

Comparisons

MOL1	Final energy/eV	
Orientation	ORIG_TOL	VAR_TOL
45degACW	-242687.8589	-242687.7679
45degCW	-242687.048	-242687.0955
BRC	-242687.9253	-242687.8573
EGC	-242687.5019	-242687.5712
EGSMGC	-242687.4572	-242687.3615
F_EGS	-242687.4328	-242687.3362
F_MGS	-242687.8033	-242687.706
HGC	-242688.0088	-242687.8262
MGC	-242687.295	-242687.2006
MGSMGC	-242687.5793	-242687.4877
SRC	-242686.8331	-242686.7407
UR	-242687.2566	-242687.1647

MOL3	Final energy/eV	
Orientation	ORIG_TOL	VAR_TOL
45degACW	-243244.3209	-243244.2275
45degCW	-243238.385	-243238.2614
BRC	-243244.3119	-243244.6808
EGC	-243242.3428	-243242.3344
EGSMGC	-243244.034	-243243.923
F_EGS	-243244.1335	-243244.4042
F_MGS	-243242.7921	-243242.6871
HGC	-243243.3946	-243243.2726
MGC	-243244.2097	-243244.1139
MGSMGC	-243244.0282	-243243.923
NGC	-243243.6494	-243243.6015
SRC	-243242.3014	-243242.1999
UR	-243244.1936	-243244.0932

MOL2	Final energy/eV	
Orientation	ORIG_TOL	VAR_TOL
45degACW	-242401.6421	-242401.5388
45degCW	-242401.5818	-242401.4909
BRC	-242401.8278	-242401.7794
EGC	-242402.2186	-242402.8274
F_EGS	-242401.5555	-242401.0451
F_SS	-242400.4775	-242400.456
HGC	-242402.5019	-242402.5228
SC	-242401.087	-242400.9687
SRC	-242401.1535	-242401.0347
UR	-242400.5759	-242400.465

MOL4	Final energy/eV	
Orientation	ORIG_TOL	VAR_TOL
45degACW	-242959.5255	-242959.4148
45degCW	-242958.2866	-242958.0882
BRC	-242958.6154	-242959.9571
EGC	-242959.5623	-242959.371
F_EGS	-242958.4609	-242958.1257
F_SS	-242958.515	-242958.3895
HGC	-242959.301	-242959.2114
NGC	-242958.6342	-242961.9789
SRC	-242953.2197	-242953.0997
SC	-242959.9199	-242961.6275
UR	-242958.5079	-242958.4016

Most negative
Least negative
Unconverged value
Finished unconverged after re-run

Differences in final energy between tolerances	
MOL1	MOL3
-0.0909694	-0.0933444
-0.0475059	-0.1236002
-0.0680038	-0.3688918
-0.0692621	-0.0084342
-0.0956635	-0.1110386
-0.0966442	-0.270756
-0.097272	-0.1050374
-0.1826428	-0.1219842
-0.0943352	-0.0957978
-0.0915991	-0.1051974
-0.0923886	-0.0479285
-0.091978	-0.1014775
	-0.100336

MOL2	MOL4
-0.1033236	-0.1107258
-0.0908663	-0.1983209
-0.0483895	-1.3417103
-0.6088242	-0.191207
-0.5104019	-0.3351571
-0.0214793	-0.1254742
-0.0208933	-0.0895904
-0.118244	-3.3447308
-0.1187994	-0.1199764
-0.1108902	-1.7075924
	-0.1063227

Differences between most negative value and other values		
MOL1 ORIG_TOL: HGC		
Value subtracted by	subtracted	/326
BRC	-0.0835031	-0.000256144
45degACW	-0.1499168	-0.000459867
F_MGS	-0.205559	-0.000630549
MGSMGC	-0.4295347	-0.001317591
EGC	-0.5069229	-0.001554978
EGSMGC	-0.5516391	-0.001692144
F_EGS	-0.575998	-0.001766865
MGC	-0.7138731	-0.002189795
UR	-0.752189	-0.002307328
45degCW	-0.9608074	-0.002947262
SRC	-1.1757447	-0.003606579

Differences between most negative value and other values		
MOL1 VAR_TOL: BRC		
Value subtracted by	subtracted	/326
HGC	-0.0311359	-9.55089E-05
45degACW	-0.0893793	-0.00027417
F_MGS	-0.1513241	-0.000464184
EGC	-0.2861539	-0.000877773
MGSMGC	-0.3696269	-0.001133825
EGSMGC	-0.4957957	-0.001520846
F_EGS	-0.5211353	-0.001598575
MGC	-0.6567014	-0.002014421
UR	-0.6926601	-0.002124724
45degCW	-0.7617946	-0.002336793
SRC	-1.1166264	-0.003425234

First value under -0.001
Most negative value (difference tables)

Differences between most negative value and other values		
MOL2 ORIG_TOL: HGC		
Value subtracted by	subtracted	/318
EGC	-0.2833105	-0.00089
BRC	-0.674081	-0.00212
45degACW	-0.8598378	-0.0027
45degCW	-0.9201044	-0.00289
F_EGS	-0.94642	-0.00298
SRC	-1.3484063	-0.00424
SC	-1.4149623	-0.00445
UR	-1.9260446	-0.00606
F_SS	-2.0243924	-0.00637

Differences between most negative value and other values		
MOL2 VAR_TOL: EGC		
Value subtracted by	subtracted	/318
HGC	-0.3046204	-0.00096
BRC	-1.0479842	-0.0033
45degACW	-1.2886751	-0.00405
45degCW	-1.3364844	-0.0042
F_EGS	-1.7823356	-0.0056
SRC	-1.7927194	-0.00564
SC	-1.85872	-0.00585
UR	-2.3624485	-0.00743
F_SS	-2.3713854	-0.00746

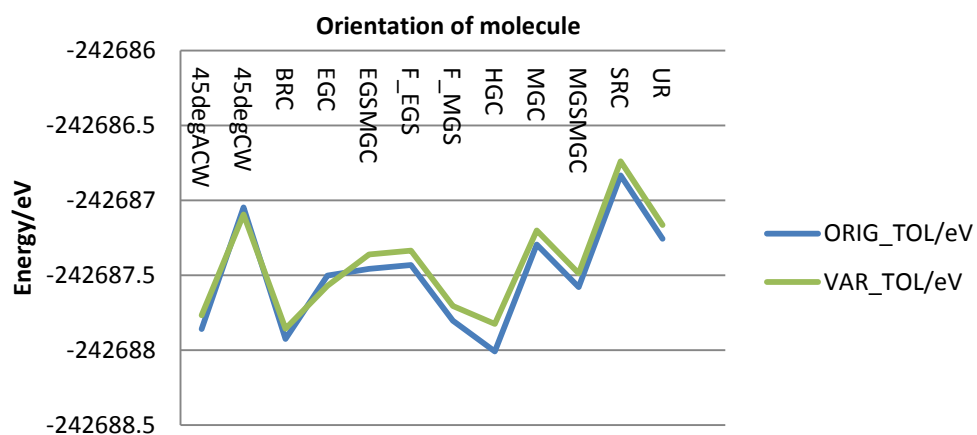
Differences between most negative value and other values		
MOL3 ORIG_TOL: 45degACW		
Value subtracted by	subtracted	/330
BRC	-0.0090124	-2.7E-05
MGC	-0.111208	-0.00034
UR	-0.1273212	-0.00039
F_EGS	-0.1874273	-0.00057
EGSMGC	-0.2868744	-0.00087
MGSMGC	-0.292657	-0.00089
NGC	-0.6715043	-0.00203
HGC	-0.9263008	-0.00281
F_MGS	-1.528752	-0.00463
EGC	-1.9780384	-0.00599
SRC	-2.0194661	-0.00612
45degCW	-5.9358507	-0.01799
Differences between most negative value and other values		
MOL3 VAR_TOL: BRC		
Value subtracted by	subtracted	/330
F_EGS	-0.2765507	-0.00084
45degACW	-0.4532238	-0.00137
MGC	-0.5668852	-0.00172
UR	-0.5875366	-0.00178
MGSMGC	-0.7577338	-0.0023
EGSMGC	-0.7577924	-0.0023
NGC	-1.0793122	-0.00327
HGC	-1.4081644	-0.00427
F_MGS	-1.9936688	-0.00604
EGC	-2.346352	-0.00711
SRC	-2.480823	-0.00752
45degCW	-6.4193303	-0.01945

Differences between most negative value and other values		
MOL4 ORIG_TOL: SS(SC)		
Value subtracted by	subtracted	/322
EGC	-0.3576235	-0.00111
45degACW	-0.3943784	-0.00122
HGC	-0.6188423	-0.00192
NGC	-1.2856724	-0.00399
BRC	-1.3044907	-0.00405
F_SS	-1.4048591	-0.00436
UR	-1.4119817	-0.00439
F_EGS	-1.4590026	-0.00453
45degCW	-1.6333188	-0.00507
SRC	-6.7002213	-0.02081

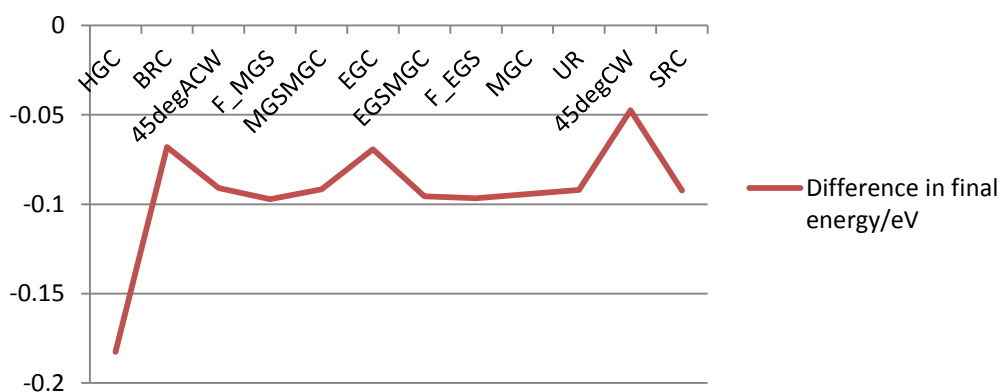
Differences between most negative value and other values		
MOL4 VAR_TOL: NGC		
Value subtracted by	subtracted	/322
SS(SC)	-0.351466	-0.00109
BRC	-2.0218388	-0.00628
45degACW	-2.5641626	-0.00796
EGC	-2.6078889	-0.0081
HGC	-2.7674911	-0.00859
UR	-3.5773628	-0.01111
F_SS	-3.5893917	-0.01115
F_EGS	-3.8532181	-0.01197
45degCW	-3.8906981	-0.01208
SRC	-8.8792561	-0.02758

The results for the energy convergence comparisons are varied between both molecule and tolerance at more negative values, however between tolerances the less negative values show similar differences from the most negative orientation.

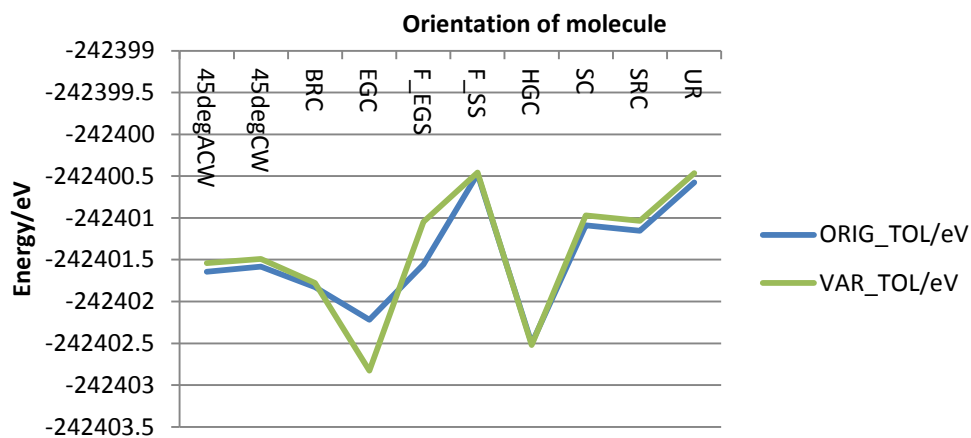
MOL1 final energies



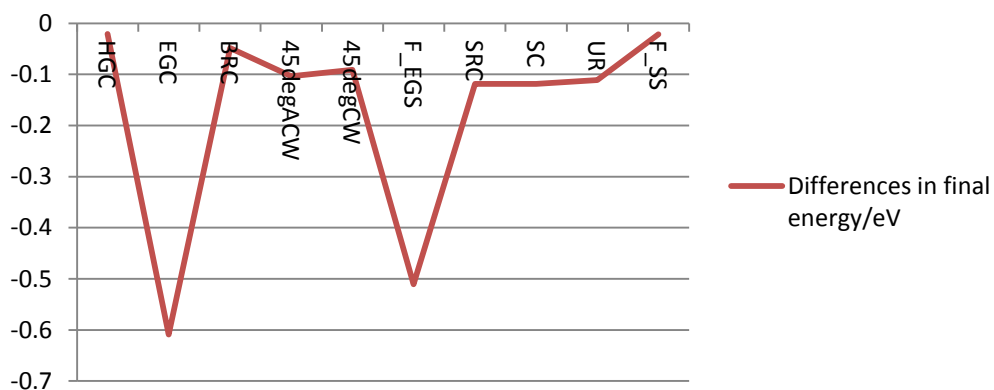
Differences in final energy between tolerances MOL1



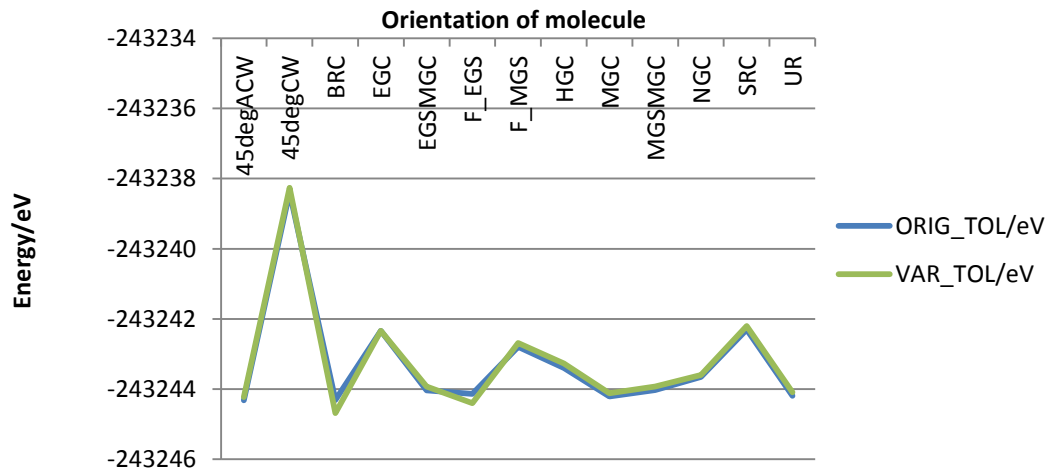
MOL2 final energies



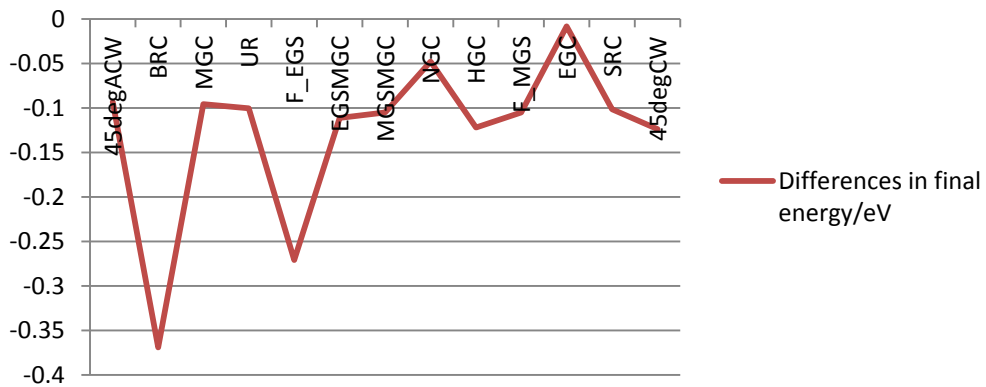
Differences in final energy between tolerances MOL2



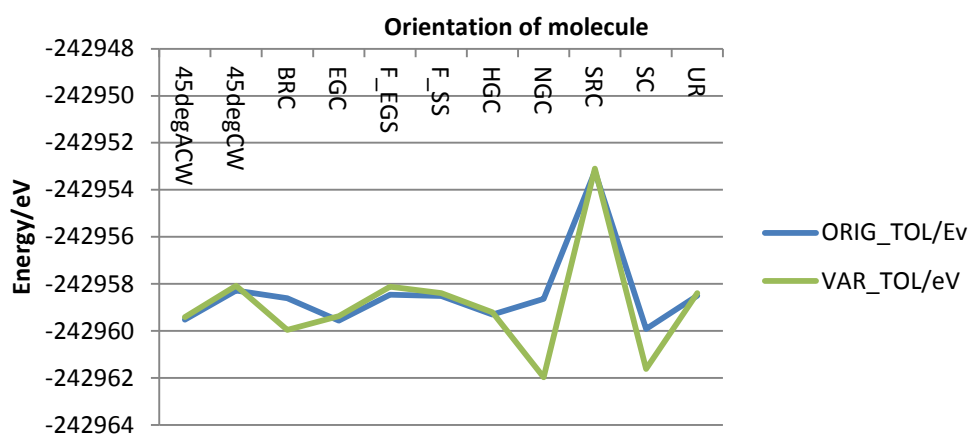
MOL3 final energies



Differences in final energy between tolerances MOL3



MOL4 final energies



Differences in final energy between tolerances MOL4

