652.272858	-652.141638	0	67.4	0.43
ax RM06-2X /6-311+G(2df,2p)	-652.272408	-652.140956	0.428	32.6	
eq RMP2(FC)/6-311+G(2df,2p)	-650.460948	-650.329728	0	73.4	0.60
ax RMP2(FC)/6-311+G(2df,2p)	-650.460226	-650.328773	0.599	26.6	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-D/6-31G*	-2809.135404		0.121202		
ax R ω B97X-D/6-31G*	-2809.134411		0.121337		

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-2809.182351	-2809.061147	0	70.7	0.52
ax R ω B97X-V/6-311+G(2df,2p)	-2809.181658	-2809.060317	0.521	29.3	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G(d)	-248.284094		0.130969		
ax RM06-2X/6-31G(d)	-248.284078		0.131297		

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298501	-652.167531	0	73.9	0.61
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297850	-652.166553	0.614	26.1	
eq R ω B97X-D/6-311+G(2df,2p)	-652.2134149	-652.082445	0	81.3	0.87
ax R ω B97X-D/6-311+G(2df,2p)	-652.212362	-652.081065	0.866	18.7	
eq RM06-2X/6-311+G(2df,2p)	-652.272989	-652.142019	0	68.7	0.46
ax RM06-2X /6-311+G(2df,2p)	-652.272578	-652.141281	0.463	31.3	
eq RMP2(FC)/6-311+G(2df,2p)	-650.461194	-650.330224	0	72.5	0.57
ax RMP2(FC)/6-311+G(2df,2p)	-650.460607	-650.329310	0.574	27.5	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
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eq RM06-2X/6-31G* -2809.050141 0.130813

ax RM06-2X/6-31G* -2809.049728 0.130875

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-2809.182405	-2809.051594	0	69.0	0.47
ax R ω B97X-V/6-311+G(2df,2p)	-2809.181718	-2809.050840	0.473	31.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-V/6-31G*	-2808.848559	0.131148			
ax R ω B97X-V/6-31G*	-2808.847975	0.131363			

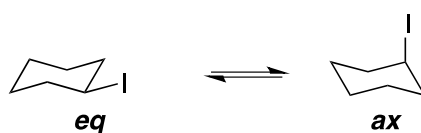
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.297987	-652.166838	0	70.5	0.52
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297382	-652.166017	0.515	29.5	
eq R ω B97X-D/6-311+G(2df,2p)	-652.213002	-652.081853	0	77.7	0.74
ax R ω B97X-D/6-311+G(2df,2p)	-652.212044	-652.080679	0.737	22.3	
eq RM06-2X/6-311+G(2df,2p)	-652.272555	-652.141406	0	66.4	0.40
ax RM06-2X /6-311+G(2df,2p)	-652.272130	-652.140765	0.402	33.6	
eq R ω B97X-V/6-311+G(2df,2p)	-2809.182218	-2809.051069	0	72.2	0.56
ax R ω B97X-V/6-311+G(2df,2p)	-2809.181534	-2809.050169	0.565	27.8	
eq RMP2(FC)/6-311+G(2df,2p)	-650.460955	-650.329806	0	70.4	0.51
ax RMP2(FC)/6-311+G(2df,2p)	-650.460355	-650.328990	0.512	29.6	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-247.463042	0.133097			
ax RMP2(FC)/6-31G(d)	-247.461905	0.133430			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-652.298348	-652.165250	0	75.6	0.67
ax RB3LYP-D3/6-311+G(2df,2p)	-652.297615	-652.164185	0.668	24.4	
eq R ω B97X-D/6-311+G(2df,2p)	-652.213447	-652.080349	0	81.7	0.88
ax R ω B97X-D/6-311+G(2df,2p)	-652.212371	-652.078941	0.883	18.3	
eq RM06-2X/6-311+G(2df,2p)	-652.272980	-652.139882	0	69.5	0.49
ax RM06-2X /6-311+G(2df,2p)	-652.272538	-652.139108	0.485	30.5	
eq RMP2(FC)/6-311+G(2df,2p)	-650.461305	-650.328208	0	72.1	0.56

ax RMP2(FC)/6-311+G(2df,2p)	-650.460745	-650.327315	0.560	27.9	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-2806.639420		0.132763		
ax RMP2(FC)/6-31G*	-2806.638331		0.133056		
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-2809.182381	-2809.049621	0	73.9	0.61
ax RωB97X-V/6-311+G(2df,2p)	-2809.181693	-2809.048642	0.614	26.1	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-649.197351	-649.058972	0	89.3	1.25
ax RHF/6-311+G(d,p)	-649.195536	-649.056977	1.252	10.7	
eq RB3LYP/6-311+G(d,p)	-652.269001	-652.141425	0	86.1	1.08
ax RB3LYP/6-311+G(d,p)	-652.267397	-652.139707	1.078	13.9	
eq RB3LYP-D3/6-311+G(d,p)	-652.285581	-652.157485	0	67.3	0.43
ax RB3LYP-D3/6-311+G(d,p)	-652.285166	-652.156806	0.426	32.7	
eq RωB97X-D/6-311+G(d,p)	-652.201169	-652.200381	0	74.5	0.63
ax RωB97X-D/6-311+G(d,p)	-652.071738	-652.070727	0.634	25.5	
eq RM06-2X/6-311+G(d,p)	-652.260120	-652.130637	0	64.2	0.35
ax RM06-2X/6-311+G(d,p)	-652.259920	-652.130087	0.345	35.8	
eq RωB97X-V/6-311+G**	-2809.170054	-2809.040932	0	68.6	0.46
ax RωB97X-V/6-311+G**	-2809.169503	-2809.040195	0.462	31.4	
eq RMP2(FC)/6-311+G(d,p)	-650.331851	-650.201964	0	61.4	0.27
ax RMP2(FC)/6-311+G(d,p)	-650.331786	-650.201528	0.274	38.6	

Iodocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-244.789103	0.139255			
ax RHF/6-31G(d)	-244.786960	0.139476			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178194	-533.038939	0	70.4	0.51
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177600	-533.038123	0.512	29.6	
eq Rwb97X-D/6-311+G(2df,2p)	-533.073099	-532.933844	0	78.0	0.75
ax Rwb97X-D/6-311+G(2df,2p)	-533.072129	-532.932652	0.748	22.0	
eq RM06-2X/6-311+G(2df,2p)	-532.869381	-532.730126	0	69.9	0.50
ax RM06-2X /6-311+G(2df,2p)	-532.868811	-532.729334	0.497	30.1	
eq RMP2(FC)/6-311+G(2df,2p)	-531.745099	-531.605844	0	79.2	0.79
ax RMP2(FC)/6-311+G(2df,2p)	-531.744062	-531.604586	0.790	20.8	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G*	-244.790347	0.138923			
ax RHF/6-31G*	-244.788238	0.139113			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq Rwb97X-V/6-311+G(2df,2p)	-7154.396256	-7154.257333	0	71.2	0.54
ax Rwb97X-V/6-311+G(2df,2p)	-7154.395592	-7154.256479	0.536	28.8	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G(d)	-246.665175	0.128098			
ax RB3LYP/6-31G(d)	-246.663405	0.128252			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178233	-533.050134	0	67.1	0.42
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177713	-533.049462	0.422	32.9	
eq Rwb97X-D/6-311+G(2df,2p)	-533.072554	-532.944455	0	75.8	0.67
ax Rwb97X-D/6-311+G(2df,2p)	-533.071634	-532.943383	0.673	24.2	

eq RM06-2X/6-311+G(2df,2p)	-532.868797	-532.740699	0	65.7	
ax RM06-2X /6-311+G(2df,2p)	-532.868340	-532.740089	0.383	34.3	0.38
eq RMP2(FC)/6-311+G(2df,2p)	-531.876838	-531.748739	0	79.0	
ax RMP2(FC)/6-311+G(2df,2p)	-531.875746	-531.747495	0.781	21.0	0.78
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP/6-31G*	-246.669360	0.119607			
ax RB3LYP/6-31G*	-246.667591	0.119699			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RwB97X-V/6-311+G(2df,2p)	-7154.396312	-7154.276705	0	67.3	
ax RwB97X-V/6-311+G(2df,2p)	-7154.395726	-7154.276027	0.425	32.7	0.43
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G(d)	-246.682226	0.128671			
ax RB3LYP-D3/6-31G(d)	-246.681821	0.128939			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178252	-533.049581	0	69.7	
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177737	-533.048798	0.491	30.3	0.49
eq RwB97X-D/6-311+G(2df,2p)	-533.072592	-532.943921	0	78.7	
ax RwB97X-D/6-311+G(2df,2p)	-533.071627	-532.942688	0.774	21.3	0.77
eq RM06-2X/6-311+G(2df,2p)	-532.868889	-532.740218	0	67.2	
ax RM06-2X /6-311+G(2df,2p)	-532.868480	-532.739541	0.425	32.8	0.42
eq RMP2(FC)/6-311+G(2df,2p)	-531.876952	-531.748280	0	80.3	
ax RMP2(FC)/6-311+G(2df,2p)	-531.875899	-531.746960	0.828	19.7	0.83
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RB3LYP-D3/6-31G*	-246.686403	0.128214			
ax RB3LYP-D3/6-31G*	-246.685999	0.128440			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RwB97X-V/6-311+G(2df,2p)	-7154.396374	-7154.268160	0	70.2	
ax RwB97X-V/6-311+G(2df,2p)	-7154.395792	-7154.267352	0.507	29.8	0.51
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq RωB97X-D/6-31G(d) -246.608488 0.130037

ax RωB97X-D/6-31G(d) -246.607685 0.130267

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178280	-533.048244	0	69.6	0.49
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177731	-533.047464	0.490	30.4	
eq RωB97X-D/6-311+G(2df,2p)	-533.073282	-532.943245	0	77.8	0.74
ax RωB97X-D/6-311+G(2df,2p)	-533.072332	-532.942065	0.741	22.2	
eq RM06-2X/6-311+G(2df,2p)	-532.869567	-532.739531	0	66.6	0.41
ax RM06-2X /6-311+G(2df,2p)	-532.869147	-532.738880	0.409	33.4	
eq RMP2(FC)/6-311+G(2df,2p)	-531.878086	-531.748049	0	78.2	0.75
ax RMP2(FC)/6-311+G(2df,2p)	-531.877114	-531.746847	0.754	21.8	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq RωB97X-D/6-31G*	-246.611787	0.119910	
ax RωB97X-D/6-31G*	-246.610977	0.120027	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-7154.396903	-7154.276993	0	67.8	0.44
ax RωB97X-V/6-311+G(2df,2p)	-7154.396317	-7154.276290	0.441	32.2	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq RM06-2X/6-31G(d)	-246.497503	0.129710	
ax RM06-2X/6-31G(d)	-246.497147	0.130005	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178174	-533.048464	0	72.7	0.58
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177547	-533.047542	0.579	27.3	
eq RωB97X-D/6-311+G(2df,2p)	-533.073349	-532.943639	0	80.1	0.82
ax RωB97X-D/6-311+G(2df,2p)	-533.072334	-532.942329	0.822	19.9	
eq RM06-2X/6-311+G(2df,2p)	-532.869712	-532.740002	0	66.5	0.40
ax RM06-2X /6-311+G(2df,2p)	-532.869362	-532.739357	0.405	33.5	
eq RMP2(FC)/6-311+G(2df,2p)	-531.878391	-531.748681	0	76.2	0.69
ax RMP2(FC)/6-311+G(2df,2p)	-531.877592	-531.747587	0.686	23.8	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RM06-2X/6-31G*	-246.500112	0.129406			
ax RM06-2X/6-31G*	-246.499729	0.129538			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-7154.396952	-7154.267546	0	67.8	0.44
ax R ω B97X-V/6-311+G(2df,2p)	-7154.396384	-7154.266846	0.439	32.2	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq R ω B97X-V/6-31G*	-246.601810	0.129812			
ax R ω B97X-V/6-31G*	-246.601231	0.130035			

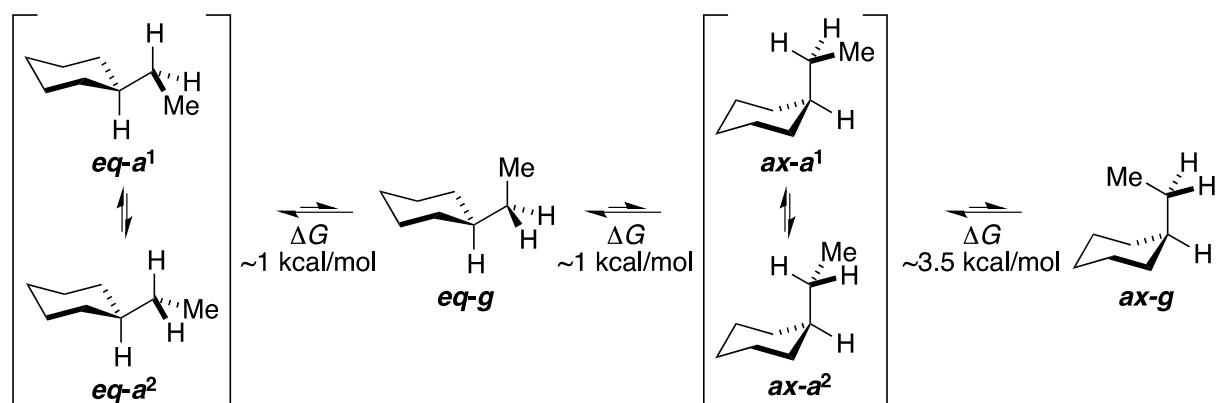
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-7154.906266	-7154.776454	0	71.4	0.54
ax RB3LYP-D3/6-311+G(2df,2p)	-7154.905627	-7154.775592	0.541	28.6	
eq R ω B97X-D/6-311+G(2df,2p)	-7154.967255	-7154.837443	0	78.6	0.77
ax R ω B97X-D/6-311+G(2df,2p)	-7154.966255	-7154.836220	0.767	21.4	
eq RM06-2X/6-311+G(2df,2p)	-7155.158474	-7155.028662	0	65.0	0.37
ax RM06-2X /6-311+G(2df,2p)	-7155.158115	-7155.028080	0.365	35.0	
eq R ω B97X-V/6-311+G(2df,2p)	-7154.396780	-7154.266968	0	70.0	0.50
ax R ω B97X-V/6-311+G(2df,2p)	-7154.396250	-7154.266170	0.501	30.0	
eq RMP2(FC)/6-311+G(2df,2p)	-531.878019	-531.748207	0	75.2	0.65
ax RMP2(FC)/6-311+G(2df,2p)	-531.877198	-531.747163	0.655	24.8	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G(d)	-245.671411	0.131769			
ax RMP2(FC)/6-31G(d)	-245.669958	0.132088			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-533.178175	-533.046406	0	74.4	0.63
ax RB3LYP-D3/6-311+G(2df,2p)	-533.177492	-533.045404	0.629	25.6	
eq R ω B97X-D/6-311+G(2df,2p)	-533.073326	-532.941557	0	80.3	0.83
ax R ω B97X-D/6-311+G(2df,2p)	-533.072324	-532.940237	0.828	19.7	
eq RM06-2X/6-311+G(2df,2p)	-532.869662	-532.737893	0	67.4	0.43
ax RM06-2X /6-311+G(2df,2p)	-532.869299	-532.737211	0.428	32.6	

eq RMP2(FC)/6-311+G(2df,2p)	-531.746220	-531.614450	0	73.8	0.61
ax RMP2(FC)/6-311+G(2df,2p)	-531.745564	-531.613477	0.611	26.2	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RMP2(FC)/6-31G*	-245.683776	0.131355			
ax RMP2(FC)/6-31G*	-245.682506	0.131682			
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-7154.396922	-7154.265567	0	72.1	0.56
ax RωB97X-V/6-311+G(2df,2p)	-7154.396357	-7154.264675	0.560	27.9	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq RHF/6-311+G(d,p)	-530.344502	-530.207910	0	92.6	1.50
ax RHF/6-311+G(d,p)	-530.342793	-530.205527	1.495	7.4	
eq RB3LYP/6-311+G(d,p)	-533.148193	-533.021857	0	88.2	1.19
ax RB3LYP/6-311+G(d,p)	-533.146387	-533.019966	1.87	11.8	
eq RB3LYP-D3/6-311+G(d,p)	-533.165219	-533.038450	0	69.7	0.49
ax RB3LYP-D3/6-311+G(d,p)	-533.164770	-533.037667	0.491	30.3	
eq RωB97X-D/6-311+G(d,p)	-533.060892	-532.932677	0	75.9	0.68
ax RωB97X-D/6-311+G(d,p)	-533.060059	-532.931596	0.678	24.1	
eq RM06-2X/6-311+G(d,p)	-532.856712	-532.728456	0	63.9	0.34
ax RM06-2X/6-311+G(d,p)	-532.856491	-532.727919	0.337	36.1	
eq RωB97X-V/6-311+G**	-7154.384267	-7154.256469	0	66.3	0.40
ax RωB97X-V/6-311+G**	-7154.383876	-7154.255832	0.400	33.7	
eq RMP2(FC)/6-311+G(d,p)	-531.746423	-531.617804	0	73.7	0.61
ax RMP2(FC)/6-311+G(d,p)	-531.745794	-531.616832	0.610	26.3	

Ethylcyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G(d)	-312.276376	0.210477
eq-g RHF/6-31G(d)	-312.274627	0.210716
ax-a RHF/6-31G(d)	-312.272626	0.210864
ax-g RHF/6-31G(d)	-312.265866	0.210883

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-D/6-311+G(2df,2p)	-314.515403	-314.30426	0	42.6	1.76
eq-g Rwb97X-D/6-311+G(2df,2p)	-314.514278	-314.303562	0.856	10.0	
ax-a Rwb97X-D/6-311+G(2df,2p)	-314.513091	-314.302227	1.693	2.4	
ax-g Rwb97X-D/6-311+G(2df,2p)	-314.507598	-314.296715	5.152	0.007	
eq-a RM06-2X/6-311+G(2df,2p)	-314.443178	-314.232700	0	43.7	1.93
eq-g RM06-2X /6-311+G(2df,2p)	-314.441925	-314.231209	0.936	9.0	
ax-a RM06-2X/6-311+G(2df,2p)	-314.440576	-314.229712	1.875	1.8	
ax-g RM06-2X /6-311+G(2df,2p)	-314.434338	-314.223455	5.801	0.002	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G*	-312.276375	0.209883
eq-g RHF/6-31G*	-312.274627	0.210133
ax-a RHF/6-31G*	-312.272625	0.210250
ax-g RHF/6-31G*	-312.265866	0.210256

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-314.522646	-314.589138	0	43.7	1.89
eq-g Rwb97X-V/6-311+G(2df,2p)	-314.521366	-314.587608	0.960	8.6	

ax-a Rwb97X-V/6-311+G(2df,2p)	-314.520085	-314.586210	1.837	1.9	3.9
ax-g Rwb97X-V/6-311+G(2df,2p)	-314.514112	-314.580231	5.589	0.002	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP/6-31G(d)	-314.507808	0.195074			
eq-g RB3LYP/6-31G(d)	-314.506199	0.195343			
ax-a RB3LYP/6-31G(d)	-314.504319	0.195420			
ax-g RB3LYP/6-31G(d)	-314.498536	0.195677			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RB3LYP-D3/6-311+G(2df,2p)	-314.631105	-314.436032	0	44.1	96.7
eq-g RB3LYP-D3/6-311+G(2df,2p)	-314.629819	-314.434485	0.971	8.5	
ax-a RB3LYP-D3/6-311+G(2df,2p)	-314.628401	-314.432925	1.950	1.6	2.00
ax-g RB3LYP-D3/6-311+G(2df,2p)	-314.622826	-314.427215	5.533	0.004	3.3
eq-a Rwb97X-D/6-311+G(2df,2p)	-314.515090	-314.320017	0	42.6	95.1
eq-g Rwb97X-D/6-311+G(2df,2p)	-314.513988	-314.318653	0.856	10.0	
ax-a Rwb97X-D/6-311+G(2df,2p)	-314.512805	-314.317329	1.687	2.4	1.75
ax-g Rwb97X-D/6-311+G(2df,2p)	-314.507373	-314.311762	5.180	0.007	4.9
eq-a RM06-2X/6-311+G(2df,2p)	-314.442790	-314.247717	0	43.6	96.2
eq-g RM06-2X/6-311+G(2df,2p)	-314.441573	-314.246239	0.927	9.1	
ax-a RM06-2X/6-311+G(2df,2p)	-314.440231	-314.244755	1.859	1.9	1.92
ax-g RM06-2X/6-311+G(2df,2p)	-314.434050	-314.238438	5.822	0.002	3.8

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP/6-31G*	-314.507818	0.183156			
eq-g RB3LYP/6-31G*	-314.506203	0.183434			
ax-a RB3LYP/6-31G*	-314.504324	0.183477			
ax-g RB3LYP/6-31G*	-314.498537	0.183724			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-314.523131	-314.339975	0	43.6	95.8
eq-g Rwb97X-V/6-311+G(2df,2p)	-314.521871	-314.338437	0.965	8.5	
ax-a Rwb97X-V/6-311+G(2df,2p)	-314.520607	-314.337130	1.785	2.1	1.84
ax-g Rwb97X-V/6-311+G(2df,2p)	-314.514692	-314.330968	5.652	0.003	4.2

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP-D3/6-31G(d)	-314.527898	0.195902			
eq-g RB3LYP-D3/6-31G(d)	-314.526736	0.196220			
ax-a RB3LYP-D3/6-31G(d)	-314.525284	0.196340			
ax-g RB3LYP-D3/6-31G(d)	-314.519768	0.196100			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-314.442976	-314.247073	0	43.5	95.8
eq-g RM06-2X /6-311+G(2df,2p)	-314.441801	-314.245581	0.9367	8.9	
ax-a RM06-2X/6-311+G(2df,2p)	-314.440550	-314.244210	1.797	2.1	4.2
ax-g RM06-2X /6-311+G(2df,2p)	-314.434296	-314.238196	5.571	0.003	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RwB97X-D/6-31G(d)	-314.421265	0.197654			
eq-g RwB97X-D/6-31G(d)	-314.420268	0.197784			
ax-a RwB97X-D/6-31G(d)	-314.419106	0.198003			
ax-g RwB97X-D/6-31G(d)	-314.413624	0.197566			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RwB97X-D/6-311+G(2df,2p)	-314.515603	-314.317950	0	41.5	94.4
eq-g RwB97X-D/6-311+G(2df,2p)	-314.514525	-314.316741	0.759	11.59	
ax-a RwB97X-D/6-311+G(2df,2p)	-314.513405	-314.315403	1.598	2.8	5.5
ax-g RwB97X-D/6-311+G(2df,2p)	-314.507972	-314.310406	4.733	0.01	

eq-a RM06-2X/6-311+G(2df,2p)	-314.443421	-314.245767	0	42.4	95.2
eq-g RM06-2X /6-311+G(2df,2p)	-314.442236	-314.244452	0.825	10.5	
ax-a RM06-2X/6-311+G(2df,2p)	-314.441057	-314.243054	1.702	2.4	4.8
ax-g RM06-2X /6-311+G(2df,2p)	-314.434736	-314.237170	5.395	0.005	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RwB97X-D/6-31G*	-314.421272	0.183204			
eq-g RwB97X-D/6-31G*	-314.420266	0.183330			
ax-a RwB97X-D/6-31G*	-314.41910	0.183605			
ax-g RwB97X-D/6-31G*	-314.413620	0.182854			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-314.523478	-314.340274	0	42.8	95.8 1.85
eq-g R ω B97X-V/6-311+G(2df,2p)	-314.522252	-314.338922	0.848	10.2	
ax-a R ω B97X-V/6-311+G(2df,2p)	-314.521030	-314.337425	1788	2.1	
ax-g R ω B97X-V/6-311+G(2df,2p)	-314.515060	-314.332206	5.063	0.008	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RM06-2X/6-31G(d)	-314.339710	0.197193			
eq-g RM06-2X/9-31G(d)	-314.338577	0.197253			
ax-a RM06-2X/6-31G(d)	-314.337370	0.197878			
ax-g RM06-2X/6-31G(d)	-314.331069	0.197689			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-314.443548	-314.246354	0	42.6	96.5 1.97
eq-g RM06-2X /6-311+G(2df,2p)	-314.442355	-314.245102	0.786	11.3	
ax-a RM06-2X/6-311+G(2df,2p)	-314.441217	-314.243339	1.892	1.7	
ax-g RM06-2X /6-311+G(2df,2p)	-314.434904	-314.237215	5.735	0.003	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a R ω B97X-V/6-31G*	-314.427702	0.197090			
eq-g R ω B97X-V/6-31G*	-314.426580	0.197277			
ax-a R ω B97X-V/6-31G*	-314.425339	0.197531			
ax-g R ω B97X-V/6-31G*	-314.419452	0.197008			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-314.443631	-314.246541	0	42.8	95.7 1.83
eq-g RM06-2X /6-311+G(2df,2p)	-314.442453	-314.245176	0.857	10.0	
ax-a RM06-2X/6-311+G(2df,2p)	-314.441258	-314.243727	1.766	2.2	
ax-g RM06-2X /6-311+G(2df,2p)	-314.434952	-314.237944	5.395	0.005	
eq-a R ω B97X-V/6-311+G(2df,2p)	-314.523297	-314.326207	0	43.2	96.0 1.88
eq-g R ω B97X-V/6-311+G(2df,2p)	-314.522067	-314.324790	0.889	9.6	
ax-a R ω B97X-V/6-311+G(2df,2p)	-314.520847	-314.323316	1.814	2.0	
ax-g R ω B97X-V/6-311+G(2df,2p)	-314.514875	-314.317867	5.233	0.006	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq-a RMP2(FC)/6-31G(d)	-313.326482	0.200335
eq-g RMP2(FC)/6-31G(d)	-313.325160	0.200509
ax-a RMP2(FC)/6-31G(d)	-313.323774	0.200786
ax-g RMP2(FC)/6-31G(d)	-313.317047	0.200286

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-314.443538	-314.243204	0	42.8	95.8 1.85
eq-g RM06-2X /6-311+G(2df,2p)	-314.442362	-314.241853	0.848	10.2	
ax-a RM06-2X/6-311+G(2df,2p)	-314.441151	-314.240365	1.782	2.1	
ax-g RM06-2X /6-311+G(2df,2p)	-314.434822	-314.234536	5.439	0.004	
eq-a RMP2(FC)/6-311+G(2df,2p)	-313.740428	-313.540094	0	43.0	95.4 1.80
eq-a RMP2(FC)/6-311+G(2df,2p)	-313.739171	-313.538662	0.898	9.4	
eq-a RMP2(FC)/6-311+G(2df,2p)	-313.738114	-313.537328	1.736	2.3	
eq-a RMP2(FC)/6-311+G(2df,2p)	-313.731461	-313.531174	5.597	0.003	

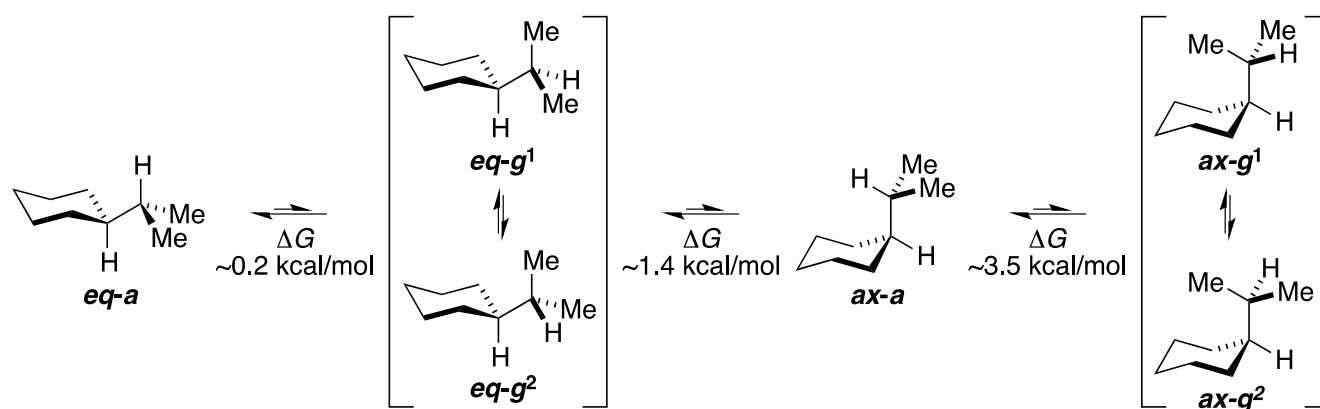
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RMP2(FC)/6-31G*	-313.326482	0.199764			
eq-g RMP2(FC)/6-31G*	-313.325160	0.199948			
ax-a RMP2(FC)/6-31G*	-313.323774	0.200210			
ax-g RMP2(FC)/6-31G*	-313.317047	0.199693			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-314.523501	-314.323737	0	43.3	96.1 1.89
eq-g Rwb97X-V/6-311+G(2df,2p)	-314.522262	-314.322314	0.893	9.5	
ax-a Rwb97X-V/6-311+G(2df,2p)	-314.521040	-314.320830	1.824	2.0	
ax-g Rwb97X-V/6-311+G(2df,2p)	-314.515055	-314.315362	5.255	0.006	

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RHF/6-311+G(d,p)	-312.351909	-312.144780	0	46.9	98.9 2.66
eq-g RHF/6-311+G(d,p)	-312.350098	-312.142706	1.301	5.2	
ax-a RHF/6-311+G(d,p)	-312.348157	-312.140595	2.626	0.5	
ax-g RHF/6-311+G(d,p)	-312.341451	-312.133859	6.852	0.0004	
eq-a RB3LYP/6-311+G(d,p)	-314.593501	-314.401054	0	47.2	98.3 2.39
eq-g RB3LYP/6-311+G(d,p)	-314.591839	-314.398682	1.488	3.8	

ax-a RB3LYP/6-311+G(d,p)	-314.590098	-314.397280	2.368	0.9		
ax-g RB3LYP/6-311+G(d,p)	-314.584290	-314.391238	6.160	0.001	1.7	
eq-a RB3LYP-D3/6-311+G(d,p)	-314.613591	-314.420291	0	44.0	96.4	
eq-g RB3LYP-D3/6-311+G(d,p)	-314.612374	-314.418738	0.9745	8.4		1.93
ax-a RB3LYP-D3/6-311+G(d,p)	-314.611061	-314.417292	1.882	1.8	3.6	
ax-g RB3LYP-D3/6-311+G(d,p)	-314.605529	-314.411973	5.220	0.006		
eq-a RωB97X-D/6-311+G(d,p)	-314.499033	-314.304079	0	40.3	93.2	
eq-g RωB97X-D/6-311+G(d,p)	-314.498014	-314.302985	0.686	12.6		1.55
ax-a RωB97X-D/6-311+G(d,p)	-314.497020	-314.301745	1.465	3.4	6.8	
ax-g RωB97X-D/6-311+G(d,p)	-314.491582	-314.296557	4.720	0.01		
eq-a RM06-2X/6-311+G(d,p)	-314.425966	-314.230994	0	42.3	96.0	
eq-g RM06-2X/6-311+G(d,p)	-314.424828	-314.229769	0.769	11.5		1.88
ax-a RM06-2X/6-311+G(d,p)	-314.423821	-314.228120	1.803	2.0	4.0	
ax-g RM06-2X/6-311+G(d,p)	-314.417461	-314.221849	5.727	0.003		
eq-a RωB97X-V/6-311+G**	-314.508209	-314.314295	0	43.1	95.6	
eq-g RωB97X-V/6-311+G**	-314.507025	-314.312870	0.894	9.5		1.82
ax-a RωB97X-V/6-311+G**	-314.505948	-314.311498	1.755	2.2	4.4	
ax-g RωB97X-V/6-311+G**	-314.499981	-314.306242	5.053	0.008		
eq-a RMP2(FC)/6-311+G(d,p)	-313.565686	-313.369903	0	42.7	96.0	
eq-g RMP2(FC)/6-311+G(d,p)	-313.564463	-313.368577	0.832	10.4		1.87
ax-a RMP2(FC)/6-311+G(d,p)	-313.563511	-313.367032	1.802	2.0	4.0	
ax-g RMP2(FC)/6-311+G(d,p)	-313.556861	-313.361828	5.0667	0.008		

Isopropylcyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G(d)	-351.307183	0.238919
eq-g RHF/6-31G(d)	-351.307380	0.239245
ax-a RHF/6-31G(d)	-351.303462	0.239372
ax-g RHF/6-31G(d)	-351.298128	0.239758

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-D/6-311+G(2df,2p)	-353.829919	-353.590675	0	32.4	97.2
eq-g Rwb97X-D/6-311+G(2df,2p)	-353.829593	-353.590674	0.0003	32.4	
ax-a Rwb97X-D/6-311+G(2df,2p)	-353.827716	-353.588344	1.463	2.7	2.8
ax-g Rwb97X-D/6-311+G(2df,2p)	-353.823025	-353.583297	4.649	0.01	
eq-a RM06-2X/6-311+G(2df,2p)	-353.748710	-353.509466	0.243	27.2	97.5
eq-g RM06-2X /6-311+G(2df,2p)	-353.748820	-353.509901	0	43.1	
ax-a RM06-2X/6-311+G(2df,2p)	-353.746596	-353.507224	1.680	2.5	2.16
ax-g RM06-2X /6-311+G(2df,2p)	-353.741009	-353.501251	5.428	0.004	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G*	-351.307379	0.238544
eq-g RHF/6-31G*	-351.307182	0.238146
ax-a RHF/6-31G*	-351.303461	0.238510
ax-g RHF/6-31G*	-351.298128	0.239054

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-353.837921	-353.599377	0.144	29.7	97.3

eq-g Rwb97X-V/6-311+G(2df,2p)	-353.837752	-353.599606	0	37.9	
ax-a Rwb97X-V/6-311+G(2df,2p)	-353.835631	-353.597121	1.559	2.7	
ax-g Rwb97X-V/6-311+G(2df,2p)	-353.830480	-353.591426	5.133	0.006	2.7

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP/6-31G(d)	-353.818893	0.221527			
eq-g RB3LYP/6-31G(d)	-353.818858	0.221865			
ax-a RB3LYP/6-31G(d)	-353.815415	0.221829			
ax-g RB3LYP/6-31G(d)	-353.810838	0.222273			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RB3LYP-D3/6-311+G(2df,2p)	-353.959624	-353.737759	0.001	32.6	
eq-g RB3LYP-D3/6-311+G(2df,2p)	-353.959288	-353.737761	0	32.7	98.0
ax-a RB3LYP-D3/6-311+G(2df,2p)	-353.956965	-353.735137	1.647	2.0	2.29
ax-g RB3LYP-D3/6-311+G(2df,2p)	-353.952363	-353.730090	4.814	0.009	2.0
eq-a Rwb97X-D/6-311+G(2df,2p)	-353.829608	-353.607743	0	32.4	
eq-g Rwb97X-D/6-311+G(2df,2p)	-353.829254	-353.607727	0.010	31.9	96.7
ax-a Rwb97X-D/6-311+G(2df,2p)	-353.827423	-353.605594	1.348	3.3	1.99
ax-g Rwb97X-D/6-311+G(2df,2p)	-353.822772	-353.600498	4.546	0.02	3.3
eq-a RM06-2X/6-311+G(2df,2p)	-353.748329	-353.526464	0.250	27.5	
eq-g RM06-2X /6-311+G(2df,2p)	-353.748390	-353.526863	0	42.0	96.9
ax-a RM06-2X/6-311+G(2df,2p)	-353.746230	-353.524402	1.545	3.1	2.04
ax-g RM06-2X /6-311+G(2df,2p)	-353.740654	-353.518381	5.323	0.005	3.1

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP/6-31G*	-353.818855	0.208322			
eq-g RB3LYP/6-31G*	-353.818877	0.207858			
ax-a RB3LYP/6-31G*	-353.815414	0.208195			
ax-g RB3LYP/6-31G*	-353.810839	0.208759			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-353.837921	-353.629599	0.185	28.8	
eq-g Rwb97X-V/6-311+G(2df,2p)	-353.937752	-353.629894	0	39.4	97.1
ax-a Rwb97X-V/6-311+G(2df,2p)	-353.835631	-353.627436	1.542	2.9	2.9

ax-g R**w**B97X-V/6-311+G(2df,2p) -353.830480 -353.621721 5.129 0.007

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RB3LYP-D3/6-31G(d)	-353.843347	0.222296	
eq-g RB3LYP-D3/6-31G(d)	-353.843734	0.222890	
ax-a RB3LYP-D3/6-31G(d)	-353.841108	0.222451	
ax-g RB3LYP-D3/6-31G(d)	-353.836494	0.223255	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-353.748585	-353.525695	0.373	24.6	95.3
eq-g RM06-2X /6-311+G(2df,2p)	-353.748585	-353.526290	0	46.2	
ax-a RM06-2X/6-311+G(2df,2p)	-353.746590	-353.524139	1.350	4.7	4.7
ax-g RM06-2X /6-311+G(2df,2p)	-353.741025	-353.517770	5.346	0.005	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a R w B97X-D/6-31G(d)	-353.724080	0.224524	
eq-g R w B97X-D/6-31G(d)	-353.723675	0.224232	
ax-a R w B97X-D/6-31G(d)	-353.721952	0.224716	
ax-g R w B97X-D/6-31G(d)	-353.717219	0.225478	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R w B97X-D/6-311+G(2df,2p)	-353.830226	-353.605701	0	33.4	97.1
eq-g R w B97X-D/6-311+G(2df,2p)	-353.829838	-353.605606	0.060	30.2	
ax-a R w B97X-D/6-311+G(2df,2p)	-353.828121	-353.603404	1.441	2.9	2.9
ax-g R w B97X-D/6-311+G(2df,2p)	-353.823474	-353.597996	4.835	0.009	
eq-a RM06-2X/6-311+G(2df,2p)	-353.749088	-353.524563	0.189	28.7	97.1
eq-g RM06-2X/6-311+G(2df,2p)	-353.749096	-353.524864	0	39.6	
ax-a RM06-2X/6-311+G(2df,2p)	-353.747132	-353.522242	1.537	2.9	2.9
ax-g RM06-2X/6-311+G(2df,2p)	-353.741588	-353.516110	5.493	0.004	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a R w B97X-D/6-31G*	-353.724079	0.208245	
eq-g R w B97X-D/6-31G*	-353.723675	0.207682	
ax-a R w B97X-D/6-31G*	-353.721949	0.208307	
ax-g R w B97X-D/6-31G*	-353.717217	0.209041	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-353.838954	-353.630709	0.206	28.5	2.13
eq-g R ω B97X-V/6-311+G(2df,2p)	-353.838720	-353.631038	0	40.4	
ax-a R ω B97X-V/6-311+G(2df,2p)	-353.836769	-353.628462	1.616	2.6	
ax-g R ω B97X-V/6-311+G(2df,2p)	-353.831611	-353.622570	5.314	0.005	
97.4					
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RM06-2X/6-31G(d)	-353.632436	0.223923			
eq-g RM06-2X/9-31G(d)	-353.632427	0.224014			
ax-a RM06-2X/6-31G(d)	-353.630435	0.224264			
ax-g RM06-2X/6-31G(d)	-353.624880	0.224932			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-353.749240	-353.525317	0	33.4	2.06
eq-g RM06-2X /6-311+G(2df,2p)	-353.749239	-353.525225	0.058	30.3	
ax-a RM06-2X/6-311+G(2df,2p)	-353.747298	-353.523035	1.432	3.0	
ax-g RM06-2X /6-311+G(2df,2p)	-353.741786	-353.516855	5.310	0.004	
97.0					
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a R ω B97X-V/6-31G*	-353.731194	0.224038			
eq-g R ω B97X-V/6-31G*	-353.730946	0.223657			
ax-a R ω B97X-V/6-31G*	-353.728998	0.224161			
ax-g R ω B97X-V/6-31G*	-353.723867	0.224787			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-353.749333	-353.525295	0.222	28.0	2.01
eq-g RM06-2X /6-311+G(2df,2p)	-353.749305	-353.525648	0	40.8	
ax-a RM06-2X/6-311+G(2df,2p)	-353.747412	-353.523251	1.504	3.2	
ax-g RM06-2X /6-311+G(2df,2p)	-353.741859	-353.517072	5.381	0.005	
96.8					
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-353.838749	-353.614711	0.097	30.6	2.13
eq-g R ω B97X-V/6-311+G(2df,2p)	-353.838523	-353.614866	0	36.1	
ax-a R ω B97X-V/6-311+G(2df,2p)	-353.836565	-353.612404	1.545	2.6	
ax-g R ω B97X-V/6-311+G(2df,2p)	-353.831411	-353.606624	5.172	0.006	
97.3					
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq-a RMP2(FC)/6-31G(d)	-352.492483	0.227689
eq-g RMP2(FC)/6-31G(d)	-352.492289	0.227363
ax-a RMP2(FC)/6-31G(d)	-352.490121	0.228009
ax-g RMP2(FC)/6-31G(d)	-352.484182	0.228384

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-353.749244	-353.521554	0.210	28.4	97.4 2.15
eq-g RM06-2X /6-311+G(2df,2p)	-353.749251	-353.521888	0	40.6	
ax-a RM06-2X/6-311+G(2df,2p)	-353.747298	-353.519289	1.631	2.6	
ax-g RM06-2X /6-311+G(2df,2p)	-353.741708	-353.513323	5.375	0.005	
eq-a RMP2(FC)/6-311+G(2df,2p)	-352.959147	-352.731457	0.134	29.7	96.5 1.96
eq-a RMP2(FC)/6-311+G(2df,2p)	-352.959033	-352.731670	0	37.2	
eq-a RMP2(FC)/6-311+G(2df,2p)	-352.957444	-352.729435	1.403	3.5	
eq-a RMP2(FC)/6-311+G(2df,2p)	-352.951446	-352.723061	5.402	0.004	

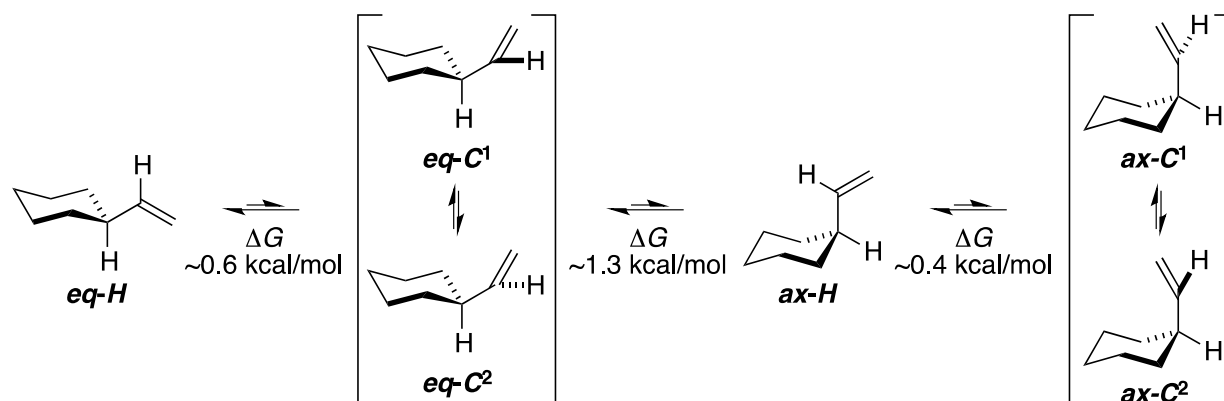
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RMP2(FC)/6-31G*	-352.492482	0.227049	
eq-g RMP2(FC)/6-31G*	-352.492289	0.226619	
ax-a RMP2(FC)/6-31G*	-352.490121	0.227273	
ax-g RMP2(FC)/6-31G*	-352.484182	0.227760	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-353.838974	-353.611925	0.134	30.0	97.7 2.21
eq-g Rwb97X-V/6-311+G(2df,2p)	-353.836784	-353.610165	0	37.7	
ax-a Rwb97X-V/6-311+G(2df,2p)	-353.836784	-353.609511	1.650	2.3	
ax-g Rwb97X-V/6-311+G(2df,2p)	-353.831622	-353.603862	5.194	0.006	

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RHF/6-311+G(d,p)	-351.392424	-351.156980	0.092	31.4	99.6 3.20
eq-g RHF/6-311+G(d,p)	-351.392244	-351.157126	0	36.7	
ax-a RHF/6-311+G(d,p)	-351.388567	-351.152955	2.617	0.4	
ax-g RHF/6-311+G(d,p)	-351.383302	-351.147310	6.160	0.001	
eq-a RB3LYP/6-311+G(d,p)	-353.915165	-353.696250	0.243	28.3	99.2 2.83
eq-g RB3LYP/6-311+G(d,p)	-353.915190	-353.696637	0	42.6	

ax-a RB3LYP/6-311+G(d,p)	-353.911844	-353.692915	2.336	0.8		
ax-g RB3LYP/6-311+G(d,p)	-353.907264	-353.687929	5.464	0.004	0.8	
eq-a RB3LYP-D3/6-311+G(d,p)	-353.940045	-353.720079	0.149	29.5	97.1	
eq-g RB3LYP-D3/6-311+G(d,p)	-353.939654	-353.720317	0	38.0		2.07
ax-a RB3LYP-D3/6-311+G(d,p)	-353.937545	-353.717893	1.521	2.9	2.9	
ax-g RB3LYP-D3/6-311+G(d,p)	-353.932923	-353.712695	4.783	0.01		
eq-a RωB97X-D/6-311+G(d,p)	-353.811752	-353.590121	0.101	30.2	96.3	
eq-g RωB97X-D/6-311+G(d,p)	-353.811346	-353.590282	0	35.8		1.92
ax-a RωB97X-D/6-311+G(d,p)	-353.809828	-353.588146	1.340	3.7	3.7	
ax-g RωB97X-D/6-311+G(d,p)	-353.805116	-353.582795	4.698	0.01		
eq-a RM06-2X/6-311+G(d,p)	-353.729618	-353.508139	0	32.6	96.7	
eq-g RM06-2X/6-311+G(d,p)	-353.729580	-353.508107	0.020	31.5		1.99
ax-a RM06-2X/6-311+G(d,p)	-353.727839	-353.505985	1.352	3.3	3.3	
ax-g RM06-2X/6-311+G(d,p)	-353.722245	-353.499503	5.419	0.003		
eq-a RωB97X-V/6-311+G**	-353.821898	-353.601460	0.155	29.4	96.9	
eq-g RωB97X-V/6-311+G**	-353.821646	-353.601707	0	38.2		2.03
ax-a RωB97X-V/6-311+G**	-353.819898	-353.599344	1.483	3.1	3.1	
ax-g RωB97X-V/6-311+G**	-353.814695	-353.593423	5.198	0.006		
eq-a RMP2(FC)/6-311+G(d,p)	-352.762493	-352.540045	0.167	29.1	96.9	
eq-g RMP2(FC)/6-311+G(d,p)	-352.762395	-352.540311	0	38.7		2.04
ax-a RMP2(FC)/6-311+G(d,p)	-352.761000	-352.537924	1.498	3.1	3.1	
ax-g RMP2(FC)/6-311+G(d,p)	-352.754926	-352.531504	5.526	0.003		

Cyclohexylethen



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RHF/6-31G(d)	-311.086009	0.185962
eq-C RHF/6-31G(d)	-311.084308	0.186392
ax-H RHF/6-31G(d)	-311.082411	0.186311
ax-C RHF/6-31G(d)	-311.081083	0.186819

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RωB97X-D/6-311+G(2df,2p)	-313.277100	-313.091138	0	55.2	1.76
eq-C RωB97X-D/6-311+G(2df,2p)	-313.276575	-313.090184	0.599	20.0	
ax-H RωB97X-D/6-311+G(2df,2p)	-313.274521	-313.088210	1.838	2.5	
ax-C RωB97X-D/6-311+G(2df,2p)	-313.274347	-313.087528	2.266	1.2	
eq-H RM06-2X/6-311+G(2df,2p)	-313.216279	-313.030318	0	47.4	1.83
eq-C RM06-2X /6-311+G(2df,2p)	-313.216076	-313.029685	0.397	24.2	
ax-H RM06-2X/6-311+G(2df,2p)	-313.213536	-313.027225	1.941	1.8	
ax-C RM06-2X /6-311+G(2df,2p)	-313.213725	-313.026906	2.141	1.3	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RHF/6-31G*	-311.086009	0.185415
eq-C RHF/6-31G*	-311.084308	0.185904
ax-H RHF/6-31G*	-311.082411	0.185740
ax-C RHF/6-31G*	-311.081083	0.186289

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RωB97X-V/6-311+G(2df,2p)	-313.288314	-313.102899	0	60.5	1.82

eq-C RωB97X-V/6-311+G(2df,2p)	-313.287690	-313.101786	0.698	18.5	
ax-H RωB97X-V/6-311+G(2df,2p)	-313.285631	-313.099891	1.888	2.5	
ax-C RωB97X-V/6-311+G(2df,2p)	-313.285331	-313.099042	2.420	1.0	4.5

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-H RB3LYP/6-31G(d)	-313.272421			0.171712	
eq-C RB3LYP/6-31G(d)	-313.271200			0.172137	
ax-H RB3LYP/6-31G(d)	-313.268990			0.172014	
ax-C RB3LYP/6-31G(d)	-313.268167			0.172478	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RB3LYP-D3/6-311+G(2df,2p)	-313.396031	-313.224320	0	63.4	
eq-C RB3LYP-D3/6-311+G(2df,2p)	-313.395197	-313.223060	0.791	16.6	96.7
ax-H RB3LYP-D3/6-311+G(2df,2p)	-313.393084	-313.221070	2.039	2.0	
ax-C RB3LYP-D3/6-311+G(2df,2p)	-313.392501	-313.220022	2.697	0.7	3.3
eq-H RωB97X-D/6-311+G(2df,2p)	-313.276839	-313.105127	0	53.3	
eq-C RωB97X-D/6-311+G(2df,2p)	-313.276374	-313.104236	0.559	20.7	94.7
ax-H RωB97X-D/6-311+G(2df,2p)	-313.274291	-313.102277	1.789	2.6	
ax-C RωB97X-D/6-311+G(2df,2p)	-313.274159	-313.101680	2.163	1.4	5.3
eq-H RM06-2X/6-311+G(2df,2p)	-313.215975	-313.044263	0	46.2	
eq-C RM06-2X /6-311+G(2df,2p)	-313.215859	-313.043722	0.340	26.0	95.0
ax-H RM06-2X/6-311+G(2df,2p)	-313.213282	-313.041268	1.880	1.9	
ax-C RM06-2X /6-311+G(2df,2p)	-313.213545	-313.041067	2.006	1.5	5.0

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-H RB3LYP/6-31G*	-313.273423			0.162024	
eq-C RB3LYP/6-31G*	-313.271202			0.161462	
ax-H RB3LYP/6-31G*	-313.268990			0.161291	
ax-C RB3LYP/6-31G*	-313.268180			0.161820	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RωB97X-V/6-311+G(2df,2p)	-313.288879	-313.126855	0.004	31.8	
eq-C RωB97X-V/6-311+G(2df,2p)	-313.288323	-313.126861	0	32.0	92.1
ax-H RωB97X-V/6-311+G(2df,2p)	-313.286251	-313.124960	1.193	4.2	7.9

ax-C RωB97X-V/6-311+G(2df,2p) -313.285989 -313.124169 1.689 1.8

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RB3LYP-D3/6-31G(d)	-313.290155	0.172318
eq-C RB3LYP-D3/6-31G(d)	-313.289384	0.172895
ax-H RB3LYP-D3/6-31G(d)	-313.287401	0.172672
ax-C RB3LYP-D3/6-31G(d)	-313.287281	0.173289

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RM06-2X/6-311+G(2df,2p)	-313.216125	-313.043807	0	49.0	1.76
eq-C RM06-2X /6-311+G(2df,2p)	-313.215993	-313.043098	0.445	23.1	
ax-H RM06-2X/6-311+G(2df,2p)	-313.214743	-313.040802	1.885	2.0	
ax-C RM06-2X /6-311+G(2df,2p)	-313.213747	-313.040458	2.102	1.4	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RωB97X-D/6-31G(d)	-313.180401	0.173943
eq-C RωB97X-D/6-31G(d)	-313.179868	0.174494
ax-H RωB97X-D/6-31G(d)	-313.178004	0.174386
ax-C RωB97X-D/6-31G(d)	-313.178182	0.174967

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RωB97X-D/6-311+G(2df,2p)	-313.277334	-313.103391	0	57.3	1.79
eq-C RωB97X-D/6-311+G(2df,2p)	-313.276847	-313.102354	0.651	19.0	
ax-H RωB97X-D/6-311+G(2df,2p)	-313.274797	-313.100411	1.870	2.4	
ax-C RωB97X-D/6-311+G(2df,2p)	-313.274627	-313.099660	2.341	1.1	
eq-H RM06-2X/6-311+G(2df,2p)	-313.216540	-313.042597	0	49.4	1.81
eq-C RM06-2X /6-311+G(2df,2p)	-313.216427	-313.041934	0.416	24.4	
ax-H RM06-2X/6-311+G(2df,2p)	-313.213881	-313.039495	1.946	1.8	
ax-C RM06-2X /6-311+G(2df,2p)	-313.214182	-313.039216	2.122	1.4	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RωB97X-D/6-31G*	-313.180401	0.160975
eq-C RωB97X-D/6-31G*	-313.179872	0.161715
ax-H RωB97X-D/6-31G*	-313.178004	0.161442
ax-C RωB97X-D/6-31G*	-313.178191	0.162152

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-H R ω B97X-V/6-311+G(2df,2p)	-313.289223	-313.128248	0	65.2	1.86
eq-C R ω B97X-V/6-311+G(2df,2p)	-313.288650	-313.126935	0.824	16.2	
ax-H R ω B97X-V/6-311+G(2df,2p)	-313.286607	-313.125165	1.935	2.5	
ax-C R ω B97X-V/6-311+G(2df,2p)	-313.286317	-313.124169	2.562	0.9	
geometry method		E (au)	Thermal correction to Gibbs Free Energy (au/Particle)		
eq-H RM06-2X/6-31G(d)	-313.110050	0.173716			
eq-C RM06-2X/6-31G(d)	-313.109913	0.174230			
ax-H RM06-2X/6-31G(d)	-313.107533	0.174049			
ax-C RM06-2X/6-31G(d)	-313.108213	0.174742			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RM06-2X/6-311+G(2df,2p)	-313.216639	-313.042923	0	48.2	1.80
eq-C RM06-2X /6-311+G(2df,2p)	-313.216530	-313.042301	0.390	24.9	
ax-H RM06-2X/6-311+G(2df,2p)	-313.214003	-313.039954	1.863	2.1	
ax-C RM06-2X /6-311+G(2df,2p)	-313.214268	-313.039526	2.132	1.3	
geometry method		E (au)	Thermal correction to Gibbs Free Energy (au/Particle)		
eq-H R ω B97X-V/6-31G*	-313.190093	0.173587			
eq-C R ω B97X-V/6-31G*	-313.189514	0.174233			
ax-H R ω B97X-V/6-31G*	-313.187629	0.173959			
ax-C R ω B97X-V/6-31G*	-313.187842	0.174651			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RM06-2X/6-311+G(2df,2p)	-313.217457	-313.043870	0	50.6	1.76
eq-C RM06-2X /6-311+G(2df,2p)	-313.217331	-313.043098	0.484	22.3	
ax-H RM06-2X/6-311+G(2df,2p)	-313.214879	-313.040920	1.851	2.2	
ax-C RM06-2X /6-311+G(2df,2p)	-313.215085	-313.040434	2.156	1.3	
eq-H R ω B97X-V/6-311+G(2df,2p)	-313.289061	-313.115474	0	61.9	1.82
eq-C R ω B97X-V/6-311+G(2df,2p)	-313.288482	-313.114249	0.769	16.9	
ax-H R ω B97X-V/6-311+G(2df,2p)	-313.286447	-313.112488	1.874	2.6	
ax-C R ω B97X-V/6-311+G(2df,2p)	-313.286136	-313.111485	2.503	0.9	
geometry method		E (au)	Thermal correction to Gibbs Free Energy (au/Particle)		

eq-H RMP2(FC)/6-31G(d)	-312.123120	0.175794
eq-C RMP2(FC)/6-31G(d)	-312.121864	0.176313
ax-H RMP2(FC)/6-31G(d)	-312.120665	0.176219
ax-C RMP2(FC)/6-31G(d)	-312.119941	0.176784

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RM06-2X/6-311+G(2df,2p)	-313.216436	-313.040642	0	46.9	95.8 1.84
eq-C RM06-2X /6-311+G(2df,2p)	-313.216340	-313.040027	0.386	24.4	
ax-H RM06-2X/6-311+G(2df,2p)	-313.214019	-313.037800	1.783	2.3	
ax-C RM06-2X /6-311+G(2df,2p)	-313.213781	-313.036996	2.288	1.0	
eq-H RMP2(FC)/6-311+G(2df,2p)	-312.520412	-312.344618	0	63.9	95.2 1.78
eq-C RMP2(FC)/6-311+G(2df,2p)	-312.519667	-312.343353	0.794	16.7	
ax-H RMP2(FC)/6-311+G(2df,2p)	-312.517876	-312.341657	1.858	2.7	
ax-C RMP2(FC)/6-311+G(2df,2p)	-312.517502	-312.340718	2.448	1.0	

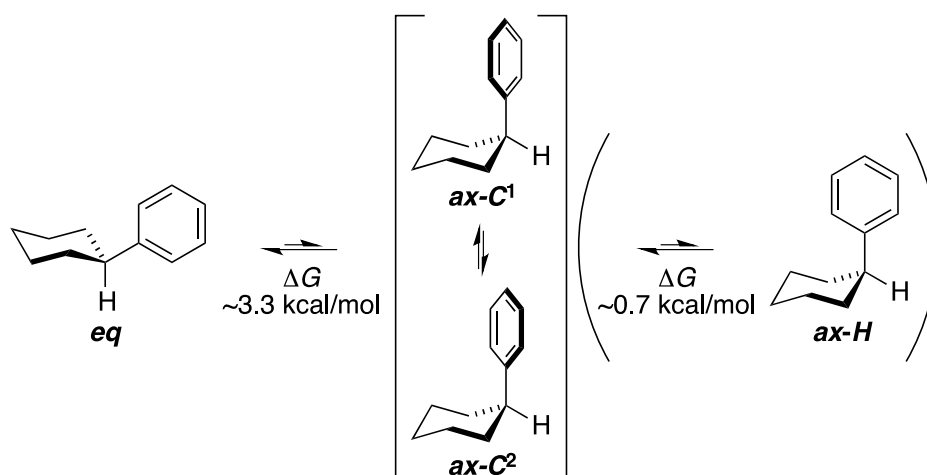
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-H RMP2(FC)/6-31G*	-312.123120	0.175365
eq-C RMP2(FC)/6-31G*	-312.121864	0.176001
ax-H RMP2(FC)/6-31G*	-312.120665	0.175804
ax-C RMP2(FC)/6-31G*	-312.119941	0.176435

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RωB97X-V/6-311+G(2df,2p)	-313.289102	-313.113737	0	62.9	96.0 1.88
eq-C RωB97X-V/6-311+G(2df,2p)	-313.288527	-313.112526	0.760	17.4	
ax-H RωB97X-V/6-311+G(2df,2p)	-313.286455	-313.110651	1.936	2.4	
ax-C RωB97X-V/6-311+G(2df,2p)	-313.286105	-313.109670	2.552	0.8	

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-H RHF/6-311+G(d,p)	-311.163503	-310.980521	0	82.3	98.8 2.58
eq-C RHF/6-311+G(d,p)	-311.161745	-310.978354	1.360	8.2	
ax-H RHF/6-311+G(d,p)	-311.159793	-310.976425	2.570	1.1	
ax-C RHF/6-311+G(d,p)	-311.157912	-310.9741148	3.999	0.09	
eq-H RB3LYP/6-311+G(d,p)	-313.360268	-313.190781	0	74.0	98.2 2.35
eq-C RB3LYP/6-311+G(d,p)	-313.358939	-313.189074	1.071	12.1	

ax-H RB3LYP/6-311+G(d,p)	-313.356788	-313.187032	2.353	1.4		
ax-C RB3LYP/6-311+G(d,p)	-313.355511	-313.185333	3.419	0.2	1.8	
eq-H RB3LYP-D3/6-311+G(d,p)	-313.378001	-313.207984	0	69.1	96.6	
eq-C RB3LYP-D3/6-311+G(d,p)	-313.377115	-313.206467	0.952	13.8		1.98
ax-H RB3LYP-D3/6-311+G(d,p)	-313.375203	-313.204689	2.068	2.1	3.4	
ax-C RB3LYP-D3/6-311+G(d,p)	-313.374561	-313.203586	2.760	0.6		
eq-H R ω B97X-D/6-311+G(d,p)	-313.260373	-313.088864	0	61.2	94.8	
eq-C R ω B97X-D/6-311+G(d,p)	-313.259802	-313.087646	0.764	16.8		1.71
ax-H R ω B97X-D/6-311+G(d,p)	-313.257990	-313.085896	1.862	2.6	5.2	
ax-C R ω B97X-D/6-311+G(d,p)	-313.257762	-313.0835247	2.270	1.3		
eq-H RM06-2X/6-311+G(d,p)	-313.198445	-313.026664	0	50.7	94.5	
eq-C RM06-2X/6-311+G(d,p)	-313.198183	-313.025874	0.496	21.9		1.68
ax-H RM06-2X/6-311+G(d,p)	-313.195974	-313.023804	1.795	2.4	5.5	
ax-C RM06-2X/6-311+G(d,p)	-313.196112	-313.023370	2.067	1.5		
eq-H R ω B97X-V/6-311+G**	-313.273341	-313.102658	0	62.9	95.3	
eq-C R ω B97X-V/6-311+G**	-313.272627	-313.101384	0.799	16.2		1.78
ax-H R ω B97X-V/6-311+G**	-313.270888	-313.099697	1.858	2.7	4.7	
ax-C R ω B97X-V/6-311+G**	-313.270498	-313.098742	2.457	1.0		
eq-H RMP2(FC)/6-311+G(d,p)	-312.347633	-312.175707	0	74.2	95.5	
eq-C RMP2(FC)/6-311+G(d,p)	-312.346232	-312.173880	1.146	10.7		1.81
ax-H RMP2(FC)/6-311+G(d,p)	-312.345146	-312.172736	1.864	3.2	4.5	
ax-C RMP2(FC)/6-311+G(d,p)	-312.344117	-312.171266	2.787	0.7		

Cyclohexylbenzene



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-463.752980	0.233754			
ax-C RHF/6-31G(d)	-463.746037	0.234722			
ax-H RHF/6-31G(d)	-463.744797	0.233744			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-D/6-311+G(2df,2p)	-466.925240	-466.691486	0	99.1	99.1
ax-C RωB97X-D/6-311+G(2df,2p)	-466.920906	-466.686184	3.327	0.4	2.79
ax-H RωB97X-D/6-311+G(2df,2p)	-466.919243	-466.685499	3.757	0.2	0.9

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RM06-2X/6-311+G(2df,2p)	-466.859231	-466.625477	0	99.1	99.1
ax-C RM06-2X/6-311+G(2df,2p)	-466.855037	-466.620315	3.239	0.4	2.78
ax-H RM06-2X /6-311+G(2df,2p)	-466.852388	-466.618644	4.288	1.4,	0.9

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-463.752980	0.232781			
ax-C RHF/6-31G(d)	-463.746037	0.233805			
ax-H RHF/6-31G(d)	-463.744797	0.232757			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RωB97X-V/6-311+G(2df,2p)	-466.949464	-466.716683	0	99.4	99.4
ax-C RωB97X-V/6-311+G(2df,2p)	-466.944911	-466.711106	3.500	0.3	2.99
ax-H RωB97X-V/6-311+G(2df,2p)	-466.942898	-466.710141	4.105	0.1	0.6

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq RHF/6-31G(d)	-463.752980	0.232781			
ax-C RHF/6-31G(d)	-463.746037	0.233805			
ax-H RHF/6-31G(d)	-463.744797	0.232757			

eq RB3LYP/6-31G(d)	-466.930334	0.216050
ax-C RB3LYP/6-31G(d)	-466.924413	0.216918
ax-H RB3LYP/6-31G(d)	-466.923330	0.216226

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RB3LYP-D3/6-311+G(2df,2p)	-467.104036	-466.887985	0	99.5	99.5
ax-C RB3LYP-D3/6-311+G(2df,2p)	-467.099079	-466.882161	3.654	0.2	3.11
ax-H RB3LYP-D3/6-311+G(2df,2p)	-467.097765	-466.881539	4.045	0.1	0.5
eq R ω B97X-D/6-311+G(2df,2p)	-466.924617	-466.708567	0	99.0	99.0
ax-C R ω B97X-D/6-311+G(2df,2p)	-466.920357	-466.703440	3.217	0.4	2.71
ax-H R ω B97X-D/6-311+G(2df,2p)	-466.918710	-466.702484	3.817	0.2	1.0
eq RM06-2X/6-311+G(2df,2p)	-466.858709	-466.642658	0	98.9	98.9
ax-C RM06-2X/6-311+G(2df,2p)	-466.854633	-466.637716	3.101	0.5	2.66
ax-H RM06-2X /6-311+G(2df,2p)	-466.851984	-466.635758	4.330	0.06	1.1

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP/6-31G(d)	-466.930335	0.202451
ax-C RB3LYP/6-31G(d)	-466.924415	0.203409
ax-H RB3LYP/6-31G(d)	-466.923328	0.202545

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-466.950076	-466.747625	0	99.4	99.4
ax-C R ω B97X-V/6-311+G(2df,2p)	-466.945634	-466.742225	3.389	0.3	2.90
ax-H R ω B97X-V/6-311+G(2df,2p)	-466.943603	-466.741058	4.121	0.09	0.6

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq RB3LYP-D3/6-31G(d)	-466.954824	0.216841
ax-C RB3LYP-D3/6-31G(d)	-466.950213	0.217536
ax-H RB3LYP-D3/6-31G(d)	-466.948780	0.216560

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RM06-2X/6-311+G(2df,2p)	-466.858904	-466.642063	0	98.5	98.5
ax-C RM06-2X/6-311+G(2df,2p)	-466.854920	-466.637384	2.936	0.7	2.48
ax-H RM06-2X /6-311+G(2df,2p)	-466.852206	-466.635646	4.027	0.1	1.5

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq R ω B97X-D/6-31G(d)	-466.788558	0.219132	
ax-C R ω B97X-D/6-31G(d)	-466.784477	0.219916	
ax-H R ω B97X-D/6-31G(d)	-466.782743	0.219386	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-D/6-311+G(2df,2p)	-466.925424	-466.706292	0	98.8	98.8
ax-C R ω B97X-D/6-311+G(2df,2p)	-466.921208	-466.701292	3.138	0.5	2.59
ax-H R ω B97X-D/6-311+G(2df,2p)	-466.920089	-466.700704	3.507	0.2	1.2
eq RM06-2X/6-311+G(2df,2p)	-466.859541	-466.640409	0	98.6	98.6
ax-C RM06-2X/6-311+G(2df,2p)	-466.855596	-466.635680	2.967	0.6	2.53
ax-H RM06-2X /6-311+G(2df,2p)	-466.852820	-466.633434	4.377	0.06	1.4

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq R ω B97X-D/6-31G*	-466.788559	0.202778	
ax-C R ω B97X-D/6-31G*	-466.784480	0.203927	
ax-H R ω B97X-D/6-31G*	-466.782730	0.205904	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq R ω B97X-V/6-311+G(2df,2p)	-466.950578	-466.747800	0	99.4	99.4
ax-C R ω B97X-V/6-311+G(2df,2p)	-466.946225	-466.742298	3.453	0.3	3.04
ax-H R ω B97X-V/6-311+G(2df,2p)	-466.944091	-466.738187	6.032	0.004	0.6

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq RM06-2X/6-31G(d)	-466.708648	0.218689	
ax-C RM06-2X/6-31G(d)	-466.704894	0.219553	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq RM06-2X/6-311+G(2df,2p)	-466.859607	-466.640918	0	98.8	98.8
ax-C RM06-2X /6-311+G(2df,2p)	-466.855682	-466.636129	3.005	0.6	2.60

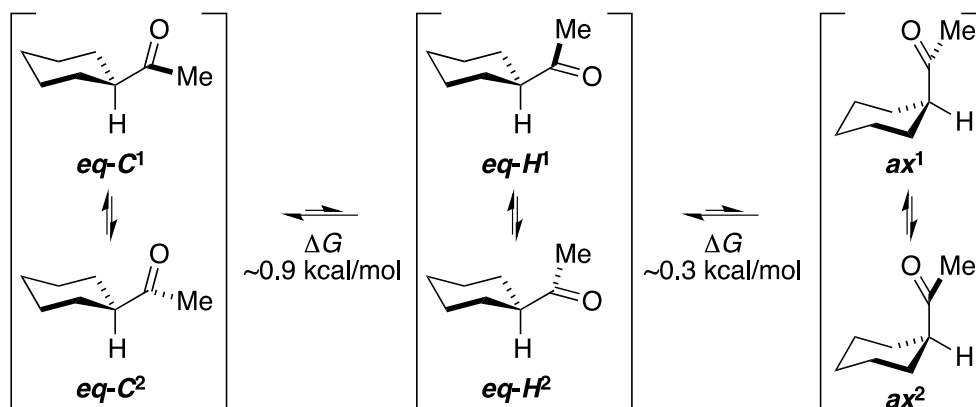
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq R ω B97X-V/6-31G*	-466.811130	0.218374	
ax-C R ω B97X-V/6-31G*	-466.807065	0.219446	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
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eq RM06-2X/6-311+G(2df,2p)	-466.860105	-466.641731	0	99.0	99.0	
ax-C RM06-2X /6-311+G(2df,2p)	-466.856152	-466.636706	3.153	0.5	1.0	2.74
eq R ω B97X-V/6-311+G(2df,2p)	-466.950307	-466.731933	0	99.4	99.4	
ax-C R ω B97X-V/6-311+G(2df,2p)	-466.945945	-466.726499	3.410	0.3	0.6	3.00
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RMP2(FC)/6-31G(d)	-465.297337	0.219212				
ax-C RMP2(FC)/6-31G(d)	-465.292752	0.220248				
ax-H RMP2(FC)/6-31G(d)	-465.290732	0.219172				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RM06-2X/6-311+G(2df,2p)	-466.859262	-466.640050	0	99.0	99.0	
ax-C RM06-2X/6-311+G(2df,2p)	-466.855255	-466.635007	3.164	0.5		2.71
ax-H RM06-2X /6-311+G(2df,2p)	-466.852523	-466.633351	4.203	0.08	1.0	
eq RMP2(FC)/6-311+G(2df,2p)	-465.844075	-465.624862	0	98.9	98.9	
ax-C RMP2(FC)/6-311+G(2df,2p)	-465.840130	-465.619883	3.124	0.5		2.65
ax-H RMP2(FC)/6-311+G(2df,2p)	-465.837672	-465.618500	3.992	0.1	1.1	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq RMP2(FC)/6-31G*	-465.297337	0.218429				
ax-C RMP2(FC)/6-31G*	-465.292752	0.219643				
ax-H RMP2(FC)/6-31G*	-465.290732	0.218866				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq R ω B97X-V/6-311+G(2df,2p)	-466.950366	-466.731937	0	99.5	99.5	
ax-C R ω B97X-V/6-311+G(2df,2p)	-466.945900	-466.726257	3.564	0.2		3.08
ax-H R ω B97X-V/6-311+G(2df,2p)	-466.943848	-466.724982	4.364	0.06	0.5	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq RHF/6-311+G(d,p)	-463.859050	-463.628528	0	100.0	100.0	
ax-C RHF/6-311+G(d,p)	-463.851875	-463.620354	5.129	0.02		4.53
ax-H RHF/6-311+G(d,p)	-463.850801	-463.620114	5.280	0.01	0.01	
eq RB3LYP/6-311+G(d,p)	-467.051575	-466.837822	0	99.8	99.8	
ax-C RB3LYP/6-311+G(d,p)	-467.045427	-466.830859	4.369	0.1		3.76
ax-H RB3LYP/6-311+G(d,p)	-467.044504	-466.830664	4.492	0.05	0.2	

eq RB3LYP-D3/6-311+G(d,p)	-467.076060	-466.861491	0	99.2	99.2	
ax-C RB3LYP-D3/6-311+G(d,p)	-467.071200	-466.856013	3.437	0.3		2.82
ax-H RB3LYP-D3/6-311+G(d,p)	-467.069942	-466.855852	3.538	0.2	0.8	
eq R ω B97X-D/6-311+G(d,p)	-466.899383	-466.682620	0	98.7	98.7	
ax-C R ω B97X-D/6-311+G(d,p)	-466.895235	-466.677788	3.032	0.6		2.55
ax-H R ω B97X-D/6-311+G(d,p)	-466.893638	-466.676566	3.799	0.2	1.3	
eq RM06-2X/6-311+G(d,p)	-466.831406	-466.614651	0	98.8	98.8	
ax-C RM06-2X/6-311+G(d,p)	-466.827497	-466.609851	3.012	0.6	1.2	2.60
eq R ω B97X-V/6-311+G**	-466.925568	-466.710092	0	99.3	99.3	
ax-C R ω B97X-V/6-311+G**	-466.921319	-466.704795	3.324	0.4	0.7	2.91
eq RMP2(FC)/6-311+G(d,p)	-465.587367	-465.372337	0	99.3	99.3	
ax-C RMP2(FC)/6-311+G(d,p)	-465.582813	-465.366917	3.401	0.3		2.90
ax-H RMP2(FC)/6-311+G(d,p)	-465.580860	-465.365840	4.077	0.1	0.7	

1-Cyclohexylethanone



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-C RHF/6-31G(d)	-385.976158	0.188521			
eq-H RHF/6-31G(d)	-385.973923	0.188929			
ax RHF/6-31G(d)	-385.973768	0.189513			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-C R ω B97X-D/6-311+G(2df,2p)	-388.530013	-388.341491	0	36.0	
eq-H R ω B97X-D/6-311+G(2df,2p)	-388.529158	-388.340230	0.7915	9.4	90.9
ax R ω B97X-D/6-311+G(2df,2p)	-388.529062	-388.339549	1.219	4.6	9.1

eq-C RM06-2X/6-311+G(2df,2p)	-388.468269	-388.279748	0	36.3		
eq-H RM06-2X /6-311+G(2df,2p)	-388.467315	-388.278386	0.854	8.5	89.7	1.28
ax RM06-2X/6-311+G(2df,2p)	-388.467423	-388.277910	1.153	5.2	10.3	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-C RHF/6-31G*	-385.976158	0.187570				
eq-H RHF/6-31G*	-385.973923	0.188023				
ax RHF/6-31G*	-385.973768	0.188640				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq-C RωB97X-V/6-311+G(2df,2p)	-388.545331	-388.357761	0	38.7		
eq-H RωB97X-V/6-311+G(2df,2p)	-388.544305	-388.356282	0.928	8.0	93.5	1.57
ax RωB97X-V/6-311+G(2df,2p)	-388.544073	-388.355433	1.461	3.3	6.5	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-C RB3LYP/6-31G(d)	-388.520270	0.173597				
eq-H RB3LYP/6-31G(d)	-388.518052	0.173979				
ax RB3LYP/6-31G(d)	-388.518132	0.174534				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq-C RB3LYP-D3/6-311+G(2df,2p)	-388.674861	-388.501265	0	37.5		
eq-H RB3LYP-D3/6-311+G(2df,2p)	-388.674005	-388.500027	0.777	10.1	95.1	1.76
ax RB3LYP-D3/6-311+G(2df,2p)	-388.673221	-388.498687	1.617	2.4	4.9	
eq-C RωB97X-D/6-311+G(2df,2p)	-388.532628	-388.359031	0	33.4		
eq-H RωB97X-D/6-311+G(2df,2p)	-388.532122	-388.358143	0.557	13.0	92.7	1.50
ax RωB97X-D/6-311+G(2df,2p)	-388.531480	-388.356946	1.309	3.6	7.3	
eq-C RM06-2X/6-311+G(2df,2p)	-388.467932	-388.294336	0	34.7		
eq-H RM06-2X /6-311+G(2df,2p)	-388.467084	-388.293105	0.772	9.4	88.2	1.19
ax RM06-2X/6-311+G(2df,2p)	-388.467200	-388.292666	1.048	5.9	11.8	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-C RB3LYP/6-31G*	-388.520279	0.162288				
eq-H RB3LYP/6-31G*	-388.518063	0.162628				
ax RB3LYP/6-31G*	-388.518132	0.163184				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	

eq-C R ω B97X-V/6-311+G(2df,2p)	-388.546228	-388.383940	0	36.7	92.0	
eq-H R ω B97X-V/6-311+G(2df,2p)	-388.545274	-388.382646	0.812	9.3		1.44
ax R ω B97X-V/6-311+G(2df,2p)	-388.545038	-388.381854	1.309	4.0	8.0	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-C RB3LYP-D3/6-31G(d)	-388.540456	0.174460	
eq-H RB3LYP-D3/6-31G(d)	-388.538629	0.174938	
ax RB3LYP-D3/6-31G(d)	-388.539641	0.175603	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-C RM06-2X/6-311+G(2df,2p)	-388.468182	-388.293721	0	35.3	88.5
eq-H RM06-2X /6-311+G(2df,2p)	-388.467373	-388.292435	0.807	9.0	1.21
ax RM06-2X/6-311+G(2df,2p)	-388.467615	-388.292012	1.073	5.7	11.5

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-C R ω B97X-D/6-31G(d)	-388.409026	0.176113	
eq-H R ω B97X-D/6-31G(d)	-388.407701	0.176537	
ax R ω B97X-D/6-31G(d)	-388.408639	0.177447	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-C R ω B97X-D/6-311+G(2df,2p)	-388.533325	-388.357213	0	34.5	94.7
eq-H R ω B97X-D/6-311+G(2df,2p)	-388.532822	-388.356286	0.582	12.9	1.70
ax R ω B97X-D/6-311+G(2df,2p)	-388.532253	-388.354807	1.510	2.7	5.3
eq-C RM06-2X/6-311+G(2df,2p)	-388.468748	-388.292635	0	35.7	90.2
eq-H RM06-2X /6-311+G(2df,2p)	-388.467923	-388.291386	0.784	9.5	1.31
ax RM06-2X/6-311+G(2df,2p)	-388.468208	-388.290762	1.175	4.9	9.8

wgeometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-C R ω B97X-D/6-31G*	-388.409041	0.162480	
eq-H R ω B97X-D/6-31G*	-388.407713	0.163071	
ax R ω B97X-D/6-31G*	-388.408633	0.163718	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-C R ω B97X-V/6-311+G(2df,2p)	-388.546700	-388.384220	0	38.9	93.4
eq-H R ω B97X-V/6-311+G(2df,2p)	-388.545774	-388.382703	0.952	7.8	1.56

ax RωB97X-V/6-311+G(2df,2p) -388.545618 -388.381900 1.456 3.3 6.6

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-C RM06-2X/6-31G(d)	-388.333156	0.175972			
eq-H RM06-2X/6-31G(d)	-388.331496	0.176220			
ax RM06-2X/6-31G(d)	-388.333340	0.177358			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-C RM06-2X/6-311+G(2df,2p)	-388.468869	-388.292897	0	34.3	91.0
eq-H RM06-2X /6-311+G(2df,2p)	-388.468066	-388.291846	0.660	11.2	
ax RM06-2X/6-311+G(2df,2p)	-388.468346	-388.290988	1.198	4.5	9.0

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-C RωB97X-V/6-31G*	-388.418294	0.175337			
eq-H RωB97X-V/6-31G*	-388.416451	0.175817			
ax RωB97X-V/6-31G*	-388.418115	0.176716			

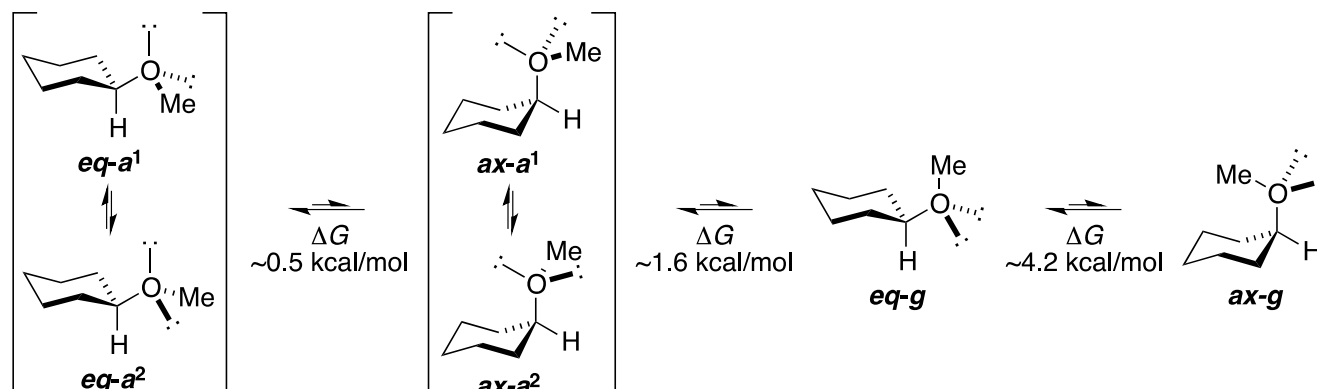
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-C RM06-2X/6-311+G(2df,2p)	-388.470246	-388.294909	0	36.6	91.5
eq-H RM06-2X /6-311+G(2df,2p)	-388.469417	-388.293600	0.821	9.1	
ax RM06-2X/6-311+G(2df,2p)	-388.469593	-388.292877	1.275	4.2	8.5
eq-C RωB97X-V/6-311+G(2df,2p)	-388.546472	-388.371135	0	38.5	94.6
eq-H RωB97X-V/6-311+G(2df,2p)	-388.545566	-388.369749	0.870	8.8	
ax RωB97X-V/6-311+G(2df,2p)	-388.545355	-388.368639	1.566	2.7	5.4

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-C RMP2(FC)/6-31G(d)	-387.191073	0.178156			
eq-H RMP2(FC)/6-31G(d)	-387.189048	0.178635			
ax RMP2(FC)/6-31G(d)	-387.190510	0.179456			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-C RM06-2X/6-311+G(2df,2p)	-388.468123	-388.289967	0	35.7	90.5
eq-H RM06-2X /6-311+G(2df,2p)	-388.467366	-388.288731	0.776	9.6	
ax RM06-2X/6-311+G(2df,2p)	-388.467522	-388.288066	1.193	4.7	9.5
eq-C RMP2(FC)/6-311+G(2df,2p)	-387.667214	-387.879058	0	37.9	93.7
eq-H RMP2(FC)/6-311+G(2df,2p)	-387.666327	-387.487692	0.857	8.9	

ax RMP2(FC)/6-311+G(2df,2p)	-387.666175	-387.486719	1.468	3.2	6.3	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-C RMP2(FC)/6-31G*	-387.191073	0.176986				
eq-H RMP2(FC)/6-31G*	-387.189048	0.177706				
ax RMP2(FC)/6-31G*	-387.190510	0.178629				
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq-C RωB97X-V/6-311+G(2df,2p)	-388.546331	-388.369345	0	40.5	96.2	
eq-H RωB97X-V/6-311+G(2df,2p)	-388.545473	-388.367767	0.990	7.6	1.90	
ax RωB97X-V/6-311+G(2df,2p)	-388.545102	-388.366473	1.802	1.9	3.8	
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)	
eq-C RHF/6-311+G(d,p)	-386.076651	-385.890709	0	42.4	98.8	
eq-H RHF/6-311+G(d,p)	-386.075208	-385.889016	1.062	7.0	2.61	
ax RHF/6-311+G(d,p)	-386.073555	-385.886695	2.519	0.6	1.2	
eq-C RB3LYP/6-311+G(d,p)	-388.633563	-388.461916	0	40.3	98.2	
eq-H RB3LYP/6-311+G(d,p)	-388.632343	-388.460486	0.897	8.8	2.36	
ax RB3LYP/6-311+G(d,p)	-388.630809	-388.458346	2.240	0.9	1.8	
eq-C RB3LYP-D3/6-311+G(d,p)	-388.653763	-388.481248	0	35.3	95.3	
eq-H RB3LYP-D3/6-311+G(d,p)	-388.652936	-388.480257	0.622	12.3	1.78	
ax RB3LYP-D3/6-311+G(d,p)	-388.652294	-388.478690	1.605	2.3	4.7	
eq-C RωB97X-D/6-311+G(d,p)	-388.513106	-388.338934	0	31.6	92.6	
eq-H RωB97X-D/6-311+G(d,p)	-388.512641	-388.338219	0.449	14.8	1.50	
ax RωB97X-D/6-311+G(d,p)	-388.512218	-388.336911	1.269	3.7	7.4	
eq-C RM06-2X/6-311+G(d,p)	-388.447733	-388.273365	0	33.2	88.7	
eq-H RM06-2X/6-311+G(d,p)	-388.446969	-388.272344	0.641	11.2	1.22	
ax RM06-2X/6-311+G(d,p)	-388.447384	-388.271698	1.046	5.6	11.3	
eq-C RωB97X-V/6-311+G**	-388.527406	-388.354660	0	38.8	93.8	
eq-H RωB97X-V/6-311+G**	-388.526521	-388.353179	0.929	8.1	1.61	
ax RωB97X-V/6-311+G**	-388.526449	-388.352279	1.494	3.1	6.2	
eq-C RMP2(FC)/6-311+G(d,p)	-387.456941	-387.282320	0	38.2	95.2	
eq-H RMP2(FC)/6-311+G(d,p)	-387.456094	-387.281004	0.826	9.4	1.76	

Methoxycyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G(d)	-348.086252	0.185354
eq-g RHF/6-31G(d)	-348.081857	0.186885
ax-a RHF/6-31G(d)	-348.085905	0.185686
ax-g RHF/6-31G(d)	-348.073645	0.185972

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-D/6-311+G(2df,2p)	-350.409321	-350.223966	0	38.5	77.5
eq-g Rwb97X-D/6-311+G(2df,2p)	-350.406579	-350.219694	2.681	0.4	
ax-a Rwb97X-D/6-311+G(2df,2p)	-350.408493	-350.222807	0.728	11.2	22.5
ax-g Rwb97X-D/6-311+G(2df,2p)	-350.400323	-350.214351	6.033	0.001	
eq-a RM06-2X/6-311+G(2df,2p)	-350.348030	-350.162675	0	35.7	71.8
eq-g RM06-2X /6-311+G(2df,2p)	-350.345186	-350.158302	2.745	0.3	
ax-a RM06-2X/6-311+G(2df,2p)	-350.347485	-350.161799	0.550	14.1	28.2
ax-g RM06-2X /6-311+G(2df,2p)	-350.338236	-350.152264	6.533	0.0006	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G*	-348.086251	0.184678
eq-g RHF/6-31G*	-348.081857	0.187045
ax-a RHF/6-31G*	-348.085905	0.184981
ax-g RHF/6-31G*	-348.073644	0.185297

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)	
eq-a R w B97X-V/6-311+G(2df,2p)	-350.417838	-350.233160	0	36.0	72.2 0.56 27.8	
eq-g R w B97X-V/6-311+G(2df,2p)	-350.414666	-350.227621	3.476	0.1		
ax-a R w B97X-V/6-311+G(2df,2p)	-350.417245	-350.232264	0.562	13.9		
ax-g R w B97X-V/6-311+G(2df,2p)	-350.407866	-350.222569	6.646	0.0005		
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-a RB3LYP/6-31G(d)	-350.397463	0.171029				
eq-g RB3LYP/6-31G(d)	-350.393780	0.171352				
ax-a RB3LYP/6-31G(d)	-350.397064	0.171475				
ax-g RB3LYP/6-31G(d)	-350.386523	0.171233				
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)	
eq-a RB3LYP-D3/6-311+G(2df,2p)	-350.537390	-350.366317	0	37.3	76.0 0.68 24.0	
eq-g RB3LYP-D3/6-311+G(2df,2p)	-350.534322	-350.363289	1.900	1.5		
ax-a RB3LYP-D3/6-311+G(2df,2p)	-350.536566	-350.365249	0.670	12.0		
ax-g RB3LYP-D3/6-311+G(2df,2p)	-350.527906	-350.357066	5.805	0.002		
eq-a R w B97X-D/6-311+G(2df,2p)	-350.409288	-350.238215	0	37.2	76.4 0.69 23.6	
eq-g R w B97X-D/6-311+G(2df,2p)	-350.406509	-350.235476	1.719	2.0		
ax-a R w B97X-D/6-311+G(2df,2p)	-350.408450	-350.237133	0.679	11.8		
ax-g R w B97X-D/6-311+G(2df,2p)	-350.400261	-350.229421	5.518	0.003		
eq-a RM06-2X/6-311+G(2df,2p)	-350.347990	-350.176917	0	34.4	70.4 0.51 29.6	
eq-g RM06-2X /6-311+G(2df,2p)	-350.345095	-350.174062	1.792	1.7		
ax-a RM06-2X/6-311+G(2df,2p)	-350.347440	-350.176122	0.499	14.8		
ax-g RM06-2X /6-311+G(2df,2p)	-350.338100	-350.167260	6.060	0.001		
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)				
eq-a RB3LYP/6-31G*	-350.397503	0.160233				
eq-g RB3LYP/6-31G*	-350.393783	0.160186				
ax-a RB3LYP/6-31G*	-350.397012	0.160527				
ax-g RB3LYP/6-31G*	-350.386503	0.160262				
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)	
eq-a R w B97X-V/6-311+G(2df,2p)	-350.418897	-350.258664	0	35.4	72.0	0.56

eq-g RwB97X-V/6-311+G(2df,2p)	-350.415708	-350.255522	1.972	1.3	
ax-a RwB97X-V/6-311+G(2df,2p)	-350.418319	-350.257792	0.547	14.0	
ax-g RwB97X-V/6-311+G(2df,2p)	-350.408927	-350.248665	6.274	0.0009	28.0

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RB3LYP-D3/6-31G(d)	-350.415596	0.171562	
eq-g RB3LYP-D3/6-31G(d)	-350.412549	0.171251	
ax-a RB3LYP-D3/6-31G(d)	-350.415853	0.171867	
ax-g RB3LYP-D3/6-31G(d)	-350.406216	0.172148	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-350.348114	-350.176552	0	32.7	
eq-g RM06-2X /6-311+G(2df,2p)	-350.345252	-350.174002	1.600	2.2	67.5
ax-a RM06-2X/6-311+G(2df,2p)	-350.347763	-350.175896	0.412	16.3	0.43
ax-g RM06-2X /6-311+G(2df,2p)	-350.338446	-350.166297	6.435	0.0006	32.5

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RwB97X-D/6-31G(d)	-350.297087	0.173396	
eq-g RwB97X-D/6-31G(d)	-350.294334	0.172691	
ax-a RwB97X-D/6-31G(d)	-350.297268	0.173981	
ax-g RwB97X-D/6-31G(d)	-350.288147	0.174530	

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RwB97X-D/6-311+G(2df,2p)	-350.409825	-350.236429	0	38.6	
eq-g RwB97X-D/6-311+G(2df,2p)	-350.407058	-350.234367	1.294	4.3	81.6
ax-a RwB97X-D/6-311+G(2df,2p)	-350.409060	-350.235078	0.848	9.2	0.88
ax-g RwB97X-D/6-311+G(2df,2p)	-350.400882	-350.226352	6.323	0.0009	18.4
eq-a RM06-2X/6-311+G(2df,2p)	-350.348618	-350.175222	0	34.4	
eq-g RM06-2X /6-311+G(2df,2p)	-350.345776	-350.173085	1.341	3.6	72.4
ax-a RM06-2X/6-311+G(2df,2p)	-350.348345	-350.174363	0.539	13.8	0.57
ax-g RM06-2X /6-311+G(2df,2p)	-350.338930	-350.164400	6.791	0.0003	27.6

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RwB97X-D/6-31G*	-350.297087	0.160205	
eq-g RwB97X-D/6-31G*	-350.294334	0.162711	

ax-a RωB97X-D/6-31G* -350.297268 0.160867
ax-g RωB97X-D/6-31G* -350.288147 0.161161

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RωB97X-V/6-311+G(2df,2p)	-350.419133	-350.258928	0	39.2	0.76
eq-g RωB97X-V/6-311+G(2df,2p)	-350.415987	-350.253276	3.547	0.1	
ax-a RωB97X-V/6-311+G(2df,2p)	-350.418582	-350.257715	0.761	10.8	
ax-g RωB97X-V/6-311+G(2df,2p)	-350.409225	-350.248064	6.817	0.0004	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RM06-2X/6-31G(d)	-350.225516	0.173354
eq-g RM06-2X/6-31G(d)	-350.222624	0.174696
ax-a RM06-2X/6-31G(d)	-350.226264	0.174026
ax-g RM06-2X/6-31G(d)	-350.215830	0.174033

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-350.348876	-350.175406	0	36.7	0.61
eq-g RM06-2X /6-311+G(2df,2p)	-350.345911	-350.171215	2.630	0.4	
ax-a RM06-2X/6-311+G(2df,2p)	-350.348463	-350.174463	0.608	13.1	
ax-g RM06-2X /6-311+G(2df,2p)	-350.339097	-350.165064	6.490	0.0006	

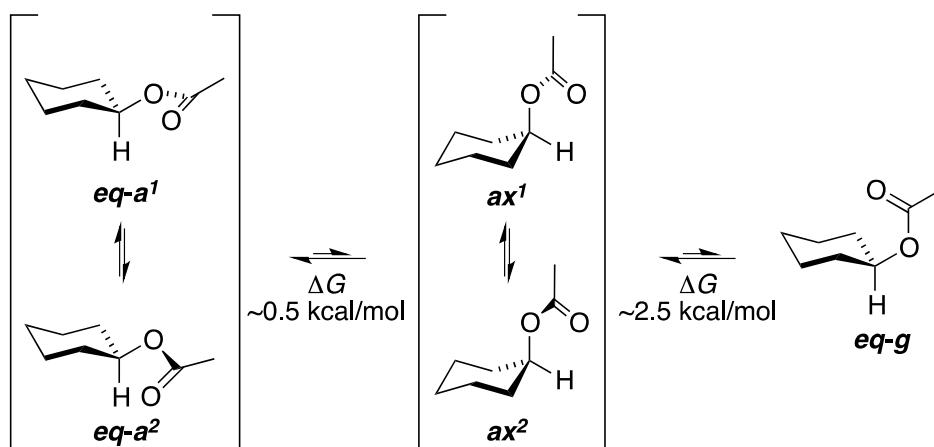
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RωB97X-V/6-31G*	-350.302920	0.172899
eq-g RωB97X-V/6-31G*	-350.299786	0.172346
ax-a RωB97X-V/6-31G*	-350.303646	0.173419
ax-g RωB97X-V/6-31G*	-350.293174	0.173634

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-350.349709	-350.176810	0	35.5	0.62
eq-g RM06-2X /6-311+G(2df,2p)	-350.346893	-350.174547	1.420	3.2	
ax-a RM06-2X/6-311+G(2df,2p)	-350.349278	-350.175859	0.597	12.9	
ax-g RM06-2X /6-311+G(2df,2p)	-350.340062	-350.166428	6.515	0.0006	
eq-a RωB97X-V/6-311+G(2df,2p)	-350.419058	-350.246159	0	37.6	0.73
eq-g RωB97X-V/6-311+G(2df,2p)	-350.415928	-350.243582	1.617	2.4	
ax-a RωB97X-V/6-311+G(2df,2p)	-350.418442	-350.245023	0.713	11.2	

ax-g Rwb97X-V/6-311+G(2df,2p)	-350.409166	-350.235532	6.668	0.0005	
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RMP2(FC)/6-31G(d)	-349.177392			0.175548	
eq-g RMP2(FC)/6-31G(d)	-349.173576			0.176987	
ax-a RMP2(FC)/6-31G(d)	-349.178422			0.176145	
ax-g RMP2(FC)/6-31G(d)	-349.166095			0.176366	
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-350.348485	-350.172938	0	37.0	
eq-g RM06-2X /6-311+G(2df,2p)	-350.345689	-350.168702	2.658	0.4	74.4
ax-a RM06-2X/6-311+G(2df,2p)	-350.348082	-350.171937	0.628	12.8	0.63
ax-g RM06-2X /6-311+G(2df,2p)	-350.338884	-350.162518	6.538	0.0006	25.6
eq-a RMP2(FC)/6-311+G(2df,2p)	-349.623121	-349.447574	0	35.6	
eq-g RMP2(FC)/6-311+G(2df,2p)	-349.619914	-349.442927	2.916	0.3	71.4
ax-a RMP2(FC)/6-311+G(2df,2p)	-349.622859	-349.442927	0.539	14.3	0.54
ax-g RMP2(FC)/6-311+G(2df,2p)	-349.612448	-349.436083	7.211	0.0001	28.6
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RMP2(FC)/6-31G*	-349.177392			0.174889	
eq-g RMP2(FC)/6-31G*	-349.173576			0.177197	
ax-a RMP2(FC)/6-31G*	-349.178422			0.175533	
ax-g RMP2(FC)/6-31G*	-349.166095			0.175772	
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-350.419159	-350.244270	0	40.3	
eq-g Rwb97X-V/6-311+G(2df,2p)	-350.416061	-350.238864	3.392	0.1	80.8
ax-a Rwb97X-V/6-311+G(2df,2p)	-350.418452	-350.244921	0.846	9.6	0.85
ax-g Rwb97X-V/6-311+G(2df,2p)	-350.409299	-350.235527	6.741	0.0004	19.2
geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RHF/6-311+G(d,p)	-348.177698	-347.995238	0	40.9	
eq-g RHF/6-311+G(d,p)	-348.173379	-347.989302	3.725	0.07	81.8
ax-a RHF/6-311+G(d,p)	-348.176447	-347.993822	0.889	9.1	0.89
ax-g RHF/6-311+G(d,p)	-348.165173	-347.982046	8.278	0.00003	18.2

eq-a RB3LYP/6-311+G(d,p)	-350.499247	-350.330472	0	40.6		
eq-g RB3LYP/6-311+G(d,p)	-350.495541	-350.326765	2.326	0.8	82.1	
ax-a RB3LYP/6-311+G(d,p)	-350.497897	-350.329049	0.893	9.0		0.90
ax-g RB3LYP/6-311+G(d,p)	-350.488367	-350.319504	6.882	0.0004	17.9	
eq-a RB3LYP-D3/6-311+G(d,p)	-350.517319	-350.348048	0	36.0		
eq-g RB3LYP-D3/6-311+G(d,p)	-350.514294	-350.345300	1.724	1.9	73.9	
ax-a RB3LYP-D3/6-311+G(d,p)	-350.516644	-350.347091	0.601	13.0		0.62
ax-g RB3LYP-D3/6-311+G(d,p)	-350.508040	-350.338208	6.175	0.001	26.1	
eq-a RωB97X-D/6-311+G(d,p)	-350.390575	-350.219497	0	38.2		
eq-g RωB97X-D/6-311+G(d,p)	-350.387859	-350.215281	2.646	0.4	76.9	
ax-a RωB97X-D/6-311+G(d,p)	-350.389976	-350.218372	0.706	11.6		0.71
ax-g RωB97X-D/6-311+G(d,p)	-350.381852	-350.209534	6.252	0.001	23.1	
eq-a RM06-2X/6-311+G(d,p)	-350.328616	-350.157025	0	33.2	68.0	
eq-g RM06-2X/6-311+G(d,p)	-350.325826	-350.154102	1.834	1.5		0.44
ax-a RM06-2X/6-311+G(d,p)	-350.328525	-350.156338	0.431	16.0	32.0	
ax-g RM06-2X/6-311+G(d,p)	-350.319133	-350.146865	6.375	0.0007		
eq-a RωB97X-V/6-311+G**	-350.401059	-350.230857	0	33.5		
eq-g RωB97X-V/6-311+G**	-350.397958	-350.228500	1.479	2.7	69.8	
ax-a RωB97X-V/6-311+G**	-350.400680	-350.23107	0.471	15.1		0.49
ax-g RωB97X-V/6-311+G**	-350.391428	-350.220343	6.598	0.0005	30.1	
eq-a RMP2(FC)/6-311+G(d,p)	-349.429881	-349.257788	0	34.6		
eq-g RMP2(FC)/6-311+G(d,p)	-349.426423	-349.254161	2.276	0.7	70.0	
ax-a RMP2(FC)/6-311+G(d,p)	-349.429743	-349.257002	0.493	15.0		0.50
ax-g RMP2(FC)/6-311+G(d,p)	-349.419107	-349.246128	7.317	0.0001	30.0	

Cyclohexyl Acetate



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RHF/6-31G(d)	-460.859794	0.193092			
eq-g RHF/6-31G(d)	-460.854951	0.193690			
ax RHF/6-31G(d)	-460.859089	0.193343			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-D/6-311+G(2df,2p)	-463.778899	-463.585807	0	37.2	74.7
eq-g R ω B97X-D/6-311+G(2df,2p)	-463.774604	-463.580914	3.071	0.2	
ax R ω B97X-D/6-311+G(2df,2p)	-463.778134	-463.584791	0.638	12.7	
eq-a RM06-2X/6-311+G(2df,2p)	-463.715173	-463.522081	0	36.1	72.5
eq-g RM06-2X /6-311+G(2df,2p)	-463.711049	-463.517359	2.963	0.2	
ax RM06-2X/6-311+G(2df,2p)	-463.714516	-463.521173	0.570	13.8	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RHF/6-31G*	-460.859794	0.191878			
eq-g RHF/6-31G*	-460.854951	0.192533			
ax RHF/6-31G*	-460.859089	0.192096			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-463.792365	-463.600487	0	34.2	68.6
eq-g R ω B97X-V/6-311+G(2df,2p)	-463.787860	-463.595327	3.238	0.1	
ax R ω B97X-V/6-311+G(2df,2p)	-463.791848	-463.599752	0.461	15.7	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP/6-31G(d)	-463.762502	0.177138			

eq-g RB3LYP/6-31G(d) -463.758348 0.177953

ax RB3LYP/6-31G(d) -463.761623 0.177352

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RB3LYP-D3/6-311+G(2df,2p)	-463.946333	-463.769196	0	36.8	73.7
eq-g RB3LYP-D3/6-311+G(2df,2p)	-463.942273	-463.764320	3.060	0.2	
ax RB3LYP-D3/6-311+G(2df,2p)	-463.945578	-463.768226	0.608	13.1	26.3
eq-a RωB97X-D/6-311+G(2df,2p)	-463.778698	-460.601560	0	37.5	75.1
eq-g RωB97X-D/6-311+G(2df,2p)	-463.774398	-463.596445	3.210	0.2	
ax RωB97X-D/6-311+G(2df,2p)	-463.777874	-463.600522	0.651	12.4	24.9
eq-a RM06-2X/6-311+G(2df,2p)	-463.714852	-463.537714	0	35.9	71.9
eq-g RM06-2X /6-311+G(2df,2p)	-463.710788	-463.532834	3.062	0.2	
ax RM06-2X/6-311+G(2df,2p)	-463.714182	-463.536830	0.554	14.0	28.1

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RB3LYP/6-31G*	-463.762492	0.165056
eq-g RB3LYP/6-31G*	-463.758355	0.166005
ax RB3LYP/6-31G*	-463.761625	0.165302

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RωB97X-V/6-311+G(2df,2p)	-463.793645	-463.628589	0	34.8	69.8
eq-g RωB97X-V/6-311+G(2df,2p)	-463.789148	-463.623143	3.417	0.1	
ax RωB97X-V/6-311+G(2df,2p)	-463.793106	-463.627804	0.493	15.1	30.2

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RB3LYP-D3/6-31G(d)	-463.783193	0.178052
eq-g RB3LYP-D3/6-31G(d)	-463.780098	0.178793
ax RB3LYP-D3/6-31G(d)	-463.783149	0.178327

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-463.715111	-463.537058	0	36.1	72.4
eq-g RM06-2X /6-311+G(2df,2p)	-463.710967	-463.532173	3.065	0.2	
ax RM06-2X/6-311+G(2df,2p)	-463.714479	-463.536152	0.569	13.8	27.6

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
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eq-a RωB97X-D/6-31G(d)	-463.627880	0.179649
eq-g RωB97X-D/6-31G(d)	-463.624420	0.180170
ax RωB97X-D/6-31G(d)	-463.627633	0.180340

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RωB97X-D/6-311+G(2df,2p)	-463.779488	-463.599838	0	41.6	83.5 0.96
eq-g RωB97X-D/6-311+G(2df,2p)	-463.775173	-463.595002	3.034	0.2	
ax RωB97X-D/6-311+G(2df,2p)	-463.778657	-463.598317	0.955	8.3	
eq-a RM06-2X/6-311+G(2df,2p)	-463.715821	-463.536172	0	39.9	80.1 0.82
eq-g RM06-2X /6-311+G(2df,2p)	-463.711722	-463.531551	2.899	0.3	
ax RM06-2X/6-311+G(2df,2p)	-463.715203	-463.534863	0.821	9.9	

wgeometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RωB97X-D/6-31G*	-463.627882	0.165650
eq-g RωB97X-D/6-31G*	-463.624439	0.166471
ax RωB97X-D/6-31G*	-463.627629	0.165779

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RωB97X-V/6-311+G(2df,2p)	-463.794124	-463.628474	0	33.5	67.1 0.42
eq-g RωB97X-V/6-311+G(2df,2p)	-463.789602	-463.623131	3.353	0.1	
ax RωB97X-V/6-311+G(2df,2p)	-463.793582	-463.627803	0.421	16.4	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RM06-2X/6-31G(d)	-463.550782	0.180121
eq-g RM06-2X/6-31G(d)	-463.547505	0.180633
ax RM06-2X/6-31G(d)	-463.550848	0.180456

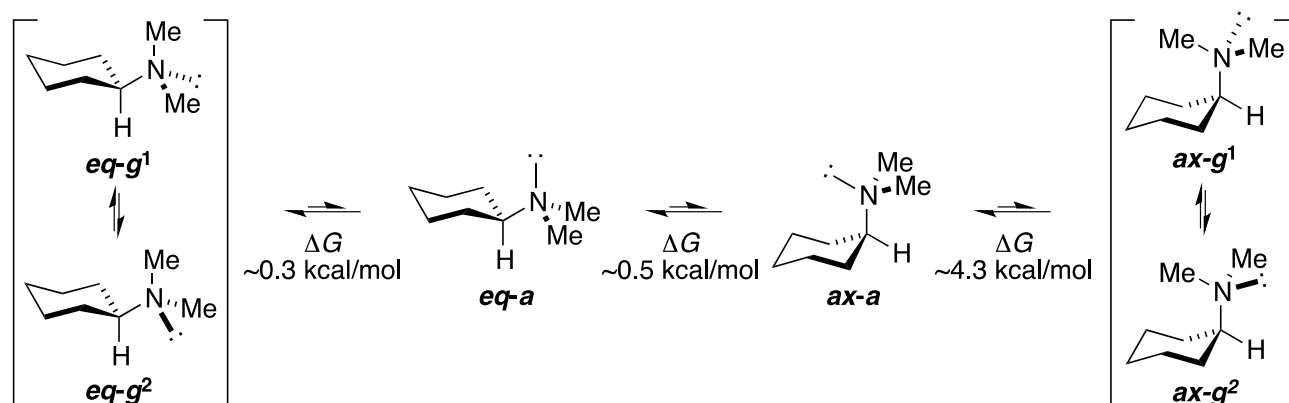
energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-463.715942	-463.535821	0	37.2	74.6 0.64
eq-g RM06-2X /6-311+G(2df,2p)	-463.711834	-463.531201	2.899	0.3	
ax RM06-2X/6-311+G(2df,2p)	-463.715267	-463.534812	0.633	12.7	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RωB97X-V/6-31G*	-463.637209	0.179110
eq-g RωB97X-V/6-31G*	-463.633814	0.179904
ax RωB97X-V/6-31G*	-463.637511	0.179505

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-463.717365	-463.538255	0	38.0	76.1 0.68
eq-g RM06-2X /6-311+G(2df,2p)	-463.713173	-463.533269	3.129	0.2	
ax RM06-2X/6-311+G(2df,2p)	-463.716671	-463.537166	0.683	11.9	
eq-a R ω B97X-V/6-311+G(2df,2p)	-463.793872	-463.614762	0	36.9	74.0 0.62
eq-g R ω B97X-V/6-311+G(2df,2p)	-463.789357	-463.609453	3.331	0.1	
ax R ω B97X-V/6-311+G(2df,2p)	-463.793283	-463.613778	0.617	13.0	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RMP2(FC)/6-31G(d)	-462.248944	0.182127			
eq-g RMP2(FC)/6-31G(d)	-462.244874	0.182739			
ax RMP2(FC)/6-31G(d)	-462.249520	0.182459			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-463.714935	-463.532809	0	37.5	75.3 0.66
eq-g RM06-2X /6-311+G(2df,2p)	-463.710843	-463.528104	2.952	0.3	
ax RM06-2X/6-311+G(2df,2p)	-463.714221	-463.531762	0.657	12.3	
eq-a RMP2(FC)/6-311+G(2df,2p)	-462.805574	-462.623447	0	34.3	68.7 0.46
eq-g RMP2(FC)/6-311+G(2df,2p)	-462.801007	-462.618268	3.250	0.1	
ax RMP2(FC)/6-311+G(2df,2p)	-462.805170	-462.622711	0.462	15.7	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RMP2(FC)/6-31G*	-462.248944	0.181038			
eq-g RMP2(FC)/6-31G*	-462.244874	0.181700			
ax RMP2(FC)/6-31G*	-462.249520	0.181347			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-463.793552	-463.612514	0	37.0	74.1 0.62
eq-g R ω B97X-V/6-311+G(2df,2p)	-463.789039	-463.607339	3.247	0.2	
ax R ω B97X-V/6-311+G(2df,2p)	-463.792872	-463.611525	0.621	12.9	
geometry method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RHF/6-311+G(d,p)	-460.982028	-460.792143	0	40.2	80.4 0.83
eq-g RHF/6-311+G(d,p)	-460.976403	-460.785876	3.933	0.05	

ax RHF/6-311+G(d,p)	-460.980821	-460.790815	0.833	9.8	19.6	
eq-a RB3LYP/6-311+G(d,p)	-463.899507	-463.725269	0	38.0	76.0	
eq-g RB3LYP/6-311+G(d,p)	-463.894426	-463.719557	3.584	0.09		0.68
ax RB3LYP/6-311+G(d,p)	-463.898146	-463.724183	0.681	12.0	24.0	
eq-a RB3LYP-D3/6-311+G(d,p)	-463.920083	-463.745167	0	37.0	74.2	
eq-g RB3LYP-D3/6-311+G(d,p)	-463.916103	-463.740124	3.164	0.2		0.62
ax RB3LYP-D3/6-311+G(d,p)	-463.919509	-463.744176	0.622	12.9	25.8	
eq-a RωB97X-D/6-311+G(d,p)	-463.754065	-463.577011	0	34.7	69.8	
eq-g RωB97X-D/6-311+G(d,p)	-463.749880	-463.572811	2.636	0.4		0.50
ax RωB97X-D/6-311+G(d,p)	-463.753423	-463.576226	0.493	15.1	30.2	
eq-a RM06-2X/6-311+G(d,p)	-463.689507	-463.511498	0	31.7	63.8	
eq-g RM06-2X/6-311+G(d,p)	-463.685528	-463.507360	2.597	0.4		0.33
ax RM06-2X/6-311+G(d,p)	-463.689079	-463.510970	0.331	18.1	36.2	
eq-a RωB97X-V/6-311+G**	-463.769412	-463.593772	0	30.4	61.0	
eq-g RωB97X-V/6-311+G**	-463.765042	-463.588851	3.088	0.2		0.26
ax RωB97X-V/6-311+G**	-463.769083	-463.593355	0.262	19.5	39.0	
eq-a RMP2(FC)/6-311+G(d,p)	-462.554022	-462.375884	0	34.3	69.0	
eq-g RMP2(FC)/6-311+G(d,p)	-462.549157	-462.371587	2.696	0.4		0.47
ax RMP2(FC)/6-311+G(d,p)	-462.553805	-462.375135	0.470	15.5	31.0	

N,N-Dimethylaminocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g RHF/6-31G(d)	-367.280676	0.227805			
eq-a RHF/6-31G(d)	-367.278790	0.227571			
ax-a RHF/6-31G(d)	-367.278080	0.228649			
ax-g RHF/6-31G(d)	-367.271387	0.228010			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g Rwb97X-D/6-311+G(2df,2p)	-369.848748	-369.620943	0	39.3	95.7
eq-a Rwb97X-D/6-311+G(2df,2p)	-369.847728	-369.620157	0.494	17.0	
ax-a Rwb97X-D/6-311+G(2df,2p)	-369.847510	-369.618860	1.307	4.3	4.3
ax-g Rwb97X-D/6-311+G(2df,2p)	-369.841805	-369.613795	4.485	0.02	
eq-g RM06-2X/6-311+G(2df,2p)	-369.774741	-369.546906	0.012	30.1	91.0
eq-a RM06-2X /6-311+G(2df,2p)	-369.774497	-369.546925	0	30.8	
ax-a RM06-2X/6-311+G(2df,2p)	-369.774417	-369.545767	0.727	9.0	1.37
ax-g RM06-2X /6-311+G(2df,2p)	-369.766984	-369.538974	4.989	0.007	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g RHF/6-31G*	-367.280676	0.227142			
eq-a RHF/6-31G*	-367.278790	0.226770			
ax-a RHF/6-31G*	-367.278080	0.227886			
ax-g RHF/6-31G*	-367.271387	0.227322			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)	
eq-g Rwb97X-V/6-311+G(2df,2p)	-369.858434	-369.631292	0	32.3	93.3	1.55

eq-a R w B97X-V/6-311+G(2df,2p)	-369.857946	-369.631176	0.073	28.6	
ax-a R w B97X-V/6-311+G(2df,2p)	-369.857696	-369.629810	0.930	6.7	
ax-g R w B97X-V/6-311+G(2df,2p)	-369.850899	-369.623577	4.841	0.009	6.7

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g RB3LYP/6-31G(d)	-369.837228	0.210561			
eq-a RB3LYP/6-31G(d)	-369.836097	0.210239			
ax-a RB3LYP/6-31G(d)	-369.835149	0.211065			
ax-g RB3LYP/6-31G(d)	-369.829356	0.210744			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RB3LYP-D3/6-311+G(2df,2p)	-369.983888	-369.773328	0	39.3	
eq-a RB3LYP-D3/6-311+G(2df,2p)	-369.982796	-369.772557	0.484	17.3	96.0
ax-a RB3LYP-D3/6-311+G(2df,2p)	-369.982233	-369.771168	1.355	4.0	1.88
ax-g RB3LYP-D3/6-311+G(2df,2p)	-369.976706	-369.765962	4.622	0.02	4.0
eq-g R w B97X-D/6-311+G(2df,2p)	-369.848520	-369.637959	0	38.3	
eq-a R w B97X-D/6-311+G(2df,2p)	-369.847478	-369.637240	0.466	17.8	94.4
ax-a R w B97X-D/6-311+G(2df,2p)	-369.847215	-369.636150	1.135	5.6	1.66
ax-g R w B97X-D/6-311+G(2df,2p)	-369.841625	-369.630881	4.442	0.02	5.6
eq-g RM06-2X/6-311+G(2df,2p)	-369.774471	-369.563910	0.028	29.1	
eq-a RM06-2X /6-311+G(2df,2p)	-369.774193	-369.563954	0	30.5	88.7
ax-a RM06-2X/6-311+G(2df,2p)	-369.774084	-369.563019	0.587	11.3	1.22
ax-g RM06-2X /6-311+G(2df,2p)	-369.766790	-369.556046	4.962	0.007	11.3

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g RB3LYP/6-31G*	-369.837227	0.197662			
eq-a RB3LYP/6-31G*	-369.836097	0.197218			
ax-a RB3LYP/6-31G*	-369.835149	0.198029			
ax-g RB3LYP/6-31G*	-369.829353	0.197762			

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-g R w B97X-V/6-311+G(2df,2p)	-369.859231	-369.661569	0	31.1	
eq-a R w B97X-V/6-311+G(2df,2p)	-369.858708	-369.661490	0.050	28.6	90.9
ax-a R w B97X-V/6-311+G(2df,2p)	-369.858440	-369.660411	0.727	9.1	9.1

ax-g R ω B97X-V/6-311+G(2df,2p) -369.851740 -369.653978 4.763 0.01

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-g RB3LYP-D3/6-31G(d)	-369.860609	0.211393
eq-a RB3LYP-D3/6-31G(d)	-369.858908	0.210734
ax-a RB3LYP-D3/6-31G(d)	-369.859457	0.211956
ax-g RB3LYP-D3/6-31G(d)	-369.853545	0.211356

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RM06-2X/6-311+G(2df,2p)	-369.774740	-369.563348	0.170	27.0	1.30
eq-a RM06-2X /6-311+G(2df,2p)	-369.774353	-369.563618	0	36.0	
ax-a RM06-2X/6-311+G(2df,2p)	-369.774358	-369.562402	0.764	9.9	
ax-g RM06-2X /6-311+G(2df,2p)	-369.767109	-369.555753	4.936	0.008	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-g R ω B97X-D/6-31G(d)	-369.735569	0.213498
eq-a R ω B97X-D/6-31G(d)	-369.733865	0.213584
ax-a R ω B97X-D/6-31G(d)	-369.734719	0.213791
ax-g R ω B97X-D/6-31G(d)	-369.728748	0.213813

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g R ω B97X-D/6-311+G(2df,2p)	-369.849182	-369.635684	0	40.8	1.54
eq-a R ω B97X-D/6-311+G(2df,2p)	-369.848075	-369.634490	0.749	11.5	
ax-a R ω B97X-D/6-311+G(2df,2p)	-369.847798	-369.634007	1.053	6.9	
ax-g R ω B97X-D/6-311+G(2df,2p)	-369.842336	-369.628523	4.494	0.02	
eq-g RM06-2X/6-311+G(2df,2p)	-369.775227	-369.561767	0	32.2	0.98
eq-a RM06-2X /6-311+G(2df,2p)	-369.774885	-369.561300	0.293	19.6	
ax-a RM06-2X/6-311+G(2df,2p)	-369.774899	-369.561108	0.414	16.0	
ax-g RM06-2X /6-311+G(2df,2p)	-369.767650	-369.553837	4.976	0.007	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-g R ω B97X-D/6-31G*	-369.735568	0.197792
eq-a R ω B97X-D/6-31G*	-369.733865	0.197849
ax-a R ω B97X-D/6-31G*	-369.734717	0.198203
ax-g R ω B97X-D/6-31G*	-369.728747	0.198184

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g R ω B97X-V/6-311+G(2df,2p)	-369.859697	-369.661905	0	36.7	91.1 1.37
eq-a R ω B97X-V/6-311+G(2df,2p)	-369.859074	-369.661225	0.427	17.8	
ax-a R ω B97X-V/6-311+G(2df,2p)	-369.858774	-369.660571	0.837	8.9	
ax-g R ω B97X-V/6-311+G(2df,2p)	-369.852210	-369.654026	4.944	0.008	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g RM06-2X/6-31G(d)	-369.650573	0.213214			
eq-a RM06-2X/6-31G(d)	-369.649669	0.213172			
ax-a RM06-2X/6-31G(d)	-369.650860	0.214212			
ax-g RM06-2X/6-31G(d)	-369.643061	0.213594			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RM06-2X/6-311+G(2df,2p)	-369.775428	-369.562214	0	34.5	92.2 1.46
eq-a RM06-2X /6-311+G(2df,2p)	-369.775015	-369.561843	0.233	23.3	
ax-a RM06-2X/6-311+G(2df,2p)	-369.775020	-369.560808	0.883	7.7	
ax-g RM06-2X /6-311+G(2df,2p)	-369.767824	-369.554230	5.011	0.007	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-g R ω B97X-V/6-31G*	-369.743074	0.213015			
eq-a R ω B97X-V/6-31G*	-369.741772	0.212594			
ax-a R ω B97X-V/6-31G*	-369.742946	0.213759			
ax-g R ω B97X-V/6-31G*	-369.735788	0.213294			
energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RM06-2X/6-311+G(2df,2p)	-369.776292	-369.563277	0.022	30.4	92.2 1.46
eq-a RM06-2X /6-311+G(2df,2p)	-369.775906	-369.563312	0	31.5	
ax-a RM06-2X/6-311+G(2df,2p)	-369.775755	-369.561996	0.826	7.8	
ax-g RM06-2X /6-311+G(2df,2p)	-369.768672	-369.555378	4.979	0.007	
eq-g R ω B97X-V/6-311+G(2df,2p)	-369.859565	-369.646550	0	33.8	94.6 1.69
eq-a R ω B97X-V/6-311+G(2df,2p)	-369.858934	-369.646340	0.131	27.0	
ax-a R ω B97X-V/6-311+G(2df,2p)	-369.858576	-369.644817	1.087	5.4	
ax-g R ω B97X-V/6-311+G(2df,2p)	-369.852077	-369.638783	4.874	0.009	
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq-g RMP2(FC)/6-31G(d)	-368.495037	0.216191
eq-a RMP2(FC)/6-31G(d)	-368.494294	0.215998
ax-a RMP2(FC)/6-31G(d)	-368.495760	0.217154
ax-g RMP2(FC)/6-31G(d)	-368.486785	0.216506

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RM06-2X/6-311+G(2df,2p)	-369.775348	-369.559157	0	33.5	92.9 1.52
eq-a RM06-2X/6-311+G(2df,2p)	-369.774915	-369.558916	0.151	25.9	
ax-a RM06-2X/6-311+G(2df,2p)	-369.774845	-369.557690	0.9200	7.1	
ax-g RM06-2X/6-311+G(2df,2p)	-369.767709	-369.551203	4.991	0.007	
eq-g RMP2(FC)/6-311+G(2df,2p)	-368.973753	-368.757562	0.162	25.8	85.5 1.05
eq-a RMP2(FC)/6-311+G(2df,2p)	-368.973818	-368.757819	0	33.9	
ax-a RMP2(FC)/6-311+G(2df,2p)	-368.974174	-368.757020	0.501	14.5	
ax-g RMP2(FC)/6-311+G(2df,2p)	-368.965784	-368.749287	5.360	0.004	

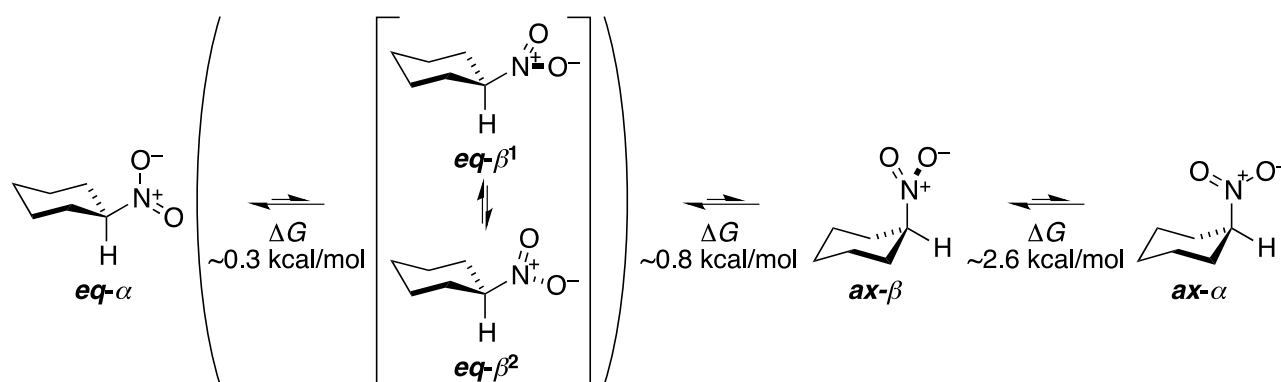
geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-g RMP2(FC)/6-31G*	-368.495037	0.215614
eq-a RMP2(FC)/6-31G*	-368.494294	0.215305
ax-a RMP2(FC)/6-31G*	-368.495760	0.216512
ax-g RMP2(FC)/6-31G*	-368.486785	0.215941

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-g Rwb97X-V/6-311+G(2df,2p)	-369.859725	-369.644111	0	35.6	95.8 1.85
eq-a Rwb97X-V/6-311+G(2df,2p)	-369.859068	-369.643763	0.218	24.6	
ax-a Rwb97X-V/6-311+G(2df,2p)	-369.858609	-369.642097	1.264	4.2	
ax-g Rwb97X-V/6-311+G(2df,2p)	-369.852232	-369.636291	4.907	0.009	

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-g RHF/6-311+G(d,p)	-367.372837	-367.148546	0	43.6	99.2 2.85
eq-a RHF/6-311+G(d,p)	-367.371412	-367.147327	0.765	11.9	
ax-a RHF/6-311+G(d,p)	-367.369687	-367.144781	2.363	0.8	
ax-g RHF/6-311+G(d,p)	-367.363586	-367.139012	5.983	0.002	
eq-g RB3LYP/6-311+G(d,p)	-369.939806	-369.732019	0	36.8	97.9 2.26
eq-a RB3LYP/6-311+G(d,p)	-369.939167	-369.731627	0.246	24.3	

ax-a RB3LYP/6-311+G(d,p)	-369.937362	-369.729338	1.682	2.1		
ax-g RB3LYP/6-311+G(d,p)	-369.931953	-369.724015	5.023	0.00	2.1	
eq-g RB3LYP-D3/6-311+G(d,p)	-369.963201	-369.754564	0	37.8	94.2	
eq-a RB3LYP-D3/6-311+G(d,p)	-369.961980	-369.753902	0.415	18.7		1.65
ax-a RB3LYP-D3/6-311+G(d,p)	-369.961556	-369.752790	1.113	5.7	5.8	
ax-g RB3LYP-D3/6-311+G(d,p)	-369.956165	-369.747569	4.389	0.02		
eq-g RωB97X-D/6-311+G(d,p)	-369.829560	-369.618909	0	40.2	90.8	
eq-a RωB97X-D/6-311+G(d,p)	-369.828363	-369.617644	0.794	10.5		1.35
ax-a RωB97X-D/6-311+G(d,p)	-369.828270	-369.617517	0.873	9.2	9.2	
ax-g RωB97X-D/6-311+G(d,p)	-369.822884	-369.611675	4.539	0.02		
eq-g RM06-2X/6-311+G(d,p)	-369.754526	-369.543561	0	35.4	89.9	
eq-a RM06-2X/6-311+G(d,p)	-369.753966	-369.542974	0.368	19.0		1.29
ax-a RM06-2X/6-311+G(d,p)	-369.754203	-369.542379	0.742	10.1	10.1	
ax-g RM06-2X/6-311+G(d,p)	-369.747080	-369.535615	4.986	0.008		
eq-g RωB97X-V/6-311+G**	-369.841457	-369.631677	0	34.0	91.4	
eq-a RωB97X-V/6-311+G**	-369.840693	-369.631325	0.221	23.4		1.40
ax-a RωB97X-V/6-311+G**	-369.840583	-369.630379	0.814	8.6	8.6	
ax-g RωB97X-V/6-311+G**	-369.834177	-369.624047	4.788	0.01		
eq-g RMP2(FC)/6-311+G(d,p)	-368.768125	-368.556449	0.071	25.3	79.2	
eq-a RMP2(FC)/6-311+G(d,p)	-368.768147	-368.556562	0	28.6		0.79
ax-a RMP2(FC)/6-311+G(d,p)	-368.768554	-368.556263	0.188	20.8	20.8	
ax-g RMP2(FC)/6-311+G(d,p)	-368.760394	-368.548248	5.217	0.004		

Nitrocyclohexane



geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-α RHF/6-31G(d)	-437.684901	0.153806			
ax-β RHF/6-31G(d)	-437.682219	0.153276			
ax-α RHF/6-31G(d)	-437.681436	0.155931			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α Rwb97X-D/6-311+G(2df,2p)	-440.401212	-440.247406	0	79.8	79.8
ax-β Rwb97X-D/6-311+G(2df,2p)	-440.399378	-440.246102	0.818	20.0	0.81
ax-α Rwb97X-D/6-311+G(2df,2p)	-440.397854	-440.241923	3.44	0.2	20.2

eq-α RM06-2X/6-311+G(2df,2p)	-440.343176	-440.18970	0	65.7	65.7
ax-β RM06-2X/6-311+G(2df,2p)	-440.342025	-440.188749	0.389	34.0	0.39
ax-α RM06-2X /6-311+G(2df,2p)	-440.340012	-440.184081	3.319	0.2	34.3

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-α RHF/6-31G*	-437.684901	0.153088			
ax-β RHF/6-31G*	-437.682218	0.152538			
ax-α RHF/6-31G*	-437.681436	0.156113			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α Rwb97X-V/6-311+G(2df,2p)	-440.414361	-440.261273	0	71.7	71.7
ax-β Rwb97X-V/6-311+G(2df,2p)	-440.412932	-440.260394	0.552	28.2	0.55
ax-α Rwb97X-V/6-311+G(2df,2p)	-440.411091	-440.254978	3.950	0.1	28.3

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-α RB3LYP/6-31G(d)	-440.382826	0.140461			
ax-β RB3LYP/6-31G(d)	-440.381235	0.139718			

ax- α RB3LYP/6-31G(d) -440.380038 0.142699

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RB3LYP-D3/6-311+G(2df,2p)	-440.559090	-440.418628	0	78.8	78.8
ax-β RB3LYP-D3/6-311+G(2df,2p)	-440.557098	-440.417379	0.784	20.9	0.78
ax-α RB3LYP-D3/6-311+G(2df,2p)	-440.556030	-440.413331	3.324	0.3	21.2
eq-α R ω B97X-D/6-311+G(2df,2p)	-440.401483	-440.261021	0	67.2	67.2
ax-β R ω B97X-D/6-311+G(2df,2p)	-440.399621	-440.259902	0.702	20.5	0.42
ax-α R ω B97X-D/6-311+G(2df,2p)	-440.402127	-440.259428	1.000	12.4	32.8
eq-α RM06-2X/6-311+G(2df,2p)	-440.342874	-440.202413	0	59.8	59.8
ax-β RM06-2X/6-311+G(2df,2p)	-440.341752	-440.202034	0.238	40.0	0.23
ax-α RM06-2X /6-311+G(2df,2p)	-440.339829	-440.197130	3.315	0.2	40.2

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RB3LYP/6-31G*	-440.382826	0.130932
ax-β RB3LYP/6-31G*	-440.381235	0.130072
ax-α RB3LYP/6-31G*	-440.380038	0.134244

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α R ω B97X-V/6-311+G(2df,2p)	-440.415692	-440.284760	0	65.1	65.1
ax-β R ω B97X-V/6-311+G(2df,2p)	-440.414243	-440.284171	0.370	34.8	0.37
ax-α R ω B97X-V/6-311+G(2df,2p)	-440.412530	-440.278286	4.062	0.1	34.9

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RB3LYP-D3/6-31G(d)	-440.400738	0.141125
ax-β RB3LYP-D3/6-31G(d)	-440.400304	0.140968
ax-α RB3LYP-D3/6-31G(d)	-440.398956	0.143380

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RM06-2X/6-311+G(2df,2p)	-440.343013	-440.201888	0	70.7	70.7
ax-β RM06-2X/6-311+G(2df,2p)	-440.342020	-440.201053	0.524	29.1	0.52
ax-α RM06-2X /6-311+G(2df,2p)	-440.339944	-440.196564	3.341	0.2	29.3

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α R ω B97X-D/6-31G(d)	-440.254573	0.142748

ax-β RωB97X-D/6-31G(d) -440.253943 0.143236

ax-α RωB97X-D/6-31G(d) -440.252315 0.145165

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RωB97X-D/6-311+G(2df,2p)	-440.402499	-440.259751	0	92.6	92.6
ax-β RωB97X-D/6-311+G(2df,2p)	-440.400586	-440.257350	1.507	7.2	1.49
ax-α RωB97X-D/6-311+G(2df,2p)	-440.399148	-440.253983	3.620	0.2	7.4
eq-α RM06-2X/6-311+G(2df,2p)	-440.344095	-440.201347	0	83.8	83.8
ax-β RM06-2X/6-311+G(2df,2p)	-440.343022	-440.199786	0.980	16.0	0.97
ax-α RM06-2X /6-311+G(2df,2p)	-440.341000	-440.195835	3.459	0.2	16.2

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RωB97X-D/6-31G*	-440.254573	0.131140
ax-β RωB97X-D/6-31G*	-440.253943	0.131568
ax-α RωB97X-D/6-31G*	-440.252315	0.134360

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RωB97X-V/6-311+G(2df,2p)	-440.416504	-440.285364	0	88.0	88.0
ax-β RωB97X-V/6-311+G(2df,2p)	-440.415047	-440.283479	1.183	11.9	1.18
ax-α RωB97X-V/6-311+G(2df,2p)	-440.413241	-440.278881	4.068	0.09	12.0

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RM06-2X/6-31G(d)	-440.182932	0.142426
ax-β RM06-2X/6-31G(d)	-440.182942	0.142637
ax-β RM06-2X/6-31G(d)	-440.183429	0.143372
ax-α RM06-2X/6-31G(d)	-440.181080	0.144956

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RM06-2X/6-311+G(2df,2p)	-440.344321	-440.201895	0	43.6	94.7
ax-β RM06-2X/6-311+G(2df,2p)	-440.344030	-440.201392	0.315	25.6	1.71
ax-β RM06-2X/6-311+G(2df,2p)	-440.343258	-440.199886	1.260	5.2	5.3
ax-α RM06-2X/6-311+G(2df,2p)	-440.341207	-440.196252	3.541	0.1	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RωB97X-V/6-31G*	-440.263086	0.142148

eq-β RωB97X-V/6-31G*	-440.262902	0.142177
ax-β RωB97X-V/6-31G*	-440.263180	0.142859
ax-α RωB97X-V/6-31G*	-440.261203	0.145468

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RM06-2X/6-311+G(2df,2p)	-440.345854	-440.203706	0	34.8	1.68
ax-β RM06-2X/6-311+G(2df,2p)	-440.345737	-440.203560	0.092	29.8	
ax-β RM06-2X/6-311+G(2df,2p)	-440.344821	-440.201962	1.094	5.5	
ax-α RM06-2X/6-311+G(2df,2p)	-440.342719	-440.197251	4.051	0.04	
eq-α RωB97X-V/6-311+G(2df,2p)	-440.416314	-440.274166	0	41.6	1.87
eq-β RωB97X-V/6-311+G(2df,2p)	-440.415943	-440.273766	0.251	27.2	
ax-β RωB97X-V/6-311+G(2df,2p)	-440.414820	-440.271961	1.384	4.0	
ax-α RωB97X-V/6-311+G(2df,2p)	-440.413038	-440.267570	4.139	0.04	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RMP2(FC)/6-31G(d)	-439.007337	0.144252
ax-β RMP2(FC)/6-31G(d)	-439.006927	0.144838
ax-α RMP2(FC)/6-31G(d)	-439.005181	0.146627

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RM06-2X/6-311+G(2df,2p)	-440.341345	-440.197094	0	85.9	1.07
ax-β RM06-2X/6-311+G(2df,2p)	-440.340217	-440.195379	1.076	13.9	
ax-α RM06-2X/6-311+G(2df,2p)	-440.338206	-440.191579	3.461	0.2	
eq-α MP2(FC)/6-311+G(2df,2p)	-439.524151	-439.379900	0	93.1	1.53
ax-β RMP2(FC)/6-311+G(2df,2p)	-439.522270	-439.377432	1.548	6.8	
ax-α RMP2(FC)/6-311+G(2df,2p)	-439.520650	-439.374023	3.688	0.2	

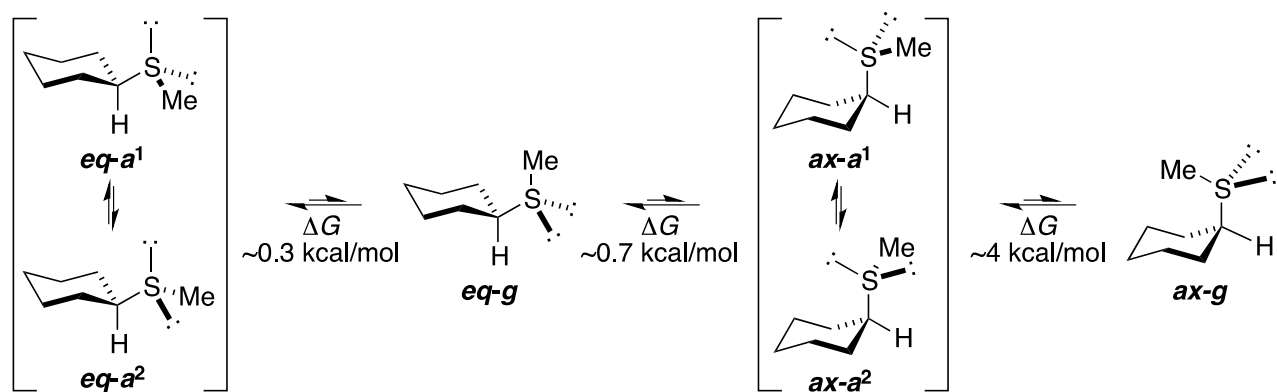
geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-α RMP2(FC)/6-31G*	-439.007337	0.143550
ax-β RMP2(FC)/6-31G*	-439.006927	0.144303
ax-α RMP2(FC)/6-31G*	-439.005181	0.146814

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RωB97X-V/6-311+G(2df,2p)	-440.414282	-440.270732	0	92.4	1.47
ax-β RωB97X-V/6-311+G(2df,2p)	-440.412679	-440.268376	1.478	7.6	

ax- α R ω B97X-V/6-311+G(2df,2p) -440.410933 -440.264119 4.150 0.08

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-α RHF/6-311+G(d,p)	-437.805809	-437.654475	0	99.6	99.6
ax-β RHF/6-311+G(d,p)	-437.802097	-437.648753	3.591	0.2	3.33
ax-α RHF/6-311+G(d,p)	-437.801648	-437.648210	3.931	0.1	
eq-α RB3LYP/6-311+G(d,p)	-440.516654	-440.378084	0	99.2	99.2
ax-β RB3LYP/6-311+G(d,p)	-440.513863	-440.373286	3.011	0.6	2.85
ax-α RB3LYP/6-311+G(d,p)	-440.512914	-440.372181	3.704	0.2	
eq-α RB3LYP-D3/6-311+G(d,p)	-440.534531	-440.395297	0	87.0	87.0
ax-β RB3LYP-D3/6-311+G(d,p)	-440.532811	-440.391573	2.337	1.7	1.13
ax-α RB3LYP-D3/6-311+G(d,p)	-440.532866	-440.393374	1.207	11.3	
eq-α R ω B97X-D/6-311+G(d,p)	-440.378192	-440.237322	0	97.9	97.9
ax-β R ω B97X-D/6-311+G(d,p)	-440.376539	-440.233461	2.423	1.6	2.28
ax-α R ω B97X-D/6-311+G(d,p)	-440.375159	-440.232249	3.183	0.4	
eq-α RM06-2X/6-311+G(d,p)	-440.318030	-440.177064	0	68.5	68.5
ax-β RM06-2X/6-311+G(d,p)	-440.317238	-440.176325	0.464	31.2	0.46
ax-α RM06-2X/6-311+G(d,p)	-440.315285	-440.171938	3.217	0.3	
eq-α R ω B97X-V/6-311+G**	-440.392309	-440.252051	0	73.4	0.60
ax-β R ω B97X-V/6-311+G**	-440.391122	-440.251097	0.599	26.6	
eq-α RMP2(FC)/6-311+G(d,p)	-439.288435	-439.146845	0	98.6	98.6
ax-β RMP2(FC)/6-311+G(d,p)	-439.286436	-439.142635	2.642	1.1	2.52
ax-α RMP2(FC)/6-311+G(d,p)	-439.285023	-439.141277	3.494	0.3	

Methylthiocyclohexane



geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G(d)	-670.749949	0.180240
eq-g RHF/6-31G(d)	-670.748567	0.180280
ax-a RHF/6-31G(d)	-670.747342	0.180467
ax-g RHF/6-31G(d)	-670.739696	0.181004

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-D/6-311+G(2df,2p)	-673.402324	-673.222084	0	34.2	92.7
eq-g Rwb97X-D/6-311+G(2df,2p)	-673.402044	-673.221764	0.201	24.3	
ax-a Rwb97X-D/6-311+G(2df,2p)	-673.400439	-673.219973	1.325	3.6	7.3
ax-g Rwb97X-D/6-311+G(2df,2p)	-673.395433	-673.214429	4.804	0.01	
eq-a RM06-2X/6-311+G(2df,2p)	-673.328778	-673.148538	0	35.9	88.1
eq-g RM06-2X /6-311+G(2df,2p)	-673.328083	-673.147803	0.461	16.4	
ax-a RM06-2X/6-311+G(2df,2p)	-673.327311	-673.146845	1.062	5.9	11.9
ax-g RM06-2X /6-311+G(2df,2p)	-673.320957	-673.139954	5.387	0.004	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RHF/6-31G*	-670.749949	0.179413
eq-g RHF/6-31G*	-670.748567	0.179493
ax-a RHF/6-31G*	-670.747342	0.179633
ax-g RHF/6-31G*	-670.739696	0.180277

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-673.354397	-673.174984	0	36.4	89.5
eq-g Rwb97X-V/6-311+G(2df,2p)	-673.353743	-673.174250	0.461	16.7	

ax-a Rwb97X-V/6-311+G(2df,2p) -673.352793 -673.173160 1.145 5.2
ax-g Rwb97X-V/6-311+G(2df,2p) -673.346664 -673.166387 5.395 0.004 10.5

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RB3LYP/6-31G(d)	-673.379582	0.166070	
eq-g RB3LYP/6-31G(d)	-673.378583	0.166183	
ax-a RB3LYP/6-31G(d)	-673.377409	0.166279	
ax-g RB3LYP/6-31G(d)	-673.370778	0.166405	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RB3LYP-D3/6-311+G(2df,2p)	-673.524049	-673.357978	0	34.1	90.2
eq-g RB3LYP-D3/6-311+G(2df,2p)	-673.523742	-673.357560	0.263	21.9	
ax-a RB3LYP-D3/6-311+G(2df,2p)	-673.522449	-673.356153	1.145	4.9	9.8
ax-g RB3LYP-D3/6-311+G(2df,2p)	-673.517003	-673.350598	4.631	0.01	
eq-a Rwb97X-D/6-311+G(2df,2p)	-673.401729	-673.235658	0	34.5	92.1
eq-g Rwb97X-D/6-311+G(2df,2p)	-673.401462	-673.235280	0.237	23.1	
ax-a Rwb97X-D/6-311+G(2df,2p)	-673.399909	-673.233614	1.283	3.9	7.9
ax-g Rwb97X-D/6-311+G(2df,2p)	-673.394821	-673.228416	4.545	0.02	
eq-a RM06-2X/6-311+G(2df,2p)	-673.328114	-673.162044	0	35.6	86.8
eq-g RM06-2X /6-311+G(2df,2p)	-673.327453	-673.161270	0.486	15.6	
ax-a RM06-2X/6-311+G(2df,2p)	-673.326751	-673.160455	0.997	6.6	13.2
ax-g RM06-2X /6-311+G(2df,2p)	-673.320171	-673.153766	5.195	0.005	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)	
eq-a RB3LYP/6-31G*	-673.379586	0.155188	
eq-g RB3LYP/6-31G*	-673.378582	0.155297	
ax-a RB3LYP/6-31G*	-673.377399	0.155325	
ax-g RB3LYP/6-31G-	-673.370778	0.155670	

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-673.354379	-673.199191	0	35.8	87.7
eq-g Rwb97X-V/6-311+G(2df,2p)	-673.353742	-673.198445	0.468	16.2	
ax-a Rwb97X-V/6-311+G(2df,2p)	-673.352856	-673.197531	1.042	6.1	12.3
ax-g Rwb97X-V/6-311+G(2df,2p)	-673.346626	-673.190956	5.167	0.006	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RB3LYP-D3/6-31G(d)	-673.398508	0.166727			
eq-g RB3LYP-D3/6-31G(d)	-673.398182	0.166788			
ax-a RB3LYP-D3/6-31G(d)	-673.397321	0.167019			
ax-g RB3LYP-D3/6-31G(d)	-673.391471	0.167331			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-673.328275	-673.161548	0	35.2	1.16
eq-g RM06-2X /6-311+G(2df,2p)	-673.327665	-673.160878	0.421	17.3	
ax-a RM06-2X/6-311+G(2df,2p)	-673.326919	-673.159901	1.034	6.1	
ax-g RM06-2X /6-311+G(2df,2p)	-673.320825	-673.153494	5.054	0.007	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RwB97X-D/6-31G(d)	-673.285257	0.168493			
eq-g RwB97X-D/6-31G(d)	-673.284971	0.168443			
ax-a RwB97X-D/6-31G(d)	-673.283777	0.168600			
ax-g RwB97X-D/6-31G(d)	-673.278355	0.169478			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RwB97X-D/6-311+G(2df,2p)	-673.402492	-673.233999	0	32.5	1.42
eq-g RwB97X-D/6-311+G(2df,2p)	-673.402258	-673.233815	0.116	26.7	
ax-a RwB97X-D/6-311+G(2df,2p)	-673.400634	-673.232054	1.221	4.1	
ax-g RwB97X-D/6-311+G(2df,2p)	-673.395771	-673.226293	4.836	0.009	

eq-a RM06-2X/6-311+G(2df,2p)	-673.329026	-673.160533	0	33.8	1.06
eq-g RM06-2X /6-311+G(2df,2p)	-673.328397	-673.159953	0.364	18.2	
ax-a RM06-2X/6-311+G(2df,2p)	-673.327667	-673.159067	0.920	7.1	
ax-g RM06-2X /6-311+G(2df,2p)	-673.321583	-673.152105	5.289	0.004	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a RwB97X-D/6-31G*	-673.285259	0.155583			
eq-g RwB97X-D/6-31G*	-673.284971	0.155392			
ax-a RwB97X-D/6-31G*	-673.283778	0.155571			
ax-g RwB97X-D/6-31G-	-673.278359	0.156675			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a R ω B97X-V/6-311+G(2df,2p)	-673.355112	-673.199529	0	32.8	1.12
eq-g R ω B97X-V/6-311+G(2df,2p)	-673.354523	-673.199131	0.250	21.5	
ax-a R ω B97X-V/6-311+G(2df,2p)	-673.353575	-673.198004	0.957	6.5	
ax-g R ω B97X-V/6-311+G(2df,2p)	-673.347546	-673.190871	5.433	0.003	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a R ω M06-2X/6-31G(d)	-673.199153	0.168061			
eq-g RM06-2X/6-31G(d)	-673.198508	0.167133			
ax-a RM06-2X/6-31G(d)	-673.198120	0.167640			
ax-g RM06-2X/6-31G(d)	-673.191662	0.169624			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-673.329159	-673.161098	0.181	24.3	0.89
eq-g RM06-2X /6-311+G(2df,2p)	-673.328520	-673.161387	0	33.1	
ax-a RM06-2X/6-311+G(2df,2p)	-673.327813	-673.160173	0.762	9.1	
ax-g RM06-2X /6-311+G(2df,2p)	-673.321870	-673.152246	5.736	0.002	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			
eq-a R ω B97X-V/6-31G*	-673.235685	0.168085			
eq-g R ω B97X-V/6-31G*	-673.235038	0.168015			
ax-a R ω B97X-V/6-31G*	-673.234629	0.168287			
ax-g R ω B97X-V/6-31G*	-673.228022	0.169251			

energy method	E (au)	G (au)	rel G (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-673.330465	-673.162380	0	34.1	1.15
eq-g RM06-2X/6-311+G(2df,2p)	-673.329868	-673.161853	0.331	19.5	
ax-a RM06-2X/6-311+G(2df,2p)	-673.329066	-673.160779	1.005	6.2	
ax-g RM06-2X/6-311+G(2df,2p)	-673.323139	-673.153888	5.329	0.004	

eq-a R ω B97X-V/6-311+G(2df,2p)	-673.355001	-673.186916	0	34.6	1.24
eq-g R ω B97X-V/6-311+G(2df,2p)	-673.354412	-673.186397	0.326	19.9	
ax-a R ω B97X-V/6-311+G(2df,2p)	-673.353468	-673.185181	1.089	5.5	
ax-g R ω B97X-V/6-311+G(2df,2p)	-673.347441	-673.178190	5.476	0.003	

geometry method	E (au)	Thermal correction to Gibbs Free Energy (au/Particle)			

eq-a RMP2(FC)/6-31G(d)	-671.791238	0.170988
eq-g RMP2(FC)/6-31G(d)	-671.790310	0.170858
ax-a RMP2(FC)/6-31G(d)	-671.789715	0.171123
ax-g RMP2(FC)/6-31G(d)	-671.781918	0.172095

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RM06-2X/6-311+G(2df,2p)	-673.329147	-673.158160	0	33.2	86.3 1.09
eq-g RM06-2X/6-311+G(2df,2p)	-673.328540	-673.157681	0.300	20.0	
ax-a RM06-2X/6-311+G(2df,2p)	-673.327797	-673.156674	0.932	6.8	
ax-g RM06-2X/6-311+G(2df,2p)	-673.321773	-673.149679	5.322	0.004	
eq-a RMP2(FC)/6-311+G(2df,2p)	-672.231545	-672.060560	0	34.1	86.9 1.12
eq-g RMP2(FC)/6-311+G(2df,2p)	-672.230833	-672.059974	0.368	19.5	
ax-a RMP2(FC)/6-311+G(2df,2p)	-672.230128	-672.059005	0.976	6.2	
ax-g RMP2(FC)/6-311+G(2df,2p)	-672.223293	-672.051198	5.875	0.004	

geometry method	<i>E</i> (au)	Thermal correction to Gibbs Free Energy (au/Particle)
eq-a RMP2(FC)/6-31G*	-671.791238	0.170192
eq-g RMP2(FC)/6-31G*	-671.790310	0.170106
ax-a RMP2(FC)/6-31G*	-671.789715	0.170347
ax-g RMP2(FC)/6-31G*	-671.781918	0.171408

energy method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a Rwb97X-V/6-311+G(2df,2p)	-673.355176	-673.184984	0	34.3	88.7 1.22
eq-g Rwb97X-V/6-311+G(2df,2p)	-673.354584	-673.184478	0.318	20.1	
ax-a Rwb97X-V/6-311+G(2df,2p)	-673.353631	-673.183284	1.067	5.6	
ax-g Rwb97X-V/6-311+G(2df,2p)	-673.347606	-673.176198	5.513	0.003	

geometry method	<i>E</i> (au)	<i>G</i> (au)	rel <i>G</i> (kcal/mol)	Population %	A-value (kcal/mol)
eq-a RHF/6-311+G(d,p)	-670.843248	-670.665999	0	43.8	96.7 2.00
eq-g RHF/6-311+G(d,p)	-670.841997	-670.664513	0.932	9.0	
ax-a RHF/6-311+G(d,p)	-670.840398	-670.662904	1.942	1.6	
ax-g RHF/6-311+G(d,p)	-670.833457	-670.655193	6.781	0.0005	
eq-a RB3LYP/6-311+G(d,p)	-673.484459	-673.320747	0	40.5	94.8 1.71
eq-g RB3LYP/6-311+G(d,p)	-673.483572	-673.319731	0.638	13.8	

ax-a RB3LYP/6-311+G(d,p)	-673.482069	-673.318165	1.620	2.6		
ax-g RB3LYP/6-311+G(d,p)	-673.475989	-673.311779	5.627	0.003	5.2	
eq-a RB3LYP-D3/6-311+G(d,p)	-673.503369	-673.338887	0	32.1	88.4	
eq-g RB3LYP-D3/6-311+G(d,p)	-673.503146	-673.338620	0.168	24.2		1.20
ax-a RB3LYP-D3/6-311+G(d,p)	-673.501945	-673.337275	1.012	5.8	11.6	
ax-g RB3LYP-D3/6-311+G(d,p)	-673.496650	-673.331555	4.601	0.01		
eq-a RωB97X-D/6-311+G(d,p)	-673.381974	-673.215869	0.172	27.8	92.8	
eq-g RωB97X-D/6-311+G(d,p)	-673.381850	-673.216143	0	37.2		1.51
ax-a RωB97X-D/6-311+G(d,p)	-673.380333	-673.213948	1.377	3.6	7.2	
ax-g RωB97X-D/6-311+G(d,p)	-673.375596	-673.208141	5.021	0.008		
eq-a RM06-2X/6-311+G(d,p)	-673.308386	-673.142208	0.253	24.4	86.1	
eq-g RM06-2X/6-311+G(d,p)	-673.307833	-673.142611	0	37.4		1.08
ax-a RM06-2X/6-311+G(d,p)	-673.307232	-673.141029	0.993	7.0	13.9	
ax-g RM06-2X/6-311+G(d,p)	-673.301391	-673.133651	5.622	0.003		
eq-a RωB97X-V/6-311+G**	-673.335807	-673.170562	0	33.7	85.4	
eq-g RωB97X-V/6-311+G**	-673.335291	-673.169969	0.372	18.0		1.04
ax-a RωB97X-V/6-311+G**	-673.334500	-673.169120	0.905	7.3	14.6	
ax-g RωB97X-V/6-311+G**	-673.328614	-673.161997	5.375	0.004		
eq-a RMP2(FC)/6-311+G(d,p)	-672.036808	-671.869597	0	31.1	90.6	
eq-g RMP2(FC)/6-311+G(d,p)	-672.036094	-671.869507	0.056	2.83		1.33
ax-a RMP2(FC)/6-311+G(d,p)	-672.035297	-671.867822	1.114	4.7	9.4	
ax-g RMP2(FC)/6-311+G(d,p)	-672.028501	-671.860079	5.973	0.001		

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

2. *Spartan'18* Wavefunction, Inc. Irvine, CA.