Supplemental Information for:

Dipole Moments of *trans*- and *cis*-4-methyl-cyclohexyl methanol (MCHM): Obtaining the Right Conformer for the Right Reason

Nathan J. DeYonker*, Katherine A. Charbonnet, and William A. Alexander*

Department of Chemistry
213 Smith Chemistry Building
The University of Memphis, Memphis, TN 38152

*to whom correspondence should be addressed; e-mail: ndyonker@memphis.edu (NJD);
w.alexander@memphis.edu (WAA)

Contents:

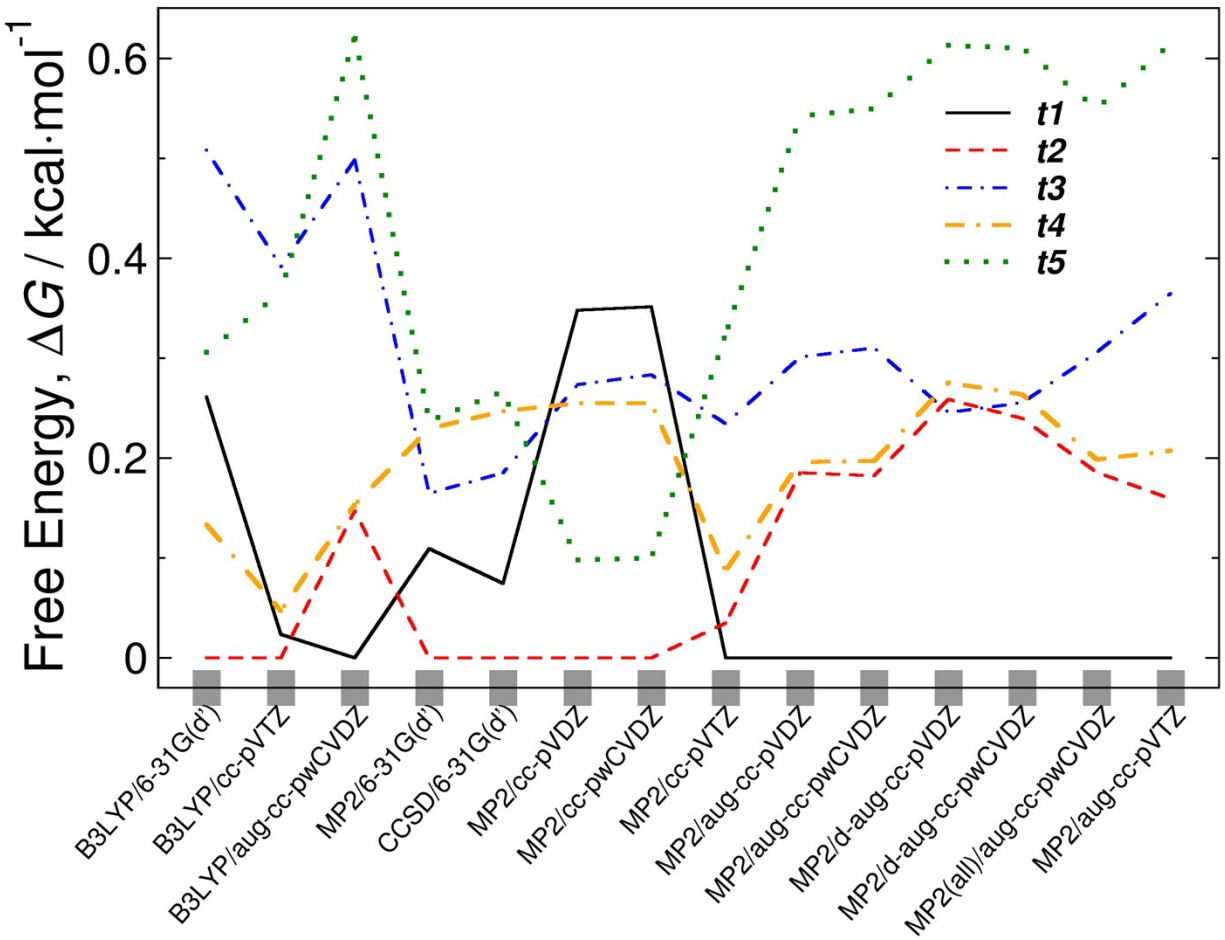

Fig. S1 Zoomed-in version of Figure 2 from the main text to show detail of methodological dependence.

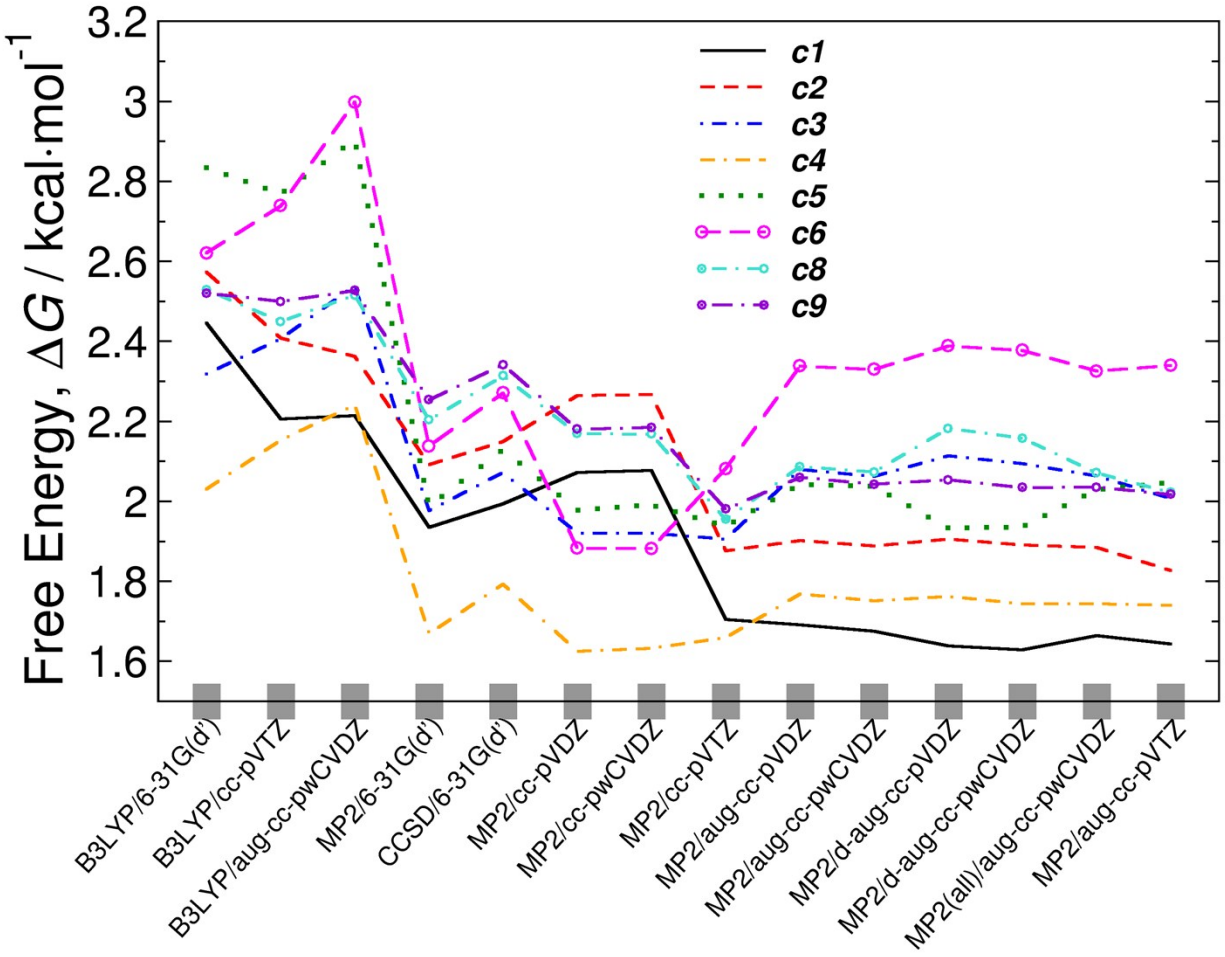

Fig. S2 Zoomed-in version of Figure 3 from the main text to show detail of methodological dependence.

Figure S3. 3D structures of *trans*-4-MCHM conformers and their conformer ID #

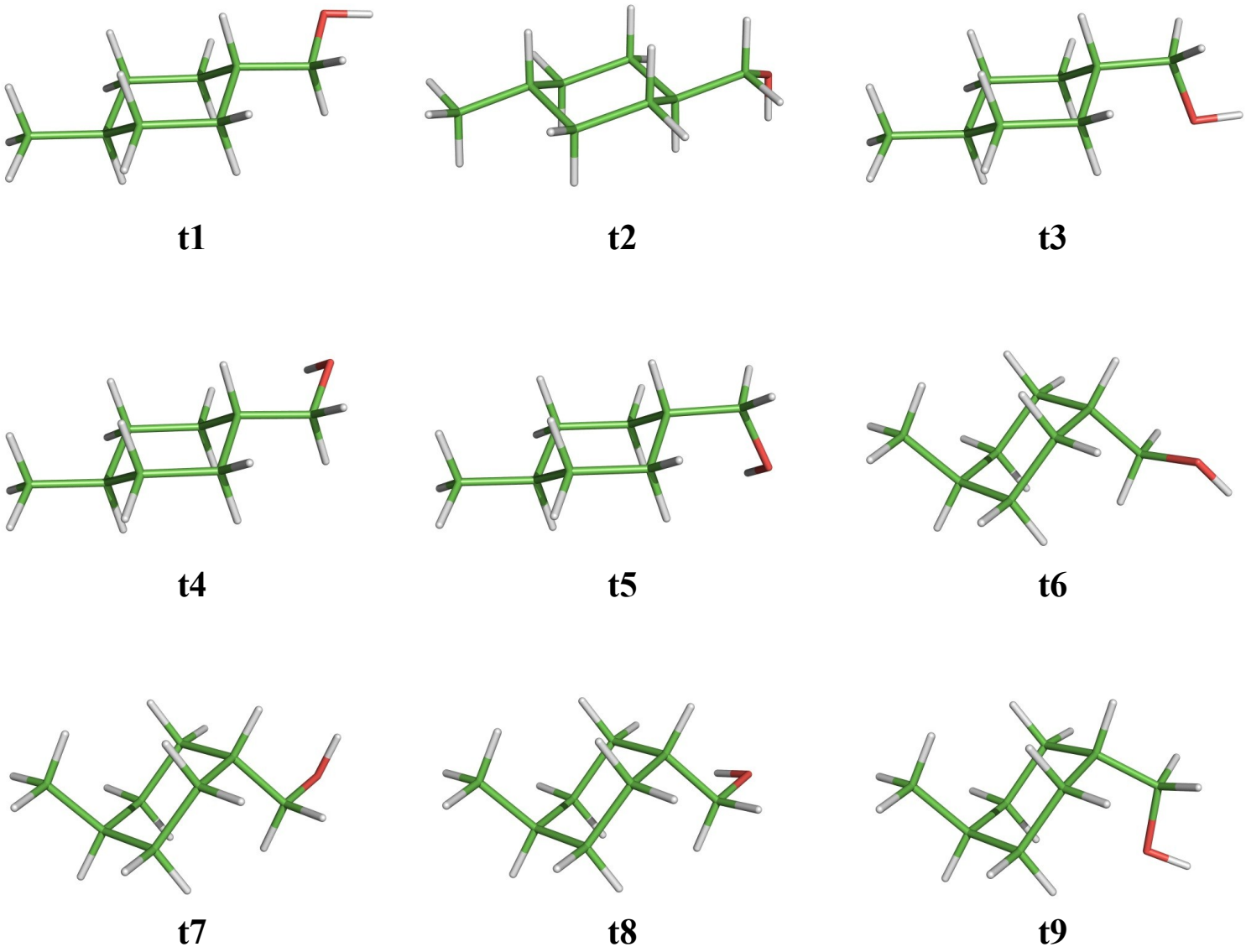

Figure S4. 3D structures of *cis*-4-MCHM conformers and their conformer ID #

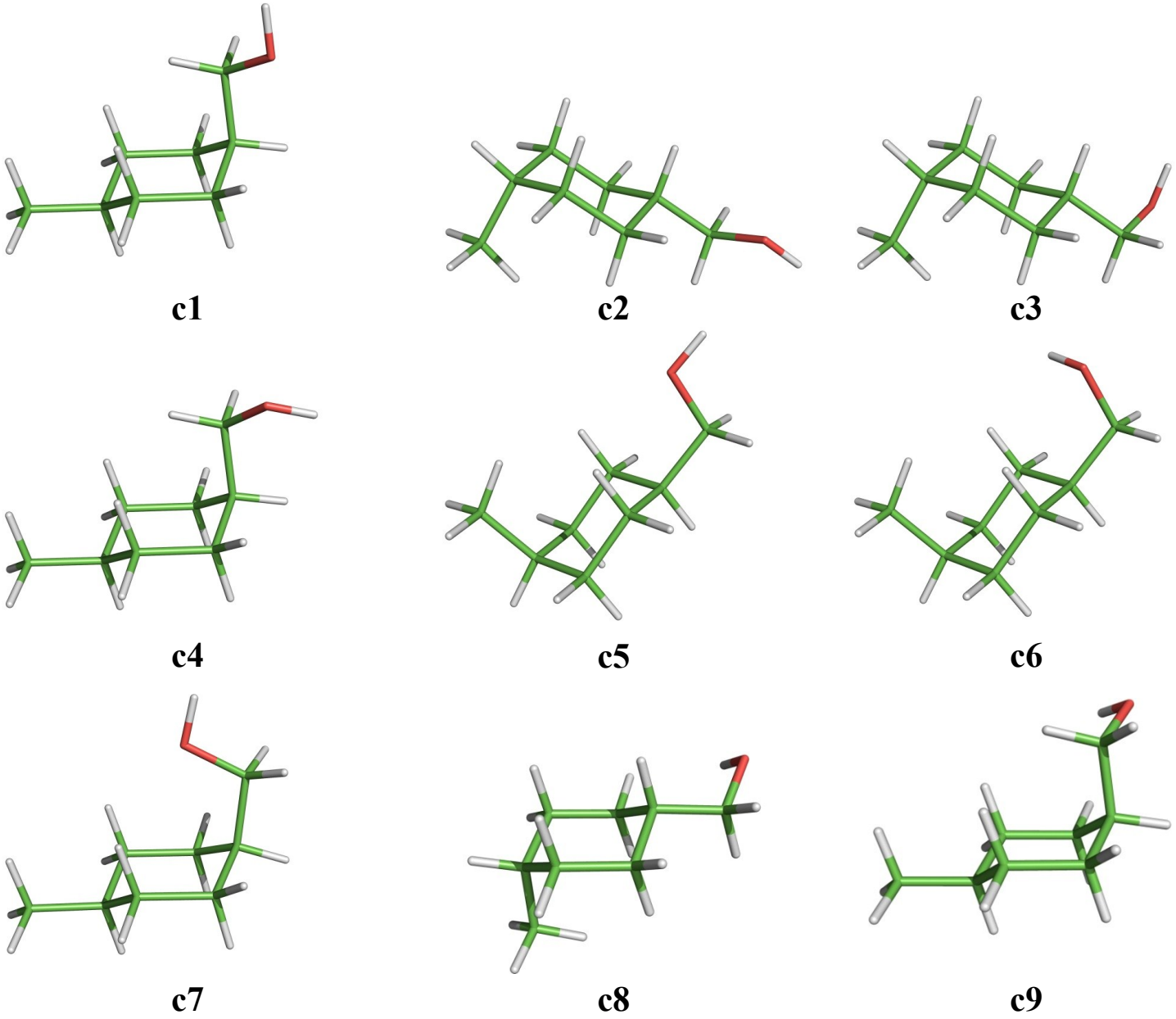

Table S1. Relative free energies (in kcal mol^{-1}) for composite methods.

	MP2 aug-cc-pVDZ (gas)	MP2 (all electron) aug-cc-pwCVDZ (gas)	CM1 (gas)	CM2 (gas)	E(CCSD) (gas)	MP2 aug-cc-pVDZ (soln)	MP2 (all electron) aug-cc-pwCVDZ (soln)	CM1 (soln)	CM2 (soln)	E(CCSD) (soln)
t1	0.00	0.00	0.00	0.00	0.00	0.12	0.10	0.72	0.10	0.07
t2	0.19	0.19	0.48	0.19	0.22	0.08	0.06	0.78	0.06	0.07
t3	0.30	0.31	0.43	0.30	0.36	0.78	0.79	1.45	0.79	0.77
t4	0.20	0.20	0.15	0.20	0.25	0.00	0.00	0.00	0.00	0.00
t5	0.54	0.55	0.44	0.55	0.61	0.46	0.42	1.05	0.42	0.46
t6	3.78	3.75	2.52	3.75	3.95	4.00	3.95	4.63	3.95	4.12
t7	3.84	3.81	3.92	3.81	4.07	3.86	3.82	4.03	3.82	4.05
t8	4.15	4.12	2.90	4.12	4.34	3.84	3.74	4.48	3.75	4.01
t9	5.50	5.49	5.79	5.49	5.69	6.56	6.54	7.37	6.54	6.65
c1	1.69	1.66	1.72	1.67	1.78	1.98	1.94	2.54	1.94	2.03
c2	1.90	1.88	1.86	1.88	1.99	1.97	1.95	2.77	1.95	2.03
c3	2.08	2.06	2.29	2.06	2.21	1.81	1.77	2.55	1.77	1.91
c4	1.77	1.74	1.92	1.74	1.93	1.69	1.62	2.58	1.62	1.81
c5	2.04	2.03	2.14	2.03	2.22	2.75	2.72	3.41	2.72	2.86
c6	2.34	2.33	2.14	2.33	2.51	2.03	1.99	2.98	1.99	2.14
c7	3.36	3.36	3.70	3.36	3.50	4.71	4.16	5.40	4.14	4.71
c8	2.09	2.07	0.86	2.07	2.23	1.98	1.94	2.41	1.94	2.09
c9	2.06	2.04	0.82	2.04	2.18	1.94	1.92	2.47	1.92	2.03

The remainder of this document contains Cartesian coordinates for all of the computed structures tabulated in the main text. The information is structured as follows:

EXAMPLE CARTESIAN COORDINATE AND ENERGY RECORD AND EXPLANATION	**AM1 gas phase**	**! Method (and basis set, gas or solution phase)**
	4mchm_1/coords	!Filenaming structure
	t1	!conformer naming scheme used in main text
	C 0.161966 1.402751 0.179936	!cartesian coordinates
	H 0.573477 2.333565 -0.290617	
	C 1.012485 0.207857 -0.222068	
	.	
	.	
	.	
	H -3.723227 -1.189821 0.278043	
	H -3.918857 0.609173 0.160313	
	el energy= -0.149093886904	!computed electronic energy
	zpe= 0.084459	!computed zero-point energy
	th energy= 0.094176	!computed thermal energy correction
	th enthalpy= 0.095121	!computed enthalpy correction
	free energy= 0.049553	!computed Gibbs Free energy correction
		(all energies in Hartree)

AM1 gas phase

4mchm_1/coords
t1
C 0.161966 1.402751 0.179936
H 0.573477 2.333565 -0.290617
C 1.012485 0.207857 -0.222068
H 1.026751 0.128332 -1.345313
C 0.430993 -1.078144 0.344275
H 1.052722 -1.942974 -0.006425
C -1.007430 -1.264308 -0.088938
H -1.422064 -2.195217 0.378082
C -1.863968 -0.072064 0.313018
H -1.861827 0.001215 1.437524
C -1.277935 1.214838 -0.249795
H -1.889273 2.086902 0.100353
C 2.446475 0.409448 0.257870
O 3.255091 -0.555281 -0.398272
C -3.289918 -0.257170 -0.156846
H 0.209015 1.536811 1.292593
H 0.485939 -1.052776 1.464347
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H 2.514430 0.274837 1.370699
H 4.152621 -0.428350 -0.070552
H -3.331119 -0.334652 -1.270151
H -3.723227 -1.189821 0.278043
H -3.918857 0.609173 0.160313
el energy= -0.149093886904
zpe= 0.084459
th energy= 0.094176
th enthalpy= 0.095121
free energy= 0.049553

4mchm_3/coords
t2
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H -0.206754 1.544578 1.289700
C -1.015468 0.229221 -0.231865
H -1.011038 0.153494 -1.356064
C -0.448739 -1.061818 0.337908

H -0.508657 -1.031696 1.457612
C 0.989018 -1.263540 -0.089879
H 1.391859 -2.198637 0.379183
C 1.856177 -0.080150 0.315806
H 1.851481 -0.008731 1.440462
C 1.285255 1.213970 -0.246160
H 1.903031 2.078998 0.110140
C -2.453136 0.439972 0.232137
O -3.322324 -0.580363 -0.220057
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H -3.227772 -0.634970 -1.178304
H 3.918260 0.580076 0.170336
H 3.703865 -1.217017 0.284295
H 3.325343 -0.355142 -1.263608
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zpe= 0.081869
th energy= 0.091459
th enthalpy= 0.092403
free energy= 0.047205

4mchm_5/coords
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H 0.814537 0.000012 1.758117
C 0.384455 1.250466 0.045380
H 0.813407 2.157735 0.544770
C -1.120896 1.248785 0.203232
H -1.387084 1.301747 1.291619
C -1.740679 -0.000003 -0.407063
H -1.518602 -0.000014 -1.511907
C -1.120896 -1.248786 0.203238
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C -3.241032 -0.000003 -0.213963
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H -3.499022 0.000054 0.872598
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H -3.692616 -0.906686 -0.683765
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zpe= 0.085672
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th enthalpy= 0.096302
free energy= 0.050958

4mchm_6/coords
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H 1.036109 -1.956525 0.000564
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C -1.272111 1.216505 -0.250565
H -1.326019 1.192787 -1.370740
C 2.452665 0.406795 0.271484
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C -3.288693 -0.250555 -0.164840
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H 3.084007 -1.348571 -0.242537
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el energy= -0.152294196755
zpe= 0.081636
th energy= 0.091177
th enthalpy= 0.092121
free energy= 0.047041

4mchm_7/coords
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C 0.408849 1.225647 -0.064859
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C 0.364458 -1.273771 -0.006524
H 0.609972 -1.309884 1.087730
C -1.139620 -1.249783 -0.179765
H -1.394318 -1.316524 -1.270038
C -1.741662 0.020748 0.402961
H -1.529707 0.037055 1.509622
C -1.096085 1.247665 -0.224590
H -1.509194 2.172328 0.256342
C 2.524579 -0.064493 -0.456490
O 2.944084 0.167766 0.873668
C -3.240124 0.042574 0.197127
H 0.855850 2.112029 -0.585932
H 0.782641 -2.201301 -0.477547
H -1.589567 -2.142700 0.327145
H -1.358846 1.288436 -1.314396
H 2.937395 -1.045929 -0.816842
H 2.992473 0.773598 -1.041405
H 2.502823 -0.481786 1.433605
H -3.711277 -0.846839 0.680591
H -3.679384 0.966005 0.645595
H -3.488939 0.026005 -0.891451
el energy= -0.151355198967
zpe= 0.082592
th energy= 0.092110
th enthalpy= 0.093055
free energy= 0.048143

4mchm_19/coords

t6
C 0.251633 -1.107177 0.630389
H -0.312398 -1.260271 1.588604
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H -0.719401 1.382068 1.513631
C -1.034415 1.203302 -0.616857
H -1.810241 2.012988 -0.599225
C -1.722163 -0.153450 -0.640527
H -2.239632 -0.255106 -1.638584
C -0.697497 -1.273165 -0.537036
H -0.108638 -1.309489 -1.492012
C 1.985636 0.402034 -0.406583
O 3.079287 -0.424305 -0.034805
C -2.781653 -0.264019 0.434528
H 1.049664 -1.894497 0.574805
H 0.410386 2.361921 0.497725
H -0.442735 1.323152 -1.563270
H -1.231426 -2.254807 -0.437633
H 1.586496 0.085495 -1.406965
H 2.329120 1.470047 -0.473762
H 3.724893 -0.360132 -0.747477
H -3.530799 0.557058 0.326335
H -3.313344 -1.242790 0.353299
H -2.326364 -0.194693 1.451777
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zpe= 0.089069
th energy= 0.098608
th enthalpy= 0.099552
free energy= 0.054439

4mchm_21/coords
t7
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C -0.921814 0.291410 0.673181
H -1.435858 0.407292 1.671310
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H 0.287112 -1.236821 1.603688
C 0.669516 -1.274101 -0.523236
H 0.076462 -1.304843 -1.475995

C 1.713393 -0.173323 -0.634430
H 2.231263 -0.293522 -1.630238
C 1.047922 1.194525 -0.625990
H 0.463151 1.316052 -1.576505
C -1.990992 0.434157 -0.407529
O -3.058545 -0.477847 -0.233384
C 2.768468 -0.290772 0.444227
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H -1.084067 -1.860416 0.592686
H 1.185530 -2.264640 -0.418424
H 1.836713 1.991739 -0.611316
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H -3.398738 -0.355756 0.660755
H 2.313027 -0.198951 1.459589
H 3.280845 -1.280836 0.376838
H 3.533928 0.513851 0.326791
el energy= -0.147628912163
zpe= 0.086521
th energy= 0.095921
th enthalpy= 0.096866
free energy= 0.052161

4mchm_22/coords
t8
C 0.098217 1.360654 0.583242
H -0.426637 2.350109 0.520491
C -0.930058 0.244167 0.664928
H -1.466604 0.332062 1.653611
C -0.244534 -1.112565 0.625507
H 0.323202 -1.251696 1.584166
C 0.707582 -1.269375 -0.541138
H 1.248321 -2.247528 -0.443249
C 1.724060 -0.141528 -0.636722
H 2.241012 -0.232889 -1.636068
C 1.027160 1.210297 -0.602274
H 1.797724 2.024667 -0.573913
C -1.984871 0.392102 -0.429387
O -3.175534 -0.306716 -0.120326
C 2.785524 -0.253187 0.436416
H 0.701826 1.361694 1.529693
H -1.019734 -1.922397 0.578395

H 0.121645 -1.306454 -1.497885
H 0.437346 1.335526 -1.549272
H -2.311371 1.464030 -0.517699
H -1.581996 0.046375 -1.418724
H -2.943424 -1.235663 -0.005477
H 3.532372 0.570140 0.328867
H 2.332379 -0.187343 1.454821
H 3.319729 -1.230297 0.351425
el energy= -0.147911829129
zpe= 0.086351
th energy= 0.095698
th enthalpy= 0.096642
free energy= 0.052058

4mchm_24/coords
t9
C -0.105580 1.255733 0.774659
H 0.623724 1.361065 1.622185
C -0.929821 0.000038 1.007467
H -1.238865 0.000075 2.095843
C -0.105589 -1.255676 0.774735
H 0.623718 -1.360961 1.622266
C 0.652246 -1.245144 -0.534935
H 1.302575 -2.156762 -0.591625
C 1.507379 -0.000025 -0.712649
H 1.892138 -0.000058 -1.773793
C 0.652260 1.245114 -0.535010
H -0.085659 1.292388 -1.381130
C -2.246864 0.000021 0.235909
O -2.008772 -0.000037 -1.161730
C 2.708479 -0.000005 0.206986
H -0.781558 2.150767 0.799527
H -0.781572 -2.150706 0.799663
H -0.085680 -1.292457 -1.381049
H 1.302602 2.156722 -0.591751
H -2.841071 -0.914311 0.512905
H -2.841048 0.914393 0.512821
H -2.876187 -0.000189 -1.583447
H 2.392411 0.000040 1.277926
H 3.334782 -0.906632 0.025302
H 3.334808 0.906590 0.025233
el energy= -0.141141014135

zpe= 0.092796
th energy= 0.102275
th enthalpy= 0.103219
free energy= 0.058503

4mchm_9/coords
c1
C -0.452224 -0.936694 0.995444
H -1.195360 -1.769709 0.880838
C -1.124669 0.371253 0.608014
H -1.894971 0.608495 1.397285
C -0.121012 1.512241 0.560480
H -0.617898 2.436289 0.164350
C 1.090759 1.188565 -0.287119
H 0.781952 1.070455 -1.359046
C 1.769174 -0.087948 0.186961
H 2.114851 0.068200 1.248094
C 0.779934 -1.243466 0.171246
H 1.276900 -2.163324 0.577069
C -1.869216 0.249976 -0.719424
O -3.011352 -0.562713 -0.490739
C 2.973416 -0.403513 -0.672373
H -0.164166 -0.881602 2.078709
H 0.212651 1.733987 1.609146
H 1.819466 2.039208 -0.238179
H 0.484786 -1.464852 -0.888130
H -2.196920 1.264450 -1.075216
H -1.215597 -0.216327 -1.504013
H -3.445042 -0.671101 -1.344544
H 2.669224 -0.560464 -1.735356
H 3.707410 0.437104 -0.635776
H 3.476557 -1.331591 -0.308696
el energy= -0.147071077173
zpe= 0.086643
th energy= 0.096259
th enthalpy= 0.097204
free energy= 0.051867

4mchm_11/coords
c2
C -0.310792 -1.103946 0.094451
H -1.017144 -1.926786 -0.191957

C -0.937174 0.231981 -0.271487
H -1.152155 0.235527 -1.376891
C 0.015494 1.371115 0.053827
H -0.439055 2.345478 -0.265146
C 1.345526 1.186240 -0.645948
H 1.190028 1.270903 -1.754376
C 1.992500 -0.158673 -0.347470
H 2.858820 -0.283765 -1.060287
C 1.016144 -1.297035 -0.607549
H 0.838661 -1.372568 -1.713234
C -2.255794 0.432219 0.469062
O -3.202786 -0.460508 -0.097817
C 2.549807 -0.210386 1.058768
H -0.162416 -1.157149 1.205101
H 0.174159 1.420303 1.163234
H 2.042316 2.009460 -0.338672
H 1.475437 -2.263638 -0.272672
H -2.131984 0.216386 1.564134
H -2.613386 1.490345 0.345174
H -4.023141 -0.336796 0.392874
H 3.055344 -1.189828 1.238586
H 3.295624 0.606983 1.210035
H 1.736915 -0.089885 1.814716
el energy= -0.146833625346
zpe= 0.086894
th energy= 0.096513
th enthalpy= 0.097457
free energy= 0.052108

4mchm_13/coords
c3
C -0.026164 1.381077 0.062516
H -0.182208 1.416328 1.172862
C 0.940567 0.258091 -0.275228
H 1.139300 0.275616 -1.384167
C 0.331036 -1.087675 0.082961
H 1.047381 -1.901729 -0.204073
C -0.993903 -1.293610 -0.618735
H -0.818190 -1.359431 -1.725295
C -1.984416 -0.169749 -0.348697
H -2.849443 -0.300150 -1.062114
C -1.355635 1.186358 -0.635599

H -2.062094 1.997306 -0.317878
C 2.263323 0.465536 0.455403
O 3.238690 -0.491837 0.090434
C -2.539907 -0.240921 1.057443
H 0.416099 2.364144 -0.246795
H 0.185597 -1.146588 1.193723
H -1.439912 -2.268412 -0.289568
H -1.205054 1.284580 -1.743559
H 2.652733 1.499885 0.251603
H 2.136581 0.328256 1.562861
H 3.317272 -0.470395 -0.870561
H -3.032164 -1.228543 1.229209
H -1.728252 -0.115850 1.813993
H -3.296575 0.565037 1.215894
el energy= -0.149698655739
zpe= 0.084298
th energy= 0.093789
th enthalpy= 0.094733
free energy= 0.049755

4mchm_15/coords
c4
C -0.477220 -0.901893 1.006173
H -0.195416 -0.833419 2.090102
C -1.131389 0.406424 0.589956
H -1.895877 0.671977 1.376682
C -0.115647 1.535542 0.527351
H -0.601288 2.453920 0.104439
C 1.100981 1.183272 -0.301618
H 0.803146 1.052284 -1.375179
C 1.759050 -0.093389 0.199640
H 2.097465 0.075621 1.261097
C 0.754895 -1.235879 0.192759
H 1.236675 -2.157298 0.612859
C -1.874738 0.265935 -0.736497
O -2.934536 -0.668556 -0.663875
C 2.966400 -0.438318 -0.643897
H -1.228077 -1.729333 0.896828
H 0.211019 1.779247 1.573301
H 1.838898 2.026278 -0.257477
H 0.459929 -1.465816 -0.864994
H -2.274175 1.266494 -1.056753

H -1.199643 -0.138127 -1.537876
H -3.504616 -0.401404 0.066712
H 2.668789 -0.611218 -1.706289
H 3.709738 0.394394 -0.616429
H 3.455731 -1.365315 -0.259219
el energy= -0.149887640587
zpe= 0.084118
th energy= 0.093594
th enthalpy= 0.094538
free energy= 0.049617

4mchm_16/coords
c5
C -0.240964 1.248720 -0.208614
H -0.742057 2.157277 -0.633771
C -0.946354 0.000078 -0.712420
H -0.924122 0.000158 -1.838814
C -0.240989 -1.248664 -0.208800
H -0.343571 -1.298392 0.907631
C 1.221803 -1.251701 -0.598067
H 1.719490 -2.155292 -0.158379
C 1.958002 -0.000003 -0.142532
H 2.970409 0.000024 -0.641416
C 1.221835 1.251786 -0.597868
H 1.305106 1.330414 -1.714500
C -2.413759 0.000069 -0.295776
O -2.484892 -0.000153 1.122168
C 2.187396 -0.000120 1.353532
H -0.343553 1.298280 0.907822
H -0.742114 -2.157139 -0.634088
H 1.305057 -1.330148 -1.714713
H 1.719539 2.155291 -0.158023
H -2.925907 0.915106 -0.699927
H -2.925983 -0.914793 -0.700218
H -3.422274 -0.000101 1.347406
H 2.765366 -0.906630 1.655710
H 2.765361 0.906347 1.655851
H 1.216560 -0.000167 1.905362
el energy= -0.145649421406
zpe= 0.088109
th energy= 0.097685
th enthalpy= 0.098629

free energy= 0.053553

4mchm_17/coords
c6
C -0.273291 1.207553 -0.294172
H -0.799242 2.067490 -0.785482
C -0.953573 -0.091528 -0.693138
H -0.922003 -0.183676 -1.815788
C -0.215553 -1.280555 -0.098835
H -0.285714 -1.248615 1.020612
C 1.241558 -1.282922 -0.510019
H 1.765182 -2.141609 -0.013998
C 1.955069 0.014413 -0.158005
H 2.960694 -0.001928 -0.670548
C 1.186667 1.214249 -0.692817
H 1.666661 2.157181 -0.321049
C -2.422767 -0.086426 -0.282461
O -2.633398 0.223663 1.080862
C 2.204991 0.129886 1.330267
H -0.372106 1.347032 0.815088
H -0.701713 -2.231848 -0.439818
H 1.309105 -1.441019 -1.619150
H 1.260888 1.216622 -1.812882
H -2.976629 0.720406 -0.835360
H -2.884264 -1.083825 -0.518468
H -2.108309 -0.394813 1.602315
H 2.782046 1.059566 1.553884
H 1.242422 0.169739 1.894803
H 2.791562 -0.748037 1.694030
el energy= -0.149094292830
zpe= 0.085017
th energy= 0.094445
th enthalpy= 0.095389
free energy= 0.050663

4mchm_23/coords
c7
C 0.452168 -1.257487 -0.932031
H 1.085268 -2.150827 -0.688875
C 1.300838 0.000168 -0.830569
H 2.004229 0.000333 -1.716684
C 0.452161 1.257848 -0.931569

H 1.085253 2.151117 -0.688130
C -0.757003 1.241799 -0.021676
H -0.418135 1.262364 1.048715
C -1.604880 0.000058 -0.252840
H -1.959520 0.000271 -1.322106
C -0.757028 -1.241789 -0.022172
H -0.418201 -1.262813 1.048223
C 2.220361 -0.000048 0.387767
O 1.463201 -0.000403 1.586329
C -2.812507 -0.000117 0.657616
H 0.109189 -1.365664 -1.995870
H 0.109150 1.366401 -1.995360
H -1.374302 2.159012 -0.206079
H -1.374340 -2.158912 -0.206982
H 2.875453 -0.914325 0.360247
H 2.875329 0.914326 0.360665
H 2.101835 -0.000169 2.309109
H -3.437389 0.906707 0.473515
H -3.437471 -0.906792 0.473057
H -2.496616 -0.000404 1.728771
el energy= -0.143357982072
zpe= 0.090457
th energy= 0.100008
th enthalpy= 0.100952
free energy= 0.056016

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.307853 -1.105304 0.101239
H 1.000251 -1.941656 -0.180583
C 0.944488 0.227271 -0.261403
H 1.164148 0.231603 -1.366063
C -0.010412 1.367191 0.054800
H -0.174478 1.418390 1.163428
C -1.337207 1.187428 -0.651656
H -1.176116 1.270089 -1.759458
C -1.990517 -0.154306 -0.353887
H -2.853551 -0.278848 -1.070790
C -1.016004 -1.295136 -0.608110
H -1.479453 -2.260555 -0.275245
C 2.259746 0.429512 0.485734
O 3.311147 -0.344677 -0.057633

C -2.554652 -0.202577 1.049721
H 0.152568 -1.156233 1.211282
H 0.449859 2.339411 -0.262998
H -2.032262 2.013804 -0.348858
H -0.832302 -1.371252 -1.712810
H 2.614136 1.490529 0.377494
H 2.130747 0.191793 1.575891
H 3.035982 -1.268429 -0.022854
H -3.299798 0.616502 1.195252
H -3.063014 -1.180692 1.228991
H -1.745665 -0.081513 1.809765
el energy= -0.150049948727
zpe= 0.084055
th energy= 0.093495
th enthalpy= 0.094439
free energy= 0.049587

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.446100 -0.959173 0.978748
H 1.171004 -1.808127 0.868143
C 1.131536 0.345786 0.602886
H 1.911329 0.565050 1.388333
C 0.132681 1.492377 0.595290
H -0.195888 1.687147 1.650781
C -1.082915 1.197289 -0.257299
H -0.776220 1.101676 -1.332133
C -1.770140 -0.084624 0.188614
H -2.116985 0.051028 1.252210
C -0.788390 -1.246077 0.150349
H -1.290228 -2.169721 0.541440
C 1.861305 0.249957 -0.735250
O 3.084641 -0.452197 -0.626215
C -2.974305 -0.375413 -0.679530
H 0.155452 -0.908216 2.061952
H 0.633576 2.424005 0.222529
H -1.805358 2.051741 -0.187177
H -0.496542 -1.450574 -0.913322
H 1.207991 -0.233447 -1.509879
H 2.163166 1.272241 -1.092034
H 2.882204 -1.335395 -0.296142
H -3.703092 0.468871 -0.626570

H -2.668858 -0.511715 -1.745014
H -3.483910 -1.307716 -0.336245
el energy= -0.150165671204
zpe= 0.083948
th energy= 0.093373
th enthalpy= 0.094317
free energy= 0.049505

AM1-SMD

4mchm_1/coords
t1
C 0.161703 1.401322 0.172070
H 0.569111 2.332115 -0.302031
C 1.013239 0.208165 -0.235166
H 1.025048 0.136075 -1.358335
C 0.430330 -1.079383 0.326884
H 1.041455 -1.949060 -0.029062
C -1.010391 -1.264406 -0.097770
H -1.419949 -2.198936 0.366501
C -1.863728 -0.074943 0.317320
H -1.852939 -0.008212 1.442039
C -1.281729 1.214268 -0.243956
H -1.888845 2.084899 0.116950
C 2.443554 0.416697 0.253273
O 3.274925 -0.540496 -0.394667
C -3.292179 -0.257809 -0.142683
H 0.220886 1.537352 1.283907
H 0.494314 -1.061089 1.446679
H -1.063546 -1.392304 -1.210656
H -1.352471 1.198106 -1.363214
H 2.802912 1.446224 -0.017639
H 2.505114 0.292036 1.366406
H 4.105779 -0.561814 0.098992
H -3.348137 -0.306194 -1.257006
H -3.717951 -1.203601 0.271079
H -3.924973 0.594904 0.202897
el energy= -0.152537901925
zpe= 0.080522
th energy= 0.090412
th enthalpy= 0.091357
free energy= 0.045305

4mchm_3/coords
t2
C -0.156352 1.413212 0.170901
H -0.216010 1.549033 1.282735
C -1.015788 0.227880 -0.240076
H -1.014689 0.150487 -1.364308
C -0.450580 -1.063022 0.330664
H -0.519477 -1.039397 1.449838
C 0.989966 -1.264174 -0.087585
H 1.389334 -2.198996 0.384851
C 1.855461 -0.080655 0.320046
H 1.849875 -0.010260 1.444507
C 1.285856 1.213525 -0.242741
H 1.900627 2.078637 0.118386
C -2.450226 0.450781 0.222836
O -3.330850 -0.576545 -0.204713
C 3.280337 -0.278030 -0.145735
H -0.555635 2.347610 -0.302943
H -1.071399 -1.925817 -0.026764
H 1.044431 -1.400942 -1.199427
H 1.357639 1.196195 -1.361952
H -2.521186 0.441170 1.343774
H -2.825873 1.437304 -0.162377
H -3.155486 -0.743531 -1.141006
H 3.922912 0.568774 0.196379
H 3.698740 -1.227685 0.266494
H 3.330946 -0.327324 -1.260347
el energy= -0.155146326212
zpe= 0.078095
th energy= 0.087918
th enthalpy= 0.088862
free energy= 0.042979

4mchm_5/coords
t3
C -0.386307 1.245029 0.038442
H -0.825157 2.147546 0.537785
C -1.005096 -0.012356 0.628617
H -0.792537 -0.024521 1.735679
C -0.383945 -1.252975 0.007955
H -0.814403 -2.168361 0.491424

C 1.120808 -1.254977 0.171476
H 1.379914 -1.335706 1.259868
C 1.748145 0.006182 -0.404401
H 1.549347 0.024334 -1.513248
C 1.117367 1.245734 0.213717
H 1.548276 2.162270 -0.267055
C -2.520677 -0.017238 0.474454
O -2.960671 -0.052807 -0.873638
C 3.243611 0.004612 -0.181136
H -0.630889 1.313472 -1.054556
H -0.648330 -1.291552 -1.081415
H 1.550878 -2.153555 -0.342628
H 1.370953 1.288888 1.305228
H -2.955058 -0.946549 0.934141
H -2.954572 0.886346 0.982003
H -2.593905 0.722229 -1.320253
H 3.482830 -0.008896 0.909724
H 3.708379 -0.894414 -0.653003
H 3.706199 0.916861 -0.629333
el energy= -0.154262162667
zpe= 0.079373
th energy= 0.089005
th enthalpy= 0.089949
free energy= 0.044478

4mchm_6/coords
t4
C 0.172988 1.392823 0.190293
H 0.213382 1.532005 1.302426
C 1.020277 0.191397 -0.198376
H 1.040847 0.111843 -1.321507
C 0.419754 -1.087429 0.365511
H 1.028410 -1.967309 0.029087
C -1.015992 -1.263615 -0.080097
H -1.051887 -1.404747 -1.192074
C -1.867633 -0.063003 0.306048
H -1.881012 0.013619 1.430079
C -1.263667 1.217131 -0.252625
H -1.312247 1.193506 -1.372985
C 2.449983 0.384240 0.296422
O 3.375495 -0.408362 -0.430528
C -3.287237 -0.237204 -0.184014

H 0.597076 2.318713 -0.279034
H 0.464775 -1.057934 1.486128
H -1.441452 -2.188897 0.388492
H -1.869820 2.095846 0.089622
H 2.790625 1.441341 0.122920
H 2.527158 0.147836 1.390944
H 3.088999 -1.329178 -0.357494
H -3.915330 0.633670 0.122987
H -3.316767 -0.314175 -1.297783
H -3.737557 -1.165279 0.243443
el energy= -0.155183164615
zpe= 0.078393
th energy= 0.088055
th enthalpy= 0.088999
free energy= 0.043597

4mchm_7/coords
t5
C 0.383759 1.253184 -0.007309
H 0.647683 1.291470 1.082168
C 1.005052 0.012808 -0.628272
H 0.792251 0.025274 -1.735350
C 0.386372 -1.244798 -0.038324
H 0.630578 -1.313203 1.054754
C -1.117276 -1.245644 -0.214139
H -1.370366 -1.288204 -1.305778
C -1.748219 -0.006331 0.404336
H -1.549387 -0.024810 1.513155
C -1.120999 1.255006 -0.171335
H -1.551354 2.153548 0.342562
C 2.520674 0.017655 -0.474609
O 2.961185 0.051927 0.873313
C -3.243644 -0.004981 0.181064
H 0.814244 2.168782 -0.490319
H 0.825514 -2.147223 -0.537569
H -1.548321 -2.162387 0.266030
H -1.379688 1.335646 -1.259826
H 2.954566 -0.885477 -0.983118
H 2.954960 0.947304 -0.933608
H 2.592944 -0.722766 1.319545
H -3.706273 -0.916551 0.630565
H -3.708358 0.894753 0.651639

H -3.482794 0.007031 -0.909825
el energy= -0.154262566737
zpe= 0.079370
th energy= 0.089004
th enthalpy= 0.089948
free energy= 0.044456

4mchm_19/coords
t6
C 0.247351 -1.091074 0.668726
H -0.338855 -1.218687 1.617653
C 0.919368 0.272315 0.696605
H 1.438338 0.381799 1.691390
C -0.116486 1.379393 0.575095
H -0.733335 1.394342 1.512674
C -1.025382 1.198137 -0.621346
H -1.806911 2.002405 -0.615435
C -1.703387 -0.163208 -0.651157
H -2.195975 -0.275992 -1.660422
C -0.676224 -1.277029 -0.515606
H -0.067953 -1.322656 -1.457864
C 1.979178 0.418476 -0.391359
O 3.061340 -0.451162 -0.073761
C -2.786982 -0.272791 0.398733
H 1.033628 -1.890542 0.652906
H 0.400735 2.371842 0.499939
H -0.424045 1.322249 -1.561242
H -1.206360 -2.260620 -0.415397
H 1.563727 0.149814 -1.398688
H 2.357614 1.475805 -0.426429
H 3.678900 -0.399215 -0.816071
H -3.542900 0.538497 0.265062
H -3.309715 -1.256503 0.315828
H -2.362228 -0.188559 1.428028
el energy= -0.148436237041
zpe= 0.085635
th energy= 0.094958
th enthalpy= 0.095903
free energy= 0.051632

4mchm_21/coords
t7

C 0.108122 1.378053 0.564141
H -0.409888 2.369595 0.480998
C -0.927695 0.270476 0.666964
H -1.457536 0.376518 1.657887
C -0.260206 -1.095038 0.639344
H 0.302302 -1.237963 1.600124
C 0.688669 -1.273863 -0.525844
H 0.100558 -1.312674 -1.481211
C 1.719055 -0.159987 -0.633215
H 2.235365 -0.269129 -1.630905
C 1.038473 1.200209 -0.615827
H 0.453449 1.322719 -1.566171
C -1.983255 0.412318 -0.425499
O -3.083426 -0.460378 -0.217560
C 2.777234 -0.272231 0.441931
H 0.708966 1.394513 1.512114
H -1.051499 -1.889179 0.594793
H 1.215943 -2.258495 -0.420927
H 1.818013 2.006117 -0.595709
H -2.352555 1.472380 -0.467630
H -1.575814 0.121063 -1.430637
H -3.448271 -0.264915 0.656493
H 2.327353 -0.196121 1.461228
H 3.305419 -1.253578 0.365866
H 3.533220 0.542548 0.332204
el energy= -0.151103078696
zpe= 0.083204
th energy= 0.092442
th enthalpy= 0.093386
free energy= 0.049335

4mchm_22/coords
t8
C 0.068673 1.332198 0.596586
H -0.476368 2.311379 0.548216
C -0.934561 0.191855 0.639077
H -1.483357 0.248216 1.623521
C -0.224620 -1.152088 0.578669
H 0.320435 -1.311022 1.546888
C 0.756766 -1.260330 -0.568839
H 1.318712 -2.227123 -0.478655
C 1.746999 -0.106862 -0.624724

H 2.282500 -0.165730 -1.616507
C 1.016761 1.226679 -0.577435
H 1.765075 2.060092 -0.525211
C -1.975281 0.327053 -0.469400
O -3.227700 -0.226924 -0.093007
C 2.792013 -0.214452 0.463629
H 0.657594 1.326666 1.552301
H -0.988612 -1.969353 0.487007
H 0.193588 -1.295779 -1.539302
H 0.435262 1.353775 -1.529327
H -2.198847 1.407041 -0.685240
H -1.625885 -0.168873 -1.414172
H -3.059100 -1.087968 0.314097
H 3.521439 0.628010 0.389381
H 2.324496 -0.183236 1.477278
H 3.354169 -1.175022 0.368408
el energy= -0.151122226951
zpe= 0.082974
th energy= 0.092390
th enthalpy= 0.093334
free energy= 0.048735

4mchm_24/coords
t9
C -0.065473 1.367599 0.552120
H 0.647428 1.594341 1.390635
C -0.911836 0.174213 0.963643
H -1.174187 0.328695 2.055101
C -0.139964 -1.131406 0.879282
H 0.556175 -1.184600 1.759492
C 0.665755 -1.304327 -0.389425
H 1.296496 -2.227523 -0.300688
C 1.556193 -0.111808 -0.700858
H 1.978680 -0.261112 -1.736715
C 0.730465 1.164727 -0.717746
H 0.027754 1.125489 -1.592220
C -2.270159 0.127162 0.270543
O -2.154686 -0.290336 -1.083677
C 2.723539 -0.013430 0.255647
H -0.726973 2.265963 0.430440
H -0.859030 -1.987696 0.973901
H -0.034808 -1.461063 -1.252669

H 1.406552 2.045850 -0.873496
H -2.934556 -0.605449 0.807707
H -2.749722 1.142626 0.312006
H -3.016270 -0.124056 -1.490752
H 2.373364 0.125844 1.306819
H 3.340077 -0.943857 0.213650
H 3.375394 0.852848 -0.013042
el energy= -0.143997506445
zpe= 0.089512
th energy= 0.099125
th enthalpy= 0.100070
free energy= 0.054942

4mchm_9/coords
c1
C -0.451815 -0.912528 1.024902
H -1.189935 -1.753022 0.945280
C -1.126734 0.386502 0.613088
H -1.893380 0.640880 1.399863
C -0.118597 1.524017 0.548747
H -0.614012 2.443779 0.140920
C 1.088884 1.185393 -0.298564
H 0.776433 1.060955 -1.368835
C 1.765122 -0.088722 0.184682
H 2.124549 0.078594 1.239366
C 0.770608 -1.239765 0.194889
H 1.265095 -2.156489 0.610527
C -1.865214 0.256164 -0.715812
O -2.984897 -0.599521 -0.511263
C 2.956367 -0.422825 -0.684052
H -0.152604 -0.832436 2.103772
H 0.216952 1.759773 1.593430
H 1.820606 2.033978 -0.260403
H 0.465338 -1.476325 -0.858291
H -2.227442 1.261989 -1.060891
H -1.200210 -0.180212 -1.507633
H -3.424192 -0.685283 -1.368047
H 2.642661 -0.591167 -1.742531
H 3.698377 0.411429 -0.667344
H 3.459216 -1.349693 -0.316358
el energy= -0.150798236312
zpe= 0.083067

th energy= 0.092494
th enthalpy= 0.093438
free energy= 0.048868

4mchm_11/coords
c2
C -0.316959 -1.095920 0.073761
H -1.016123 -1.921787 -0.219630
C -0.938724 0.243427 -0.288020
H -1.139364 0.258718 -1.395356
C 0.016392 1.375595 0.056735
H -0.430026 2.354081 -0.260938
C 1.355638 1.191937 -0.624410
H 1.219921 1.298494 -1.733426
C 1.993563 -0.160122 -0.340838
H 2.861779 -0.280347 -1.052048
C 1.013437 -1.290010 -0.620480
H 0.845016 -1.354883 -1.728124
C -2.258514 0.450258 0.447961
O -3.208527 -0.466863 -0.084643
C 2.545296 -0.235646 1.065661
H -0.177544 -1.155939 1.185332
H 0.156684 1.417016 1.169037
H 2.051883 2.006450 -0.293094
H 1.463195 -2.263563 -0.292518
H -2.129760 0.277803 1.548937
H -2.637098 1.495503 0.285676
H -3.938133 -0.505362 0.548111
H 3.020779 -1.230705 1.243427
H 3.317478 0.555469 1.224824
H 1.738760 -0.093157 1.824719
el energy= -0.150360750776
zpe= 0.082971
th energy= 0.092705
th enthalpy= 0.093649
free energy= 0.048031

4mchm_13/coords
c3
C -0.019271 1.378710 0.058272
H -0.167317 1.419574 1.169624
C 0.943722 0.252117 -0.280335

H 1.149601 0.267030 -1.387834
C 0.328956 -1.090664 0.078587
H 1.034838 -1.910697 -0.216386
C -0.999417 -1.292275 -0.617592
H -0.827563 -1.361655 -1.724469
C -1.985989 -0.165612 -0.347040
H -2.849443 -0.292087 -1.062981
C -1.353057 1.188620 -0.631195
H -2.054928 2.001125 -0.307014
C 2.261425 0.467592 0.454386
O 3.242699 -0.493508 0.099055
C -2.545851 -0.238636 1.056328
H 0.424759 2.359341 -0.256253
H 0.188511 -1.153229 1.189806
H -1.446387 -2.265937 -0.286104
H -1.210316 1.292411 -1.739573
H 2.654537 1.497474 0.237962
H 2.131128 0.345802 1.563241
H 3.332866 -0.474945 -0.863552
H -3.031189 -1.229636 1.229827
H -1.742129 -0.104813 1.819932
H -3.311673 0.559193 1.212867
el energy= -0.152876005776
zpe= 0.080569
th energy= 0.090297
th enthalpy= 0.091241
free energy= 0.045402

4mchm_15/coords
c4
C -0.484564 -0.871061 1.031394
H -0.192355 -0.775336 2.110680
C -1.135966 0.428799 0.587219
H -1.907235 0.708852 1.362356
C -0.113493 1.551256 0.509074
H -0.592839 2.464799 0.068957
C 1.104101 1.180151 -0.309710
H 0.811018 1.046554 -1.384348
C 1.752027 -0.097914 0.201226
H 2.100526 0.078573 1.258044
C 0.737628 -1.231471 0.215216
H 1.211889 -2.152611 0.644035

C -1.870708 0.275979 -0.740769
O -2.894695 -0.704837 -0.681536
C 2.948595 -0.464490 -0.647104
H -1.237945 -1.699456 0.962390
H 0.208512 1.812017 1.552115
H 1.848675 2.017489 -0.268809
H 0.435451 -1.472307 -0.837927
H -2.321203 1.260283 -1.041938
H -1.182408 -0.079598 -1.553750
H -3.431676 -0.518851 0.100969
H 2.646178 -0.640280 -1.707672
H 3.705194 0.356566 -0.630424
H 3.430048 -1.395488 -0.261669
el energy= -0.153308274856
zpe= 0.080639
th energy= 0.090053
th enthalpy= 0.090997
free energy= 0.046352

4mchm_16/coords
c5
C -0.236958 1.247752 -0.187888
H -0.744149 2.158086 -0.601547
C -0.943925 0.000041 -0.691228
H -0.908586 0.000093 -1.818520
C -0.236977 -1.247719 -0.187998
H -0.321036 -1.298082 0.929392
C 1.221160 -1.252925 -0.593999
H 1.723774 -2.155505 -0.158087
C 1.965139 0.000000 -0.154928
H 2.966257 0.000014 -0.676217
C 1.221177 1.252973 -0.593890
H 1.289425 1.338507 -1.710922
C -2.418553 0.000044 -0.309018
O -2.542668 -0.000093 1.108600
C 2.231072 -0.000068 1.334161
H -0.321017 1.298014 0.929508
H -0.744181 -2.158009 -0.601739
H 1.289411 -1.338363 -1.711038
H 1.723804 2.155509 -0.157902
H -2.922848 0.914590 -0.722903
H -2.922891 -0.914401 -0.723080

H -3.490856 -0.000040 1.297544
H 2.817020 -0.905444 1.625135
H 2.816947 0.905324 1.625231
H 1.277464 -0.000138 1.915087
el energy= -0.148803085239
zpe= 0.084342
th energy= 0.094247
th enthalpy= 0.095191
free energy= 0.048659

4mchm_17/coords
c6
C -0.245587 1.253748 -0.159354
H -0.752843 2.173833 -0.550989
C -0.952471 0.018945 -0.693379
H -0.919665 0.048330 -1.819898
C -0.240338 -1.240685 -0.226787
H -0.308827 -1.326278 0.890188
C 1.216107 -1.231114 -0.639518
H 1.721115 -2.146852 -0.234692
C 1.957281 0.008009 -0.158233
H 2.961540 0.025558 -0.672790
C 1.212911 1.272018 -0.563184
H 1.714129 2.162680 -0.101787
C -2.424083 0.008449 -0.298073
O -2.640184 0.041375 1.103607
C 2.212521 -0.036353 1.332103
H -0.332484 1.273377 0.959118
H -0.748561 -2.140194 -0.662254
H 1.282336 -1.278815 -1.758698
H 1.282707 1.388666 -1.677330
H -2.937314 0.932421 -0.680496
H -2.925492 -0.900429 -0.727982
H -2.180369 -0.717764 1.487215
H 2.788924 0.864218 1.655153
H 1.254685 -0.062177 1.905635
H 2.803549 -0.945677 1.599294
el energy= -0.152079772531
zpe= 0.081654
th energy= 0.091270
th enthalpy= 0.092214
free energy= 0.046465

4mchm_23/coords
c7
C 0.451327 -0.759982 -1.305976
H 1.118289 -1.657840 -1.395040
C 1.257043 0.400356 -0.745126
H 1.891837 0.798360 -1.595031
C 0.375042 1.553837 -0.294459
H 0.988078 2.278149 0.304322
C -0.832826 1.137685 0.514308
H -0.505043 0.737142 1.509411
C -1.646128 0.077811 -0.211708
H -1.992372 0.504149 -1.195332
C -0.769321 -1.131506 -0.492806
H -0.454176 -1.589813 0.481505
C 2.280933 -0.024988 0.303070
O 1.675318 -0.795257 1.332973
C -2.859640 -0.315178 0.599263
H 0.120615 -0.487766 -2.344399
H 0.020772 2.099198 -1.210750
H -1.475401 2.034927 0.712425
H -1.360938 -1.905495 -1.048296
H 3.080229 -0.644658 -0.189467
H 2.762806 0.883732 0.756718
H 2.392175 -1.065939 1.923286
H -3.520147 0.569701 0.765756
H -3.448837 -1.099884 0.066134
H -2.559004 -0.720123 1.595573
el energy= -0.146643259582
zpe= 0.087041
th energy= 0.096588
th enthalpy= 0.097532
free energy= 0.052570

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.285841 -1.123648 0.135847
H 0.972920 -1.971415 -0.124909
C 0.947805 0.194706 -0.233852
H 1.182580 0.180815 -1.335376
C 0.008111 1.354793 0.050467
H -0.169807 1.427453 1.155553

C -1.309425 1.184499 -0.674590
H -1.129994 1.248365 -1.780747
C -1.990752 -0.140989 -0.368411
H -2.841058 -0.261779 -1.100786
C -1.032724 -1.303424 -0.584381
H -1.516440 -2.253213 -0.235248
C 2.253063 0.376565 0.534691
O 3.338606 -0.280593 -0.100821
C -2.584152 -0.155821 1.022941
H 0.117635 -1.158006 1.244784
H 0.487834 2.315093 -0.274703
H -1.995088 2.027793 -0.398353
H -0.839622 -1.410971 -1.684652
H 2.555656 1.458682 0.559090
H 2.152006 -0.000624 1.587118
H 3.073940 -1.198036 -0.254223
H -3.314879 0.680366 1.143401
H -3.119009 -1.118810 1.207606
H -1.792122 -0.041050 1.801745
el energy= -0.153107950883
zpe= 0.080622
th energy= 0.090260
th enthalpy= 0.091204
free energy= 0.045769

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.426457 -1.022612 0.927345
H 1.138837 -1.874537 0.766435
C 1.128396 0.287275 0.601057
H 1.912625 0.463023 1.393083
C 0.150606 1.450399 0.642823
H -0.169358 1.610201 1.706647
C -1.071903 1.208146 -0.215428
H -0.767769 1.144842 -1.293432
C -1.780870 -0.075444 0.189248
H -2.119428 0.028816 1.258860
C -0.822167 -1.253407 0.103054
H -1.337859 -2.180527 0.466882
C 1.848502 0.221157 -0.743469
O 3.141912 -0.352879 -0.624084
C -2.994626 -0.311097 -0.680418

H 0.151713 -1.017730 2.015464
H 0.664798 2.388038 0.305066
H -1.777528 2.073342 -0.115291
H -0.546138 -1.429353 -0.970008
H 1.252581 -0.366555 -1.491623
H 2.036167 1.250918 -1.152463
H 3.052609 -1.177293 -0.126559
H -3.705159 0.546649 -0.599805
H -2.701316 -0.422744 -1.752122
H -3.526440 -1.240555 -0.363734
el energy= -0.153389277633
zpe= 0.080622
th energy= 0.090008
th enthalpy= 0.090952
free energy= 0.046279

PM3 gas phase

4mchm_1/coords
t1
C 0.169785 1.392931 0.190645
H 0.587544 2.321125 -0.246477
C 1.019452 0.189616 -0.219150
H 1.014551 0.114340 -1.335386
C 0.418023 -1.092731 0.354920
H 1.020729 -1.965750 0.038089
C -1.023728 -1.266421 -0.094262
H -1.446358 -2.192893 0.341010
C -1.875303 -0.064943 0.313930
H -1.871992 0.007915 1.429720
C -1.272821 1.218804 -0.255490
H -1.875143 2.091650 0.063708
C 2.462840 0.390105 0.264448
O 3.288190 -0.522752 -0.422973
C -3.308046 -0.238502 -0.158072
H 0.214160 1.528563 1.290184
H 0.469839 -1.073135 1.462597
H -1.066018 -1.402323 -1.193892
H -1.328226 1.201530 -1.362826
H 2.801054 1.424874 0.054672
H 2.538519 0.235578 1.359595
H 4.155605 -0.429139 -0.054029

H -3.369278 -0.316197 -1.252178
H -3.757954 -1.147967 0.261020
H -3.933758 0.610685 0.146160
el energy= -0.128152118208
zpe= 0.098368
th energy= 0.108303
th enthalpy= 0.109247
free energy= 0.063507

4mchm_3/coords
t2
C -0.163116 1.401965 0.186279
H -0.214267 1.532989 1.286069
C -1.018901 0.207454 -0.232369
H -1.003893 0.136671 -1.349333
C -0.432341 -1.080817 0.341435
H -0.492838 -1.061394 1.448540
C 1.010655 -1.266158 -0.098816
H 1.422297 -2.196879 0.337879
C 1.869529 -0.072531 0.317380
H 1.860364 -0.003144 1.433362
C 1.281070 1.218266 -0.251054
H 1.887917 2.084987 0.076106
C -2.467215 0.419277 0.237951
O -3.365454 -0.548131 -0.233617
C 3.303395 -0.256525 -0.147146
H -0.572355 2.334634 -0.249370
H -1.042118 -1.947970 0.020888
H 1.059817 -1.400836 -1.198324
H 1.344497 1.205501 -1.358021
H -2.560001 0.329908 1.334965
H -2.820209 1.429696 -0.049901
H -3.292067 -0.568996 -1.179864
H 3.934318 0.586437 0.163571
H 3.743314 -1.171052 0.271543
H 3.370393 -0.331088 -1.241134
el energy= -0.131538917748
zpe= 0.095584
th energy= 0.105283
th enthalpy= 0.106227
free energy= 0.061124

4mchm_5/coords
t3
C 0.375491 -1.252295 0.001704
H 0.818156 -2.157962 0.460205
C 1.001872 0.000001 0.612546
H 0.781194 -0.000007 1.710316
C 0.375482 1.252293 0.001703
H 0.818151 2.157961 0.460204
C -1.132114 1.252348 0.199332
H -1.376056 1.313529 1.279283
C -1.765472 -0.000002 -0.405858
H -1.564497 -0.000001 -1.505887
C -1.132103 -1.252357 0.199329
H -1.573550 -2.157497 -0.261322
C 2.529974 0.000005 0.476771
O 2.893440 0.000022 -0.884551
C -3.267575 -0.000001 -0.184658
H 0.615822 -1.309920 -1.078779
H 0.615816 1.309920 -1.078776
H -1.573569 2.157486 -0.261316
H -1.376049 -1.313542 1.279279
H 2.953789 0.893617 0.977470
H 2.953798 -0.893603 0.977464
H 3.840529 -0.000129 -0.904665
H -3.521579 0.000045 0.884144
H -3.736394 0.885522 -0.633250
H -3.736400 -0.885554 -0.633182
el energy= -0.126564507113
zpe= 0.099932
th energy= 0.109840
th enthalpy= 0.110784
free energy= 0.065226

4mchm_6/coords
t4
C 0.152937 1.425855 0.186389
H 0.213704 1.552627 1.286267
C 1.015647 0.245996 -0.250645
H 0.986245 0.176884 -1.366742
C 0.457206 -1.052031 0.331928
H 1.097084 -1.903310 0.013414
C -0.981738 -1.264373 -0.105187

H -1.031980 -1.394163 -1.205127
C -1.856709 -0.085151 0.321822
H -1.844790 -0.023858 1.438268
C -1.292908 1.220995 -0.238277
H -1.366520 1.218251 -1.344704
C 2.471667 0.450807 0.195554
O 3.344387 -0.528612 -0.302569
C -3.289043 -0.289314 -0.139127
H 0.547002 2.364619 -0.249338
H 0.518315 -1.028505 1.439109
H -1.376103 -2.203742 0.328701
H -1.911169 2.073884 0.103364
H 2.889105 1.392429 -0.201282
H 2.544328 0.487382 1.300997
H 2.921034 -1.370677 -0.158017
H -3.932292 0.541219 0.179683
H -3.358584 -0.357184 -1.233399
H -3.712823 -1.213666 0.274618
el energy= -0.132200279341
zpe= 0.095085
th energy= 0.104604
th enthalpy= 0.105548
free energy= 0.061044

4mchm_7/coords
t5
C 0.370976 1.276056 -0.007476
H 0.625387 1.318375 1.071186
C 1.018208 0.050234 -0.648161
H 0.830769 0.087330 -1.749182
C 0.403254 -1.234541 -0.093252
H 0.686784 -1.343678 0.977994
C -1.107501 -1.243557 -0.247841
H -1.376182 -1.276426 -1.323230
C -1.741298 -0.016990 0.406453
H -1.513572 -0.041891 1.500864
C -1.138126 1.256504 -0.184398
H -1.586752 2.146020 0.299244
C 2.541338 0.049374 -0.437555
O 2.949401 -0.025986 0.902915
C -3.248409 -0.031907 0.222377
H 0.793840 2.197647 -0.453025

H 0.839312 -2.112942 -0.608552
H -1.526622 -2.167285 0.196740
H -1.398077 1.333471 -1.259551
H 3.002274 -0.786745 -0.999788
H 2.999377 0.989401 -0.791552
H 2.377901 -0.659378 1.329563
H -3.694428 -0.935144 0.658760
H -3.716994 0.835218 0.705823
H -3.528876 -0.007123 -0.839492
el energy= -0.131677614040
zpe= 0.095840
th energy= 0.105280
th enthalpy= 0.106224
free energy= 0.061972

4mchm_19/coords
t6
C 0.200685 -1.114749 0.695896
H -0.409568 -1.203881 1.616948
C 0.933478 0.226851 0.695682
H 1.484696 0.330195 1.663320
C -0.084040 1.364394 0.607703
H -0.678698 1.385498 1.543664
C -1.015446 1.228047 -0.586946
H -1.775317 2.033639 -0.560483
C -1.707892 -0.133668 -0.656916
H -2.186357 -0.219098 -1.664353
C -0.678823 -1.257069 -0.536043
H -0.020973 -1.240443 -1.435000
C 1.945767 0.297986 -0.460073
O 3.135404 -0.329390 -0.036870
C -2.812901 -0.260901 0.378148
H 0.932450 -1.944881 0.735676
H 0.438415 2.340607 0.563438
H -0.438417 1.387232 -1.520730
H -1.185939 -2.240271 -0.533753
H 1.529602 -0.210287 -1.360703
H 2.157964 1.349488 -0.737495
H 3.707891 -0.353028 -0.791187
H -3.574639 0.518408 0.243431
H -3.317079 -1.233344 0.302290
H -2.432226 -0.170062 1.405183

el energy= -0.124923936563
zpe= 0.101591
th energy= 0.111313
th enthalpy= 0.112257
free energy= 0.067126

4mchm_21/coords
t7
C 0.105551 1.378064 0.573579
H -0.400807 2.362098 0.513054
C -0.931329 0.261804 0.681534
H -1.443880 0.370746 1.671219
C -0.244760 -1.102082 0.660010
H 0.321954 -1.234700 1.604089
C 0.690160 -1.275495 -0.525851
H 0.096551 -1.317406 -1.462356
C 1.723621 -0.156167 -0.642490
H 2.227731 -0.262231 -1.635447
C 1.033830 1.206969 -0.617586
H 0.458456 1.338464 -1.556522
C -2.000547 0.394753 -0.417709
O -3.108983 -0.443599 -0.232276
C 2.802076 -0.265989 0.422601
H 0.702010 1.405244 1.508362
H -1.009250 -1.904018 0.650078
H 1.204425 -2.253916 -0.451502
H 1.794648 2.012266 -0.614105
H -2.336399 1.447625 -0.502390
H -1.620208 0.081697 -1.407267
H -3.465902 -0.260840 0.628247
H 2.393168 -0.176533 1.438774
H 3.319778 -1.232578 0.364301
H 3.557975 0.521742 0.305152
el energy= -0.127937284463
zpe= 0.098654
th energy= 0.108403
th enthalpy= 0.109347
free energy= 0.063998

4mchm_22/coords
t8
C 0.132110 1.408338 0.550628

H -0.361278 2.397115 0.467100
C -0.923521 0.316465 0.692929
H -1.410581 0.440842 1.692728
C -0.284012 -1.070968 0.657613
H 0.268220 -1.241065 1.603313
C 0.648638 -1.274079 -0.525068
H 1.136748 -2.265527 -0.445048
C 1.711342 -0.183258 -0.643227
H 2.220597 -0.312542 -1.630817
C 1.055484 1.196467 -0.637718
H 1.836695 1.982103 -0.644102
C -2.023276 0.459673 -0.374597
O -3.099840 -0.418796 -0.177752
C 2.777402 -0.310603 0.432220
H 0.732074 1.449655 1.482649
H -1.088169 -1.840333 0.632288
H 0.058017 -1.304247 -1.463546
H 0.486532 1.330012 -1.580353
H -2.496461 1.456399 -0.334965
H -1.613925 0.321241 -1.395612
H -2.721925 -1.281004 -0.023375
H 3.554631 0.455771 0.312772
H 2.362620 -0.199234 1.443825
H 3.269918 -1.291028 0.388473
el energy= -0.129022317083
zpe= 0.098338
th energy= 0.107709
th enthalpy= 0.108653
free energy= 0.064483

4mchm_24/coords
t9
C -0.103297 1.262539 0.745032
H 0.593529 1.393581 1.598698
C -0.928100 0.000007 0.985730
H -1.204376 0.000013 2.072207
C -0.103300 -1.262530 0.745049
H 0.593522 -1.393561 1.598721
C 0.691606 -1.251080 -0.549202
H 1.332808 -2.154023 -0.593682
C 1.551520 -0.000006 -0.711667
H 1.955045 -0.000014 -1.755004

C 0.691600 1.251067 -0.549223
H 0.001751 1.328228 -1.413338
C -2.285038 0.000009 0.264686
O -2.133740 0.000013 -1.134063
C 2.744158 0.000003 0.230515
H -0.767198 2.149663 0.761939
H -0.767204 -2.149650 0.761965
H 0.001765 -1.328263 -1.413323
H 1.332796 2.154014 -0.593727
H -2.867152 -0.893210 0.570937
H -2.867142 0.893241 0.570919
H -3.010632 -0.000193 -1.493045
H 2.439720 0.000027 1.286462
H 3.373894 -0.885719 0.073649
H 3.373908 0.885709 0.073612
el energy= -0.119665015888
zpe= 0.106435
th energy= 0.116314
th enthalpy= 0.117258
free energy= 0.071780

4mchm_9/coords
c1
C -0.422714 -0.898877 1.097963
H -1.132788 -1.747978 1.120592
C -1.136243 0.365125 0.615515
H -1.927554 0.631497 1.359508
C -0.141045 1.524789 0.548344
H -0.639034 2.432043 0.152995
C 1.081335 1.198533 -0.295925
H 0.788695 1.090259 -1.360499
C 1.766583 -0.080442 0.185286
H 2.133874 0.085043 1.228267
C 0.760811 -1.230500 0.202843
H 1.250522 -2.164439 0.536557
C -1.801155 0.128508 -0.751046
O -3.052621 -0.481272 -0.527395
C 2.952518 -0.417703 -0.700792
H -0.082924 -0.757281 2.143054
H 0.179236 1.781660 1.578185
H 1.796821 2.043354 -0.265428
H 0.387924 -1.420411 -0.829763

H -1.944901 1.084113 -1.293002
H -1.150784 -0.521631 -1.381200
H -3.398544 -0.701941 -1.381171
H 2.645382 -0.599390 -1.739784
H 3.685859 0.399138 -0.713398
H 3.468651 -1.320460 -0.348889
el energy= -0.126749730460
zpe= 0.099979
th energy= 0.109677
th enthalpy= 0.110621
free energy= 0.065535

4mchm_11/coords
c2
C -0.296609 -1.117504 0.111169
H -0.976572 -1.954715 -0.139907
C -0.946312 0.211544 -0.269052
H -1.138828 0.211054 -1.371151
C 0.003544 1.362519 0.059820
H -0.453387 2.329275 -0.230470
C 1.334831 1.193042 -0.653856
H 1.178068 1.282480 -1.747775
C 2.005220 -0.148028 -0.355360
H 2.858894 -0.265271 -1.068582
C 1.031767 -1.300108 -0.604717
H 0.851982 -1.391767 -1.694865
C -2.275709 0.412032 0.472543
O -3.238919 -0.433566 -0.114185
C 2.584320 -0.190356 1.049130
H -0.149274 -1.166996 1.209693
H 0.160022 1.420239 1.156375
H 2.015358 2.021864 -0.376271
H 1.495777 -2.256344 -0.292775
H -2.164758 0.186185 1.552181
H -2.609740 1.465968 0.390165
H -4.024712 -0.345953 0.407509
H 3.098899 -1.141860 1.237711
H 3.313641 0.616029 1.202652
H 1.809670 -0.080514 1.820937
el energy= -0.126368254666
zpe= 0.100007
th energy= 0.109924

th enthalpy= 0.110868
free energy= 0.065144

4mchm_13/coords
c3
C -0.013043 1.370776 0.065705
H -0.163406 1.415224 1.163737
C 0.946050 0.233494 -0.278563
H 1.129386 0.246356 -1.382721
C 0.313130 -1.105147 0.092504
H 1.001978 -1.932907 -0.167041
C -1.017061 -1.296308 -0.617594
H -0.843339 -1.377729 -1.709544
C -2.001018 -0.156509 -0.352939
H -2.857024 -0.276258 -1.062928
C -1.346630 1.194575 -0.642126
H -2.034024 2.013269 -0.351747
C 2.281371 0.442688 0.454222
O 3.282195 -0.466095 0.083234
C -2.571975 -0.218036 1.054179
H 0.433753 2.344606 -0.216613
H 0.173922 -1.163702 1.191526
H -1.468928 -2.259831 -0.310311
H -1.198018 1.297174 -1.736023
H 2.643160 1.479499 0.304060
H 2.184001 0.274047 1.541467
H 3.374838 -0.419470 -0.860399
H -3.076422 -1.176231 1.236146
H -1.794204 -0.108231 1.822874
H -3.308176 0.579748 1.219322
el energy= -0.129766394357
zpe= 0.097210
th energy= 0.106892
th enthalpy= 0.107836
free energy= 0.062744

4mchm_15/coords
c4
C -0.449717 -0.921764 1.025383
H -0.153980 -0.844984 2.091098
C -1.136636 0.377123 0.605967
H -1.893354 0.631885 1.391038

C -0.126233 1.522407 0.550557
H -0.613346 2.440165 0.165434
C 1.091200 1.191153 -0.296941
H 0.797787 1.075932 -1.360363
C 1.772213 -0.084441 0.195277
H 2.112543 0.079022 1.247785
C 0.774242 -1.240686 0.182329
H 1.259410 -2.162047 0.559771
C -1.880044 0.235357 -0.734462
O -2.985337 -0.625479 -0.679221
C 2.982197 -0.410821 -0.662109
H -1.171561 -1.760136 0.968602
H 0.198849 1.764435 1.582605
H 1.807675 2.035457 -0.272234
H 0.472854 -1.466121 -0.861621
H -2.197516 1.230342 -1.105564
H -1.247314 -0.228690 -1.513072
H -3.560435 -0.310029 0.007121
H 2.703555 -0.581089 -1.711026
H 3.714687 0.406721 -0.645594
H 3.489502 -1.317001 -0.306218
el energy= -0.129750184098
zpe= 0.097034
th energy= 0.106769
th enthalpy= 0.107713
free energy= 0.062383

4mchm_16/coords
c5
C -0.233061 1.249832 -0.165588
H -0.743240 2.157220 -0.544136
C -0.945639 0.000002 -0.676483
H -0.893811 0.000005 -1.794936
C -0.233061 -1.249829 -0.165593
H -0.303014 -1.302671 0.939799
C 1.224052 -1.256902 -0.599920
H 1.729738 -2.155458 -0.195144
C 1.979382 0.000000 -0.166515
H 2.966339 0.000001 -0.692924
C 1.224053 1.256906 -0.599912
H 1.279792 1.349322 -1.703389
C -2.435573 0.000002 -0.311206

O -2.589491 -0.000007 1.089450
C 2.264790 -0.000005 1.326259
H -0.303016 1.302671 0.939804
H -0.743242 -2.157216 -0.544142
H 1.279790 -1.349310 -1.703397
H 1.729739 2.155458 -0.195129
H -2.930210 0.893605 -0.742145
H -2.930211 -0.893597 -0.742155
H -3.522685 0.000014 1.252268
H 2.843833 -0.885609 1.619699
H 2.843829 0.885599 1.619707
H 1.342635 -0.000009 1.924357
el energy= -0.124769300172
zpe= 0.101557
th energy= 0.111453
th enthalpy= 0.112397
free energy= 0.066840

4mchm_17/coords
c6
C -0.224488 1.284547 -0.092537
H -0.712204 2.228005 -0.407521
C -0.959468 0.095387 -0.704969
H -0.938600 0.200701 -1.817318
C -0.266737 -1.212410 -0.325648
H -0.384498 -1.385750 0.768340
C 1.201641 -1.202396 -0.713001
H 1.682059 -2.142088 -0.376373
C 1.962805 -0.002226 -0.150965
H 2.965292 0.024104 -0.646481
C 1.239210 1.297981 -0.500145
H 1.752678 2.153323 -0.018772
C -2.434201 0.066446 -0.270374
O -2.637869 -0.092917 1.108880
C 2.203289 -0.133817 1.343786
H -0.313313 1.255993 1.013035
H -0.776715 -2.064390 -0.817462
H 1.286274 -1.197100 -1.818499
H 1.316670 1.473015 -1.592172
H -2.941262 1.021015 -0.495089
H -2.972804 -0.739647 -0.806773
H -2.003532 -0.739440 1.408070

H 2.783452 0.715392 1.728392
H 1.264331 -0.171459 1.913816
H 2.762816 -1.049405 1.576887
el energy= -0.129920608241
zpe= 0.097456
th energy= 0.106878
th enthalpy= 0.107822
free energy= 0.063582

4mchm_23/coords
c7
C 0.418299 -1.265191 -0.911737
H 1.043862 -2.150074 -0.681154
C 1.273050 -0.000210 -0.843699
H 1.918614 -0.000429 -1.760107
C 0.418314 1.264745 -0.912328
H 1.043889 2.149736 -0.682192
C -0.794007 1.246219 0.002631
H -0.479525 1.291450 1.064696
C -1.643568 -0.000038 -0.232792
H -1.991619 -0.000263 -1.295510
C -0.794054 -1.246228 0.003174
H -0.479614 -1.291031 1.065269
C 2.283024 0.000065 0.314469
O 1.641171 0.000314 1.566337
C -2.859826 0.000183 0.676545
H 0.077274 -1.401678 -1.958479
H 0.077262 1.400739 -1.959127
H -1.402897 2.155896 -0.169407
H -1.402973 -2.155954 -0.168502
H 2.936309 -0.893091 0.236741
H 2.936294 0.893193 0.236322
H 2.331444 0.001003 2.215466
H -3.485587 0.885759 0.505094
H -3.485664 -0.885402 0.505425
H -2.573826 0.000368 1.737193
el energy= -0.121462609899
zpe= 0.104816
th energy= 0.114691
th enthalpy= 0.115636
free energy= 0.070135

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.341018 -1.075350 0.078723
H 1.061172 -1.881976 -0.180099
C 0.943808 0.278583 -0.291490
H 1.113416 0.304133 -1.396913
C -0.028088 1.393426 0.079032
H -0.169215 1.422891 1.178871
C -1.364139 1.198039 -0.620572
H -1.226656 1.321835 -1.713742
C -1.988237 -0.171869 -0.349719
H -2.842997 -0.299563 -1.059774
C -0.983654 -1.290355 -0.632178
H -1.415062 -2.266283 -0.335063
C 2.290132 0.479409 0.421389
O 3.272592 -0.435482 0.012952
C -2.554947 -0.264599 1.057508
H 0.201551 -1.141186 1.177467
H 0.400973 2.376888 -0.196021
H -2.067183 1.996281 -0.311476
H -0.809868 -1.355195 -1.725120
H 2.735511 1.459864 0.179075
H 2.165974 0.426388 1.521582
H 2.861151 -1.295730 0.012710
H -3.310996 0.512212 1.232799
H -3.034681 -1.237243 1.229437
H -1.779182 -0.143158 1.826487
el energy= -0.130456269462
zpe= 0.096716
th energy= 0.106207
th enthalpy= 0.107152
free energy= 0.062691

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.486737 -0.889651 1.010307
H 1.238212 -1.706228 0.925414
C 1.138709 0.431962 0.602607
H 1.877438 0.705511 1.397348
C 0.106553 1.553436 0.521128
H -0.219269 1.815485 1.548038
C -1.109392 1.184808 -0.312833

H -0.824839 1.063916 -1.378111
C -1.758577 -0.098900 0.200093
H -2.085780 0.065951 1.256539
C -0.738534 -1.235097 0.180182
H -1.201605 -2.164896 0.565047
C 1.915757 0.293431 -0.718978
O 2.988990 -0.606856 -0.635577
C -2.974692 -0.456273 -0.636096
H 0.207733 -0.842614 2.081410
H 0.579217 2.467919 0.111435
H -1.843967 2.013619 -0.291254
H -0.444630 -1.457317 -0.866278
H 1.245725 -0.004219 -1.550685
H 2.401470 1.243503 -1.002558
H 2.649328 -1.396716 -0.222331
H -3.722818 0.346861 -0.614157
H -2.708890 -0.628787 -1.687972
H -3.458610 -1.369429 -0.265738
el energy= -0.130854766884
zpe= 0.096689
th energy= 0.106055
th enthalpy= 0.107000
free energy= 0.062807

PM3-SMD

4mchm_1/coords
t1
C 0.174001 1.391472 0.197173
H 0.596979 2.317921 -0.238262
C 1.021387 0.187087 -0.208116
H 1.020114 0.112677 -1.324028
C 0.415943 -1.093726 0.365223
H 1.016012 -1.972738 0.056154
C -1.023867 -1.266245 -0.088887
H -1.449402 -2.190288 0.348382
C -1.875175 -0.061604 0.310440
H -1.881482 0.012585 1.425774
C -1.266315 1.220474 -0.255719
H -1.867639 2.095028 0.059888
C 2.463441 0.381556 0.283267
O 3.399924 -0.406585 -0.415988
C -3.302887 -0.231804 -0.174408

H 0.216030 1.529011 1.296324
H 0.464189 -1.071984 1.472967
H -1.062360 -1.409177 -1.187597
H -1.317577 1.205508 -1.363207
H 2.820061 1.410055 0.094806
H 2.548979 0.190531 1.370814
H 3.108980 -1.309820 -0.351253
H -3.358056 -0.308713 -1.268968
H -3.762252 -1.139247 0.238963
H -3.931135 0.618072 0.123311
el energy= -0.133912528433
zpe= 0.093474
th energy= 0.103241
th enthalpy= 0.104185
free energy= 0.058956

4mchm_3/coords
t2
C -0.161415 1.404632 0.180812
H -0.219176 1.538988 1.279841
C -1.017957 0.212281 -0.242391
H -1.001669 0.138838 -1.359227
C -0.438044 -1.076990 0.335940
H -0.505872 -1.060458 1.442388
C 1.006446 -1.266491 -0.096444
H 1.412743 -2.198520 0.342091
C 1.867119 -0.075302 0.322040
H 1.856981 -0.006980 1.437704
C 1.284260 1.217416 -0.247490
H 1.890935 2.082280 0.084279
C -2.463780 0.437447 0.220119
O -3.368629 -0.553793 -0.210937
C 3.299840 -0.262046 -0.141692
H -0.566041 2.337664 -0.257838
H -1.043867 -1.944379 0.008908
H 1.059705 -1.403778 -1.195333
H 1.355011 1.208239 -1.353914
H -2.557389 0.406149 1.320452
H -2.829568 1.425802 -0.120377
H -3.207749 -0.705546 -1.135375
H 3.936886 0.572185 0.180416
H 3.736977 -1.183634 0.264431

H 3.372314 -0.322189 -1.236306
el energy= -0.133701385476
zpe= 0.093530
th energy= 0.103407
th enthalpy= 0.104351
free energy= 0.058787

4mchm_5/coords
t3
C 0.362442 -1.284242 -0.013891
H 0.779917 -2.215021 0.417159
C 1.016200 -0.070562 0.642565
H 0.828391 -0.122844 1.742854
C 0.410066 1.225116 0.103675
H 0.850386 2.093166 0.632373
C -1.100122 1.241438 0.257599
H -1.370365 1.269667 1.332505
C -1.743135 0.025308 -0.406862
H -1.520822 0.060664 -1.501666
C -1.145631 -1.258377 0.166961
H -1.599949 -2.140386 -0.324661
C 2.537984 -0.078287 0.441851
O 2.958005 0.066867 -0.896838
C -3.248128 0.047020 -0.214478
H 0.611751 -1.313310 -1.093705
H 0.695733 1.351909 -0.965317
H -1.511875 2.171706 -0.179858
H -1.402507 -1.347974 1.241758
H 3.009246 0.724342 1.041563
H 2.985928 -1.038551 0.752320
H 2.390186 0.727290 -1.290148
H -3.526829 0.014706 0.847754
H -3.693402 0.956275 -0.639411
H -3.727896 -0.811047 -0.703337
el energy= -0.133953072298
zpe= 0.094151
th energy= 0.103551
th enthalpy= 0.104496
free energy= 0.060316

4mchm_6/coords
t4

C 0.174121 1.391366 0.197070
H 0.216267 1.529014 1.296204
C 1.021415 0.186900 -0.208160
H 1.020121 0.112497 -1.324073
C 0.415875 -1.093911 0.365045
H 1.015784 -1.972920 0.055693
C -1.024006 -1.266251 -0.088930
H -1.062554 -1.409206 -1.187641
C -1.875223 -0.061543 0.310443
H -1.881478 0.012586 1.425788
C -1.266273 1.220541 -0.255647
H -1.317696 1.205716 -1.363121
C 2.463415 0.381502 0.283339
O 3.400131 -0.406368 -0.415882
C -3.303013 -0.231657 -0.174339
H 0.597171 2.317716 -0.238515
H 0.464262 -1.072387 1.472784
H -1.449618 -2.190247 0.348381
H -1.867414 2.095153 0.060170
H 2.819821 1.410145 0.095151
H 2.548735 0.190294 1.370881
H 3.109556 -1.309687 -0.351166
H -3.930827 0.619028 0.122000
H -3.358099 -0.310248 -1.268783
H -3.762956 -1.138192 0.240377
el energy= -0.133912436534
zpe= 0.093470
th energy= 0.103238
th enthalpy= 0.104183
free energy= 0.058951

4mchm_7/coords
t5
C 0.362427 1.284186 0.014151
H 0.611786 1.313187 1.093948
C 1.016080 0.070530 -0.642398
H 0.827950 0.122700 -1.742637
C 0.410065 -1.225054 -0.103230
H 0.695363 -1.351382 0.965902
C -1.100100 -1.241466 -0.257601
H -1.370039 -1.269527 -1.332584
C -1.743273 -0.025386 0.406857

H -1.521236 -0.060822 1.501714
C -1.145661 1.258385 -0.166679
H -1.599924 2.140286 0.325191
C 2.537916 0.078432 -0.442107
O 2.958547 -0.067061 0.896385
C -3.248262 -0.047015 0.214113
H 0.779867 2.214959 -0.416937
H 0.850627 -2.093205 -0.631529
H -1.511890 -2.171834 0.179608
H -1.402529 1.348219 -1.241463
H 3.009174 -0.723933 -1.042163
H 2.985551 1.038883 -0.752473
H 2.390252 -0.726842 1.290076
H -3.693574 -0.956720 0.638052
H -3.728178 0.810537 0.703717
H -3.526727 -0.013686 -0.848148
el energy= -0.133953181525
zpe= 0.094147
th energy= 0.103548
th enthalpy= 0.104492
free energy= 0.060313

4mchm_19/coords
t6
C 0.202088 -1.127130 0.672882
H -0.401372 -1.231641 1.596586
C 0.935874 0.213771 0.688776
H 1.493012 0.302666 1.654145
C -0.076965 1.354949 0.622546
H -0.665594 1.368569 1.562428
C -1.014469 1.237763 -0.568383
H -1.770058 2.046528 -0.527451
C -1.711888 -0.120240 -0.652097
H -2.199304 -0.189878 -1.656040
C -0.685157 -1.247884 -0.555452
H -0.032832 -1.221251 -1.458318
C 1.939881 0.293514 -0.474971
O 3.210073 -0.229244 -0.157500
C -2.807699 -0.259823 0.390019
H 0.930749 -1.961943 0.695450
H 0.450447 2.328668 0.588180
H -0.441699 1.407901 -1.502690

H -1.194331 -2.229784 -0.565684
H 1.535929 -0.230106 -1.371359
H 2.163175 1.335810 -0.762727
H 3.072811 -1.067755 0.269726
H -3.563031 0.530479 0.285197
H -3.327163 -1.222752 0.295191
H -2.421309 -0.201077 1.417444
el energy= -0.131136608144
zpe= 0.096863
th energy= 0.106201
th enthalpy= 0.107145
free energy= 0.063155

4mchm_21/coords
t7
C 0.099870 1.375684 0.576371
H -0.408832 2.358328 0.517119
C -0.934472 0.256733 0.679455
H -1.456803 0.364129 1.664010
C -0.239005 -1.102990 0.660873
H 0.330539 -1.228921 1.604146
C 0.694021 -1.274490 -0.526311
H 0.099865 -1.318351 -1.462300
C 1.723745 -0.151911 -0.642614
H 2.226590 -0.254632 -1.636076
C 1.030743 1.209314 -0.612943
H 0.456713 1.344253 -1.552102
C -1.992701 0.386950 -0.427708
O -3.114457 -0.442971 -0.224958
C 2.802830 -0.262591 0.420684
H 0.692885 1.404179 1.513157
H -0.993553 -1.913669 0.660371
H 1.210369 -2.251849 -0.454293
H 1.789422 2.016307 -0.606254
H -2.325808 1.438356 -0.528009
H -1.613192 0.057600 -1.412483
H -3.486383 -0.212697 0.618996
H 2.398855 -0.184877 1.439967
H 3.329353 -1.224211 0.355117
H 3.555460 0.529634 0.311466
el energy= -0.130549254127
zpe= 0.096598

th energy= 0.106290
th enthalpy= 0.107234
free energy= 0.062092

4mchm_22/coords
t8
C 0.077134 1.355096 0.622722
H -0.450149 2.328857 0.588301
C -0.935763 0.214091 0.689091
H -1.492790 0.303147 1.654527
C -0.202182 -1.126919 0.673225
H 0.401319 -1.231595 1.596862
C 0.684834 -1.247956 -0.555207
H 1.193945 -2.229923 -0.565249
C 1.711594 -0.120406 -0.652220
H 2.198723 -0.190140 -1.656289
C 1.014331 1.237654 -0.568443
H 1.769974 2.046344 -0.527828
C -1.939614 0.293900 -0.474737
O -3.209778 -0.229970 -0.158569
C 2.807692 -0.260010 0.389600
H 0.665845 1.368724 1.562513
H -0.931030 -1.961546 0.695769
H 0.032563 -1.221540 -1.458030
H 0.441258 1.407647 -1.502550
H -2.163330 1.336210 -0.762138
H -1.535417 -0.229183 -1.371254
H -3.072494 -1.066028 0.273559
H 3.563646 0.529540 0.283699
H 2.421720 -0.199997 1.417088
H 3.326295 -1.223455 0.295378
el energy= -0.131136782681
zpe= 0.096887
th energy= 0.106214
th enthalpy= 0.107158
free energy= 0.063196

4mchm_24/coords
t9
C -0.105578 1.319793 0.662673
H 0.585870 1.502550 1.510987
C -0.943096 0.083839 0.980503

H -1.231094 0.159241 2.060143
C -0.129773 -1.199844 0.826511
H 0.558412 -1.286139 1.692118
C 0.676634 -1.280120 -0.458983
H 1.309588 -2.189360 -0.439177
C 1.547510 -0.049895 -0.700333
H 1.955107 -0.121524 -1.739329
C 0.702730 1.219208 -0.619472
H 0.027348 1.259112 -1.497412
C -2.290666 0.039135 0.244469
O -2.245004 -0.051797 -1.159922
C 2.735450 -0.001157 0.244433
H -0.760844 2.212382 0.618153
H -0.802868 -2.077973 0.894353
H -0.005466 -1.417930 -1.326932
H 1.356484 2.109418 -0.710831
H -2.897872 -0.806288 0.624654
H -2.867223 0.966981 0.411918
H -1.594125 -0.716178 -1.377990
H 2.432114 0.074892 1.297971
H 3.355573 -0.902726 0.151176
H 3.379764 0.862160 0.030772
el energy= -0.129851032967
zpe= 0.098417
th energy= 0.107635
th enthalpy= 0.108579
free energy= 0.064769

4mchm_9/coords
c1
C -0.432973 -0.915757 1.074872
H -1.143140 -1.766509 1.079253
C -1.138149 0.360534 0.613430
H -1.933995 0.616153 1.355584
C -0.141014 1.517840 0.573219
H -0.635127 2.432096 0.189729
C 1.085713 1.204715 -0.268509
H 0.800733 1.121742 -1.337359
C 1.763166 -0.086236 0.190362
H 2.127405 0.055686 1.237560
C 0.753290 -1.232495 0.178710
H 1.236863 -2.175687 0.494432

C -1.794130 0.148100 -0.762126
O -3.082475 -0.418791 -0.683922
C 2.950297 -0.409561 -0.697247
H -0.099318 -0.797904 2.124597
H 0.171369 1.758042 1.609284
H 1.803082 2.046595 -0.215287
H 0.384408 -1.399722 -0.859337
H -1.971830 1.101117 -1.290169
H -1.143494 -0.486805 -1.406019
H -3.017186 -1.189934 -0.131071
H 2.651240 -0.565924 -1.742711
H 3.690334 0.401395 -0.688337
H 3.461259 -1.322847 -0.365041
el energy= -0.133005725656
zpe= 0.095117
th energy= 0.104444
th enthalpy= 0.105388
free energy= 0.061300

4mchm_11/coords
c2
C -0.342719 -1.078369 0.087337
H -1.063832 -1.884947 -0.170239
C -0.944499 0.274741 -0.285992
H -1.117354 0.295625 -1.390849
C 0.025924 1.393212 0.075466
H -0.404081 2.374814 -0.204469
C 1.359151 1.194815 -0.627491
H 1.218362 1.314593 -1.720515
C 1.986242 -0.172456 -0.353303
H 2.835417 -0.302613 -1.069062
C 0.982748 -1.295516 -0.620448
H 0.809798 -1.375943 -1.712252
C -2.284799 0.477310 0.433256
O -3.277483 -0.427606 0.002411
C 2.564538 -0.254553 1.048865
H -0.205687 -1.142620 1.186361
H 0.168527 1.431139 1.174639
H 2.062140 1.995905 -0.326023
H 1.415803 -2.267170 -0.311987
H -2.168558 0.396752 1.531742
H -2.720141 1.467571 0.212860

H -2.859609 -1.285799 -0.033222
H 3.044641 -1.226220 1.226286
H 3.325385 0.520143 1.213830
H 1.799537 -0.125489 1.827475
el energy= -0.132336512705
zpe= 0.095208
th energy= 0.104763
th enthalpy= 0.105707
free energy= 0.061104

4mchm_13/coords
c3
C -0.003199 1.364586 0.065393
H -0.154623 1.417720 1.162808
C 0.949014 0.218946 -0.270392
H 1.145681 0.227302 -1.371987
C 0.302000 -1.113588 0.099714
H 0.981168 -1.949551 -0.157790
C -1.026865 -1.296064 -0.614220
H -0.849905 -1.384859 -1.704834
C -2.002586 -0.147745 -0.358405
H -2.854298 -0.261081 -1.074008
C -1.335527 1.196905 -0.645271
H -2.016805 2.022019 -0.358886
C 2.274955 0.422871 0.476578
O 3.292958 -0.457550 0.058863
C -2.584033 -0.203616 1.043638
H 0.451339 2.333590 -0.220928
H 0.158264 -1.172941 1.198148
H -1.486970 -2.254932 -0.304660
H -1.183502 1.298753 -1.738573
H 2.624082 1.468836 0.372671
H 2.178701 0.206249 1.555489
H 3.450959 -0.286401 -0.862488
H -3.104909 -1.153995 1.221454
H -1.814350 -0.106985 1.822360
H -3.311058 0.602910 1.208117
el energy= -0.132000624254
zpe= 0.095280
th energy= 0.105039
th enthalpy= 0.105983
free energy= 0.060665

4mchm_15/coords
c4
C -0.447896 -0.928953 1.015721
H -0.154581 -0.858910 2.082538
C -1.137643 0.371258 0.605189
H -1.896492 0.619081 1.390830
C -0.128077 1.517462 0.555959
H -0.615530 2.436651 0.175018
C 1.090729 1.192395 -0.291244
H 0.799500 1.084598 -1.356033
C 1.773113 -0.084328 0.195435
H 2.111669 0.073632 1.249173
C 0.777927 -1.242632 0.174298
H 1.263137 -2.165229 0.548619
C -1.880505 0.244292 -0.734178
O -2.993420 -0.619807 -0.681345
C 2.984630 -0.404505 -0.660020
H -1.165640 -1.770482 0.959455
H 0.193801 1.756037 1.589574
H 1.805547 2.037759 -0.261363
H 0.481719 -1.465248 -0.871445
H -2.211206 1.239214 -1.091470
H -1.252709 -0.205116 -1.525268
H -3.531270 -0.343408 0.052504
H 2.713630 -0.570808 -1.711575
H 3.718156 0.412116 -0.638578
H 3.493968 -1.311367 -0.308177
el energy= -0.132241662008
zpe= 0.095223
th energy= 0.104828
th enthalpy= 0.105772
free energy= 0.060887

4mchm_16/coords
c5
C 0.212669 -1.295542 -0.040372
H 0.692303 -2.254598 -0.318156
C 0.957110 -0.135771 -0.696151
H 0.938599 -0.286315 -1.803431
C 0.274186 1.191533 -0.371065
H 0.391237 1.413802 0.714267

C -1.193806 1.176834 -0.758619
H -1.666656 2.132028 -0.457200
C -1.963201 0.004690 -0.150961
H -2.967078 -0.034548 -0.641759
C -1.249664 -1.312772 -0.451029
H -1.326097 -1.527536 -1.535846
C 2.431277 -0.103745 -0.268116
O 2.644841 0.165029 1.099985
C -2.198271 0.194747 1.337384
H 0.295527 -1.226848 1.063484
H 0.791618 2.017616 -0.897567
H -1.280774 1.133130 -1.862822
H -1.770967 -2.146925 0.058022
H 2.921090 -1.081475 -0.421088
H 2.986899 0.649864 -0.859028
H 2.010078 0.833864 1.350544
H -2.774704 1.108010 1.536734
H -2.761565 -0.646338 1.763159
H -1.260045 0.276199 1.904385
el energy= -0.132383061663
zpe= 0.095614
th energy= 0.104975
th enthalpy= 0.105919
free energy= 0.061784

4mchm_17/coords
c6
C -0.212544 1.295603 -0.039887
H -0.692144 2.254784 -0.317261
C -0.957120 0.136100 -0.696039
H -0.938552 0.287010 -1.803250
C -0.274251 -1.191375 -0.371258
H -0.391376 -1.413725 0.714089
C 1.193666 -1.176657 -0.758962
H 1.666491 -2.131998 -0.457981
C 1.963224 -0.004759 -0.151031
H 2.967012 0.034516 -0.642022
C 1.249763 1.312837 -0.450660
H 1.771173 2.146805 0.058600
C -2.431297 0.104084 -0.268051
O -2.645035 -0.165680 1.099792
C 2.198433 -0.195178 1.337236

H -0.295367 1.226472 1.063946
H -0.791772 -2.017367 -0.897813
H 1.280432 -1.132582 -1.863174
H 1.326134 1.527908 -1.535425
H -2.920729 1.082090 -0.420437
H -2.987316 -0.648755 -0.859629
H -2.009875 -0.834242 1.350162
H 2.762393 0.645459 1.763030
H 1.260233 -0.276036 1.904365
H 2.774294 -1.108841 1.536379
el energy= -0.132383580389
zpe= 0.095615
th energy= 0.104976
th enthalpy= 0.105920
free energy= 0.061783

4mchm_23/coords
c7
C 0.447330 -1.054258 -1.132443
H 1.075705 -1.964957 -1.068391
C 1.292694 0.177328 -0.810737
H 1.956449 0.356967 -1.694563
C 0.431008 1.427766 -0.649132
H 1.047763 2.254418 -0.244338
C -0.797856 1.234340 0.222520
H -0.506560 1.093830 1.282914
C -1.633611 0.045896 -0.245318
H -1.979103 0.242761 -1.289967
C -0.776633 -1.216989 -0.246739
H -0.475851 -1.473366 0.793334
C 2.276522 -0.051030 0.346533
O 1.718227 -0.298194 1.615282
C -2.849944 -0.134909 0.644182
H 0.119558 -0.990978 -2.189626
H 0.106850 1.763013 -1.655299
H -1.411821 2.156525 0.207556
H -1.376906 -2.079661 -0.596726
H 2.958625 -0.888839 0.099827
H 2.897917 0.845924 0.521946
H 1.029867 -0.950107 1.498317
H -3.481685 0.763154 0.647560
H -3.473652 -0.972501 0.305288

H -2.570030 -0.339498 1.686729
el energy= -0.132017115587
zpe= 0.096645
th energy= 0.105779
th enthalpy= 0.106723
free energy= 0.063172

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.282984 -1.128320 0.136183
H 0.953946 -1.978325 -0.100410
C 0.950802 0.191282 -0.245716
H 1.157273 0.180492 -1.345083
C 0.010088 1.354315 0.057919
H -0.157648 1.427669 1.151619
C -1.312348 1.191547 -0.672477
H -1.140402 1.268584 -1.764938
C -2.002586 -0.137814 -0.369668
H -2.845557 -0.253439 -1.095179
C -1.040344 -1.304974 -0.589172
H -1.518267 -2.250203 -0.264793
C 2.271838 0.376829 0.516820
O 3.360061 -0.285369 -0.086826
C -2.604572 -0.156301 1.024637
H 0.125147 -1.168358 1.233685
H 0.481898 2.312409 -0.237008
H -1.986512 2.031850 -0.415135
H -0.852492 -1.420227 -1.675477
H 2.596865 1.432724 0.517615
H 2.179285 0.054679 1.572274
H 3.099536 -1.189814 -0.222194
H -3.324222 0.662240 1.160059
H -3.139377 -1.096139 1.216229
H -1.845129 -0.050575 1.812187
el energy= -0.132266847298
zpe= 0.094928
th energy= 0.104796
th enthalpy= 0.105740
free energy= 0.059824

4mchm-1000rej-h-rmsd_20/coords
c9

C 0.433029 -0.915738 1.074910
H 1.143221 -1.766499 1.079119
C 1.138208 0.360583 0.613433
H 1.934209 0.616112 1.355483
C 0.140971 1.517823 0.573374
H -0.171609 1.757713 1.609468
C -1.085608 1.204716 -0.268589
H -0.800422 1.121676 -1.337398
C -1.763131 -0.086198 0.190314
H -2.127409 0.055850 1.237515
C -0.753344 -1.232504 0.178913
H -1.236997 -2.175596 0.494907
C 1.794126 0.148340 -0.762136
O 3.082236 -0.419013 -0.684032
C -2.950181 -0.409576 -0.697347
H 0.099537 -0.797991 2.124707
H 0.635051 2.432276 0.190286
H -1.802988 2.046626 -0.215652
H -0.384618 -1.400125 -0.859119
H 1.143422 -0.486165 -1.406317
H 1.972214 1.101515 -1.289799
H 3.016568 -1.190441 -0.131655
H -3.690586 0.401041 -0.688015
H -2.651161 -0.565313 -1.742922
H -3.460749 -1.323246 -0.365578
el energy= -0.133005629895
zpe= 0.095111
th energy= 0.104440
th enthalpy= 0.105384
free energy= 0.061290

PM6 gas phase

4mchm_1/coords
t1
C 0.167739 1.424970 0.193936
H 0.580273 2.345860 -0.258159
C 1.031870 0.209686 -0.191007
H 1.062175 0.118187 -1.307043
C 0.436115 -1.088746 0.383901
H 1.059053 -1.946062 0.059691
C -1.012777 -1.280220 -0.078575

H -1.429529 -2.203173 0.363946
C -1.884278 -0.068372 0.310600
H -1.894880 0.014455 1.425188
C -1.282376 1.229379 -0.267835
H -1.893730 2.097602 0.038630
C 2.477725 0.409826 0.295361
O 3.253238 -0.541575 -0.466899
C -3.325095 -0.258491 -0.176560
H 0.193998 1.578756 1.289200
H 0.481790 -1.076652 1.488354
H -1.041399 -1.429844 -1.174468
H -1.323986 1.202184 -1.373236
H 2.854898 1.422809 0.070831
H 2.600629 0.197512 1.370091
H 4.180597 -0.530290 -0.169911
H -3.377707 -0.347395 -1.267103
H -3.771835 -1.164716 0.246223
H -3.959793 0.585172 0.114027
el energy= -0.125405056848
zpe= 0.085678
th energy= 0.096011
th enthalpy= 0.096955
free energy= 0.049943

4mchm_3/coords
t2
C -0.155969 1.437770 0.183163
H -0.197734 1.579870 1.280042
C -1.029318 0.236658 -0.226083
H -1.024005 0.157197 -1.340779
C -0.457380 -1.069330 0.355609
H -0.516356 -1.050712 1.460470
C 0.994466 -1.279780 -0.088283
H 1.392610 -2.208984 0.359068
C 1.876581 -0.080903 0.317938
H 1.875153 -0.005677 1.433325
C 1.298925 1.229267 -0.257592
H 1.915490 2.086902 0.068464
C -2.479691 0.450237 0.242022
O -3.344154 -0.589546 -0.242537
C 3.320328 -0.286549 -0.153554
H -0.551320 2.368779 -0.263130

H -1.088233 -1.922252 0.038122
H 1.038727 -1.427748 -1.183333
H 1.359664 1.213462 -1.361990
H -2.592144 0.362568 1.338689
H -2.882370 1.423301 -0.090016
H -3.282674 -0.661389 -1.213954
H 3.962545 0.546595 0.151088
H 3.750417 -1.201189 0.268705
H 3.385815 -0.368573 -1.243789
el energy= -0.128543316833
zpe= 0.082962
th energy= 0.093048
th enthalpy= 0.093993
free energy= 0.047883

4mchm_5/coords
t3
C 0.399043 -1.266091 0.058745
H 0.827559 -2.170220 0.526340
C 1.025416 0.000006 0.672975
H 0.833842 0.000008 1.774209
C 0.399035 1.266087 0.058727
H 0.827564 2.170232 0.526304
C -1.125548 1.265146 0.216096
H -1.396033 1.328256 1.286363
C -1.747835 0.000001 -0.409751
H -1.517463 0.000000 -1.503908
C -1.125543 -1.265157 0.216079
H -1.551002 -2.167807 -0.259666
C 2.551332 0.000003 0.465777
O 2.771815 0.000018 -0.962021
C -3.270533 0.000001 -0.232427
H 0.676078 -1.317823 -1.015042
H 0.676055 1.317793 -1.015061
H -1.551023 2.167802 -0.259624
H -1.396044 -1.328292 1.286340
H 3.021571 0.902188 0.893487
H 3.021571 -0.902176 0.893485
H 3.728028 -0.000102 -1.148046
H -3.557558 0.000048 0.824303
H -3.724924 0.882280 -0.695363
H -3.724953 -0.882297 -0.695280

el energy= -0.123979033763
zpe= 0.087170
th energy= 0.097443
th enthalpy= 0.098387
free energy= 0.051734

4mchm_6/coords
t4
C 0.168574 1.421242 0.195062
H 0.200629 1.570220 1.291099
C 1.034089 0.209856 -0.199290
H 1.052619 0.129201 -1.315342
C 0.436448 -1.088488 0.375992
H 1.044119 -1.956970 0.061570
C -1.013953 -1.277952 -0.085899
H -1.045200 -1.420901 -1.182593
C -1.885129 -0.068216 0.310972
H -1.894498 0.008880 1.426111
C -1.283643 1.231724 -0.261646
H -1.330963 1.213332 -1.366976
C 2.481250 0.414428 0.282642
O 3.387017 -0.448857 -0.422252
C -3.326062 -0.257130 -0.175378
H 0.581324 2.344293 -0.253788
H 0.476642 -1.067727 1.481869
H -1.430702 -2.202790 0.353155
H -1.891985 2.099139 0.053860
H 2.868183 1.419167 0.026691
H 2.598155 0.244394 1.366559
H 3.120657 -1.382599 -0.316722
H -3.960644 0.585144 0.120519
H -3.381012 -0.339621 -1.266325
H -3.772899 -1.165087 0.243593
el energy= -0.128749799434
zpe= 0.082727
th energy= 0.092826
th enthalpy= 0.093771
free energy= 0.047524

4mchm_7/coords
t5
C 0.410098 1.257065 -0.070819

H 0.690757 1.340405 0.998234
C 1.030920 -0.019506 -0.667417
H 0.839297 -0.026521 -1.769056
C 0.389342 -1.279878 -0.054727
H 0.651964 -1.349696 1.019173
C -1.135558 -1.262948 -0.214522
H -1.402981 -1.322753 -1.286387
C -1.747018 0.009066 0.408275
H -1.518056 0.011851 1.502406
C -1.114680 1.265501 -0.224088
H -1.532509 2.174532 0.246633
C 2.555690 -0.027278 -0.453718
O 2.925791 0.102214 0.928153
C -3.269160 0.019779 0.230069
H 0.843044 2.149874 -0.559574
H 0.804603 -2.186684 -0.532638
H -1.572529 -2.161732 0.257948
H -1.386720 1.326135 -1.294549
H 3.019623 -0.949855 -0.846555
H 3.043848 0.851838 -0.914880
H 2.401564 -0.515647 1.477775
H -3.732170 -0.856243 0.696602
H -3.717315 0.908158 0.688194
H -3.556555 0.017819 -0.826859
el energy= -0.128120732743
zpe= 0.083318
th energy= 0.093386
th enthalpy= 0.094330
free energy= 0.048277

4mchm_19/coords
t6
C 0.232778 -1.150490 0.602273
H -0.309471 -1.305005 1.554669
C 0.941475 0.215703 0.643693
H 1.502883 0.283883 1.613173
C -0.080790 1.364589 0.584024
H -0.663053 1.372180 1.526929
C -1.040390 1.235552 -0.604654
H -1.783962 2.053623 -0.571129
C -1.765041 -0.126708 -0.637032
H -2.301368 -0.202048 -1.617186

C -0.743536 -1.281046 -0.572409
H -0.176686 -1.315040 -1.522589
C 1.986922 0.345503 -0.477717
O 3.158023 -0.324734 0.043239
C -2.813601 -0.236394 0.475769
H 0.995074 -1.953094 0.550509
H 0.439024 2.339772 0.545593
H -0.482414 1.371097 -1.550206
H -1.275530 -2.248273 -0.504006
H 1.671867 -0.141533 -1.414443
H 2.259129 1.396515 -0.676659
H 3.811914 -0.457456 -0.664566
H -3.552946 0.567999 0.409169
H -3.352831 -1.187704 0.422817
H -2.352713 -0.177302 1.468348
el energy= -0.122318171097
zpe= 0.088632
th energy= 0.098960
th enthalpy= 0.099904
free energy= 0.052704

4mchm_21/coords
t7
C 0.117836 1.398654 0.570335
H -0.375873 2.386469 0.513263
C -0.935778 0.280591 0.673174
H -1.460001 0.387551 1.655874
C -0.271517 -1.108380 0.642039
H 0.276336 -1.271874 1.589025
C 0.684383 -1.286078 -0.543250
H 0.100769 -1.317476 -1.484275
C 1.740174 -0.166404 -0.641677
H 2.261540 -0.276699 -1.626756
C 1.057351 1.217272 -0.627389
H 0.491805 1.351238 -1.569035
C -1.991903 0.417895 -0.438996
O -3.110735 -0.452448 -0.202332
C 2.799107 -0.287177 0.460215
H 0.714851 1.412715 1.503935
H -1.061834 -1.885459 0.598065
H 1.185724 -2.269081 -0.468030
H 1.825187 2.013369 -0.619497

H -2.364575 1.452286 -0.532416
H -1.620802 0.069027 -1.420730
H -3.509259 -0.271727 0.668932
H 2.353463 -0.197486 1.457132
H 3.309494 -1.254879 0.416907
H 3.561131 0.493375 0.369562
el energy= -0.124969854263
zpe= 0.086424
th energy= 0.096483
th enthalpy= 0.097427
free energy= 0.051294

4mchm_22/coords
t8
C 0.114264 1.394284 0.584876
H -0.381517 2.381994 0.537349
C -0.939252 0.275861 0.678232
H -1.477249 0.378021 1.655479
C -0.262795 -1.107549 0.647834
H 0.307585 -1.248608 1.587150
C 0.678251 -1.281921 -0.550042
H 1.182431 -2.264254 -0.484947
C 1.732909 -0.160042 -0.649375
H 2.244429 -0.262628 -1.640498
C 1.051520 1.223942 -0.616435
H 1.820788 2.018769 -0.600786
C -1.992033 0.421999 -0.435301
O -3.170229 -0.340589 -0.125837
C 2.802390 -0.290637 0.440934
H 0.711298 1.402559 1.518377
H -1.031116 -1.903285 0.640286
H 0.088182 -1.305901 -1.486447
H 0.484631 1.371092 -1.555331
H -2.386693 1.452651 -0.502798
H -1.612190 0.107651 -1.422182
H -2.944541 -1.285240 -0.020707
H 3.567418 0.486657 0.344531
H 2.368594 -0.200145 1.443107
H 3.308254 -1.260237 0.389779
el energy= -0.125660459149
zpe= 0.085702
th energy= 0.095757

th enthalpy= 0.096701
free energy= 0.050416

4mchm_24/coords
t9
C -0.108486 1.268991 0.815927
H 0.628223 1.357461 1.637894
C -0.953425 -0.000004 1.038843
H -1.282136 -0.000006 2.112737
C -0.108480 -1.268993 0.815924
H 0.628239 -1.357452 1.637885
C 0.625485 -1.259931 -0.529800
H 1.243386 -2.168781 -0.628470
C 1.492457 0.000000 -0.726470
H 1.854845 0.000003 -1.785937
C 0.625491 1.259933 -0.529791
H -0.131051 1.295227 -1.344977
C -2.256174 -0.000006 0.215305
O -1.933321 0.000035 -1.192633
C 2.725061 -0.000005 0.186008
H -0.751098 2.166534 0.879104
H -0.751081 -2.166543 0.879114
H -0.131068 -1.295202 -1.344980
H 1.243404 2.168780 -0.628442
H -2.856478 -0.903226 0.427096
H -2.856495 0.903199 0.427120
H -2.758162 -0.000168 -1.712879
H 2.440958 0.000021 1.243721
H 3.346742 -0.883891 0.013217
H 3.346773 0.883854 0.013183
el energy= -0.117684907345
zpe= 0.093681
th energy= 0.103779
th enthalpy= 0.104724
free energy= 0.058764

4mchm_9/coords
c1
C -0.438832 -1.003790 0.966678
H -1.154977 -1.841299 0.848771
C -1.142250 0.314935 0.594481
H -1.939607 0.508533 1.360155

C -0.149601 1.491787 0.607720
H -0.648444 2.417877 0.266704
C 1.093067 1.219710 -0.248567
H 0.811610 1.150452 -1.315314
C 1.797431 -0.078769 0.195721
H 2.127000 0.044763 1.256780
C 0.816723 -1.266643 0.126758
H 1.315485 -2.187933 0.479796
C -1.855345 0.209397 -0.764871
O -3.114491 -0.434506 -0.461591
C 3.034610 -0.346167 -0.668971
H -0.171702 -0.980487 2.040323
H 0.158017 1.686489 1.654219
H 1.793183 2.072044 -0.174270
H 0.533511 -1.460960 -0.924679
H -2.078593 1.199599 -1.198508
H -1.296951 -0.399523 -1.493876
H -3.548551 -0.726731 -1.281512
H 2.774547 -0.475073 -1.724893
H 3.750828 0.480003 -0.606807
H 3.555763 -1.254467 -0.347857
el energy= -0.124623646510
zpe= 0.086359
th energy= 0.096703
th enthalpy= 0.097647
free energy= 0.050366

4mchm_11/coords
c2
C -0.310281 -1.119429 0.132630
H -1.015033 -1.936728 -0.118774
C -0.951291 0.229957 -0.238580
H -1.187711 0.218966 -1.333354
C 0.015661 1.389847 0.060693
H -0.436970 2.353284 -0.238337
C 1.345457 1.194665 -0.678929
H 1.174016 1.269150 -1.770332
C 2.011478 -0.162726 -0.367484
H 2.862667 -0.293574 -1.083312
C 1.017685 -1.319064 -0.606168
H 0.825024 -1.412225 -1.692539
C -2.276153 0.432765 0.516971

O -3.215228 -0.435937 -0.154813
C 2.588633 -0.196540 1.052415
H -0.145894 -1.179309 1.224308
H 0.201944 1.458268 1.149227
H 2.036860 2.018504 -0.422305
H 1.474729 -2.277006 -0.296493
H -2.211736 0.143033 1.578572
H -2.645729 1.469917 0.436274
H -4.071697 -0.423231 0.308322
H 3.093179 -1.146940 1.254348
H 3.317678 0.605181 1.206502
H 1.803365 -0.076646 1.807111
el energy= -0.123146032459
zpe= 0.087903
th energy= 0.098216
th enthalpy= 0.099160
free energy= 0.052145

4mchm_13/coords
c3
C -0.032109 1.402645 0.065279
H -0.201038 1.446122 1.158443
C 0.950615 0.265736 -0.270561
H 1.150000 0.279892 -1.369933
C 0.336586 -1.097536 0.095210
H 1.049778 -1.905336 -0.159485
C -0.997808 -1.312311 -0.627032
H -0.822659 -1.389837 -1.717016
C -2.008008 -0.176711 -0.357198
H -2.866542 -0.311413 -1.063478
C -1.370882 1.197687 -0.655291
H -2.072048 2.004077 -0.370328
C 2.282708 0.478343 0.470157
O 3.262940 -0.494433 0.074587
C -2.564509 -0.243212 1.069524
H 0.398885 2.379953 -0.219774
H 0.187240 -1.164999 1.189755
H -1.433508 -2.281628 -0.320857
H -1.221713 1.296273 -1.747700
H 2.698420 1.485729 0.292439
H 2.198827 0.303712 1.558885
H 3.377652 -0.490745 -0.894582

H -3.051186 -1.204743 1.262988
H -1.771089 -0.123323 1.815927
H -3.304091 0.543885 1.247495
el energy= -0.126292857312
zpe= 0.085174
th energy= 0.095241
th enthalpy= 0.096185
free energy= 0.050075

4mchm_15/coords
c4
C -0.479115 -0.927939 1.013282
H -0.212198 -0.877715 2.085437
C -1.148159 0.394713 0.593366
H -1.920325 0.647077 1.362711
C -0.125221 1.545504 0.548707
H -0.601382 2.465775 0.162360
C 1.109305 1.204894 -0.294526
H 0.826034 1.097206 -1.357943
C 1.780287 -0.090975 0.205018
H 2.113417 0.068246 1.260088
C 0.768572 -1.253661 0.183670
H 1.242928 -2.174455 0.570134
C -1.865470 0.247389 -0.761349
O -2.994758 -0.634996 -0.656077
C 3.009464 -0.426347 -0.647057
H -1.215400 -1.751554 0.912016
H 0.190765 1.782187 1.584041
H 1.830901 2.041665 -0.256753
H 0.476151 -1.481373 -0.859372
H -2.212127 1.217785 -1.155805
H -1.237396 -0.256618 -1.519764
H -3.620063 -0.314873 0.020043
H 2.744659 -0.594699 -1.696506
H 3.746562 0.383084 -0.621229
H 3.507551 -1.333231 -0.287504
el energy= -0.127235891754
zpe= 0.084208
th energy= 0.094266
th enthalpy= 0.095210
free energy= 0.049069

4mchm_16/coords
c5
C -0.249760 1.264835 -0.225816
H -0.744873 2.170250 -0.619264
C -0.962129 0.000035 -0.739750
H -0.939704 0.000074 -1.857230
C -0.249773 -1.264807 -0.225903
H -0.356965 -1.312936 0.878159
C 1.232665 -1.266924 -0.613956
H 1.722760 -2.165927 -0.196187
C 1.974119 -0.000001 -0.136492
H 2.988199 0.000009 -0.610750
C 1.232679 1.266962 -0.613868
H 1.329475 1.349949 -1.713042
C -2.439473 0.000032 -0.304106
O -2.442222 -0.000056 1.140821
C 2.168447 -0.000056 1.383819
H -0.356952 1.312890 0.878250
H -0.744897 -2.170190 -0.619416
H 1.329462 -1.349834 -1.713138
H 1.722783 2.165931 -0.196033
H -2.968908 0.902442 -0.655486
H -2.968926 -0.902335 -0.655599
H -3.359604 -0.000120 1.468230
H 2.720741 -0.883978 1.716889
H 2.720727 0.883853 1.716951
H 1.203808 -0.000083 1.907532
el energy= -0.121746334311
zpe= 0.089360
th energy= 0.099601
th enthalpy= 0.100546
free energy= 0.053942

4mchm_17/coords
c6
C -0.264668 1.254097 -0.251363
H -0.768471 2.142774 -0.675270
C -0.969199 -0.027578 -0.731048
H -0.947437 -0.049881 -1.848606
C -0.241722 -1.279161 -0.203683
H -0.333516 -1.328234 0.899469
C 1.239944 -1.271704 -0.596901

H 1.741667 -2.160407 -0.170691
C 1.971690 0.009172 -0.143485
H 2.983260 0.009050 -0.624077
C 1.217787 1.260891 -0.638903
H 1.700558 2.171453 -0.237144
C -2.443861 -0.029812 -0.287962
O -2.598991 0.106732 1.133709
C 2.178339 0.037398 1.374972
H -0.374279 1.347087 0.847843
H -0.726466 -2.193016 -0.594783
H 1.331060 -1.369062 -1.695978
H 1.312910 1.327644 -1.739708
H -2.994995 0.848354 -0.673704
H -2.963857 -0.953165 -0.600536
H -1.993734 -0.506121 1.599467
H 2.748823 0.920133 1.682392
H 1.222747 0.065818 1.910489
H 2.723800 -0.846103 1.721391
el energy= -0.125875712315
zpe= 0.085522
th energy= 0.095573
th enthalpy= 0.096517
free energy= 0.050458

4mchm_23/coords
c7
C 0.491627 -1.270812 -0.960927
H 1.103824 -2.166024 -0.745489
C 1.352548 0.000216 -0.821572
H 2.089259 0.000426 -1.669232
C 0.491618 1.271310 -0.960291
H 1.103807 2.166426 -0.744431
C -0.734459 1.256485 -0.039686
H -0.391623 1.266501 1.018019
C -1.594237 0.000075 -0.283313
H -1.940291 0.000341 -1.345071
C -0.734455 -1.256454 -0.040323
H -0.391621 -1.267016 1.017379
C 2.207729 -0.000107 0.460632
O 1.339525 -0.000501 1.614662
C -2.826139 -0.000163 0.629699
H 0.163898 -1.367470 -2.014048

H 0.163877 1.368486 -2.013362
H -1.333846 2.170201 -0.188711
H -1.333840 -2.170093 -0.189818
H 2.842456 -0.903269 0.510949
H 2.842401 0.903062 0.511444
H 1.880918 -0.000198 2.425889
H -3.449533 0.883003 0.458199
H -3.449574 -0.883200 0.457679
H -2.541703 -0.000481 1.687997
el energy= -0.119617958901
zpe= 0.091808
th energy= 0.101908
th enthalpy= 0.102852
free energy= 0.056860

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.312279 -1.116161 0.123203
H 1.001313 -1.945256 -0.122180
C 0.954593 0.233415 -0.248392
H 1.178218 0.233100 -1.344762
C -0.015343 1.388437 0.060508
H -0.194608 1.452327 1.150764
C -1.349158 1.198224 -0.672472
H -1.185113 1.281362 -1.764376
C -2.012596 -0.160990 -0.365723
H -2.865961 -0.290129 -1.079498
C -1.017627 -1.314372 -0.614320
H -1.473119 -2.274504 -0.308482
C 2.281625 0.441110 0.502723
O 3.331963 -0.349265 -0.076196
C -2.584797 -0.203464 1.055631
H 0.142418 -1.167751 1.215842
H 0.436145 2.353880 -0.235750
H -2.039219 2.020298 -0.405778
H -0.828574 -1.400066 -1.701888
H 2.670794 1.470362 0.385344
H 2.206164 0.200237 1.576768
H 3.083799 -1.293945 -0.083442
H -3.318352 0.593725 1.214172
H -3.084226 -1.156806 1.256475
H -1.799241 -0.079909 1.809422

el energy= -0.126529163966
zpe= 0.084911
th energy= 0.094990
th enthalpy= 0.095934
free energy= 0.049693

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.474684 -0.928509 1.019421
H 1.201676 -1.760025 0.958843
C 1.150540 0.390821 0.598798
H 1.935518 0.636587 1.359190
C 0.126709 1.540727 0.568623
H -0.188467 1.767169 1.606367
C -1.106842 1.209251 -0.279950
H -0.822693 1.119370 -1.344812
C -1.777434 -0.094579 0.198502
H -2.120508 0.051800 1.252430
C -0.762543 -1.255592 0.174386
H -1.239080 -2.179695 0.550247
C 1.861531 0.258528 -0.760241
O 3.069423 -0.509082 -0.630074
C -2.997702 -0.424980 -0.667928
H 0.186137 -0.859657 2.086731
H 0.604059 2.465332 0.193122
H -1.830104 2.044186 -0.230186
H -0.463355 -1.471885 -0.868483
H 1.222315 -0.207491 -1.529337
H 2.236173 1.230589 -1.130792
H 2.867864 -1.403569 -0.293010
H -3.737607 0.382167 -0.639033
H -2.724119 -0.579311 -1.717238
H -3.496859 -1.336916 -0.323124
el energy= -0.127919297030
zpe= 0.083492
th energy= 0.093550
th enthalpy= 0.094494
free energy= 0.048191

PM6-SMD

4mchm_1/coords

t1
C 0.191791 1.397176 0.209505
H 0.631435 2.311209 -0.234337
C 1.039038 0.165924 -0.160740
H 1.075999 0.083283 -1.276152
C 0.404173 -1.119337 0.402968
H 1.000756 -2.000758 0.097314
C -1.044969 -1.280376 -0.069060
H -1.484747 -2.190606 0.380687
C -1.895455 -0.047463 0.299506
H -1.923639 0.039912 1.413758
C -1.254899 1.234596 -0.270247
H -1.848929 2.119232 0.026767
C 2.475251 0.336407 0.356741
O 3.418633 -0.348313 -0.499569
C -3.329198 -0.207909 -0.210411
H 0.215000 1.560683 1.304326
H 0.439932 -1.106714 1.509951
H -1.072177 -1.450010 -1.161698
H -1.288382 1.217236 -1.376082
H 2.825491 1.385579 0.318547
H 2.612636 -0.043532 1.384865
H 3.095444 -1.261139 -0.709328
H -3.373880 -0.326160 -1.299063
H -3.819129 -1.086203 0.225861
H -3.949274 0.660385 0.041567
el energy= -0.137860711222
zpe= 0.072321
th energy= 0.082564
th enthalpy= 0.083508
free energy= 0.036784

4mchm_3/coords
t2
C -0.163668 1.428855 0.179708
H -0.216429 1.588946 1.274227
C -1.031487 0.221381 -0.222002
H -1.033568 0.135244 -1.338431
C -0.451558 -1.078950 0.364150
H -0.514313 -1.061206 1.469236
C 1.003306 -1.281203 -0.074216
H 1.405849 -2.206097 0.379958

C 1.881323 -0.075680 0.319674
H 1.890027 0.002505 1.434767
C 1.292688 1.229752 -0.253565
H 1.900886 2.093866 0.074195
C -2.475138 0.452006 0.244738
O -3.371967 -0.564164 -0.259622
C 3.319494 -0.273549 -0.164937
H -0.565338 2.355782 -0.273200
H -1.063870 -1.943067 0.043671
H 1.050715 -1.445508 -1.167271
H 1.361378 1.224746 -1.357960
H -2.598096 0.379285 1.341133
H -2.867134 1.429200 -0.094551
H -3.140043 -0.798827 -1.193409
H 3.966240 0.559596 0.134118
H 3.765235 -1.186868 0.245639
H 3.384434 -0.349956 -1.256445
el energy= -0.137915958691
zpe= 0.072222
th energy= 0.082472
th enthalpy= 0.083416
free energy= 0.037029

4mchm_5/coords
t3
C -0.369151 -1.307366 0.009221
H -0.770646 -2.241792 -0.428789
C -1.031920 -0.089693 -0.659957
H -0.850882 -0.152660 -1.763705
C -0.428853 1.228795 -0.139152
H -0.865269 2.086464 -0.687203
C 1.095863 1.251313 -0.277574
H 1.376810 1.279782 -1.347513
C 1.747604 0.033835 0.408534
H 1.522627 0.082997 1.502338
C 1.154170 -1.274470 -0.151227
H 1.603407 -2.145238 0.362311
C -2.553172 -0.104193 -0.447223
O -2.930165 0.102108 0.934906
C 3.266542 0.060931 0.224767
H -0.634808 -1.343458 1.082654
H -0.719380 1.381060 0.922977

H 1.495058 2.187705 0.156637
H 1.425311 -1.389800 -1.217843
H -3.055297 0.681831 -1.041765
H -3.007237 -1.083439 -0.688649
H -2.385195 0.837973 1.327034
H 3.560138 0.021124 -0.830407
H 3.709201 0.972022 0.644343
H 3.750987 -0.786341 0.723999
el energy= -0.137573304844
zpe= 0.072801
th energy= 0.082837
th enthalpy= 0.083781
free energy= 0.037944

4mchm_6/coords
t4
C 0.191988 1.396950 0.209798
H 0.215019 1.560350 1.304631
C 1.039054 0.165570 -0.160381
H 1.076077 0.082949 -1.275800
C 0.403875 -1.119609 0.403199
H 1.000338 -2.001112 0.097576
C -1.045223 -1.280349 -0.069077
H -1.072241 -1.449909 -1.161730
C -1.895545 -0.047282 0.299386
H -1.923890 0.040078 1.413627
C -1.254668 1.234684 -0.270224
H -1.287970 1.217365 -1.376062
C 2.475287 0.335664 0.357195
O 3.418746 -0.347380 -0.500349
C -3.329257 -0.207545 -0.210744
H 0.631881 2.310925 -0.233902
H 0.439460 -1.107012 1.510177
H -1.485269 -2.190505 0.380551
H -1.848551 2.119426 0.026753
H 2.825242 1.384997 0.320639
H 2.612922 -0.045829 1.384718
H 3.096337 -1.260398 -0.710600
H -3.948547 0.662059 0.038625
H -3.373578 -0.328724 -1.299086
H -3.820277 -1.084116 0.227759
el energy= -0.137861054568

zpe= 0.072319
th energy= 0.082562
th enthalpy= 0.083506
free energy= 0.036755

4mchm_7/coords
t5
C 0.369132 1.307398 0.009210
H 0.634737 1.343389 1.082666
C 1.031939 0.089766 -0.660029
H 0.851007 0.152824 -1.763765
C 0.428909 -1.228797 -0.139383
H 0.719636 -1.381265 0.922694
C -1.095827 -1.251314 -0.277537
H -1.376915 -1.279880 -1.347439
C -1.747533 -0.033816 0.408545
H -1.522526 -0.082914 1.502346
C -1.154190 1.274471 -0.151298
H -1.603460 2.145253 0.362171
C 2.553184 0.104230 -0.447103
O 2.929950 -0.102148 0.935038
C -3.266476 -0.060975 0.224833
H 0.770629 2.241854 -0.428691
H 0.865225 -2.086356 -0.687688
H -1.494928 -2.187665 0.156901
H -1.425302 1.389683 -1.217928
H 3.055313 -0.681770 -1.041694
H 3.007324 1.083476 -0.688437
H 2.384870 -0.838250 1.326953
H -3.709163 -0.971570 0.645423
H -3.750838 0.786878 0.723143
H -3.560046 -0.022275 -0.830385
el energy= -0.137573184422
zpe= 0.072804
th energy= 0.082838
th enthalpy= 0.083782
free energy= 0.037948

4mchm_19/coords
t6
C 0.235093 -1.158502 0.601374
H -0.304075 -1.316202 1.555928

C 0.953785 0.202852 0.649019
H 1.513286 0.264588 1.618445
C -0.064420 1.356499 0.611804
H -0.632317 1.365003 1.563303
C -1.035394 1.248563 -0.567686
H -1.776981 2.068087 -0.514557
C -1.759751 -0.111811 -0.633376
H -2.272803 -0.169006 -1.628340
C -0.743894 -1.271027 -0.572011
H -0.178712 -1.303111 -1.524819
C 1.977318 0.337660 -0.487987
O 3.250062 -0.244790 -0.115225
C -2.837502 -0.239769 0.446822
H 0.979675 -1.977061 0.548502
H 0.461896 2.329923 0.578273
H -0.486432 1.411780 -1.515971
H -1.279056 -2.237880 -0.518408
H 1.653126 -0.156163 -1.421872
H 2.238988 1.388398 -0.711622
H 3.113611 -1.074689 0.407232
H -3.579413 0.563642 0.375717
H -3.382085 -1.187150 0.363317
H -2.420615 -0.198637 1.458918
el energy= -0.135203389086
zpe= 0.075590
th energy= 0.085454
th enthalpy= 0.086399
free energy= 0.041112

4mchm_21/coords
t7
C 0.097254 1.391830 0.582700
H -0.405442 2.376562 0.523244
C -0.949115 0.265434 0.671445
H -1.492196 0.367954 1.647001
C -0.263766 -1.113100 0.652378
H 0.287064 -1.252527 1.603623
C 0.695236 -1.287126 -0.529696
H 0.117076 -1.335350 -1.473390
C 1.738650 -0.156185 -0.639844
H 2.237083 -0.257055 -1.638625
C 1.048304 1.222728 -0.606289

H 0.489835 1.370372 -1.551637
C -1.986620 0.409877 -0.452091
O -3.128029 -0.448600 -0.217103
C 2.826978 -0.275960 0.431034
H 0.678651 1.417770 1.525401
H -1.025562 -1.914763 0.638332
H 1.207503 -2.264758 -0.451060
H 1.810188 2.024874 -0.589712
H -2.357195 1.446685 -0.544057
H -1.615668 0.066403 -1.434866
H -3.506009 -0.277984 0.682439
H 2.421978 -0.198307 1.445826
H 3.351629 -1.236031 0.367750
H 3.583770 0.509961 0.328724
el energy= -0.134920207323
zpe= 0.075696
th energy= 0.085624
th enthalpy= 0.086568
free energy= 0.041147

4mchm_22/coords
t8
C 0.064483 1.356539 0.611770
H -0.461793 2.329959 0.578263
C -0.953759 0.202926 0.649016
H -1.513181 0.264746 1.618505
C -0.235166 -1.158469 0.601360
H 0.303917 -1.316318 1.555934
C 0.743832 -1.271065 -0.571964
H 1.278987 -2.237935 -0.518274
C 1.759719 -0.111891 -0.633378
H 2.272750 -0.169151 -1.628346
C 1.035418 1.248531 -0.567723
H 1.777027 2.068028 -0.514666
C -1.977294 0.337783 -0.487948
O -3.249995 -0.244844 -0.115193
C 2.837473 -0.239790 0.446830
H 0.632403 1.364984 1.563275
H -0.979834 -1.976978 0.548448
H 0.178682 -1.303206 -1.524785
H 0.486426 1.411732 -1.516000
H -2.239073 1.388473 -0.711588

H -1.653200 -0.156011 -1.421891
H -3.113432 -1.074907 0.406945
H 3.580336 0.562651 0.374566
H 2.420762 -0.196810 1.458926
H 3.380955 -1.187894 0.364455
el energy= -0.135203537831
zpe= 0.075593
th energy= 0.085455
th enthalpy= 0.086399
free energy= 0.041121

4mchm_24/coords
t9
C 0.102047 1.409502 -0.553233
H -0.584193 1.660095 -1.387935
C 0.966527 0.209996 -0.981525
H 1.267178 0.394429 -2.051860
C 0.163162 -1.103225 -0.961451
H -0.534060 -1.106635 -1.823538
C -0.628497 -1.317464 0.332036
H -1.227945 -2.244376 0.255607
C -1.537596 -0.126498 0.692760
H -1.926158 -0.301211 1.729675
C -0.719873 1.179973 0.718611
H -0.051673 1.169754 1.600803
C 2.294774 0.108387 -0.215210
O 2.176643 -0.246170 1.180295
C -2.747208 -0.025347 -0.240123
H 0.739971 2.305947 -0.426919
H 0.838695 -1.963963 -1.132817
H 0.079920 -1.503505 1.175844
H -1.395682 2.042160 0.879963
H 2.959040 -0.648847 -0.675250
H 2.829036 1.077193 -0.182274
H 1.448106 -0.927690 1.304425
H -2.456542 0.136356 -1.283879
H -3.353842 -0.937869 -0.214867
H -3.405002 0.805573 0.039479
el energy= -0.134896500726
zpe= 0.076297
th energy= 0.085800
th enthalpy= 0.086744

free energy= 0.042526

4mchm_9/coords
c1
C -0.465157 -0.922239 1.035990
H -1.189914 -1.756698 0.987524
C -1.147041 0.391079 0.608813
H -1.920971 0.643257 1.378268
C -0.125654 1.543723 0.554637
H -0.606011 2.463777 0.168502
C 1.104532 1.204830 -0.294183
H 0.816577 1.109730 -1.358316
C 1.782134 -0.091950 0.192493
H 2.136462 0.068281 1.240649
C 0.771254 -1.256430 0.195226
H 1.251469 -2.173264 0.586262
C -1.862171 0.262303 -0.743716
O -3.013240 -0.593491 -0.508183
C 2.992619 -0.430465 -0.680211
H -0.181066 -0.848327 2.104738
H 0.188443 1.792716 1.587799
H 1.824582 2.044046 -0.260525
H 0.472894 -1.500257 -0.841762
H -2.234027 1.233139 -1.117700
H -1.237106 -0.205480 -1.523532
H -3.475092 -0.764939 -1.365887
H 2.719014 -0.599704 -1.727908
H 3.736598 0.374521 -0.672945
H 3.500971 -1.337979 -0.333988
el energy= -0.134683033451
zpe= 0.075553
th energy= 0.085701
th enthalpy= 0.086645
free energy= 0.040541

4mchm_11/coords
c2
C -0.274063 -1.152101 0.171447
H -0.943657 -2.005472 -0.051393
C -0.964721 0.171488 -0.205867
H -1.210385 0.145497 -1.297172
C -0.025456 1.362012 0.057267

H -0.512817 2.308685 -0.246007
C 1.297453 1.198936 -0.698333
H 1.113251 1.263806 -1.788715
C 2.013966 -0.131517 -0.388623
H 2.840455 -0.248205 -1.136637
C 1.052814 -1.323916 -0.574903
H 0.856955 -1.464665 -1.655826
C -2.274392 0.345309 0.578348
O -3.385757 -0.240724 -0.138176
C 2.651332 -0.123697 1.003215
H -0.097851 -1.189417 1.264082
H 0.165084 1.463066 1.143208
H 1.965307 2.050052 -0.465595
H 1.544970 -2.258413 -0.243901
H -2.240569 -0.109486 1.584458
H -2.579708 1.404099 0.680875
H -3.150316 -1.148381 -0.456934
H 3.208484 -1.047023 1.198316
H 3.357564 0.706378 1.119909
H 1.907705 -0.023813 1.801431
el energy= -0.135985858296
zpe= 0.074387
th energy= 0.084522
th enthalpy= 0.085466
free energy= 0.039206

4mchm_13/coords
c3
C -0.000925 1.384952 0.065285
H -0.166564 1.459350 1.157554
C 0.960944 0.223423 -0.244886
H 1.186429 0.224666 -1.340690
C 0.309976 -1.122904 0.120962
H 0.995622 -1.954894 -0.126247
C -1.022941 -1.311878 -0.610783
H -0.840590 -1.413192 -1.698450
C -2.012215 -0.152320 -0.371969
H -2.850893 -0.270293 -1.106001
C -1.339015 1.205600 -0.658927
H -2.023110 2.030613 -0.382669
C 2.278840 0.428444 0.517198
O 3.302429 -0.462943 0.020068

C -2.619208 -0.203740 1.032536
H 0.455809 2.349359 -0.230068
H 0.150177 -1.183745 1.214851
H -1.483796 -2.269288 -0.301558
H -1.185911 1.308148 -1.751218
H 2.652667 1.465045 0.430944
H 2.208445 0.159628 1.587273
H 3.501322 -0.257257 -0.927930
H -3.158279 -1.142282 1.204891
H -1.858867 -0.122183 1.817034
H -3.334634 0.610400 1.195250
el energy= -0.135725494873
zpe= 0.074579
th energy= 0.084748
th enthalpy= 0.085693
free energy= 0.039398

4mchm_15/coords
c4
C -0.466094 -0.956721 0.989330
H -0.198550 -0.913243 2.063954
C -1.148865 0.364700 0.590493
H -1.926165 0.596100 1.366053
C -0.135999 1.524884 0.568586
H -0.619809 2.447103 0.191730
C 1.108408 1.211948 -0.269223
H 0.836444 1.135111 -1.338897
C 1.787044 -0.089379 0.203232
H 2.116715 0.050171 1.262426
C 0.784418 -1.260086 0.157550
H 1.264894 -2.184773 0.529127
C -1.869099 0.256540 -0.761585
O -3.032658 -0.599907 -0.663121
C 3.019633 -0.398849 -0.648590
H -1.185584 -1.793172 0.905941
H 0.162379 1.759442 1.609785
H 1.821595 2.055477 -0.209076
H 0.503054 -1.476130 -0.890325
H -2.211167 1.241187 -1.129228
H -1.264547 -0.233855 -1.545439
H -3.570244 -0.357516 0.133301
H 2.770137 -0.557916 -1.703840

H 3.751635 0.416517 -0.615810
H 3.533798 -1.303479 -0.303497
el energy= -0.137067988613
zpe= 0.073444
th energy= 0.083419
th enthalpy= 0.084363
free energy= 0.038731

4mchm_16/coords
c5
C -0.217175 1.320780 -0.001046
H -0.685772 2.292066 -0.251040
C -0.972223 0.177708 -0.703203
H -0.958864 0.371626 -1.806422
C -0.293295 -1.178944 -0.435514
H -0.407952 -1.450106 0.636503
C 1.190160 -1.157621 -0.814098
H 1.653344 -2.127218 -0.548689
C 1.970645 -0.004504 -0.150226
H 2.976555 0.049398 -0.640867
C 1.261118 1.341735 -0.401768
H 1.353057 1.604171 -1.473963
C -2.444985 0.133924 -0.268020
O -2.610692 -0.233581 1.121730
C 2.198282 -0.259867 1.341870
H -0.306760 1.218530 1.096984
H -0.810122 -1.979152 -0.999700
H 1.290857 -1.076929 -1.914264
H 1.783255 2.150899 0.143213
H -2.937962 1.122043 -0.329297
H -3.025534 -0.593038 -0.866286
H -1.979574 -0.967308 1.356997
H 2.782707 -1.171452 1.510512
H 2.746302 0.563097 1.814443
H 1.256843 -0.377250 1.890066
el energy= -0.135590903885
zpe= 0.074826
th energy= 0.084801
th enthalpy= 0.085745
free energy= 0.039995

4mchm_17/coords

c6
C -0.217162 1.320843 -0.000918
H -0.685742 2.292134 -0.250918
C -0.972208 0.177816 -0.703158
H -0.958856 0.371861 -1.806362
C -0.293309 -1.178861 -0.435583
H -0.407877 -1.450035 0.636447
C 1.190128 -1.157543 -0.814244
H 1.653294 -2.127186 -0.548989
C 1.970636 -0.004516 -0.150226
H 2.976547 0.049466 -0.640896
C 1.261126 1.341768 -0.401633
H 1.783299 2.150859 0.143424
C -2.444976 0.133932 -0.268010
O -2.610686 -0.233697 1.121699
C 2.198289 -0.260046 1.341842
H -0.306760 1.218528 1.097091
H -0.810181 -1.979009 -0.999801
H 1.290792 -1.076719 -1.914396
H 1.353063 1.604292 -1.473815
H -2.938008 1.121999 -0.329172
H -3.025390 -0.593016 -0.866447
H -1.979695 -0.967644 1.356852
H 2.746570 0.562744 1.814430
H 1.256870 -0.377212 1.890123
H 2.782421 -1.171836 1.510411
el energy= -0.135591036725
zpe= 0.074829
th energy= 0.084802
th enthalpy= 0.085746
free energy= 0.039999

4mchm_23/coords
c7
C 0.493267 -0.803842 -1.331020
H 1.122516 -1.704814 -1.467673
C 1.333921 0.343784 -0.743159
H 2.027928 0.694939 -1.558981
C 0.459584 1.553363 -0.362040
H 1.061536 2.283212 0.214254
C -0.812023 1.209985 0.420655
H -0.558074 0.919947 1.456930

C -1.622495 0.087642 -0.256682
H -1.970995 0.456558 -1.252867
C -0.733457 -1.150285 -0.482775
H -0.411393 -1.575157 0.496764
C 2.265591 -0.124535 0.385495
O 1.601770 -0.662525 1.550530
C -2.849214 -0.274141 0.583396
H 0.168737 -0.522520 -2.353390
H 0.178377 2.085283 -1.294116
H -1.438145 2.117135 0.523853
H -1.314065 -1.956159 -0.969824
H 2.960462 -0.907860 0.026081
H 2.857368 0.712927 0.802841
H 0.829610 -1.242450 1.270080
H -3.499312 0.592929 0.748286
H -3.460784 -1.043730 0.097863
H -2.578960 -0.661875 1.572438
el energy= -0.137277764045
zpe= 0.073810
th energy= 0.083396
th enthalpy= 0.084340
free energy= 0.039744

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.273975 -1.151995 0.171647
H 0.943575 -2.005489 -0.050553
C 0.964695 0.171543 -0.205778
H 1.210238 0.145682 -1.297101
C 0.025476 1.362093 0.057350
H -0.164849 1.463462 1.143270
C -1.297498 1.199043 -0.698124
H -1.113489 1.264375 -1.788509
C -2.013960 -0.131544 -0.388731
H -2.840401 -0.248248 -1.136681
C -1.052646 -1.323814 -0.575110
H -1.544837 -2.258444 -0.244596
C 2.274444 0.345281 0.578343
O 3.385591 -0.240919 -0.138305
C -2.651235 -0.123975 1.003156
H 0.097521 -1.189025 1.264275
H 0.512961 2.308695 -0.246143

H -1.965442 2.050064 -0.465077
H -0.856500 -1.464216 -1.656034
H 2.579929 1.404053 0.680602
H 2.240666 -0.109366 1.584476
H 3.149705 -1.148504 -0.457405
H -3.356368 0.706934 1.120521
H -3.209540 -1.046745 1.197529
H -1.907400 -0.025666 1.801350
el energy= -0.135986014939
zpe= 0.074396
th energy= 0.084526
th enthalpy= 0.085470
free energy= 0.039223

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.435958 -1.032394 0.945224
H 1.137998 -1.880529 0.821875
C 1.145650 0.290037 0.598700
H 1.936467 0.469315 1.372693
C 0.158696 1.470751 0.645610
H -0.134601 1.652249 1.698770
C -1.090775 1.229095 -0.207314
H -0.818241 1.201433 -1.279316
C -1.798582 -0.079884 0.196405
H -2.133471 0.015121 1.258811
C -0.821209 -1.268993 0.101069
H -1.322891 -2.198281 0.430583
C 1.843206 0.212667 -0.768029
O 3.172563 -0.346407 -0.632981
C -3.030285 -0.319618 -0.679248
H 0.170684 -1.029998 2.020774
H 0.661280 2.402469 0.320929
H -1.785894 2.083420 -0.103746
H -0.541686 -1.445530 -0.955203
H 1.294078 -0.404262 -1.501172
H 2.037973 1.207019 -1.211004
H 3.148467 -1.161379 -0.070456
H -3.742896 0.510949 -0.613643
H -2.774464 -0.434119 -1.738736
H -3.569252 -1.226593 -0.381812
el energy= -0.137367342258

zpe= 0.073236
th energy= 0.083168
th enthalpy= 0.084112
free energy= 0.038527

B3LYP 6-31G(d') gas phase

4mchm_1/coords
t1

C	0.160027	1.430557	0.178119
H	0.550863	2.359928	-0.262048
C	1.040155	0.236528	-0.232715
H	1.039556	0.171623	-1.333359
C	0.459880	-1.076802	0.321690
H	1.076970	-1.919649	-0.011043
C	-1.004783	-1.274528	-0.097223
H	-1.399677	-2.203956	0.338740
C	-1.894573	-0.085345	0.310361
H	-1.879280	-0.021889	1.412207
C	-1.305936	1.228479	-0.237257
H	-1.913403	2.081235	0.099751
C	2.490458	0.448901	0.195493
O	3.279770	-0.616314	-0.324522
C	-3.349282	-0.283141	-0.133366
H	0.212267	1.559324	1.271866
H	0.523757	-1.056218	1.422715
H	-1.057806	-1.401178	-1.191181
H	-1.372829	1.217312	-1.337545
H	2.849482	1.423636	-0.181512
H	2.549669	0.482566	1.299092
H	4.185169	-0.505239	-0.007407
H	-3.421287	-0.353125	-1.228087
H	-3.773240	-1.205587	0.285718
H	-3.984051	0.553828	0.187655

el energy= -389.701445275
zpe= -389.469812
th energy= -389.460122
th enthalpy= -389.459178
free energy= -389.503976

4mchm_3/coords
t2

C	-0.159234	1.432255	0.177284

H -0.211363 1.561249 1.270716
C -1.041396 0.237446 -0.227335
H -1.028940 0.174619 -1.332088
C -0.459660 -1.074106 0.327418
H -0.521201 -1.048594 1.427912
C 1.003129 -1.275300 -0.095445
H 1.398217 -2.203843 0.341893
C 1.894582 -0.085496 0.307958
H 1.881542 -0.020837 1.409605
C 1.306234 1.228708 -0.239701
H 1.914702 2.080910 0.096611
C -2.498422 0.450785 0.203293
O -3.371168 -0.602742 -0.189154
C 3.348065 -0.285359 -0.138669
H -0.551617 2.361231 -0.262322
H -1.080953 -1.919332 0.006365
H 1.054616 -1.404519 -1.189453
H 1.372710 1.217613 -1.340157
H -2.565519 0.484943 1.298665
H -2.861125 1.423633 -0.175334
H -3.365618 -0.645821 -1.155401
H 3.984175 0.551296 0.180195
H 3.771951 -1.207644 0.280690
H 3.417981 -0.356560 -1.233478
el energy= -389.701995934
zpe= -389.470276
th energy= -389.460636
th enthalpy= -389.459691
free energy= -389.504392

4mchm_5/coords
t3
C 0.390987 -1.266748 0.043654
H 0.816594 -2.160742 0.523682
C 1.038495 -0.000008 0.634754
H 0.857055 0.000009 1.723946
C 0.390989 1.266743 0.043642
H 0.816634 2.160720 0.523682
C -1.136955 1.260651 0.205523
H -1.393172 1.312279 1.277086
C -1.782381 -0.000008 -0.398136
H -1.563657 0.000001 -1.479680

C -1.136975 -1.260664 0.205502
H -1.567079 -2.160996 -0.257436
C 2.557719 0.000001 0.458112
O 2.862551 0.000019 -0.934499
C -3.305905 0.000018 -0.220609
H 0.652736 -1.330651 -1.021504
H 0.652739 1.330640 -1.021513
H -1.567104 2.160977 -0.257386
H -1.393217 -1.312331 1.277062
H 2.986665 0.890917 0.951059
H 2.986682 -0.890913 0.951042
H 3.822869 -0.000065 -1.034069
H -3.579000 0.000056 0.844422
H -3.762478 0.887327 -0.679559
H -3.762523 -0.887293 -0.679498
el energy= -389.701075060
zpe= -389.469461
th energy= -389.459790
th enthalpy= -389.458846
free energy= -389.503582

4mchm_6/coords
t4
C 0.158217 1.429384 0.178316
H 0.219785 1.546481 1.272879
C 1.042937 0.245667 -0.252610
H 1.041053 0.192823 -1.353652
C 0.464036 -1.075938 0.285592
H 1.059245 -1.926495 -0.078425
C -1.005831 -1.271427 -0.118659
H -1.068937 -1.383028 -1.213308
C -1.891827 -0.088813 0.314245
H -1.863600 -0.038273 1.416431
C -1.311235 1.231293 -0.225896
H -1.389740 1.232182 -1.325334
C 2.498651 0.464296 0.184039
O 3.397693 -0.531206 -0.289074
C -3.350878 -0.286447 -0.114955
H 0.545288 2.363902 -0.253620
H 0.542328 -1.081350 1.386193
H -1.393075 -2.207477 0.309529
H -1.916144 2.079131 0.127278

H 2.872639 1.409643 -0.228831
H 2.547361 0.549079 1.285652
H 3.184473 -1.362105 0.155016
H -3.983326 0.545240 0.223230
H -3.435444 -0.343668 -1.209447
H -3.767868 -1.214526 0.298573
el energy= -389.701743954
zpe= -389.469990
th energy= -389.460316
th enthalpy= -389.459372
free energy= -389.504180

4mchm_7/coords
t5
C 0.386024 1.273650 -0.022265
H 0.655103 1.322552 1.042603
C 1.040507 0.022053 -0.634446
H 0.856384 0.032688 -1.723077
C 0.393894 -1.255586 -0.065345
H 0.629311 -1.332279 1.009280
C -1.133948 -1.255891 -0.230293
H -1.383375 -1.287620 -1.303624
C -1.785437 -0.009593 0.396799
H -1.570658 -0.031651 1.479085
C -1.142618 1.265876 -0.178478
H -1.574453 2.153676 0.306192
C 2.568047 0.026784 -0.456669
O 2.994893 0.043710 0.902049
C -3.308125 -0.012676 0.214440
H 0.807196 2.177135 -0.487171
H 0.826794 -2.145474 -0.547256
H -1.560598 -2.167590 0.212872
H -1.402247 1.341729 -1.247577
H 3.006899 -0.833859 -0.992819
H 2.991061 0.937336 -0.899454
H 2.759724 -0.804898 1.299544
H -3.762968 -0.910871 0.653452
H -3.769344 0.863105 0.690163
H -3.578031 0.008647 -0.851063
el energy= -389.701541928
zpe= -389.469782
th energy= -389.460160

th enthalpy= -389.459216
free energy= -389.503905

4mchm_19/coords
t6
C 0.281202 -1.086341 0.662962
H -0.279228 -1.221872 1.599481
C 0.941993 0.309704 0.686423
H 1.445418 0.430653 1.657206
C -0.125682 1.417189 0.552326
H -0.715398 1.443557 1.479750
C -1.072498 1.208104 -0.645236
H -1.839991 1.995884 -0.649546
C -1.744898 -0.183514 -0.646646
H -2.248925 -0.307074 -1.617770
C -0.665639 -1.284041 -0.534981
H -0.077567 -1.297399 -1.465138
C 2.047415 0.453027 -0.365549
O 3.059600 -0.507598 -0.078232
C -2.830103 -0.312356 0.436889
H 1.063319 -1.854639 0.654938
H 0.357588 2.402591 0.475244
H -0.509737 1.328922 -1.583195
H -1.144104 -2.271974 -0.467513
H 1.649447 0.306027 -1.383690
H 2.456298 1.478522 -0.321285
H 3.728685 -0.460061 -0.772969
H -3.603936 0.456840 0.310446
H -3.322597 -1.292421 0.381120
H -2.426819 -0.207401 1.451657
el energy= -389.694614631
zpe= -389.462473
th energy= -389.452903
th enthalpy= -389.451959
free energy= -389.496519

4mchm_21/coords
t7
C 0.124654 1.420022 0.548954
H -0.361959 2.403158 0.463580
C -0.942093 0.310547 0.677969
H -1.438842 0.438064 1.656177

C -0.286578 -1.087352 0.656964
H 0.264287 -1.233503 1.597418
C 0.667013 -1.283467 -0.535828
H 0.083027 -1.294028 -1.468028
C 1.748300 -0.184404 -0.637997
H 2.259860 -0.308998 -1.604844
C 1.076385 1.207190 -0.643729
H 0.517696 1.325672 -1.584149
C -2.049725 0.454816 -0.381855
O -3.082350 -0.515436 -0.249853
C 2.824049 -0.313386 0.454820
H 0.709397 1.453027 1.479298
H -1.072662 -1.852404 0.631639
H 1.142742 -2.272427 -0.466842
H 1.843468 1.995188 -0.646039
H -2.463679 1.478418 -0.337424
H -1.657877 0.311830 -1.395057
H -3.466801 -0.418285 0.632639
H 2.412376 -0.207576 1.466246
H 3.316397 -1.293724 0.403764
H 3.599334 0.455279 0.334658
el energy= -389.695562069
zpe= -389.463280
th energy= -389.453775
th enthalpy= -389.452831
free energy= -389.497230

4mchm_22/coords
t8
C 0.124556 1.422977 0.545748
H -0.361040 2.406138 0.458587
C -0.945682 0.318331 0.689827
H -1.446846 0.445163 1.660850
C -0.274974 -1.073576 0.680108
H 0.292733 -1.195413 1.613498
C 0.662458 -1.286271 -0.523075
H 1.139508 -2.274373 -0.450718
C 1.741684 -0.187002 -0.645465
H 2.241132 -0.319308 -1.617512
C 1.069897 1.204788 -0.651707
H 1.838511 1.991116 -0.661840
C -2.058279 0.458964 -0.366527

O -3.152073 -0.426326 -0.152779
C 2.830912 -0.310330 0.434687
H 0.715092 1.460562 1.472474
H -1.040950 -1.863405 0.706079
H 0.071157 -1.302505 -1.451496
H 0.506392 1.320164 -1.589452
H -2.488516 1.466351 -0.302723
H -1.660093 0.344633 -1.388661
H -2.854201 -1.325496 -0.341680
H 3.607650 0.453309 0.294938
H 2.434142 -0.190291 1.450400
H 3.318485 -1.293324 0.387915
el energy= -389.694481691
zpe= -389.462338
th energy= -389.452739
th enthalpy= -389.451794
free energy= -389.496460

4mchm_24/coords
t9
C -0.111744 1.273243 0.771950
H 0.587001 1.374748 1.615751
C -0.960311 0.000112 1.002887
H -1.266412 0.000206 2.062178
C -0.111769 -1.273075 0.772170
H 0.586987 -1.374443 1.615980
C 0.680656 -1.262692 -0.548117
H 1.310686 -2.163384 -0.602138
C 1.555610 -0.000070 -0.714540
H 1.941867 -0.000162 -1.745649
C 0.680708 1.262615 -0.548322
H -0.027199 1.312283 -1.383704
C -2.295170 0.000056 0.249147
O -2.099284 -0.000152 -1.164065
C 2.779390 -0.000022 0.218744
H -0.759183 2.161880 0.808856
H -0.759224 -2.161693 0.809245
H -0.027270 -1.312455 -1.383480
H 1.310781 2.163271 -0.602472
H -2.874522 -0.889707 0.555484
H -2.874463 0.889942 0.555239
H -2.967437 -0.000250 -1.587829

H 2.500382 0.000078 1.280053
H 3.404005 -0.886906 0.045818
H 3.404049 0.886802 0.045666
el energy= -389.693686457
zpe= -389.461446
th energy= -389.451944
th enthalpy= -389.450999
free energy= -389.495200

4mchm_9/coords
c1
C -0.489650 -0.876238 1.050624
H -1.225957 -1.687903 1.016419
C -1.158423 0.438141 0.592614
H -1.910860 0.716516 1.345359
C -0.113865 1.571754 0.508131
H -0.575283 2.485596 0.104996
C 1.126368 1.194651 -0.321165
H 0.850022 1.068019 -1.380154
C 1.788453 -0.102514 0.181154
H 2.123363 0.077742 1.217499
C 0.752718 -1.242010 0.221493
H 1.214568 -2.152041 0.631772
C -1.932824 0.276988 -0.720156
O -2.964818 -0.682555 -0.510598
C 3.018121 -0.475783 -0.655407
H -0.190692 -0.763376 2.104272
H 0.210057 1.818412 1.530641
H 1.852638 2.020359 -0.294833
H 0.457900 -1.493510 -0.809933
H -2.358992 1.254224 -1.010495
H -1.265453 -0.041513 -1.538503
H -3.415832 -0.831560 -1.351453
H 2.740495 -0.668199 -1.701624
H 3.764179 0.330351 -0.653284
H 3.503007 -1.382608 -0.269626
el energy= -389.698175289
zpe= -389.466358
th energy= -389.456740
th enthalpy= -389.455796
free energy= -389.500494

4mchm_11/coords
c2
C -0.340245 -1.103494 0.056080
H -1.036739 -1.899633 -0.231938
C -0.960583 0.266165 -0.276356
H -1.159382 0.294947 -1.360693
C 0.024126 1.400599 0.060317
H -0.401893 2.371491 -0.232821
C 1.380882 1.202018 -0.637870
H 1.230115 1.288679 -1.725193
C 2.024579 -0.170184 -0.336865
H 2.878589 -0.291403 -1.021008
C 1.014358 -1.298097 -0.645121
H 0.845450 -1.331589 -1.732802
C -2.302172 0.475257 0.421927
O -3.211841 -0.522720 -0.029765
C 2.584373 -0.256122 1.093911
H -0.214374 -1.183116 1.147798
H 0.167143 1.446327 1.151421
H 2.070523 2.011044 -0.356256
H 1.444089 -2.272329 -0.370114
H -2.162813 0.416728 1.517292
H -2.683832 1.487018 0.194083
H -4.043639 -0.413512 0.448609
H 3.076636 -1.223157 1.263559
H 3.328304 0.532180 1.271864
H 1.804641 -0.148769 1.858175
el energy= -389.698024431
zpe= -389.466174
th energy= -389.456541
th enthalpy= -389.455597
free energy= -389.500292

4mchm_13/coords
c3
C -0.025124 1.401696 0.061946
H -0.170984 1.445697 1.152451
C 0.961669 0.267028 -0.268146
H 1.152051 0.300286 -1.358047
C 0.339874 -1.101960 0.060253
H 1.039483 -1.900410 -0.216395
C -1.010810 -1.298885 -0.647370

H -0.838307 -1.333132 -1.734748
C -2.022672 -0.170888 -0.343270
H -2.873567 -0.292923 -1.031002
C -1.379380 1.202364 -0.641330
H -2.070800 2.010243 -0.361143
C 2.307866 0.475921 0.437113
O 3.278361 -0.516532 0.123066
C -2.588310 -0.257504 1.085213
H 0.402687 2.372825 -0.227716
H 0.209485 -1.179054 1.151068
H -1.441080 -2.272983 -0.373234
H -1.225620 1.290682 -1.728260
H 2.692702 1.487495 0.213461
H 2.176291 0.413117 1.525324
H 3.448494 -0.472066 -0.828043
H -3.079722 -1.225231 1.252917
H -1.812385 -0.148501 1.853049
H -3.334294 0.529588 1.259335
el energy= -389.698594192
zpe= -389.466650
th energy= -389.457070
th enthalpy= -389.456126
free energy= -389.500697

4mchm_15/coords
c4
C -0.494425 -0.883821 1.040634
H -0.206211 -0.784961 2.098566
C -1.158815 0.433267 0.586252
H -1.907746 0.716268 1.346863
C -0.117400 1.570973 0.511396
H -0.580487 2.482614 0.105037
C 1.126139 1.196459 -0.313540
H 0.853895 1.071839 -1.373588
C 1.787429 -0.100774 0.189201
H 2.115034 0.076370 1.228493
C 0.753593 -1.242163 0.216767
H 1.213536 -2.153810 0.625128
C -1.931697 0.276417 -0.736040
O -2.942038 -0.724477 -0.680680
C 3.023022 -0.468763 -0.640890
H -1.229099 -1.696955 0.985512

H 0.201117 1.819190 1.535237
H 1.850668 2.023348 -0.282397
H 0.463368 -1.488316 -0.816732
H -2.360906 1.252924 -1.024730
H -1.271019 -0.036186 -1.552284
H -3.559571 -0.481135 0.023135
H 2.752246 -0.657883 -1.689365
H 3.767283 0.338908 -0.630896
H 3.507114 -1.375970 -0.255212
el energy= -389.699091461
zpe= -389.467111
th energy= -389.457558
th enthalpy= -389.456613
free energy= -389.501157

4mchm_16/coords
c5
C -0.242946 1.267632 -0.215158
H -0.734854 2.160107 -0.630246
C -0.973741 -0.000003 -0.698255
H -0.961827 -0.000008 -1.802462
C -0.242944 -1.267633 -0.215147
H -0.345362 -1.339794 0.875202
C 1.241673 -1.261765 -0.618004
H 1.738778 -2.164288 -0.233308
C 1.992870 0.000000 -0.138709
H 2.983107 -0.000004 -0.620205
C 1.241674 1.261763 -0.618011
H 1.311273 1.315102 -1.716234
C -2.448351 -0.000002 -0.292036
O -2.538419 -0.000009 1.130541
C 2.232884 0.000004 1.381211
H -0.345363 1.339806 0.875192
H -0.734856 -2.160107 -0.630233
H 1.311268 -1.315109 -1.716228
H 1.738778 2.164287 -0.233315
H -2.947016 0.890909 -0.714549
H -2.947016 -0.890919 -0.714558
H -3.472403 0.000093 1.375040
H 2.804538 -0.886713 1.686782
H 2.804547 0.886719 1.686772
H 1.297044 0.000014 1.952678

el energy= -389.697809086
zpe= -389.465873
th energy= -389.456286
th enthalpy= -389.455342
free energy= -389.499875

4mchm_17/coords
c6
C -0.237350 1.285519 -0.130254
H -0.724654 2.206084 -0.483528
C -0.978089 0.058838 -0.693403
H -0.963619 0.123593 -1.795768
C -0.250799 -1.239922 -0.294161
H -0.324942 -1.377803 0.796139
C 1.232527 -1.219845 -0.702168
H 1.724750 -2.148934 -0.379922
C 1.993924 0.003990 -0.146276
H 2.979749 0.028732 -0.635614
C 1.247332 1.299642 -0.533484
H 1.749800 2.169838 -0.086656
C -2.460161 0.042553 -0.284288
O -2.673388 -0.016512 1.122930
C 2.248841 -0.097725 1.367827
H -0.342500 1.287475 0.962949
H -0.749612 -2.107535 -0.752340
H 1.292452 -1.202589 -1.801606
H 1.315790 1.431065 -1.625014
H -2.945679 0.972039 -0.607601
H -2.976528 -0.791834 -0.792160
H -2.391356 -0.887786 1.430923
H 2.840123 0.757261 1.721801
H 1.319688 -0.113619 1.950583
H 2.806297 -1.012186 1.611608
el energy= -389.698174462
zpe= -389.466160
th energy= -389.456591
th enthalpy= -389.455647
free energy= -389.500216

4mchm_23/coords
c7
C 0.455932 -1.270776 -0.944729

H 1.067282 -2.163006 -0.743781
C 1.329408 -0.000228 -0.827309
H 2.021059 -0.000455 -1.685904
C 0.455946 1.270271 -0.945387
H 1.067311 2.162596 -0.744903
C -0.783672 1.262332 -0.034849
H -0.466257 1.315659 1.014323
C -1.643080 -0.000058 -0.236762
H -1.998114 -0.000326 -1.282943
C -0.783685 -1.262351 -0.034194
H -0.466269 -1.315141 1.015004
C 2.267491 0.000083 0.384783
O 1.538905 0.000429 1.611219
C -2.873199 0.000186 0.678930
H 0.122827 -1.356835 -1.991120
H 0.122850 1.355794 -1.991825
H -1.388802 2.159384 -0.235839
H -1.388822 -2.159502 -0.234721
H 2.920337 -0.889682 0.327405
H 2.920369 0.889791 0.326922
H 2.174765 0.000795 2.338483
H -3.498021 0.887722 0.509624
H -3.498034 -0.887429 0.510082
H -2.574568 0.000455 1.736547
el energy= -389.697349432
zpe= -389.465286
th energy= -389.455739
th enthalpy= -389.454795
free energy= -389.499137

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.347262 -1.096918 0.016019
H 1.027150 -1.897130 -0.312204
C 0.963280 0.280621 -0.295317
H 1.158341 0.325787 -1.379531
C -0.027417 1.402571 0.065709
H -0.157439 1.434217 1.158910
C -1.392047 1.210121 -0.618368
H -1.256730 1.313252 -1.706164
C -2.026189 -0.168415 -0.327733
H -2.889176 -0.284990 -1.001001

C -1.016893 -1.286738 -0.669604
H -1.437328 -2.267733 -0.405048
C 2.309849 0.490243 0.411650
O 3.313131 -0.441799 0.027851
C -2.563580 -0.279309 1.109843
H 0.238370 -1.207103 1.107312
H 0.393092 2.378259 -0.218376
H -2.080842 2.011978 -0.315439
H -0.860914 -1.300054 -1.759282
H 2.716530 1.475545 0.151186
H 2.159476 0.480009 1.507360
H 3.049262 -1.313663 0.349367
H -3.310249 0.500884 1.309446
H -3.046463 -1.252113 1.273263
H -1.773715 -0.175823 1.864206
el energy= -389.698356837
zpe= -389.466288
th energy= -389.456703
th enthalpy= -389.455758
free energy= -389.500362

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.485524 -0.865385 1.059621
H 1.212827 -1.691391 1.061353
C 1.163498 0.442351 0.594839
H 1.914647 0.720245 1.348809
C 0.116647 1.574662 0.508893
H -0.206987 1.827378 1.530190
C -1.123826 1.196574 -0.320106
H -0.848030 1.070109 -1.378866
C -1.786634 -0.100287 0.181764
H -2.123019 0.078736 1.217757
C -0.750637 -1.239518 0.224393
H -1.211900 -2.150294 0.633279
C 1.942983 0.282896 -0.724380
O 3.032132 -0.628264 -0.627572
C -3.014118 -0.476082 -0.656751
H 0.179560 -0.744612 2.109847
H 0.579750 2.485251 0.100975
H -1.850469 2.021642 -0.293078
H -0.453206 -1.488056 -0.807282

H 1.274099 0.001837 -1.554989
H 2.397207 1.245086 -0.992478
H 2.672091 -1.519785 -0.535087
H -3.760474 0.329487 -0.655477
H -2.734746 -0.667706 -1.702529
H -3.499040 -1.383082 -0.271481
el energy= -389.698070734
zpe= -389.466208
th energy= -389.456580
th enthalpy= -389.455636
free energy= -389.500375

B3LYP-SMD 6-31G(d')
4mchm_1/coords
t1
C 0.162868 1.422509 0.178680
H 0.560261 2.347890 -0.262776
C 1.039384 0.225634 -0.232622
H 1.036103 0.164588 -1.333810
C 0.449319 -1.084030 0.322153
H 1.051610 -1.939490 -0.010214
C -1.016291 -1.275043 -0.096129
H -1.414350 -2.201929 0.342311
C -1.899258 -0.081559 0.311242
H -1.884933 -0.017937 1.412462
C -1.303207 1.227781 -0.237455
H -1.905708 2.083543 0.100509
C 2.485814 0.442859 0.204265
O 3.307728 -0.601397 -0.335445
C -3.352498 -0.271937 -0.137038
H 0.216888 1.549070 1.271978
H 0.515133 -1.062390 1.422323
H -1.069511 -1.400779 -1.189983
H -1.369598 1.215037 -1.337610
H 2.841554 1.424377 -0.150611
H 2.549693 0.447747 1.305241
H 4.203948 -0.472222 0.004836
H -3.421903 -0.337574 -1.232494
H -3.783402 -1.193471 0.278144
H -3.984399 0.567429 0.184678
el energy= -389.707393005
zpe= -389.476599

th energy= -389.466794
th enthalpy= -389.465850
free energy= -389.510893

4mchm_3/coords
t2
C -0.162694 1.426868 0.176392
H -0.213698 1.556835 1.269519
C -1.042267 0.229581 -0.226552
H -1.041600 0.165261 -1.329159
C -0.454483 -1.079146 0.329163
H -0.515882 -1.054734 1.429595
C 1.008995 -1.275203 -0.093867
H 1.406856 -2.201945 0.345042
C 1.895505 -0.082439 0.308751
H 1.882779 -0.016030 1.409834
C 1.302340 1.227416 -0.242199
H 1.907963 2.082145 0.092864
C -2.491913 0.450163 0.214906
O -3.382488 -0.594964 -0.197979
C 3.347783 -0.277613 -0.140739
H -0.559634 2.351835 -0.266573
H -1.063444 -1.931968 0.001676
H 1.058489 -1.402948 -1.187706
H 1.366790 1.212045 -1.342432
H -2.556706 0.472652 1.310921
H -2.853069 1.422998 -0.157911
H -3.353181 -0.629777 -1.165325
H 3.982138 0.560984 0.178093
H 3.776748 -1.199165 0.276369
H 3.415753 -0.346234 -1.236100
el energy= -389.708591082
zpe= -389.477647
th energy= -389.467880
th enthalpy= -389.466936
free energy= -389.511980

4mchm_5/coords
t3
C 0.384531 -1.266085 0.026232
H 0.814668 -2.160099 0.501332
C 1.031725 -0.000010 0.618632

H 0.837468 0.000002 1.704310
C 0.384531 1.266077 0.026226
H 0.814710 2.160072 0.501335
C -1.142255 1.261357 0.197660
H -1.388605 1.313713 1.270930
C -1.792391 -0.000006 -0.399060
H -1.586038 0.000007 -1.482705
C -1.142273 -1.261368 0.197637
H -1.574825 -2.160438 -0.265368
C 2.553043 -0.000003 0.473941
O 2.912246 0.000018 -0.914523
C -3.312562 0.000019 -0.202500
H 0.630469 -1.330446 -1.043872
H 0.630467 1.330432 -1.043877
H -1.574851 2.160423 -0.265314
H -1.388644 -1.313765 1.270904
H 2.973546 0.888912 0.972445
H 2.973563 -0.888920 0.972422
H 3.878052 -0.000008 -0.963790
H -3.572021 0.000084 0.866188
H -3.775992 0.887219 -0.655735
H -3.776025 -0.887218 -0.655621
el energy= -389.706750553
zpe= -389.476012
th energy= -389.466224
th enthalpy= -389.465279
free energy= -389.510348

4mchm_6/coords
t4
C 0.159529 1.427443 0.181065
H 0.218864 1.544843 1.275137
C 1.041238 0.239789 -0.245463
H 1.037465 0.187410 -1.346857
C 0.460221 -1.078269 0.298855
H 1.058685 -1.931728 -0.051689
C -1.007580 -1.272816 -0.111624
H -1.066881 -1.388060 -1.206151
C -1.893386 -0.087518 0.313130
H -1.871516 -0.033778 1.414713
C -1.308139 1.229637 -0.228138
H -1.381540 1.226129 -1.327865

C 2.492117 0.462270 0.194964
O 3.405781 -0.520473 -0.310104
C -3.348729 -0.281643 -0.126630
H 0.550432 2.358757 -0.254063
H 0.534548 -1.071759 1.398687
H -1.397784 -2.205766 0.320701
H -1.912882 2.079191 0.121365
H 2.857302 1.423086 -0.189630
H 2.549070 0.503219 1.295685
H 3.186485 -1.366113 0.105249
H -3.982953 0.549943 0.210225
H -3.426130 -0.334282 -1.222239
H -3.771041 -1.210658 0.280618
el energy= -389.708383616
zpe= -389.477685
th energy= -389.467801
th enthalpy= -389.466857
free energy= -389.512138

4mchm_7/coords
t5
C 0.385074 1.269958 -0.017237
H 0.637883 1.319469 1.052282
C 1.035983 0.014457 -0.625159
H 0.846883 0.025134 -1.712045
C 0.389415 -1.260622 -0.051404
H 0.629404 -1.339000 1.021174
C -1.137707 -1.257004 -0.219616
H -1.385224 -1.293295 -1.293145
C -1.788800 -0.006249 0.397982
H -1.579354 -0.022405 1.480874
C -1.142450 1.265021 -0.181745
H -1.574610 2.156107 0.296882
C 2.562809 0.017290 -0.470063
O 3.019413 0.060747 0.889820
C -3.309261 -0.006857 0.205591
H 0.811389 2.171676 -0.481296
H 0.821387 -2.148800 -0.535716
H -1.567197 -2.164169 0.230101
H -1.393957 1.333589 -1.252872
H 2.991140 -0.859885 -0.981915
H 2.982715 0.914259 -0.943002

H 2.768914 -0.773004 1.312134
H -3.768849 -0.904142 0.642647
H -3.774219 0.869802 0.677353
H -3.571993 0.012727 -0.862105
el energy= -389.708075849
zpe= -389.476930
th energy= -389.467301
th enthalpy= -389.466357
free energy= -389.510964

4mchm_19/coords
t6
C 0.264815 -1.091995 0.670367
H -0.305155 -1.214518 1.602441
C 0.940653 0.297255 0.692756
H 1.442374 0.418776 1.665180
C -0.122819 1.409348 0.560558
H -0.717770 1.431107 1.484523
C -1.061294 1.208990 -0.644104
H -1.823988 2.001313 -0.650644
C -1.743985 -0.176835 -0.651721
H -2.242729 -0.296497 -1.625648
C -0.673929 -1.285109 -0.534449
H -0.078757 -1.301051 -1.459540
C 2.038399 0.444612 -0.365185
O 3.085844 -0.494582 -0.081766
C -2.833832 -0.299632 0.426487
H 1.030466 -1.878675 0.673613
H 0.367816 2.390966 0.488703
H -0.488875 1.325679 -1.576091
H -1.160495 -2.269137 -0.466723
H 1.647546 0.274188 -1.379195
H 2.436168 1.472533 -0.335823
H 3.729007 -0.438197 -0.802209
H -3.598674 0.479516 0.302474
H -3.338918 -1.273282 0.361266
H -2.432830 -0.205871 1.443548
el energy= -389.700907529
zpe= -389.469111
th energy= -389.459615
th enthalpy= -389.458670
free energy= -389.503030

4mchm_21/coords
t7
C 0.115725 1.407855 0.557248
H -0.377844 2.387724 0.479568
C -0.945701 0.291934 0.671496
H -1.457444 0.409398 1.641030
C -0.273341 -1.097756 0.648099
H 0.279711 -1.235188 1.588115
C 0.683302 -1.281867 -0.543971
H 0.101906 -1.289983 -1.477863
C 1.754682 -0.172622 -0.637510
H 2.269513 -0.287027 -1.603595
C 1.070149 1.212147 -0.635226
H 0.509691 1.330080 -1.574396
C -2.039439 0.439909 -0.398166
O -3.111308 -0.497988 -0.233249
C 2.826210 -0.299529 0.458416
H 0.698227 1.431492 1.489114
H -1.045058 -1.878810 0.628019
H 1.168621 -2.266534 -0.477091
H 1.831482 2.005767 -0.629749
H -2.432849 1.469630 -0.377300
H -1.650853 0.258782 -1.406602
H -3.487365 -0.349837 0.647345
H 2.407844 -0.210914 1.468920
H 3.333423 -1.272271 0.397099
H 3.591941 0.481166 0.351061
el energy= -389.702260178
zpe= -389.470481
th energy= -389.460984
th enthalpy= -389.460040
free energy= -389.504421

4mchm_22/coords
t8
C 0.130033 1.429418 0.542914
H -0.353367 2.413271 0.451283
C -0.942661 0.328815 0.697358
H -1.439247 0.466856 1.669941
C -0.277925 -1.065469 0.693768
H 0.296882 -1.177511 1.623933

C 0.649046 -1.286980 -0.514901
H 1.122466 -2.276743 -0.439319
C 1.732554 -0.194112 -0.648958
H 2.226968 -0.332903 -1.622545
C 1.067574 1.200351 -0.658101
H 1.840457 1.982579 -0.673963
C -2.048514 0.470518 -0.361926
O -3.138088 -0.441967 -0.163033
C 2.823959 -0.317472 0.427626
H 0.725093 1.465927 1.466494
H -1.046973 -1.850778 0.724185
H 0.047417 -1.303969 -1.435968
H 0.498238 1.312307 -1.592342
H -2.491234 1.472198 -0.291456
H -1.650588 0.358949 -1.381156
H -2.817933 -1.330987 -0.370369
H 3.600438 0.447456 0.288666
H 2.428228 -0.201496 1.444449
H 3.313463 -1.299838 0.375752
el energy= -389.701704442
zpe= -389.469975
th energy= -389.460406
th enthalpy= -389.459462
free energy= -389.503999

4mchm_24/coords
t9
C -0.105104 1.272899 0.759565
H 0.591163 1.376397 1.604541
C -0.953081 -0.000304 0.993027
H -1.246058 -0.000566 2.055095
C -0.105021 -1.273342 0.758970
H 0.591223 -1.377192 1.603922
C 0.700812 -1.263860 -0.552875
H 1.335735 -2.161447 -0.596569
C 1.573580 0.000192 -0.717473
H 1.966313 0.000441 -1.745803
C 0.700679 1.264075 -0.552315
H 0.008741 1.329097 -1.401557
C -2.305138 -0.000172 0.271999
O -2.171428 0.000456 -1.157023
C 2.789055 0.000050 0.224298

H -0.753715 2.160684 0.791048
H -0.753572 -2.161188 0.790024
H 0.008907 -1.328595 -1.402162
H 1.335502 2.161749 -0.595642
H -2.876859 -0.888147 0.589203
H -2.877076 0.887398 0.589946
H -3.064905 0.000448 -1.528472
H 2.501149 -0.000204 1.283162
H 3.415139 -0.886647 0.053932
H 3.415039 0.886894 0.054333
el energy= -389.698525952
zpe= -389.467234
th energy= -389.457577
th enthalpy= -389.456633
free energy= -389.501299

4mchm_9/coords
c1
C -0.476042 -0.881947 1.059994
H -1.200359 -1.706697 1.039005
C -1.156318 0.426636 0.600653
H -1.908854 0.705437 1.354150
C -0.115814 1.564423 0.519256
H -0.584873 2.476401 0.122034
C 1.118955 1.194956 -0.319755
H 0.832671 1.066504 -1.375332
C 1.791026 -0.098503 0.177368
H 2.133886 0.082118 1.210546
C 0.762149 -1.243510 0.223436
H 1.230487 -2.150143 0.634016
C -1.921146 0.270134 -0.716904
O -2.990665 -0.666271 -0.521376
C 3.013233 -0.465652 -0.670527
H -0.170766 -0.762367 2.110680
H 0.212427 1.804184 1.541745
H 1.841583 2.023831 -0.295711
H 0.461259 -1.494140 -0.805922
H -2.328095 1.248450 -1.021831
H -1.262516 -0.076416 -1.526920
H -3.418627 -0.801386 -1.378289
H 2.728209 -0.655521 -1.715434
H 3.757328 0.342773 -0.671376

H 3.505293 -1.372086 -0.291473
el energy= -389.704341969
zpe= -389.473062
th energy= -389.463438
th enthalpy= -389.462494
free energy= -389.507207

4mchm_11/coords
c2
C -0.329397 -1.109166 0.054902
H -1.011195 -1.919534 -0.234057
C -0.959387 0.255607 -0.281438
H -1.151310 0.285191 -1.367335
C 0.019928 1.394281 0.057909
H -0.412524 2.361209 -0.237354
C 1.378128 1.203330 -0.637756
H 1.228538 1.288025 -1.725253
C 2.029514 -0.163919 -0.334937
H 2.885468 -0.280488 -1.016872
C 1.026908 -1.297293 -0.644968
H 0.858820 -1.330765 -1.732616
C -2.297275 0.470998 0.420189
O -3.236375 -0.515385 -0.029615
C 2.583068 -0.247594 1.097310
H -0.204545 -1.183261 1.146480
H 0.158846 1.437005 1.149060
H 2.062538 2.015949 -0.353662
H 1.460780 -2.268830 -0.366776
H -2.164782 0.401045 1.512747
H -2.676703 1.482170 0.198080
H -4.053401 -0.389006 0.472583
H 3.083382 -1.211173 1.266386
H 3.319914 0.546673 1.280468
H 1.798246 -0.148593 1.857769
el energy= -389.704111959
zpe= -389.472966
th energy= -389.463259
th enthalpy= -389.462315
free energy= -389.507216

4mchm_13/coords
c3

C -0.021033 1.397049 0.056956
H -0.163106 1.440506 1.147735
C 0.961530 0.259152 -0.275922
H 1.158626 0.289922 -1.362292
C 0.334325 -1.106788 0.055197
H 1.021691 -1.913112 -0.232768
C -1.019237 -1.297477 -0.649001
H -0.848331 -1.328558 -1.736317
C -2.025194 -0.166667 -0.339542
H -2.880335 -0.285542 -1.022086
C -1.377498 1.202695 -0.641526
H -2.064799 2.013204 -0.358211
C 2.298825 0.478817 0.436958
O 3.287574 -0.513594 0.131636
C -2.579632 -0.252269 1.092379
H 0.410693 2.364663 -0.237521
H 0.206246 -1.184362 1.146213
H -1.451942 -2.270362 -0.373649
H -1.226582 1.288025 -1.728781
H 2.686605 1.483280 0.199471
H 2.161386 0.427221 1.525226
H 3.448642 -0.474435 -0.822640
H -3.075862 -1.217987 1.261358
H -1.795958 -0.149622 1.853511
H -3.320076 0.538841 1.274667
el energy= -389.705316525
zpe= -389.473944
th energy= -389.464322
th enthalpy= -389.463378
free energy= -389.508071

4mchm_15/coords
c4
C -0.487493 -0.883308 1.047804
H -0.192080 -0.771788 2.102130
C -1.160842 0.427077 0.588093
H -1.918698 0.705177 1.338912
C -0.121412 1.566877 0.516905
H -0.587622 2.477402 0.112495
C 1.121593 1.197102 -0.310120
H 0.846467 1.072510 -1.369113
C 1.787221 -0.099192 0.188466

H 2.120463 0.076443 1.225638
C 0.756454 -1.242998 0.219461
H 1.219916 -2.152963 0.628140
C -1.918653 0.275057 -0.740212
O -2.949206 -0.720419 -0.688765
C 3.016793 -0.464352 -0.649647
H -1.215454 -1.704712 1.014150
H 0.196181 1.810226 1.541906
H 1.845191 2.024782 -0.276330
H 0.462800 -1.486501 -0.813721
H -2.348396 1.248978 -1.027419
H -1.254512 -0.040398 -1.552582
H -3.549855 -0.473757 0.029954
H 2.740942 -0.650272 -1.697736
H 3.761706 0.343284 -0.641230
H 3.504637 -1.372636 -0.269574
el energy= -389.705696908
zpe= -389.474186
th energy= -389.464678
th enthalpy= -389.463733
free energy= -389.508028

4mchm_16/coords
c5
C -0.235440 1.266768 -0.201874
H -0.731871 2.159715 -0.609481
C -0.967325 0.000006 -0.685438
H -0.944929 0.000011 -1.788385
C -0.235441 -1.266761 -0.201885
H -0.319093 -1.338175 0.891256
C 1.246025 -1.262088 -0.615889
H 1.746206 -2.163584 -0.232790
C 2.000255 -0.000001 -0.142885
H 2.987408 -0.000003 -0.629505
C 1.246029 1.262093 -0.615875
H 1.304786 1.315308 -1.714216
C -2.447980 0.000005 -0.307158
O -2.589951 -0.000017 1.121153
C 2.249421 -0.000009 1.374521
H -0.319091 1.338177 0.891268
H -0.731880 -2.159700 -0.609503
H 1.304777 -1.315287 -1.714231

H 1.746212 2.163582 -0.232760
H -2.941389 0.888933 -0.733633
H -2.941383 -0.888924 -0.733653
H -3.536977 0.000032 1.318142
H 2.823135 -0.886917 1.677169
H 2.823164 0.886881 1.677170
H 1.317267 0.000007 1.952844
el energy= -389.703524036
zpe= -389.472198
th energy= -389.462581
th enthalpy= -389.461637
free energy= -389.506328

4mchm_17/coords
c6
C -0.238487 1.277507 -0.157626
H -0.731886 2.187485 -0.529852
C -0.973711 0.033577 -0.690022
H -0.958210 0.074857 -1.792659
C -0.242440 -1.253298 -0.261160
H -0.318693 -1.372873 0.830377
C 1.239902 -1.233963 -0.672621
H 1.737570 -2.152217 -0.328305
C 1.995328 0.005537 -0.145038
H 2.983308 0.024021 -0.629570
C 1.244423 1.287563 -0.566210
H 1.744790 2.171165 -0.143524
C -2.456999 0.020868 -0.296701
O -2.690888 0.028162 1.119354
C 2.241804 -0.058753 1.371597
H -0.327495 1.304107 0.937321
H -0.739892 -2.128511 -0.704372
H 1.298605 -1.239840 -1.772144
H 1.307381 1.387931 -1.660981
H -2.951734 0.925110 -0.673698
H -2.957474 -0.848007 -0.754777
H -2.356840 -0.806911 1.476097
H 2.818827 0.812324 1.711390
H 1.308741 -0.078264 1.948208
H 2.811186 -0.959906 1.638347
el energy= -389.704839300
zpe= -389.473168

th energy= -389.463643
th enthalpy= -389.462699
free energy= -389.507143

4mchm_23/coords
c7
C 0.428186 -1.318170 -0.868024
H 1.042420 -2.196176 -0.619867
C 1.304003 -0.043758 -0.838953
H 1.960182 -0.087573 -1.722676
C 0.430980 1.224429 -0.990420
H 1.047556 2.120644 -0.828325
C -0.805051 1.258441 -0.075469
H -0.494309 1.365006 0.973036
C -1.666482 -0.009505 -0.217664
H -2.015403 -0.058572 -1.263571
C -0.809848 -1.261719 0.043982
H -0.501674 -1.270784 1.098825
C 2.303872 0.012350 0.320065
O 1.661080 0.084247 1.600662
C -2.898708 0.036498 0.692454
H 0.083381 -1.466818 -1.902924
H 0.085441 1.273608 -2.034475
H -1.409671 2.146024 -0.314749
H -1.417387 -2.165703 -0.111807
H 2.947732 -0.881957 0.278558
H 2.955894 0.890953 0.183283
H 2.358893 0.120530 2.270366
H -3.520437 0.917556 0.481066
H -3.526952 -0.855307 0.560831
H -2.606022 0.083189 1.751312
el energy= -389.702068452
zpe= -389.470657
th energy= -389.461087
th enthalpy= -389.460143
free energy= -389.504528

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.343693 -1.099144 0.024921
H 1.024487 -1.903082 -0.290524
C 0.961403 0.275780 -0.292453

H 1.151674 0.321596 -1.377836
C -0.025825 1.400801 0.068509
H -0.157583 1.428143 1.161076
C -1.387866 1.209675 -0.620003
H -1.247492 1.311329 -1.707237
C -2.025848 -0.166904 -0.331494
H -2.886500 -0.281096 -1.007849
C -1.017145 -1.287419 -0.666967
H -1.440517 -2.266640 -0.400097
C 2.303462 0.491984 0.414536
O 3.320856 -0.438087 0.019231
C -2.566410 -0.275758 1.104070
H 0.230288 -1.197391 1.115915
H 0.397571 2.375084 -0.216054
H -2.076552 2.012501 -0.318788
H -0.856955 -1.302736 -1.756066
H 2.701882 1.483087 0.162612
H 2.162925 0.459399 1.507924
H 3.058310 -1.312447 0.339263
H -3.309125 0.508869 1.304049
H -3.056088 -1.246333 1.264046
H -1.775959 -0.179679 1.859007
el energy= -389.705194764
zpe= -389.473430
th energy= -389.463930
th enthalpy= -389.462986
free energy= -389.507323

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.486926 -0.862714 1.065630
H 1.212990 -1.688840 1.063888
C 1.162260 0.444452 0.595765
H 1.914722 0.729757 1.346530
C 0.115298 1.576489 0.507969
H -0.208757 1.826645 1.529414
C -1.122656 1.194911 -0.321677
H -0.842705 1.064026 -1.378513
C -1.784192 -0.101009 0.182858
H -2.124815 0.080386 1.216621
C -0.747171 -1.238517 0.229713
H -1.207956 -2.147995 0.642282

C 1.929952 0.284978 -0.726954
O 3.031610 -0.629618 -0.630125
C -3.006588 -0.479404 -0.659974
H 0.179585 -0.734925 2.114603
H 0.578910 2.486098 0.098495
H -1.850303 2.019306 -0.296329
H -0.443860 -1.487914 -0.799289
H 1.264038 -0.017153 -1.548423
H 2.376193 1.247927 -1.006151
H 2.667243 -1.521081 -0.539364
H -3.756004 0.324056 -0.661001
H -2.723584 -0.670633 -1.705174
H -3.491548 -1.387825 -0.276564
el energy= -389.705180673
zpe= -389.473623
th energy= -389.464114
th enthalpy= -389.463170
free energy= -389.507513

B3LYP aug-cc-pwCVDZ gas phase

4mchm_1/coords
t1
C 0.159736 1.424122 0.177992
H 0.552951 2.350833 -0.266027
C 1.037838 0.230227 -0.228896
H 1.039963 0.165522 -1.330145
C 0.453570 -1.078641 0.324048
H 1.064023 -1.926659 -0.009751
C -1.008262 -1.271795 -0.096082
H -1.405379 -2.198964 0.343307
C -1.894886 -0.083379 0.307093
H -1.881460 -0.018861 1.409398
C -1.302923 1.225588 -0.238879
H -1.908339 2.079368 0.100164
C 2.482338 0.447815 0.204995
O 3.291965 -0.609668 -0.328326
C -3.346902 -0.278158 -0.136285
H 0.210416 1.553710 1.272091
H 0.516748 -1.056129 1.425382
H -1.060012 -1.399031 -1.190540
H -1.368708 1.213035 -1.339717

H 2.839082 1.423482 -0.166227
H 2.543415 0.458380 1.307545
H 4.204394 -0.474888 -0.050541
H -3.415121 -0.348780 -1.231994
H -3.771777 -1.199998 0.284892
H -3.978972 0.561654 0.184848
el energy= -389.780246395
zpe= -389.550642
th energy= -389.540851
th enthalpy= -389.539907
free energy= -389.584922

4mchm_3/coords
t2
C -0.161696 1.421648 0.178426
H -0.211898 1.551834 1.272310
C -1.039746 0.224945 -0.221594
H -1.034686 0.162216 -1.326040
C -0.449307 -1.080414 0.330925
H -0.508175 -1.053031 1.431994
C 1.010860 -1.272779 -0.094654
H 1.411265 -2.198240 0.345134
C 1.896708 -0.081749 0.303777
H 1.886675 -0.016360 1.405911
C 1.300544 1.225942 -0.241235
H 1.905171 2.080929 0.096082
C -2.488472 0.442947 0.219405
O -3.385937 -0.588885 -0.205760
C 3.347407 -0.274408 -0.144301
H -0.559110 2.346867 -0.265053
H -1.061007 -1.932416 0.008037
H 1.060212 -1.401881 -1.189227
H 1.364627 1.213380 -1.342306
H -2.551640 0.442804 1.316273
H -2.843478 1.426741 -0.132656
H -3.435188 -0.574404 -1.169098
H 3.979041 0.566758 0.173960
H 3.775422 -1.194959 0.276441
H 3.412482 -0.345952 -1.240175
el energy= -389.780111702
zpe= -389.550455
th energy= -389.540702

th enthalpy= -389.539758
free energy= -389.584688

4mchm_5/coords
t3
C 0.385879 -1.263964 0.029663
H 0.814719 -2.157837 0.507436
C 1.031182 -0.000013 0.620876
H 0.838888 0.000000 1.708950
C 0.385880 1.263955 0.029658
H 0.814765 2.157807 0.507439
C -1.138259 1.258591 0.200469
H -1.388761 1.311320 1.273803
C -1.787288 -0.000005 -0.395703
H -1.577029 0.000011 -1.479382
C -1.138281 -1.258601 0.200441
H -1.569982 -2.157154 -0.265028
C 2.550360 -0.000005 0.474329
O 2.895083 0.000030 -0.918956
C -3.306747 0.000019 -0.208895
H 0.638178 -1.325312 -1.038579
H 0.638176 1.325297 -1.038583
H -1.570008 2.157140 -0.264968
H -1.388800 -1.311374 1.273772
H 2.969090 0.893299 0.968632
H 2.969107 -0.893319 0.968595
H 3.854386 -0.000060 -1.002672
H -3.569954 0.000053 0.859411
H -3.764878 0.888215 -0.666136
H -3.764915 -0.888187 -0.666073
el energy= -389.779446495
zpe= -389.549868
th energy= -389.540089
th enthalpy= -389.539145
free energy= -389.584128

4mchm_6/coords
t4
C 0.159605 1.421952 0.180011
H 0.216873 1.542108 1.274846
C 1.040607 0.235243 -0.242566
H 1.042307 0.181049 -1.344099

C 0.455225 -1.078243 0.299294
H 1.046321 -1.935898 -0.055197
C -1.010129 -1.269924 -0.111937
H -1.068278 -1.386199 -1.206918
C -1.893459 -0.085387 0.309164
H -1.872053 -0.031058 1.411795
C -1.305533 1.228111 -0.229726
H -1.379086 1.225449 -1.330020
C 2.489068 0.457341 0.199174
O 3.410694 -0.511829 -0.310979
C -3.348153 -0.278936 -0.125645
H 0.551559 2.352155 -0.257300
H 0.527058 -1.072812 1.400557
H -1.402814 -2.201451 0.321883
H -1.908848 2.078352 0.121420
H 2.851018 1.421013 -0.182305
H 2.542804 0.495548 1.301766
H 3.216149 -1.367467 0.087964
H -3.978452 0.557228 0.207708
H -3.424312 -0.339510 -1.221368
H -3.769185 -1.204817 0.290487
el energy= -389.780036198
zpe= -389.550394
th energy= -389.540605
th enthalpy= -389.539660
free energy= -389.584678

4mchm_7/coords
t5
C 0.378950 1.272720 -0.005876
H 0.634538 1.320158 1.062889
C 1.032986 0.024330 -0.617550
H 0.840874 0.038056 -1.705833
C 0.390331 -1.253071 -0.053213
H 0.621185 -1.333727 1.022015
C -1.134084 -1.254086 -0.225680
H -1.379165 -1.286641 -1.300565
C -1.789872 -0.010414 0.394427
H -1.582567 -0.031652 1.478633
C -1.145525 1.263312 -0.174439
H -1.581610 2.149261 0.310387
C 2.558801 0.029372 -0.472123

O 3.025072 0.042146 0.882932
C -3.308565 -0.015009 0.203997
H 0.802838 2.176453 -0.468457
H 0.825080 -2.139093 -0.541173
H -1.561991 -2.164342 0.219935
H -1.397481 1.338120 -1.245983
H 2.987297 -0.831516 -1.013530
H 2.971552 0.941907 -0.921913
H 2.825864 -0.809640 1.287654
H -3.763584 -0.914542 0.641732
H -3.772115 0.861287 0.678074
H -3.569423 0.005820 -0.864582
el energy= -389.779269106
zpe= -389.549678
th energy= -389.539916
th enthalpy= -389.538972
free energy= -389.583931

4mchm_19/coords
t6
C 0.273530 -1.089689 0.660240
H -0.287136 -1.219619 1.597723
C 0.940669 0.300719 0.683565
H 1.443273 0.418593 1.655780
C -0.123450 1.409677 0.555828
H -0.711037 1.433048 1.484939
C -1.069540 1.208433 -0.639741
H -1.836153 1.997594 -0.638181
C -1.745166 -0.178579 -0.645138
H -2.246108 -0.297706 -1.618753
C -0.672007 -1.281481 -0.535860
H -0.084964 -1.297117 -1.466926
C 2.040110 0.450436 -0.368910
O 3.075457 -0.500541 -0.077993
C -2.831535 -0.306673 0.433272
H 1.048147 -1.866564 0.653466
H 0.363118 2.393956 0.481071
H -0.508317 1.331751 -1.578539
H -1.155603 -2.267183 -0.467045
H 1.650153 0.283360 -1.385337
H 2.443942 1.476089 -0.325587
H 3.759326 -0.433657 -0.753085

H -3.601771 0.466658 0.304967
H -3.327001 -1.285469 0.370468
H -2.429180 -0.206464 1.449446
el energy= -389.773294449
zpe= -389.543123
th energy= -389.533442
th enthalpy= -389.532497
free energy= -389.577318

4mchm_21/coords
t7
C 0.117294 1.407043 0.555694
H -0.375193 2.388118 0.476841
C -0.943035 0.292555 0.673798
H -1.443418 0.413204 1.650610
C -0.273528 -1.096075 0.652963
H 0.278535 -1.232657 1.594592
C 0.681445 -1.281567 -0.536848
H 0.100429 -1.298110 -1.471215
C 1.751072 -0.174458 -0.636247
H 2.259589 -0.290815 -1.606099
C 1.069001 1.209218 -0.635649
H 0.510947 1.328781 -1.576607
C -2.039857 0.442439 -0.390042
O -3.108231 -0.499485 -0.240930
C 2.829388 -0.298758 0.450469
H 0.700044 1.434821 1.487813
H -1.047010 -1.874724 0.630625
H 1.167803 -2.265615 -0.465550
H 1.831276 2.002403 -0.631304
H -2.433219 1.473177 -0.365771
H -1.650881 0.265378 -1.399425
H -3.529435 -0.351907 0.614642
H 2.418537 -0.203271 1.463789
H 3.330955 -1.274505 0.389432
H 3.596202 0.479218 0.330246
el energy= -389.773449575
zpe= -389.543206
th energy= -389.533571
th enthalpy= -389.532626
free energy= -389.577313

4mchm_22/coords
t8
C 0.120862 1.412686 0.551626
H -0.369274 2.394382 0.469309
C -0.944806 0.304854 0.686153
H -1.446785 0.427849 1.657854
C -0.268692 -1.081570 0.672026
H 0.296258 -1.202666 1.607702
C 0.671383 -1.282984 -0.527338
H 1.155129 -2.268213 -0.454842
C 1.743418 -0.179744 -0.643182
H 2.241861 -0.304649 -1.617133
C 1.066351 1.206354 -0.643722
H 1.832695 1.995522 -0.646147
C -2.047260 0.453080 -0.372260
O -3.170735 -0.407284 -0.149105
C 2.831922 -0.302995 0.433570
H 0.708865 1.445775 1.480361
H -1.027771 -1.878626 0.689997
H 0.083280 -1.300641 -1.457870
H 0.504716 1.324931 -1.582464
H -2.457024 1.470359 -0.325371
H -1.655222 0.304615 -1.390718
H -2.901980 -1.320014 -0.303015
H 3.603453 0.467239 0.296248
H 2.433536 -0.192318 1.450260
H 3.325068 -1.283362 0.377437
el energy= -389.772755415
zpe= -389.542661
th energy= -389.532923
th enthalpy= -389.531979
free energy= -389.576926

4mchm_24/coords
t9
C -0.107764 1.273620 0.753861
H 0.585670 1.388748 1.600525
C -0.949262 0.000035 0.993978
H -1.235097 0.000064 2.059446
C -0.107772 -1.273568 0.753930
H 0.585662 -1.388654 1.600601
C 0.692616 -1.259064 -0.558267

H 1.322355 -2.160429 -0.608721
C 1.569507 -0.000022 -0.711843
H 1.967309 -0.000051 -1.738864
C 0.692629 1.259037 -0.558333
H -0.005331 1.305665 -1.403335
C -2.300197 0.000020 0.276708
O -2.145389 -0.000041 -1.151818
C 2.779117 -0.000006 0.235035
H -0.762470 2.157717 0.776909
H -0.762482 -2.157661 0.777031
H -0.005350 -1.305724 -1.403264
H 1.322380 2.160393 -0.608831
H -2.868959 -0.892492 0.590283
H -2.868941 0.892570 0.590209
H -3.020586 -0.000128 -1.554884
H 2.485942 0.000023 1.292980
H 3.404878 -0.887722 0.067042
H 3.404888 0.887695 0.066999
el energy= -389.770878829
zpe= -389.540671
th energy= -389.531033
th enthalpy= -389.530089
free energy= -389.574633

4mchm_9/coords
c1
C -0.480423 -0.881660 1.049019
H -1.210885 -1.699710 1.019840
C -1.154159 0.428569 0.594463
H -1.904477 0.703879 1.351314
C -0.113183 1.563078 0.515014
H -0.577480 2.477640 0.116145
C 1.123524 1.193387 -0.316951
H 0.846555 1.071010 -1.376541
C 1.789036 -0.101670 0.176460
H 2.126513 0.075861 1.212888
C 0.758204 -1.241195 0.217321
H 1.224349 -2.149135 0.628115
C -1.925577 0.278179 -0.717513
O -2.981901 -0.672119 -0.513233
C 3.015649 -0.468264 -0.661750
H -0.178514 -0.764490 2.101789

H 0.211105 1.803292 1.539309
H 1.848886 2.020096 -0.284418
H 0.462855 -1.492243 -0.814403
H -2.345935 1.257064 -1.004108
H -1.267986 -0.058976 -1.534114
H -3.453561 -0.798050 -1.343673
H 2.733456 -0.658085 -1.707990
H 3.758815 0.341438 -0.657178
H 3.503080 -1.375183 -0.277494
el energy= -389.776917075
zpe= -389.547121
th energy= -389.537396
th enthalpy= -389.536451
free energy= -389.581393

4mchm_11/coords
c2
C -0.333374 -1.105970 0.061463
H -1.023151 -1.908444 -0.227488
C -0.958583 0.257803 -0.272686
H -1.159366 0.284296 -1.357276
C 0.022190 1.394295 0.058180
H -0.408087 2.361575 -0.241254
C 1.375836 1.199383 -0.640579
H 1.223595 1.282700 -1.728354
C 2.023352 -0.167069 -0.337392
H 2.874763 -0.287260 -1.025585
C 1.018547 -1.296862 -0.640124
H 0.847830 -1.334262 -1.727792
C -2.293921 0.472010 0.429157
O -3.226095 -0.515473 -0.033450
C 2.588262 -0.247453 1.088841
H -0.207308 -1.181655 1.153572
H 0.166005 1.444521 1.149186
H 2.063152 2.010906 -0.359102
H 1.451837 -2.268503 -0.360309
H -2.159376 0.389242 1.522031
H -2.671194 1.484586 0.206893
H -4.069786 -0.381231 0.411530
H 3.084775 -1.213394 1.256015
H 3.331046 0.544457 1.258856
H 1.810176 -0.140568 1.855522

el energy= -389.776806192
zpe= -389.546919
th energy= -389.537185
th enthalpy= -389.536241
free energy= -389.581158

4mchm_13/coords
c3
C -0.019393 1.392014 0.059452
H -0.166252 1.441994 1.149902
C 0.960650 0.252221 -0.263477
H 1.157171 0.281395 -1.351949
C 0.328580 -1.108315 0.067269
H 1.018311 -1.915591 -0.210074
C -1.019374 -1.297467 -0.641971
H -0.844137 -1.336160 -1.729115
C -2.022853 -0.164550 -0.344836
H -2.870727 -0.282942 -1.037594
C -1.370755 1.200554 -0.644927
H -2.057452 2.013547 -0.366374
C 2.297780 0.465018 0.448649
O 3.296313 -0.503811 0.109299
C -2.595372 -0.243159 1.078300
H 0.415671 2.358064 -0.237123
H 0.195514 -1.179496 1.158452
H -1.456664 -2.267606 -0.363563
H -1.214109 1.284048 -1.732209
H 2.670331 1.484227 0.247824
H 2.165314 0.370104 1.535098
H 3.514734 -0.404078 -0.825064
H -3.093872 -1.208313 1.243805
H -1.821664 -0.136220 1.849362
H -3.338250 0.549628 1.243480
el energy= -389.776706746
zpe= -389.546734
th energy= -389.537053
th enthalpy= -389.536109
free energy= -389.580876

4mchm_15/coords
c4
C -0.479230 -0.899796 1.035528

H -0.186995 -0.798376 2.092655
C -1.155111 0.411838 0.590272
H -1.904429 0.683883 1.354078
C -0.120823 1.554237 0.527735
H -0.590173 2.468279 0.133469
C 1.119276 1.197247 -0.304075
H 0.844975 1.080288 -1.364789
C 1.790726 -0.097098 0.182967
H 2.121352 0.074487 1.222655
C 0.766945 -1.243313 0.207886
H 1.235819 -2.151811 0.614048
C -1.921341 0.271352 -0.732769
O -2.974396 -0.697798 -0.679419
C 3.023870 -0.449232 -0.651691
H -1.204231 -1.722596 0.985253
H 0.199054 1.789178 1.554748
H 1.839333 2.028132 -0.264512
H 0.478407 -1.487501 -0.826997
H -2.323018 1.255634 -1.028767
H -1.267646 -0.070976 -1.543229
H -3.618147 -0.414363 -0.018863
H 2.748371 -0.631910 -1.700875
H 3.761910 0.364964 -0.636213
H 3.514723 -1.356339 -0.272430
el energy= -389.777042728
zpe= -389.547158
th energy= -389.537476
th enthalpy= -389.536532
free energy= -389.581351

4mchm_16/coords
c5
C -0.238351 1.265267 -0.203962
H -0.733075 2.156950 -0.617916
C -0.967364 -0.000002 -0.686098
H -0.946429 -0.000008 -1.790942
C -0.238349 -1.265268 -0.203952
H -0.331815 -1.337731 0.887613
C 1.241173 -1.260035 -0.615298
H 1.740391 -2.161451 -0.229852
C 1.993426 0.000000 -0.141928
H 2.979431 -0.000003 -0.632922

C 1.241174 1.260033 -0.615304
H 1.304829 1.314124 -1.714231
C -2.445559 -0.000003 -0.306750
O -2.571469 -0.000010 1.123303
C 2.246570 0.000004 1.373153
H -0.331816 1.337743 0.887604
H -0.733078 -2.156949 -0.617903
H 1.304823 -1.314128 -1.714226
H 1.740391 2.161450 -0.229856
H -2.935377 0.893423 -0.730588
H -2.935373 -0.893435 -0.730596
H -3.506480 0.000100 1.353617
H 2.822014 -0.887580 1.671070
H 2.822030 0.887582 1.671059
H 1.314964 0.000016 1.952480
el energy= -389.776144502
zpe= -389.546175
th energy= -389.536488
th enthalpy= -389.535544
free energy= -389.580294

4mchm_17/coords
c6
C -0.230454 1.283771 -0.119665
H -0.720126 2.202875 -0.474310
C -0.970208 0.058407 -0.678852
H -0.949561 0.123978 -1.782115
C -0.247302 -1.239302 -0.282213
H -0.318699 -1.381993 0.807466
C 1.231660 -1.219945 -0.697096
H 1.725817 -2.147684 -0.372756
C 1.994392 0.002805 -0.148495
H 2.976734 0.026666 -0.645821
C 1.248617 1.296227 -0.533272
H 1.754909 2.165915 -0.089004
C -2.454806 0.044401 -0.299062
O -2.704200 -0.013009 1.111055
C 2.259666 -0.096610 1.361258
H -0.323791 1.288976 0.974842
H -0.748787 -2.102785 -0.745971
H 1.287043 -1.204627 -1.797266
H 1.310082 1.424966 -1.625952

H -2.932756 0.974433 -0.633985
H -2.961788 -0.792669 -0.809153
H -2.462970 -0.888686 1.433619
H 2.851654 0.761525 1.708229
H 1.333448 -0.115537 1.949392
H 2.823008 -1.009803 1.598724
el energy= -389.775898504
zpe= -389.545972
th energy= -389.536268
th enthalpy= -389.535324
free energy= -389.580144

4mchm_23/coords
c7
C 0.441126 -1.269820 -0.935399
H 1.054996 -2.159185 -0.727980
C 1.313062 0.000141 -0.833514
H 1.983497 0.000289 -1.709684
C 0.441102 1.270129 -0.934997
H 1.054970 2.159442 -0.727314
C -0.793905 1.258451 -0.022965
H -0.478724 1.308746 1.028001
C -1.652543 0.000027 -0.226267
H -2.004684 0.000188 -1.273851
C -0.793886 -1.258452 -0.023358
H -0.478718 -1.309066 1.027604
C 2.287114 -0.000038 0.345600
O 1.598647 -0.000313 1.606335
C -2.883272 -0.000109 0.683508
H 0.102889 -1.364088 -1.979760
H 0.102883 1.364739 -1.979340
H -1.399595 2.155573 -0.222722
H -1.399561 -2.155520 -0.223385
H 2.932591 -0.892491 0.272841
H 2.932521 0.892493 0.273178
H 2.253329 -0.000175 2.313260
H -3.506630 0.888517 0.510510
H -3.506644 -0.888678 0.510258
H -2.585087 -0.000265 1.742051
el energy= -389.774614882
zpe= -389.544598
th energy= -389.534940

th enthalpy= -389.533996
free energy= -389.578594

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.337619 -1.100787 0.033118
H 1.012076 -1.910624 -0.283183
C 0.961739 0.267577 -0.286356
H 1.159613 0.307629 -1.370782
C -0.023497 1.394954 0.063866
H -0.157992 1.433083 1.156505
C -1.382639 1.206377 -0.625504
H -1.240987 1.303166 -1.713478
C -2.024326 -0.164798 -0.332154
H -2.881261 -0.280468 -1.013934
C -1.020289 -1.288273 -0.659344
H -1.447808 -2.264702 -0.387996
C 2.300582 0.482363 0.422852
O 3.330840 -0.422556 0.012529
C -2.574926 -0.264790 1.098144
H 0.221470 -1.196570 1.125067
H 0.403724 2.365906 -0.227211
H -2.069332 2.012548 -0.327907
H -0.857835 -1.310161 -1.748368
H 2.689673 1.481545 0.187304
H 2.157901 0.431161 1.516978
H 3.094204 -1.312747 0.296631
H -3.320806 0.520528 1.283494
H -3.064136 -1.235380 1.259894
H -1.790798 -0.160201 1.859016
el energy= -389.776642447
zpe= -389.546691
th energy= -389.536962
th enthalpy= -389.536018
free energy= -389.580913

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.477379 -0.877326 1.053298
H 1.198046 -1.709406 1.050409
C 1.159378 0.428485 0.597793
H 1.909139 0.702257 1.355489

C 0.117049 1.563041 0.519811
H -0.206868 1.807052 1.543499
C -1.120137 1.195871 -0.312830
H -0.843877 1.075842 -1.372516
C -1.787444 -0.099256 0.177449
H -2.125317 0.075095 1.214216
C -0.757484 -1.239717 0.216516
H -1.224073 -2.148736 0.624090
C 1.932281 0.283355 -0.721104
O 3.052505 -0.604900 -0.630476
C -3.013156 -0.464648 -0.662474
H 0.171104 -0.758157 2.104233
H 0.584188 2.475073 0.118930
H -1.844926 2.022744 -0.277784
H -0.461394 -1.485742 -0.816354
H 1.271616 -0.025727 -1.546167
H 2.363426 1.254989 -0.995065
H 2.729190 -1.506651 -0.524182
H -3.755684 0.345367 -0.656222
H -2.730412 -0.651544 -1.708986
H -3.501385 -1.372095 -0.280535
el energy= -389.776394536
zpe= -389.546617
th energy= -389.536862
th enthalpy= -389.535918
free energy= -389.580895

B3LYP-SMD aug-cc-pwCVDZ

4mchm_1/coords
t1
C 0.163173 1.415406 0.178613
H 0.563487 2.337721 -0.266888
C 1.036962 0.217960 -0.228975
H 1.036130 0.158064 -1.330614
C 0.442438 -1.086812 0.324377
H 1.037742 -1.947058 -0.009569
C -1.020332 -1.272371 -0.095735
H -1.421601 -2.196664 0.345871
C -1.899480 -0.079292 0.307913
H -1.886583 -0.014859 1.409555
C -1.299495 1.224911 -0.239062

H -1.899496 2.081824 0.101272
C 2.476263 0.440644 0.214256
O 3.320819 -0.594350 -0.338573
C -3.350112 -0.265622 -0.139760
H 0.215643 1.542097 1.272352
H 0.506739 -1.062393 1.424900
H -1.072232 -1.397198 -1.190266
H -1.364432 1.210145 -1.339769
H 2.830051 1.423183 -0.134222
H 2.542263 0.421753 1.313870
H 4.225315 -0.429998 -0.041507
H -3.415629 -0.331218 -1.236267
H -3.782079 -1.186572 0.277326
H -3.978370 0.577024 0.182775
el energy= -389.785640112
zpe= -389.556966
th energy= -389.547088
th enthalpy= -389.546143
free energy= -389.591319

4mchm_3/coords
t2
C -0.166451 1.415252 0.178431
H -0.214539 1.546729 1.271943
C -1.041288 0.214888 -0.217781
H -1.049146 0.151806 -1.320401
C -0.442456 -1.086882 0.335159
H -0.499860 -1.059209 1.436014
C 1.018038 -1.272933 -0.092497
H 1.422816 -2.195455 0.349659
C 1.897740 -0.077583 0.303827
H 1.888822 -0.009759 1.405292
C 1.294737 1.224621 -0.244837
H 1.895906 2.082881 0.090178
C -2.481735 0.439037 0.236281
O -3.398682 -0.577353 -0.221989
C 3.346994 -0.264078 -0.148302
H -0.570369 2.335131 -0.269127
H -1.041040 -1.947651 0.007816
H 1.064600 -1.400540 -1.186960
H 1.354995 1.206410 -1.345762
H -2.545122 0.415650 1.332325

H -2.832678 1.426243 -0.102985
H -3.404091 -0.551026 -1.188758
H 3.975474 0.580478 0.168804
H 3.781422 -1.182899 0.270935
H 3.408798 -0.333904 -1.244751
el energy= -389.786160586
zpe= -389.557325
th energy= -389.547527
th enthalpy= -389.546582
free energy= -389.591555

4mchm_5/coords
t3
C 0.378583 -1.263500 0.009956
H 0.812543 -2.157026 0.482864
C 1.023963 -0.000004 0.601397
H 0.819306 -0.000008 1.686012
C 0.378585 1.263493 0.009959
H 0.812550 2.157012 0.482877
C -1.144009 1.259236 0.192617
H -1.382798 1.311183 1.268132
C -1.798295 0.000002 -0.396400
H -1.600790 -0.000001 -1.482136
C -1.144009 -1.259238 0.192614
H -1.579707 -2.156388 -0.271713
C 2.543942 -0.000001 0.490715
O 2.950343 0.000009 -0.896353
C -3.313672 0.000004 -0.189216
H 0.612943 -1.324571 -1.063452
H 0.612950 1.324569 -1.063445
H -1.579694 2.156391 -0.271710
H -1.382805 -1.311188 1.268129
H 2.953150 0.891698 0.990689
H 2.953155 -0.891701 0.990678
H 3.915735 -0.000013 -0.918932
H -3.561825 0.000037 0.882998
H -3.778987 0.888251 -0.640037
H -3.778994 -0.888264 -0.639987
el energy= -389.784499966
zpe= -389.555916
th energy= -389.546044
th enthalpy= -389.545100

free energy= -389.590377

4mchm_6/coords
t4
C 0.160090 1.423719 0.180741
H 0.217472 1.543074 1.275061
C 1.039324 0.235133 -0.239997
H 1.035645 0.181458 -1.341735
C 0.455593 -1.076147 0.309055
H 1.052312 -1.934888 -0.032606
C -1.007252 -1.270545 -0.106979
H -1.062220 -1.388177 -1.201982
C -1.892063 -0.085876 0.309260
H -1.874737 -0.029781 1.411254
C -1.303930 1.226767 -0.230536
H -1.374894 1.220375 -1.330902
C 2.482845 0.461014 0.204104
O 3.411512 -0.512900 -0.318860
C -3.343352 -0.279326 -0.133428
H 0.552771 2.351528 -0.260467
H 0.523906 -1.057917 1.409465
H -1.399890 -2.200330 0.330507
H -1.908160 2.076528 0.120174
H 2.845238 1.429095 -0.164026
H 2.541988 0.471237 1.304498
H 3.167153 -1.380214 0.031124
H -3.976630 0.554765 0.201162
H -3.413777 -0.334001 -1.230215
H -3.765807 -1.207992 0.276251
el energy= -389.786379507
zpe= -389.557575
th energy= -389.547761
th enthalpy= -389.546817
free energy= -389.591807

4mchm_7/coords
t5
C 0.376974 1.272292 0.000083
H 0.615894 1.319253 1.073369
C 1.030189 0.022620 -0.609715
H 0.835694 0.038624 -1.696490
C 0.388880 -1.255402 -0.045730

H 0.624538 -1.341548 1.027477
C -1.134737 -1.254170 -0.220054
H -1.377997 -1.287234 -1.295160
C -1.791308 -0.009079 0.395231
H -1.587331 -0.027146 1.479563
C -1.146486 1.262967 -0.175954
H -1.584427 2.150029 0.305378
C 2.554342 0.025364 -0.483343
O 3.044606 0.047393 0.875399
C -3.308024 -0.013534 0.197461
H 0.804092 2.175286 -0.461059
H 0.823922 -2.137088 -0.539619
H -1.563529 -2.162000 0.229550
H -1.390898 1.331395 -1.249220
H 2.972770 -0.848224 -1.007217
H 2.966268 0.929110 -0.950009
H 2.789003 -0.781091 1.302528
H -3.764791 -0.914939 0.630643
H -3.775838 0.860922 0.672010
H -3.563203 0.009160 -0.872811
el energy= -389.785356144
zpe= -389.556420
th energy= -389.546705
th enthalpy= -389.545761
free energy= -389.590503

4mchm_19/coords
t6
C 0.255984 -1.098411 0.664973
H -0.313434 -1.215430 1.598446
C 0.939581 0.284247 0.688392
H 1.442012 0.401952 1.661324
C -0.119094 1.399336 0.565843
H -0.711937 1.415351 1.491515
C -1.057192 1.210382 -0.636962
H -1.817804 2.005167 -0.636146
C -1.745422 -0.169573 -0.649928
H -2.242281 -0.282687 -1.625938
C -0.683624 -1.282472 -0.537004
H -0.090696 -1.300410 -1.463814
C 2.028488 0.437552 -0.371795
O 3.108108 -0.479375 -0.075932

C -2.835499 -0.290730 0.424312
H 1.013459 -1.893812 0.666295
H 0.376135 2.379218 0.498481
H -0.485535 1.329181 -1.569515
H -1.177971 -2.262850 -0.467884
H 1.647475 0.232487 -1.381619
H 2.413385 1.468829 -0.354780
H 3.756399 -0.412547 -0.789129
H -3.594877 0.494542 0.300180
H -3.345176 -1.262066 0.350960
H -2.433359 -0.203905 1.442093
el energy= -389.779096887
zpe= -389.549391
th energy= -389.539792
th enthalpy= -389.538847
free energy= -389.583489

4mchm_21/coords
t7
C 0.107380 1.393934 0.564938
H -0.392837 2.371248 0.494947
C -0.947169 0.272711 0.665856
H -1.463748 0.384044 1.633587
C -0.260288 -1.107383 0.643105
H 0.294053 -1.233326 1.584435
C 0.697828 -1.279596 -0.545882
H 0.118871 -1.292828 -1.481534
C 1.756835 -0.161775 -0.635758
H 2.268924 -0.267088 -1.604694
C 1.061760 1.214772 -0.626223
H 0.501316 1.333916 -1.565619
C -2.028563 0.427477 -0.408541
O -3.137282 -0.479298 -0.224235
C 2.830482 -0.284154 0.454632
H 0.687443 1.409615 1.498763
H -1.017514 -1.903287 0.624448
H 1.194831 -2.258630 -0.476619
H 1.818116 2.013497 -0.612667
H -2.400947 1.463777 -0.405744
H -1.646522 0.210505 -1.412150
H -3.519105 -0.300757 0.646734
H 2.412295 -0.203720 1.466487

H 3.344945 -1.253182 0.384568
H 3.588544 0.504686 0.346178
el energy= -389.779751372
zpe= -389.550002
th energy= -389.540458
th enthalpy= -389.539514
free energy= -389.583905

4mchm_22/coords
t8
C 0.126244 1.418330 0.549111
H -0.362252 2.400384 0.462468
C -0.941993 0.314336 0.692472
H -1.438534 0.447755 1.666189
C -0.272297 -1.074921 0.682179
H 0.298267 -1.188461 1.615134
C 0.659182 -1.283394 -0.521893
H 1.139497 -2.270180 -0.446441
C 1.735408 -0.186083 -0.646250
H 2.230834 -0.316601 -1.620818
C 1.064760 1.202444 -0.649506
H 1.835351 1.987536 -0.656140
C -2.037532 0.465994 -0.368135
O -3.158034 -0.422107 -0.158160
C 2.823762 -0.309921 0.429432
H 0.718359 1.448746 1.475000
H -1.035307 -1.867321 0.700974
H 0.061999 -1.299698 -1.446087
H 0.497322 1.317321 -1.584878
H -2.459320 1.477411 -0.314195
H -1.645205 0.318125 -1.383706
H -2.858977 -1.327596 -0.315799
H 3.594465 0.462501 0.295056
H 2.423399 -0.204354 1.446143
H 3.319170 -1.289423 0.367926
el energy= -389.779716367
zpe= -389.550088
th energy= -389.540438
th enthalpy= -389.539494
free energy= -389.584167

4mchm_24/coords

t9
C -0.100410 1.275627 0.727897
H 0.588169 1.401733 1.576212
C -0.936427 -0.000026 0.978995
H -1.197632 -0.000045 2.049744
C -0.100404 -1.275662 0.727847
H 0.588165 -1.401803 1.576165
C 0.717766 -1.258585 -0.572914
H 1.350241 -2.158435 -0.612869
C 1.596184 0.000017 -0.713119
H 2.015982 0.000035 -1.731050
C 0.717750 1.258601 -0.572872
H 0.041293 1.312013 -1.436436
C -2.310861 -0.000013 0.311580
O -2.233705 0.000045 -1.132724
C 2.783119 0.000005 0.259756
H -0.761179 2.155169 0.738020
H -0.761164 -2.155212 0.737937
H 0.041317 -1.311982 -1.436484
H 1.350213 2.158459 -0.612809
H -2.868222 -0.891114 0.641276
H -2.868239 0.891052 0.641347
H -3.139138 -0.000029 -1.469489
H 2.465244 -0.000021 1.310370
H 3.412153 -0.887892 0.103400
H 3.412135 0.887921 0.103444
el energy= -389.774947573
zpe= -389.545677
th energy= -389.535937
th enthalpy= -389.534993
free energy= -389.579830

4mchm_9/coords
c1
C -0.464628 -0.893940 1.055341
H -1.181457 -1.726032 1.035632
C -1.151661 0.410746 0.603383
H -1.903016 0.683801 1.360726
C -0.116604 1.551488 0.532219
H -0.590248 2.465211 0.143995
C 1.114540 1.195091 -0.311856
H 0.826304 1.073135 -1.368036

C 1.792546 -0.096405 0.172135
H 2.138088 0.079195 1.205670
C 0.771076 -1.243859 0.215497
H 1.246332 -2.148062 0.624194
C -1.910659 0.268341 -0.714517
O -3.016261 -0.645177 -0.523660
C 3.011820 -0.451889 -0.679208
H -0.156875 -0.772317 2.105507
H 0.212610 1.779137 1.557502
H 1.834876 2.026031 -0.279097
H 0.470379 -1.490715 -0.815169
H -2.300718 1.250819 -1.022029
H -1.264586 -0.109049 -1.519062
H -3.460739 -0.753850 -1.374405
H 2.721420 -0.636002 -1.724439
H 3.751413 0.361558 -0.675051
H 3.507735 -1.358880 -0.304621
el energy= -389.782564199
zpe= -389.553436
th energy= -389.543724
th enthalpy= -389.542780
free energy= -389.587695

4mchm_11/coords
c2
C -0.320077 -1.113835 0.063748
H -0.994233 -1.931427 -0.224647
C -0.957480 0.243536 -0.275549
H -1.152908 0.269922 -1.361237
C 0.016467 1.386490 0.054802
H -0.422322 2.348337 -0.248130
C 1.370569 1.200069 -0.643314
H 1.217041 1.278224 -1.731158
C 2.028600 -0.159555 -0.336621
H 2.881530 -0.274743 -1.023167
C 1.033129 -1.297335 -0.637697
H 0.862547 -1.336833 -1.725153
C -2.287411 0.463465 0.431402
O -3.254941 -0.502101 -0.039701
C 2.588689 -0.233647 1.090767
H -0.192790 -1.181059 1.155612
H 0.158081 1.435114 1.145567

H 2.051588 2.016918 -0.362000
H 1.472998 -2.264472 -0.352410
H -2.161271 0.357132 1.520476
H -2.658257 1.479253 0.224966
H -4.080918 -0.351148 0.438038
H 3.095984 -1.194504 1.258251
H 3.322149 0.566840 1.263719
H 1.805395 -0.135878 1.853652
el energy= -389.782368639
zpe= -389.553336
th energy= -389.543526
th enthalpy= -389.542581
free energy= -389.587711

4mchm_13/coords
c3
C -0.013599 1.386027 0.055989
H -0.162187 1.437754 1.145805
C 0.961162 0.240403 -0.262403
H 1.166151 0.264464 -1.347485
C 0.320250 -1.114731 0.074203
H 0.997716 -1.932618 -0.206211
C -1.027291 -1.298665 -0.637900
H -0.848327 -1.339598 -1.723989
C -2.024025 -0.159390 -0.345974
H -2.872273 -0.275534 -1.038133
C -1.363415 1.199516 -0.650692
H -2.045996 2.017125 -0.375237
C 2.289121 0.463251 0.456889
O 3.310232 -0.494288 0.103407
C -2.593889 -0.230387 1.077702
H 0.429070 2.346416 -0.246297
H 0.183372 -1.179599 1.165077
H -1.470686 -2.264856 -0.354862
H -1.202667 1.275814 -1.737628
H 2.657624 1.480670 0.252537
H 2.158561 0.361196 1.542293
H 3.484721 -0.401845 -0.843649
H -3.100931 -1.191513 1.244415
H -1.816175 -0.129193 1.845839
H -3.329708 0.569480 1.243382
el energy= -389.782889326

zpe= -389.553880
th energy= -389.544015
th enthalpy= -389.543071
free energy= -389.588566

4mchm_15/coords
c4
C -0.471331 -0.903305 1.041656
H -0.173084 -0.789516 2.095456
C -1.157021 0.401634 0.592285
H -1.917063 0.668064 1.345198
C -0.126377 1.547625 0.537312
H -0.600325 2.460760 0.147586
C 1.113130 1.198914 -0.298220
H 0.834605 1.083249 -1.357707
C 1.790466 -0.094331 0.182198
H 2.127764 0.074700 1.219557
C 0.771690 -1.244680 0.209376
H 1.246060 -2.150611 0.615273
C -1.904414 0.268382 -0.738686
O -2.984815 -0.688135 -0.688941
C 3.016801 -0.441189 -0.662531
H -1.187126 -1.736142 1.009602
H 0.192501 1.773784 1.566223
H 1.831245 2.031252 -0.254264
H 0.479423 -1.484822 -0.825306
H -2.301807 1.251971 -1.034040
H -1.248975 -0.083523 -1.542744
H -3.603243 -0.397379 -0.004201
H 2.734138 -0.620295 -1.710774
H 3.754095 0.374244 -0.648939
H 3.512641 -1.348955 -0.289729
el energy= -389.783169926
zpe= -389.554157
th energy= -389.544354
th enthalpy= -389.543409
free energy= -389.588822

4mchm_16/coords
c5
C -0.230666 1.264062 -0.185644
H -0.731076 2.156433 -0.590111

C -0.960377 0.000017 -0.668861
H -0.927330 0.000046 -1.772404
C -0.230678 -1.264042 -0.185690
H -0.301747 -1.332554 0.908910
C 1.244376 -1.260589 -0.612620
H 1.748089 -2.160437 -0.229421
C 2.001574 -0.000003 -0.149166
H 2.981727 -0.000005 -0.650501
C 1.244392 1.260604 -0.612576
H 1.293075 1.314657 -1.711744
C -2.444464 0.000022 -0.323615
O -2.631509 -0.000052 1.110874
C 2.271162 -0.000029 1.361976
H -0.301732 1.332545 0.908960
H -0.731103 -2.156393 -0.590188
H 1.293061 -1.314604 -1.711790
H 1.748118 2.160432 -0.229347
H -2.927608 0.891751 -0.752657
H -2.927626 -0.891663 -0.752753
H -3.581877 0.000057 1.283913
H 2.850171 -0.887946 1.653553
H 2.850241 0.887843 1.653561
H 1.345787 0.000008 1.952203
el energy= -389.781263002
zpe= -389.551990
th energy= -389.542289
th enthalpy= -389.541345
free energy= -389.586252

4mchm_17/coords
c6
C -0.224678 1.286565 -0.104666
H -0.715564 2.208366 -0.450660
C -0.966778 0.065447 -0.670267
H -0.942842 0.140917 -1.771768
C -0.248135 -1.237541 -0.282318
H -0.319917 -1.391143 0.805474
C 1.229006 -1.217261 -0.702614
H 1.723104 -2.146199 -0.381586
C 1.995227 0.001584 -0.151013
H 2.977099 0.027513 -0.648321
C 1.251309 1.297752 -0.528366

H 1.763110 2.164477 -0.084262
C -2.452668 0.050194 -0.309764
O -2.723555 -0.023728 1.107344
C 2.259707 -0.105056 1.357485
H -0.298388 1.284054 0.992081
H -0.755285 -2.092297 -0.754362
H 1.280178 -1.195660 -1.802728
H 1.303085 1.427048 -1.621139
H -2.930228 0.979910 -0.644321
H -2.950913 -0.789607 -0.819162
H -2.411035 -0.880307 1.427696
H 2.841039 0.758192 1.711570
H 1.332449 -0.142283 1.943618
H 2.834615 -1.013263 1.588268
el energy= -389.782077286
zpe= -389.552784
th energy= -389.543052
th enthalpy= -389.542108
free energy= -389.587055

4mchm_23/coords
c7
C 0.414931 -1.272226 -0.916718
H 1.034403 -2.155566 -0.701789
C 1.286279 0.000630 -0.844697
H 1.918017 0.001259 -1.747846
C 0.414882 1.273553 -0.914971
H 1.034291 2.156618 -0.698736
C -0.818215 1.257197 -0.000184
H -0.512942 1.308795 1.055151
C -1.676226 0.000112 -0.207603
H -2.018144 0.000771 -1.257361
C -0.818084 -1.257152 -0.001800
H -0.512707 -1.310016 1.053442
C 2.323492 -0.000167 0.276437
O 1.726350 -0.001206 1.593102
C -2.912668 -0.000538 0.692283
H 0.065706 -1.382312 -1.955233
H 0.065737 1.385094 -1.953356
H -1.424482 2.154195 -0.197486
H -1.424297 -2.153960 -0.200141
H 2.962796 -0.891010 0.171399

H 2.962757 0.890859 0.172747
H 2.447143 -0.001368 2.236959
H -3.535087 0.888079 0.514036
H -3.535169 -0.888798 0.512557
H -2.625169 -0.001455 1.754355
el energy= -389.778549700
zpe= -389.549513
th energy= -389.539741
th enthalpy= -389.538797
free energy= -389.583774

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.337519 -1.100291 0.036491
H 1.014331 -1.911226 -0.270664
C 0.959860 0.267614 -0.287108
H 1.149799 0.310816 -1.373039
C -0.023143 1.395228 0.067777
H -0.157115 1.425360 1.160192
C -1.381003 1.206931 -0.623115
H -1.237339 1.305717 -1.710577
C -2.022630 -0.164582 -0.334381
H -2.878715 -0.278058 -1.017212
C -1.017753 -1.287205 -0.660360
H -1.445646 -2.263331 -0.388246
C 2.294357 0.489789 0.420868
O 3.331317 -0.427857 0.011543
C -2.572259 -0.267792 1.095284
H 0.217992 -1.186660 1.128007
H 0.404625 2.366005 -0.222737
H -2.068418 2.011336 -0.322037
H -0.852532 -1.307038 -1.749043
H 2.683722 1.487560 0.182165
H 2.159030 0.429076 1.512582
H 3.075755 -1.316051 0.294737
H -3.316297 0.519095 1.284437
H -3.064109 -1.238465 1.252054
H -1.785302 -0.169436 1.854300
el energy= -389.783168602
zpe= -389.553677
th energy= -389.544037
th enthalpy= -389.543093

free energy= -389.587744

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.477700 -0.876647 1.058979
H 1.196268 -1.709862 1.051582
C 1.158443 0.428646 0.599750
H 1.908421 0.709288 1.355390
C 0.116509 1.563651 0.520689
H -0.208595 1.803258 1.544626
C -1.117688 1.194531 -0.314122
H -0.835817 1.069416 -1.371479
C -1.785215 -0.099096 0.178195
H -2.127583 0.077710 1.212564
C -0.755632 -1.239088 0.221353
H -1.222998 -2.146119 0.632636
C 1.919227 0.286796 -0.722816
O 3.052841 -0.605381 -0.634379
C -3.005526 -0.466036 -0.666910
H 0.170239 -0.750831 2.108643
H 0.585211 2.474491 0.119244
H -1.842938 2.021149 -0.280789
H -0.454115 -1.485012 -0.809308
H 1.261509 -0.043942 -1.538137
H 2.342136 1.258765 -1.006138
H 2.721236 -1.507335 -0.532041
H -3.749939 0.342972 -0.663714
H -2.717922 -0.653232 -1.712360
H -3.494753 -1.374196 -0.286396
el energy= -389.783230087
zpe= -389.553883
th energy= -389.544260
th enthalpy= -389.543316
free energy= -389.587969

B3LYP cc-pVTZ gas phase

4mchm_1/coords
t1
C 0.159908 1.423320 0.177104
H 0.550136 2.343820 -0.265388
C 1.036228 0.231515 -0.228466

H 1.037989 0.166440 -1.323027
C 0.454091 -1.075505 0.324076
H 1.063663 -1.916611 -0.006008
C -1.005348 -1.270465 -0.092763
H -1.399539 -2.191497 0.344767
C -1.891564 -0.083798 0.308228
H -1.881260 -0.020285 1.403698
C -1.301183 1.224416 -0.235081
H -1.903303 2.071946 0.102956
C 2.479710 0.445198 0.202183
O 3.282272 -0.606533 -0.333271
C -3.339451 -0.279197 -0.139507
H 0.213160 1.555065 1.264023
H 0.518156 -1.053545 1.418704
H -1.058229 -1.399847 -1.180042
H -1.369419 1.214464 -1.328973
H 2.831200 1.418741 -0.161359
H 2.539033 0.457750 1.298643
H 4.184163 -0.496559 -0.021463
H -3.404765 -0.349088 -1.228231
H -3.763324 -1.195354 0.276259
H -3.970179 0.553932 0.176965
el energy= -389.864976864
zpe= -389.637292
th energy= -389.627415
th enthalpy= -389.626471
free energy= -389.671647

4mchm_3/coords
t2
C -0.160408 1.422523 0.176556
H -0.213633 1.553566 1.263369
C -1.037790 0.229323 -0.224183
H -1.030787 0.166419 -1.322050
C -0.452364 -1.075571 0.327552
H -0.514343 -1.050707 1.421829
C 1.005904 -1.271045 -0.092608
H 1.401491 -2.191252 0.345157
C 1.892291 -0.083256 0.305664
H 1.883640 -0.019293 1.400992
C 1.300456 1.224721 -0.237064
H 1.902534 2.072430 0.100428

C -2.485937 0.444782 0.212079
O -3.372406 -0.593598 -0.198134
C 3.339373 -0.278356 -0.144444
H -0.552943 2.342805 -0.264433
H -1.063558 -1.919334 0.005681
H 1.057825 -1.401552 -1.180048
H 1.368298 1.215108 -1.331123
H -2.546375 0.461442 1.302434
H -2.840858 1.418377 -0.148057
H -3.418942 -0.590315 -1.158900
H 3.970234 0.555112 0.170637
H 3.764315 -1.194054 0.271121
H 3.403198 -0.348692 -1.233268
el energy= -389.865191953
zpe= -389.637412
th energy= -389.627596
th enthalpy= -389.626651
free energy= -389.671684

4mchm_5/coords
t3
C 0.387368 -1.262992 0.042348
H 0.809266 -2.150041 0.523159
C 1.032990 -0.000010 0.629584
H 0.850148 0.000009 1.712165
C 0.387367 1.262988 0.042336
H 0.809311 2.150017 0.523155
C -1.135145 1.256428 0.201774
H -1.391728 1.309315 1.266645
C -1.779480 -0.000009 -0.397470
H -1.565079 0.000006 -1.473321
C -1.135169 -1.256438 0.201749
H -1.561814 -2.149768 -0.261902
C 2.547914 -0.000001 0.462843
O 2.869925 0.000024 -0.929095
C -3.297149 0.000019 -0.217273
H 0.647138 -1.330524 -1.016700
H 0.647137 1.330508 -1.016710
H -1.561845 2.149748 -0.261848
H -1.391769 -1.309369 1.266617
H 2.969835 0.886671 0.951981
H 2.969853 -0.886675 0.951956

H 3.825345 -0.000074 -1.024830
H -3.564407 0.000055 0.842620
H -3.751468 0.882055 -0.672814
H -3.751509 -0.882028 -0.672746
el energy= -389.864427836
zpe= -389.636735
th energy= -389.626868
th enthalpy= -389.625923
free energy= -389.671060

4mchm_6/coords
t4
C 0.158372 1.421979 0.178160
H 0.219793 1.542320 1.265951
C 1.038426 0.239216 -0.246507
H 1.038803 0.186807 -1.341515
C 0.458333 -1.075300 0.290676
H 1.048181 -1.922362 -0.069025
C -1.006094 -1.267972 -0.112920
H -1.068525 -1.383163 -1.200946
C -1.888861 -0.087294 0.311635
H -1.866741 -0.035904 1.407513
C -1.305756 1.226910 -0.224233
H -1.384081 1.228164 -1.317377
C 2.486210 0.459765 0.190976
O 3.395946 -0.519176 -0.303605
C -3.340865 -0.282169 -0.122689
H 0.545207 2.347583 -0.256220
H 0.535196 -1.077025 1.384999
H -1.393915 -2.195055 0.317206
H -1.905892 2.069761 0.128347
H 2.846587 1.412456 -0.200137
H 2.537770 0.517679 1.286430
H 3.227227 -1.351030 0.146786
H -3.969544 0.546038 0.209780
H -3.417840 -0.340061 -1.211294
H -3.758386 -1.203609 0.287758
el energy= -389.865005158
zpe= -389.637253
th energy= -389.627387
th enthalpy= -389.626442
free energy= -389.671609

4mchm_7/coords
t5
C 0.381343 1.270013 -0.017069
H 0.643665 1.321488 1.042897
C 1.034011 0.022050 -0.625511
H 0.848524 0.034870 -1.707924
C 0.390863 -1.252155 -0.061430
H 0.626317 -1.333750 1.005801
C -1.131767 -1.252126 -0.225134
H -1.381032 -1.286412 -1.291999
C -1.782840 -0.009711 0.395784
H -1.573616 -0.030429 1.472686
C -1.141546 1.261302 -0.175216
H -1.571806 2.142299 0.307994
C 2.556102 0.027479 -0.463177
O 3.000752 0.045844 0.892443
C -3.299623 -0.013507 0.209161
H 0.799654 2.166940 -0.481432
H 0.819478 -2.133561 -0.547382
H -1.555600 -2.156240 0.219591
H -1.398324 1.337039 -1.238501
H 2.987906 -0.829078 -0.995368
H 2.969407 0.932277 -0.911473
H 2.813936 -0.809915 1.287335
H -3.752008 -0.906310 0.645144
H -3.759406 0.857278 0.680203
H -3.562374 0.006678 -0.851557
el energy= -389.864577572
zpe= -389.636807
th energy= -389.626986
th enthalpy= -389.626042
free energy= -389.671101

4mchm_19/coords
t6
C 0.277369 -1.085694 0.657372
H -0.276064 -1.220172 1.590345
C 0.939519 0.304070 0.681222
H 1.438448 0.422624 1.647428
C -0.122572 1.410287 0.550587
H -0.704337 1.438987 1.475026

C -1.071200 1.205615 -0.639031
H -1.834445 1.988145 -0.636871
C -1.743343 -0.180218 -0.642615
H -2.242468 -0.300395 -1.608974
C -0.670214 -1.279461 -0.533323
H -0.088647 -1.295337 -1.459619
C 2.040792 0.449778 -0.366569
O 3.066949 -0.499758 -0.075073
C -2.826860 -0.308914 0.434920
H 1.051672 -1.852844 0.645894
H 0.361909 2.387301 0.471064
H -0.516223 1.328223 -1.573491
H -1.149516 -2.259293 -0.463570
H 1.650589 0.289819 -1.377284
H 2.440537 1.470347 -0.324206
H 3.730838 -0.459963 -0.768157
H -3.594405 0.457074 0.307823
H -3.317342 -1.282400 0.375557
H -2.427078 -0.206827 1.444246
el energy= -389.858038049
zpe= -389.629763
th energy= -389.620005
th enthalpy= -389.619060
free energy= -389.664009

4mchm_21/coords
t7
C 0.118390 1.410159 0.549318
H -0.370400 2.384617 0.463915
C -0.941418 0.299915 0.672779
H -1.436200 0.422010 1.644532
C -0.279368 -1.089222 0.651446
H 0.266807 -1.230246 1.587740
C 0.675468 -1.279093 -0.534133
H 0.098665 -1.293850 -1.462941
C 1.747732 -0.178311 -0.634119
H 2.253846 -0.297278 -1.596828
C 1.072462 1.205821 -0.635758
H 0.521480 1.325835 -1.572677
C -2.042122 0.447053 -0.384492
O -3.091762 -0.507164 -0.244095
C 2.823290 -0.305304 0.451400

H 0.695584 1.444070 1.476517
H -1.053793 -1.856895 0.626476
H 1.154991 -2.258572 -0.462874
H 1.833325 1.990519 -0.630756
H -2.442389 1.467798 -0.348188
H -1.652031 0.291431 -1.389899
H -3.504865 -0.378367 0.615337
H 2.415935 -0.205001 1.457972
H 3.316618 -1.277488 0.394942
H 3.589913 0.462625 0.330842
el energy= -389.858488127
zpe= -389.630125
th energy= -389.620422
th enthalpy= -389.619478
free energy= -389.664267

4mchm_22/coords
t8
C 0.121380 1.416209 0.543387
H -0.365342 2.391056 0.453607
C -0.942720 0.312289 0.685455
H -1.439633 0.438393 1.651527
C -0.272749 -1.073695 0.675600
H 0.288158 -1.194141 1.605674
C 0.666552 -1.282749 -0.519605
H 1.145328 -2.262280 -0.443794
C 1.739300 -0.184549 -0.641469
H 2.233726 -0.313976 -1.608836
C 1.067708 1.201411 -0.646638
H 1.831875 1.982774 -0.651992
C -2.049556 0.456115 -0.366342
O -3.154346 -0.418483 -0.146167
C 2.827549 -0.306146 0.432194
H 0.704790 1.456933 1.466522
H -1.032958 -1.859353 0.696576
H 0.082132 -1.303352 -1.444345
H 0.511175 1.317415 -1.580620
H -2.464253 1.463654 -0.308694
H -1.659231 0.327205 -1.381161
H -2.891460 -1.313421 -0.376311
H 3.597342 0.454850 0.291084
H 2.434504 -0.188950 1.442543

H 3.313831 -1.282255 0.382068
el energy= -389.857634801
zpe= -389.629413
th energy= -389.619601
th enthalpy= -389.618656
free energy= -389.663744

4mchm_24/coords
t9
C -0.110855 1.270367 0.761042
H 0.579031 1.379497 1.602455
C -0.953919 0.000071 0.995875
H -1.246823 0.000131 2.052011
C -0.110871 -1.270261 0.761182
H 0.579018 -1.379307 1.602604
C 0.687319 -1.258212 -0.549371
H 1.315253 -2.152310 -0.598470
C 1.560127 -0.000045 -0.710538
H 1.947168 -0.000103 -1.734012
C 0.687349 1.258162 -0.549502
H -0.008842 1.309239 -1.386586
C -2.293994 0.000038 0.262695
O -2.121855 -0.000093 -1.157150
C 2.776213 -0.000013 0.223884
H -0.758743 2.150650 0.788595
H -0.758771 -2.150532 0.788839
H -0.008883 -1.309353 -1.386443
H 1.315309 2.152238 -0.598686
H -2.863238 -0.885737 0.571481
H -2.863201 0.885892 0.571327
H -2.989418 -0.000193 -1.570088
H 2.494798 0.000048 1.277691
H 3.396969 -0.881701 0.052484
H 3.396994 0.881641 0.052391
el energy= -389.856297629
zpe= -389.627993
th energy= -389.618292
th enthalpy= -389.617348
free energy= -389.661966

4mchm_9/coords
c1

C -0.483328 -0.878317 1.044349
H -1.212386 -1.687914 1.008251
C -1.152652 0.431731 0.591749
H -1.897676 0.706756 1.343857
C -0.112966 1.563110 0.508827
H -0.574316 2.469254 0.106711
C 1.124573 1.191328 -0.315995
H 0.852213 1.068681 -1.369703
C 1.786590 -0.102060 0.179126
H 2.122026 0.074459 1.209113
C 0.755909 -1.238511 0.219025
H 1.216786 -2.141537 0.627908
C -1.926874 0.277701 -0.715526
O -2.972930 -0.672265 -0.509221
C 3.010314 -0.470563 -0.657755
H -0.188281 -0.767986 2.092487
H 0.206352 1.809161 1.525825
H 1.845837 2.012330 -0.284039
H 0.464560 -1.488618 -0.806838
H -2.344515 1.251188 -1.000432
H -1.270160 -0.049824 -1.528433
H -3.421466 -0.824617 -1.344904
H 2.730672 -0.658816 -1.697453
H 3.750929 0.331635 -0.654254
H 3.493465 -1.372544 -0.277122
el energy= -389.861687122
zpe= -389.633808
th energy= -389.623981
th enthalpy= -389.623037
free energy= -389.668169

4mchm_11/coords
c2
C -0.334438 -1.102775 0.061334
H -1.022605 -1.898761 -0.222915
C -0.958078 0.259331 -0.271362
H -1.158774 0.285835 -1.349248
C 0.020868 1.393499 0.058556
H -0.406392 2.354863 -0.238770
C 1.373287 1.198479 -0.636651
H 1.223802 1.285094 -1.717507
C 2.019340 -0.167094 -0.338226

H 2.863694 -0.286156 -1.023858
C 1.014982 -1.294961 -0.638189
H 0.845531 -1.334402 -1.718914
C -2.292430 0.468831 0.428454
O -3.218474 -0.511473 -0.038775
C 2.587356 -0.249386 1.083852
H -0.208104 -1.178235 1.146746
H 0.162598 1.444568 1.143040
H 2.057556 2.002945 -0.355093
H 1.446226 -2.259870 -0.359623
H -2.156124 0.385773 1.514887
H -2.663312 1.479074 0.215398
H -4.045323 -0.408133 0.439102
H 3.080030 -1.209474 1.249164
H 3.326649 0.536063 1.252849
H 1.817015 -0.142941 1.848334
el energy= -389.861499776
zpe= -389.633539
th energy= -389.623717
th enthalpy= -389.622773
free energy= -389.667847

4mchm_13/coords
c3
C -0.020177 1.392832 0.060283
H -0.164103 1.441282 1.144408
C 0.959666 0.257563 -0.264902
H 1.153936 0.287894 -1.347155
C 0.332709 -1.103049 0.063531
H 1.021772 -1.901832 -0.212517
C -1.013656 -1.294703 -0.641694
H -0.841246 -1.333664 -1.722223
C -2.018302 -0.166077 -0.344321
H -2.860114 -0.284178 -1.033148
C -1.370852 1.199746 -0.639108
H -2.055664 2.003905 -0.358236
C 2.296731 0.467149 0.443291
O 3.282306 -0.508998 0.114575
C -2.591219 -0.249515 1.075626
H 0.409431 2.354510 -0.232719
H 0.202104 -1.176999 1.148135
H -1.446621 -2.259307 -0.365180

H -1.218844 1.288243 -1.719599
H 2.671025 1.477335 0.235811
H 2.161384 0.387343 1.524036
H 3.498602 -0.418723 -0.818358
H -3.084286 -1.209758 1.238481
H -1.823917 -0.143340 1.843155
H -3.331303 0.535598 1.242269
el energy= -389.861731054
zpe= -389.633654
th energy= -389.623904
th enthalpy= -389.622959
free energy= -389.667848

4mchm_15/coords
c4
C -0.484606 -0.890736 1.033484
H -0.197835 -0.793114 2.085207
C -1.153907 0.420633 0.586924
H -1.897051 0.695158 1.345931
C -0.118919 1.558103 0.517212
H -0.583246 2.463270 0.116110
C 1.122105 1.194293 -0.305411
H 0.853567 1.075918 -1.360383
C 1.786852 -0.099000 0.186072
H 2.115825 0.072757 1.219004
C 0.760570 -1.239704 0.212105
H 1.222121 -2.143799 0.617520
C -1.924246 0.274454 -0.730736
O -2.954742 -0.709177 -0.677288
C 3.016429 -0.457438 -0.646472
H -1.209828 -1.703739 0.979851
H 0.195835 1.801913 1.536264
H 1.839861 2.017959 -0.267069
H 0.474666 -1.483771 -0.816297
H -2.337421 1.249393 -1.017534
H -1.269592 -0.046446 -1.540429
H -3.592443 -0.443401 -0.007633
H 2.743078 -0.640301 -1.688679
H 3.753631 0.347767 -0.633844
H 3.501108 -1.359768 -0.268787
el energy= -389.862113259
zpe= -389.634049

th energy= -389.624320
th enthalpy= -389.623376
free energy= -389.668252

4mchm_16/coords
c5
C -0.240661 1.263762 -0.213212
H -0.729229 2.149549 -0.628819
C -0.968952 0.000000 -0.693079
H -0.954571 -0.000006 -1.791008
C -0.240659 -1.263763 -0.213205
H -0.341132 -1.339009 0.870763
C 1.238911 -1.257932 -0.613883
H 1.733268 -2.153170 -0.227911
C 1.988108 0.000000 -0.138596
H 2.970164 -0.000002 -0.621420
C 1.238912 1.257931 -0.613887
H 1.309219 1.313398 -1.705340
C -2.440794 -0.000002 -0.297614
O -2.548195 -0.000014 1.127074
C 2.234025 0.000003 1.375093
H -0.341132 1.339019 0.870757
H -0.729232 -2.149545 -0.628814
H 1.309213 -1.313401 -1.705337
H 1.733268 2.153168 -0.227913
H -2.931894 0.886746 -0.717296
H -2.931891 -0.886753 -0.717312
H -3.478073 0.000114 1.366669
H 2.804104 -0.881501 1.674959
H 2.804112 0.881505 1.674951
H 1.306024 0.000010 1.946778
el energy= -389.861107032
zpe= -389.633062
th energy= -389.623276
th enthalpy= -389.622332
free energy= -389.667271

4mchm_17/coords
c6
C -0.233807 1.280965 -0.127523
H -0.718670 2.194628 -0.481441
C -0.972054 0.056921 -0.685020

H -0.955464 0.121536 -1.781412
C -0.248910 -1.237502 -0.287344
H -0.324300 -1.377668 0.795614
C 1.229349 -1.218490 -0.694392
H 1.719773 -2.139260 -0.368416
C 1.989635 0.003269 -0.147109
H 2.966600 0.027150 -0.639174
C 1.244720 1.293947 -0.532617
H 1.745833 2.157934 -0.088758
C -2.451097 0.043136 -0.291572
O -2.682110 -0.010850 1.115702
C 2.252286 -0.094646 1.360562
H -0.332549 1.286841 0.959790
H -0.744683 -2.097377 -0.747401
H 1.289559 -1.206760 -1.787354
H 1.311197 1.423968 -1.617820
H -2.927851 0.966172 -0.625376
H -2.959521 -0.788886 -0.794076
H -2.456286 -0.890469 1.429847
H 2.839048 0.758178 1.706891
H 1.331499 -0.113688 1.944049
H 2.811961 -1.001093 1.599509
el energy= -389.861184250
zpe= -389.633103
th energy= -389.623340
th enthalpy= -389.622396
free energy= -389.667319

4mchm_23/coords
c7
C 0.447007 -1.267700 -0.936850
H 1.056108 -2.152010 -0.730916
C 1.317644 -0.000323 -0.829167
H 1.992378 -0.000645 -1.692770
C 0.447033 1.266993 -0.937773
H 1.056156 2.151440 -0.732487
C -0.789085 1.257583 -0.031748
H -0.477266 1.311950 1.012887
C -1.645977 -0.000078 -0.231116
H -2.000587 -0.000452 -1.270574
C -0.789105 -1.257604 -0.030828
H -0.477280 -1.311216 1.013843

C 2.273557 0.000101 0.362022
O 1.569763 0.000613 1.606881
C -2.869928 0.000262 0.683294
H 0.115258 -1.360363 -1.976166
H 0.115297 1.358908 -1.977160
H -1.391090 2.148206 -0.233504
H -1.391120 -2.148368 -0.231932
H 2.917724 -0.885687 0.295696
H 2.917792 0.885785 0.295010
H 2.212525 0.001099 2.321034
H -3.490816 0.882631 0.515344
H -3.490829 -0.882221 0.515987
H -2.569226 0.000639 1.733651
el energy= -389.860081687
zpe= -389.631927
th energy= -389.622212
th enthalpy= -389.621267
free energy= -389.665942

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.341601 -1.096967 0.023890
H 1.015177 -1.895496 -0.297912
C 0.960134 0.272376 -0.289107
H 1.156216 0.315774 -1.367069
C -0.023922 1.395141 0.065275
H -0.153757 1.431344 1.151811
C -1.383437 1.206498 -0.617261
H -1.247850 1.309661 -1.698397
C -2.020550 -0.165397 -0.330238
H -2.873165 -0.279174 -1.006228
C -1.016638 -1.284178 -0.661941
H -1.439899 -2.255502 -0.394042
C 2.298983 0.484082 0.416463
O 3.315637 -0.430100 0.015216
C -2.568218 -0.272426 1.098070
H 0.230449 -1.200647 1.109019
H 0.398024 2.361648 -0.222221
H -2.067268 2.003822 -0.315438
H -0.859129 -1.304004 -1.744719
H 2.688179 1.474082 0.173719
H 2.154560 0.449148 1.504582

H 3.096693 -1.301365 0.356108
H -3.309679 0.505844 1.288272
H -3.052968 -1.237728 1.256227
H -1.788402 -0.171381 1.853653
el energy= -389.861560229
zpe= -389.633496
th energy= -389.623694
th enthalpy= -389.622749
free energy= -389.667781

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.480821 -0.866443 1.055646
H 1.202443 -1.687924 1.054159
C 1.157618 0.436571 0.594750
H 1.901856 0.713327 1.346711
C 0.116103 1.567036 0.507687
H -0.203819 1.820933 1.522731
C -1.121128 1.192556 -0.316960
H -0.848582 1.068046 -1.370058
C -1.783811 -0.099648 0.179932
H -2.121589 0.077998 1.208881
C -0.752850 -1.235795 0.225331
H -1.213922 -2.138298 0.634871
C 1.934773 0.283454 -0.718650
O 3.034921 -0.618917 -0.622045
C -3.004877 -0.472338 -0.658970
H 0.178290 -0.746235 2.100261
H 0.579148 2.469521 0.099726
H -1.842883 2.012942 -0.286683
H -0.459103 -1.485828 -0.800148
H 1.275780 -0.007724 -1.543068
H 2.374263 1.245831 -0.985355
H 2.695741 -1.517012 -0.584665
H -3.745732 0.329379 -0.658993
H -2.722665 -0.662471 -1.697534
H -3.488479 -1.373517 -0.277072
el energy= -389.861315736
zpe= -389.633378
th energy= -389.623563
th enthalpy= -389.622619
free energy= -389.667701

B3LYP-SMD cc-pVTZ

4mchm_1/coords
t1
C 0.162974 1.415198 0.177812
H 0.559785 2.331860 -0.265732
C 1.035347 0.220316 -0.228920
H 1.033793 0.159741 -1.323961
C 0.443786 -1.083023 0.324142
H 1.038793 -1.935945 -0.006316
C -1.016690 -1.270978 -0.092269
H -1.414495 -2.189428 0.347482
C -1.895918 -0.080083 0.309205
H -1.886174 -0.016723 1.404074
C -1.298173 1.223741 -0.234983
H -1.895325 2.074106 0.104510
C 2.474025 0.439257 0.210096
O 3.309580 -0.592672 -0.342152
C -3.342360 -0.267700 -0.142843
H 0.218129 1.543771 1.264452
H 0.509433 -1.059476 1.417972
H -1.069975 -1.398273 -1.179630
H -1.365917 1.211940 -1.328782
H 2.822852 1.418253 -0.133860
H 2.538451 0.425677 1.303584
H 4.203980 -0.456492 -0.011294
H -3.405068 -0.332147 -1.232425
H -3.772811 -1.183503 0.268290
H -3.970048 0.567650 0.175410
el energy= -389.870236211
zpe= -389.643462
th energy= -389.633488
th enthalpy= -389.632544
free energy= -389.677907

4mchm_3/coords
t2
C -0.164903 1.416336 0.177162
H -0.215636 1.548756 1.263697
C -1.039214 0.219626 -0.219726
H -1.044798 0.155974 -1.315842
C -0.445561 -1.081686 0.332755

H -0.505830 -1.056089 1.426907
C 1.012961 -1.271284 -0.089649
H 1.412902 -2.188535 0.350687
C 1.893643 -0.079137 0.305581
H 1.886962 -0.012560 1.400292
C 1.294803 1.223474 -0.240523
H 1.893808 2.074461 0.094209
C -2.479382 0.440385 0.228737
O -3.384649 -0.582717 -0.215823
C 3.338857 -0.268373 -0.149719
H -0.563946 2.331595 -0.267517
H -1.044388 -1.933981 0.006974
H 1.061920 -1.401086 -1.176947
H 1.358536 1.208309 -1.334533
H -2.540150 0.432133 1.318852
H -2.830498 1.418226 -0.116398
H -3.395330 -0.560215 -1.179716
H 3.967311 0.568250 0.163620
H 3.770466 -1.182544 0.263793
H 3.398637 -0.337008 -1.239208
el energy= -389.870980706
zpe= -389.643976
th energy= -389.634114
th enthalpy= -389.633170
free energy= -389.678248

4mchm_5/coords
t3
C 0.380637 -1.262535 0.024264
H 0.807173 -2.149110 0.501088
C 1.026055 -0.000010 0.611945
H 0.831346 -0.000001 1.691358
C 0.380636 1.262524 0.024257
H 0.807220 2.149079 0.501092
C -1.140595 1.256993 0.194331
H -1.386495 1.309346 1.261246
C -1.789671 -0.000004 -0.398231
H -1.587165 0.000008 -1.476107
C -1.140613 -1.257003 0.194306
H -1.570472 -2.149096 -0.268742
C 2.542369 -0.000003 0.478209
O 2.921315 0.000019 -0.908256

C -3.303782 0.000018 -0.199239
H 0.623761 -1.330551 -1.039773
H 0.623758 1.330530 -1.039777
H -1.570494 2.149084 -0.268690
H -1.386534 -1.309397 1.261220
H 2.955348 0.884926 0.973260
H 2.955368 -0.884931 0.973236
H 3.883252 -0.000001 -0.948762
H -3.557284 0.000088 0.864373
H -3.764741 0.882117 -0.649074
H -3.764775 -0.882119 -0.648950
el energy= -389.869372979
zpe= -389.642610
th energy= -389.632668
th enthalpy= -389.631724
free energy= -389.677096

4mchm_6/coords
t4
C 0.159242 1.421286 0.180084
H 0.220112 1.540127 1.267544
C 1.036957 0.236101 -0.242853
H 1.033129 0.184972 -1.338229
C 0.456650 -1.076136 0.299960
H 1.049720 -1.925553 -0.048188
C -1.005960 -1.268863 -0.108192
H -1.065684 -1.385333 -1.196304
C -1.888913 -0.087045 0.311488
H -1.871172 -0.034000 1.406801
C -1.303641 1.225499 -0.224965
H -1.378822 1.223255 -1.318302
C 2.479676 0.461165 0.197454
O 3.400578 -0.514341 -0.316457
C -3.337621 -0.279626 -0.131236
H 0.548448 2.344494 -0.256976
H 0.530716 -1.067022 1.393529
H -1.395143 -2.193881 0.325233
H -1.903806 2.068820 0.126605
H 2.835951 1.422281 -0.175620
H 2.537831 0.486477 1.291157
H 3.211139 -1.357023 0.110209
H -3.968356 0.547161 0.202774

H -3.408870 -0.330824 -1.220986
H -3.758162 -1.203504 0.271975
el energy= -389.870989916
zpe= -389.644260
th energy= -389.634251
th enthalpy= -389.633307
free energy= -389.678775

4mchm_7/coords
t5
C 0.379287 1.269315 -0.010573
H 0.625988 1.320305 1.053839
C 1.030903 0.020086 -0.617290
H 0.841628 0.034975 -1.698025
C 0.388952 -1.254582 -0.052892
H 0.628477 -1.341064 1.012558
C -1.132781 -1.252422 -0.218980
H -1.380400 -1.287257 -1.286100
C -1.785285 -0.008432 0.396789
H -1.579955 -0.026141 1.473946
C -1.142496 1.260917 -0.176005
H -1.574399 2.143134 0.303932
C 2.551688 0.023471 -0.474767
O 3.022225 0.051833 0.883585
C -3.299726 -0.011682 0.201745
H 0.801079 2.165760 -0.473174
H 0.818241 -2.132287 -0.543656
H -1.557897 -2.154219 0.229385
H -1.392450 1.330907 -1.240943
H 2.973364 -0.844871 -0.990975
H 2.963243 0.919687 -0.941007
H 2.787649 -0.785315 1.298818
H -3.754943 -0.906112 0.632859
H -3.764244 0.857538 0.672569
H -3.556436 0.010275 -0.860866
el energy= -389.870381917
zpe= -389.643210
th energy= -389.633453
th enthalpy= -389.632509
free energy= -389.677308

4mchm_19/coords

t6
C 0.260582 -1.092595 0.664101
H -0.302905 -1.213173 1.592632
C 0.938373 0.289907 0.687247
H 1.436372 0.408858 1.654592
C -0.119080 1.401363 0.559744
H -0.706581 1.423589 1.480561
C -1.059176 1.206853 -0.637345
H -1.817265 1.994323 -0.637023
C -1.742516 -0.172671 -0.647817
H -2.236855 -0.288087 -1.616846
C -0.679477 -1.280572 -0.533402
H -0.090894 -1.298451 -1.454818
C 2.030204 0.439750 -0.367196
O 3.094399 -0.484484 -0.077501
C -2.830343 -0.294743 0.424873
H 1.018398 -1.877849 0.663250
H 0.373105 2.374533 0.486588
H -0.493693 1.324937 -1.565596
H -1.168168 -2.255862 -0.463603
H 1.647214 0.252150 -1.372933
H 2.416286 1.463788 -0.343096
H 3.732202 -0.432721 -0.797630
H -3.588023 0.482215 0.300866
H -3.334081 -1.261457 0.355653
H -2.431710 -0.204674 1.436178
el energy= -389.863657427
zpe= -389.635781
th energy= -389.626122
th enthalpy= -389.625178
free energy= -389.669880

4mchm_21/coords
t7
C 0.109173 1.397507 0.558454
H -0.386568 2.368737 0.481827
C -0.945418 0.280987 0.665197
H -1.456562 0.393738 1.627936
C -0.266558 -1.100002 0.642195
H 0.282027 -1.231061 1.578144
C 0.691269 -1.277257 -0.542744
H 0.116365 -1.288628 -1.472802

C 1.753469 -0.166167 -0.633743
H 2.263013 -0.274554 -1.595599
C 1.065578 1.211106 -0.626705
H 0.511930 1.330572 -1.561965
C -2.030748 0.432006 -0.402724
O -3.120150 -0.487937 -0.227105
C 2.824508 -0.291337 0.455310
H 0.684231 1.419519 1.487199
H -1.025950 -1.884006 0.621264
H 1.180756 -2.252184 -0.473689
H 1.820681 2.001327 -0.613287
H -2.409777 1.458973 -0.389737
H -1.645936 0.235708 -1.402688
H -3.503930 -0.320147 0.641956
H 2.409736 -0.207552 1.460648
H 3.331758 -1.256361 0.388828
H 3.581783 0.488364 0.347365
el energy= -389.864473795
zpe= -389.636590
th energy= -389.626962
th enthalpy= -389.626018
free energy= -389.670573

4mchm_22/coords
t8
C 0.126132 1.420771 0.542233
H -0.359123 2.396073 0.449786
C -0.940485 0.320371 0.691320
H -1.432976 0.455665 1.659124
C -0.275433 -1.067898 0.684485
H 0.291288 -1.180939 1.611815
C 0.655249 -1.282391 -0.515622
H 1.130881 -2.263484 -0.438229
C 1.731825 -0.189629 -0.644487
H 2.223468 -0.323447 -1.612514
C 1.065721 1.198331 -0.651131
H 1.833565 1.976219 -0.659885
C -2.039597 0.466899 -0.363558
O -3.143541 -0.430737 -0.156175
C 2.819568 -0.312525 0.428226
H 0.713671 1.457676 1.462679
H -1.037593 -1.851024 0.706052

H 0.061607 -1.300719 -1.433925
H 0.503466 1.311230 -1.581752
H -2.464511 1.469536 -0.301842
H -1.648424 0.336058 -1.375073
H -2.846390 -1.322338 -0.367814
H 3.588457 0.451080 0.291332
H 2.424384 -0.201727 1.438810
H 3.308678 -1.287547 0.372037
el energy= -389.864224034
zpe= -389.636544
th energy= -389.626763
th enthalpy= -389.625819
free energy= -389.670805

4mchm_24/coords
t9
C -0.103951 1.271230 0.741362
H 0.582006 1.386365 1.584614
C -0.944043 -0.000022 0.983086
H -1.218302 -0.000039 2.043401
C -0.103945 -1.271261 0.741320
H 0.582004 -1.386423 1.584574
C 0.710271 -1.258594 -0.558919
H 1.342381 -2.150254 -0.596496
C 1.582783 0.000014 -0.712594
H 1.983792 0.000029 -1.730399
C 0.710259 1.258608 -0.558883
H 0.033339 1.320851 -1.412412
C -2.304617 -0.000011 0.291752
O -2.202858 0.000040 -1.143846
C 2.783602 0.000005 0.239013
H -0.755533 2.148859 0.759675
H -0.755521 -2.148896 0.759605
H 0.033358 -1.320825 -1.412454
H 1.342358 2.150273 -0.596442
H -2.864314 -0.884240 0.614433
H -2.864330 0.884187 0.614495
H -3.099261 -0.000031 -1.496570
H 2.485184 -0.000015 1.288138
H 3.406782 -0.881823 0.074880
H 3.406769 0.881845 0.074912
el energy= -389.860344970

zpe= -389.633085
th energy= -389.623242
th enthalpy= -389.622298
free energy= -389.667363

4mchm_9/coords
c1
C -0.469380 -0.884946 1.054145
H -1.186333 -1.707472 1.031666
C -1.150765 0.418824 0.600113
H -1.896538 0.694079 1.352216
C -0.115619 1.555014 0.521376
H -0.584890 2.459508 0.125902
C 1.116426 1.191948 -0.313637
H 0.833466 1.067391 -1.363892
C 1.789042 -0.097764 0.175277
H 2.133030 0.078782 1.201932
C 0.765658 -1.240225 0.220879
H 1.234022 -2.139577 0.629609
C -1.913102 0.269801 -0.712439
O -2.998487 -0.655190 -0.521035
C 3.004647 -0.459190 -0.674190
H -0.167230 -0.766508 2.099078
H 0.208122 1.792635 1.538739
H 1.833927 2.016260 -0.283583
H 0.467858 -1.488365 -0.803154
H -2.310021 1.244541 -1.013358
H -1.264690 -0.087650 -1.515745
H -3.428878 -0.783325 -1.373211
H 2.716325 -0.644231 -1.712366
H 3.743009 0.345661 -0.673629
H 3.495274 -1.360992 -0.301073
el energy= -389.867158278
zpe= -389.639887
th energy= -389.630075
th enthalpy= -389.629131
free energy= -389.674237

4mchm_11/coords
c2
C -0.322664 -1.109375 0.062267
H -0.996180 -1.919504 -0.222005

C -0.956827 0.247115 -0.275253
H -1.150916 0.274078 -1.354594
C 0.016033 1.386504 0.056196
H -0.418544 2.343533 -0.243186
C 1.369146 1.199488 -0.637893
H 1.219207 1.282670 -1.718881
C 2.024140 -0.160297 -0.337180
H 2.870183 -0.274535 -1.021009
C 1.028118 -1.294778 -0.636942
H 0.858896 -1.335112 -1.717571
C -2.286663 0.462828 0.427954
O -3.243719 -0.502492 -0.040633
C 2.586613 -0.238450 1.086255
H -0.195696 -1.177309 1.147504
H 0.155114 1.434246 1.140645
H 2.047998 2.008165 -0.355163
H 1.464865 -2.256044 -0.354059
H -2.158318 0.364938 1.511354
H -2.653728 1.473642 0.223262
H -4.057632 -0.376163 0.458833
H 3.089416 -1.194031 1.250908
H 3.317008 0.554910 1.259803
H 1.810693 -0.141763 1.846790
el energy= -389.866921902
zpe= -389.639712
th energy= -389.629856
th enthalpy= -389.628912
free energy= -389.674085

4mchm_13/coords
c3
C -0.015585 1.388077 0.056408
H -0.158034 1.435865 1.140529
C 0.959932 0.248956 -0.268883
H 1.160494 0.276109 -1.348171
C 0.326610 -1.107799 0.063899
H 1.003865 -1.915488 -0.219057
C -1.020922 -1.294212 -0.641200
H -0.847534 -1.331813 -1.721312
C -2.019810 -0.161770 -0.342837
H -2.864158 -0.277201 -1.028555
C -1.366875 1.199668 -0.641100

H -2.047977 2.006713 -0.358926
C 2.288178 0.469467 0.445547
O 3.292186 -0.504352 0.117915
C -2.585066 -0.242414 1.079387
H 0.419164 2.345690 -0.241255
H 0.195254 -1.178582 1.148493
H -1.457580 -2.256657 -0.362207
H -1.214934 1.284175 -1.721689
H 2.663474 1.474034 0.225252
H 2.151121 0.395511 1.526152
H 3.475194 -0.428395 -0.825946
H -3.084522 -1.199998 1.242697
H -1.811213 -0.143028 1.841671
H -3.318882 0.548043 1.251685
el energy= -389.867653775
zpe= -389.640375
th energy= -389.630521
th enthalpy= -389.629577
free energy= -389.674834

4mchm_15/coords
c4
C -0.477762 -0.890273 1.041893
H -0.183942 -0.778221 2.089910
C -1.156117 0.413931 0.588672
H -1.909394 0.684433 1.336931
C -0.123703 1.553939 0.523426
H -0.591457 2.457743 0.124138
C 1.116616 1.194972 -0.301779
H 0.843884 1.075567 -1.355339
C 1.786178 -0.096943 0.185589
H 2.121704 0.073675 1.216076
C 0.763313 -1.240335 0.215831
H 1.228913 -2.142360 0.621742
C -1.908908 0.272532 -0.736032
O -2.960289 -0.705041 -0.686933
C 3.008743 -0.452795 -0.656284
H -1.195190 -1.712258 1.009116
H 0.190127 1.792076 1.543813
H 1.833103 2.019696 -0.261395
H 0.472876 -1.481316 -0.812050
H -2.322702 1.245280 -1.020695

H -1.250899 -0.052529 -1.540790
H -3.576740 -0.435250 0.003948
H 2.728355 -0.633001 -1.697497
H 3.746303 0.352690 -0.646370
H 3.497211 -1.356065 -0.283965
el energy= -389.867958685
zpe= -389.640568
th energy= -389.630826
th enthalpy= -389.629882
free energy= -389.674714

4mchm_16/coords
c5
C -0.233039 1.262744 -0.197502
H -0.726837 2.149061 -0.604818
C -0.962075 -0.000016 -0.678146
H -0.936691 -0.000026 -1.774950
C -0.233033 -1.262751 -0.197466
H -0.313049 -1.335104 0.889453
C 1.242810 -1.258358 -0.611568
H 1.741120 -2.152285 -0.227586
C 1.995908 0.000000 -0.144047
H 2.973840 -0.000010 -0.634029
C 1.242808 1.258342 -0.611602
H 1.300291 1.313281 -1.703355
C -2.439631 -0.000009 -0.313620
O -2.603381 0.000012 1.116047
C 2.253399 0.000021 1.366578
H -0.313054 1.335136 0.889417
H -0.726833 -2.149080 -0.604759
H 1.300290 -1.313324 -1.703320
H 1.741117 2.152279 -0.227640
H -2.924773 0.884981 -0.738028
H -2.924763 -0.885032 -0.737999
H -3.548312 0.000094 1.302587
H 2.826051 -0.881810 1.662366
H 2.826075 0.881851 1.662331
H 1.329693 0.000048 1.946199
el energy= -389.866122450
zpe= -389.638730
th energy= -389.628952
th enthalpy= -389.628008

free energy= -389.673019

4mchm_17/coords
c6
C -0.227812 1.283357 -0.114347
H -0.714097 2.199258 -0.460729
C -0.968238 0.062727 -0.676780
H -0.948129 0.135620 -1.771686
C -0.249248 -1.236280 -0.286016
H -0.325030 -1.386239 0.795261
C 1.227350 -1.216626 -0.698293
H 1.717932 -2.138241 -0.374795
C 1.990757 0.001934 -0.149178
H 2.967590 0.027229 -0.640702
C 1.247772 1.294741 -0.529231
H 1.754212 2.156426 -0.086550
C -2.448674 0.047806 -0.302290
O -2.701974 -0.018475 1.111525
C 2.251764 -0.101126 1.357544
H -0.307560 1.282912 0.975275
H -0.750280 -2.088395 -0.753290
H 1.283634 -1.199905 -1.791295
H 1.304946 1.424090 -1.614737
H -2.925054 0.969866 -0.638300
H -2.948660 -0.787531 -0.803008
H -2.415889 -0.883929 1.423395
H 2.827598 0.757304 1.710262
H 1.329639 -0.137619 1.938680
H 2.822923 -1.002245 1.591561
el energy= -389.867077934
zpe= -389.639591
th energy= -389.629820
th enthalpy= -389.628876
free energy= -389.673854

4mchm_23/coords
c7
C 0.420971 -1.301354 -0.878387
H 1.034152 -2.173740 -0.637517
C 1.292674 -0.030522 -0.840104
H 1.932726 -0.060988 -1.728168
C 0.423219 1.236841 -0.962852

H 1.038069 2.122124 -0.780514
C -0.810433 1.254909 -0.053527
H -0.506706 1.345838 0.992254
C -1.668281 -0.006544 -0.213355
H -2.015379 -0.040684 -1.253690
C -0.813333 -1.256723 0.029561
H -0.510359 -1.279274 1.079394
C 2.307396 0.007070 0.298281
O 1.688173 0.059606 1.595788
C -2.895530 0.025202 0.694234
H 0.078497 -1.441546 -1.908299
H 0.080760 1.308874 -1.999710
H -1.412214 2.139013 -0.282008
H -1.417110 -2.152588 -0.140289
H 2.942144 -0.883115 0.235973
H 2.950576 0.883759 0.168573
H 2.393826 0.081977 2.251748
H -3.514329 0.903019 0.495072
H -3.518115 -0.860760 0.550991
H -2.602017 0.057968 1.746781
el energy= -389.863994178
zpe= -389.636692
th energy= -389.626911
th enthalpy= -389.625967
free energy= -389.670828

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.340369 -1.096856 0.031143
H 1.015584 -1.898881 -0.278015
C 0.958888 0.270979 -0.287829
H 1.148319 0.315755 -1.367227
C -0.023274 1.394888 0.068355
H -0.154131 1.424464 1.154465
C -1.380479 1.206211 -0.617570
H -1.240958 1.308953 -1.698218
C -2.018990 -0.165036 -0.333475
H -2.869565 -0.277379 -1.011937
C -1.014251 -1.284229 -0.660603
H -1.438842 -2.254563 -0.390757
C 2.292795 0.488950 0.417480
O 3.318913 -0.431543 0.012061

C -2.568025 -0.272176 1.093256
H 0.224316 -1.188375 1.115993
H 0.400085 2.360847 -0.218816
H -2.065242 2.002857 -0.315451
H -0.852867 -1.304202 -1.742883
H 2.680083 1.479992 0.177346
H 2.155973 0.438762 1.503231
H 3.074421 -1.307550 0.330084
H -3.307067 0.508847 1.285013
H -3.056944 -1.236640 1.247771
H -1.786669 -0.176927 1.848375
el energy= -389.867741418
zpe= -389.640042
th energy= -389.630366
th enthalpy= -389.629422
free energy= -389.674094

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.481845 -0.867360 1.058028
H 1.200616 -1.691020 1.050385
C 1.157084 0.436285 0.595691
H 1.901998 0.718513 1.345765
C 0.115479 1.566939 0.509929
H -0.204711 1.815492 1.525908
C -1.119370 1.191577 -0.316211
H -0.842300 1.063587 -1.367483
C -1.781778 -0.100042 0.181132
H -2.122613 0.077969 1.208583
C -0.750718 -1.235474 0.226997
H -1.211749 -2.137323 0.638370
C 1.921998 0.286836 -0.721292
O 3.035993 -0.617611 -0.626821
C -2.998510 -0.472596 -0.662035
H 0.179116 -0.743207 2.102076
H 0.579764 2.468873 0.102265
H -1.841644 2.011678 -0.285933
H -0.452035 -1.482956 -0.796992
H 1.265277 -0.025845 -1.536182
H 2.353037 1.249841 -0.997899
H 2.688347 -1.513603 -0.561911
H -3.741551 0.327910 -0.662086

H -2.713129 -0.660433 -1.700521
H -3.482555 -1.375577 -0.283208
el energy= -389.867780876
zpe= -389.640326
th energy= -389.630609
th enthalpy= -389.629665
free energy= -389.674500

MP2 6-31G(d') gas phase

4mchm_1/coords
t1
C 0.156868 1.428729 0.179232
H 0.546676 2.363856 -0.253034
C 1.033776 0.242160 -0.242133
H 1.030900 0.177599 -1.343895
C 0.465440 -1.066871 0.319126
H 1.088070 -1.909128 -0.009419
C -0.995656 -1.268184 -0.101383
H -1.389949 -2.202867 0.327350
C -1.882089 -0.087004 0.316601
H -1.860779 -0.022860 1.419173
C -1.304511 1.221626 -0.240126
H -1.919105 2.074146 0.089109
C 2.478836 0.454956 0.189263
O 3.256287 -0.626095 -0.311375
C -3.333390 -0.289199 -0.127744
H 0.207094 1.542427 1.275438
H 0.526796 -1.034861 1.420759
H -1.048666 -1.380385 -1.197686
H -1.366988 1.196165 -1.341180
H 2.846248 1.421265 -0.201903
H 2.526843 0.502936 1.293128
H 4.163696 -0.511568 -0.003993
H -3.394246 -0.357895 -1.223060
H -3.752685 -1.214426 0.290535
H -3.969839 0.547070 0.192661
el energy= -388.34830457023
zpe= -388.112911
th energy= -388.103371
th enthalpy= -388.102427
free energy= -388.146911

4mchm_3/coords
t2
C -0.156898 1.428917 0.178497
H -0.206726 1.543350 1.274440
C -1.034895 0.240738 -0.235529
H -1.020014 0.178038 -1.341025
C -0.462892 -1.065987 0.325857
H -0.520959 -1.028582 1.426988
C 0.996262 -1.269227 -0.099568
H 1.392060 -2.202534 0.330486
C 1.883131 -0.086351 0.313688
H 1.864529 -0.020831 1.416094
C 1.303974 1.221783 -0.243092
H 1.918678 2.074592 0.084909
C -2.486060 0.453266 0.200740
O -3.352677 -0.607603 -0.181801
C 3.333293 -0.288866 -0.134116
H -0.549421 2.363151 -0.253282
H -1.088383 -1.912005 0.010503
H 1.047502 -1.383987 -1.195939
H 1.365599 1.196138 -1.344342
H -2.541418 0.491206 1.297050
H -2.854993 1.422625 -0.182229
H -3.356330 -0.641706 -1.146840
H 3.970130 0.548012 0.183640
H 3.753907 -1.213242 0.284593
H 3.391771 -0.359036 -1.229495
el energy= -388.34865678363
zpe= -388.113143
th energy= -388.103659
th enthalpy= -388.102715
free energy= -388.147085

4mchm_5/coords
t3
C 0.393989 -1.260289 0.033099
H 0.827056 -2.158305 0.502029
C 1.029837 -0.000001 0.635999
H 0.834506 0.000019 1.724301
C 0.393993 1.260288 0.033077
H 0.827093 2.158291 0.502013

C -1.130081 1.255778 0.205674
H -1.379548 1.295612 1.280052
C -1.770234 -0.000009 -0.401235
H -1.552361 -0.000010 -1.483919
C -1.130101 -1.255790 0.205664
H -1.566961 -2.158033 -0.250594
C 2.545333 0.000008 0.465116
O 2.837351 0.000006 -0.928081
C -3.289877 0.000015 -0.212385
H 0.649066 -1.306104 -1.035433
H 0.649071 1.306091 -1.035450
H -1.566979 2.158011 -0.250569
H -1.379592 -1.295645 1.280040
H 2.973753 0.892578 0.956540
H 2.973770 -0.892541 0.956553
H 3.796357 -0.000095 -1.033509
H -3.544658 0.000056 0.856955
H -3.748243 0.888803 -0.667238
H -3.748291 -0.888778 -0.667176
el energy= -388.34833421569
zpe= -388.112882
th energy= -388.103372
th enthalpy= -388.102428
free energy= -388.146823

4mchm_6/coords
t4
C 0.155946 1.425221 0.180760
H 0.215038 1.526714 1.277821
C 1.036239 0.248608 -0.261047
H 1.032432 0.197356 -1.363343
C 0.467070 -1.068927 0.281578
H 1.064542 -1.919215 -0.081760
C -0.999580 -1.264953 -0.124155
H -1.062993 -1.360390 -1.221170
C -1.880352 -0.089767 0.320328
H -1.845865 -0.039162 1.423243
C -1.309057 1.224674 -0.228205
H -1.382893 1.211857 -1.328662
C 2.486467 0.468261 0.178154
O 3.379665 -0.537638 -0.281565
C -3.336331 -0.289721 -0.109347

H 0.543917 2.365138 -0.242260
H 0.543078 -1.066252 1.383245
H -1.387769 -2.206200 0.295387
H -1.919873 2.073226 0.117460
H 2.865676 1.408934 -0.242433
H 2.525224 0.560907 1.279823
H 3.179120 -1.348903 0.199579
H -3.969327 0.542001 0.228651
H -3.410199 -0.345147 -1.204557
H -3.749834 -1.220141 0.303098
el energy= -388.34828898222
zpe= -388.112721
th energy= -388.103212
th enthalpy= -388.102268
free energy= -388.146720

4mchm_7/coords
t5
C 0.388007 1.267952 -0.010786
H 0.652128 1.299538 1.056698
C 1.031675 0.023502 -0.635334
H 0.834238 0.035729 -1.723132
C 0.396284 -1.248653 -0.056090
H 0.622425 -1.307129 1.021600
C -1.127643 -1.250710 -0.232647
H -1.370513 -1.268703 -1.308575
C -1.773805 -0.010840 0.400084
H -1.559425 -0.034741 1.483334
C -1.137036 1.260965 -0.176591
H -1.575858 2.149792 0.303081
C 2.554762 0.030955 -0.463075
O 2.970888 0.040556 0.897696
C -3.292903 -0.013808 0.207258
H 0.815574 2.175349 -0.465502
H 0.836706 -2.142561 -0.527292
H -1.560832 -2.164963 0.202370
H -1.390419 1.326729 -1.248585
H 2.995657 -0.827376 -1.002342
H 2.975338 0.946373 -0.899989
H 2.771682 -0.826464 1.270507
H -3.748917 -0.914292 0.640894
H -3.755837 0.862587 0.680753

H -3.545108 0.009505 -0.862304
el energy= -388.34843066971
zpe= -388.112786
th energy= -388.103330
th enthalpy= -388.102386
free energy= -388.146707

4mchm_19/coords
t6
C 0.279597 -1.070837 0.689608
H -0.305986 -1.196386 1.612964
C 0.926883 0.324974 0.703034
H 1.440266 0.458735 1.669015
C -0.144794 1.420308 0.557094
H -0.753318 1.440602 1.473474
C -1.057959 1.198251 -0.659967
H -1.837114 1.976271 -0.685641
C -1.712937 -0.195737 -0.659220
H -2.216931 -0.331424 -1.630652
C -0.629537 -1.282884 -0.530251
H -0.018717 -1.291701 -1.446536
C 2.012165 0.462444 -0.363438
O 3.008266 -0.518598 -0.096149
C -2.788798 -0.323793 0.428709
H 1.068582 -1.833826 0.711652
H 0.333423 2.410550 0.489261
H -0.475682 1.319217 -1.586673
H -1.103690 -2.275175 -0.472109
H 1.594882 0.329294 -1.375401
H 2.437824 1.481458 -0.314487
H 3.681144 -0.459021 -0.785137
H -3.570495 0.436532 0.293681
H -3.269055 -1.310945 0.384016
H -2.378988 -0.201752 1.438351
el energy= -388.34282039622
zpe= -388.106761
th energy= -388.097386
th enthalpy= -388.096442
free energy= -388.140601

4mchm_21/coords
t7

C 0.142046 1.420597 0.555796
H -0.340828 2.408163 0.481824
C -0.926999 0.321629 0.694151
H -1.433949 0.460445 1.667323
C -0.282232 -1.074978 0.682583
H 0.292998 -1.211291 1.610763
C 0.635064 -1.282557 -0.531891
H 0.028778 -1.290040 -1.450739
C 1.717764 -0.194161 -0.650450
H 2.229633 -0.329018 -1.617681
C 1.059835 1.198066 -0.657337
H 0.480261 1.315502 -1.585991
C -2.012304 0.459502 -0.382000
O -3.037935 -0.519053 -0.263958
C 2.784302 -0.320648 0.446687
H 0.746208 1.446371 1.474908
H -1.072938 -1.837500 0.685092
H 1.109005 -2.274675 -0.472090
H 1.836691 1.978239 -0.681313
H -2.434694 1.480644 -0.343512
H -1.601681 0.317170 -1.387648
H -3.439066 -0.410710 0.608087
H 2.365567 -0.201249 1.453068
H 3.267655 -1.306343 0.404673
H 3.564979 0.442012 0.319661
el energy= -388.34357712783
zpe= -388.107330
th energy= -388.098029
th enthalpy= -388.097085
free energy= -388.141056

4mchm_22/coords
t8
C 0.143995 1.429124 0.545282
H -0.337301 2.416593 0.462403
C -0.929283 0.337071 0.708006
H -1.437356 0.479656 1.675403
C -0.272072 -1.054554 0.712094
H 0.324038 -1.162109 1.630324
C 0.624400 -1.286879 -0.513779
H 1.096462 -2.279635 -0.449026
C 1.708486 -0.202284 -0.658253

H 2.207182 -0.350546 -1.630316
C 1.054621 1.192080 -0.671390
H 1.835128 1.968095 -0.706545
C -2.024789 0.469593 -0.359504
O -3.099564 -0.443243 -0.168792
C 2.788892 -0.321254 0.426190
H 0.754370 1.466069 1.460118
H -1.044957 -1.836186 0.775953
H 0.010555 -1.299677 -1.428728
H 0.471197 1.304368 -1.598069
H -2.476311 1.468120 -0.288429
H -1.609471 0.374352 -1.376409
H -2.786461 -1.321888 -0.413182
H 3.574333 0.431549 0.273518
H 2.386647 -0.178266 1.436143
H 3.262952 -1.311936 0.395307
el energy= -388.34236515732
zpe= -388.106212
th energy= -388.096842
th enthalpy= -388.095898
free energy= -388.140074

4mchm_24/coords
t9
C -0.104495 1.270143 0.767371
H 0.605806 1.374678 1.602132
C -0.944966 -0.000294 1.006252
H -1.245416 -0.000544 2.069435
C -0.104426 -1.270583 0.766795
H 0.605842 -1.375469 1.601539
C 0.667930 -1.257828 -0.561675
H 1.299615 -2.158483 -0.625603
C 1.540444 0.000183 -0.720689
H 1.944129 0.000423 -1.746883
C 0.667786 1.258025 -0.561144
H -0.049193 1.301188 -1.390040
C -2.275635 -0.000144 0.255558
O -2.069452 0.000425 -1.153949
C 2.741428 0.000057 0.236301
H -0.756779 2.156811 0.811924
H -0.756666 -2.157306 0.810916
H -0.049004 -1.300744 -1.390617

H 1.299360 2.158781 -0.624735
H -2.853948 -0.891628 0.561040
H -2.854116 0.891000 0.561714
H -2.936225 0.000456 -1.579408
H 2.437429 -0.000165 1.290153
H 3.368237 -0.887805 0.073533
H 3.368146 0.888049 0.073883
el energy -388.34166137878
zpe= -388.105480
th energy= -388.096155
th enthalpy= -388.095211
free energy= -388.139067

4mchm_9/coords
c1
C -0.500208 -0.832668 1.088060
H -1.245669 -1.638503 1.092743
C -1.156335 0.465523 0.588916
H -1.926315 0.765835 1.317913
C -0.110189 1.588885 0.485595
H -0.568988 2.500042 0.069522
C 1.117824 1.183012 -0.343906
H 0.836388 1.030515 -1.398585
C 1.765141 -0.103532 0.187802
H 2.107203 0.095724 1.219223
C 0.724229 -1.230149 0.252039
H 1.183739 -2.137725 0.674030
C -1.893767 0.264321 -0.733449
O -2.903744 -0.715744 -0.520141
C 2.978869 -0.506697 -0.653946
H -0.180894 -0.683118 2.132272
H 0.223679 1.847798 1.503051
H 1.855406 2.000980 -0.339786
H 0.417576 -1.492950 -0.773604
H -2.336794 1.226601 -1.049294
H -1.201367 -0.055352 -1.529862
H -3.353347 -0.871499 -1.359561
H 2.676711 -0.714680 -1.690238
H 3.732591 0.292375 -0.677624
H 3.456652 -1.412262 -0.255736
el energy= -388.34575088651
zpe= -388.110028

th energy= -388.100587
th enthalpy= -388.099643
free energy= -388.144001

4mchm_11/coords
c2
C -0.343449 -1.094946 0.048900
H -1.047445 -1.885748 -0.241050
C -0.947753 0.274365 -0.287378
H -1.145004 0.307222 -1.373013
C 0.037557 1.398620 0.060756
H -0.384867 2.374582 -0.226065
C 1.387174 1.193218 -0.642548
H 1.230330 1.273223 -1.730534
C 2.014944 -0.177535 -0.330604
H 2.887178 -0.305781 -0.992959
C 1.006395 -1.294950 -0.653932
H 0.835981 -1.315887 -1.742804
C -2.282305 0.484967 0.415314
O -3.180485 -0.527416 -0.022311
C 2.527794 -0.261969 1.113936
H -0.220104 -1.171415 1.141631
H 0.180365 1.431826 1.152795
H 2.086138 1.998292 -0.366643
H 1.433642 -2.274104 -0.386465
H -2.129866 0.436892 1.509783
H -2.673471 1.491336 0.178300
H -4.013812 -0.415414 0.450987
H 3.007836 -1.232840 1.298573
H 3.271454 0.523050 1.309169
H 1.723401 -0.146514 1.850117
el energy= -388.34556251869
zpe= -388.109844
th energy= -388.100388
th enthalpy= -388.099444
free energy= -388.143752

4mchm_13/coords
c3
C -0.037240 1.398448 0.061828
H -0.182738 1.430591 1.153353
C 0.948716 0.272678 -0.278900

H 1.136633 0.309032 -1.369894
C 0.340555 -1.095051 0.054040
H 1.045896 -1.890299 -0.222609
C -1.005113 -1.295771 -0.656045
H -0.830814 -1.317684 -1.744545
C -2.013912 -0.176891 -0.337414
H -2.883130 -0.304891 -1.003657
C -1.384467 1.193910 -0.646600
H -2.084034 1.998899 -0.372341
C 2.287197 0.482204 0.432020
O 3.251907 -0.517572 0.127838
C -2.533178 -0.260935 1.104874
H 0.388236 2.374062 -0.221700
H 0.211711 -1.167735 1.145886
H -1.434408 -2.274164 -0.389556
H -1.224473 1.275132 -1.734202
H 2.678473 1.491278 0.205618
H 2.142386 0.423096 1.519259
H 3.430139 -0.465715 -0.819814
H -3.013465 -1.231933 1.287850
H -1.732706 -0.144284 1.845085
H -3.278312 0.523639 1.295755
el energy= -388.34592472692
zpe= -388.110087
th energy= -388.100688
th enthalpy= -388.099744
free energy= -388.143936

4mchm_15/coords
c4
C -0.502663 -0.844718 1.077133
H -0.194632 -0.710931 2.126742
C -1.156239 0.456756 0.584148
H -1.922155 0.759876 1.322186
C -0.114687 1.585500 0.493135
H -0.576316 2.495396 0.077328
C 1.116048 1.185689 -0.334724
H 0.837059 1.035956 -1.390302
C 1.765192 -0.100538 0.195064
H 2.100306 0.094794 1.229593
C 0.728127 -1.231102 0.245303
H 1.187375 -2.140124 0.664056

C -1.891118 0.261486 -0.748421
O -2.886213 -0.753227 -0.688830
C 2.985113 -0.495351 -0.641643
H -1.244042 -1.655094 1.058953
H 0.214936 1.842844 1.512410
H 1.850636 2.006133 -0.325849
H 0.426261 -1.487953 -0.782877
H -2.328272 1.225621 -1.067876
H -1.206481 -0.061215 -1.540466
H -3.522801 -0.491936 -0.010930
H 2.689560 -0.699111 -1.680562
H 3.736066 0.306460 -0.656611
H 3.463556 -1.401243 -0.245128
el energy= -388.34646679245
zpe= -388.110567
th energy= -388.101197
th enthalpy= -388.100253
free energy= -388.144426

4mchm_16/coords
c5
C -0.239230 1.263469 -0.213717
H -0.734846 2.156720 -0.626539
C -0.959697 0.000003 -0.706433
H -0.937731 -0.000001 -1.811946
C -0.239229 -1.263465 -0.213717
H -0.342649 -1.327216 0.877588
C 1.240761 -1.257371 -0.621359
H 1.743379 -2.160611 -0.241307
C 1.980650 -0.000001 -0.130876
H 2.985404 -0.000002 -0.585462
C 1.240763 1.257375 -0.621354
H 1.306912 1.301627 -1.721166
C -2.429076 -0.000002 -0.298203
O -2.496222 -0.000020 1.123939
C 2.169314 -0.000003 1.392609
H -0.342651 1.327222 0.877589
H -0.734852 -2.156711 -0.626542
H 1.306904 -1.301617 -1.721172
H 1.743381 2.160611 -0.241294
H -2.929942 0.892550 -0.715615
H -2.929941 -0.892547 -0.715637

H -3.426205 0.000115 1.380791
H 2.731601 -0.887779 1.713631
H 2.731612 0.887765 1.713630
H 1.213872 0.000005 1.930229
el energy= -388.34587637837
zpe= -388.110068
th energy= -388.100651
th enthalpy= -388.099707
free energy= -388.143917

4mchm_17/coords
c6
C -0.232919 1.281977 -0.118482
H -0.723791 2.205698 -0.463225
C -0.963831 0.064236 -0.699561
H -0.938851 0.136720 -1.802764
C -0.245752 -1.232993 -0.298588
H -0.315585 -1.365266 0.792347
C 1.231944 -1.210061 -0.714504
H 1.729783 -2.142133 -0.404471
C 1.983368 0.004073 -0.139401
H 2.982832 0.030784 -0.604252
C 1.247096 1.299314 -0.526540
H 1.755380 2.167074 -0.077854
C -2.440815 0.048391 -0.290869
O -2.636755 -0.025711 1.116968
C 2.191094 -0.109198 1.377451
H -0.340242 1.267658 0.974973
H -0.749052 -2.100279 -0.756352
H 1.286785 -1.175514 -1.814802
H 1.311289 1.430216 -1.619375
H -2.924117 0.984385 -0.601227
H -2.962001 -0.780564 -0.803774
H -2.397126 -0.916528 1.398725
H 2.775749 0.742195 1.751875
H 1.243574 -0.124727 1.929057
H 2.738299 -1.028463 1.628338
el energy= -388.34582915937
zpe= -388.109855
th energy= -388.100487
th enthalpy= -388.099543
free energy= -388.143678

4mchm_23/coords
c7
C 0.461901 -1.265762 -0.944873
H 1.076915 -2.158549 -0.749029
C 1.330507 0.000970 -0.823306
H 2.030884 0.001940 -1.677729
C 0.461853 1.267943 -0.942037
H 1.076831 2.160310 -0.744182
C -0.773034 1.256642 -0.029616
H -0.456582 1.294716 1.020844
C -1.626786 0.000259 -0.247840
H -1.972945 0.001403 -1.297801
C -0.772953 -1.256545 -0.032387
H -0.456471 -1.296909 1.017980
C 2.248556 -0.000394 0.397763
O 1.494902 -0.001949 1.606600
C -2.856317 -0.000785 0.664889
H 0.123007 -1.346514 -1.991009
H 0.122991 1.351029 -1.987998
H -1.379827 2.155708 -0.223946
H -1.379692 -2.155221 -0.228679
H 2.901184 -0.891485 0.348246
H 2.900987 0.890955 0.350393
H 2.118921 -0.002577 2.343444
H -3.479704 0.888323 0.496613
H -3.479641 -0.889567 0.494668
H -2.548438 -0.001930 1.719828
el energy= -388.34460946799
zpe= -388.108761
th energy= -388.099364
th enthalpy= -388.098420
free energy= -388.142484

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.346480 -1.091636 0.008789
H 1.030516 -1.887528 -0.323774
C 0.949739 0.284514 -0.304832
H 1.143799 0.333735 -1.390268
C -0.039098 1.398102 0.067026
H -0.169353 1.417998 1.160989

C -1.396948 1.202404 -0.622659
H -1.255122 1.298523 -1.711292
C -2.017985 -0.173443 -0.321428
H -2.899367 -0.295378 -0.972485
C -1.013135 -1.282907 -0.679013
H -1.433509 -2.268048 -0.423399
C 2.289460 0.496294 0.405106
O 3.288848 -0.442023 0.028534
C -2.508012 -0.282374 1.129359
H 0.239035 -1.200162 1.101055
H 0.380643 2.377727 -0.210481
H -2.093147 2.002047 -0.325305
H -0.855418 -1.282585 -1.769681
H 2.699999 1.480298 0.142721
H 2.128919 0.487898 1.499717
H 3.035993 -1.299399 0.390285
H -3.251688 0.496419 1.347161
H -2.981507 -1.257774 1.306897
H -1.693591 -0.173304 1.855496
el energy= -388.34556191225
zpe= -388.109668
th energy= -388.100244
th enthalpy= -388.099300
free energy= -388.143573

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.495716 -0.815538 1.102022
H 1.233757 -1.631250 1.150530
C 1.161434 0.473752 0.591196
H 1.928542 0.776450 1.322090
C 0.113380 1.595161 0.479928
H -0.220522 1.865995 1.494429
C -1.114626 1.183639 -0.347565
H -0.833508 1.027242 -1.401421
C -1.762251 -0.100894 0.188417
H -2.106303 0.100693 1.218662
C -0.720536 -1.226392 0.259865
H -1.179549 -2.133574 0.682967
C 1.906815 0.270120 -0.735085
O 2.967060 -0.673795 -0.636514
C -2.973237 -0.510353 -0.654141

H 0.166134 -0.652574 2.140481
H 0.573944 2.500663 0.053936
H -1.853105 2.000537 -0.346377
H -0.411855 -1.489156 -0.765784
H 1.214069 -0.006246 -1.547098
H 2.385350 1.214274 -1.027557
H 2.573803 -1.551435 -0.566264
H -3.727693 0.287622 -0.681671
H -2.669039 -0.720887 -1.689249
H -3.450678 -1.414962 -0.253386
el energy= -388.34531509116
zpe= -388.109497
th energy= -388.100061
th enthalpy= -388.099117
free energy= -388.143493

MP2-SMD 6-31G(d')

4mchm_1/coords
t1
C 0.160612 1.419143 0.179713
H 0.558385 2.350181 -0.253183
C 1.033021 0.229415 -0.243102
H 1.026475 0.169779 -1.345499
C 0.453794 -1.075477 0.318632
H 1.059536 -1.931805 -0.009319
C -1.008751 -1.268642 -0.100883
H -1.407342 -2.200652 0.329872
C -1.887156 -0.082655 0.317922
H -1.865894 -0.018483 1.420026
C -1.301229 1.220916 -0.240257
H -1.910346 2.077061 0.089711
C 2.474072 0.448391 0.197659
O 3.286800 -0.609763 -0.321053
C -3.337290 -0.276169 -0.130719
H 0.213257 1.529321 1.275729
H 0.517229 -1.041674 1.419549
H -1.062839 -1.378356 -1.197267
H -1.363488 1.192952 -1.341189
H 2.836900 1.422874 -0.170916
H 2.524967 0.467834 1.299784
H 4.185194 -0.473169 0.010002

H -3.394921 -0.339869 -1.226843
H -3.764009 -1.200525 0.283312
H -3.969943 0.563098 0.190857
el energy= -388.35517364498
zpe= -388.120795
th energy= -388.111116
th enthalpy= -388.110172
free energy= -388.155001

4mchm_3/coords
t2
C -0.161141 1.422345 0.177554
H -0.209978 1.536921 1.273401
C -1.036054 0.231309 -0.235042
H -1.033852 0.167408 -1.338837
C -0.457010 -1.072232 0.327185
H -0.515441 -1.035801 1.428321
C 1.003248 -1.268923 -0.098133
H 1.402886 -2.200294 0.332993
C 1.884247 -0.082587 0.314879
H 1.865102 -0.014994 1.416823
C 1.299422 1.220472 -0.245996
H 1.911081 2.076404 0.079824
C -2.479655 0.452471 0.212368
O -3.365363 -0.597934 -0.189981
C 3.333361 -0.279703 -0.135674
H -0.559722 2.352261 -0.257254
H -1.068157 -1.926844 0.004293
H 1.052875 -1.380892 -1.194538
H 1.358752 1.189038 -1.347004
H -2.531175 0.479330 1.309638
H -2.845159 1.422756 -0.165009
H -3.338947 -0.629919 -1.156774
H 3.967782 0.559708 0.181941
H 3.759328 -1.203262 0.280839
H 3.389020 -0.347267 -1.231662
el energy= -388.35627973282
zpe= -388.121709
th energy= -388.112078
th enthalpy= -388.111134
free energy= -388.155909

4mchm_5/coords
t3
C 0.386570 -1.259706 0.013285
H 0.825191 -2.157737 0.476515
C 1.022734 -0.000004 0.616971
H 0.813221 -0.000002 1.701507
C 0.386565 1.259702 0.013285
H 0.825194 2.157728 0.476519
C -1.136295 1.256409 0.197369
H -1.374846 1.295766 1.273769
C -1.781962 -0.000003 -0.402230
H -1.577195 0.000002 -1.487196
C -1.136296 -1.256415 0.197363
H -1.577051 -2.157291 -0.257918
C 2.540808 0.000001 0.482081
O 2.894018 0.000011 -0.904884
C -3.297875 0.000005 -0.192507
H 0.623217 -1.305766 -1.060440
H 0.623214 1.305765 -1.060437
H -1.577063 2.157283 -0.257906
H -1.374848 -1.295784 1.273763
H 2.958800 0.890527 0.981427
H 2.958808 -0.890525 0.981417
H 3.859859 -0.000027 -0.954930
H -3.536913 0.000034 0.880766
H -3.763608 0.888895 -0.640764
H -3.763620 -0.888901 -0.640721
el energy= -388.35484568006
zpe= -388.120260
th energy= -388.110667
th enthalpy= -388.109723
free energy= -388.154322

4mchm_6/coords
t4
C 0.157291 1.422822 0.183700
H 0.216176 1.521655 1.280574
C 1.033896 0.242994 -0.256881
H 1.025228 0.193380 -1.359653
C 0.463874 -1.071455 0.291935
H 1.065629 -1.924523 -0.057228
C -1.001047 -1.266337 -0.119555

H -1.061737 -1.362439 -1.216768
C -1.881405 -0.089348 0.320030
H -1.851456 -0.037389 1.422574
C -1.306599 1.223149 -0.228440
H -1.377082 1.207040 -1.329080
C 2.479716 0.468325 0.184611
O 3.386364 -0.529140 -0.298353
C -3.334178 -0.285192 -0.118943
H 0.548861 2.360439 -0.241090
H 0.536627 -1.056325 1.392805
H -1.392137 -2.205376 0.302509
H -1.917268 2.072556 0.115839
H 2.849420 1.422202 -0.215430
H 2.526086 0.525753 1.285562
H 3.193073 -1.348187 0.176851
H -3.968387 0.546007 0.219949
H -3.401050 -0.333891 -1.215303
H -3.752180 -1.217529 0.285968
el energy= -388.35601347407
zpe= -388.121657
th energy= -388.111915
th enthalpy= -388.110971
free energy= -388.156183

4mchm_7/coords
t5
C 0.387607 1.262516 -0.007599
H 0.632080 1.295215 1.065047
C 1.027344 0.012614 -0.625349
H 0.825742 0.023150 -1.711660
C 0.390402 -1.255980 -0.040634
H 0.623327 -1.317274 1.035033
C -1.132967 -1.252073 -0.219309
H -1.374400 -1.275531 -1.295429
C -1.777510 -0.005666 0.401522
H -1.567638 -0.021086 1.485380
C -1.136032 1.259660 -0.183498
H -1.575290 2.153513 0.286927
C 2.550185 0.017289 -0.475758
O 2.997447 0.064734 0.884034
C -3.294251 -0.005270 0.198974
H 0.822577 2.167215 -0.461418

H 0.829055 -2.148423 -0.514712
H -1.570459 -2.160505 0.223830
H -1.380808 1.313936 -1.257807
H 2.978472 -0.862785 -0.984409
H 2.967508 0.915006 -0.951888
H 2.775798 -0.783034 1.292504
H -3.755831 -0.902886 0.634018
H -3.759650 0.874542 0.665120
H -3.538737 0.012531 -0.872898
el energy= -388.35593889510
zpe= -388.120989
th energy= -388.111539
th enthalpy= -388.110595
free energy= -388.154826

4mchm_19/coords
t6
C 0.260170 -1.078370 0.696464
H -0.337062 -1.187769 1.614113
C 0.925781 0.309255 0.709647
H 1.436495 0.442635 1.677868
C -0.140075 1.410909 0.566544
H -0.753816 1.426569 1.479482
C -1.044210 1.199902 -0.658336
H -1.817025 1.984108 -0.687013
C -1.712601 -0.187027 -0.664788
H -2.210927 -0.317366 -1.639567
C -0.640912 -1.284519 -0.530298
H -0.024056 -1.297650 -1.442235
C 2.004033 0.452423 -0.362211
O 3.037709 -0.504255 -0.099728
C -2.793915 -0.307675 0.417366
H 1.029199 -1.862635 0.732293
H 0.347515 2.396534 0.504490
H -0.450176 1.315310 -1.577852
H -1.126106 -2.271564 -0.471106
H 1.594793 0.295492 -1.371274
H 2.415869 1.475541 -0.327688
H 3.683542 -0.432846 -0.816214
H -3.563737 0.465924 0.285735
H -3.289880 -1.287040 0.360610
H -2.385924 -0.200581 1.429849

el energy= -388.35013124053
zpe= -388.114602
th energy= -388.105268
th enthalpy= -388.104324
free energy= -388.148364

4mchm_21/coords
t7
C 0.131622 1.407372 0.564827
H -0.360407 2.390649 0.498743
C -0.930596 0.300459 0.686720
H -1.453296 0.426908 1.651443
C -0.267543 -1.087487 0.670893
H 0.310805 -1.213719 1.598274
C 0.654621 -1.281316 -0.542314
H 0.053297 -1.286727 -1.464627
C 1.725643 -0.180517 -0.649704
H 2.242433 -0.303474 -1.615745
C 1.052365 1.203849 -0.648544
H 0.469368 1.318709 -1.575363
C -2.003459 0.444036 -0.397547
O -3.069050 -0.500531 -0.246316
C 2.786499 -0.304333 0.452123
H 0.732995 1.424067 1.485970
H -1.042920 -1.866755 0.679520
H 1.140481 -2.268052 -0.484157
H 1.822311 1.991159 -0.665375
H -2.403256 1.472453 -0.379544
H -1.597443 0.265653 -1.399814
H -3.458537 -0.344903 0.626345
H 2.358671 -0.206794 1.457358
H 3.287930 -1.281000 0.397597
H 3.555065 0.473709 0.341181
el energy= -388.35138165966
zpe= -388.115827
th energy= -388.106496
th enthalpy= -388.105552
free energy= -388.149647

4mchm_22/coords
t8
C 0.147894 1.431981 0.544662

H -0.333175 2.419491 0.460085
C -0.926531 0.342109 0.713186
H -1.430599 0.493525 1.682058
C -0.272709 -1.050914 0.720360
H 0.329113 -1.150267 1.635835
C 0.615882 -1.287235 -0.509498
H 1.086985 -2.280443 -0.441707
C 1.701761 -0.206093 -0.661334
H 2.197365 -0.357771 -1.634368
C 1.051204 1.189231 -0.675619
H 1.834141 1.962842 -0.714888
C -2.014850 0.477404 -0.357911
O -3.091620 -0.450617 -0.174721
C 2.782178 -0.324378 0.421968
H 0.762019 1.465045 1.457018
H -1.046195 -1.831334 0.783615
H -0.007245 -1.301015 -1.417549
H 0.460977 1.298091 -1.598138
H -2.469354 1.475003 -0.286884
H -1.601886 0.374014 -1.372154
H -2.761585 -1.325066 -0.420860
H 3.565570 0.432281 0.273297
H 2.377635 -0.188553 1.432378
H 3.260221 -1.313531 0.385142
el energy= -388.35085803963
zpe= -388.115044
th energy= -388.105793
th enthalpy= -388.104848
free energy= -388.148582

4mchm_24/coords
t9
C -0.096105 1.270825 0.752278
H 0.613319 1.379163 1.586836
C -0.934752 -0.000025 0.996381
H -1.220076 -0.000047 2.062981
C -0.096094 -1.270860 0.752231
H 0.613327 -1.379221 1.586788
C 0.687647 -1.259060 -0.569358
H 1.324179 -2.156802 -0.624118
C 1.558691 0.000015 -0.724788
H 1.974351 0.000036 -1.746075

C 0.687633 1.259076 -0.569314
H -0.014282 1.315669 -1.411431
C -2.284069 -0.000014 0.280888
O -2.143343 0.000044 -1.143865
C 2.746375 0.000005 0.246458
H -0.750982 2.155804 0.791334
H -0.750963 -2.155846 0.791258
H -0.014265 -1.315632 -1.411479
H 1.324155 2.156826 -0.624047
H -2.854321 -0.889424 0.599976
H -2.854340 0.889361 0.600046
H -3.037391 -0.000021 -1.514613
H 2.428188 -0.000010 1.296085
H 3.374946 -0.888077 0.089349
H 3.374940 0.888096 0.089375
el energy= -388.34706471667
zpe= -388.111913
th energy= -388.102414
th enthalpy= -388.101470
free energy= -388.145858

4mchm_9/coords
c1
C -0.483836 -0.841688 1.096363
H -1.215154 -1.661806 1.115797
C -1.154137 0.450475 0.598659
H -1.923111 0.749920 1.330078
C -0.113425 1.579425 0.498942
H -0.581794 2.488247 0.089401
C 1.109135 1.183353 -0.341612
H 0.816818 1.028545 -1.392645
C 1.769198 -0.098788 0.183562
H 2.118707 0.100254 1.212194
C 0.737069 -1.232504 0.252214
H 1.204823 -2.136273 0.673657
C -1.883873 0.257394 -0.728304
O -2.934430 -0.696458 -0.531984
C 2.975632 -0.492856 -0.671070
H -0.157096 -0.685512 2.137051
H 0.225203 1.831160 1.516512
H 1.841753 2.005769 -0.339878
H 0.426206 -1.492974 -0.772417

H -2.303995 1.223399 -1.056604
H -1.201085 -0.091153 -1.517422
H -3.362974 -0.832227 -1.388379
H 2.665089 -0.693515 -1.706556
H 3.727034 0.308949 -0.694030
H 3.460437 -1.399984 -0.283414
el energy= -388.35289535946
zpe= -388.117856
th energy= -388.108392
th enthalpy= -388.107448
free energy= -388.151834

4mchm_11/coords
c2
C -0.331135 -1.101879 0.044056
H -1.017670 -1.908680 -0.248304
C -0.946564 0.262006 -0.295946
H -1.136357 0.296690 -1.383229
C 0.032432 1.390967 0.056237
H -0.397319 2.362726 -0.232828
C 1.385303 1.195012 -0.641927
H 1.232201 1.272769 -1.730567
C 2.021142 -0.170376 -0.326289
H 2.898431 -0.293360 -0.982572
C 1.021803 -1.293387 -0.655556
H 0.854269 -1.312231 -1.744871
C -2.276576 0.480206 0.411935
O -3.206519 -0.519306 -0.018836
C 2.521665 -0.252559 1.121699
H -0.209798 -1.172388 1.136942
H 0.168939 1.420224 1.148767
H 2.077611 2.004279 -0.361290
H 1.453695 -2.269912 -0.385506
H -2.127949 0.422655 1.503853
H -2.664656 1.486624 0.180191
H -4.023158 -0.388268 0.482536
H 3.006272 -1.221379 1.308497
H 3.259598 0.536849 1.323173
H 1.709622 -0.142097 1.850650
el energy= -388.35263524986
zpe= -388.117718
th energy= -388.108181

th enthalpy= -388.107237
free energy= -388.151795

4mchm_13/coords
c3
C -0.032346 1.392637 0.053539
H -0.171923 1.424725 1.145711
C 0.948667 0.262936 -0.290031
H 1.145816 0.297458 -1.377444
C 0.334044 -1.101574 0.044601
H 1.024608 -1.905428 -0.247330
C -1.016497 -1.293963 -0.659167
H -0.846324 -1.310944 -1.748152
C -2.017555 -0.172029 -0.330764
H -2.894606 -0.296724 -0.987047
C -1.383734 1.194257 -0.647072
H -2.077733 2.002682 -0.367984
C 2.276474 0.484602 0.431674
O 3.261288 -0.512604 0.140093
C -2.518361 -0.254163 1.117252
H 0.398095 2.364040 -0.236198
H 0.209725 -1.175742 1.136919
H -1.448451 -2.271185 -0.391636
H -1.229310 1.271257 -1.735588
H 2.669299 1.487470 0.191910
H 2.121466 0.437496 1.518546
H 3.430781 -0.469032 -0.811701
H -3.000635 -1.224024 1.304786
H -1.706957 -0.141045 1.846458
H -3.258303 0.533609 1.317807
el energy= -388.35372850465
zpe= -388.118589
th energy= -388.109136
th enthalpy= -388.108192
free energy= -388.152533

4mchm_15/coords
c4
C -0.494714 -0.847252 1.081964
H -0.179488 -0.701438 2.127614
C -1.158444 0.447727 0.585884
H -1.934514 0.743315 1.314056

C -0.120007 1.579732 0.500618
H -0.585959 2.488160 0.086979
C 1.110912 1.186589 -0.329374
H 0.829065 1.036925 -1.384032
C 1.765943 -0.098646 0.194799
H 2.105889 0.094005 1.227836
C 0.733287 -1.232833 0.246177
H 1.197114 -2.140009 0.664568
C -1.878733 0.259855 -0.752738
O -2.896444 -0.745581 -0.696903
C 2.980134 -0.487693 -0.651152
H -1.229185 -1.665127 1.085236
H 0.207938 1.831585 1.521660
H 1.843803 2.008646 -0.316855
H 0.430794 -1.485052 -0.783070
H -2.313280 1.223696 -1.069159
H -1.191597 -0.066959 -1.541429
H -3.511312 -0.482437 0.002693
H 2.678726 -0.683105 -1.690350
H 3.731542 0.314330 -0.663495
H 3.461761 -1.396773 -0.264100
el energy= -388.35416588606
zpe= -388.119004
th energy= -388.109599
th enthalpy= -388.108655
free energy= -388.152780

4mchm_16/coords
c5
C -0.232104 1.262191 -0.195699
H -0.733703 2.156277 -0.598802
C -0.953476 0.000023 -0.689855
H -0.918820 0.000028 -1.794301
C -0.232112 -1.262173 -0.195737
H -0.313023 -1.323254 0.898610
C 1.243629 -1.258301 -0.618744
H 1.750465 -2.160169 -0.240661
C 1.988990 -0.000005 -0.138915
H 2.988310 0.000000 -0.604465
C 1.243640 1.258317 -0.618699
H 1.294611 1.303831 -1.718886
C -2.430387 0.000018 -0.314177

O -2.555288 -0.000046 1.112291
C 2.196876 -0.000029 1.381180
H -0.313020 1.323244 0.898651
H -0.733738 -2.156225 -0.598882
H 1.294593 -1.303763 -1.718934
H 1.750488 2.160159 -0.240567
H -2.924412 0.890758 -0.738100
H -2.924401 -0.890713 -0.738165
H -3.500471 0.000046 1.317769
H 2.763229 -0.888312 1.695134
H 2.763288 0.888218 1.695137
H 1.248569 0.000000 1.932018
el energy= -388.35240361602
zpe= -388.117284
th energy= -388.107837
th enthalpy= -388.106893
free energy= -388.151212

4mchm_17/coords
c6
C -0.234591 1.271644 -0.152258
H -0.733779 2.182117 -0.520294
C -0.959382 0.031950 -0.693871
H -0.931534 0.072452 -1.797993
C -0.236838 -1.250067 -0.253898
H -0.308918 -1.357513 0.839351
C 1.239603 -1.229938 -0.674802
H 1.744520 -2.147953 -0.335353
C 1.985252 0.005687 -0.140123
H 2.985580 0.023472 -0.603078
C 1.242640 1.283485 -0.569551
H 1.749231 2.168085 -0.152335
C -2.438975 0.021626 -0.304347
O -2.660568 0.031015 1.110716
C 2.189500 -0.057302 1.379289
H -0.321103 1.288178 0.943454
H -0.738876 -2.127949 -0.690725
H 1.290936 -1.227872 -1.775834
H 1.298323 1.375007 -1.666590
H -2.931769 0.927784 -0.682165
H -2.940615 -0.849121 -0.759576
H -2.351421 -0.817154 1.456324

H 2.758132 0.815585 1.729920
H 1.240127 -0.076409 1.928100
H 2.752453 -0.959335 1.658434
el energy= -388.35349144792
zpe= -388.118048
th energy= -388.108669
th enthalpy= -388.107725
free energy= -388.151882

4mchm_23/coords
c7
C 0.436645 -1.220504 -0.990119
H 1.057422 -2.116661 -0.831914
C 1.304565 0.043936 -0.835913
H 1.970218 0.087429 -1.715575
C 0.432405 1.314140 -0.868903
H 1.050592 2.193208 -0.626937
C -0.798010 1.254972 0.047663
H -0.487635 1.248971 1.101791
C -1.650895 0.010056 -0.227584
H -1.992952 0.061011 -1.276748
C -0.795957 -1.254210 -0.074536
H -0.488666 -1.351928 0.975847
C 2.285012 -0.011036 0.333505
O 1.618432 -0.085799 1.597901
C -2.880624 -0.034308 0.682203
H 0.085880 -1.265409 -2.033962
H 0.079482 1.456705 -1.903274
H -1.407608 2.160787 -0.100052
H -1.403119 -2.142160 -0.312938
H 2.940414 -0.889452 0.204291
H 2.926753 0.886296 0.300776
H 2.307258 -0.124149 2.276908
H -3.506336 0.859727 0.550536
H -3.501991 -0.916431 0.472462
H -2.575997 -0.079824 1.737686
el energy= -388.34979472405
zpe= -388.114950
th energy= -388.105404
th enthalpy= -388.104460
free energy= -388.148929

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.341118 -1.094849 0.019401
H 1.025680 -1.896996 -0.296230
C 0.947978 0.277568 -0.302212
H 1.137362 0.326697 -1.388883
C -0.036755 1.395202 0.068321
H -0.168938 1.410509 1.161738
C -1.391893 1.201576 -0.626389
H -1.244382 1.294407 -1.714597
C -2.018098 -0.171422 -0.325233
H -2.898547 -0.291061 -0.977877
C -1.014763 -1.284321 -0.675779
H -1.439308 -2.267010 -0.416949
C 2.282360 0.495909 0.409960
O 3.298312 -0.434548 0.018988
C -2.509493 -0.275759 1.124485
H 0.227744 -1.187479 1.111607
H 0.387257 2.372850 -0.209841
H -2.087524 2.003018 -0.331772
H -0.852289 -1.286755 -1.765895
H 2.681033 1.488851 0.161442
H 2.129551 0.459312 1.502239
H 3.045113 -1.300224 0.366149
H -3.248804 0.508309 1.341080
H -2.989756 -1.248737 1.300586
H -1.693411 -0.172730 1.849978
el energy= -388.35354512641
zpe= -388.118110
th energy= -388.108740
th enthalpy= -388.107796
free energy= -388.151941

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.497438 -0.817003 1.102912
H 1.232528 -1.635419 1.140590
C 1.160447 0.473376 0.591520
H 1.928837 0.781825 1.319580
C 0.112404 1.594813 0.482137
H -0.221266 1.860544 1.497895
C -1.113706 1.182501 -0.346128

H -0.828702 1.022759 -1.398272
C -1.760952 -0.101521 0.190307
H -2.107436 0.100040 1.219466
C -0.718980 -1.225918 0.261298
H -1.177369 -2.132368 0.686994
C 1.893713 0.271674 -0.738721
O 2.970298 -0.669141 -0.638417
C -2.967703 -0.510498 -0.656923
H 0.169656 -0.652227 2.141735
H 0.574069 2.499903 0.056366
H -1.852479 1.999354 -0.344276
H -0.406139 -1.487066 -0.762790
H 1.203863 -0.031925 -1.539833
H 2.357954 1.219181 -1.044560
H 2.577199 -1.547474 -0.548090
H -3.725984 0.284753 -0.680412
H -2.660026 -0.713522 -1.692798
H -3.443056 -1.419775 -0.262677
el energy= -388.35361346540
zpe= -388.118380
th energy= -388.108952
th enthalpy= -388.108008
free energy= -388.152293

MP2 cc-pVDZ gas phase

4mchm_1/coords
t1
C 0.155310 1.430934 0.180861
H 0.547038 2.369685 -0.253221
C 1.033931 0.245424 -0.237980
H 1.026163 0.178118 -1.345322
C 0.465845 -1.064046 0.323712
H 1.095887 -1.908205 -0.001134
C -0.992480 -1.268755 -0.101047
H -1.389069 -2.207421 0.328456
C -1.881726 -0.088173 0.314337
H -1.858969 -0.023249 1.422401
C -1.304582 1.221997 -0.240637
H -1.924372 2.076374 0.089098
C 2.481993 0.455453 0.185638
O 3.251577 -0.631328 -0.316378

C -3.331883 -0.291922 -0.128929
H 0.203331 1.542893 1.282828
H 0.522116 -1.025873 1.430927
H -1.041399 -1.378146 -1.203336
H -1.363626 1.193500 -1.347319
H 2.845789 1.425702 -0.212200
H 2.529624 0.510365 1.294380
H 4.151317 -0.513532 0.015584
H -3.391828 -0.360776 -1.229983
H -3.751457 -1.222171 0.291179
H -3.971612 0.547888 0.192947
el energy= -388.48743149407
zpe= -388.254328
th energy= -388.244662
th enthalpy= -388.243717
free energy= -388.288452

4mchm_3/coords
t2
C -0.155015 1.432220 0.179829
H -0.202726 1.544581 1.281610
C -1.035586 0.246023 -0.232607
H -1.015992 0.181444 -1.343531
C -0.465806 -1.062360 0.328063
H -0.520630 -1.021236 1.434843
C 0.991114 -1.269525 -0.099593
H 1.388058 -2.207344 0.331191
C 1.881302 -0.088123 0.312208
H 1.860148 -0.021782 1.420103
C 1.304178 1.221940 -0.243429
H 1.924769 2.076156 0.084987
C -2.489053 0.457322 0.193065
O -3.345200 -0.616303 -0.178373
C 3.330622 -0.293284 -0.133060
H -0.548353 2.370604 -0.253605
H -1.098878 -1.908616 0.013092
H 1.039311 -1.381040 -1.201957
H 1.362723 1.192898 -1.350284
H -2.543973 0.515676 1.294334
H -2.855818 1.425888 -0.206806
H -3.308128 -0.662080 -1.144330
H 3.971033 0.546718 0.186707

H 3.750417 -1.222989 0.287909
H 3.389090 -0.363722 -1.234125
el energy= -388.48833098728
zpe= -388.255019
th energy= -388.245456
th enthalpy= -388.244512
free energy= -388.289006

4mchm_5/coords
t3
C 0.394313 -1.261178 0.041559
H 0.828501 -2.161492 0.515720
C 1.033506 0.000007 0.640839
H 0.841941 0.000034 1.734768
C 0.394319 1.261184 0.041521
H 0.828541 2.161486 0.515686
C -1.129114 1.255539 0.210975
H -1.381051 1.289607 1.290610
C -1.766552 -0.000010 -0.399641
H -1.537457 -0.000016 -1.485712
C -1.129140 -1.255556 0.210965
H -1.567942 -2.161782 -0.246453
C 2.548439 0.000011 0.457341
O 2.821322 -0.000004 -0.941185
C -3.286525 0.000016 -0.223399
H 0.651904 -1.308241 -1.032025
H 0.651906 1.308232 -1.032060
H -1.567975 2.161755 -0.246410
H -1.381118 -1.289654 1.290591
H 2.979664 0.896509 0.949646
H 2.979674 -0.896465 0.949668
H 3.782784 -0.000107 -1.037821
H -3.549639 0.000069 0.849760
H -3.742870 0.893244 -0.683766
H -3.742921 -0.893228 -0.683680
el energy= -388.48774712645
zpe= -388.254541
th energy= -388.244921
th enthalpy= -388.243977
free energy= -388.288570

4mchm_6/coords

t4
C 0.154861 1.426879 0.181861
H 0.211458 1.524542 1.284842
C 1.036956 0.251812 -0.258793
H 1.029014 0.198286 -1.366552
C 0.468901 -1.066841 0.283014
H 1.072467 -1.918620 -0.080617
C -0.996057 -1.265143 -0.124585
H -1.057250 -1.357755 -1.227530
C -1.879119 -0.090500 0.318318
H -1.841660 -0.038986 1.426641
C -1.308554 1.225159 -0.229353
H -1.379209 1.208772 -1.335488
C 2.488167 0.468948 0.175551
O 3.374826 -0.544018 -0.281599
C -3.334437 -0.292049 -0.108569
H 0.545030 2.371238 -0.241124
H 0.542965 -1.060412 1.390295
H -1.386156 -2.210319 0.296221
H -1.924362 2.075810 0.116603
H 2.863786 1.413642 -0.252732
H 2.523391 0.573114 1.281562
H 3.144212 -1.344615 0.207670
H -3.970374 0.543365 0.231201
H -3.408545 -0.348179 -1.209418
H -3.747688 -1.227335 0.306546
el energy= -388.48772913853
zpe= -388.254470
th energy= -388.244828
th enthalpy= -388.243884
free energy= -388.288600

4mchm_7/coords
t5
C 0.392291 1.264627 -0.022776
H 0.658531 1.298120 1.049727
C 1.035622 0.015234 -0.638921
H 0.840722 0.020920 -1.732145
C 0.394407 -1.252884 -0.055778
H 0.620641 -1.307359 1.027948
C -1.128828 -1.251335 -0.231017
H -1.373074 -1.268792 -1.312292

C -1.770626 -0.006876 0.398169
H -1.547139 -0.026179 1.485313
C -1.131801 1.260450 -0.186955
H -1.570461 2.156539 0.289822
C 2.557342 0.018952 -0.457362
O 2.959089 0.056448 0.907824
C -3.289514 -0.006907 0.214764
H 0.824272 2.172154 -0.484145
H 0.835214 -2.152442 -0.526281
H -1.566673 -2.166293 0.209314
H -1.386985 1.316937 -1.264716
H 2.995980 -0.855284 -0.982335
H 2.982163 0.927501 -0.916799
H 2.704826 -0.795606 1.286778
H -3.746965 -0.908379 0.657571
H -3.749188 0.877588 0.688132
H -3.547946 0.011423 -0.859239
el energy= -388.48817850515
zpe= -388.254832
th energy= -388.245256
th enthalpy= -388.244312
free energy= -388.288850

4mchm_19/coords
t6
C 0.280541 -1.068621 0.692822
H -0.310568 -1.193316 1.618785
C 0.925367 0.329434 0.704247
H 1.439724 0.465408 1.674713
C -0.147997 1.422811 0.556098
H -0.761956 1.441625 1.475027
C -1.057886 1.197291 -0.662968
H -1.841604 1.977193 -0.693480
C -1.710748 -0.198507 -0.659967
H -2.216782 -0.337123 -1.634959
C -0.624120 -1.283265 -0.529852
H -0.006889 -1.286058 -1.448122
C 2.012880 0.464877 -0.361471
O 3.002876 -0.523800 -0.096102
C -2.784923 -0.327040 0.428695
H 1.075750 -1.831939 0.716468
H 0.331494 2.417590 0.487945

H -0.469164 1.314884 -1.592079
H -1.097410 -2.281340 -0.475022
H 1.587405 0.340044 -1.376894
H 2.439685 1.488296 -0.306764
H 3.656457 -0.460619 -0.805020
H -3.572456 0.434576 0.292301
H -3.264146 -1.320680 0.387703
H -2.371228 -0.200014 1.442583
el energy= -388.48214262989
zpe= -388.248393
th energy= -388.238875
th enthalpy= -388.237931
free energy= -388.282383

4mchm_21/coords
t7
C 0.145515 1.423992 0.553252
H -0.337732 2.416506 0.478257
C -0.926141 0.327768 0.694215
H -1.433757 0.469477 1.671601
C -0.285011 -1.071487 0.684960
H 0.295723 -1.207050 1.615820
C 0.628275 -1.282685 -0.531996
H 0.016336 -1.282350 -1.453409
C 1.715733 -0.197954 -0.650725
H 2.230430 -0.336467 -1.621023
C 1.061420 1.196863 -0.660681
H 0.477026 1.311616 -1.592755
C -2.015249 0.465107 -0.378004
O -3.028619 -0.527459 -0.268059
C 2.779595 -0.325957 0.448002
H 0.754121 1.448258 1.475599
H -1.083046 -1.833021 0.689708
H 1.099906 -2.281316 -0.475995
H 1.843758 1.978073 -0.688423
H -2.442569 1.488724 -0.326918
H -1.596230 0.341575 -1.389336
H -3.404100 -0.425750 0.618442
H 2.356418 -0.200119 1.458207
H 3.260329 -1.318980 0.410814
H 3.567516 0.436616 0.319754
el energy= -388.48333520396

zpe= -388.249333
th energy= -388.239932
th enthalpy= -388.238988
free energy= -388.283126

4mchm_22/coords
t8
C 0.146439 1.431938 0.545502
H -0.335147 2.424573 0.463120
C -0.929104 0.342207 0.709291
H -1.439106 0.486121 1.680617
C -0.274274 -1.051298 0.715785
H 0.327155 -1.158312 1.636871
C 0.617404 -1.286784 -0.512860
H 1.088358 -2.285464 -0.451127
C 1.704877 -0.204758 -0.659203
H 2.204685 -0.355604 -1.635342
C 1.054029 1.191844 -0.673102
H 1.839691 1.969150 -0.712204
C -2.023835 0.471663 -0.359297
O -3.091576 -0.450717 -0.173806
C 2.784464 -0.325513 0.425034
H 0.762048 1.465864 1.463060
H -1.053331 -1.833359 0.782904
H -0.004204 -1.294044 -1.428830
H 0.464399 1.302106 -1.602087
H -2.477494 1.474655 -0.282779
H -1.597848 0.388367 -1.378631
H -2.738340 -1.321273 -0.399280
H 3.575579 0.428838 0.271619
H 2.378743 -0.179110 1.439527
H 3.257423 -1.322578 0.396121
el energy= -388.48195627761
zpe= -388.248165
th energy= -388.238636
th enthalpy= -388.237692
free energy= -388.282203

4mchm_24/coords
t9
C -0.104308 1.269414 0.773915
H 0.613180 1.367323 1.610254

C -0.947496 -0.000705 1.008591
H -1.255494 -0.001309 2.073948
C -0.104136 -1.270469 0.772534
H 0.613279 -1.369217 1.608834
C 0.663490 -1.259480 -0.559162
H 1.300033 -2.162280 -0.624201
C 1.534516 0.000442 -0.721718
H 1.935699 0.001020 -1.753629
C 0.663151 1.259957 -0.557879
H -0.061118 1.303741 -1.387079
C -2.273727 -0.000342 0.247997
O -2.052902 0.001008 -1.161252
C 2.738432 0.000133 0.230639
H -0.757594 2.160889 0.825257
H -0.757312 -2.162085 0.822840
H -0.060676 -1.302664 -1.388473
H 1.299432 2.163000 -0.622099
H -2.854644 -0.895941 0.553699
H -2.855043 0.894451 0.555300
H -2.926163 0.001136 -1.577123
H 2.435177 -0.000415 1.290911
H 3.367573 -0.892145 0.065603
H 3.367351 0.892727 0.066466
el energy= -388.48196767507
zpe= -388.248032
th energy= -388.238599
th enthalpy= -388.237655
free energy= -388.281669

4mchm_9/coords
c1
C -0.502154 -0.828851 1.090376
H -1.253409 -1.635576 1.094367
C -1.156046 0.470274 0.587844
H -1.928647 0.773974 1.319712
C -0.108706 1.592241 0.482093
H -0.569399 2.506019 0.061903
C 1.117510 1.181955 -0.347354
H 0.832078 1.022818 -1.405855
C 1.763232 -0.104711 0.187058
H 2.103057 0.097780 1.224567
C 0.719752 -1.229308 0.252928

H 1.180052 -2.142207 0.674708
C -1.895622 0.264901 -0.733743
O -2.898297 -0.722955 -0.517620
C 2.978021 -0.510504 -0.649588
H -0.178640 -0.676192 2.137980
H 0.229297 1.852396 1.503199
H 1.860021 2.001730 -0.347392
H 0.409065 -1.489051 -0.778426
H -2.342206 1.231968 -1.046745
H -1.194158 -0.047138 -1.532653
H -3.323445 -0.879593 -1.371108
H 2.675575 -0.721198 -1.691303
H 3.735494 0.291972 -0.673285
H 3.455724 -1.420047 -0.246397
el energy= -388.48502528845
zpe= -388.251593
th energy= -388.242021
th enthalpy= -388.241077
free energy= -388.285704

4mchm_11/coords
c2
C -0.343297 -1.092506 0.054837
H -1.054504 -1.885760 -0.228584
C -0.947411 0.277248 -0.281733
H -1.140509 0.308220 -1.374060
C 0.039609 1.399833 0.064417
H -0.384897 2.380579 -0.220732
C 1.386846 1.193683 -0.643033
H 1.223533 1.272345 -1.735209
C 2.013494 -0.179029 -0.333231
H 2.887186 -0.308789 -1.000733
C 1.002306 -1.295934 -0.653924
H 0.824850 -1.312962 -1.746753
C -2.286524 0.485954 0.413357
O -3.178152 -0.531000 -0.029360
C 2.529796 -0.264227 1.109466
H -0.213013 -1.163023 1.152878
H 0.186067 1.428921 1.161796
H 2.091619 2.000165 -0.367891
H 1.431961 -2.279447 -0.387580
H -2.133345 0.442710 1.513143

H -2.674483 1.497251 0.170587
H -3.998971 -0.419110 0.467969
H 3.009130 -1.241206 1.294988
H 3.279261 0.522879 1.303557
H 1.722413 -0.144909 1.850575
el energy= -388.48477941743
zpe= -388.251363
th energy= -388.241772
th enthalpy= -388.240828
free energy= -388.285398

4mchm_13/coords
c3
C -0.040332 1.400613 0.066012
H -0.189814 1.428064 1.162855
C 0.948563 0.277789 -0.273499
H 1.132132 0.313332 -1.371030
C 0.342947 -1.091496 0.058730
H 1.056555 -1.887078 -0.213564
C -0.998836 -1.296558 -0.656369
H -0.817857 -1.313405 -1.748868
C -2.011306 -0.179602 -0.339297
H -2.882423 -0.309861 -1.009951
C -1.384717 1.193722 -0.646730
H -2.091219 1.999301 -0.373859
C 2.291525 0.487348 0.426678
O 3.245577 -0.524746 0.127675
C -2.532335 -0.265193 1.101669
H 0.385814 2.381702 -0.215387
H 0.208329 -1.160325 1.155964
H -1.429336 -2.279981 -0.391705
H -1.218049 1.273284 -1.738480
H 2.682646 1.497805 0.184706
H 2.145663 0.445999 1.520454
H 3.382325 -0.484392 -0.829569
H -3.011164 -1.242613 1.285589
H -1.727939 -0.144661 1.845750
H -3.283335 0.521059 1.292535
el energy= -388.48567945504
zpe= -388.252049
th energy= -388.242563
th enthalpy= -388.241619

free energy= -388.285945

4mchm_15/coords
c4
C -0.506073 -0.839672 1.078061
H -0.193164 -0.702366 2.130881
C -1.156489 0.462846 0.581281
H -1.924724 0.769910 1.321834
C -0.112911 1.589576 0.487718
H -0.575356 2.502239 0.066937
C 1.117201 1.184585 -0.338090
H 0.836130 1.028879 -1.398164
C 1.762852 -0.102531 0.194898
H 2.094282 0.095312 1.236092
C 0.722000 -1.230076 0.244871
H 1.180760 -2.145528 0.662381
C -1.895673 0.264763 -0.748327
O -2.875792 -0.764809 -0.688001
C 2.984704 -0.500761 -0.635054
H -1.254543 -1.649543 1.059850
H 0.219454 1.848495 1.511015
H 1.857355 2.006293 -0.331817
H 0.416556 -1.481799 -0.789678
H -2.342115 1.232645 -1.059673
H -1.201489 -0.041148 -1.547154
H -3.492337 -0.503283 0.011035
H 2.690146 -0.706777 -1.679846
H 3.740029 0.303880 -0.648793
H 3.461691 -1.411121 -0.233042
el energy= -388.48618610051
zpe= -388.252502
th energy= -388.243044
th enthalpy= -388.242099
free energy= -388.286416

4mchm_16/coords
c5
C -0.239067 1.263454 -0.217818
H -0.737132 2.160348 -0.632245
C -0.961453 0.000005 -0.709859
H -0.939981 0.000009 -1.820176
C -0.239067 -1.263450 -0.217828

H -0.345436 -1.324489 0.879123
C 1.241227 -1.257716 -0.622561
H 1.745796 -2.164847 -0.241131
C 1.979408 0.000000 -0.128108
H 2.990301 0.000001 -0.579802
C 1.241229 1.257723 -0.622548
H 1.308241 1.297637 -1.727465
C -2.429790 0.000002 -0.294923
O -2.483224 -0.000025 1.129185
C 2.159857 -0.000007 1.395797
H -0.345438 1.324485 0.879134
H -0.737135 -2.160339 -0.632262
H 1.308237 -1.297617 -1.727478
H 1.745798 2.164850 -0.241107
H -2.931746 0.896475 -0.715046
H -2.931750 -0.896456 -0.715075
H -3.417990 0.000099 1.373863
H 2.722257 -0.892339 1.721927
H 2.722263 0.892318 1.721934
H 1.195446 -0.000006 1.929410
el energy= -388.48544740780
zpe= -388.251907
th energy= -388.242365
th enthalpy= -388.241421
free energy= -388.285854

4mchm_17/coords
c6
C -0.237346 1.276012 -0.141600
H -0.734217 2.196914 -0.499939
C -0.966343 0.047028 -0.702141
H -0.940982 0.099431 -1.811412
C -0.242942 -1.240595 -0.278790
H -0.311831 -1.351292 0.820563
C 1.234335 -1.221064 -0.695297
H 1.737650 -2.150004 -0.368936
C 1.981716 0.005243 -0.139196
H 2.986114 0.026775 -0.604203
C 1.242108 1.292099 -0.549886
H 1.750353 2.172415 -0.114600
C -2.441835 0.033069 -0.289514
O -2.628292 0.003210 1.122018

C 2.185457 -0.081288 1.379367
H -0.345845 1.272922 0.957483
H -0.747303 -2.120884 -0.721347
H 1.287404 -1.201141 -1.801067
H 1.304495 1.401604 -1.650175
H -2.930937 0.960021 -0.634118
H -2.957886 -0.817846 -0.781347
H -2.336722 -0.871118 1.413262
H 2.769850 0.781714 1.742838
H 1.230345 -0.088207 1.929768
H 2.734947 -1.000011 1.649435
el energy= -388.48573350607
zpe= -388.252077
th energy= -388.242577
th enthalpy= -388.241633
free energy= -388.286006

4mchm_23/coords
c7
C 0.465475 -1.264578 -0.949435
H 1.083650 -2.161501 -0.756602
C 1.334439 0.001978 -0.821012
H 2.043564 0.003965 -1.673564
C 0.465382 1.269058 -0.943614
H 1.083486 2.165128 -0.746635
C -0.768925 1.257906 -0.030486
H -0.449923 1.293900 1.025114
C -1.622421 0.000536 -0.248314
H -1.967614 0.002904 -1.304441
C -0.768771 -1.257702 -0.036189
H -0.449712 -1.298427 1.019227
C 2.242980 -0.000839 0.408436
O 1.474080 -0.003971 1.609858
C -2.852577 -0.001599 0.661637
H 0.122955 -1.338992 -2.000171
H 0.122917 1.348285 -1.994014
H -1.379812 2.159516 -0.226096
H -1.379556 -2.158494 -0.235842
H 2.898550 -0.895678 0.359164
H 2.898181 0.894498 0.363556
H 2.106601 -0.005412 2.341631
H -3.478129 0.892102 0.492803

H -3.478012 -0.894612 0.488776
H -2.543285 -0.003970 1.722087
el energy= -388.48486368340
zpe= -388.251247
th energy= -388.241752
th enthalpy= -388.240808
free energy= -388.285013

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.348126 -1.089395 0.012225
H 1.038855 -1.887181 -0.317588
C 0.949996 0.287706 -0.301121
H 1.140396 0.335079 -1.392997
C -0.040988 1.398995 0.069811
H -0.174715 1.413159 1.169091
C -1.396546 1.202730 -0.623557
H -1.248842 1.296747 -1.716643
C -2.016166 -0.174873 -0.323190
H -2.899996 -0.298516 -0.978127
C -1.008800 -1.283673 -0.679230
H -1.431064 -2.273205 -0.424034
C 2.291846 0.497720 0.403445
O 3.284814 -0.447412 0.026591
C -2.507299 -0.284331 1.126568
H 0.237022 -1.193830 1.110244
H 0.380478 2.384000 -0.204678
H -2.098399 2.004001 -0.327099
H -0.845973 -1.279604 -1.774204
H 2.699478 1.486689 0.133520
H 2.127289 0.499734 1.502802
H 3.000526 -1.296004 0.390783
H -3.255176 0.497590 1.345294
H -2.981220 -1.265238 1.305116
H -1.688185 -0.173394 1.856098
el energy= -388.48508186473
zpe= -388.251510
th energy= -388.241947
th enthalpy= -388.241003
free energy= -388.285549

4mchm-1000rej-h-rmsd_20/coords

c9
C 0.499133 -0.811107 1.104077
H 1.243516 -1.627361 1.152762
C 1.162379 0.478674 0.589402
H 1.933085 0.783699 1.322341
C 0.112950 1.598708 0.477130
H -0.224609 1.869555 1.495741
C -1.113774 1.183194 -0.349815
H -0.829304 1.021145 -1.407763
C -1.759258 -0.102075 0.187962
H -2.101265 0.101949 1.224399
C -0.714706 -1.225349 0.261073
H -1.174162 -2.137854 0.684377
C 1.905963 0.269842 -0.737070
O 2.957694 -0.683752 -0.638443
C -2.971002 -0.514183 -0.649985
H 0.166220 -0.645527 2.146414
H 0.574662 2.507547 0.047625
H -1.857373 2.001724 -0.351536
H -0.400952 -1.485433 -0.769828
H 1.201966 0.004475 -1.550345
H 2.388041 1.218968 -1.027655
H 2.532014 -1.545881 -0.543167
H -3.729464 0.286963 -0.677613
H -2.665954 -0.727189 -1.690383
H -3.448085 -1.422992 -0.244472
el energy= -388.48484654724
zpe= -388.251370
th energy= -388.241787
th enthalpy= -388.240843
free energy= -388.285531

MP2-SMD cc-pVDZ

4mchm_1/coords
t1
C 0.158126 1.423453 0.180746
H 0.556168 2.358543 -0.254561
C 1.033269 0.235685 -0.239185
H 1.022669 0.172317 -1.346974
C 0.456745 -1.070564 0.322600
H 1.073066 -1.925854 -0.003080

C -1.002781 -1.269204 -0.100804
H -1.402469 -2.205589 0.330902
C -1.885381 -0.084873 0.315805
H -1.862195 -0.020049 1.423341
C -1.302021 1.221176 -0.240679
H -1.917500 2.078173 0.090176
C 2.477413 0.450747 0.192604
O 3.275138 -0.619137 -0.322805
C -3.334339 -0.281646 -0.130878
H 0.208607 1.532502 1.282432
H 0.515352 -1.031628 1.429146
H -1.052924 -1.376267 -1.203130
H -1.361274 1.190249 -1.347173
H 2.838890 1.426529 -0.188115
H 2.527995 0.483049 1.299828
H 4.169756 -0.480724 0.023486
H -3.392115 -0.345361 -1.232653
H -3.760000 -1.211598 0.284943
H -3.971310 0.560154 0.192620
el energy= -388.49196612987
zpe= -388.259928
th energy= -388.250110
th enthalpy= -388.249166
free energy= -388.294297

4mchm_3/coords
t2
C -0.158291 1.427032 0.178312
H -0.205840 1.539353 1.279914
C -1.036281 0.238843 -0.233585
H -1.027935 0.172797 -1.342838
C -0.461308 -1.067023 0.327759
H -0.517023 -1.027414 1.434510
C 0.996628 -1.269299 -0.098878
H 1.396192 -2.205418 0.333529
C 1.881848 -0.085331 0.313690
H 1.859655 -0.017596 1.421079
C 1.300725 1.220699 -0.245497
H 1.918820 2.077055 0.082224
C -2.482818 0.457419 0.202474
O -3.354978 -0.609107 -0.182905
C 3.330130 -0.286169 -0.133436

H -0.556154 2.361719 -0.258290
H -1.082327 -1.920012 0.004689
H 1.044221 -1.378238 -1.201184
H 1.358216 1.186845 -1.352018
H -2.534341 0.507190 1.304544
H -2.848147 1.425597 -0.194170
H -3.299525 -0.652302 -1.150845
H 3.968968 0.555296 0.187211
H 3.754142 -1.215747 0.284897
H 3.387105 -0.353293 -1.235054
el energy= -388.49339951766
zpe= -388.261017
th energy= -388.251357
th enthalpy= -388.250413
free energy= -388.295157

4mchm_5/coords
t3
C 0.388172 -1.260579 0.025889
H 0.826416 -2.160651 0.496340
C 1.027346 -0.000007 0.625782
H 0.824258 0.000010 1.716613
C 0.388187 1.260569 0.025870
H 0.826481 2.160621 0.496329
C -1.134124 1.256083 0.203935
H -1.377010 1.289866 1.285209
C -1.775546 -0.000003 -0.400797
H -1.557333 -0.000001 -1.488876
C -1.134160 -1.256099 0.203903
H -1.575487 -2.161069 -0.253659
C 2.544285 -0.000006 0.471703
O 2.866978 0.000016 -0.922863
C -3.292322 0.000026 -0.207255
H 0.630258 -1.308403 -1.052064
H 0.630261 1.308386 -1.052084
H -1.575502 2.161054 -0.253578
H -1.377089 -1.289926 1.285169
H 2.967754 0.894772 0.969645
H 2.967759 -0.894791 0.969619
H 3.834942 -0.000024 -0.974648
H -3.542632 0.000100 0.869260
H -3.754943 0.893265 -0.662345

H -3.754991 -0.893249 -0.662217
el energy= -388.49199168745
zpe= -388.259745
th energy= -388.250034
th enthalpy= -388.249090
free energy= -388.293918

4mchm_6/coords
t4
C 0.156128 1.425494 0.184723
H 0.211448 1.522842 1.287337
C 1.035180 0.246919 -0.252037
H 1.024419 0.193190 -1.360081
C 0.465778 -1.068025 0.296850
H 1.074310 -1.923028 -0.050658
C -0.996610 -1.266553 -0.118176
H -1.053450 -1.361261 -1.221212
C -1.880048 -0.089823 0.317435
H -1.848670 -0.035875 1.425331
C -1.305660 1.223510 -0.230674
H -1.371717 1.202923 -1.336996
C 2.482329 0.467720 0.184008
O 3.379756 -0.535238 -0.300903
C -3.331549 -0.287984 -0.120267
H 0.549692 2.366787 -0.241744
H 0.534595 -1.047974 1.403385
H -1.389689 -2.209059 0.305961
H -1.921914 2.075095 0.112490
H 2.850454 1.425148 -0.222438
H 2.526187 0.534719 1.290131
H 3.140011 -1.352955 0.160423
H -3.969301 0.547167 0.218461
H -3.397815 -0.338747 -1.222223
H -3.749891 -1.224618 0.287891
el energy= -388.49296701729
zpe= -388.260917
th energy= -388.251031
th enthalpy= -388.250087
free energy= -388.295696

4mchm_7/coords
t5

C 0.392245 1.260839 -0.019278
H 0.641426 1.294761 1.057701
C 1.032180 0.007546 -0.630867
H 0.833055 0.012953 -1.722545
C 0.391025 -1.258334 -0.043562
H 0.623852 -1.316642 1.038295
C -1.131669 -1.252190 -0.219855
H -1.374883 -1.274066 -1.301229
C -1.772590 -0.002879 0.399434
H -1.553787 -0.015210 1.487192
C -1.130712 1.259612 -0.191747
H -1.569946 2.159201 0.278232
C 2.553149 0.008184 -0.468573
O 2.979344 0.073002 0.896686
C -3.289259 -0.000858 0.206364
H 0.829769 2.166261 -0.480143
H 0.829987 -2.155871 -0.518147
H -1.572406 -2.162273 0.227743
H -1.378004 1.306996 -1.271457
H 2.980733 -0.883505 -0.968644
H 2.977918 0.901921 -0.956634
H 2.675403 -0.748773 1.311642
H -3.751527 -0.900208 0.649622
H -3.752286 0.886023 0.673243
H -3.540274 0.012900 -0.869853
el energy= -388.49324443965
zpe= -388.260952
th energy= -388.251227
th enthalpy= -388.250283
free energy= -388.295097

4mchm_19/coords
t6
C 0.264745 -1.073150 0.699945
H -0.337155 -1.183775 1.620509
C 0.924221 0.318211 0.710214
H 1.436473 0.454479 1.682415
C -0.144751 1.416144 0.563556
H -0.763669 1.431127 1.479125
C -1.046117 1.198196 -0.662305
H -1.825262 1.982471 -0.695850
C -1.709270 -0.192082 -0.664993

H -2.209878 -0.327108 -1.642993
C -0.632070 -1.284970 -0.528810
H -0.008863 -1.291998 -1.442741
C 2.005555 0.457878 -0.359819
O 3.023536 -0.515373 -0.101095
C -2.788259 -0.314770 0.418337
H 1.044190 -1.853442 0.736555
H 0.342376 2.407037 0.498642
H -0.446228 1.310505 -1.584433
H -1.114528 -2.278627 -0.471218
H 1.587108 0.317394 -1.373591
H 2.425016 1.482796 -0.313581
H 3.661077 -0.435840 -0.827002
H -3.565082 0.459099 0.286020
H -3.282156 -1.301184 0.365215
H -2.376027 -0.202694 1.434945
el energy= -388.48717747402
zpe= -388.254027
th energy= -388.244549
th enthalpy= -388.243605
free energy= -388.287948

4mchm_21/coords
t7
C 0.139247 1.416324 0.558877
H -0.350347 2.405705 0.487045
C -0.928279 0.315534 0.691177
H -1.446904 0.448583 1.662359
C -0.274806 -1.077574 0.678829
H 0.310795 -1.204317 1.607675
C 0.639226 -1.282068 -0.538479
H 0.029236 -1.279917 -1.461376
C 1.719504 -0.189827 -0.651232
H 2.236870 -0.321269 -1.620930
C 1.055854 1.200089 -0.655739
H 0.467565 1.312142 -1.585543
C -2.008166 0.458463 -0.386271
O -3.045978 -0.518506 -0.260129
C 2.779127 -0.316813 0.450549
H 0.746948 1.434719 1.481870
H -1.062242 -1.850891 0.691986
H 1.118725 -2.277209 -0.481992

H 1.834707 1.985000 -0.679152
H -2.427598 1.483540 -0.340041
H -1.591693 0.319421 -1.396860
H -3.409561 -0.398013 0.631985
H 2.348954 -0.209029 1.460180
H 3.274120 -1.302925 0.402210
H 3.558014 0.457733 0.335353
el energy= -388.48866366735
zpe= -388.255581
th energy= -388.246035
th enthalpy= -388.245090
free energy= -388.289874

4mchm_22/coords
t8
C 0.149207 1.433051 0.545343
H -0.333288 2.425124 0.461428
C -0.926451 0.344177 0.711933
H -1.433974 0.494177 1.684308
C -0.273943 -1.050234 0.719366
H 0.331733 -1.150868 1.638348
C 0.612703 -1.286831 -0.511652
H 1.083924 -2.285313 -0.446711
C 1.700867 -0.206624 -0.661319
H 2.200031 -0.358808 -1.637472
C 1.051194 1.189906 -0.675935
H 1.838017 1.966066 -0.717370
C -2.015106 0.477211 -0.358998
O -3.087868 -0.453542 -0.175069
C 2.778248 -0.326637 0.423926
H 0.767662 1.462929 1.460971
H -1.053510 -1.831518 0.782316
H -0.015894 -1.294601 -1.422226
H 0.455130 1.296372 -1.601010
H -2.468860 1.480481 -0.284325
H -1.593236 0.381993 -1.376518
H -2.726858 -1.323809 -0.401693
H 3.566023 0.433547 0.278066
H 2.367998 -0.190666 1.438414
H 3.257733 -1.320884 0.388035
el energy= -388.48800422815
zpe= -388.254606

th energy= -388.245197
th enthalpy= -388.244253
free energy= -388.288307

4mchm_24/coords
t9
C -0.096588 1.270096 0.763492
H 0.622708 1.370513 1.597549
C -0.938412 0.000163 1.002729
H -1.236560 0.000305 2.070188
C -0.096622 -1.269849 0.763816
H 0.622697 -1.370061 1.597878
C 0.676534 -1.260227 -0.564199
H 1.316208 -2.161143 -0.624117
C 1.546636 -0.000105 -0.726171
H 1.956101 -0.000238 -1.754715
C 0.676617 1.260115 -0.564496
H -0.038395 1.312414 -1.402128
C -2.277788 0.000083 0.267519
O -2.107588 -0.000224 -1.154862
C 2.740625 -0.000034 0.236414
H -0.751726 2.160314 0.811014
H -0.751777 -2.160041 0.811594
H -0.038510 -1.312663 -1.401799
H 1.316356 2.160972 -0.624600
H -2.853496 -0.893267 0.583023
H -2.853402 0.893624 0.582654
H -3.003972 -0.000342 -1.526568
H 2.426501 0.000103 1.293427
H 3.370950 -0.892607 0.075544
H 3.371010 0.892457 0.075334
el energy= -388.48530467864
zpe= -388.252405
th energy= -388.242827
th enthalpy= -388.241883
free energy= -388.286337

4mchm_9/coords
c1
C -0.489256 -0.836250 1.095731
H -1.229973 -1.653955 1.109511
C -1.153936 0.458464 0.595067

H -1.926196 0.761156 1.328569
C -0.110838 1.584675 0.492967
H -0.579116 2.496339 0.077489
C 1.110850 1.182099 -0.345130
H 0.816054 1.020882 -1.400347
C 1.766566 -0.101064 0.184086
H 2.112220 0.100755 1.219402
C 0.730185 -1.231409 0.252461
H 1.196791 -2.141119 0.674444
C -1.887227 0.259767 -0.729741
O -2.922277 -0.708295 -0.526094
C 2.975208 -0.499370 -0.663089
H -0.160864 -0.680090 2.141091
H 0.230925 1.838241 1.514332
H 1.849541 2.005249 -0.346231
H 0.416385 -1.488231 -0.778306
H -2.317023 1.229145 -1.052190
H -1.194628 -0.075788 -1.523678
H -3.341685 -0.838688 -1.390243
H 2.666602 -0.703179 -1.704566
H 3.731335 0.304887 -0.685332
H 3.458542 -1.410714 -0.269304
el energy= -388.48987335396
zpe= -388.257174
th energy= -388.247577
th enthalpy= -388.246633
free energy= -388.291282

4mchm_11/coords
c2
C -0.333777 -1.096913 0.051107
H -1.031319 -1.902765 -0.234645
C -0.946449 0.268534 -0.288561
H -1.132453 0.300883 -1.382311
C 0.035749 1.394157 0.061728
H -0.394328 2.371674 -0.224992
C 1.385403 1.195406 -0.641580
H 1.225254 1.273142 -1.734217
C 2.018036 -0.173460 -0.330119
H 2.895516 -0.298985 -0.993079
C 1.013676 -1.294244 -0.655816
H 0.837922 -1.308783 -1.748910

C -2.281862 0.483199 0.409892
O -3.196651 -0.527106 -0.025222
C 2.524480 -0.258323 1.115022
H -0.204319 -1.162397 1.149117
H 0.177059 1.418439 1.159443
H 2.085137 2.004437 -0.361040
H 1.446718 -2.275724 -0.387195
H -2.133370 0.435561 1.507765
H -2.669806 1.492557 0.167832
H -4.008534 -0.395476 0.487528
H 3.005525 -1.234850 1.301506
H 3.271302 0.530516 1.314295
H 1.711363 -0.141521 1.850652
el energy= -388.48955769589
zpe= -388.256862
th energy= -388.247240
th enthalpy= -388.246296
free energy= -388.290999

4mchm_13/coords
c3
C -0.035748 1.395586 0.059678
H -0.181065 1.422618 1.156906
C 0.948508 0.269406 -0.281991
H 1.140424 0.302258 -1.376233
C 0.337277 -1.096711 0.052664
H 1.038647 -1.899783 -0.232059
C -1.007914 -1.295398 -0.658175
H -0.829458 -1.309098 -1.750874
C -2.013973 -0.175350 -0.334738
H -2.890832 -0.302844 -0.998136
C -1.383072 1.194026 -0.647410
H -2.084927 2.002387 -0.370220
C 2.282126 0.488625 0.427453
O 3.253737 -0.519946 0.136189
C -2.521585 -0.258886 1.110219
H 0.394917 2.372889 -0.227226
H 0.204776 -1.165458 1.150164
H -1.441097 -2.277226 -0.391148
H -1.220102 1.269922 -1.739771
H 2.674102 1.494276 0.175772
H 2.129183 0.454587 1.520758

H 3.382197 -0.486292 -0.825259
H -3.001917 -1.235588 1.297442
H -1.709294 -0.140486 1.846419
H -3.269170 0.529619 1.307759
el energy= -388.49094872863
zpe= -388.258156
th energy= -388.248565
th enthalpy= -388.247621
free energy= -388.292263

4mchm_15/coords
c4
C -0.500378 -0.842758 1.079564
H -0.183388 -0.698505 2.130067
C -1.158212 0.455346 0.581917
H -1.935959 0.754933 1.313525
C -0.117043 1.584436 0.494362
H -0.582789 2.495861 0.075107
C 1.113485 1.185353 -0.332621
H 0.830089 1.029988 -1.391909
C 1.763591 -0.101173 0.195372
H 2.098536 0.093486 1.235574
C 0.726453 -1.231797 0.244457
H 1.188634 -2.145710 0.662144
C -1.884670 0.263665 -0.752695
O -2.885919 -0.756418 -0.693336
C 2.980871 -0.493913 -0.642068
H -1.244016 -1.658160 1.075422
H 0.213470 1.837767 1.519471
H 1.852413 2.008197 -0.321865
H 0.421496 -1.478529 -0.791483
H -2.328114 1.231322 -1.062467
H -1.189696 -0.048797 -1.548472
H -3.477973 -0.496899 0.030760
H 2.682544 -0.691871 -1.687669
H 3.736865 0.310695 -0.652358
H 3.460653 -1.407385 -0.248891
el energy= -388.49140100567
zpe= -388.258424
th energy= -388.248965
th enthalpy= -388.248021
free energy= -388.292202

4mchm_16/coords
c5
C -0.233435 1.262094 -0.204960
H -0.735828 2.159892 -0.611592
C -0.956779 0.000008 -0.698349
H -0.925308 0.000014 -1.807577
C -0.233438 -1.262087 -0.204976
H -0.321786 -1.320090 0.894519
C 1.243852 -1.258260 -0.620505
H 1.751410 -2.163857 -0.239253
C 1.985878 -0.000001 -0.133685
H 2.993277 -0.000001 -0.592268
C 1.243857 1.258268 -0.620486
H 1.299615 1.299046 -1.725626
C -2.430423 0.000005 -0.307867
O -2.527733 -0.000022 1.121086
C 2.178994 -0.000011 1.387733
H -0.321786 1.320084 0.894535
H -0.735836 -2.159877 -0.611617
H 1.299609 -1.299021 -1.725645
H 1.751417 2.163857 -0.239220
H -2.928275 0.894877 -0.731257
H -2.928274 -0.894854 -0.731288
H -3.475084 0.000054 1.326674
H 2.744130 -0.892736 1.709398
H 2.744155 0.892697 1.709404
H 1.219396 0.000002 1.930691
el energy= -388.48979028194
zpe= -388.256889
th energy= -388.247347
th enthalpy= -388.246403
free energy= -388.290849

4mchm_17/coords
c6
C -0.237024 1.269271 -0.163400
H -0.738963 2.181732 -0.536676
C -0.962682 0.026855 -0.698349
H -0.936350 0.060219 -1.807644
C -0.237506 -1.251434 -0.250961
H -0.309536 -1.348040 0.849094

C 1.238974 -1.233537 -0.669907
H 1.746286 -2.153139 -0.323720
C 1.982725 0.005569 -0.138693
H 2.988871 0.021097 -0.599652
C 1.240456 1.281019 -0.577843
H 1.747893 2.171707 -0.162667
C -2.439205 0.017022 -0.299398
O -2.643674 0.039069 1.117833
C 2.180198 -0.048110 1.381328
H -0.328134 1.285675 0.937507
H -0.741566 -2.136659 -0.682300
H 1.290806 -1.233320 -1.775897
H 1.296870 1.363654 -1.680545
H -2.934968 0.923944 -0.685796
H -2.942707 -0.860631 -0.751216
H -2.300000 -0.804065 1.450752
H 2.753919 0.828618 1.730375
H 1.222506 -0.057586 1.927651
H 2.738845 -0.955683 1.671400
el energy= -388.49102016815
zpe= -388.257962
th energy= -388.248442
th enthalpy= -388.247498
free energy= -388.291920

4mchm_23/coords
c7
C 0.447796 -1.264009 -0.945741
H 1.068865 -2.158751 -0.752777
C 1.317730 0.003191 -0.831055
H 2.006357 0.006351 -1.699231
C 0.447496 1.270942 -0.936812
H 1.068398 2.164461 -0.737755
C -0.783362 1.257617 -0.019279
H -0.467988 1.297642 1.037976
C -1.637164 0.000807 -0.234849
H -1.980893 0.004690 -1.290552
C -0.783356 -1.257540 -0.028465
H -0.468381 -1.305498 1.028574
C 2.264146 -0.000900 0.368406
O 1.550185 -0.006541 1.609863
C -2.865007 -0.002425 0.676327

H 0.094847 -1.343174 -1.992261
H 0.094254 1.357317 -1.982667
H -1.396198 2.158535 -0.211544
H -1.396046 -2.157033 -0.227732
H 2.918124 -0.893401 0.299386
H 2.916694 0.893175 0.306545
H 2.229370 -0.008393 2.302740
H -3.491342 0.891339 0.508757
H -3.491098 -0.895264 0.503000
H -2.556122 -0.005773 1.737441
el energy= -388.48795127616
zpe= -388.255343
th energy= -388.245700
th enthalpy= -388.244756
free energy= -388.289416

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.342090 -1.092986 0.025430
H 1.032798 -1.897641 -0.286739
C 0.948699 0.279829 -0.296262
H 1.136254 0.325605 -1.389002
C -0.038136 1.395928 0.070937
H -0.175076 1.407421 1.169459
C -1.390447 1.201779 -0.628288
H -1.236050 1.291925 -1.720785
C -2.016188 -0.172546 -0.328048
H -2.897987 -0.294008 -0.985996
C -1.010320 -1.285484 -0.674613
H -1.437378 -2.272050 -0.415466
C 2.285653 0.495951 0.409791
O 3.294897 -0.438199 0.015141
C -2.511646 -0.276179 1.119685
H 0.223251 -1.181193 1.123134
H 0.388224 2.378252 -0.205524
H -2.091430 2.005281 -0.335211
H -0.841273 -1.285273 -1.768757
H 2.681533 1.493772 0.154461
H 2.129861 0.468649 1.507536
H 3.010949 -1.298934 0.357786
H -3.256025 0.510773 1.334833
H -2.992297 -1.254621 1.296883

H -1.692750 -0.170112 1.850468
el energy= -388.49058842097
zpe= -388.257649
th energy= -388.248091
th enthalpy= -388.247147
free energy= -388.291687

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.498887 -0.818438 1.099557
H 1.239426 -1.638433 1.133862
C 1.160789 0.473894 0.589538
H 1.933060 0.780640 1.320973
C 0.112223 1.595101 0.483328
H -0.224694 1.857635 1.504133
C -1.113419 1.182986 -0.345174
H -0.825478 1.020535 -1.401952
C -1.759828 -0.102571 0.189515
H -2.102627 0.098455 1.225919
C -0.716278 -1.226242 0.256673
H -1.175622 -2.139107 0.679536
C 1.895745 0.271991 -0.739740
O 2.968160 -0.671647 -0.637797
C -2.969182 -0.509669 -0.652479
H 0.168565 -0.654854 2.143030
H 0.575487 2.504525 0.056792
H -1.856202 2.002410 -0.343196
H -0.399954 -1.480733 -0.774088
H 1.196992 -0.022066 -1.544483
H 2.360861 1.226361 -1.041186
H 2.550264 -1.538133 -0.521127
H -3.730308 0.289879 -0.672667
H -2.663359 -0.712811 -1.694887
H -3.445316 -1.423441 -0.255594
el energy= -388.49068111473
zpe= -388.257616
th energy= -388.248156
th enthalpy= -388.247212
free energy= -388.291506

MP2 cc-pwCVDZ gas phase

4mchm_1/coords
t1
C 0.155044 1.429645 0.180649
H 0.546298 2.367637 -0.253019
C 1.032977 0.245316 -0.238045
H 1.025314 0.178059 -1.344319
C 0.465529 -1.062844 0.323590
H 1.095061 -1.906298 -0.000687
C -0.991564 -1.267543 -0.100876
H -1.387662 -2.205427 0.328257
C -1.880094 -0.088141 0.314357
H -1.857226 -0.023146 1.421320
C -1.303596 1.220729 -0.240598
H -1.922889 2.074387 0.088647
C 2.479399 0.455523 0.185774
O 3.249230 -0.631020 -0.316584
C -3.328944 -0.291898 -0.128917
H 0.202947 1.540928 1.281642
H 0.521529 -1.023862 1.429752
H -1.040415 -1.376320 -1.202176
H -1.362378 1.191503 -1.346224
H 2.842926 1.425051 -0.211437
H 2.526446 0.509609 1.293609
H 4.148135 -0.513767 0.017554
H -3.388104 -0.360721 -1.229050
H -3.748099 -1.221420 0.290762
H -3.968236 0.547217 0.192437
el energy= -388.51842502580
zpe= -388.285427
th energy= -388.275764
th enthalpy= -388.274820
free energy= -388.319543

4mchm_3/coords
t2
C -0.154702 1.430922 0.179689
H -0.202298 1.542509 1.280503
C -1.034577 0.245929 -0.232716
H -1.014917 0.181393 -1.342559
C -0.465486 -1.061147 0.327885

H -0.520043 -1.019258 1.433613
C 0.990200 -1.268296 -0.099466
H 1.386640 -2.205356 0.330910
C 1.879705 -0.088117 0.312226
H 1.858459 -0.021749 1.419022
C 1.303234 1.220673 -0.243332
H 1.923334 2.074152 0.084629
C -2.486461 0.457383 0.193095
O -3.342897 -0.616205 -0.178196
C 3.327703 -0.293281 -0.133083
H -0.547547 2.368595 -0.253248
H -1.098039 -1.906686 0.013448
H 1.038342 -1.379157 -1.200846
H 1.361518 1.190955 -1.349131
H -2.540764 0.515083 1.293466
H -2.853048 1.425120 -0.206220
H -3.306304 -0.660433 -1.144170
H 3.967695 0.546002 0.186189
H 3.747082 -1.222283 0.287407
H 3.385370 -0.363638 -1.233230
el energy= -388.51933734886
zpe= -388.286126
th energy= -388.276569
th enthalpy= -388.275625
free energy= -388.320103

4mchm_5/coords
t3
C 0.394098 -1.259997 0.041380
H 0.827917 -2.159519 0.515102
C 1.032463 0.000009 0.640577
H 0.840464 0.000039 1.733379
C 0.394101 1.260005 0.041340
H 0.827955 2.159518 0.515062
C -1.128096 1.254356 0.210762
H -1.379688 1.287774 1.289426
C -1.764898 -0.000012 -0.399607
H -1.535927 -0.000018 -1.484591
C -1.128120 -1.254372 0.210756
H -1.566518 -2.159847 -0.246168
C 2.545974 0.000015 0.457696
O 2.818680 -0.000008 -0.940915

C -3.283616 0.000014 -0.223088
H 0.651351 -1.306420 -1.031208
H 0.651352 1.306409 -1.031247
H -1.566553 2.159818 -0.246133
H -1.379750 -1.287816 1.289412
H 2.976749 0.895930 0.949329
H 2.976762 -0.895873 0.949360
H 3.780099 -0.000114 -1.036906
H -3.545776 0.000069 0.849319
H -3.739635 0.892541 -0.682904
H -3.739684 -0.892531 -0.682814
el energy= -388.51872784200
zpe= -388.285630
th energy= -388.276014
th enthalpy= -388.275069
free energy= -388.319652

4mchm_6/coords
t4
C 0.154475 1.425639 0.181708
H 0.210956 1.522447 1.283721
C 1.035929 0.251869 -0.259055
H 1.027929 0.198584 -1.365750
C 0.468725 -1.065645 0.282421
H 1.071676 -1.916510 -0.081307
C -0.995087 -1.263903 -0.124603
H -1.056381 -1.355736 -1.226560
C -1.877440 -0.090555 0.318408
H -1.839711 -0.039045 1.425629
C -1.307681 1.223874 -0.229231
H -1.378116 1.206792 -1.334319
C 2.485564 0.469215 0.175360
O 3.372322 -0.544136 -0.281151
C -3.331507 -0.292149 -0.108289
H 0.544094 2.369338 -0.240702
H 0.542869 -1.058858 1.388664
H -1.384588 -2.208383 0.295746
H -1.923048 2.073750 0.116288
H 2.861135 1.412775 -0.253066
H 2.520255 0.573495 1.280357
H 3.142719 -1.343227 0.210918
H -3.967004 0.542510 0.231128

H -3.404996 -0.348148 -1.208223
H -3.744238 -1.226763 0.306371
el energy= -388.51873941014
zpe= -388.285579
th energy= -388.275944
th enthalpy= -388.275000
free energy= -388.319697

4mchm_7/coords
t5
C 0.391884 1.263611 -0.021984
H 0.657815 1.296098 1.049520
C 1.034466 0.015691 -0.638497
H 0.838812 0.021714 -1.730544
C 0.394303 -1.251386 -0.055584
H 0.619933 -1.305021 1.027206
C -1.127636 -1.250109 -0.231074
H -1.371383 -1.266682 -1.311404
C -1.769050 -0.007124 0.398130
H -1.545888 -0.026745 1.484218
C -1.130948 1.259279 -0.186226
H -1.569375 2.154371 0.290355
C 2.554771 0.019578 -0.457975
O 2.956652 0.055578 0.907348
C -3.286627 -0.007260 0.214158
H 0.823332 2.170583 -0.482605
H 0.834986 -2.150102 -0.525546
H -1.565009 -2.164477 0.208490
H -1.385699 1.315490 -1.263029
H 2.993164 -0.853260 -0.983369
H 2.978823 0.928202 -0.915696
H 2.704100 -0.797986 1.283846
H -3.743736 -0.908223 0.656028
H -3.746157 0.876325 0.687185
H -3.543908 0.011408 -0.859128
el energy= -388.51918658961
zpe= -388.285939
th energy= -388.276370
th enthalpy= -388.275426
free energy= -388.319944

4mchm_19/coords

t6
C 0.280292 -1.067614 0.692281
H -0.310556 -1.192301 1.617167
C 0.924262 0.329304 0.703820
H 1.438399 0.465305 1.673236
C -0.148316 1.421510 0.555741
H -0.762035 1.440018 1.473575
C -1.057043 1.196109 -0.662649
H -1.840296 1.975057 -0.693109
C -1.709091 -0.198534 -0.659664
H -2.214889 -0.337130 -1.633599
C -0.623269 -1.282139 -0.529659
H -0.006351 -1.284715 -1.446887
C 2.010205 0.464914 -0.361374
O 3.000775 -0.523224 -0.095618
C -2.781832 -0.327000 0.428670
H 1.075019 -1.829959 0.715887
H 0.330698 2.415419 0.487713
H -0.468575 1.313662 -1.590687
H -1.096130 -2.279305 -0.474849
H 1.584813 0.339157 -1.375613
H 2.436341 1.487589 -0.307098
H 3.653062 -0.460408 -0.805646
H -3.568759 0.433923 0.292649
H -3.260470 -1.319869 0.387918
H -2.367718 -0.199956 1.441292
el energy= -388.51312193328
zpe= -388.279483
th energy= -388.269969
th enthalpy= -388.269025
free energy= -388.313469

4mchm_21/coords
t7
C 0.145922 1.422799 0.552805
H -0.336812 2.414461 0.477858
C -0.924984 0.327779 0.693906
H -1.432202 0.469598 1.670321
C -0.284737 -1.070328 0.684673
H 0.295847 -1.205758 1.614418
C 0.627319 -1.281613 -0.531613
H 0.015590 -1.281183 -1.451921

C 1.714000 -0.198088 -0.650468
H 2.228366 -0.336712 -1.619738
C 1.060565 1.195604 -0.660502
H 0.476351 1.310253 -1.591467
C -2.012629 0.465171 -0.377771
O -3.026297 -0.527264 -0.267893
C 2.776526 -0.325941 0.447842
H 0.754372 1.446832 1.474008
H -1.082284 -1.830888 0.689563
H 1.098493 -2.279345 -0.475544
H 1.842476 1.975821 -0.688337
H -2.439525 1.487903 -0.327063
H -1.593614 0.340948 -1.387937
H -3.402104 -0.423836 0.618193
H 2.353032 -0.199932 1.456794
H 3.256619 -1.318225 0.410975
H 3.563871 0.435879 0.319795
el energy= -388.51431798368
zpe= -388.280425
th energy= -388.271029
th enthalpy= -388.270085
free energy= -388.314211

4mchm_22/coords
t8
C 0.147024 1.431230 0.544713
H -0.333913 2.423040 0.461923
C -0.927894 0.342928 0.709311
H -1.437370 0.487512 1.679647
C -0.274150 -1.049479 0.716415
H 0.327693 -1.155691 1.636067
C 0.615642 -1.285789 -0.511857
H 1.085850 -2.283703 -0.450019
C 1.702653 -0.205372 -0.659061
H 2.201746 -0.356805 -1.634297
C 1.053173 1.190340 -0.673276
H 1.838688 1.966349 -0.712765
C -2.021193 0.472134 -0.358731
O -3.088168 -0.451508 -0.174087
C 2.781269 -0.325971 0.424407
H 0.762555 1.465307 1.461058
H -1.052772 -1.830386 0.784809

H -0.006095 -1.292921 -1.426505
H 0.463713 1.300488 -1.601134
H -2.475625 1.473683 -0.281570
H -1.595099 0.389726 -1.376941
H -2.734098 -1.320629 -0.403481
H 3.572149 0.427115 0.270447
H 2.375732 -0.178587 1.437737
H 3.253044 -1.322559 0.396194
el energy= -388.51294889009
zpe= -388.279264
th energy= -388.269741
th enthalpy= -388.268797
free energy= -388.313290

4mchm_24/coords
t9
C -0.103978 1.268396 0.773018
H 0.613104 1.366562 1.608287
C -0.946127 -0.000719 1.007964
H -1.253146 -0.001335 2.072568
C -0.103803 -1.269471 0.771610
H 0.613206 -1.368492 1.606839
C 0.662801 -1.258293 -0.559249
H 1.298807 -2.160244 -0.624425
C 1.533130 0.000450 -0.721399
H 1.934467 0.001040 -1.752134
C 0.662457 1.258781 -0.557940
H -0.061441 1.302161 -1.386072
C -2.271496 -0.000349 0.248877
O -2.051104 0.001027 -1.160526
C 2.735354 0.000135 0.231117
H -0.757080 2.158775 0.824067
H -0.756794 -2.159993 0.821603
H -0.060991 -1.301062 -1.387493
H 1.298196 2.160979 -0.622281
H -2.851643 -0.895348 0.554337
H -2.852050 0.893828 0.555969
H -2.924826 0.001157 -1.575229
H 2.431262 -0.000425 1.290104
H 3.363980 -0.891420 0.066601
H 3.363754 0.892012 0.067482
el energy= -388.51291684276

zpe= -388.279089
th energy= -388.269661
th enthalpy= -388.268717
free energy= -388.312720

4mchm_9/coords
c1
C -0.501861 -0.827607 1.089846
H -1.252571 -1.633457 1.093993
C -1.154994 0.470249 0.587312
H -1.927235 0.773986 1.318000
C -0.108449 1.591039 0.481431
H -0.568670 2.503921 0.061371
C 1.116573 1.180624 -0.347415
H 0.831189 1.020807 -1.404714
C 1.761680 -0.104636 0.187190
H 2.101149 0.097975 1.223627
C 0.718938 -1.228047 0.253060
H 1.178683 -2.140079 0.674713
C -1.892967 0.264700 -0.733435
O -2.896419 -0.722434 -0.516933
C 2.975140 -0.510545 -0.649065
H -0.178375 -0.674661 2.136338
H 0.229535 1.850890 1.501508
H 1.858484 1.999603 -0.347811
H 0.408540 -1.487323 -0.777359
H -2.338650 1.230883 -1.047028
H -1.191770 -0.048404 -1.530752
H -3.319842 -0.879982 -1.371016
H 2.672158 -0.721175 -1.689619
H 3.732049 0.291164 -0.673210
H 3.452311 -1.419344 -0.246126
el energy= -388.51601008649
zpe= -388.282687
th energy= -388.273118
th enthalpy= -388.272174
free energy= -388.316792

4mchm_11/coords
c2
C -0.342990 -1.091342 0.054885
H -1.053637 -1.883865 -0.228065

C -0.946424 0.277142 -0.281786
H -1.139479 0.308141 -1.373036
C 0.039906 1.398498 0.064306
H -0.384057 2.378453 -0.220545
C 1.385936 1.192415 -0.642722
H 1.222518 1.270796 -1.733862
C 2.011809 -0.179107 -0.332979
H 2.884923 -0.308944 -0.999491
C 1.001405 -1.294877 -0.653425
H 0.823921 -1.311744 -1.745212
C -2.283851 0.486016 0.413252
O -3.175893 -0.530514 -0.029835
C 2.526756 -0.264053 1.108888
H -0.212630 -1.161084 1.151900
H 0.186271 1.426990 1.160643
H 2.090222 1.998025 -0.367759
H 1.430594 -2.277486 -0.387117
H -2.130280 0.441878 1.511969
H -2.671359 1.496604 0.171110
H -3.995513 -0.419327 0.469447
H 3.005402 -1.240252 1.294593
H 3.275515 0.522368 1.303035
H 1.719445 -0.144604 1.848556
el energy= -388.51577032423
zpe= -388.282461
th energy= -388.272874
th enthalpy= -388.271930
free energy= -388.316490

4mchm_13/coords
c3
C -0.040650 1.399280 0.066011
H -0.190017 1.426013 1.161819
C 0.947543 0.277706 -0.273604
H 1.130882 0.313290 -1.370088
C 0.342641 -1.090310 0.058699
H 1.055673 -1.885156 -0.213173
C -0.997939 -1.295453 -0.655937
H -0.816938 -1.312087 -1.747401
C -2.009647 -0.179663 -0.339064
H -2.880179 -0.309955 -1.008753
C -1.383837 1.192505 -0.646314

H -2.089852 1.997193 -0.373554
C 2.288899 0.487397 0.426458
O 3.243287 -0.524544 0.127536
C -2.529360 -0.265112 1.101057
H 0.384921 2.379623 -0.214992
H 0.207953 -1.158424 1.154907
H -1.427964 -2.277993 -0.391362
H -1.217066 1.271894 -1.737023
H 2.679720 1.497023 0.185018
H 2.142628 0.445340 1.519190
H 3.380266 -0.482669 -0.829539
H -3.007501 -1.241772 1.285074
H -1.725055 -0.144499 1.843734
H -3.279671 0.520433 1.292021
el energy= -388.51668304231
zpe= -388.283156
th energy= -388.273676
th enthalpy= -388.272732
free energy= -388.317043

4mchm_15/coords
c4
C -0.505795 -0.838076 1.077854
H -0.192793 -0.700230 2.129510
C -1.155423 0.463064 0.580811
H -1.923153 0.770345 1.320259
C -0.112579 1.588567 0.486808
H -0.574511 2.500276 0.065979
C 1.116273 1.183188 -0.338385
H 0.835184 1.026624 -1.397216
C 1.761252 -0.102461 0.195004
H 2.092443 0.095687 1.235055
C 0.721073 -1.228745 0.245311
H 1.179259 -2.143261 0.662870
C -1.893097 0.264527 -0.747927
O -2.873394 -0.765022 -0.687421
C 2.981679 -0.501047 -0.634598
H -1.253743 -1.647059 1.060076
H 0.219851 1.847382 1.509001
H 1.855889 2.004049 -0.332663
H 0.415809 -1.480242 -0.788213
H -2.339029 1.231303 -1.059887

H -1.199070 -0.042151 -1.545219
H -3.490362 -0.501614 0.010435
H 2.686470 -0.707204 -1.678163
H 3.736493 0.302782 -0.649025
H 3.458120 -1.410610 -0.232698
el energy= -388.51717341125
zpe= -388.283596
th energy= -388.274142
th enthalpy= -388.273198
free energy= -388.317502

4mchm_16/coords
c5
C -0.238733 1.262257 -0.217715
H -0.736218 2.158271 -0.632029
C -0.960104 0.000002 -0.709903
H -0.938168 -0.000004 -1.819238
C -0.238732 -1.262254 -0.217711
H -0.345112 -1.322907 0.878160
C 1.240364 -1.256494 -0.622074
H 1.744436 -2.162768 -0.240912
C 1.977557 -0.000001 -0.127623
H 2.988012 -0.000003 -0.577742
C 1.240366 1.256496 -0.622072
H 1.307160 1.295954 -1.725966
C -2.426976 -0.000002 -0.295584
O -2.479864 -0.000020 1.128651
C 2.155516 -0.000001 1.395303
H -0.345114 1.322914 0.878158
H -0.736225 -2.158262 -0.632029
H 1.307152 -1.295949 -1.725968
H 1.744439 2.162766 -0.240904
H -2.928555 0.895904 -0.714716
H -2.928556 -0.895901 -0.714739
H -3.414710 0.000127 1.372735
H 2.716904 -0.891602 1.721815
H 2.716916 0.891594 1.721810
H 1.191009 0.000009 1.926632
el energy= -388.51642870566
zpe= -388.282988
th energy= -388.273451
th enthalpy= -388.272507

free energy= -388.316929

4mchm_17/coords
c6
C -0.236843 1.275180 -0.139508
H -0.733078 2.195852 -0.496281
C -0.965200 0.048296 -0.701720
H -0.939089 0.102184 -1.809879
C -0.242878 -1.238750 -0.279830
H -0.311341 -1.349815 0.818400
C 1.233075 -1.219134 -0.696377
H 1.735820 -2.147701 -0.371427
C 1.980021 0.005176 -0.139094
H 2.983611 0.027107 -0.603347
C 1.241356 1.291595 -0.547661
H 1.749384 2.170317 -0.111421
C -2.439406 0.034132 -0.290137
O -2.625784 0.001087 1.121465
C 2.182768 -0.083367 1.378228
H -0.345231 1.270043 0.958484
H -0.747075 -2.117691 -0.722822
H 1.285768 -1.197600 -1.801111
H 1.303419 1.402369 -1.646813
H -2.927486 0.961515 -0.631997
H -2.955374 -0.814755 -0.783311
H -2.336587 -0.875061 1.409328
H 2.766888 0.778189 1.742668
H 1.228091 -0.090477 1.927365
H 2.731197 -1.001947 1.647033
el energy= -388.51674207889
zpe= -388.283187
th energy= -388.273693
th enthalpy= -388.272749
free energy= -388.317104

4mchm_23/coords
c7
C 0.465135 -1.263555 -0.948556
H 1.082912 -2.159480 -0.755493
C 1.333262 0.001952 -0.820486
H 2.041514 0.003912 -1.672473
C 0.465044 1.267974 -0.942811

H 1.082751 2.163056 -0.745658
C -0.768206 1.256648 -0.030333
H -0.449403 1.291897 1.024215
C -1.621013 0.000530 -0.248464
H -1.965550 0.002867 -1.303664
C -0.768056 -1.256448 -0.035961
H -0.449196 -1.296365 1.018409
C 2.241172 -0.000828 0.407576
O 1.472258 -0.003918 1.609086
C -2.850081 -0.001577 0.660888
H 0.122762 -1.338032 -1.998254
H 0.122726 1.347201 -1.992177
H -1.378484 2.157538 -0.225604
H -1.378234 -2.156531 -0.235222
H 2.895962 -0.895060 0.358439
H 2.895601 0.893894 0.362772
H 2.105467 -0.005337 2.340151
H -3.475038 0.891424 0.492240
H -3.474923 -0.893899 0.488267
H -2.540482 -0.003916 1.720248
el energy= -388.51581222162
zpe= -388.282303
th energy= -388.272812
th enthalpy= -388.271868
free energy= -388.316062

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.347979 -1.088165 0.011785
H 1.038157 -1.884927 -0.318243
C 0.948906 0.287820 -0.301342
H 1.139065 0.335477 -1.392160
C -0.041451 1.397732 0.069849
H -0.175016 1.411107 1.168086
C -1.395835 1.201495 -0.623024
H -1.248119 1.295345 -1.715082
C -2.014500 -0.175009 -0.322791
H -2.897872 -0.298712 -0.976573
C -1.007882 -1.282504 -0.678960
H -1.429544 -2.271235 -0.423951
C 2.289190 0.497981 0.403021
O 3.282246 -0.447395 0.026518

C -2.503951 -0.284496 1.126209
H 0.237166 -1.192315 1.108802
H 0.379351 2.382036 -0.204195
H -2.097257 2.001800 -0.326622
H -0.845218 -1.278010 -1.772924
H 2.696738 1.485936 0.133057
H 2.124329 0.499923 1.501310
H 2.998481 -1.294852 0.393572
H -3.251071 0.496692 1.345320
H -2.977139 -1.264664 1.304843
H -1.684757 -0.173563 1.854127
el energy= -388.51609038244
zpe= -388.282620
th energy= -388.273063
th enthalpy= -388.272119
free energy= -388.316648

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.499183 -0.808113 1.104810
H 1.243326 -1.623079 1.155279
C 1.161423 0.479890 0.588729
H 1.931616 0.785897 1.320249
C 0.112573 1.598449 0.475041
H -0.224947 1.870156 1.492318
C -1.112919 1.181586 -0.350795
H -0.828580 1.018134 -1.407443
C -1.757305 -0.102108 0.188172
H -2.099195 0.102737 1.223320
C -0.713032 -1.223707 0.262440
H -1.171691 -2.135195 0.686206
C 1.903367 0.269574 -0.736772
O 2.953709 -0.685715 -0.637815
C -2.967427 -0.515532 -0.649214
H 0.165618 -0.640833 2.145580
H 0.573604 2.505971 0.044549
H -1.856232 1.999032 -0.353470
H -0.399182 -1.483993 -0.767256
H 1.199304 0.004878 -1.548761
H 2.386648 1.216906 -1.027612
H 2.525778 -1.546963 -0.545342
H -3.725641 0.284517 -0.678108

H -2.661599 -0.729247 -1.688220
H -3.443684 -1.423435 -0.243244
el energy= -388.51584645608
zpe= -388.282472
th energy= -388.272897
th enthalpy= -388.271953
free energy= -388.316621

MP2-SMD cc-pwCVDZ

4mchm_1/coords
t1
C 0.157886 1.422119 0.180490
H 0.555505 2.356455 -0.254345
C 1.032322 0.235526 -0.239401
H 1.021790 0.172311 -1.346126
C 0.456431 -1.069457 0.322275
H 1.072084 -1.924103 -0.003000
C -1.001928 -1.267984 -0.100739
H -1.401151 -2.203594 0.330571
C -1.883741 -0.084821 0.315868
H -1.860292 -0.019950 1.422305
C -1.301036 1.219919 -0.240651
H -1.915986 2.076211 0.089749
C 2.474780 0.450862 0.192715
O 3.272893 -0.618831 -0.322706
C -3.331450 -0.281566 -0.130694
H 0.208298 1.530376 1.281210
H 0.514885 -1.029778 1.427763
H -1.052097 -1.374302 -1.202086
H -1.360077 1.188214 -1.346085
H 2.836022 1.425836 -0.187528
H 2.524687 0.482529 1.299007
H 4.166702 -0.480674 0.025484
H -3.388531 -0.345090 -1.231553
H -3.756612 -1.210871 0.284611
H -3.967952 0.559491 0.192478
el energy= -388.52302254750
zpe= -388.291103
th energy= -388.281287
th enthalpy= -388.280343
free energy= -388.325466

4mchm_3/coords
t2
C -0.158031 1.425666 0.178200
H -0.205448 1.537154 1.278842
C -1.035287 0.238626 -0.233665
H -1.026945 0.172654 -1.341847
C -0.460913 -1.065920 0.327610
H -0.516431 -1.025558 1.433303
C 0.995828 -1.268073 -0.098723
H 1.394963 -2.203399 0.333289
C 1.880293 -0.085259 0.313719
H 1.857993 -0.017469 1.420012
C 1.299737 1.219446 -0.245438
H 1.917304 2.075111 0.081781
C -2.480220 0.457420 0.202617
O -3.352821 -0.608868 -0.182845
C 3.327261 -0.286056 -0.133503
H -0.555504 2.359606 -0.257883
H -1.081231 -1.918289 0.004950
H 1.043355 -1.376309 -1.200052
H 1.356914 1.184826 -1.350901
H -2.531098 0.506356 1.303788
H -2.845274 1.424845 -0.193359
H -3.297915 -0.650380 -1.150807
H 3.965670 0.554684 0.186690
H 3.750853 -1.214971 0.284266
H 3.383362 -0.353015 -1.234214
el energy= -388.52445896860
zpe= -388.292195
th energy= -388.282537
th enthalpy= -388.281593
free energy= -388.326333

4mchm_5/coords
t3
C 0.387894 -1.259394 0.025456
H 0.825848 -2.158687 0.495375
C 1.026250 -0.000005 0.625295
H 0.822554 0.000012 1.714967
C 0.387907 1.259386 0.025435
H 0.825912 2.158660 0.495360

C -1.133159 1.254910 0.203669
H -1.375563 1.288008 1.284004
C -1.774020 -0.000004 -0.400749
H -1.556044 -0.000002 -1.487772
C -1.133193 -1.254926 0.203639
H -1.574196 -2.159129 -0.253393
C 2.541813 -0.000004 0.472234
O 2.864881 0.000013 -0.922296
C -3.289526 0.000025 -0.206740
H 0.629410 -1.306503 -1.051563
H 0.629410 1.306485 -1.051584
H -1.574213 2.159113 -0.253318
H -1.375639 -1.288066 1.283967
H 2.964696 0.894188 0.969614
H 2.964702 -0.894198 0.969595
H 3.832784 -0.000028 -0.973079
H -3.538725 0.000100 0.869052
H -3.751865 0.892576 -0.661212
H -3.751912 -0.892565 -0.661082
el energy= -388.52303448820
zpe= -388.290907
th energy= -388.281201
th enthalpy= -388.280257
free energy= -388.325071

4mchm_6/coords
t4
C 0.155540 1.424450 0.184358
H 0.211530 1.520150 1.286033
C 1.033984 0.247616 -0.253714
H 1.022429 0.194585 -1.360716
C 0.466256 -1.066642 0.294513
H 1.074293 -1.920298 -0.053887
C -0.995189 -1.265217 -0.119276
H -1.052716 -1.358233 -1.221380
C -1.877999 -0.090349 0.317873
H -1.845520 -0.037164 1.424688
C -1.305272 1.222336 -0.229760
H -1.372076 1.201834 -1.334984
C 2.479597 0.469141 0.182011
O 3.376353 -0.537040 -0.297874
C -3.328520 -0.288718 -0.118702

H 0.548074 2.365465 -0.241148
H 0.535773 -1.046855 1.399988
H -1.387214 -2.207461 0.303866
H -1.921036 2.072695 0.114181
H 2.848480 1.423589 -0.228206
H 2.522633 0.540486 1.286843
H 3.140644 -1.349712 0.174204
H -3.965931 0.544967 0.221235
H -3.395030 -0.338041 -1.219747
H -3.745540 -1.225386 0.288215
el energy= -388.52403263044
zpe= -388.292083
th energy= -388.282219
th enthalpy= -388.281275
free energy= -388.326780

4mchm_7/coords
t5
C 0.391850 1.259817 -0.018518
H 0.640498 1.292682 1.057517
C 1.031060 0.007968 -0.630433
H 0.831190 0.013634 -1.720922
C 0.390988 -1.256922 -0.043362
H 0.623208 -1.314672 1.037567
C -1.130457 -1.250975 -0.219843
H -1.373163 -1.271984 -1.300278
C -1.770985 -0.003068 0.399384
H -1.552453 -0.015617 1.486086
C -1.129841 1.258463 -0.191170
H -1.568863 2.157100 0.278522
C 2.550621 0.008698 -0.469188
O 2.976905 0.072248 0.896223
C -3.286363 -0.001173 0.205771
H 0.828972 2.164652 -0.478573
H 0.829766 -2.153556 -0.517559
H -1.570750 -2.160430 0.227046
H -1.376652 1.305407 -1.269937
H 2.977843 -0.881837 -0.969423
H 2.974770 0.902384 -0.955713
H 2.672862 -0.750297 1.309358
H -3.748259 -0.900013 0.648125
H -3.749228 0.884831 0.672271

H -3.536215 0.012870 -0.869728
el energy= -388.52430581190
zpe= -388.292115
th energy= -388.282402
th enthalpy= -388.281458
free energy= -388.326244

4mchm_19/coords
t6
C 0.264562 -1.071736 0.700332
H -0.337431 -1.181769 1.619662
C 0.923313 0.318400 0.710106
H 1.435484 0.454958 1.681150
C -0.144987 1.415095 0.563464
H -0.763669 1.429788 1.477917
C -1.045058 1.197059 -0.661875
H -1.823909 1.980193 -0.695424
C -1.707170 -0.192229 -0.664826
H -2.206795 -0.327371 -1.642141
C -0.630803 -1.283979 -0.527912
H -0.007581 -1.291139 -1.440556
C 2.002673 0.457989 -0.359804
O 3.020769 -0.515585 -0.101608
C -2.785690 -0.314938 0.417288
H 1.043341 -1.851216 0.737594
H 0.341664 2.405098 0.498508
H -0.445196 1.309478 -1.582735
H -1.112890 -2.276675 -0.470001
H 1.583874 0.317280 -1.372306
H 2.422345 1.481770 -0.313729
H 3.658261 -0.434416 -0.827262
H -3.561744 0.458301 0.284740
H -3.278989 -1.300561 0.363811
H -2.373944 -0.203002 1.432997
el energy= -388.51822477486
zpe= -388.285199
th energy= -388.275723
th enthalpy= -388.274779
free energy= -388.319113

4mchm_21/coords
t7

C 0.139424 1.414881 0.558687
H -0.349847 2.403324 0.487116
C -0.927191 0.315092 0.690704
H -1.445809 0.448082 1.660734
C -0.274278 -1.076737 0.678357
H 0.311181 -1.203187 1.606098
C 0.638704 -1.281002 -0.538236
H 0.029071 -1.278820 -1.460122
C 1.717926 -0.189651 -0.650940
H 2.234999 -0.320934 -1.619630
C 1.054763 1.198972 -0.655371
H 0.466461 1.310794 -1.583960
C -2.005279 0.457945 -0.386535
O -3.044284 -0.517818 -0.259416
C 2.776220 -0.316389 0.450448
H 0.746898 1.432843 1.480586
H -1.061013 -1.849326 0.691593
H 1.118043 -2.275102 -0.481672
H 1.832983 1.983097 -0.678874
H -2.423420 1.482529 -0.341795
H -1.588855 0.316748 -1.395752
H -3.408955 -0.393459 0.631636
H 2.345664 -0.208879 1.458849
H 3.270920 -1.301583 0.402164
H 3.554222 0.457752 0.335674
el energy= -388.51970599662
zpe= -388.286740
th energy= -388.277199
th enthalpy= -388.276255
free energy= -388.321029

4mchm_22/coords
t8
C 0.149518 1.432053 0.545084
H -0.332538 2.423212 0.461015
C -0.925333 0.344332 0.711874
H -1.432731 0.494701 1.683092
C -0.273414 -1.048816 0.719816
H 0.332710 -1.148585 1.637330
C 0.611339 -1.285716 -0.511029
H 1.082057 -2.283341 -0.446191
C 1.698752 -0.206826 -0.661281

H 2.197184 -0.359163 -1.636611
C 1.050173 1.188728 -0.675704
H 1.836710 1.963733 -0.717270
C -2.012164 0.477201 -0.358919
O -3.085195 -0.453545 -0.175272
C 2.775204 -0.326889 0.423216
H 0.767721 1.461781 1.459617
H -1.052162 -1.829371 0.783689
H -0.017597 -1.293275 -1.420131
H 0.454066 1.295284 -1.599482
H -2.465771 1.479523 -0.284578
H -1.590052 0.381477 -1.375164
H -2.723699 -1.323273 -0.402829
H 3.562529 0.432333 0.277195
H 2.364976 -0.190535 1.436563
H 3.253711 -1.320555 0.387587
el energy= -388.51906398249
zpe= -388.285777
th energy= -388.276375
th enthalpy= -388.275431
free energy= -388.319464

4mchm_24/coords
t9
C -0.096183 1.269157 0.762307
H 0.622744 1.369985 1.595241
C -0.936879 0.000192 1.002074
H -1.233795 0.000358 2.068843
C -0.096223 -1.268868 0.762687
H 0.622728 -1.369457 1.595628
C 0.675883 -1.259021 -0.564527
H 1.314951 -2.159136 -0.624631
C 1.545397 -0.000123 -0.725889
H 1.955437 -0.000279 -1.753092
C 0.675980 1.258889 -0.564876
H -0.038657 1.310528 -1.401492
C -2.275541 0.000098 0.268674
O -2.106041 -0.000265 -1.153864
C 2.737304 -0.000039 0.237317
H -0.751228 2.158215 0.809466
H -0.751290 -2.157895 0.810144
H -0.038789 -1.310823 -1.401106

H 1.315123 2.158936 -0.625199
H -2.850434 -0.892633 0.584028
H -2.850323 0.893055 0.583593
H -3.002872 -0.000389 -1.524242
H 2.421936 0.000120 1.292906
H 3.367154 -0.891913 0.077231
H 3.367222 0.891741 0.076986
el energy= -388.51631045335
zpe= -388.283535
th energy= -388.273960
th enthalpy= -388.273016
free energy= -388.317463

4mchm_9/coords
c1
C -0.488939 -0.834729 1.095626
H -1.229043 -1.651625 1.110010
C -1.152939 0.458564 0.594638
H -1.924845 0.761480 1.326876
C -0.110650 1.583617 0.492175
H -0.578511 2.494270 0.076633
C 1.109756 1.180716 -0.345381
H 0.814862 1.018568 -1.399309
C 1.764936 -0.100952 0.184207
H 2.110339 0.101181 1.218382
C 0.729275 -1.230099 0.252917
H 1.195380 -2.138862 0.674900
C -1.884365 0.259475 -0.729442
O -2.920004 -0.708106 -0.525706
C 2.972127 -0.499558 -0.662707
H -0.160361 -0.677870 2.139744
H 0.231168 1.837062 1.512440
H 1.847856 2.003064 -0.347076
H 0.415621 -1.486570 -0.776844
H -2.313449 1.227836 -1.052550
H -1.191875 -0.077004 -1.521653
H -3.337727 -0.839236 -1.390455
H 2.662785 -0.703350 -1.702949
H 3.727742 0.303885 -0.685548
H 3.454889 -1.410174 -0.269147
el energy= -388.52092315528
zpe= -388.288348

th energy= -388.278751
th enthalpy= -388.277807
free energy= -388.322455

4mchm_11/coords
c2
C -0.333433 -1.095827 0.050860
H -1.030260 -1.901022 -0.234620
C -0.945447 0.268372 -0.288870
H -1.131396 0.300833 -1.381543
C 0.036064 1.392782 0.061439
H -0.393478 2.369498 -0.225013
C 1.384611 1.194123 -0.641294
H 1.224501 1.271501 -1.732926
C 2.016431 -0.173536 -0.329691
H 2.893569 -0.299160 -0.991347
C 1.012942 -1.293186 -0.655425
H 0.837348 -1.307444 -1.747515
C -2.279083 0.483317 0.409713
O -3.194372 -0.526700 -0.025313
C 2.520993 -0.258079 1.114808
H -0.204050 -1.160568 1.147855
H 0.177134 1.416424 1.158129
H 2.083796 2.002308 -0.360844
H 1.445495 -2.273771 -0.386823
H -2.130080 0.435040 1.506501
H -2.666698 1.491855 0.168084
H -4.005374 -0.394903 0.488602
H 3.001044 -1.233925 1.301771
H 3.267223 0.529943 1.314251
H 1.707737 -0.140811 1.848697
el energy= -388.52061537221
zpe= -388.288032
th energy= -388.278417
th enthalpy= -388.277472
free energy= -388.322160

4mchm_13/coords
c3
C -0.036078 1.394209 0.059467
H -0.181133 1.420519 1.155678
C 0.947480 0.269251 -0.282322

H 1.139296 0.302198 -1.375496
C 0.336935 -1.095627 0.052356
H 1.037584 -1.898004 -0.232219
C -1.007187 -1.294302 -0.657841
H -0.828880 -1.307674 -1.749538
C -2.012392 -0.175411 -0.334329
H -2.888900 -0.302968 -0.996447
C -1.382307 1.192782 -0.647046
H -2.083612 2.000277 -0.369872
C 2.279372 0.488717 0.427225
O 3.251438 -0.519644 0.136283
C -2.518149 -0.258714 1.109978
H 0.394031 2.370737 -0.227115
H 0.204553 -1.163729 1.148845
H -1.439882 -2.275253 -0.390884
H -1.219385 1.268413 -1.738397
H 2.671046 1.493514 0.175989
H 2.125821 0.454088 1.519458
H 3.380265 -0.484706 -0.824985
H -2.997475 -1.234755 1.297615
H -1.705728 -0.139878 1.844455
H -3.265160 0.528953 1.307725
el energy= -388.52200909925
zpe= -388.289334
th energy= -388.279747
th enthalpy= -388.278803
free energy= -388.323432

4mchm_15/coords
c4
C -0.500036 -0.841003 1.079703
H -0.182765 -0.695842 2.128926
C -1.157200 0.455594 0.581564
H -1.934559 0.755444 1.311916
C -0.116813 1.583515 0.493412
H -0.582128 2.493878 0.073972
C 1.112381 1.183927 -0.333040
H 0.828822 1.027491 -1.391012
C 1.761943 -0.101052 0.195469
H 2.096731 0.094062 1.234479
C 0.725502 -1.230452 0.245149
H 1.187185 -2.143348 0.662986

C -1.881846 0.263305 -0.752319
O -2.883238 -0.756806 -0.692991
C 2.977698 -0.494240 -0.641766
H -1.243103 -1.655570 1.076397
H 0.213823 1.836877 1.517368
H 1.850756 2.005946 -0.323036
H 0.420645 -1.477040 -0.789724
H -2.324820 1.229805 -1.062789
H -1.186823 -0.049899 -1.546365
H -3.476283 -0.495195 0.029425
H 2.678533 -0.692303 -1.686093
H 3.733217 0.309526 -0.652812
H 3.456897 -1.406959 -0.248742
el energy= -388.52244544270
zpe= -388.289592
th energy= -388.280135
th enthalpy= -388.279191
free energy= -388.323368

4mchm_16/coords
c5
C -0.233105 1.260893 -0.204307
H -0.735164 2.157902 -0.610409
C -0.955575 0.000008 -0.697841
H -0.923221 0.000014 -1.806016
C -0.233109 -1.260886 -0.204323
H -0.321043 -1.318118 0.894153
C 1.242870 -1.257176 -0.619977
H 1.750121 -2.161829 -0.238941
C 1.984223 -0.000001 -0.133657
H 2.990787 -0.000001 -0.591563
C 1.242875 1.257184 -0.619959
H 1.298112 1.297782 -1.724109
C -2.428005 0.000005 -0.308682
O -2.525739 -0.000022 1.120321
C 2.176341 -0.000011 1.386637
H -0.321042 1.318112 0.894168
H -0.735172 -2.157887 -0.610434
H 1.298106 -1.297758 -1.724127
H 1.750127 2.161828 -0.238908
H -2.925176 0.894286 -0.731613
H -2.925176 -0.894264 -0.731643

H -3.473211 0.000053 1.324835
H 2.740795 -0.892024 1.708203
H 2.740820 0.891985 1.708209
H 1.217154 0.000002 1.928273
el energy= -388.52083365513
zpe= -388.288054
th energy= -388.278516
th enthalpy= -388.277572
free energy= -388.322005

4mchm_17/coords
c6
C -0.236293 1.268739 -0.160427
H -0.737530 2.181298 -0.531478
C -0.961503 0.028831 -0.697895
H -0.934337 0.064386 -1.806072
C -0.237647 -1.249312 -0.252707
H -0.309325 -1.346952 0.846184
C 1.237542 -1.231364 -0.671652
H 1.744135 -2.150861 -0.327298
C 1.981030 0.005408 -0.138619
H 2.986373 0.021435 -0.598814
C 1.239879 1.280799 -0.575000
H 1.747358 2.169629 -0.158536
C -2.436767 0.018552 -0.300095
O -2.641187 0.035960 1.117308
C 2.177404 -0.051110 1.380202
H -0.326982 1.282318 0.939463
H -0.741723 -2.132824 -0.685028
H 1.288944 -1.228991 -1.776635
H 1.295768 1.365155 -1.676576
H -2.931438 0.926424 -0.682930
H -2.940183 -0.856716 -0.754181
H -2.299325 -0.809395 1.446151
H 2.750509 0.824207 1.730777
H 1.220090 -0.061499 1.925137
H 2.735282 -0.958552 1.668529
el energy= -388.52208147724
zpe= -388.289161
th energy= -388.279637
th enthalpy= -388.278693
free energy= -388.323132

4mchm_23/coords
c7
C 0.447463 -1.262392 -0.945424
H 1.068315 -2.156152 -0.752770
C 1.316437 0.003835 -0.830584
H 2.003846 0.007677 -1.698460
C 0.447133 1.270726 -0.934652
H 1.067792 2.162985 -0.734566
C -0.782799 1.256378 -0.017944
H -0.467795 1.294767 1.038361
C -1.635847 0.000968 -0.234904
H -1.978689 0.005604 -1.289803
C -0.782790 -1.256291 -0.028961
H -0.468181 -1.304112 1.027066
C 2.262598 -0.001096 0.367065
O 1.549087 -0.007841 1.608748
C -2.863026 -0.002909 0.675310
H 0.094617 -1.341096 -1.990885
H 0.094006 1.358178 -1.979333
H -1.394951 2.156769 -0.209206
H -1.394796 -2.154984 -0.228498
H 2.915926 -0.892816 0.297141
H 2.914269 0.892472 0.305764
H 2.229088 -0.010225 2.300714
H -3.488650 0.890298 0.508380
H -3.488461 -0.894901 0.501299
H -2.554054 -0.007048 1.735388
el energy= -388.51895365231
zpe= -388.286467
th energy= -388.276824
th enthalpy= -388.275880
free energy= -388.320544

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.341945 -1.091744 0.024864
H 1.032105 -1.895449 -0.287405
C 0.947591 0.279981 -0.296651
H 1.134984 0.326076 -1.388319
C -0.038659 1.394697 0.070798
H -0.175342 1.405404 1.168284

C -1.389845 1.200494 -0.627851
H -1.235534 1.290394 -1.719343
C -2.014529 -0.172745 -0.327547
H -2.896076 -0.294354 -0.984058
C -1.009435 -1.284361 -0.674425
H -1.435844 -2.270129 -0.415393
C 2.282840 0.496228 0.409474
O 3.292244 -0.438114 0.015200
C -2.507819 -0.276308 1.119614
H 0.223382 -1.179547 1.121567
H 0.387028 2.376303 -0.205303
H -2.090404 2.003006 -0.334775
H -0.840657 -1.283683 -1.767579
H 2.678663 1.493078 0.154326
H 2.126541 0.468597 1.506112
H 3.008311 -1.298020 0.359714
H -3.251514 0.509826 1.335227
H -2.987493 -1.254084 1.297187
H -1.688634 -0.169960 1.848511
el energy= -388.52165425827
zpe= -388.288830
th energy= -388.279275
th enthalpy= -388.278331
free energy= -388.322862

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.498747 -0.816213 1.099815
H 1.238835 -1.635206 1.135208
C 1.159802 0.474572 0.589049
H 1.931532 0.781957 1.319231
C 0.111926 1.594476 0.481834
H -0.225025 1.857479 1.501394
C -1.112430 1.181462 -0.345873
H -0.824451 1.017723 -1.401321
C -1.758037 -0.102524 0.189685
H -2.100535 0.099084 1.224914
C -0.714983 -1.224765 0.257481
H -1.173661 -2.136681 0.680525
C 1.893102 0.271782 -0.739350
O 2.964976 -0.672654 -0.637179
C -2.965943 -0.510423 -0.651795

H 0.167998 -0.651522 2.141896
H 0.574707 2.502658 0.054683
H -1.854769 1.999953 -0.344742
H -0.398678 -1.479082 -0.772201
H 1.194405 -0.022338 -1.542654
H 2.358557 1.224768 -1.041141
H 2.545632 -1.538674 -0.522954
H -3.726695 0.288175 -0.672790
H -2.659451 -0.713863 -1.692930
H -3.441312 -1.423404 -0.254761
el energy= -388.52174281603
zpe= -388.288797
th energy= -388.279340
th enthalpy= -388.278396
free energy= -388.322677

MP2 aug-cc-pVDZ

4mchm_1/coords
t1
C 0.156102 1.427388 0.181781
H 0.551414 2.364718 -0.249067
C 1.032610 0.238478 -0.242081
H 1.026806 0.173621 -1.348009
C 0.462104 -1.069988 0.324519
H 1.084464 -1.918859 -0.000049
C -0.999209 -1.269275 -0.102833
H -1.398475 -2.206496 0.324366
C -1.884797 -0.085963 0.316773
H -1.860477 -0.019863 1.423305
C -1.305080 1.221627 -0.244769
H -1.922883 2.077377 0.081355
C 2.475022 0.459114 0.195380
O 3.272263 -0.626284 -0.313966
C -3.336652 -0.286981 -0.128930
H 0.201686 1.533198 1.283231
H 0.518450 -1.027676 1.430301
H -1.047725 -1.373663 -1.204532
H -1.361458 1.187022 -1.350298
H 2.843692 1.424850 -0.198402
H 2.524243 0.490849 1.301352
H 4.186316 -0.483844 -0.034017

H -3.392415 -0.356707 -1.229039
H -3.758441 -1.214828 0.291458
H -3.973907 0.554164 0.190744
el energy= -388.56882616745
zpe= -388.337859
th energy= -388.328085
th enthalpy= -388.327141
free energy= -388.372103

4mchm_3/coords
t2
C -0.158216 1.424429 0.182164
H -0.203589 1.531532 1.283394
C -1.034316 0.232046 -0.234067
H -1.020973 0.168720 -1.342970
C -0.456463 -1.072523 0.332442
H -0.507589 -1.024565 1.437908
C 1.002932 -1.270497 -0.101188
H 1.406088 -2.205829 0.326298
C 1.887366 -0.084136 0.313365
H 1.866876 -0.017177 1.419771
C 1.302553 1.221830 -0.247196
H 1.919120 2.079224 0.076851
C -2.480582 0.453025 0.209944
O -3.372282 -0.600952 -0.192262
C 3.337849 -0.282239 -0.137615
H -0.558114 2.359739 -0.248894
H -1.079895 -1.925839 0.020281
H 1.048704 -1.376728 -1.203042
H 1.357169 1.186994 -1.352935
H -2.533053 0.468703 1.310872
H -2.845385 1.429935 -0.160588
H -3.405739 -0.597920 -1.159175
H 3.974290 0.560628 0.178972
H 3.763497 -1.208587 0.282130
H 3.390115 -0.352824 -1.237867
el energy= -388.56858761740
zpe= -388.337593
th energy= -388.327842
th enthalpy= -388.326898
free energy= -388.371808

4mchm_5/coords
t3
C 0.391713 -1.261388 0.021134
H 0.832581 -2.162101 0.485437
C 1.025420 -0.000006 0.628903
H 0.818894 0.000007 1.719288
C 0.391717 1.261379 0.021119
H 0.832630 2.162073 0.485431
C -1.132756 1.256854 0.205481
H -1.374851 1.288593 1.286307
C -1.774702 -0.000005 -0.402033
H -1.557258 0.000001 -1.488988
C -1.132778 -1.256869 0.205456
H -1.575736 -2.161334 -0.248712
C 2.544242 0.000000 0.482355
O 2.860697 0.000023 -0.922726
C -3.294345 0.000019 -0.206367
H 0.636190 -1.298044 -1.054884
H 0.636190 1.298031 -1.054897
H -1.575760 2.161315 -0.248653
H -1.374905 -1.288648 1.286278
H 2.967665 0.897807 0.971388
H 2.967682 -0.897807 0.971366
H 3.822878 -0.000080 -1.012228
H -3.541235 0.000063 0.869524
H -3.755778 0.892480 -0.660603
H -3.755828 -0.892447 -0.660536
el energy= -388.56845711602
zpe= -388.337436
th energy= -388.327689
th enthalpy= -388.326745
free energy= -388.371624

4mchm_6/coords
t4
C 0.156941 1.423030 0.183591
H 0.210161 1.517281 1.285809
C 1.035624 0.241784 -0.258428
H 1.029754 0.189276 -1.364717
C 0.462445 -1.071959 0.294465
H 1.061118 -1.931654 -0.056030
C -1.003504 -1.266914 -0.121598

H -1.060304 -1.358207 -1.223739
C -1.883585 -0.087487 0.319353
H -1.849182 -0.032987 1.426179
C -1.307360 1.224622 -0.234572
H -1.373207 1.201168 -1.339742
C 2.480810 0.467688 0.188883
O 3.399466 -0.526816 -0.292731
C -3.339106 -0.285372 -0.115368
H 0.552022 2.364124 -0.238824
H 0.530400 -1.051313 1.400587
H -1.398488 -2.208857 0.298901
H -1.921459 2.077449 0.105561
H 2.855517 1.420980 -0.215621
H 2.519116 0.529941 1.294439
H 3.170567 -1.366482 0.128185
H -3.973089 0.552425 0.218773
H -3.405065 -0.343664 -1.215521
H -3.757177 -1.217306 0.299658
el energy= -388.56861590615
zpe= -388.337565
th energy= -388.327805
th enthalpy= -388.326861
free energy= -388.371791

4mchm_7/coords
t5
C 0.384316 1.270751 0.002066
H 0.634669 1.293135 1.077594
C 1.027180 0.025600 -0.626701
H 0.821618 0.039061 -1.717428
C 0.395493 -1.249650 -0.045932
H 0.615562 -1.303470 1.037651
C -1.129321 -1.252109 -0.232570
H -1.366181 -1.262227 -1.314482
C -1.777663 -0.011274 0.400869
H -1.562253 -0.034123 1.488091
C -1.140852 1.261841 -0.178073
H -1.588047 2.152988 0.297256
C 2.551840 0.030771 -0.478662
O 2.995274 0.040315 0.889892
C -3.296858 -0.015492 0.202942
H 0.819245 2.181173 -0.447759

H 0.843514 -2.143221 -0.518524
H -1.568020 -2.168659 0.200640
H -1.385707 1.317245 -1.257174
H 2.985702 -0.832664 -1.018217
H 2.969710 0.949454 -0.919797
H 2.793264 -0.825470 1.269710
H -3.754561 -0.919824 0.636861
H -3.763205 0.864477 0.675714
H -3.542319 0.006980 -0.872905
el energy= -388.56811533457
zpe= -388.337067
th energy= -388.327341
th enthalpy= -388.326397
free energy= -388.371239

4mchm_19/coords
t6
C 0.272090 -1.071183 0.704606
H -0.330838 -1.182872 1.623086
C 0.922951 0.326125 0.713206
H 1.438693 0.464919 1.681323
C -0.152674 1.421339 0.564912
H -0.772977 1.430740 1.478068
C -1.051528 1.198928 -0.665950
H -1.834646 1.977609 -0.700783
C -1.705661 -0.198265 -0.667196
H -2.206195 -0.336423 -1.643876
C -0.619907 -1.285662 -0.530402
H 0.006090 -1.288517 -1.441096
C 1.997575 0.467983 -0.364519
O 3.012131 -0.521561 -0.106392
C -2.784051 -0.325468 0.420708
H 1.057795 -1.842360 0.744672
H 0.324988 2.416227 0.506045
H -0.454654 1.317558 -1.588083
H -1.094616 -2.281908 -0.479039
H 1.574572 0.323608 -1.374187
H 2.429569 1.485292 -0.314433
H 3.694360 -0.434500 -0.785600
H -3.568034 0.437546 0.282507
H -3.263538 -1.317371 0.377207
H -2.370389 -0.199844 1.433136

el energy= -388.56356536277
zpe= -388.331984
th energy= -388.322361
th enthalpy= -388.321417
free energy= -388.366075

4mchm_21/coords
t7
C 0.144962 1.415976 0.566430
H -0.340596 2.406975 0.505660
C -0.925229 0.313230 0.701014
H -1.439834 0.451700 1.673604
C -0.270572 -1.081887 0.692107
H 0.320271 -1.203415 1.617223
C 0.635690 -1.286041 -0.534609
H 0.018484 -1.290783 -1.450991
C 1.715335 -0.191229 -0.657258
H 2.226267 -0.323924 -1.629184
C 1.050385 1.200717 -0.660406
H 0.455998 1.313573 -1.584873
C -1.997431 0.456849 -0.386838
O -3.054357 -0.510417 -0.265770
C 2.783394 -0.313306 0.441224
H 0.760111 1.428743 1.483139
H -1.055109 -1.856036 0.710931
H 1.115812 -2.279444 -0.480304
H 1.826858 1.985997 -0.692026
H -2.408342 1.484463 -0.363777
H -1.579562 0.288995 -1.389730
H -3.477428 -0.369921 0.593275
H 2.358265 -0.196752 1.450118
H 3.272812 -1.300383 0.397990
H 3.561646 0.457681 0.315120
el energy= -388.56362786514
zpe= -388.331986
th energy= -388.322405
th enthalpy= -388.321460
free energy= -388.365985

4mchm_22/coords
t8
C 0.149336 1.426251 0.556926

H -0.333051 2.418035 0.486647
C -0.926868 0.331943 0.716247
H -1.439541 0.476428 1.684970
C -0.265076 -1.060525 0.718672
H 0.344970 -1.160423 1.633464
C 0.618758 -1.287659 -0.520356
H 1.092555 -2.284017 -0.465471
C 1.704079 -0.200687 -0.665158
H 2.202449 -0.346548 -1.641611
C 1.048468 1.195688 -0.672512
H 1.831551 1.973984 -0.711698
C -2.006911 0.469947 -0.364812
O -3.111809 -0.431512 -0.178449
C 2.783923 -0.321432 0.421963
H 0.770034 1.449708 1.469788
H -1.033472 -1.851264 0.791802
H -0.007925 -1.291198 -1.431226
H 0.452427 1.308316 -1.595562
H -2.448576 1.477423 -0.309234
H -1.583016 0.348399 -1.377107
H -2.792520 -1.328040 -0.348501
H 3.571499 0.435277 0.271222
H 2.374545 -0.178839 1.433933
H 3.258292 -1.316294 0.390357
el energy= -388.56296669207
zpe= -388.331399
th energy= -388.321759
th enthalpy= -388.320815
free energy= -388.365490

4mchm_24/coords
t9
C -0.098023 1.275276 0.756083
H 0.618860 1.388235 1.589034
C -0.933266 0.000168 1.006652
H -1.219981 0.000313 2.077319
C -0.098058 -1.275023 0.756416
H 0.618845 -1.387775 1.589379
C 0.671342 -1.258572 -0.577054
H 1.302982 -2.163072 -0.645343
C 1.549064 -0.000107 -0.724497
H 1.969255 -0.000245 -1.747659

C 0.671428 1.258456 -0.577358
H -0.047326 1.292354 -1.410949
C -2.279271 0.000087 0.281934
O -2.092534 -0.000231 -1.148405
C 2.733206 -0.000033 0.255639
H -0.758813 2.160256 0.795983
H -0.758865 -2.159979 0.796574
H -0.047443 -1.292606 -1.410615
H 1.303137 2.162893 -0.645837
H -2.851538 -0.896728 0.587854
H -2.851450 0.897088 0.587475
H -2.968798 -0.000353 -1.557670
H 2.405030 0.000100 1.306821
H 3.363892 -0.891965 0.104096
H 3.363950 0.891820 0.103890
el energy= -388.56114802916
zpe= -388.329503
th energy= -388.319923
th enthalpy= -388.318979
free energy= -388.363342

4mchm_9/coords
c1
C -0.497788 -0.821348 1.109766
H -1.244110 -1.631108 1.135946
C -1.156230 0.472556 0.593903
H -1.931140 0.782417 1.319061
C -0.107753 1.596906 0.482196
H -0.569553 2.508904 0.062483
C 1.113617 1.179923 -0.355432
H 0.820369 1.012081 -1.408964
C 1.762776 -0.103436 0.186861
H 2.108289 0.105134 1.219761
C 0.718232 -1.228430 0.262717
H 1.180588 -2.138378 0.685459
C -1.877734 0.263090 -0.737093
O -2.902355 -0.728114 -0.530170
C 2.971308 -0.516239 -0.658959
H -0.163946 -0.650419 2.150268
H 0.235104 1.855566 1.500858
H 1.856196 1.997999 -0.365882
H 0.399938 -1.490973 -0.764107

H -2.327182 1.220645 -1.061448
H -1.178254 -0.071784 -1.523100
H -3.362122 -0.862884 -1.369691
H 2.657077 -0.732278 -1.694836
H 3.728332 0.284768 -0.693952
H 3.450697 -1.422903 -0.254257
el energy= -388.56645830937
zpe= -388.335194
th energy= -388.325516
th enthalpy= -388.324572
free energy= -388.369408

4mchm_11/coords
c2
C -0.337539 -1.098158 0.055776
H -1.041367 -1.896964 -0.227012
C -0.944694 0.270211 -0.288759
H -1.137976 0.301320 -1.379456
C 0.041131 1.396319 0.061690
H -0.386078 2.374993 -0.221697
C 1.389126 1.193461 -0.650067
H 1.224163 1.266857 -1.741264
C 2.018024 -0.177897 -0.331860
H 2.895968 -0.307778 -0.991952
C 1.010407 -1.299009 -0.655451
H 0.832664 -1.316015 -1.747157
C -2.275908 0.489451 0.418181
O -3.195167 -0.526320 -0.024722
C 2.520283 -0.256747 1.118571
H -0.207258 -1.162333 1.152642
H 0.189348 1.421815 1.157380
H 2.090849 2.001621 -0.376628
H 1.441612 -2.280031 -0.387281
H -2.126410 0.426063 1.513776
H -2.668283 1.495232 0.177024
H -4.038471 -0.384471 0.425705
H 2.999561 -1.230912 1.310869
H 3.263910 0.533042 1.316598
H 1.704126 -0.137664 1.847741
el energy= -388.56620296161
zpe= -388.334915
th energy= -388.325218

th enthalpy= -388.324274
free energy= -388.369072

4mchm_13/coords
c3
C -0.037364 1.393299 0.062019
H -0.187853 1.419445 1.157323
C 0.946824 0.262816 -0.279999
H 1.135592 0.295946 -1.374479
C 0.331062 -1.101822 0.061459
H 1.033862 -1.906392 -0.209009
C -1.013187 -1.299689 -0.657231
H -0.831108 -1.318571 -1.748445
C -2.018437 -0.174450 -0.339256
H -2.893200 -0.301688 -1.003980
C -1.383591 1.195052 -0.654461
H -2.083596 2.005489 -0.383391
C 2.279294 0.481116 0.437002
O 3.271391 -0.510342 0.120276
C -2.528649 -0.251152 1.108519
H 0.395576 2.370035 -0.219472
H 0.193791 -1.161273 1.157407
H -1.449232 -2.278804 -0.390117
H -1.214976 1.268837 -1.745237
H 2.664016 1.495960 0.220155
H 2.132232 0.401743 1.526593
H 3.477347 -0.422364 -0.820947
H -3.010337 -1.224375 1.299446
H -1.716615 -0.132094 1.842247
H -3.272332 0.539818 1.301381
el energy= -388.56598263241
zpe= -388.334668
th energy= -388.324997
th enthalpy= -388.324053
free energy= -388.368789

4mchm_15/coords
c4
C -0.494746 -0.846811 1.092458
H -0.173357 -0.696738 2.140023
C -1.156158 0.450985 0.591516
H -1.930072 0.754245 1.325506

C -0.115689 1.585065 0.501058
H -0.583808 2.498090 0.090557
C 1.108646 1.185025 -0.339833
H 0.816440 1.023904 -1.394620
C 1.766423 -0.097976 0.192658
H 2.104677 0.102615 1.229561
C 0.731009 -1.232347 0.248924
H 1.197619 -2.143159 0.664825
C -1.874193 0.256797 -0.750015
O -2.901784 -0.747397 -0.697324
C 2.982568 -0.491837 -0.651104
H -1.234474 -1.663963 1.091617
H 0.223502 1.834210 1.523426
H 1.844662 2.008901 -0.342655
H 0.421131 -1.485879 -0.782397
H -2.294687 1.224299 -1.085372
H -1.182557 -0.092464 -1.529828
H -3.558053 -0.455821 -0.048524
H 2.675849 -0.698530 -1.691034
H 3.733497 0.315336 -0.672530
H 3.466739 -1.399275 -0.253940
el energy= -388.56647457276
zpe= -388.335152
th energy= -388.325509
th enthalpy= -388.324565
free energy= -388.369285

4mchm_16/coords
c5
C -0.233548 1.264949 -0.206248
H -0.735995 2.160603 -0.614596
C -0.952645 0.000006 -0.703550
H -0.920517 0.000010 -1.812912
C -0.233548 -1.264940 -0.206258
H -0.327380 -1.322494 0.890636
C 1.245926 -1.259669 -0.623968
H 1.752955 -2.165299 -0.245588
C 1.984271 -0.000001 -0.129046
H 2.994813 -0.000001 -0.578945
C 1.245930 1.259677 -0.623950
H 1.305173 1.296773 -1.728338
C -2.428408 0.000002 -0.316345

O -2.514506 -0.000030 1.122163
C 2.158867 -0.000011 1.397970
H -0.327382 1.322496 0.890647
H -0.736005 -2.160584 -0.614617
H 1.305161 -1.296745 -1.728356
H 1.752962 2.165299 -0.245551
H -2.924876 0.897952 -0.730622
H -2.924875 -0.897938 -0.730658
H -3.449694 0.000122 1.365598
H 2.719044 -0.891864 1.724689
H 2.719063 0.891829 1.724693
H 1.192532 0.000000 1.924986
el energy= -388.56611861912
zpe= -388.334755
th energy= -388.325096
th enthalpy= -388.324152
free energy= -388.368848

4mchm_17/coords
c6
C -0.226008 1.283958 -0.114873
H -0.723368 2.208340 -0.459528
C -0.955643 0.062773 -0.695643
H -0.923831 0.133118 -1.803232
C -0.240538 -1.236740 -0.290168
H -0.305642 -1.366726 0.805614
C 1.237726 -1.214535 -0.713573
H 1.739866 -2.147956 -0.402463
C 1.986444 0.003237 -0.135962
H 2.993229 0.027634 -0.593146
C 1.253265 1.299867 -0.533877
H 1.767015 2.171762 -0.091186
C -2.437306 0.046140 -0.308188
O -2.656043 -0.019604 1.112587
C 2.174916 -0.105618 1.385581
H -0.321864 1.267896 0.983778
H -0.750525 -2.104334 -0.748264
H 1.287677 -1.175273 -1.817918
H 1.310531 1.418252 -1.632484
H -2.920888 0.982803 -0.627850
H -2.951136 -0.792145 -0.816353
H -2.399372 -0.903754 1.407624

H 2.755389 0.750898 1.766263
H 1.214159 -0.119969 1.922818
H 2.719973 -1.028207 1.645861
el energy= -388.56569767725
zpe= -388.334312
th energy= -388.324676
th enthalpy= -388.323731
free energy= -388.368377

4mchm_23/coords
c7
C 0.454064 -1.271127 -0.938823
H 1.075595 -2.162202 -0.736320
C 1.322328 0.000465 -0.831621
H 2.011928 0.000932 -1.699412
C 0.454030 1.272157 -0.937484
H 1.075545 2.163032 -0.734037
C -0.778004 1.255681 -0.017266
H -0.459590 1.282238 1.038005
C -1.633223 0.000113 -0.244702
H -1.969359 0.000649 -1.302290
C -0.777952 -1.255656 -0.018561
H -0.459533 -1.283295 1.036685
C 2.267061 -0.000167 0.370198
O 1.525938 -0.000944 1.607628
C -2.869052 -0.000366 0.660726
H 0.105377 -1.358934 -1.985195
H 0.105383 1.361079 -1.983779
H -1.387366 2.158674 -0.204426
H -1.387272 -2.158482 -0.206651
H 2.914011 -0.896818 0.317156
H 2.913900 0.896623 0.318194
H 2.166530 -0.001066 2.332218
H -3.492696 0.892409 0.487011
H -3.492660 -0.892995 0.486131
H -2.562805 -0.000888 1.720884
el energy= -388.56410003328
zpe= -388.332774
th energy= -388.323130
th enthalpy= -388.322186
free energy= -388.366742

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.339005 -1.095686 0.023045
H 1.023104 -1.903562 -0.292888
C 0.948015 0.276687 -0.304642
H 1.139634 0.322161 -1.394837
C -0.040242 1.394770 0.066284
H -0.177548 1.408259 1.163612
C -1.395476 1.201920 -0.633814
H -1.243340 1.288934 -1.725770
C -2.020590 -0.173098 -0.324857
H -2.905763 -0.296843 -0.976137
C -1.017211 -1.289268 -0.676189
H -1.443707 -2.274513 -0.416414
C 2.281115 0.496206 0.411977
O 3.308796 -0.429745 0.022824
C -2.504967 -0.271970 1.130379
H 0.221543 -1.183341 1.120207
H 0.386065 2.376057 -0.208779
H -2.094046 2.006363 -0.342218
H -0.850044 -1.290210 -1.769413
H 2.683808 1.490380 0.162174
H 2.120447 0.460923 1.507751
H 3.040293 -1.309017 0.321890
H -3.247582 0.513658 1.347149
H -2.980291 -1.249327 1.316358
H -1.680825 -0.159328 1.851629
el energy= -388.56603314762
zpe= -388.334655
th energy= -388.324981
th enthalpy= -388.324037
free energy= -388.368778

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.493318 -0.815086 1.115390
H 1.230015 -1.636406 1.175311
C 1.161914 0.473122 0.597522
H 1.935449 0.781138 1.324689
C 0.112550 1.597678 0.485308
H -0.229467 1.862470 1.502847
C -1.110026 1.182687 -0.351954

H -0.818511 1.017088 -1.405979
C -1.761070 -0.100776 0.187572
H -2.106670 0.104338 1.221057
C -0.717256 -1.226712 0.261922
H -1.179944 -2.138280 0.680499
C 1.886527 0.267285 -0.739013
O 2.975277 -0.668232 -0.653390
C -2.968771 -0.512455 -0.659792
H 0.152463 -0.640218 2.152635
H 0.577415 2.506161 0.061573
H -1.852094 2.001024 -0.359208
H -0.398568 -1.482808 -0.766875
H 1.184703 -0.036713 -1.535351
H 2.350136 1.216622 -1.050464
H 2.598243 -1.546671 -0.509119
H -3.725270 0.288894 -0.692798
H -2.654422 -0.725496 -1.696162
H -3.448817 -1.419745 -0.257260
el energy= -388.56585188740
zpe= -388.334598
th energy= -388.324901
th enthalpy= -388.323957
free energy= -388.368821

MP2-SMD aug-cc-pVDZ

4mchm_1/coords
t1
C 0.160271 1.417460 0.182667
H 0.563916 2.350022 -0.249721
C 1.031771 0.224550 -0.242242
H 1.022949 0.164986 -1.348557
C 0.449942 -1.079301 0.324802
H 1.055238 -1.941640 -0.000560
C -1.012735 -1.269835 -0.102071
H -1.416858 -2.203803 0.327852
C -1.889919 -0.081182 0.317873
H -1.866395 -0.014892 1.423805
C -1.301007 1.220927 -0.245121
H -1.912985 2.080552 0.081667
C 2.468827 0.451353 0.204976
O 3.303122 -0.610174 -0.323211

C -3.340337 -0.272850 -0.132965
H 0.207553 1.520071 1.283887
H 0.508200 -1.035454 1.429842
H -1.061844 -1.371783 -1.203838
H -1.356296 1.183261 -1.350501
H 2.833253 1.425373 -0.166102
H 2.521944 0.453283 1.309054
H 4.211509 -0.429831 -0.035570
H -3.392308 -0.338256 -1.233902
H -3.770412 -1.199217 0.283696
H -3.973316 0.571982 0.187115
el energy= -388.57449126073
zpe= -388.344614
th energy= -388.334710
th enthalpy= -388.333765
free energy= -388.379053

4mchm_3/coords
t2
C -0.163672 1.416975 0.182229
H -0.206649 1.525540 1.283211
C -1.036065 0.220434 -0.229977
H -1.036577 0.156650 -1.337354
C -0.448637 -1.079832 0.337224
H -0.498426 -1.031443 1.442519
C 1.011255 -1.270586 -0.098660
H 1.419536 -2.202720 0.331358
C 1.888819 -0.079313 0.313581
H 1.869556 -0.009563 1.419384
C 1.296058 1.220399 -0.251191
H 1.908887 2.081693 0.069722
C -2.474014 0.448570 0.227549
O -3.386204 -0.587787 -0.209580
C 3.337764 -0.270477 -0.142096
H -0.571180 2.346584 -0.253136
H -1.057333 -1.943233 0.020600
H 1.054111 -1.375157 -1.200460
H 1.346478 1.178907 -1.356676
H -2.526313 0.439513 1.328233
H -2.832950 1.430671 -0.128918
H -3.375894 -0.574057 -1.179784
H 3.970703 0.576421 0.172588

H 3.770768 -1.194670 0.276366
H 3.385866 -0.339856 -1.242963
el energy= -388.57494619459
zpe= -388.344846
th energy= -388.335020
th enthalpy= -388.334076
free energy= -388.379125

4mchm_5/coords
t3
C 0.384260 -1.260972 0.001668
H 0.830686 -2.161214 0.460862
C 1.018283 -0.000003 0.609501
H 0.799272 -0.000006 1.696348
C 0.384257 1.260965 0.001671
H 0.830690 2.161201 0.460873
C -1.138888 1.257467 0.197854
H -1.369258 1.287652 1.280807
C -1.786030 0.000000 -0.402937
H -1.580908 0.000002 -1.491919
C -1.138886 -1.257471 0.197848
H -1.586201 -2.160446 -0.254935
C 2.538198 0.000000 0.498719
O 2.917345 0.000012 -0.900166
C -3.301770 0.000004 -0.187331
H 0.609963 -1.297047 -1.079368
H 0.609965 1.297045 -1.079362
H -1.586201 2.160445 -0.254925
H -1.369263 -1.287667 1.280802
H 2.951742 0.896344 0.994251
H 2.951750 -0.896346 0.994237
H 3.886326 -0.000022 -0.930034
H -3.533527 0.000033 0.892275
H -3.770159 0.892577 -0.635294
H -3.770171 -0.892584 -0.635253
el energy= -388.57371341565
zpe= -388.343672
th energy= -388.333853
th enthalpy= -388.332909
free energy= -388.378006

4mchm_6/coords

t4
C 0.158300 1.423736 0.187509
H 0.209402 1.518033 1.289325
C 1.034054 0.238867 -0.250248
H 1.022141 0.185206 -1.356646
C 0.460273 -1.070435 0.312895
H 1.064812 -1.933423 -0.019086
C -1.002035 -1.268080 -0.111877
H -1.052610 -1.363393 -1.214013
C -1.884014 -0.086531 0.318392
H -1.858581 -0.028326 1.424697
C -1.303859 1.223158 -0.236333
H -1.363164 1.194023 -1.341732
C 2.475516 0.467989 0.196773
O 3.401219 -0.522768 -0.312604
C -3.334195 -0.283470 -0.130975
H 0.556387 2.361402 -0.239301
H 0.521513 -1.032576 1.418045
H -1.399341 -2.206773 0.313760
H -1.919443 2.076638 0.099706
H 2.846097 1.431209 -0.186611
H 2.523940 0.490864 1.301135
H 3.132102 -1.380866 0.050460
H -3.971735 0.554332 0.198258
H -3.388271 -0.339290 -1.232333
H -3.757251 -1.216320 0.278343
el energy= -388.57530825794
zpe= -388.345081
th energy= -388.335311
th enthalpy= -388.334366
free energy= -388.379246

4mchm_7/coords
t5
C 0.382587 1.268485 0.008005
H 0.613039 1.291183 1.088551
C 1.023890 0.020588 -0.616840
H 0.815428 0.035045 -1.706113
C 0.392214 -1.254127 -0.035211
H 0.617882 -1.314413 1.046613
C -1.131809 -1.252451 -0.223724
H -1.366525 -1.264795 -1.305987

C -1.780259 -0.008257 0.401956
H -1.569279 -0.025661 1.489674
C -1.141287 1.261208 -0.181779
H -1.590057 2.154913 0.287734
C 2.547524 0.023339 -0.491013
O 3.019702 0.051872 0.878716
C -3.297143 -0.011479 0.194931
H 0.822981 2.177362 -0.440047
H 0.839390 -2.143989 -0.513947
H -1.572867 -2.165246 0.215179
H -1.377348 1.307796 -1.262881
H 2.969802 -0.856206 -1.009091
H 2.963177 0.930667 -0.956271
H 2.763519 -0.787981 1.290386
H -3.758139 -0.915645 0.627154
H -3.767421 0.868989 0.664365
H -3.535498 0.009168 -0.882999
el energy= -388.57443791438
zpe= -388.344311
th energy= -388.334521
th enthalpy= -388.333577
free energy= -388.378512

4mchm_19/coords
t6
C 0.252790 -1.080938 0.707640
H -0.359165 -1.178292 1.621628
C 0.922623 0.307637 0.717694
H 1.437439 0.444553 1.687139
C -0.146391 1.410395 0.575500
H -0.770540 1.413761 1.486007
C -1.037464 1.201732 -0.662323
H -1.813070 1.987732 -0.698531
C -1.707131 -0.187434 -0.671896
H -2.203407 -0.318197 -1.651429
C -0.634722 -1.287242 -0.532047
H -0.005522 -1.295292 -1.440335
C 1.988055 0.455234 -0.366060
O 3.046337 -0.502293 -0.104887
C -2.789999 -0.307326 0.411201
H 1.018983 -1.872596 0.757610
H 0.341691 2.400096 0.523298

H -0.428912 1.314096 -1.577321
H -1.122687 -2.277084 -0.478187
H 1.575044 0.276061 -1.371895
H 2.401307 1.479080 -0.337564
H 3.696541 -0.408310 -0.818204
H -3.559927 0.471787 0.279701
H -3.288360 -1.289782 0.352392
H -2.376683 -0.201631 1.426531
el energy= -388.56972313555
zpe= -388.338828
th energy= -388.329231
th enthalpy= -388.328286
free energy= -388.372879

4mchm_21/coords
t7
C 0.132446 1.401007 0.578507
H -0.363118 2.387113 0.527774
C -0.930175 0.289432 0.691905
H -1.463656 0.415677 1.654362
C -0.255153 -1.095965 0.679992
H 0.338096 -1.205163 1.604806
C 0.656747 -1.284326 -0.545120
H 0.044170 -1.288112 -1.464655
C 1.722688 -0.175201 -0.656383
H 2.237450 -0.294000 -1.627850
C 1.040788 1.207968 -0.648939
H 0.441617 1.318049 -1.570642
C -1.985774 0.438446 -0.407453
O -3.087907 -0.487753 -0.246425
C 2.786689 -0.295104 0.445176
H 0.743828 1.401435 1.497709
H -1.021478 -1.889226 0.702848
H 1.151136 -2.271002 -0.491878
H 1.809369 2.001238 -0.672336
H -2.370246 1.474382 -0.409714
H -1.576297 0.224437 -1.404707
H -3.477792 -0.307215 0.624283
H 2.353818 -0.204779 1.453819
H 3.296270 -1.271704 0.385273
H 3.550561 0.493362 0.336192
el energy= -388.57029740941

zpe= -388.339263
th energy= -388.329744
th enthalpy= -388.328799
free energy= -388.373097

4mchm_22/coords
t8
C 0.154290 1.432450 0.552752
H -0.327289 2.424135 0.476356
C -0.924109 0.341868 0.722100
H -1.430112 0.497578 1.693093
C -0.268119 -1.053064 0.729161
H 0.347680 -1.144076 1.640881
C 0.607169 -1.288975 -0.513308
H 1.078901 -2.286047 -0.451757
C 1.695688 -0.207342 -0.668107
H 2.190712 -0.359679 -1.645103
C 1.045671 1.191013 -0.679569
H 1.832620 1.965205 -0.724545
C -1.998795 0.483423 -0.359961
O -3.096002 -0.448223 -0.186818
C 2.775460 -0.326895 0.418100
H 0.778205 1.454783 1.463254
H -1.039122 -1.840463 0.803915
H -0.027752 -1.295242 -1.417965
H 0.442787 1.298790 -1.598533
H -2.454965 1.483342 -0.294414
H -1.577438 0.365809 -1.371369
H -2.748376 -1.335413 -0.367918
H 3.562021 0.432185 0.269365
H 2.364324 -0.188966 1.430438
H 3.252276 -1.321027 0.381843
el energy= -388.57041057257
zpe= -388.339295
th energy= -388.329767
th enthalpy= -388.328823
free energy= -388.373121

4mchm_24/coords
t9
C -0.089290 1.276504 0.736506
H 0.626471 1.396978 1.568861

C -0.920029 -0.000032 0.995466
H -1.187708 -0.000057 2.070280
C -0.089280 -1.276546 0.736446
H 0.626474 -1.397059 1.568801
C 0.691379 -1.258006 -0.590061
H 1.324993 -2.161521 -0.652762
C 1.570399 0.000020 -0.727626
H 2.009915 0.000045 -1.742520
C 0.691362 1.258028 -0.590007
H -0.012860 1.296529 -1.436984
C -2.286015 -0.000017 0.312112
O -2.169162 0.000050 -1.133742
C 2.734219 0.000006 0.274381
H -0.755183 2.157862 0.768378
H -0.755163 -2.157915 0.768278
H -0.012839 -1.296482 -1.437041
H 1.324964 2.161552 -0.652676
H -2.848912 -0.895676 0.631956
H -2.848930 0.895602 0.632037
H -3.074508 -0.000003 -1.482295
H 2.385434 -0.000018 1.318792
H 3.367342 -0.892153 0.131746
H 3.367332 0.892176 0.131786
el energy= -388.56512564705
zpe= -388.334589
th energy= -388.324837
th enthalpy= -388.323892
free energy= -388.368797

4mchm_9/coords
c1
C -0.480350 -0.834459 1.114561
H -1.212116 -1.658508 1.153201
C -1.153937 0.454131 0.603956
H -1.927484 0.761116 1.332479
C -0.111620 1.585201 0.498418
H -0.583562 2.495529 0.087516
C 1.104762 1.181113 -0.350925
H 0.801094 1.012635 -1.401108
C 1.767772 -0.098489 0.182276
H 2.119642 0.107599 1.213022
C 0.732989 -1.231843 0.259110

H 1.204431 -2.138148 0.679893
C -1.868248 0.256691 -0.730907
O -2.936749 -0.705463 -0.541189
C 2.969973 -0.498912 -0.676400
H -0.139770 -0.658886 2.151856
H 0.235801 1.833531 1.517903
H 1.841523 2.004351 -0.360838
H 0.411590 -1.489367 -0.767748
H -2.292927 1.219513 -1.066133
H -1.180786 -0.109426 -1.510561
H -3.381075 -0.809568 -1.396803
H 2.649046 -0.703754 -1.712751
H 3.724647 0.305075 -0.706195
H 3.455889 -1.408596 -0.284753
el energy= -388.57242050398
zpe= -388.341886
th energy= -388.332210
th enthalpy= -388.331266
free energy= -388.376096

4mchm_11/coords
c2
C -0.324659 -1.106446 0.051444
H -1.010908 -1.920510 -0.235542
C -0.943925 0.256001 -0.296763
H -1.131772 0.288732 -1.388475
C 0.034887 1.388328 0.055609
H -0.400524 2.361592 -0.232527
C 1.386159 1.194917 -0.650876
H 1.224544 1.264132 -1.742787
C 2.024447 -0.170159 -0.327478
H 2.907760 -0.294731 -0.980979
C 1.026993 -1.298236 -0.655843
H 0.852718 -1.314390 -1.748082
C -2.268588 0.482607 0.417136
O -3.222776 -0.516170 -0.022487
C 2.515037 -0.244551 1.126261
H -0.196908 -1.164830 1.148460
H 0.177221 1.412067 1.151714
H 2.080253 2.008346 -0.373401
H 1.463653 -2.275759 -0.383222
H -2.122674 0.404459 1.509985

H -2.656769 1.490128 0.185460
H -4.050789 -0.348927 0.453736
H 2.999137 -1.216409 1.321587
H 3.253184 0.549997 1.328341
H 1.691973 -0.129309 1.848695
el energy= -388.57208479468
zpe= -388.341712
th energy= -388.331913
th enthalpy= -388.330969
free energy= -388.376102

4mchm_13/coords
c3
C -0.031673 1.387439 0.054437
H -0.178132 1.414543 1.150086
C 0.947461 0.252118 -0.287420
H 1.144441 0.282307 -1.378737
C 0.324260 -1.108227 0.057920
H 1.012134 -1.923072 -0.223536
C -1.023089 -1.298768 -0.657793
H -0.842423 -1.314494 -1.749046
C -2.021136 -0.169579 -0.334693
H -2.901741 -0.294221 -0.991797
C -1.380682 1.194873 -0.656714
H -2.075093 2.009146 -0.382195
C 2.269534 0.484048 0.438602
O 3.282101 -0.503416 0.128122
C -2.517607 -0.242404 1.117193
H 0.407086 2.359190 -0.234158
H 0.189166 -1.165977 1.154106
H -1.462743 -2.275833 -0.388296
H -1.215317 1.263376 -1.748096
H 2.654300 1.493186 0.205944
H 2.117961 0.413753 1.527857
H 3.447441 -0.443613 -0.826399
H -2.999651 -1.215262 1.312656
H -1.697836 -0.123126 1.842700
H -3.258820 0.550421 1.314733
el energy= -388.57252442365
zpe= -388.342025
th energy= -388.332266
th enthalpy= -388.331322

free energy= -388.376362

4mchm_15/coords
c4
C -0.485860 -0.850115 1.098190
H -0.157423 -0.685847 2.141197
C -1.158686 0.440144 0.593319
H -1.943333 0.736413 1.316558
C -0.122081 1.578369 0.510010
H -0.595026 2.489848 0.102439
C 1.102564 1.186654 -0.333613
H 0.807356 1.026631 -1.387583
C 1.767096 -0.095321 0.192100
H 2.111499 0.102343 1.227002
C 0.737047 -1.234055 0.250449
H 1.209297 -2.141855 0.667101
C -1.859165 0.254028 -0.755546
O -2.912853 -0.738243 -0.706409
C 2.976359 -0.483107 -0.662511
H -1.215570 -1.676925 1.119250
H 0.215281 1.820062 1.534500
H 1.836258 2.012657 -0.331059
H 0.425601 -1.483897 -0.781373
H -2.276029 1.221809 -1.087974
H -1.167039 -0.103476 -1.530684
H -3.545670 -0.440568 -0.033307
H 2.662536 -0.680240 -1.702547
H 3.728216 0.323849 -0.680782
H 3.463226 -1.394436 -0.275854
el energy= -388.57297787399
zpe= -388.342432
th energy= -388.332760
th enthalpy= -388.331816
free energy= -388.376549

4mchm_16/coords
c5
C -0.226056 1.263368 -0.184848
H -0.735056 2.160176 -0.581665
C -0.945985 -0.000006 -0.683800
H -0.899721 -0.000009 -1.791805
C -0.226058 -1.263369 -0.184829

H -0.294905 -1.315109 0.915209
C 1.248223 -1.260662 -0.621179
H 1.760611 -2.164237 -0.244944
C 1.993409 -0.000003 -0.139237
H 2.997244 -0.000011 -0.602924
C 1.248228 1.260649 -0.621197
H 1.289369 1.299101 -1.725957
C -2.428866 -0.000001 -0.333961
O -2.580586 -0.000005 1.108505
C 2.191537 0.000013 1.383905
H -0.294901 1.315129 0.915190
H -0.735066 -2.160178 -0.581635
H 1.289363 -1.299125 -1.725938
H 1.760619 2.164225 -0.244970
H -2.917347 0.896452 -0.755776
H -2.917343 -0.896461 -0.755779
H -3.532569 0.000104 1.293422
H 2.756994 -0.892381 1.701577
H 2.757050 0.892385 1.701541
H 1.233753 0.000057 1.927292
el energy= -388.57142942972
zpe= -388.340745
th energy= -388.331090
th enthalpy= -388.330146
free energy= -388.374863

4mchm_17/coords
c6
C -0.222080 1.282568 -0.114053
H -0.723453 2.204835 -0.458952
C -0.952227 0.057538 -0.686238
H -0.916657 0.124407 -1.793055
C -0.239012 -1.241178 -0.274255
H -0.304684 -1.371361 0.821339
C 1.237390 -1.220015 -0.703593
H 1.741465 -2.149662 -0.384116
C 1.987927 0.002517 -0.139329
H 2.994076 0.024595 -0.597352
C 1.253427 1.295480 -0.545685
H 1.771096 2.170907 -0.114056
C -2.436231 0.041538 -0.320434
O -2.680074 -0.008968 1.107207

C 2.177873 -0.093567 1.382078
H -0.294109 1.270930 0.987111
H -0.752724 -2.105992 -0.731823
H 1.282205 -1.188318 -1.808324
H 1.299110 1.400954 -1.645870
H -2.922471 0.968682 -0.661843
H -2.936488 -0.812945 -0.810693
H -2.340142 -0.859531 1.425500
H 2.743503 0.775922 1.757482
H 1.217226 -0.125839 1.919449
H 2.740233 -1.005127 1.646601
el energy= -388.57218041162
zpe= -388.341654
th energy= -388.331886
th enthalpy= -388.330942
free energy= -388.376012

4mchm_23/coords
c7
C 0.424590 -1.316319 -0.865959
H 1.050080 -2.193150 -0.619263
C 1.295351 -0.041984 -0.843678
H 1.950152 -0.083263 -1.736024
C 0.429276 1.228810 -0.979632
H 1.057733 2.121790 -0.810522
C -0.799701 1.253349 -0.055350
H -0.489438 1.330127 1.000959
C -1.656665 -0.009136 -0.225430
H -1.986249 -0.057193 -1.282913
C -0.801905 -1.252465 0.058961
H -0.488350 -1.231467 1.117002
C 2.301384 0.008108 0.304103
O 1.649446 0.081928 1.597510
C -2.894425 0.031878 0.674474
H 0.061564 -1.463355 -1.900265
H 0.068877 1.285144 -2.023671
H -1.408672 2.147556 -0.281473
H -1.413507 -2.162381 -0.081034
H 2.936142 -0.895829 0.267059
H 2.951209 0.892383 0.173760
H 2.357231 0.114162 2.260680
H -3.515210 0.918686 0.461783

H -3.520658 -0.865183 0.532821
H -2.593904 0.073102 1.736093
el energy= -388.56786270756
zpe= -388.337564
th energy= -388.327802
th enthalpy= -388.326858
free energy= -388.371736

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.336553 -1.097218 0.028235
H 1.021757 -1.908337 -0.275952
C 0.946272 0.273394 -0.304479
H 1.130838 0.321613 -1.395953
C -0.038906 1.393415 0.069254
H -0.176132 1.399800 1.166269
C -1.392593 1.202204 -0.633319
H -1.237412 1.289261 -1.724822
C -2.019830 -0.171958 -0.327234
H -2.905055 -0.293216 -0.978694
C -1.016679 -1.288731 -0.676454
H -1.445133 -2.272951 -0.415607
C 2.274457 0.501146 0.412101
O 3.312206 -0.430221 0.018487
C -2.503282 -0.271337 1.127398
H 0.214465 -1.172979 1.124975
H 0.389727 2.373573 -0.205948
H -2.090949 2.006294 -0.339678
H -0.846224 -1.288169 -1.769270
H 2.673131 1.497039 0.164044
H 2.122107 0.449637 1.505762
H 3.038677 -1.309893 0.321555
H -3.244160 0.516471 1.345048
H -2.981934 -1.248400 1.309729
H -1.677299 -0.163464 1.847636
el energy= -388.57295651280
zpe= -388.342083
th energy= -388.332488
th enthalpy= -388.331544
free energy= -388.376087

4mchm-1000rej-h-rmsd_20/coords

c9
C 0.496433 -0.817028 1.112783
H 1.231241 -1.640521 1.159716
C 1.161409 0.473692 0.596654
H 1.934498 0.787386 1.322485
C 0.111282 1.597706 0.486781
H -0.229660 1.856653 1.505883
C -1.109958 1.181644 -0.350261
H -0.815506 1.013218 -1.402907
C -1.759495 -0.101818 0.189944
H -2.105607 0.102299 1.222991
C -0.715087 -1.226458 0.260766
H -1.176199 -2.137600 0.682213
C 1.876062 0.272824 -0.742404
O 2.976013 -0.667677 -0.653250
C -2.964554 -0.512769 -0.659761
H 0.158487 -0.642432 2.150855
H 0.576715 2.505633 0.062681
H -1.852683 1.999522 -0.354839
H -0.394428 -1.479235 -0.767650
H 1.178679 -0.053479 -1.530609
H 2.333308 1.222083 -1.061942
H 2.592389 -1.542140 -0.483131
H -3.725428 0.285478 -0.685419
H -2.649483 -0.716819 -1.698030
H -3.440977 -1.425386 -0.263308
el energy= -388.57309677485
zpe= -388.342273
th energy= -388.332726
th enthalpy= -388.331782
free energy= -388.376151

MP2 aug-cc-pwCVDZ gas phase

4mchm_1/coords
t1
C 0.155809 1.426080 0.181662
H 0.550910 2.362880 -0.249009
C 1.031539 0.238288 -0.241353
H 1.026087 0.173213 -1.346686
C 0.461580 -1.068736 0.324952
H 1.083750 -1.917254 0.001176

C -0.998235 -1.268023 -0.102298
H -1.397308 -2.204741 0.324623
C -1.883114 -0.085861 0.316378
H -1.859326 -0.019599 1.422303
C -1.303911 1.220342 -0.244703
H -1.921499 2.075740 0.080704
C 2.472640 0.458820 0.195704
O 3.269628 -0.625820 -0.314925
C -3.333596 -0.286884 -0.129398
H 0.201142 1.532070 1.282521
H 0.517518 -1.026006 1.430156
H -1.046382 -1.372542 -1.203406
H -1.359911 1.185417 -1.349653
H 2.840733 1.424484 -0.197055
H 2.521970 0.489383 1.301080
H 4.183586 -0.483544 -0.034652
H -3.388782 -0.356759 -1.228889
H -3.755176 -1.214171 0.290793
H -3.970615 0.553826 0.189736
el energy= -388.59837055399
zpe= -388.367459
th energy= -388.357691
th enthalpy= -388.356747
free energy= -388.401696

4mchm_3/coords
t2
C -0.157905 1.423113 0.182084
H -0.203018 1.530268 1.282728
C -1.033229 0.231883 -0.233438
H -1.020163 0.168476 -1.341752
C -0.455966 -1.071311 0.332606
H -0.506868 -1.023175 1.437492
C 1.001993 -1.269244 -0.100739
H 1.404906 -2.204077 0.326507
C 1.885670 -0.084046 0.313000
H 1.865619 -0.016949 1.418795
C 1.301406 1.220545 -0.247099
H 1.917749 2.077569 0.076292
C -2.478147 0.452759 0.210119
O -3.369835 -0.600592 -0.192870
C 3.334816 -0.282135 -0.137943

H -0.557588 2.357951 -0.248673
H -1.079122 -1.924236 0.020973
H 1.047541 -1.375606 -1.201993
H 1.355671 1.185444 -1.352258
H -2.530813 0.467311 1.310416
H -2.842412 1.429496 -0.159534
H -3.402433 -0.596636 -1.159795
H 3.970990 0.560289 0.178182
H 3.760220 -1.207937 0.281611
H 3.386589 -0.352834 -1.237571
el energy= -388.59814456681
zpe= -388.367200
th energy= -388.357458
th enthalpy= -388.356513
free energy= -388.401406

4mchm_5/coords
t3
C 0.391299 -1.260182 0.021206
H 0.831887 -2.160446 0.485226
C 1.024302 -0.000006 0.628378
H 0.817840 0.000007 1.718189
C 0.391303 1.260173 0.021191
H 0.831936 2.160418 0.485220
C -1.131757 1.255607 0.205225
H -1.373759 1.287225 1.285481
C -1.773010 -0.000005 -0.401722
H -1.555764 0.000001 -1.488101
C -1.131779 -1.255621 0.205201
H -1.574508 -2.159678 -0.248545
C 2.541825 0.000000 0.482381
O 2.858412 0.000022 -0.922386
C -3.291402 0.000019 -0.206290
H 0.635728 -1.296850 -1.054198
H 0.635728 1.296836 -1.054212
H -1.574532 2.159660 -0.248487
H -1.373813 -1.287279 1.285453
H 2.964864 0.897347 0.971241
H 2.964880 -0.897346 0.971220
H 3.820629 -0.000081 -1.011331
H -3.538011 0.000062 0.869014
H -3.752523 0.891993 -0.660285

H -3.752573 -0.891960 -0.660217
el energy= -388.59798722713
zpe= -388.367022
th energy= -388.357283
th enthalpy= -388.356338
free energy= -388.401202

4mchm_6/coords
t4
C 0.156716 1.421577 0.183500
H 0.209631 1.516079 1.285122
C 1.034554 0.241337 -0.257562
H 1.029064 0.188683 -1.363247
C 0.461726 -1.070881 0.295012
H 1.060050 -1.930378 -0.054699
C -1.002734 -1.265673 -0.121059
H -1.059101 -1.357058 -1.222619
C -1.882004 -0.087298 0.318921
H -1.848148 -0.032620 1.425143
C -1.306121 1.223333 -0.234568
H -1.371537 1.199549 -1.339164
C 2.478327 0.467148 0.189441
O 3.397300 -0.525868 -0.293861
C -3.336160 -0.285055 -0.115922
H 0.551714 2.362075 -0.238764
H 0.529239 -1.049897 1.400565
H -1.397657 -2.207087 0.299110
H -1.919913 2.075898 0.104819
H 2.852309 1.420586 -0.213705
H 2.516770 0.527734 1.294448
H 3.168833 -1.366045 0.126206
H -3.969835 0.552392 0.217620
H -3.401503 -0.343534 -1.215461
H -3.754138 -1.216365 0.298935
el energy= -388.59815941283
zpe= -388.367162
th energy= -388.357408
th enthalpy= -388.356464
free energy= -388.401382

4mchm_7/coords
t5

C 0.383997 1.269315 0.001851
H 0.634216 1.291985 1.076786
C 1.025993 0.025142 -0.625943
H 0.820405 0.038382 -1.716087
C 0.394827 -1.248634 -0.045504
H 0.614683 -1.302184 1.037531
C -1.128551 -1.250893 -0.231999
H -1.365180 -1.261092 -1.313362
C -1.776073 -0.011089 0.400550
H -1.560929 -0.033731 1.487210
C -1.139737 1.260538 -0.178085
H -1.586605 2.151444 0.296600
C 2.549324 0.030145 -0.478849
O 2.993670 0.041202 0.889106
C -3.293996 -0.015135 0.202768
H 0.818802 2.179117 -0.447882
H 0.842496 -2.141937 -0.517527
H -1.567189 -2.166868 0.200953
H -1.384425 1.315627 -1.256641
H 2.982425 -0.833439 -1.017511
H 2.966869 0.947883 -0.920728
H 2.790967 -0.823990 1.269860
H -3.751529 -0.918821 0.636622
H -3.759919 0.864513 0.675093
H -3.539142 0.007147 -0.872503
el energy= -388.59765267132
zpe= -388.366658
th energy= -388.356939
th enthalpy= -388.355995
free energy= -388.400820

4mchm_19/coords
t6
C 0.271785 -1.070773 0.702432
H -0.330104 -1.182835 1.620842
C 0.922233 0.325062 0.711504
H 1.438177 0.463106 1.678948
C -0.152286 1.419382 0.564617
H -0.771764 1.428274 1.477623
C -1.050957 1.198047 -0.664620
H -1.833228 1.976740 -0.699053
C -1.704969 -0.197515 -0.666095

H -2.205794 -0.334990 -1.642031
C -0.620475 -1.284172 -0.530660
H 0.004394 -1.286778 -1.441423
C 1.995965 0.467315 -0.365023
O 3.011546 -0.520194 -0.104527
C -2.782125 -0.324869 0.421112
H 1.056866 -1.841768 0.741632
H 0.325092 2.413772 0.506380
H -0.454697 1.316674 -1.586461
H -1.095020 -2.279839 -0.479611
H 1.574091 0.320659 -1.374144
H 2.426032 1.484834 -0.316134
H 3.693895 -0.433155 -0.783584
H -3.565416 0.438092 0.283606
H -3.261621 -1.316063 0.377149
H -2.368296 -0.200040 1.432867
el energy= -388.59315293381
zpe= -388.361628
th energy= -388.352012
th enthalpy= -388.351068
free energy= -388.395708

4mchm_21/coords
t7
C 0.144748 1.414284 0.565897
H -0.340296 2.404882 0.505486
C -0.924428 0.312635 0.699739
H -1.438938 0.450693 1.671749
C -0.270323 -1.081086 0.690714
H 0.319714 -1.202707 1.615617
C 0.635894 -1.284803 -0.534213
H 0.019586 -1.289844 -1.450462
C 1.714266 -0.190827 -0.656355
H 2.225102 -0.323196 -1.627658
C 1.049631 1.199550 -0.659511
H 0.455594 1.312333 -1.583504
C -1.995771 0.456418 -0.386845
O -3.053187 -0.509772 -0.264756
C 2.781438 -0.312694 0.441157
H 0.759289 1.426751 1.482288
H -1.054341 -1.854903 0.709172
H 1.115861 -2.277601 -0.479783

H 1.825385 1.984683 -0.691166
H -2.405539 1.483841 -0.364507
H -1.578675 0.287191 -1.389102
H -3.476077 -0.367358 0.594045
H 2.356338 -0.196561 1.449382
H 3.270822 -1.299075 0.397711
H 3.558942 0.458184 0.315292
el energy= -388.59321995087
zpe= -388.361632
th energy= -388.352058
th enthalpy= -388.351113
free energy= -388.395619

4mchm_22/coords
t8
C 0.148872 1.424054 0.556863
H -0.333241 2.415356 0.487507
C -0.926200 0.330562 0.714601
H -1.439061 0.474175 1.682661
C -0.264604 -1.060332 0.716384
H 0.344305 -1.160636 1.631184
C 0.619625 -1.286178 -0.520693
H 1.093457 -2.281864 -0.466021
C 1.703500 -0.199742 -0.664120
H 2.202106 -0.344722 -1.639883
C 1.047774 1.194893 -0.671047
H 1.829886 1.973317 -0.709783
C -2.005190 0.469060 -0.365293
O -3.111722 -0.429602 -0.176898
C 2.782182 -0.320583 0.422232
H 0.768765 1.446735 1.469565
H -1.032166 -1.851151 0.788424
H -0.005944 -1.289656 -1.431600
H 0.452250 1.307528 -1.593736
H -2.444690 1.476900 -0.311122
H -1.582287 0.344863 -1.376974
H -2.793650 -1.327011 -0.344442
H 3.568737 0.436488 0.272498
H 2.372567 -0.179394 1.433595
H 3.256994 -1.314517 0.389748
el energy= -388.59254810760
zpe= -388.361037

th energy= -388.351403
th enthalpy= -388.350459
free energy= -388.395119

4mchm_24/coords
t9
C -0.097637 1.273956 0.755456
H 0.619097 1.386430 1.587832
C -0.932171 0.000194 1.005671
H -1.218900 0.000360 2.075791
C -0.097676 -1.273665 0.755840
H 0.619080 -1.385901 1.588229
C 0.670718 -1.257309 -0.576443
H 1.301785 -2.161448 -0.645041
C 1.547647 -0.000123 -0.723826
H 1.967334 -0.000282 -1.746520
C 0.670816 1.257175 -0.576793
H -0.047776 1.290817 -1.409734
C -2.277251 0.000100 0.282333
O -2.091674 -0.000267 -1.147901
C 2.731216 -0.000038 0.254891
H -0.757696 2.158693 0.795953
H -0.757757 -2.158373 0.796633
H -0.047909 -1.291108 -1.409350
H 1.301962 2.161242 -0.645610
H -2.848954 -0.896234 0.588518
H -2.848853 0.896648 0.588082
H -2.968511 -0.000396 -1.555937
H 2.403605 0.000115 1.305565
H 3.361421 -0.891514 0.103131
H 3.361486 0.891350 0.102895
el energy= -388.59073146227
zpe= -388.359135
th energy= -388.349566
th enthalpy= -388.348622
free energy= -388.392957

4mchm_9/coords
c1
C -0.497061 -0.822615 1.106495
H -1.242763 -1.632213 1.130893
C -1.154832 0.470822 0.593066

H -1.929292 0.779328 1.318387
C -0.107495 1.594293 0.483158
H -0.569060 2.506379 0.064960
C 1.112937 1.179023 -0.353832
H 0.819917 1.011893 -1.406951
C 1.761871 -0.103339 0.186846
H 2.106850 0.104016 1.219500
C 0.718656 -1.227654 0.260723
H 1.180695 -2.137602 0.682262
C -1.876605 0.263718 -0.736442
O -2.902775 -0.725369 -0.528328
C 2.969771 -0.514375 -0.658348
H -0.164358 -0.653627 2.147064
H 0.234879 1.851588 1.501684
H 1.854724 1.997030 -0.363679
H 0.401505 -1.488740 -0.766207
H -2.324034 1.221751 -1.060149
H -1.178851 -0.072672 -1.522457
H -3.362608 -0.859921 -1.367815
H 2.655981 -0.729269 -1.693926
H 3.726035 0.286564 -0.692239
H 3.449128 -1.420787 -0.254702
el energy= -388.59603141424
zpe= -388.364824
th energy= -388.355154
th enthalpy= -388.354209
free energy= -388.399027

4mchm_11/coords
c2
C -0.337181 -1.096947 0.056501
H -1.040649 -1.895585 -0.225294
C -0.943906 0.269922 -0.287985
H -1.137481 0.300791 -1.378048
C 0.041053 1.394926 0.061735
H -0.385894 2.373168 -0.221252
C 1.387567 1.192200 -0.649660
H 1.222264 1.265436 -1.740218
C 2.016031 -0.177747 -0.331939
H 2.892980 -0.307646 -0.992317
C 1.009248 -1.297831 -0.654371
H 0.831156 -1.315215 -1.745413

C -2.273859 0.489050 0.418456
O -3.193109 -0.525818 -0.025679
C 2.519432 -0.256369 1.116700
H -0.206432 -1.160425 1.152772
H 0.189549 1.420293 1.156811
H 2.088986 2.000033 -0.376952
H 1.440309 -2.278282 -0.386402
H -2.124512 0.424471 1.513379
H -2.665511 1.494678 0.178298
H -4.036250 -0.384131 0.425060
H 2.998660 -1.229986 1.308379
H 3.262827 0.533046 1.313660
H 1.704561 -0.137320 1.846348
el energy= -388.59576782916
zpe= -388.364537
th energy= -388.354848
th enthalpy= -388.353903
free energy= -388.398687

4mchm_13/coords
c3
C -0.037320 1.391904 0.062173
H -0.188098 1.417778 1.156852
C 0.945993 0.262554 -0.279276
H 1.134934 0.295561 -1.373135
C 0.330731 -1.100606 0.062020
H 1.033144 -1.904956 -0.207648
C -1.012055 -1.298481 -0.656215
H -0.829722 -1.317724 -1.746774
C -2.016447 -0.174287 -0.339299
H -2.890242 -0.301504 -1.004267
C -1.382053 1.193816 -0.653973
H -2.081762 2.003895 -0.383580
C 2.277205 0.480717 0.437093
O 3.269435 -0.509977 0.119531
C -2.527712 -0.250841 1.106697
H 0.395348 2.368247 -0.218784
H 0.193116 -1.159507 1.157370
H -1.447934 -2.277028 -0.389290
H -1.213098 1.267500 -1.744101
H 2.661202 1.495353 0.221152
H 2.130440 0.400114 1.525995

H 3.474555 -0.420916 -0.821757
H -3.009501 -1.223453 1.296907
H -1.716902 -0.132050 1.840855
H -3.271009 0.539856 1.298632
el energy= -388.59555932528
zpe= -388.364298
th energy= -388.354636
th enthalpy= -388.353691
free energy= -388.398409

4mchm_15/coords
c4
C -0.493920 -0.847136 1.090148
H -0.173074 -0.698008 2.137386
C -1.154759 0.449739 0.590780
H -1.928128 0.752214 1.324776
C -0.115407 1.582843 0.501293
H -0.583292 2.495729 0.091854
C 1.107911 1.183953 -0.338879
H 0.815798 1.023137 -1.393131
C 1.765302 -0.097845 0.192539
H 2.103144 0.102076 1.229048
C 0.731120 -1.231320 0.247655
H 1.197383 -2.141983 0.662680
C -1.872901 0.256987 -0.749204
O -2.901812 -0.745513 -0.695980
C 2.980708 -0.490600 -0.650500
H -1.233078 -1.663977 1.088541
H 0.223469 1.831109 1.523321
H 1.843207 2.007670 -0.341571
H 0.421923 -1.483889 -0.783480
H -2.291696 1.224615 -1.084297
H -1.182731 -0.093669 -1.528783
H -3.556632 -0.452735 -0.046280
H 2.674224 -0.696547 -1.689972
H 3.731009 0.316322 -0.671250
H 3.464655 -1.397690 -0.254005
el energy= -388.59605232688
zpe= -388.364783
th energy= -388.355148
th enthalpy= -388.354204
free energy= -388.398905

4mchm_16/coords
c5
C -0.233417 1.263652 -0.205899
H -0.735608 2.159003 -0.613627
C -0.951789 0.000005 -0.702858
H -0.919504 0.000007 -1.811645
C -0.233417 -1.263645 -0.205906
H -0.327067 -1.320817 0.890418
C 1.244604 -1.258444 -0.623282
H 1.751431 -2.163599 -0.245279
C 1.982385 -0.000001 -0.129181
H 2.992110 -0.000002 -0.579396
C 1.244609 1.258451 -0.623268
H 1.303661 1.295682 -1.727072
C -2.426381 0.000001 -0.316508
O -2.512776 -0.000028 1.121714
C 2.158131 -0.000009 1.396361
H -0.327069 1.320821 0.890426
H -0.735617 -2.158987 -0.613642
H 1.303650 -1.295658 -1.727087
H 1.751438 2.163598 -0.245247
H -2.922416 0.897489 -0.730690
H -2.922414 -0.897478 -0.730723
H -3.448115 0.000124 1.364518
H 2.718272 -0.891393 1.722339
H 2.718291 0.891363 1.722341
H 1.192815 0.000003 1.923898
el energy= -388.59566952594
zpe= -388.364364
th energy= -388.354712
th enthalpy= -388.353768
free energy= -388.398448

4mchm_17/coords
c6
C -0.225954 1.282473 -0.115223
H -0.723176 2.206228 -0.459866
C -0.954700 0.062132 -0.694805
H -0.922728 0.131887 -1.801859
C -0.240173 -1.235755 -0.289004
H -0.304984 -1.364822 0.806312

C 1.236616 -1.213673 -0.712165
H 1.738669 -2.146374 -0.400935
C 1.984622 0.003315 -0.136072
H 2.990584 0.027624 -0.593569
C 1.251857 1.298369 -0.533931
H 1.765319 2.170110 -0.092137
C -2.435204 0.045561 -0.308528
O -2.654946 -0.018561 1.111883
C 2.174242 -0.104650 1.384043
H -0.321626 1.266816 0.982849
H -0.749820 -2.103350 -0.746040
H 1.286315 -1.175125 -1.815952
H 1.308894 1.416267 -1.632005
H -2.918512 0.981340 -0.629079
H -2.948203 -0.792913 -0.815881
H -2.397435 -0.902154 1.407803
H 2.754602 0.751690 1.763505
H 1.214508 -0.118830 1.921785
H 2.719323 -1.026542 1.644115
el energy= -388.59525858423
zpe= -388.363928
th energy= -388.354299
th enthalpy= -388.353355
free energy= -388.397983

4mchm_23/coords
c7
C 0.453312 -1.269799 -0.938141
H 1.074464 -2.160538 -0.736364
C 1.320714 0.000494 -0.831047
H 2.009952 0.000989 -1.698423
C 0.453277 1.270892 -0.936719
H 1.074411 2.161419 -0.733937
C -0.777395 1.254396 -0.017152
H -0.458835 1.280598 1.037457
C -1.631832 0.000120 -0.244396
H -1.968052 0.000691 -1.301311
C -0.777341 -1.254369 -0.018527
H -0.458773 -1.281721 1.036054
C 2.265239 -0.000178 0.369076
O 1.525291 -0.001000 1.606894
C -2.866459 -0.000389 0.660526

H 0.104527 -1.357305 -1.983888
H 0.104532 1.359581 -1.982383
H -1.386342 2.157049 -0.203765
H -1.386243 -2.156845 -0.206129
H 2.911766 -0.896350 0.315510
H 2.911651 0.896142 0.316610
H 2.166907 -0.001146 2.330577
H -3.489737 0.891920 0.487060
H -3.489700 -0.892542 0.486123
H -2.559948 -0.000945 1.719945
el energy= -388.59367007756
zpe= -388.362394
th energy= -388.352759
th enthalpy= -388.351815
free energy= -388.396349

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.338450 -1.094642 0.023919
H 1.022023 -1.902555 -0.290999
C 0.947211 0.276111 -0.303819
H 1.139104 0.321319 -1.393369
C -0.040061 1.393238 0.066263
H -0.177681 1.406703 1.162965
C -1.393807 1.200648 -0.633530
H -1.241276 1.287401 -1.724850
C -2.018684 -0.172837 -0.324962
H -2.902867 -0.296525 -0.976545
C -1.016249 -1.288123 -0.675038
H -1.442726 -2.272744 -0.415465
C 2.278957 0.495571 0.412304
O 3.307159 -0.428854 0.021904
C -2.504244 -0.271301 1.128499
H 0.220494 -1.181567 1.120495
H 0.386117 2.374017 -0.208445
H -2.091965 2.004886 -0.342719
H -0.848666 -1.289466 -1.767594
H 2.680769 1.489692 0.163593
H 2.118469 0.458866 1.507422
H 3.039078 -1.308491 0.320181
H -3.246621 0.514011 1.344085
H -2.979557 -1.248064 1.313956

H -1.681401 -0.158642 1.850245
el energy= -388.59559491877
zpe= -388.364274
th energy= -388.354606
th enthalpy= -388.353662
free energy= -388.398392

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.492194 -0.816557 1.112285
H 1.228059 -1.637930 1.170640
C 1.160421 0.471034 0.596919
H 1.933442 0.777675 1.324286
C 0.112304 1.594828 0.486538
H -0.229385 1.857949 1.503969
C -1.109329 1.181820 -0.350321
H -0.817913 1.017087 -1.403902
C -1.760289 -0.100617 0.187359
H -2.105397 0.103290 1.220592
C -0.717967 -1.225959 0.259831
H -1.180498 -2.137478 0.677131
C 1.885262 0.267532 -0.738126
O 2.976558 -0.664606 -0.651932
C -2.967376 -0.510397 -0.659504
H 0.152249 -0.643407 2.149487
H 0.577061 2.503482 0.064653
H -1.850491 2.000176 -0.356982
H -0.400127 -1.480654 -0.768933
H 1.185152 -0.038529 -1.534284
H 2.346214 1.217584 -1.049221
H 2.601662 -1.543793 -0.506794
H -3.723100 0.290876 -0.691271
H -2.653346 -0.722062 -1.695577
H -3.447355 -1.417521 -0.258226
el energy= -388.59541902161
zpe= -388.364223
th energy= -388.354531
th enthalpy= -388.353587
free energy= -388.398441

MP2-SMD aug-cc-pwCVDZ

4mchm_1/coords
t1
C 0.159986 1.416154 0.182551
H 0.563454 2.348194 -0.249601
C 1.030706 0.224344 -0.241543
H 1.022221 0.164599 -1.347267
C 0.449419 -1.078093 0.325176
H 1.054515 -1.940085 0.000597
C -1.011785 -1.268598 -0.101601
H -1.415743 -2.202078 0.327981
C -1.888233 -0.081079 0.317486
H -1.865177 -0.014652 1.422812
C -1.299840 1.219653 -0.245064
H -1.911608 2.078930 0.080984
C 2.466442 0.451086 0.205291
O 3.300532 -0.609662 -0.324146
C -3.337314 -0.272732 -0.133361
H 0.207030 1.518892 1.283184
H 0.507288 -1.033851 1.429634
H -1.060535 -1.370600 -1.202785
H -1.354753 1.181639 -1.349863
H 2.830299 1.424992 -0.164805
H 2.519704 0.451899 1.308734
H 4.208726 -0.429850 -0.035673
H -3.388756 -0.338177 -1.233684
H -3.767146 -1.198590 0.283028
H -3.970051 0.571628 0.186293
el energy= -388.60405261621
zpe= -388.374240
th energy= -388.364341
th enthalpy= -388.363397
free energy= -388.408671

4mchm_3/coords
t2
C -0.163394 1.415599 0.182079
H -0.206166 1.524134 1.282480
C -1.034997 0.220185 -0.229489
H -1.035883 0.156424 -1.336279
C -0.448093 -1.078728 0.337186

H -0.497710 -1.030213 1.441898
C 1.010409 -1.269334 -0.098372
H 1.418479 -2.200998 0.331312
C 1.887129 -0.079206 0.313234
H 1.868148 -0.009374 1.418427
C 1.294910 1.219128 -0.251110
H 1.907462 2.080077 0.069176
C -2.471542 0.448282 0.227795
O -3.383902 -0.587338 -0.209971
C 3.334817 -0.270285 -0.142225
H -0.570730 2.344744 -0.252920
H -1.056401 -1.941802 0.021040
H 1.053112 -1.373891 -1.199583
H 1.345051 1.177357 -1.356008
H -2.523851 0.438151 1.327836
H -2.829945 1.430210 -0.127759
H -3.373332 -0.572474 -1.180123
H 3.967442 0.576125 0.172213
H 3.767523 -1.194000 0.275955
H 3.382575 -0.339605 -1.242475
el energy= -388.60451989506
zpe= -388.374471
th energy= -388.364656
th enthalpy= -388.363712
free energy= -388.408735

4mchm_5/coords
t3
C 0.383846 -1.259736 0.001601
H 0.830042 -2.159561 0.460388
C 1.017141 -0.000003 0.608892
H 0.798060 -0.000006 1.695147
C 0.383843 1.259729 0.001604
H 0.830045 2.159548 0.460399
C -1.137887 1.256227 0.197554
H -1.368096 1.286317 1.279949
C -1.784381 0.000000 -0.402615
H -1.579563 0.000001 -1.491039
C -1.137885 -1.256232 0.197549
H -1.584982 -2.158789 -0.254803
C 2.535734 0.000000 0.498865
O 2.915231 0.000012 -0.899685

C -3.298864 0.000004 -0.187117
H 0.609414 -1.295713 -1.078852
H 0.609417 1.295712 -1.078846
H -1.584983 2.158787 -0.254793
H -1.368101 -1.286332 1.279944
H 2.948823 0.895884 0.994255
H 2.948832 -0.895884 0.994242
H 3.884208 -0.000022 -0.928871
H -3.530271 0.000033 0.891915
H -3.766977 0.892092 -0.634795
H -3.766989 -0.892098 -0.634754
el energy= -388.60326394390
zpe= -388.373280
th energy= -388.363469
th enthalpy= -388.362525
free energy= -388.407602

4mchm_6/coords
t4
C 0.158011 1.422402 0.187386
H 0.208924 1.516841 1.288608
C 1.032947 0.238605 -0.249593
H 1.021304 0.184863 -1.355395
C 0.459694 -1.069260 0.313199
H 1.063912 -1.931973 -0.018092
C -1.001157 -1.266831 -0.111471
H -1.051382 -1.362165 -1.213030
C -1.882362 -0.086427 0.318013
H -1.857385 -0.028153 1.423720
C -1.302737 1.221913 -0.236212
H -1.361740 1.192554 -1.341031
C 2.473054 0.467633 0.197033
O 3.398880 -0.522177 -0.313314
C -3.331214 -0.283343 -0.131351
H 0.555926 2.359535 -0.239216
H 0.520576 -1.031113 1.417770
H -1.398299 -2.205057 0.313797
H -1.918061 2.075034 0.099232
H 2.843163 1.430644 -0.185557
H 2.521608 0.489508 1.300778
H 3.130294 -1.380351 0.049848
H -3.968530 0.553947 0.197531

H -3.384774 -0.339125 -1.232101
H -3.753994 -1.215726 0.277640
el energy= -388.60487315881
zpe= -388.374703
th energy= -388.364940
th enthalpy= -388.363996
free energy= -388.408861

4mchm_7/coords
t5
C 0.382166 1.267183 0.008067
H 0.612345 1.289914 1.088057
C 1.022696 0.020425 -0.616045
H 0.814156 0.034834 -1.704721
C 0.391686 -1.252982 -0.034927
H 0.617148 -1.313164 1.046344
C -1.130925 -1.251222 -0.223289
H -1.365409 -1.263546 -1.305002
C -1.778680 -0.008173 0.401625
H -1.568012 -0.025467 1.488785
C -1.140284 1.259950 -0.181627
H -1.588840 2.153315 0.287311
C 2.545010 0.023044 -0.491232
O 3.018152 0.052206 0.877889
C -3.294307 -0.011349 0.194689
H 0.822417 2.175565 -0.439653
H 0.838592 -2.142465 -0.513227
H -1.571841 -2.163525 0.215259
H -1.376089 1.306299 -1.262192
H 2.966558 -0.856304 -1.008931
H 2.960262 0.929710 -0.956686
H 2.760956 -0.786993 1.290192
H -3.755066 -0.914947 0.626757
H -3.764262 0.868728 0.663711
H -3.532295 0.009158 -0.882674
el energy= -388.60399456510
zpe= -388.373941
th energy= -388.364152
th enthalpy= -388.363208
free energy= -388.408143

4mchm_19/coords

t6
C 0.252387 -1.080527 0.705782
H -0.358660 -1.178055 1.619641
C 0.921934 0.306523 0.716088
H 1.437204 0.442751 1.684706
C -0.145983 1.408400 0.575422
H -0.769377 1.411062 1.485724
C -1.036718 1.200886 -0.660917
H -1.811469 1.986882 -0.696806
C -1.706286 -0.186645 -0.670873
H -2.202611 -0.316690 -1.649778
C -0.635200 -1.285762 -0.532144
H -0.006914 -1.293560 -1.440344
C 1.986100 0.454256 -0.366863
O 3.045999 -0.500447 -0.102956
C -2.788184 -0.306676 0.411302
H 1.017840 -1.872104 0.755029
H 0.341799 2.397599 0.523995
H -0.428613 1.313298 -1.575509
H -1.123043 -2.275000 -0.478664
H 1.574011 0.271794 -1.371771
H 2.396930 1.478471 -0.340571
H 3.695429 -0.407786 -0.817111
H -3.557322 0.472442 0.280410
H -3.286605 -1.288370 0.351880
H -2.374891 -0.201884 1.426031
el energy= -388.59933226405
zpe= -388.368493
th energy= -388.358906
th enthalpy= -388.357961
free energy= -388.402540

4mchm_21/coords
t7
C 0.132207 1.399288 0.577963
H -0.362894 2.384992 0.527596
C -0.929447 0.288770 0.690558
H -1.462767 0.414541 1.652471
C -0.254920 -1.095239 0.678353
H 0.337417 -1.204655 1.603046
C 0.657020 -1.282952 -0.544923
H 0.045332 -1.286930 -1.464357

C 1.721767 -0.174706 -0.655499
H 2.236535 -0.293049 -1.626309
C 1.040264 1.206962 -0.647836
H 0.441723 1.317334 -1.569240
C -1.984163 0.437904 -0.407597
O -3.087286 -0.486729 -0.245290
C 2.784737 -0.294682 0.445254
H 0.742823 1.399369 1.496959
H -1.020546 -1.888372 0.700635
H 1.151175 -2.269069 -0.491587
H 1.808212 2.000029 -0.670900
H -2.367156 1.473735 -0.411191
H -1.575467 0.221759 -1.404004
H -3.474796 -0.305971 0.626394
H 2.351670 -0.205089 1.453188
H 3.294331 -1.270571 0.385017
H 3.547907 0.493709 0.336960
el energy= -388.59991351473
zpe= -388.368934
th energy= -388.359427
th enthalpy= -388.358482
free energy= -388.402749

4mchm_22/coords
t8
C 0.153951 1.430546 0.552552
H -0.327288 2.421770 0.476817
C -0.923375 0.340865 0.720753
H -1.429416 0.495963 1.691137
C -0.267731 -1.052564 0.727382
H 0.347180 -1.143811 1.638968
C 0.607611 -1.287545 -0.513349
H 1.079198 -2.284033 -0.452002
C 1.694853 -0.206647 -0.667170
H 2.189884 -0.358341 -1.643561
C 1.044955 1.190100 -0.678320
H 1.831074 1.964277 -0.723062
C -1.997008 0.482749 -0.360211
O -3.095423 -0.446827 -0.185661
C 2.773671 -0.326318 0.418099
H 0.777149 1.452330 1.462828
H -1.038029 -1.839867 0.801421

H -0.026407 -1.293750 -1.417915
H 0.442513 1.297857 -1.596875
H -2.451505 1.482843 -0.295754
H -1.576327 0.363141 -1.370966
H -2.748756 -1.334674 -0.365184
H 3.559437 0.432802 0.269951
H 2.362544 -0.189304 1.429860
H 3.250572 -1.319702 0.381206
el energy= -388.60001521213
zpe= -388.368985
th energy= -388.359453
th enthalpy= -388.358509
free energy= -388.402829

4mchm_24/coords
t9
C -0.089324 1.275166 0.736310
H 0.626159 1.395063 1.568239
C -0.919466 0.000012 0.994700
H -1.187713 0.000025 2.068816
C -0.089327 -1.275148 0.736337
H 0.626157 -1.395028 1.568267
C 0.690601 -1.256928 -0.588851
H 1.323907 -2.159975 -0.651370
C 1.568601 -0.000008 -0.726841
H 2.007029 -0.000020 -1.741511
C 0.690604 1.256916 -0.588877
H -0.013266 1.295862 -1.435370
C -2.284006 0.000009 0.311825
O -2.166948 -0.000014 -1.133882
C 2.732612 0.000001 0.272992
H -0.754448 2.156326 0.768813
H -0.754453 -2.156306 0.768859
H -0.013264 -1.295896 -1.435345
H 1.323908 2.159960 -0.651420
H -2.846587 -0.895184 0.631436
H -2.846575 0.895221 0.631409
H -3.072425 -0.000060 -1.482074
H 2.384951 0.000008 1.317077
H 3.365220 -0.891708 0.129838
H 3.365219 0.891707 0.129823
el energy= -388.59473319355

zpe= -388.364251
th energy= -388.354512
th enthalpy= -388.353568
free energy= -388.398436

4mchm_9/coords
c1
C -0.479500 -0.835313 1.111887
H -1.210635 -1.659156 1.149306
C -1.152496 0.452508 0.603148
H -1.925751 0.758386 1.331540
C -0.111390 1.582741 0.499207
H -0.583140 2.493055 0.089719
C 1.104037 1.180184 -0.349528
H 0.800474 1.012302 -1.399232
C 1.766749 -0.098356 0.182198
H 2.118185 0.106763 1.212627
C 0.733256 -1.230943 0.257451
H 1.204380 -2.137252 0.677009
C -1.866687 0.256739 -0.730393
O -2.937202 -0.702665 -0.539524
C 2.968257 -0.497301 -0.675907
H -0.139697 -0.661062 2.149023
H 0.235637 1.829777 1.518489
H 1.840025 2.003318 -0.359077
H 0.412561 -1.487085 -0.769344
H -2.288947 1.219901 -1.065660
H -1.180878 -0.111380 -1.509658
H -3.381741 -0.806485 -1.395022
H 2.647517 -0.701140 -1.711839
H 3.722224 0.306524 -0.704848
H 3.454048 -1.406703 -0.285210
el energy= -388.60201335409
zpe= -388.371535
th energy= -388.361867
th enthalpy= -388.360923
free energy= -388.405738

4mchm_11/coords
c2
C -0.324307 -1.105229 0.052190
H -1.010179 -1.919163 -0.233740

C -0.943155 0.255706 -0.295994
H -1.131289 0.288205 -1.387072
C 0.034809 1.386934 0.055681
H -0.400354 2.359775 -0.231989
C 1.384606 1.193672 -0.650452
H 1.222666 1.262764 -1.741723
C 2.022463 -0.170011 -0.327589
H 2.904746 -0.294601 -0.981423
C 1.025815 -1.297056 -0.654787
H 0.851174 -1.313578 -1.746360
C -2.266532 0.482238 0.417408
O -3.220736 -0.515674 -0.023437
C 2.514230 -0.244197 1.124371
H -0.196054 -1.162868 1.148601
H 0.177405 1.410468 1.151173
H 2.078394 2.006766 -0.373683
H 1.462332 -2.274011 -0.382386
H -2.120812 0.402932 1.509566
H -2.653988 1.489578 0.186689
H -4.048583 -0.348705 0.453104
H 2.998057 -1.215605 1.319142
H 3.252327 0.549825 1.325346
H 1.692475 -0.128731 1.847284
el energy= -388.60166781750
zpe= -388.371358
th energy= -388.361568
th enthalpy= -388.360624
free energy= -388.405738

4mchm_13/coords
c3
C -0.031576 1.385981 0.054517
H -0.178275 1.412790 1.149553
C 0.946656 0.251730 -0.286771
H 1.143899 0.281814 -1.377449
C 0.323837 -1.107095 0.058433
H 1.011183 -1.921853 -0.222210
C -1.022095 -1.297564 -0.656796
H -0.841224 -1.313679 -1.747406
C -2.019217 -0.169357 -0.334720
H -2.898888 -0.293941 -0.992038
C -1.379138 1.193657 -0.656254

H -2.073181 2.007626 -0.382381
C 2.267410 0.483564 0.438769
O 3.280309 -0.502942 0.127373
C -2.516644 -0.241984 1.115455
H 0.406974 2.357316 -0.233531
H 0.188416 -1.164249 1.154025
H -1.461629 -2.274034 -0.387460
H -1.213498 1.262050 -1.747001
H 2.651358 1.492580 0.207169
H 2.116053 0.411898 1.527329
H 3.445167 -0.441786 -0.827112
H -2.998673 -1.214271 1.310321
H -1.698021 -0.122826 1.841307
H -3.257531 0.550515 1.312095
el energy= -388.60211758534
zpe= -388.371686
th energy= -388.361931
th enthalpy= -388.360987
free energy= -388.406026

4mchm_15/coords
c4
C -0.485087 -0.850123 1.096306
H -0.157087 -0.686418 2.138906
C -1.157364 0.439090 0.592613
H -1.941592 0.734704 1.315679
C -0.121866 1.576330 0.510142
H -0.594524 2.487631 0.103488
C 1.101724 1.185542 -0.332752
H 0.806499 1.025747 -1.386145
C 1.765837 -0.095192 0.191990
H 2.110052 0.101946 1.226417
C 0.737010 -1.232996 0.249574
H 1.208908 -2.140572 0.665533
C -1.857626 0.254221 -0.754866
O -2.912400 -0.736593 -0.705540
C 2.974212 -0.482092 -0.662084
H -1.214198 -1.676660 1.117004
H 0.215181 1.817260 1.534258
H 1.834741 2.011345 -0.330232
H 0.426029 -1.482115 -0.781936
H -2.273044 1.222028 -1.087035

H -1.166721 -0.104394 -1.529665
H -3.542752 -0.439359 -0.029967
H 2.660334 -0.678532 -1.701561
H 3.725519 0.324534 -0.679886
H 3.460821 -1.393082 -0.276083
el energy= -388.60257551822
zpe= -388.372103
th energy= -388.362428
th enthalpy= -388.361484
free energy= -388.406237

4mchm_16/coords
c5
C -0.225947 1.262076 -0.184334
H -0.734750 2.158596 -0.580411
C -0.945155 -0.000005 -0.682958
H -0.898596 -0.000006 -1.790380
C -0.225949 -1.262077 -0.184318
H -0.294482 -1.313336 0.915160
C 1.246872 -1.259498 -0.620466
H 1.759106 -2.162561 -0.244582
C 1.991551 -0.000003 -0.139516
H 2.994465 -0.000011 -0.603714
C 1.246877 1.259487 -0.620482
H 1.287702 1.298200 -1.724656
C -2.426899 0.000000 -0.334219
O -2.579100 -0.000007 1.107979
C 2.191148 0.000011 1.382117
H -0.294477 1.313354 0.915145
H -0.734761 -2.158597 -0.580387
H 1.287695 -1.298221 -1.724640
H 1.759115 2.162550 -0.244603
H -2.914891 0.895992 -0.756002
H -2.914887 -0.895998 -0.756007
H -3.531186 0.000100 1.292221
H 2.756612 -0.891914 1.698972
H 2.756667 0.891913 1.698939
H 1.234481 0.000053 1.926161
el energy= -388.60100237784
zpe= -388.370387
th energy= -388.360738
th enthalpy= -388.359794

free energy= -388.404496

4mchm_17/coords
c6
C -0.222020 1.281042 -0.114509
H -0.723306 2.202667 -0.459364
C -0.951276 0.056789 -0.685383
H -0.915462 0.122883 -1.791664
C -0.238631 -1.240223 -0.272837
H -0.303862 -1.369218 0.822330
C 1.236291 -1.219250 -0.702030
H 1.740320 -2.148120 -0.382340
C 1.986110 0.002590 -0.139477
H 2.991439 0.024504 -0.597804
C 1.252015 1.293919 -0.545972
H 1.769412 2.169244 -0.115388
C -2.434148 0.040773 -0.320851
O -2.679107 -0.007749 1.106415
C 2.177112 -0.092372 1.380543
H -0.293671 1.269780 0.986085
H -0.752027 -2.105159 -0.729087
H 1.280769 -1.188424 -1.806206
H 1.297408 1.398727 -1.645637
H -2.920231 0.966852 -0.663399
H -2.933447 -0.814094 -0.810049
H -2.336659 -0.856672 1.426307
H 2.742669 0.776945 1.754646
H 1.217416 -0.124275 1.918323
H 2.739371 -1.003259 1.645031
el energy= -388.60176212358
zpe= -388.371295
th energy= -388.361538
th enthalpy= -388.360594
free energy= -388.405632

4mchm_23/coords
c7
C 0.424016 -1.316735 -0.863056
H 1.049021 -2.192946 -0.615681
C 1.293986 -0.043723 -0.842873
H 1.949019 -0.086735 -1.734320
C 0.428798 1.225472 -0.981629

H 1.056841 2.118503 -0.815271
C -0.798847 1.252029 -0.058072
H -0.488398 1.330745 0.997403
C -1.654957 -0.009570 -0.225219
H -1.984779 -0.059740 -1.281900
C -0.801030 -1.251134 0.061197
H -0.487120 -1.227753 1.118453
C 2.299013 0.008532 0.303706
O 1.647560 0.085353 1.596934
C -2.891409 0.033233 0.674317
H 0.060822 -1.465005 -1.896497
H 0.068355 1.279032 -2.025177
H -1.407477 2.145364 -0.285677
H -1.412333 -2.160886 -0.076495
H 2.933161 -0.895163 0.268492
H 2.948630 0.891899 0.171425
H 2.355863 0.119176 2.259460
H -3.511678 0.919363 0.460497
H -3.517498 -0.863459 0.534527
H -2.590325 0.076156 1.735056
el energy= -388.59745568058
zpe= -388.367212
th energy= -388.357461
th enthalpy= -388.356517
free energy= -388.401369

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.336016 -1.096144 0.028893
H 1.020681 -1.907273 -0.274333
C 0.945419 0.272901 -0.303830
H 1.130200 0.320944 -1.394667
C -0.038812 1.391922 0.069211
H -0.176268 1.398136 1.165611
C -1.391068 1.200957 -0.632950
H -1.235654 1.287853 -1.723829
C -2.017935 -0.171736 -0.327250
H -2.902292 -0.292954 -0.978840
C -1.015725 -1.287538 -0.675468
H -1.444104 -2.271173 -0.414895
C 2.272241 0.500612 0.412314
O 3.310443 -0.429440 0.017729

C -2.502147 -0.270826 1.125750
H 0.213440 -1.171214 1.125037
H 0.389637 2.371611 -0.205567
H -2.089026 2.004771 -0.339938
H -0.844962 -1.287255 -1.767634
H 2.670136 1.496378 0.165236
H 2.120010 0.447866 1.505293
H 3.037374 -1.309392 0.320269
H -3.242937 0.516461 1.342445
H -2.980451 -1.247432 1.307710
H -1.677263 -0.162687 1.846240
el energy= -388.60253968801
zpe= -388.371735
th energy= -388.362144
th enthalpy= -388.361199
free energy= -388.405737

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.495559 -0.817223 1.110857
H 1.229746 -1.640482 1.157209
C 1.160014 0.472460 0.596036
H 1.932703 0.785450 1.321673
C 0.111022 1.595531 0.487128
H -0.229633 1.853538 1.505910
C -1.109162 1.180596 -0.349303
H -0.814708 1.012467 -1.401386
C -1.758383 -0.101669 0.189796
H -2.104382 0.101860 1.222341
C -0.715210 -1.225423 0.259841
H -1.176058 -2.136326 0.680548
C 1.874364 0.272792 -0.741682
O 2.975865 -0.665480 -0.652188
C -2.962456 -0.511667 -0.659527
H 0.158203 -0.643357 2.148617
H 0.576223 2.503354 0.064145
H -1.851179 1.998306 -0.353834
H -0.395038 -1.477445 -0.768282
H 1.178126 -0.055016 -1.529379
H 2.329795 1.222228 -1.061233
H 2.593496 -1.540416 -0.481868
H -3.722773 0.286264 -0.684792

H -2.647255 -0.715001 -1.697225
H -3.438675 -1.423965 -0.263824
el energy= -388.60268808477
zpe= -388.371916
th energy= -388.362379
th enthalpy= -388.361434
free energy= -388.405783

MP2(FC1) aug-cc-pwCVDZ gas phase

4mchm_1/coords
t1
C 0.155431 1.424516 0.181631
H 0.550460 2.360909 -0.248248
C 1.030148 0.238218 -0.241021
H 1.024446 0.173100 -1.345669
C 0.461093 -1.067316 0.324740
H 1.083271 -1.915168 0.001537
C -0.996893 -1.266537 -0.102382
H -1.395895 -2.202841 0.323747
C -1.880821 -0.085830 0.315921
H -1.856682 -0.019551 1.421145
C -1.302447 1.218873 -0.244666
H -1.920049 2.073672 0.079972
C 2.469739 0.458331 0.195215
O 3.266015 -0.625240 -0.314404
C -3.329781 -0.286777 -0.129011
H 0.200482 1.530032 1.281863
H 0.516803 -1.024367 1.429262
H -1.044780 -1.370607 -1.202859
H -1.358091 1.183575 -1.348940
H 2.837365 1.423461 -0.197465
H 2.518762 0.489524 1.299941
H 4.179787 -0.483829 -0.034698
H -3.385191 -0.356659 -1.227809
H -3.751063 -1.213498 0.290948
H -3.966545 0.553304 0.189945
el energy= -388.86178118851
zpe= -388.630561
th energy= -388.620810
th enthalpy= -388.619866
free energy= -388.664779

4mchm_3/coords
t2
C -0.157585 1.421546 0.181977
H -0.202456 1.528269 1.281988
C -1.031876 0.231809 -0.233151
H -1.018554 0.168331 -1.340760
C -0.455515 -1.069857 0.332435
H -0.506158 -1.021400 1.436632
C 1.000606 -1.267755 -0.100792
H 1.403456 -2.202157 0.325697
C 1.883331 -0.084001 0.312548
H 1.862932 -0.016861 1.417641
C 1.299897 1.219074 -0.247094
H 1.916236 2.075513 0.075529
C -2.475247 0.452311 0.209666
O -3.365849 -0.600107 -0.192476
C 3.330957 -0.282018 -0.137540
H -0.557197 2.355962 -0.248023
H -1.078693 -1.922154 0.021519
H 1.045902 -1.373698 -1.201410
H 1.353854 1.183586 -1.351573
H -2.527443 0.467655 1.309337
H -2.839180 1.428483 -0.159879
H -3.399232 -0.597121 -1.158913
H 3.966874 0.559786 0.178396
H 3.756070 -1.207244 0.281800
H 3.382965 -0.352739 -1.236475
el energy= -388.86154684743
zpe= -388.630295
th energy= -388.620569
th enthalpy= -388.619625
free energy= -388.664483

4mchm_5/coords
t3
C 0.390845 -1.258689 0.021118
H 0.831564 -2.158469 0.484316
C 1.022979 -0.000005 0.627743
H 0.816380 0.000010 1.716812
C 0.390848 1.258682 0.021100
H 0.831612 2.158443 0.484306

C -1.130403 1.254153 0.205253
H -1.372069 1.285366 1.284898
C -1.770800 -0.000005 -0.401160
H -1.553217 -0.000001 -1.486770
C -1.130425 -1.254167 0.205231
H -1.573232 -2.157718 -0.247776
C 2.538772 0.000001 0.481862
O 2.855094 0.000020 -0.921399
C -3.287582 0.000018 -0.206473
H 0.634910 -1.294874 -1.053687
H 0.634909 1.294860 -1.053702
H -1.573257 2.157699 -0.247721
H -1.372121 -1.285417 1.284871
H 2.961444 0.896719 0.970711
H 2.961460 -0.896713 0.970694
H 3.816740 -0.000086 -1.011422
H -3.534403 0.000063 0.868087
H -3.748415 0.891399 -0.660269
H -3.748464 -0.891370 -0.660198
el energy= -388.86140334024
zpe= -388.630131
th energy= -388.620408
th enthalpy= -388.619464
free energy= -388.664292

4mchm_6/coords
t4
C 0.156374 1.420024 0.183420
H 0.209041 1.514018 1.284413
C 1.033189 0.241304 -0.257305
H 1.027502 0.188684 -1.362306
C 0.461321 -1.069463 0.294683
H 1.059547 -1.928320 -0.054583
C -1.001336 -1.264174 -0.121182
H -1.057521 -1.355063 -1.222109
C -1.879639 -0.087271 0.318491
H -1.845369 -0.032576 1.424007
C -1.304634 1.221871 -0.234535
H -1.369747 1.197718 -1.338459
C 2.475420 0.466752 0.188939
O 3.393264 -0.525556 -0.293277
C -3.332293 -0.284968 -0.115416

H 0.551305 2.360121 -0.238025
H 0.528662 -1.048295 1.399558
H -1.396184 -2.205175 0.298195
H -1.918439 2.073839 0.104112
H 2.848935 1.419640 -0.214201
H 2.513593 0.528173 1.293262
H 3.165739 -1.365436 0.126815
H -3.965703 0.551838 0.217998
H -3.397938 -0.343441 -1.214258
H -3.749938 -1.215722 0.299228
el energy= -388.86156280587
zpe= -388.630260
th energy= -388.620522
th enthalpy= -388.619577
free energy= -388.664463

4mchm_7/coords
t5
C 0.383506 1.267886 0.002177
H 0.633394 1.289936 1.076508
C 1.024657 0.025329 -0.625270
H 0.818881 0.038718 -1.714657
C 0.394475 -1.247017 -0.045420
H 0.613857 -1.300050 1.037024
C -1.127078 -1.249421 -0.232134
H -1.363344 -1.259139 -1.312885
C -1.773853 -0.011191 0.399978
H -1.558483 -0.033948 1.485888
C -1.138414 1.259089 -0.177919
H -1.585421 2.149391 0.296179
C 2.546242 0.030341 -0.478366
O 2.990040 0.040833 0.888139
C -3.290139 -0.015287 0.202782
H 0.818402 2.177288 -0.446600
H 0.842362 -2.139786 -0.516659
H -1.565753 -2.164950 0.199983
H -1.382747 1.313966 -1.255869
H 2.979066 -0.832345 -1.017356
H 2.963332 0.947590 -0.920097
H 2.788432 -0.824063 1.268966
H -3.747396 -0.918459 0.636277
H -3.755863 0.863686 0.674981

H -3.535420 0.007126 -0.871760
el energy= -388.86105798361
zpe= -388.629758
th energy= -388.620055
th enthalpy= -388.619111
free energy= -388.663903

4mchm_19/coords
t6
C 0.271448 -1.069231 0.702286
H -0.330443 -1.181288 1.619859
C 0.920691 0.325160 0.711064
H 1.436465 0.463459 1.677819
C -0.152704 1.417973 0.564025
H -0.772249 1.426799 1.476157
C -1.049545 1.196520 -0.664327
H -1.831519 1.974508 -0.699534
C -1.702374 -0.197630 -0.665585
H -2.202837 -0.335368 -1.640920
C -0.618933 -1.282789 -0.529930
H 0.006016 -1.285341 -1.439795
C 1.993114 0.466906 -0.364393
O 3.007572 -0.519672 -0.104746
C -2.778364 -0.324889 0.420376
H 1.056273 -1.839475 0.742284
H 0.324118 2.411901 0.506289
H -0.453291 1.315087 -1.585347
H -1.092903 -2.277999 -0.479380
H 1.570919 0.320715 -1.372701
H 2.422792 1.483896 -0.315733
H 3.689839 -0.433556 -0.783337
H -3.561429 0.437333 0.282928
H -3.257403 -1.315566 0.376774
H -2.364922 -0.199848 1.431501
el energy= -388.85657873600
zpe= -388.624748
th energy= -388.615150
th enthalpy= -388.614205
free energy= -388.658808

4mchm_21/coords
t7

C 0.145094 1.412824 0.565417
H -0.339428 2.402946 0.505555
C -0.922937 0.312661 0.699302
H -1.437311 0.450892 1.670600
C -0.270023 -1.079608 0.690458
H 0.319985 -1.201287 1.614538
C 0.634354 -1.283376 -0.533595
H 0.017984 -1.288280 -1.448961
C 1.711672 -0.190877 -0.655829
H 2.222181 -0.323420 -1.626520
C 1.048160 1.198066 -0.659124
H 0.454106 1.310778 -1.582277
C -1.992853 0.456062 -0.386279
O -3.048971 -0.509263 -0.264824
C 2.777636 -0.312708 0.440466
H 0.759708 1.425191 1.480928
H -1.053773 -1.852711 0.709559
H 1.113768 -2.275709 -0.479743
H 1.823584 1.982527 -0.691525
H -2.402234 1.482948 -0.364229
H -1.575260 0.287441 -1.387680
H -3.472505 -0.367930 0.593318
H 2.352861 -0.196518 1.448049
H 3.266623 -1.298535 0.397284
H 3.554869 0.457501 0.314798
el energy= -388.85664161271
zpe= -388.624747
th energy= -388.615190
th enthalpy= -388.614246
free energy= -388.658715

4mchm_22/coords
t8
C 0.149253 1.422655 0.556237
H -0.332304 2.413496 0.487328
C -0.924679 0.330675 0.714033
H -1.437449 0.474521 1.681361
C -0.264335 -1.058795 0.716082
H 0.344620 -1.159054 1.630019
C 0.618077 -1.284768 -0.520070
H 1.091295 -2.280017 -0.465968
C 1.700958 -0.199862 -0.663535

H 2.199297 -0.345076 -1.638647
C 1.046417 1.193367 -0.670721
H 1.828237 1.971074 -0.710183
C -2.002362 0.468651 -0.364765
O -3.107537 -0.429230 -0.176760
C 2.778370 -0.320645 0.421665
H 0.769160 1.445283 1.468095
H -1.031597 -1.848846 0.789005
H -0.007452 -1.287986 -1.430160
H 0.450956 1.305926 -1.592624
H -2.441272 1.476072 -0.310984
H -1.579315 0.344802 -1.375673
H -2.790591 -1.326397 -0.345024
H 3.564798 0.435576 0.271967
H 2.369105 -0.179083 1.432347
H 3.252613 -1.314113 0.389672
el energy= -388.85596791110
zpe= -388.624152
th energy= -388.614535
th enthalpy= -388.613591
free energy= -388.658214

4mchm_24/coords
t9
C -0.097193 1.272179 0.754722
H 0.619333 1.384758 1.586374
C -0.930478 -0.000311 1.004480
H -1.216526 -0.000575 2.074102
C -0.097122 -1.272641 0.754113
H 0.619364 -1.385594 1.585746
C 0.670080 -1.255609 -0.576801
H 1.300436 -2.159359 -0.646470
C 1.546100 0.000195 -0.723095
H 1.966071 0.000447 -1.744961
C 0.669925 1.255822 -0.576243
H -0.048459 1.289011 -1.408502
C -2.274554 -0.000158 0.282840
O -2.090544 0.000447 -1.146157
C 2.727928 0.000060 0.255020
H -0.756998 2.156232 0.795738
H -0.756884 -2.156749 0.794670
H -0.048253 -1.288542 -1.409108

H 1.300160 2.159681 -0.645561
H -2.845512 -0.896174 0.589048
H -2.845679 0.895507 0.589763
H -2.966927 0.000478 -1.554066
H 2.400158 -0.000172 1.304906
H 3.358026 -0.890722 0.103499
H 3.357929 0.890972 0.103864
el energy= -388.85413217211
zpe= -388.622235
th energy= -388.612683
th enthalpy= -388.611739
free energy= -388.656036

4mchm_9/coords
c1
C -0.496702 -0.820546 1.106223
H -1.242266 -1.629305 1.131780
C -1.153336 0.471144 0.592385
H -1.927580 0.780056 1.316760
C -0.107109 1.593074 0.481902
H -0.568293 2.504638 0.063960
C 1.111451 1.177378 -0.354353
H 0.818386 1.009670 -1.406626
C 1.759324 -0.103287 0.186555
H 2.103883 0.104590 1.218506
C 0.717068 -1.226016 0.261107
H 1.178789 -2.135394 0.682447
C -1.873889 0.263052 -0.735648
O -2.898557 -0.725365 -0.527940
C 2.965937 -0.514683 -0.657229
H -0.163647 -0.650950 2.145857
H 0.235548 1.850519 1.499562
H 1.853135 1.994547 -0.365179
H 0.399771 -1.487384 -0.764947
H -2.320996 1.220297 -1.059911
H -1.175788 -0.072878 -1.520585
H -3.358275 -0.861212 -1.366746
H 2.652463 -0.730156 -1.692058
H 3.721963 0.285524 -0.691705
H 3.444898 -1.420332 -0.253249
el energy= -388.85945984216
zpe= -388.627943

th energy= -388.618291
th enthalpy= -388.617347
free energy= -388.662126

4mchm_11/coords
c2
C -0.336763 -1.095547 0.056532
H -1.040141 -1.893472 -0.224870
C -0.942475 0.269833 -0.287599
H -1.135633 0.300673 -1.377055
C 0.041384 1.393355 0.061903
H -0.385347 2.371112 -0.220448
C 1.386122 1.190771 -0.649059
H 1.220566 1.263803 -1.738908
C 2.013600 -0.177689 -0.331568
H 2.890182 -0.307632 -0.991307
C 1.007920 -1.296377 -0.653827
H 0.829665 -1.313431 -1.744163
C -2.271142 0.488590 0.417690
O -3.189496 -0.525240 -0.025604
C 2.516041 -0.256294 1.115597
H -0.206150 -1.159034 1.152112
H 0.189878 1.418462 1.156281
H 2.087385 1.998044 -0.377061
H 1.438705 -2.276377 -0.386583
H -2.121644 0.424615 1.511979
H -2.662303 1.493701 0.177534
H -4.032617 -0.384329 0.424408
H 2.994898 -1.229291 1.307447
H 3.258917 0.532579 1.312898
H 1.701482 -0.137362 1.844549
el energy= -388.85918393730
zpe= -388.627646
th energy= -388.617973
th enthalpy= -388.617029
free energy= -388.661776

4mchm_13/coords
c3
C -0.037609 1.390336 0.062290
H -0.188384 1.415967 1.156270
C 0.944601 0.262477 -0.278901

H 1.133119 0.295405 -1.372135
C 0.330353 -1.099150 0.062171
H 1.032697 -1.902847 -0.206864
C -1.010628 -1.297044 -0.655629
H -0.828080 -1.315975 -1.745468
C -2.013952 -0.174255 -0.338957
H -2.887352 -0.301555 -1.003314
C -1.380559 1.192364 -0.653423
H -2.080123 2.001878 -0.383762
C 2.274467 0.480334 0.436367
O 3.265477 -0.509488 0.119429
C -2.524299 -0.250746 1.105551
H 0.394843 2.366189 -0.218037
H 0.192762 -1.157872 1.156824
H -1.446237 -2.275129 -0.389411
H -1.211356 1.265819 -1.742841
H 2.658095 1.494409 0.220444
H 2.127391 0.400500 1.524636
H 3.471197 -0.421430 -0.821346
H -3.005639 -1.222766 1.295979
H -1.713838 -0.131948 1.839033
H -3.267153 0.539355 1.297743
el energy= -388.85896682814
zpe= -388.627398
th energy= -388.617753
th enthalpy= -388.616809
free energy= -388.661491

4mchm_15/coords
c4
C -0.493618 -0.845238 1.089765
H -0.172495 -0.695623 2.136130
C -1.153326 0.449954 0.590133
H -1.926508 0.752737 1.323189
C -0.115102 1.581548 0.500261
H -0.582614 2.493963 0.091198
C 1.106350 1.182359 -0.339249
H 0.814174 1.021053 -1.392668
C 1.762731 -0.097784 0.192266
H 2.100136 0.102564 1.228100
C 0.729537 -1.229724 0.247931
H 1.195506 -2.139841 0.662676

C -1.870078 0.256436 -0.748491
O -2.897359 -0.745469 -0.695499
C 2.976861 -0.490777 -0.649416
H -1.232590 -1.661328 1.089134
H 0.224064 1.829835 1.521457
H 1.841513 2.005278 -0.342859
H 0.420241 -1.482493 -0.782372
H -2.288545 1.223268 -1.084148
H -1.179407 -0.093581 -1.526943
H -3.552775 -0.453836 -0.046574
H 2.670706 -0.697180 -1.688174
H 3.726915 0.315437 -0.670652
H 3.460425 -1.397153 -0.252702
el energy= -388.85947596086
zpe= -388.627898
th energy= -388.618280
th enthalpy= -388.617336
free energy= -388.662000

4mchm_16/coords
c5
C -0.232965 1.262188 -0.205720
H -0.735079 2.156972 -0.612945
C -0.950305 0.000005 -0.702286
H -0.917706 0.000008 -1.810370
C -0.232965 -1.262180 -0.205727
H -0.326691 -1.319213 0.889898
C 1.243321 -1.257006 -0.622679
H 1.750011 -2.161671 -0.245327
C 1.979944 -0.000001 -0.128725
H 2.989372 -0.000002 -0.577964
C 1.243325 1.257013 -0.622664
H 1.302308 1.293905 -1.725803
C -2.423222 0.000001 -0.316353
O -2.509609 -0.000029 1.120290
C 2.154383 -0.000009 1.395248
H -0.326693 1.319217 0.889907
H -0.735088 -2.156955 -0.612961
H 1.302296 -1.293880 -1.725820
H 1.750017 2.161670 -0.245294
H -2.918886 0.896856 -0.730619
H -2.918885 -0.896844 -0.730653

H -3.444213 0.000124 1.364070
H 2.713863 -0.890810 1.721650
H 2.713882 0.890779 1.721652
H 1.189270 0.000003 1.921693
el energy= -388.85909404630
zpe= -388.627480
th energy= -388.617847
th enthalpy= -388.616902
free energy= -388.661545

4mchm_17/coords
c6
C -0.225472 1.281114 -0.114345
H -0.722595 2.204489 -0.457963
C -0.953270 0.062563 -0.694095
H -0.920974 0.132873 -1.800402
C -0.239857 -1.234063 -0.289203
H -0.304517 -1.363349 0.805374
C 1.235139 -1.211956 -0.712131
H 1.737030 -2.144317 -0.402057
C 1.982167 0.003266 -0.135775
H 2.987748 0.027688 -0.592482
C 1.250576 1.297148 -0.532749
H 1.764001 2.168157 -0.091186
C -2.432093 0.045865 -0.308332
O -2.651521 -0.019271 1.110505
C 2.170772 -0.105378 1.382693
H -0.321178 1.264762 0.983017
H -0.749554 -2.100887 -0.746008
H 1.284643 -1.172582 -1.815220
H 1.307428 1.415319 -1.630121
H -2.914951 0.981256 -0.628491
H -2.944853 -0.791523 -0.816303
H -2.394980 -0.902659 1.406363
H 2.750775 0.750023 1.762838
H 1.211350 -0.119465 1.919552
H 2.715021 -1.026971 1.642672
el energy= -388.85867166828
zpe= -388.627035
th energy= -388.617423
th enthalpy= -388.616479
free energy= -388.661073

4mchm_23/coords
c7
C 0.452307 -1.268518 -0.937129
H 1.073086 -2.158747 -0.735914
C 1.318748 0.000268 -0.830305
H 2.007579 0.000535 -1.697076
C 0.452293 1.269110 -0.936356
H 1.073060 2.159224 -0.734598
C -0.776293 1.252843 -0.017063
H -0.457406 1.278530 1.036743
C -1.629958 0.000068 -0.243889
H -1.965729 0.000377 -1.300151
C -0.776265 -1.252823 -0.017808
H -0.457371 -1.279131 1.035980
C 2.262709 -0.000099 0.368162
O 1.524309 -0.000553 1.605359
C -2.863193 -0.000213 0.659871
H 0.103000 -1.356160 -1.982033
H 0.103005 1.357390 -1.981212
H -1.384856 2.155107 -0.202674
H -1.384811 -2.154989 -0.203951
H 2.908828 -0.895732 0.314505
H 2.908762 0.895616 0.315111
H 2.165783 -0.000562 2.328531
H -3.486179 0.891477 0.486383
H -3.486155 -0.891818 0.485864
H -2.557152 -0.000519 1.718716
el energy= -388.85707313579
zpe= -388.625489
th energy= -388.615871
th enthalpy= -388.614927
free energy= -388.659424

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.338099 -1.093226 0.023888
H 1.021524 -1.900439 -0.290711
C 0.945759 0.276062 -0.303485
H 1.137297 0.321308 -1.392409
C -0.040409 1.391665 0.066385
H -0.178027 1.404838 1.162388

C -1.392368 1.199174 -0.632977
H -1.239612 1.285661 -1.723601
C -2.016194 -0.172820 -0.324534
H -2.900090 -0.296583 -0.975357
C -1.014867 -1.286670 -0.674521
H -1.441062 -2.270839 -0.415699
C 2.276170 0.495222 0.411545
O 3.303089 -0.428484 0.021907
C -2.500561 -0.271227 1.127521
H 0.220274 -1.180127 1.119774
H 0.385534 2.371970 -0.207651
H -2.090393 2.002844 -0.342894
H -0.847178 -1.287602 -1.766376
H 2.677471 1.488831 0.162799
H 2.115562 0.459266 1.506016
H 3.035984 -1.307855 0.320320
H -3.242409 0.513512 1.343525
H -2.975429 -1.247384 1.313251
H -1.677924 -0.158609 1.848433
el energy= -388.85900471923
zpe= -388.627377
th energy= -388.617725
th enthalpy= -388.616781
free energy= -388.661478

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.491885 -0.814576 1.111861
H 1.227581 -1.635067 1.171484
C 1.158954 0.471298 0.596144
H 1.931840 0.778270 1.322515
C 0.111983 1.593580 0.485362
H -0.229895 1.856821 1.501963
C -1.107867 1.180220 -0.350686
H -0.816499 1.015049 -1.403470
C -1.757727 -0.100594 0.187113
H -2.102391 0.103723 1.219677
C -0.716363 -1.224363 0.260089
H -1.178573 -2.135346 0.677121
C 1.882506 0.266872 -0.737453
O 2.972208 -0.664700 -0.651294
C -2.963571 -0.510628 -0.658339

H 0.151558 -0.640793 2.148114
H 0.576331 2.501732 0.063731
H -1.848934 1.997736 -0.358160
H -0.398484 -1.479180 -0.767876
H 1.182195 -0.038869 -1.532593
H 2.342940 1.216214 -1.049217
H 2.597990 -1.543699 -0.506406
H -3.719051 0.289928 -0.690565
H -2.649911 -0.722749 -1.693706
H -3.443164 -1.417028 -0.256817
el energy= -388.85884153468
zpe= -388.627338
th energy= -388.617663
th enthalpy= -388.616719
free energy= -388.661536

MP2-SMD (FC1) aug-cc-pwCVDZ

4mchm_1/coords
t1
C 0.159590 1.414621 0.182504
H 0.562978 2.346245 -0.248909
C 1.029322 0.224312 -0.241227
H 1.020536 0.164533 -1.346260
C 0.448967 -1.076669 0.324947
H 1.054089 -1.937980 0.000924
C -1.010406 -1.267127 -0.101707
H -1.414334 -2.200165 0.327131
C -1.885911 -0.081076 0.317036
H -1.862509 -0.014659 1.421659
C -1.298399 1.218203 -0.244992
H -1.910205 2.076833 0.080405
C 2.463559 0.450688 0.204706
O 3.296857 -0.609065 -0.323739
C -3.333467 -0.272672 -0.132945
H 0.206416 1.516920 1.282500
H 0.506603 -1.032225 1.428723
H -1.058933 -1.368688 -1.202255
H -1.353025 1.179892 -1.349109
H 2.826930 1.424073 -0.165362
H 2.516582 0.452172 1.307512
H 4.204597 -0.431066 -0.034220

H -3.385190 -0.337923 -1.232585
H -3.762914 -1.198071 0.283083
H -3.965998 0.570952 0.186741
el energy= -388.86748757396
zpe= -388.637378
th energy= -388.627492
th enthalpy= -388.626548
free energy= -388.671797

4mchm_3/coords
t2
C -0.163076 1.414020 0.181995
H -0.205540 1.522112 1.281770
C -1.033662 0.220069 -0.229121
H -1.034275 0.156228 -1.335219
C -0.447612 -1.077297 0.337116
H -0.496852 -1.028364 1.441145
C 1.009029 -1.267833 -0.098434
H 1.417121 -2.199058 0.330436
C 1.884796 -0.079139 0.312755
H 1.865440 -0.009242 1.417246
C 1.293385 1.217669 -0.251156
H 1.905949 2.078046 0.068306
C -2.468695 0.447823 0.227348
O -3.379989 -0.586799 -0.209668
C 3.330976 -0.270156 -0.141831
H -0.570395 2.342730 -0.252239
H -1.055901 -1.939793 0.021756
H 1.051400 -1.371898 -1.199021
H 1.343149 1.175441 -1.355373
H -2.520569 0.438438 1.326783
H -2.826654 1.429249 -0.128076
H -3.369442 -0.573265 -1.179398
H 3.963365 0.575565 0.172563
H 3.763305 -1.193382 0.276039
H 3.378974 -0.339352 -1.241401
el energy= -388.86795343009
zpe= -388.637602
th energy= -388.627801
th enthalpy= -388.626857
free energy= -388.671853

4mchm_5/coords
t3
C 0.383406 -1.258226 0.001494
H 0.829723 -2.157562 0.459488
C 1.015822 -0.000003 0.608262
H 0.796596 -0.000006 1.693774
C 0.383402 1.258220 0.001497
H 0.829726 2.157549 0.459498
C -1.136522 1.254761 0.197571
H -1.366418 1.284480 1.279348
C -1.782167 0.000000 -0.402056
H -1.577042 0.000002 -1.489722
C -1.136519 -1.254766 0.197566
H -1.583689 -2.156799 -0.254092
C 2.532688 0.000000 0.498271
O 2.911872 0.000012 -0.898652
C -3.295050 0.000004 -0.187262
H 0.608621 -1.293714 -1.078351
H 0.608623 1.293713 -1.078344
H -1.583692 2.156797 -0.254082
H -1.366422 -1.284496 1.279344
H 2.945342 0.895235 0.993793
H 2.945350 -0.895236 0.993780
H 3.880370 -0.000022 -0.928865
H -3.526658 0.000034 0.891034
H -3.762877 0.891505 -0.634740
H -3.762889 -0.891512 -0.634697
el energy= -388.86670158568
zpe= -388.636404
th energy= -388.626612
th enthalpy= -388.625668
free energy= -388.670699

4mchm_6/coords
t4
C 0.157791 1.420716 0.187352
H 0.208372 1.514881 1.287935
C 1.031632 0.238320 -0.249052
H 1.019982 0.184498 -1.354170
C 0.459123 -1.067973 0.313244
H 1.063040 -1.930265 -0.017459
C -0.999937 -1.265359 -0.111313

H -1.049896 -1.360552 -1.212209
C -1.880105 -0.086253 0.317477
H -1.854973 -0.027835 1.422485
C -1.301106 1.220464 -0.236293
H -1.359704 1.190727 -1.340443
C 2.470149 0.466974 0.196923
O 3.395142 -0.521403 -0.313291
C -3.327426 -0.283017 -0.131202
H 0.555820 2.357308 -0.238610
H 0.519760 -1.029594 1.417136
H -1.397130 -2.202997 0.313466
H -1.916349 2.073078 0.098374
H 2.839463 1.429915 -0.184823
H 2.518458 0.488742 1.300045
H 3.126856 -1.379940 0.048030
H -3.964498 0.553644 0.197510
H -3.381100 -0.338761 -1.231268
H -3.749959 -1.214847 0.277510
el energy= -388.86830810723
zpe= -388.637822
th energy= -388.628080
th enthalpy= -388.627135
free energy= -388.671956

4mchm_7/coords
t5
C 0.381659 1.265745 0.008513
H 0.611434 1.287716 1.087904
C 1.021339 0.020625 -0.615293
H 0.812516 0.035154 -1.703196
C 0.391322 -1.251355 -0.034754
H 0.616237 -1.310999 1.045959
C -1.129463 -1.249750 -0.223408
H -1.363493 -1.261537 -1.304532
C -1.776503 -0.008272 0.401044
H -1.565644 -0.025703 1.487464
C -1.138969 1.258511 -0.181429
H -1.587722 2.151269 0.286875
C 2.541948 0.023279 -0.490774
O 3.014672 0.051815 0.876778
C -3.290495 -0.011505 0.194617
H 0.822049 2.173734 -0.438191

H 0.838496 -2.140324 -0.512202
H -1.570462 -2.161614 0.214255
H -1.374337 1.304583 -1.261408
H 2.963104 -0.855184 -1.008949
H 2.956642 0.929465 -0.956166
H 2.758544 -0.787172 1.289136
H -3.750980 -0.914605 0.626292
H -3.760272 0.867902 0.663482
H -3.528514 0.009129 -0.882045
el energy= -388.86742780359
zpe= -388.637091
th energy= -388.627309
th enthalpy= -388.626365
free energy= -388.671294

4mchm_19/coords
t6
C 0.252019 -1.078935 0.705855
H -0.359204 -1.176259 1.618779
C 0.920423 0.306650 0.715734
H 1.435619 0.443237 1.683591
C -0.146378 1.407020 0.574915
H -0.769828 1.409588 1.484346
C -1.035270 1.199395 -0.660564
H -1.809761 1.984648 -0.697234
C -1.703596 -0.186777 -0.670396
H -2.199370 -0.317103 -1.648793
C -0.633505 -1.284342 -0.531322
H -0.005006 -1.291921 -1.438531
C 1.983166 0.453709 -0.366301
O 3.042002 -0.499883 -0.103257
C -2.784525 -0.306775 0.410346
H 1.017146 -1.869799 0.756110
H 0.340840 2.395763 0.524004
H -0.427133 1.311802 -1.574292
H -1.120751 -2.273143 -0.478501
H 1.570520 0.271500 -1.370296
H 2.393401 1.477496 -0.340577
H 3.691156 -0.408253 -0.817196
H -3.553539 0.471461 0.279235
H -3.282278 -1.288067 0.351302
H -2.371840 -0.201551 1.424516

el energy= -388.86278458904
zpe= -388.631639
th energy= -388.622069
th enthalpy= -388.621124
free energy= -388.665668

4mchm_21/coords
t7
C 0.132587 1.397830 0.577476
H -0.361988 2.383063 0.527668
C -0.927943 0.288808 0.690099
H -1.461093 0.414769 1.651324
C -0.254656 -1.093776 0.678065
H 0.337647 -1.203272 1.601943
C 0.655472 -1.281505 -0.544338
H 0.043762 -1.285226 -1.462923
C 1.719209 -0.174768 -0.654960
H 2.233662 -0.293291 -1.625158
C 1.038830 1.205475 -0.647462
H 0.440228 1.315738 -1.568005
C -1.981297 0.437521 -0.407019
O -3.083092 -0.486230 -0.245316
C 2.780958 -0.294709 0.444609
H 0.743236 1.397807 1.495626
H -1.020062 -1.886144 0.700971
H 1.149063 -2.267172 -0.491648
H 1.806437 1.997896 -0.671303
H -2.363811 1.472853 -0.410947
H -1.572075 0.221934 -1.402593
H -3.471403 -0.306293 0.625697
H 2.348215 -0.204918 1.451901
H 3.290050 -1.270112 0.384723
H 3.543914 0.492950 0.336432
el energy= -388.86336532909
zpe= -388.632074
th energy= -388.622587
th enthalpy= -388.621643
free energy= -388.665867

4mchm_22/coords
t8
C 0.154096 1.429095 0.552117

H -0.326723 2.419822 0.476853
C -0.921842 0.340740 0.720229
H -1.427983 0.496012 1.689825
C -0.267225 -1.051218 0.727165
H 0.347832 -1.142474 1.637809
C 0.606178 -1.286080 -0.512831
H 1.077179 -2.282168 -0.452327
C 1.692325 -0.206573 -0.666598
H 2.187022 -0.358316 -1.642411
C 1.043478 1.188756 -0.677840
H 1.829246 1.962295 -0.723312
C -1.994109 0.481891 -0.359854
O -3.091436 -0.446044 -0.185412
C 2.770044 -0.326297 0.417399
H 0.777231 1.450829 1.461597
H -1.037142 -1.837856 0.802007
H -0.028047 -1.291875 -1.416420
H 0.440972 1.296461 -1.595514
H -2.447414 1.481950 -0.296508
H -1.573028 0.361942 -1.369699
H -2.746603 -1.333890 -0.365964
H 3.555390 0.432335 0.269563
H 2.359266 -0.189509 1.428564
H 3.246619 -1.319091 0.380508
el energy= -388.86346878355
zpe= -388.632154
th energy= -388.622634
th enthalpy= -388.621690
free energy= -388.665988

4mchm_24/coords
t9
C -0.088856 1.273865 0.734990
H 0.626396 1.394279 1.566126
C -0.917691 0.000116 0.993628
H -1.185207 0.000217 2.067245
C -0.088884 -1.273698 0.735220
H 0.626380 -1.393971 1.566366
C 0.689599 -1.255418 -0.588779
H 1.322155 -2.158105 -0.652041
C 1.566816 -0.000074 -0.726151
H 2.005652 -0.000170 -1.739924

C 0.689651 1.255331 -0.588991
H -0.014076 1.293434 -1.434719
C -2.280993 0.000069 0.312132
O -2.165048 -0.000164 -1.132043
C 2.728895 -0.000017 0.273318
H -0.753773 2.154321 0.767607
H -0.753819 -2.154134 0.768006
H -0.014138 -1.293637 -1.434492
H 1.322243 2.157981 -0.652399
H -2.843074 -0.894404 0.632441
H -2.842993 0.894693 0.632163
H -3.069980 -0.000226 -1.480425
H 2.380812 0.000064 1.316519
H 3.361276 -0.891164 0.130901
H 3.361300 0.891092 0.130769
el energy= -388.85814924681
zpe= -388.627363
th energy= -388.617640
th enthalpy= -388.616696
free energy= -388.661528

4mchm_9/coords
c1
C -0.479182 -0.833121 1.111706
H -1.210223 -1.656061 1.150395
C -1.151023 0.452955 0.602507
H -1.923974 0.759327 1.330012
C -0.111018 1.581627 0.497799
H -0.582374 2.491369 0.088415
C 1.102533 1.178505 -0.350172
H 0.798929 1.009957 -1.399019
C 1.764170 -0.098314 0.181902
H 2.115155 0.107425 1.211628
C 0.731613 -1.229292 0.257932
H 1.202437 -2.134997 0.677351
C -1.864126 0.256153 -0.729510
O -2.932688 -0.703001 -0.539205
C 2.964434 -0.497723 -0.674750
H -0.138947 -0.658154 2.147859
H 0.236334 1.828998 1.516162
H 1.838440 2.000789 -0.360780
H 0.410789 -1.485769 -0.767989

H -2.286347 1.218498 -1.065101
H -1.177858 -0.111014 -1.507872
H -3.377231 -0.807924 -1.394066
H 2.644011 -0.702189 -1.709934
H 3.718170 0.305372 -0.704283
H 3.449784 -1.406359 -0.283628
el energy= -388.86546818054
zpe= -388.634682
th energy= -388.625032
th enthalpy= -388.624088
free energy= -388.668862

4mchm_11/coords
c2
C -0.323943 -1.103817 0.052053
H -1.009726 -1.917019 -0.233536
C -0.941736 0.255650 -0.295749
H -1.129452 0.288180 -1.386216
C 0.035123 1.385371 0.055783
H -0.399791 2.357735 -0.231300
C 1.383245 1.192275 -0.649749
H 1.221208 1.261256 -1.740328
C 2.020032 -0.169978 -0.327139
H 2.902022 -0.294614 -0.980232
C 1.024471 -1.295565 -0.654343
H 0.849752 -1.311645 -1.745227
C -2.263810 0.481804 0.416546
O -3.217008 -0.515182 -0.023171
C 2.510708 -0.244215 1.123393
H -0.195854 -1.161475 1.147781
H 0.177559 1.408673 1.150605
H 2.076856 2.004774 -0.373502
H 1.460689 -2.272095 -0.382701
H -2.117749 0.403354 1.508087
H -2.650789 1.488622 0.185740
H -4.044817 -0.348847 0.452743
H 2.993717 -1.215192 1.318491
H 3.248609 0.548978 1.324637
H 1.689295 -0.128381 1.845560
el energy= -388.86510945055
zpe= -388.634491
th energy= -388.624719

th enthalpy= -388.623775
free energy= -388.668850

4mchm_13/coords
c3
C -0.031868 1.384369 0.054490
H -0.178402 1.411022 1.148846
C 0.945353 0.251576 -0.286459
H 1.142189 0.281587 -1.376505
C 0.323485 -1.105707 0.058502
H 1.010610 -1.919874 -0.221691
C -1.020720 -1.296110 -0.656168
H -0.839751 -1.311999 -1.746081
C -2.016784 -0.169331 -0.334324
H -2.896067 -0.294051 -0.991009
C -1.377726 1.192204 -0.655684
H -2.071549 2.005608 -0.382318
C 2.264704 0.483242 0.438044
O 3.276592 -0.502311 0.127384
C -2.513259 -0.241839 1.114381
H 0.406516 2.355153 -0.233075
H 0.188190 -1.162765 1.153410
H -1.460001 -2.272096 -0.387455
H -1.212081 1.260480 -1.745750
H 2.648181 1.491736 0.206436
H 2.112971 0.412381 1.525946
H 3.440866 -0.443065 -0.826876
H -2.994267 -1.213765 1.309732
H -1.695081 -0.121964 1.839556
H -3.254176 0.549675 1.311073
el energy= -388.86555646658
zpe= -388.634820
th energy= -388.625082
th enthalpy= -388.624138
free energy= -388.669137

4mchm_15/coords
c4
C -0.484795 -0.848323 1.095804
H -0.156527 -0.684171 2.137531
C -1.155934 0.439265 0.591942
H -1.939925 0.735125 1.314151

C -0.121575 1.575018 0.509150
H -0.593856 2.485860 0.102872
C 1.100167 1.183957 -0.333082
H 0.804902 1.023718 -1.385663
C 1.763295 -0.095140 0.191720
H 2.107013 0.102402 1.225502
C 0.735484 -1.231445 0.249776
H 1.207120 -2.138457 0.665463
C -1.854952 0.253753 -0.754130
O -2.908019 -0.736519 -0.705076
C 2.970474 -0.482204 -0.660977
H -1.213766 -1.674040 1.117426
H 0.215740 1.815949 1.532452
H 1.833049 2.008972 -0.331420
H 0.424512 -1.480721 -0.780950
H -2.270078 1.220834 -1.086676
H -1.163621 -0.104072 -1.527945
H -3.538547 -0.440757 -0.029659
H 2.656961 -0.679017 -1.699775
H 3.721506 0.323748 -0.679133
H 3.456685 -1.392507 -0.274781
el energy= -388.86602984488
zpe= -388.635259
th energy= -388.625596
th enthalpy= -388.624652
free energy= -388.669379

4mchm_16/coords
c5
C -0.225575 1.260607 -0.183950
H -0.734371 2.156562 -0.579433
C -0.943735 -0.000002 -0.682232
H -0.896739 -0.000001 -1.788941
C -0.225579 -1.260605 -0.183941
H -0.294105 -1.311624 0.914845
C 1.245473 -1.258113 -0.619841
H 1.757642 -2.160638 -0.244580
C 1.989115 -0.000004 -0.139286
H 2.991575 -0.000010 -0.602875
C 1.245479 1.258104 -0.619850
H 1.286057 1.296626 -1.723366
C -2.423819 0.000003 -0.334024

O -2.576066 -0.000012 1.106507
C 2.187968 0.000006 1.380741
H -0.294100 1.311637 0.914837
H -0.734383 -2.156558 -0.579420
H 1.286049 -1.296637 -1.723358
H 1.757652 2.160628 -0.244589
H -2.911352 0.895348 -0.756073
H -2.911349 -0.895345 -0.756086
H -3.527522 0.000095 1.291614
H 2.752885 -0.891340 1.697832
H 2.752942 0.891328 1.697805
H 1.231687 0.000048 1.924029
el energy= -388.86444614484
zpe= -388.633526
th energy= -388.623894
th enthalpy= -388.622950
free energy= -388.667614

4mchm_17/coords
c6
C -0.221380 1.279868 -0.112867
H -0.722455 2.201372 -0.456170
C -0.949838 0.057850 -0.684652
H -0.913653 0.125133 -1.790148
C -0.238485 -1.238225 -0.273753
H -0.303629 -1.367998 0.820612
C 1.234667 -1.217218 -0.702660
H 1.738408 -2.145982 -0.384590
C 1.983641 0.002475 -0.139170
H 2.988599 0.024631 -0.596686
C 1.250866 1.292920 -0.544141
H 1.768417 2.167232 -0.113449
C -2.431022 0.041603 -0.320551
O -2.675533 -0.009440 1.105043
C 2.173538 -0.093981 1.379174
H -0.293014 1.267189 0.987010
H -0.752060 -2.102084 -0.730211
H 1.278950 -1.184962 -1.806123
H 1.295972 1.398444 -1.643070
H -2.916476 0.967738 -0.661800
H -2.930195 -0.811594 -0.811359
H -2.334281 -0.858754 1.423841

H 2.738669 0.774244 1.754441
H 1.214101 -0.126146 1.915959
H 2.734984 -1.004697 1.643120
el energy= -388.86520303104
zpe= -388.634455
th energy= -388.624704
th enthalpy= -388.623760
free energy= -388.668787

4mchm_23/coords
c7
C 0.425205 -1.269875 -0.923214
H 1.051951 -2.154623 -0.717118
C 1.291399 0.001417 -0.843771
H 1.944275 0.002799 -1.737002
C 0.425023 1.272790 -0.919452
H 1.051657 2.157018 -0.710801
C -0.799244 1.251234 0.005355
H -0.486679 1.275652 1.062184
C -1.653264 0.000298 -0.224537
H -1.981101 0.001920 -1.282290
C -0.799211 -1.251313 0.001515
H -0.486827 -1.279061 1.058304
C 2.297356 -0.000236 0.300848
O 1.649216 -0.002790 1.596236
C -2.889745 -0.001031 0.672910
H 0.062856 -1.370866 -1.961895
H 0.062526 1.376773 -1.957789
H -1.408911 2.153895 -0.174231
H -1.408798 -2.153430 -0.181048
H 2.939126 -0.894136 0.213796
H 2.938564 0.894377 0.217000
H 2.358078 -0.003635 2.258393
H -3.512398 0.890713 0.496219
H -3.512217 -0.892465 0.494010
H -2.590939 -0.002308 1.734454
el energy= -388.86083965669
zpe= -388.630659
th energy= -388.620736
th enthalpy= -388.619791
free energy= -388.665329

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.335588 -1.094787 0.028861
H 1.020019 -1.905319 -0.273979
C 0.943995 0.272764 -0.303519
H 1.128427 0.320823 -1.393723
C -0.039138 1.390306 0.069257
H -0.176549 1.396281 1.164969
C -1.389642 1.199487 -0.632426
H -1.234051 1.286097 -1.722617
C -2.015484 -0.171701 -0.326800
H -2.899602 -0.293012 -0.977568
C -1.014421 -1.286085 -0.674964
H -1.442555 -2.269249 -0.415129
C 2.269461 0.500182 0.411602
O 3.306469 -0.428937 0.017700
C -2.498406 -0.270665 1.124832
H 0.213124 -1.169798 1.124324
H 0.389118 2.369493 -0.204898
H -2.087427 2.002753 -0.340094
H -0.843559 -1.285376 -1.766429
H 2.666678 1.495559 0.164676
H 2.117021 0.448021 1.503936
H 3.034502 -1.308698 0.320354
H -3.238889 0.515878 1.341814
H -2.975970 -1.246778 1.307233
H -1.673757 -0.162183 1.844474
el energy= -388.86598053518
zpe= -388.634879
th energy= -388.625301
th enthalpy= -388.624356
free energy= -388.668870

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.495163 -0.815335 1.110430
H 1.229117 -1.637790 1.158053
C 1.158541 0.472629 0.595335
H 1.931038 0.785923 1.320044
C 0.110717 1.594216 0.486025
H -0.230244 1.852262 1.503963
C -1.107623 1.178992 -0.349722

H -0.813147 1.010353 -1.400984
C -1.755844 -0.101608 0.189517
H -2.101284 0.102360 1.221431
C -0.713663 -1.223839 0.259995
H -1.174220 -2.134251 0.680301
C 1.871662 0.272094 -0.740950
O 2.971654 -0.665420 -0.651500
C -2.958746 -0.511792 -0.658341
H 0.157328 -0.640855 2.147211
H 0.575566 2.501549 0.063386
H -1.849501 1.995906 -0.355139
H -0.393410 -1.475865 -0.767358
H 1.175223 -0.055474 -1.527614
H 2.326351 1.220928 -1.061161
H 2.589983 -1.540356 -0.482160
H -3.718787 0.285456 -0.683953
H -2.643959 -0.715536 -1.695364
H -3.434535 -1.423387 -0.262384
el energy= -388.86614434696
zpe= -388.635056
th energy= -388.625539
th enthalpy= -388.624595
free energy= -388.668896

CCSD 6-31G(d') gas phase

4mchm_1/coords
t1
C 0.158790 1.431854 0.177901
H 0.549214 2.367360 -0.259167
C 1.038336 0.240683 -0.241675
H 1.037447 0.176380 -1.345962
C 0.465424 -1.072999 0.317415
H 1.085934 -1.917764 -0.016002
C -1.000571 -1.272711 -0.100692
H -1.395309 -2.207890 0.332658
C -1.888926 -0.086531 0.316298
H -1.869258 -0.023003 1.421680
C -1.307547 1.226684 -0.238638
H -1.920510 2.081263 0.096209
C 2.487015 0.453240 0.192139
O 3.267540 -0.622902 -0.313470

C -3.344294 -0.287387 -0.128588
H 0.211703 1.551371 1.276279
H 0.530088 -1.046657 1.421852
H -1.055853 -1.390182 -1.199135
H -1.373833 1.206948 -1.342381
H 2.854774 1.423695 -0.195324
H 2.538176 0.495574 1.298640
H 4.173923 -0.511806 -0.004695
H -3.408985 -0.356099 -1.226984
H -3.765796 -1.214565 0.291206
H -3.981408 0.551598 0.193928
el energy= -388.44418524

4mchm_3/coords
t2
C -0.159196 1.432196 0.177389
H -0.211231 1.552719 1.275431
C -1.039869 0.239301 -0.234476
H -1.027464 0.176293 -1.342585
C -0.463318 -1.071983 0.325002
H -0.524409 -1.040120 1.428923
C 1.000651 -1.273687 -0.098388
H 1.397000 -2.207382 0.336348
C 1.889622 -0.085738 0.313226
H 1.873073 -0.020522 1.418405
C 1.306458 1.226829 -0.241900
H 1.919720 2.081757 0.091157
C -2.493987 0.451583 0.204436
O -3.360143 -0.606208 -0.185169
C 3.343668 -0.287034 -0.135631
H -0.552380 2.366680 -0.259330
H -1.086735 -1.920498 0.004561
H 1.053705 -1.394005 -1.196883
H 1.371373 1.206525 -1.345857
H -2.551447 0.485787 1.303589
H -2.864278 1.424568 -0.174809
H -3.373437 -0.632803 -1.149822
H 3.981313 0.552645 0.183717
H 3.766655 -1.213246 0.284657
H 3.405503 -0.357534 -1.234105
el energy= -388.44448212

4mchm_5/coords
t3
C 0.393996 -1.264791 0.033465
H 0.826302 -2.164003 0.506552
C 1.033960 -0.000002 0.634740
H 0.839025 0.000000 1.725496
C 0.393992 1.264789 0.033465
H 0.826300 2.163999 0.506556
C -1.134282 1.260426 0.203846
H -1.386519 1.306134 1.280206
C -1.778627 -0.000002 -0.401212
H -1.563331 0.000000 -1.487087
C -1.134280 -1.260430 0.203843
H -1.570220 -2.163579 -0.257191
C 2.553608 0.000002 0.464701
O 2.853848 0.000014 -0.926529
C -3.301857 0.000002 -0.210604
H 0.651372 -1.316038 -1.036918
H 0.651371 1.316039 -1.036915
H -1.570227 2.163573 -0.257184
H -1.386521 -1.306147 1.280203
H 2.982153 0.894174 0.958640
H 2.982157 -0.894173 0.958628
H 3.812051 -0.000069 -1.030074
H -3.559609 0.000018 0.861384
H -3.762071 0.890948 -0.666780
H -3.762082 -0.890948 -0.666761
el energy= -388.44412658

4mchm_6/coords
t4
C 0.157950 1.428856 0.179794
H 0.219153 1.536439 1.279025
C 1.041051 0.247327 -0.259566
H 1.038771 0.195927 -1.364367
C 0.467435 -1.074626 0.281687
H 1.064458 -1.926861 -0.084903
C -1.003667 -1.269680 -0.122393
H -1.068704 -1.371205 -1.221543
C -1.886979 -0.089371 0.319793
H -1.854906 -0.038904 1.425518
C -1.311663 1.229496 -0.227078

H -1.388501 1.221853 -1.330164
C 2.494410 0.467060 0.181041
O 3.387060 -0.535447 -0.285728
C -3.346697 -0.288222 -0.111341
H 0.546314 2.369110 -0.248278
H 0.546166 -1.076354 1.385967
H -1.392376 -2.211227 0.302184
H -1.921283 2.080045 0.123285
H 2.872384 1.413398 -0.234954
H 2.538254 0.553525 1.285461
H 3.199616 -1.348840 0.195940
H -3.980696 0.546254 0.227955
H -3.423580 -0.344132 -1.209614
H -3.762587 -1.220494 0.302691
el energy= -388.44408594

4mchm_7/coords
t5
C 0.389143 1.271549 -0.012002
H 0.654332 1.309310 1.057709
C 1.035927 0.021505 -0.633857
H 0.839073 0.032905 -1.724279
C 0.396087 -1.254331 -0.054901
H 0.625522 -1.318323 1.024679
C -1.131791 -1.255720 -0.229589
H -1.376839 -1.280597 -1.307719
C -1.781159 -0.009976 0.399822
H -1.569434 -0.032667 1.486370
C -1.139862 1.265383 -0.176544
H -1.577287 2.156030 0.306452
C 2.562498 0.028901 -0.463329
O 2.982778 0.044421 0.895826
C -3.303870 -0.012281 0.205236
H 0.816539 2.179511 -0.471508
H 0.835125 -2.149670 -0.530164
H -1.564567 -2.170294 0.211112
H -1.394951 1.335632 -1.250715
H 3.004082 -0.833862 -0.999793
H 2.983838 0.943369 -0.908108
H 2.789439 -0.819617 1.276966
H -3.762044 -0.914172 0.641435
H -3.768017 0.867155 0.679001

H -3.558871 0.009754 -0.867065
el energy= -388.44420953

4mchm_19/coords
t6
C 0.280884 -1.077885 0.684209
H -0.298908 -1.204235 1.614454
C 0.934884 0.319933 0.699648
H 1.447222 0.449535 1.669271
C -0.136793 1.421911 0.557653
H -0.740361 1.444989 1.480533
C -1.063395 1.204123 -0.655361
H -1.840919 1.987275 -0.673469
C -1.725383 -0.191533 -0.656873
H -2.228671 -0.323323 -1.631982
C -0.643245 -1.286566 -0.530596
H -0.038390 -1.300107 -1.454118
C 2.027307 0.458710 -0.365970
O 3.027974 -0.515664 -0.093038
C -2.809101 -0.319058 0.429623
H 1.067820 -1.846269 0.697973
H 0.345156 2.412723 0.485925
H -0.485797 1.325864 -1.588319
H -1.122131 -2.278836 -0.466698
H 1.615125 0.319660 -1.382172
H 2.450317 1.481471 -0.319205
H 3.701413 -0.459730 -0.780475
H -3.589480 0.446801 0.293794
H -3.294599 -1.306745 0.380032
H -2.402538 -0.201571 1.444760
el energy= -388.43843574

4mchm_21/coords
t7
C 0.133649 1.422357 0.556087
H -0.352472 2.410676 0.478285
C -0.935770 0.317080 0.690347
H -1.441875 0.451378 1.667190
C -0.284351 -1.081645 0.676768
H 0.285070 -1.218439 1.611804
C 0.648282 -1.286172 -0.532227
H 0.048436 -1.298313 -1.458509

C 1.730037 -0.190082 -0.647891
H 2.241332 -0.321069 -1.618742
C 1.065464 1.204073 -0.652506
H 0.491387 1.322845 -1.587784
C -2.027547 0.456471 -0.384981
O -3.054835 -0.518489 -0.259931
C 2.804383 -0.316403 0.447937
H 0.732417 1.450374 1.481911
H -1.073057 -1.849382 0.671524
H 1.126765 -2.278336 -0.466457
H 1.840980 1.989076 -0.668093
H -2.449346 1.480365 -0.347467
H -1.620022 0.312285 -1.394848
H -3.461423 -0.404987 0.608219
H 2.388913 -0.200965 1.459816
H 3.292439 -1.302930 0.401458
H 3.584247 0.451256 0.319943
el energy= -388.43908527

4mchm_22/coords
t8
C 0.135826 1.430201 0.546797
H -0.348530 2.418537 0.461259
C -0.937925 0.331603 0.704313
H -1.445619 0.470006 1.675036
C -0.274157 -1.062226 0.706376
H 0.315476 -1.170693 1.631939
C 0.637966 -1.290420 -0.514306
H 1.114881 -2.283043 -0.443848
C 1.720724 -0.197807 -0.656006
H 2.218573 -0.341663 -1.631920
C 1.059921 1.198304 -0.666016
H 1.838876 1.979492 -0.692999
C -2.039031 0.466564 -0.362854
O -3.116904 -0.440071 -0.164637
C 2.809098 -0.316734 0.426778
H 0.741126 1.468292 1.468206
H -1.045500 -1.849388 0.759747
H 0.029713 -1.308409 -1.436222
H 0.481230 1.312062 -1.598885
H -2.485444 1.470448 -0.294786
H -1.628718 0.364689 -1.384014

H -2.816946 -1.321404 -0.413380
H 3.592925 0.442086 0.274045
H 2.409902 -0.179521 1.442395
H 3.288756 -1.307832 0.390023
el energy= -388.43793751

4mchm_24/coords
t9
C -0.109648 1.274287 0.766653
H 0.596199 1.381334 1.608497
C -0.952928 0.000198 1.005727
H -1.252387 0.000367 2.071475
C -0.109692 -1.273989 0.767043
H 0.596180 -1.380791 1.608898
C 0.675980 -1.262113 -0.558579
H 1.310149 -2.164466 -0.615108
C 1.550369 -0.000124 -0.718805
H 1.951773 -0.000286 -1.748528
C 0.676081 1.261981 -0.558936
H -0.035224 1.309692 -1.395734
C -2.287810 0.000098 0.253429
O -2.084282 -0.000275 -1.156048
C 2.759259 -0.000041 0.235404
H -0.763584 2.162966 0.804340
H -0.763652 -2.162637 0.805031
H -0.035359 -1.309987 -1.395342
H 1.310329 2.164264 -0.615689
H -2.867765 -0.892979 0.559526
H -2.867655 0.893399 0.559082
H -2.948935 -0.000402 -1.583068
H 2.460312 0.000120 1.294219
H 3.387071 -0.890353 0.069706
H 3.387141 0.890173 0.069457
el energy= -388.43722974

4mchm_9/coords
c1
C -0.497818 -0.849269 1.078448
H -1.240869 -1.660268 1.071904
C -1.159690 0.456200 0.591375
H -1.926650 0.749280 1.329808
C -0.113041 1.585762 0.494862

H -0.574386 2.499749 0.081468
C 1.122706 1.190234 -0.335439
H 0.843787 1.047694 -1.395249
C 1.775666 -0.102982 0.186596
H 2.118156 0.089857 1.221947
C 0.735687 -1.237158 0.243585
H 1.198227 -2.146575 0.664471
C -1.909177 0.267574 -0.731467
O -2.926559 -0.704711 -0.519836
C 2.995353 -0.496543 -0.658115
H -0.184012 -0.709565 2.128588
H 0.217283 1.841792 1.517123
H 1.858467 2.012884 -0.321289
H 0.432688 -1.498569 -0.786561
H -2.348216 1.236586 -1.040448
H -1.223803 -0.054421 -1.536710
H -3.379934 -0.856593 -1.356863
H 2.697821 -0.698871 -1.700346
H 3.748559 0.307392 -0.673790
H 3.477237 -1.405601 -0.264430
el energy= -388.44148258

4mchm_11/coords
c2
C -0.344843 -1.100337 0.047911
H -1.046800 -1.894534 -0.245973
C -0.954425 0.272477 -0.286643
H -1.153894 0.304793 -1.374374
C 0.032342 1.402321 0.059305
H -0.392054 2.378807 -0.232112
C 1.388327 1.198795 -0.641023
H 1.235465 1.282073 -1.732088
C 2.021575 -0.175300 -0.332391
H 2.890988 -0.301452 -1.002903
C 1.011234 -1.298281 -0.652465
H 0.843451 -1.323973 -1.744396
C -2.292434 0.482038 0.418670
O -3.193331 -0.526051 -0.022318
C 2.549337 -0.260878 1.111486
H -0.223404 -1.180392 1.143501
H 0.173455 1.440782 1.154353
H 2.085641 2.006848 -0.360269

H 1.440041 -2.278144 -0.380377
H -2.142983 0.429122 1.515884
H -2.683933 1.491701 0.184887
H -4.025508 -0.418439 0.452152
H 3.033783 -1.233839 1.291405
H 3.295751 0.527032 1.301419
H 1.749966 -0.146991 1.858338
el energy= -388.44129567

4mchm_13/coords
c3
C -0.031705 1.402247 0.060417
H -0.176144 1.440086 1.154803
C 0.955821 0.270761 -0.277418
H 1.146662 0.305902 -1.370514
C 0.342371 -1.100395 0.054109
H 1.045857 -1.898948 -0.226502
C -1.009269 -1.299275 -0.654043
H -0.836996 -1.326369 -1.745505
C -2.020023 -0.174728 -0.339653
H -2.886009 -0.300849 -1.014464
C -1.384920 1.199272 -0.645683
H -2.083029 2.007320 -0.367332
C 2.296928 0.479381 0.436469
O 3.261467 -0.517827 0.126485
C -2.554928 -0.259360 1.101647
H 0.395809 2.378248 -0.227952
H 0.215020 -1.176431 1.148745
H -1.440243 -2.278263 -0.382789
H -1.228243 1.283268 -1.736308
H 2.689603 1.491201 0.213352
H 2.153745 0.417458 1.526604
H 3.448955 -0.459209 -0.818429
H -3.039836 -1.232314 1.279947
H -1.759814 -0.144201 1.852775
H -3.302715 0.528301 1.286626
el energy= -388.44159756

4mchm_15/coords
c4
C -0.500727 -0.861138 1.066747
H -0.197834 -0.736762 2.121846

C -1.160160 0.447342 0.585630
H -1.923378 0.742603 1.333052
C -0.118002 1.582188 0.502003
H -0.581869 2.494962 0.088835
C 1.121153 1.193046 -0.325694
H 0.845586 1.053837 -1.386591
C 1.775346 -0.100206 0.194149
H 2.110124 0.088151 1.232923
C 0.738921 -1.237972 0.236129
H 1.200817 -2.149260 0.653211
C -1.905894 0.264704 -0.747423
O -2.908089 -0.742025 -0.686690
C 3.001687 -0.485265 -0.644738
H -1.239991 -1.676053 1.037757
H 0.207353 1.836257 1.526321
H 1.853945 2.018027 -0.305800
H 0.440788 -1.492473 -0.796699
H -2.340374 1.234821 -1.060066
H -1.226794 -0.057743 -1.548317
H -3.544974 -0.479904 -0.010284
H 2.711402 -0.682689 -1.689807
H 3.752226 0.321174 -0.650769
H 3.483735 -1.394933 -0.252903
el energy= -388.44209375

4mchm_16/coords
c5
C -0.241952 1.267515 -0.212939
H -0.737907 2.162582 -0.627918
C -0.966503 0.000000 -0.703779
H -0.945923 -0.000003 -1.811782
C -0.241950 -1.267513 -0.212935
H -0.344455 -1.334744 0.880941
C 1.242226 -1.261669 -0.620931
H 1.744760 -2.166321 -0.237252
C 1.987991 0.000000 -0.135930
H 2.989629 -0.000001 -0.603190
C 1.242227 1.261672 -0.620930
H 1.308940 1.310747 -1.723239
C -2.439945 -0.000004 -0.295474
O -2.514721 -0.000016 1.126174
C 2.197819 0.000000 1.389326

H -0.344459 1.334751 0.880937
H -0.737908 -2.162577 -0.627914
H 1.308935 -1.310742 -1.723241
H 1.744760 2.166323 -0.237246
H -2.941648 0.894291 -0.714596
H -2.941646 -0.894297 -0.714610
H -3.444177 0.000115 1.381076
H 2.765933 -0.890129 1.703830
H 2.765942 0.890124 1.703828
H 1.247520 0.000006 1.942546
el energy= -388.44147644

4mchm_17/coords
c6
C -0.236941 1.284578 -0.125654
H -0.728884 2.207529 -0.478440
C -0.970873 0.058266 -0.697302
H -0.947877 0.124412 -1.803369
C -0.247677 -1.240156 -0.291166
H -0.318377 -1.371271 0.802774
C 1.234228 -1.218308 -0.707084
H 1.732763 -2.149750 -0.388056
C 1.990054 0.004548 -0.144035
H 2.986744 0.030165 -0.620579
C 1.247219 1.300606 -0.534151
H 1.754651 2.172869 -0.087455
C -2.451325 0.044114 -0.288530
O -2.650743 -0.016172 1.119121
C 2.217189 -0.099548 1.375228
H -0.342936 1.280650 0.970692
H -0.750537 -2.111513 -0.747354
H 1.290095 -1.194620 -1.810330
H 1.312037 1.429199 -1.629978
H -2.937273 0.977555 -0.611558
H -2.972648 -0.792529 -0.793851
H -2.414254 -0.902493 1.415223
H 2.805329 0.757932 1.738943
H 1.274178 -0.115163 1.941025
H 2.771683 -1.018197 1.625512
el energy= -388.44144242

4mchm_23/coords

c7
C 0.460868 -1.270732 -0.942258
H 1.076588 -2.164673 -0.740631
C 1.332195 0.000341 -0.826477
H 2.027093 0.000684 -1.688235
C 0.460843 1.271496 -0.941271
H 1.076551 2.165286 -0.738943
C -0.780111 1.261166 -0.030299
H -0.466417 1.306188 1.023371
C -1.636102 0.000082 -0.245042
H -1.984935 0.000476 -1.296968
C -0.780072 -1.261137 -0.031256
H -0.466368 -1.306957 1.022380
C 2.261452 -0.000132 0.391639
O 1.517864 -0.000704 1.606269
C -2.869072 -0.000273 0.669568
H 0.124413 -1.356944 -1.991567
H 0.124416 1.358528 -1.990523
H -1.387909 2.161292 -0.230408
H -1.387835 -2.161133 -0.232047
H 2.915058 -0.893207 0.339217
H 2.914961 0.893057 0.339982
H 2.143884 -0.000740 2.339824
H -3.494348 0.890920 0.499383
H -3.494323 -0.891359 0.498733
H -2.563750 -0.000659 1.728653
el energy= -388.44027072

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.348276 -1.096872 0.009710
H 1.031739 -1.895686 -0.324744
C 0.956769 0.282685 -0.302914
H 1.152849 0.330957 -1.390518
C -0.033852 1.402090 0.065879
H -0.163439 1.427252 1.162729
C -1.397261 1.207514 -0.622032
H -1.258195 1.306373 -1.713527
C -2.024049 -0.171532 -0.324118
H -2.901948 -0.291549 -0.984316
C -1.016805 -1.286809 -0.676536
H -1.438901 -2.272518 -0.415842

C 2.299444 0.494057 0.408932
O 3.298603 -0.441517 0.026672
C -2.530768 -0.280800 1.125664
H 0.242069 -1.207741 1.104723
H 0.387697 2.382303 -0.216196
H -2.092226 2.010110 -0.321068
H -0.860786 -1.292216 -1.770161
H 2.708590 1.482621 0.150332
H 2.143541 0.480623 1.506599
H 3.058062 -1.300120 0.392337
H -3.277132 0.501385 1.337134
H -3.009354 -1.257968 1.298315
H -1.721905 -0.173686 1.863327
el energy= -388.44121140

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.494144 -0.832735 1.092367
H 1.229681 -1.654492 1.127380
C 1.165204 0.464095 0.593144
H 1.929853 0.759727 1.332813
C 0.116432 1.591772 0.489760
H -0.213683 1.858499 1.509470
C -1.119413 1.190979 -0.338586
H -0.840968 1.044957 -1.397685
C -1.772596 -0.100437 0.187437
H -2.117275 0.094716 1.221547
C -0.731749 -1.233484 0.251772
H -1.193716 -2.142380 0.674061
C 1.920925 0.273989 -0.733967
O 2.988169 -0.660987 -0.634259
C -2.989383 -0.500252 -0.658387
H 0.170996 -0.679543 2.137143
H 0.579135 2.500661 0.067260
H -1.856062 2.012596 -0.326933
H -0.426412 -1.495457 -0.778123
H 1.234948 -0.005528 -1.554192
H 2.392699 1.226437 -1.020259
H 2.607938 -1.544800 -0.579910
H -3.743373 0.302572 -0.678160
H -2.689536 -0.705244 -1.699346
H -3.470958 -1.408387 -0.262229

el energy= -388.44100145

CCSD-SMD 6-31G(d')

4mchm_1/coords
t1
C 0.162458 1.422616 0.178425
H 0.560556 2.353936 -0.259541
C 1.037602 0.228296 -0.241900
H 1.033666 0.168418 -1.346808
C 0.453885 -1.081218 0.317737
H 1.058044 -1.939810 -0.015051
C -1.013334 -1.273179 -0.099584
H -1.412219 -2.205569 0.336058
C -1.893993 -0.082196 0.317433
H -1.874984 -0.018415 1.422283
C -1.304210 1.225907 -0.238886
H -1.911838 2.084059 0.096382
C 2.482364 0.446287 0.201358
O 3.297238 -0.606392 -0.324853
C -3.347944 -0.274627 -0.132285
H 0.217604 1.539083 1.276499
H 0.520486 -1.053107 1.421364
H -1.069379 -1.388774 -1.198029
H -1.369973 1.203642 -1.342510
H 2.845458 1.425332 -0.161791
H 2.536882 0.457988 1.305821
H 4.194350 -0.474818 0.007714
H -3.409037 -0.338904 -1.231451
H -3.777043 -1.200700 0.283483
H -3.981450 0.567455 0.190619
el energy= -388.45091042

4mchm_3/coords
t2
C -0.163520 1.425484 0.176491
H -0.214705 1.546545 1.274341
C -1.041088 0.229648 -0.233451
H -1.042068 0.165695 -1.339692
C -0.456992 -1.078418 0.326466
H -0.518458 -1.047729 1.430346
C 1.008005 -1.273549 -0.096686

H 1.408224 -2.205039 0.339668
C 1.891000 -0.081888 0.314193
H 1.874438 -0.014579 1.418870
C 1.301703 1.225477 -0.244771
H 1.911735 2.083649 0.086128
C -2.487527 0.449471 0.217855
O -3.373130 -0.596001 -0.195489
C 3.343828 -0.277339 -0.137835
H -0.562842 2.355428 -0.263531
H -1.066297 -1.935605 -0.001177
H 1.059661 -1.391760 -1.195104
H 1.364308 1.199670 -1.348507
H -2.541031 0.467796 1.317933
H -2.854211 1.424946 -0.151487
H -3.360547 -0.611643 -1.161818
H 3.978831 0.565195 0.180926
H 3.772796 -1.202392 0.280329
H 3.402747 -0.345490 -1.236886
el energy= -388.45194568

4mchm_5/coords
t3
C 0.387065 -1.264159 0.014666
H 0.824473 -2.163351 0.482357
C 1.026832 -0.000004 0.617097
H 0.818748 -0.000003 1.704299
C 0.387062 1.264155 0.014668
H 0.824477 2.163342 0.482362
C -1.139886 1.261096 0.195783
H -1.381287 1.306562 1.274108
C -1.789065 -0.000002 -0.402182
H -1.586567 0.000003 -1.490275
C -1.139887 -1.261102 0.195777
H -1.579182 -2.162986 -0.264581
C 2.548661 0.000000 0.481177
O 2.906180 0.000012 -0.904889
C -3.308618 0.000005 -0.191386
H 0.626732 -1.315686 -1.060979
H 0.626729 1.315685 -1.060975
H -1.579191 2.162980 -0.264566
H -1.381292 -1.306580 1.274101
H 2.968070 0.892292 0.981263

H 2.968075 -0.892297 0.981248
H 3.870563 -0.000023 -0.954897
H -3.551062 0.000035 0.884455
H -3.775852 0.891052 -0.641230
H -3.775861 -0.891061 -0.641184
el energy= -388.45052003

4mchm_6/coords
t4
C 0.159451 1.426349 0.182746
H 0.219926 1.532282 1.281668
C 1.038948 0.241296 -0.253990
H 1.032941 0.190865 -1.359242
C 0.463627 -1.077056 0.293722
H 1.064659 -1.932489 -0.058124
C -1.005541 -1.271074 -0.116589
H -1.067342 -1.374322 -1.215843
C -1.888482 -0.088493 0.319155
H -1.861966 -0.035961 1.424429
C -1.308836 1.227912 -0.227956
H -1.381627 1.216425 -1.331268
C 2.488065 0.465784 0.189605
O 3.394565 -0.525427 -0.305192
C -3.344626 -0.283267 -0.122310
H 0.551760 2.363852 -0.247605
H 0.538544 -1.065843 1.397208
H -1.397428 -2.209987 0.311108
H -1.918278 2.079706 0.120046
H 2.856056 1.426869 -0.201767
H 2.539748 0.512379 1.293181
H 3.210242 -1.349841 0.162046
H -3.979930 0.551129 0.216515
H -3.413770 -0.333430 -1.221726
H -3.765686 -1.216928 0.284606
el energy= -388.45166890

4mchm_7/coords
t5
C 0.388477 1.266957 -0.008721
H 0.635101 1.305459 1.066070
C 1.031863 0.012324 -0.624821
H 0.831528 0.022806 -1.713732

C 0.391126 -1.260618 -0.041330
H 0.627231 -1.327477 1.036113
C -1.136231 -1.256871 -0.217593
H -1.380281 -1.286567 -1.295779
C -1.784356 -0.005522 0.401239
H -1.576845 -0.020631 1.488275
C -1.139173 1.264240 -0.182447
H -1.577183 2.159267 0.292367
C 2.558120 0.016828 -0.475292
O 3.007197 0.065297 0.883777
C -3.304725 -0.005074 0.197488
H 0.822423 2.172718 -0.467039
H 0.828690 -2.154081 -0.519863
H -1.572535 -2.166242 0.230581
H -1.386259 1.324117 -1.258758
H 2.987837 -0.865636 -0.983488
H 2.976755 0.915089 -0.955172
H 2.787393 -0.779528 1.296777
H -3.767852 -0.904789 0.634203
H -3.771630 0.876967 0.665053
H -3.552546 0.012565 -0.876969
el energy= -388.45159785

4mchm_19/coords
t6
C 0.262485 -1.085322 0.690314
H -0.327731 -1.197131 1.615452
C 0.933609 0.304820 0.705837
H 1.443523 0.434039 1.677583
C -0.132626 1.412570 0.566725
H -0.741484 1.430662 1.486128
C -1.050604 1.205558 -0.653824
H -1.822089 1.994561 -0.674420
C -1.725263 -0.183244 -0.662134
H -2.223682 -0.309945 -1.640064
C -0.654146 -1.287912 -0.531035
H -0.043255 -1.304820 -1.450175
C 2.019036 0.449052 -0.365188
O 3.056944 -0.500869 -0.095701
C -2.813433 -0.303656 0.419376
H 1.030694 -1.874029 0.716017
H 0.358121 2.398969 0.500827

H -0.461945 1.322035 -1.580021
H -1.143273 -2.275280 -0.466504
H 1.614852 0.285208 -1.377962
H 2.428049 1.475790 -0.333690
H 3.702851 -0.434976 -0.810811
H -3.582601 0.474742 0.287345
H -3.313920 -1.283829 0.358650
H -2.408005 -0.200248 1.436821
el energy= -388.44558018

4mchm_21/coords
t7
C 0.123607 1.409045 0.565034
H -0.371088 2.393278 0.495255
C -0.939319 0.296273 0.682652
H -1.461340 0.418616 1.650708
C -0.270138 -1.093887 0.665160
H 0.301540 -1.221450 1.599696
C 0.667169 -1.284549 -0.542468
H 0.071677 -1.293982 -1.471706
C 1.737657 -0.176754 -0.647054
H 2.253778 -0.296094 -1.616623
C 1.058614 1.209732 -0.643447
H 0.481693 1.326697 -1.577073
C -2.018247 0.440767 -0.401362
O -3.086063 -0.499230 -0.241663
C 2.806271 -0.300708 0.453361
H 0.719609 1.427438 1.492805
H -1.043904 -1.878050 0.664689
H 1.156900 -2.271607 -0.478719
H 1.827523 2.001414 -0.651294
H -2.416847 1.471982 -0.386414
H -1.615545 0.257958 -1.407217
H -3.477237 -0.338765 0.628096
H 2.381984 -0.205679 1.463902
H 3.311224 -1.278686 0.395156
H 3.574858 0.481253 0.340781
el energy= -388.44673913

4mchm_22/coords
t8
C 0.140242 1.434076 0.545536

H -0.343344 2.422606 0.457421
C -0.935142 0.338395 0.709931
H -1.438712 0.486284 1.682155
C -0.275599 -1.057066 0.715800
H 0.320185 -1.157195 1.638365
C 0.627627 -1.290388 -0.509460
H 1.102351 -2.284096 -0.436724
C 1.713400 -0.202528 -0.659101
H 2.207887 -0.350680 -1.635972
C 1.057441 1.195225 -0.670495
H 1.839652 1.973247 -0.701150
C -2.029477 0.475298 -0.360747
O -3.106983 -0.449950 -0.172059
C 2.801948 -0.321725 0.422111
H 0.749400 1.468907 1.464374
H -1.048187 -1.842187 0.769982
H 0.009543 -1.307922 -1.424131
H 0.472766 1.306121 -1.599628
H -2.481796 1.476708 -0.290639
H -1.620849 0.368545 -1.379105
H -2.785862 -1.325863 -0.420494
H 3.584357 0.440190 0.273087
H 2.401024 -0.191184 1.438217
H 3.284810 -1.311609 0.379268
el energy= -388.44624391

4mchm_24/coords
t9
C -0.101946 1.274707 0.751478
H 0.601941 1.385485 1.593900
C -0.943529 0.000153 0.995111
H -1.227774 0.000281 2.064215
C -0.101985 -1.274482 0.751775
H 0.601912 -1.385082 1.594218
C 0.696867 -1.263268 -0.565694
H 1.335536 -2.162832 -0.612543
C 1.569742 -0.000098 -0.722110
H 1.982230 -0.000218 -1.747237
C 0.696935 1.263156 -0.565975
H 0.001522 1.324539 -1.416730
C -2.297479 0.000087 0.278792
O -2.160352 -0.000213 -1.146183

C 2.766495 -0.000027 0.244976
H -0.758363 2.161728 0.782933
H -0.758425 -2.161477 0.783458
H 0.001430 -1.324788 -1.416427
H 1.335663 2.162677 -0.613007
H -2.868911 -0.891112 0.598447
H -2.868808 0.891482 0.598085
H -3.052154 -0.000332 -1.517926
H 2.454417 0.000091 1.299827
H 3.395974 -0.890458 0.084158
H 3.396015 0.890343 0.083978
el energy= -388.44257096

4mchm_9/coords
c1
C -0.482005 -0.858752 1.085742
H -1.211189 -1.684112 1.092110
C -1.157402 0.441136 0.600519
H -1.923771 0.732950 1.341088
C -0.116086 1.576078 0.508627
H -0.586590 2.488107 0.102416
C 1.114461 1.190777 -0.332442
H 0.824939 1.046523 -1.388738
C 1.779628 -0.098339 0.182545
H 2.129468 0.093701 1.215195
C 0.748218 -1.239432 0.243120
H 1.218702 -2.145369 0.662995
C -1.898965 0.260589 -0.727018
O -2.957305 -0.684479 -0.530746
C 2.992123 -0.482574 -0.674681
H -0.161631 -0.713545 2.132808
H 0.218701 1.824003 1.531271
H 1.845409 2.017701 -0.320131
H 0.440912 -1.498000 -0.786020
H -2.314447 1.233145 -1.049317
H -1.223610 -0.091396 -1.524519
H -3.388869 -0.817978 -1.384400
H 2.686551 -0.678075 -1.716082
H 3.742880 0.324145 -0.689944
H 3.481154 -1.392868 -0.291240
el energy= -388.44846947

4mchm_11/coords
c2
C -0.332852 -1.106867 0.045258
H -1.018142 -1.916831 -0.250090
C -0.953285 0.260483 -0.293480
H -1.145484 0.293947 -1.382871
C 0.027306 1.394885 0.055775
H -0.404361 2.367243 -0.237401
C 1.385604 1.200384 -0.640885
H 1.234946 1.281240 -1.732367
C 2.027263 -0.168282 -0.329343
H 2.900176 -0.289335 -0.995758
C 1.025568 -1.297083 -0.652917
H 0.859508 -1.321826 -1.745043
C -2.287251 0.477140 0.416156
O -3.218890 -0.517855 -0.020852
C 2.545783 -0.251259 1.116969
H -0.212760 -1.180525 1.140866
H 0.163329 1.429304 1.151077
H 2.076778 2.012555 -0.356696
H 1.459192 -2.274058 -0.377774
H -2.142805 0.413257 1.510707
H -2.675238 1.487062 0.188522
H -4.034913 -0.392122 0.480227
H 3.036729 -1.221414 1.297735
H 3.285498 0.542140 1.312391
H 1.739845 -0.144201 1.858093
el energy= -388.44820327

4mchm_13/coords
c3
C -0.027086 1.396793 0.053231
H -0.166383 1.433927 1.148111
C 0.955825 0.261820 -0.287410
H 1.155140 0.295002 -1.376921
C 0.336312 -1.106175 0.046129
H 1.025767 -1.913161 -0.248565
C -1.019530 -1.297581 -0.656468
H -0.850565 -1.320432 -1.748235
C -2.023225 -0.170070 -0.333998
H -2.895722 -0.292974 -1.000618
C -1.383745 1.199601 -0.646080

H -2.076835 2.010780 -0.363567
C 2.287099 0.482183 0.436067
O 3.270611 -0.513535 0.137671
C -2.542273 -0.253184 1.112229
H 0.405101 2.368858 -0.240549
H 0.213013 -1.183268 1.141152
H -1.453073 -2.275344 -0.383941
H -1.231638 1.279702 -1.737418
H 2.681589 1.487480 0.198945
H 2.135096 0.432360 1.525970
H 3.445387 -0.465486 -0.811877
H -3.030721 -1.224514 1.293553
H -1.737116 -0.143384 1.853762
H -3.284195 0.538410 1.306629
el energy= -388.44922582

4mchm_15/coords
c4
C -0.493290 -0.861655 1.073439
H -0.183257 -0.724079 2.124583
C -1.162430 0.439961 0.587432
H -1.935874 0.729078 1.324244
C -0.122957 1.577506 0.508303
H -0.590645 2.488680 0.096482
C 1.116196 1.193732 -0.321201
H 0.837721 1.054096 -1.381071
C 1.775762 -0.098375 0.193887
H 2.116677 0.088126 1.230524
C 0.743197 -1.239192 0.239101
H 1.209426 -2.148230 0.656955
C -1.893304 0.263084 -0.751925
O -2.915616 -0.737023 -0.695232
C 2.995341 -0.479360 -0.654765
H -1.225438 -1.684667 1.066839
H 0.200839 1.826932 1.534095
H 1.847716 2.019921 -0.298305
H 0.443489 -1.490679 -0.794077
H -2.327065 1.231826 -1.061877
H -1.210809 -0.062182 -1.549159
H -3.534686 -0.471800 -0.001728
H 2.698294 -0.670707 -1.699418
H 3.746546 0.327065 -0.660820

H 3.480905 -1.391403 -0.271033
el energy= -388.44963824

4mchm_16/coords
c5
C -0.234525 1.266370 -0.196954
H -0.735882 2.162202 -0.602827
C -0.960217 0.000015 -0.688772
H -0.927811 0.000028 -1.795469
C -0.234531 -1.266356 -0.196985
H -0.315798 -1.331356 0.899920
C 1.245812 -1.262201 -0.618591
H 1.752227 -2.165521 -0.236755
C 1.995938 -0.000002 -0.142168
H 2.993237 0.000000 -0.617608
C 1.245819 1.262215 -0.618558
H 1.299296 1.311724 -1.721133
C -2.440659 0.000010 -0.311095
O -2.570498 -0.000034 1.115352
C 2.220213 -0.000021 1.380011
H -0.315793 1.331345 0.899953
H -0.735897 -2.162172 -0.602881
H 1.299285 -1.311678 -1.721168
H 1.752239 2.165521 -0.236693
H -2.936057 0.892422 -0.735789
H -2.936054 -0.892384 -0.735835
H -3.514350 0.000042 1.320222
H 2.791393 -0.890558 1.689250
H 2.791426 0.890489 1.689265
H 1.275421 -0.000007 1.943397
el energy= -388.44789089

4mchm_17/coords
c6
C -0.238151 1.275334 -0.155600
H -0.737547 2.186532 -0.528499
C -0.966653 0.029949 -0.692373
H -0.941653 0.068417 -1.798907
C -0.239644 -1.255107 -0.252335
H -0.312934 -1.364992 0.843411
C 1.241215 -1.235342 -0.672258
H 1.745960 -2.154182 -0.327256

C 1.991568 0.005945 -0.144251
H 2.989541 0.023617 -0.617870
C 1.243488 1.286548 -0.572060
H 1.749359 2.173654 -0.153135
C -2.449333 0.020032 -0.300952
O -2.671895 0.033974 1.113861
C 2.213666 -0.054140 1.377225
H -0.324484 1.298446 0.942794
H -0.741416 -2.135181 -0.690906
H 1.294450 -1.239830 -1.775861
H 1.300844 1.380042 -1.671539
H -2.944380 0.925850 -0.684037
H -2.952572 -0.854271 -0.752995
H -2.364062 -0.810598 1.466380
H 2.786776 0.822201 1.721247
H 1.268201 -0.073341 1.939221
H 2.782152 -0.957465 1.652679
el energy= -388.44897019

4mchm_23/coords
c7
C 0.429634 -1.322261 -0.859391
H 1.048485 -2.200900 -0.607315
C 1.304861 -0.047997 -0.839040
H 1.961853 -0.095486 -1.727575
C 0.434871 1.221220 -0.990362
H 1.057067 2.118663 -0.829028
C -0.803548 1.257995 -0.076042
H -0.499289 1.363241 0.977564
C -1.661681 -0.010222 -0.224288
H -2.004205 -0.064462 -1.275857
C -0.807365 -1.258931 0.054759
H -0.501356 -1.254209 1.113202
C 2.300925 0.010930 0.322761
O 1.649229 0.093309 1.594270
C -2.896668 0.037797 0.684492
H 0.079255 -1.475721 -1.895899
H 0.086037 1.269255 -2.037524
H -1.410562 2.147226 -0.320884
H -1.417812 -2.166841 -0.094208
H 2.941891 -0.889624 0.288824
H 2.957737 0.889471 0.182853

H 2.341607 0.131921 2.267327
H -3.518897 0.921800 0.469459
H -3.524622 -0.858391 0.552868
H -2.597197 0.086407 1.744698
el energy= -388.44544946

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.343579 -1.099332 0.021395
H 1.027888 -1.904193 -0.295980
C 0.955231 0.276543 -0.299487
H 1.146614 0.324259 -1.388351
C -0.031559 1.399577 0.067789
H -0.163424 1.420088 1.163986
C -1.391936 1.206702 -0.625579
H -1.246681 1.302526 -1.716554
C -2.023729 -0.169716 -0.328559
H -2.899385 -0.287682 -0.991895
C -1.017425 -1.288283 -0.672607
H -1.443508 -2.271529 -0.408525
C 2.293211 0.493966 0.413930
O 3.307566 -0.435079 0.017132
C -2.534223 -0.274691 1.119230
H 0.231191 -1.194238 1.116281
H 0.393995 2.377964 -0.214635
H -2.086752 2.010846 -0.327700
H -0.856039 -1.296931 -1.765548
H 2.691572 1.490577 0.168295
H 2.145505 0.453364 1.509136
H 3.060804 -1.302396 0.361945
H -3.276604 0.512563 1.328771
H -3.019683 -1.249492 1.289542
H -1.724914 -0.173705 1.857501
el energy= -388.44903082

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.495767 -0.835359 1.092015
H 1.228514 -1.659543 1.115785
C 1.163990 0.463021 0.593224
H 1.930320 0.763545 1.330115
C 0.115378 1.590802 0.493071

H -0.214197 1.851488 1.514312
C -1.118852 1.190165 -0.336032
H -0.836759 1.041899 -1.393617
C -1.771380 -0.101243 0.189279
H -2.118274 0.092819 1.222536
C -0.730275 -1.233289 0.251728
H -1.191579 -2.142081 0.675335
C 1.907745 0.275507 -0.738091
O 2.992634 -0.654742 -0.636325
C -2.984264 -0.499666 -0.661024
H 0.174531 -0.681473 2.137341
H 0.579119 2.499612 0.071559
H -1.855829 2.011675 -0.322893
H -0.420825 -1.492032 -0.776938
H 1.225187 -0.032145 -1.547374
H 2.364374 1.231457 -1.038018
H 2.613014 -1.538315 -0.551637
H -3.741594 0.300838 -0.676675
H -2.681444 -0.697304 -1.702816
H -3.464278 -1.412134 -0.271433
el energy= -388.44913056

MP2 d-aug-cc-pVDZ gas phase

4mchm_1/coords
t1
C 0.156135 1.427812 0.181017
H 0.550833 2.364218 -0.251589
C 1.032679 0.238730 -0.242804
H 1.027225 0.173688 -1.348371
C 0.462557 -1.070212 0.323499
H 1.083933 -1.918588 -0.003375
C -0.999193 -1.269170 -0.102802
H -1.397892 -2.205832 0.325216
C -1.884721 -0.085959 0.317298
H -1.859869 -0.019923 1.423465
C -1.305363 1.221719 -0.244487
H -1.922768 2.076954 0.082686
C 2.474703 0.459373 0.196083
O 3.271679 -0.627651 -0.311285
C -3.336549 -0.287247 -0.128676
H 0.202492 1.534504 1.282123

H 0.520374 -1.029185 1.429098
H -1.048348 -1.373734 -1.204208
H -1.362461 1.187457 -1.349760
H 2.843644 1.424306 -0.198042
H 2.522182 0.491807 1.301721
H 4.188769 -0.476349 -0.046919
H -3.391395 -0.357172 -1.228401
H -3.757937 -1.214816 0.291514
H -3.973697 0.553597 0.190358
el energy= -388.57309787841
zpe= -388.342354
th energy= -388.332558
th enthalpy= -388.331614
free energy= -388.376631

4mchm_3/coords
t2
C -0.158455 1.424721 0.181324
H -0.203938 1.533792 1.282146
C -1.034459 0.231869 -0.233739
H -1.022774 0.168366 -1.342332
C -0.456352 -1.072865 0.332319
H -0.507535 -1.025608 1.437590
C 1.003338 -1.270540 -0.101148
H 1.406529 -2.205112 0.327034
C 1.887309 -0.084017 0.313641
H 1.866278 -0.016920 1.419739
C 1.302547 1.221688 -0.247330
H 1.918356 2.078787 0.077617
C -2.480255 0.451919 0.212452
O -3.372377 -0.600392 -0.194163
C 3.337890 -0.281924 -0.137738
H -0.557895 2.358828 -0.251901
H -1.079261 -1.925821 0.019290
H 1.049200 -1.377162 -1.202732
H 1.357549 1.186859 -1.352812
H -2.531267 0.462867 1.313208
H -2.845076 1.430112 -0.153479
H -3.406798 -0.591407 -1.161002
H 3.973831 0.561098 0.177800
H 3.763661 -1.207654 0.282060
H 3.388773 -0.352993 -1.237617

el energy= -388.57269390881
zpe= -388.341967
th energy= -388.332185
th enthalpy= -388.331241
free energy= -388.376219

4mchm_5/coords
t3
C 0.392290 -1.261585 0.025119
H 0.832561 -2.161291 0.491207
C 1.026809 0.000152 0.631990
H 0.822167 0.000094 1.722100
C 0.392290 1.261812 0.025009
H 0.831883 2.161677 0.491438
C -1.132512 1.256720 0.206609
H -1.377297 1.288593 1.286501
C -1.773394 -0.000145 -0.402572
H -1.552678 -0.000350 -1.488424
C -1.132627 -1.256762 0.207202
H -1.574959 -2.160759 -0.247698
C 2.545260 0.000290 0.480369
O 2.854718 -0.000601 -0.927422
C -3.293326 -0.000078 -0.210156
H 0.637922 -1.299268 -1.050348
H 0.638093 1.299980 -1.050395
H -1.574272 2.160596 -0.248925
H -1.377449 -1.287674 1.287200
H 2.970271 0.898354 0.966226
H 2.970633 -0.896985 0.967360
H 3.816132 -0.000432 -1.023272
H -3.542204 -0.000599 0.864831
H -3.753504 0.892415 -0.664456
H -3.753778 -0.891964 -0.665391
el energy= -388.57283131312
zpe= -388.342023
th energy= -388.332259
th enthalpy= -388.331315
free energy= -388.376240

4mchm_6/coords
t4
C 0.156982 1.423446 0.183213

H 0.210778 1.518521 1.285098
C 1.035646 0.242282 -0.259123
H 1.029561 0.190642 -1.365152
C 0.462991 -1.072012 0.293005
H 1.060951 -1.930966 -0.059550
C -1.003555 -1.266707 -0.121909
H -1.061551 -1.357892 -1.223875
C -1.883356 -0.087540 0.320046
H -1.847899 -0.033033 1.426482
C -1.307438 1.224466 -0.234428
H -1.373342 1.200726 -1.339379
C 2.480654 0.468262 0.188548
O 3.398829 -0.527911 -0.291314
C -3.339075 -0.285716 -0.114544
H 0.551418 2.363821 -0.240501
H 0.531942 -1.052663 1.398895
H -1.397961 -2.208094 0.299485
H -1.921157 2.076930 0.106144
H 2.855667 1.420794 -0.216530
H 2.518666 0.531558 1.293743
H 3.168871 -1.366134 0.131821
H -3.973292 0.550979 0.220371
H -3.404227 -0.342583 -1.214379
H -3.756154 -1.218202 0.298990
el energy= -388.57272774912
zpe= -388.341933
th energy= -388.332143
th enthalpy= -388.331199
free energy= -388.376192

4mchm_7/coords
t5
C 0.384212 1.271302 0.001835
H 0.634401 1.295056 1.077121
C 1.027543 0.026217 -0.626868
H 0.821232 0.040194 -1.717082
C 0.396019 -1.249763 -0.047219
H 0.616473 -1.305952 1.035956
C -1.128955 -1.251925 -0.233515
H -1.365918 -1.261330 -1.315195
C -1.777372 -0.011607 0.401104
H -1.561352 -0.034849 1.487811

C -1.141125 1.261866 -0.177790
H -1.587818 2.152099 0.298968
C 2.552139 0.032108 -0.478363
O 2.994106 0.038554 0.891249
C -3.296708 -0.016036 0.203578
H 0.818061 2.181184 -0.449455
H 0.843212 -2.142021 -0.522359
H -1.567082 -2.168343 0.199701
H -1.386328 1.317814 -1.256552
H 2.987532 -0.829400 -1.018768
H 2.969259 0.952114 -0.916590
H 2.789460 -0.827858 1.268193
H -3.753808 -0.920164 0.637422
H -3.762713 0.863665 0.676137
H -3.541973 0.006380 -0.871880
el energy= -388.57222119350
zpe= -388.341435
th energy= -388.331673
th enthalpy= -388.330729
free energy= -388.375654

4mchm_19/coords
t6
C 0.272005 -1.069740 0.706928
H -0.333052 -1.180188 1.623909
C 0.922548 0.327829 0.714711
H 1.437158 0.467859 1.682902
C -0.153384 1.422622 0.564381
H -0.773638 1.433408 1.477260
C -1.051741 1.198731 -0.666510
H -1.836104 1.975710 -0.700949
C -1.703954 -0.199477 -0.667880
H -2.203422 -0.338664 -1.644624
C -0.617043 -1.285650 -0.529705
H 0.010831 -1.287370 -1.438916
C 1.996981 0.469633 -0.363435
O 3.007833 -0.525804 -0.110148
C -2.783041 -0.327316 0.419494
H 1.057623 -1.840400 0.750359
H 0.324471 2.416957 0.503968
H -0.455019 1.318470 -1.588393
H -1.090965 -2.281922 -0.479068

H 1.572532 0.330732 -1.372723
H 2.432209 1.484839 -0.309300
H 3.698855 -0.427654 -0.778631
H -3.568912 0.432529 0.277595
H -3.258695 -1.320757 0.378387
H -2.370762 -0.196908 1.431501
el energy= -388.56812006149
zpe= -388.336696
th energy= -388.327068
th enthalpy= -388.326124
free energy= -388.370799

4mchm_21/coords
t7
C 0.145423 1.416081 0.567395
H -0.340090 2.406731 0.507024
C -0.925026 0.313535 0.701775
H -1.441028 0.452615 1.673132
C -0.270601 -1.081772 0.693624
H 0.321352 -1.202712 1.617827
C 0.634457 -1.286446 -0.533842
H 0.016291 -1.292263 -1.449227
C 1.713805 -0.191487 -0.657917
H 2.223393 -0.324423 -1.630096
C 1.049850 1.200929 -0.660171
H 0.454948 1.315126 -1.583883
C -1.995345 0.456410 -0.388113
O -3.053513 -0.509792 -0.266174
C 2.782797 -0.313565 0.439928
H 0.760970 1.428214 1.483486
H -1.054938 -1.855672 0.713206
H 1.115253 -2.279093 -0.478986
H 1.827070 1.984966 -0.691540
H -2.404519 1.484222 -0.368137
H -1.575753 0.285726 -1.389363
H -3.477054 -0.367342 0.592248
H 2.358457 -0.195212 1.448463
H 3.270457 -1.301047 0.397254
H 3.561139 0.456380 0.311903
el energy= -388.56802950379
zpe= -388.336577
th energy= -388.326978

th enthalpy= -388.326034
free energy= -388.370591

4mchm_22/coords
t8
C 0.150379 1.427674 0.556725
H -0.331900 2.419028 0.485341
C -0.926359 0.333957 0.717434
H -1.438925 0.480159 1.685612
C -0.265834 -1.059120 0.720838
H 0.345872 -1.158373 1.634249
C 0.615888 -1.287925 -0.519430
H 1.089233 -2.284134 -0.464159
C 1.701957 -0.201937 -0.665747
H 2.199202 -0.348816 -1.642234
C 1.048488 1.195436 -0.673220
H 1.832961 1.971794 -0.712796
C -2.005669 0.471255 -0.364577
O -3.108175 -0.433927 -0.180444
C 2.782407 -0.323192 0.420970
H 0.771399 1.451797 1.468988
H -1.034417 -1.849031 0.796409
H -0.012087 -1.291570 -1.429101
H 0.451993 1.308872 -1.595585
H -2.449386 1.477360 -0.308181
H -1.581032 0.351903 -1.376476
H -2.783703 -1.329218 -0.347313
H 3.570205 0.432284 0.268675
H 2.373638 -0.179040 1.432493
H 3.254807 -1.318493 0.389673
el energy= -388.56735852114
zpe= -388.335977
th energy= -388.326318
th enthalpy= -388.325374
free energy= -388.370086

4mchm_24/coords
t9
C -0.098885 1.275346 0.757018
H 0.618233 1.387900 1.589621
C -0.934080 -0.000089 1.007569
H -1.221259 -0.000085 2.077794

C -0.099463 -1.275846 0.756655
H 0.617272 -1.389325 1.589484
C 0.670593 -1.259147 -0.576692
H 1.303250 -2.162729 -0.643686
C 1.547832 -0.000064 -0.724467
H 1.967862 0.000050 -1.747376
C 0.670690 1.259024 -0.576556
H -0.047622 1.295161 -1.410228
C -2.279111 0.000233 0.280757
O -2.086743 0.000295 -1.149528
C 2.731939 0.000097 0.255931
H -0.759613 2.159975 0.796816
H -0.760844 -2.160050 0.795777
H -0.047653 -1.294926 -1.410403
H 1.303382 2.162539 -0.643307
H -2.851717 -0.896591 0.584356
H -2.851199 0.897337 0.584465
H -2.960795 0.000509 -1.563244
H 2.403441 0.000578 1.306595
H 3.362002 -0.891782 0.104526
H 3.362115 0.891748 0.103740
el energy= -388.56611120256
zpe= -388.334590
th energy= -388.325029
th enthalpy= -388.324085
free energy= -388.368393

4mchm_9/coords
c1
C -0.498398 -0.817728 1.112569
H -1.245193 -1.626580 1.141929
C -1.156507 0.474993 0.593355
H -1.931303 0.786960 1.317329
C -0.107695 1.598904 0.479373
H -0.569330 2.509225 0.056705
C 1.114337 1.179691 -0.356458
H 0.821617 1.011026 -1.409817
C 1.762262 -0.103847 0.187350
H 2.107968 0.105372 1.219692
C 0.716390 -1.227655 0.265055
H 1.178076 -2.137170 0.688620
C -1.876927 0.262563 -0.737939

O -2.897896 -0.732976 -0.530868
C 2.969712 -0.519252 -0.658994
H -0.163542 -0.643916 2.152018
H 0.233870 1.860242 1.497528
H 1.857506 1.996782 -0.366794
H 0.396461 -1.490733 -0.760974
H -2.329237 1.218367 -1.061786
H -1.176092 -0.069826 -1.523086
H -3.365772 -0.860646 -1.366811
H 2.653883 -0.736036 -1.693773
H 3.727310 0.280481 -0.695864
H 3.447892 -1.425749 -0.253840
el energy= -388.57085606993
zpe= -388.339772
th energy= -388.330079
th enthalpy= -388.329135
free energy= -388.374019

4mchm_11/coords
c2
C -0.338549 -1.098061 0.053011
H -1.041992 -1.895671 -0.232989
C -0.944808 0.271165 -0.290532
H -1.138436 0.302429 -1.380797
C 0.041274 1.397107 0.060476
H -0.385337 2.375369 -0.224018
C 1.390257 1.193632 -0.649334
H 1.227408 1.267704 -1.740533
C 2.017992 -0.178173 -0.330695
H 2.896509 -0.308051 -0.989476
C 1.010497 -1.298820 -0.656298
H 0.834684 -1.315578 -1.748080
C -2.275193 0.490343 0.418207
O -3.193413 -0.528680 -0.020729
C 2.518267 -0.257919 1.120566
H -0.210146 -1.164132 1.149877
H 0.188535 1.422668 1.156112
H 2.091880 2.000899 -0.374137
H 1.440860 -2.279670 -0.387409
H -2.123457 0.429462 1.513220
H -2.669142 1.494592 0.175428
H -4.041943 -0.376562 0.415960

H 2.997050 -1.231946 1.312374
H 3.261212 0.531672 1.319689
H 1.701191 -0.139381 1.848207
el energy= -388.57052943204
zpe= -388.339421
th energy= -388.329714
th enthalpy= -388.328770
free energy= -388.373595

4mchm_13/coords
c3
C -0.037473 1.393509 0.061341
H -0.188670 1.420091 1.156339
C 0.946793 0.262684 -0.279841
H 1.136609 0.295476 -1.373801
C 0.331131 -1.102133 0.061508
H 1.033660 -1.906289 -0.209632
C -1.013342 -1.300096 -0.656877
H -0.831777 -1.319979 -1.747879
C -2.018212 -0.174538 -0.339254
H -2.892852 -0.301904 -1.003567
C -1.383583 1.194787 -0.655255
H -2.083654 2.004621 -0.383984
C 2.278439 0.480186 0.438950
O 3.271780 -0.509376 0.118660
C -2.528039 -0.250429 1.108878
H 0.395603 2.369621 -0.220818
H 0.193872 -1.161866 1.157265
H -1.449580 -2.278364 -0.388431
H -1.215399 1.268168 -1.745849
H 2.662369 1.495717 0.226232
H 2.130300 0.396580 1.527745
H 3.477468 -0.416857 -0.822175
H -3.009812 -1.223115 1.299661
H -1.715819 -0.131624 1.841849
H -3.270841 0.540920 1.301074
el energy= -388.57019644773
zpe= -388.339109
th energy= -388.329413
th enthalpy= -388.328468
free energy= -388.373262

4mchm_15/coords
c4
C -0.495163 -0.844484 1.095262
H -0.173248 -0.691996 2.142044
C -1.156352 0.452206 0.591189
H -1.931572 0.756620 1.322837
C -0.115998 1.586341 0.499813
H -0.584063 2.498002 0.087096
C 1.108877 1.185143 -0.340071
H 0.816846 1.024343 -1.394778
C 1.765832 -0.097982 0.193052
H 2.104899 0.103493 1.229199
C 0.730098 -1.231894 0.251738
H 1.196639 -2.141520 0.669477
C -1.871589 0.255000 -0.751500
O -2.899939 -0.748594 -0.697969
C 2.980439 -0.493813 -0.652389
H -1.234660 -1.661489 1.096112
H 0.222359 1.837174 1.521758
H 1.845285 2.008189 -0.342139
H 0.419004 -1.487256 -0.778569
H -2.290100 1.221622 -1.090215
H -1.178244 -0.096798 -1.528129
H -3.556924 -0.455106 -0.050850
H 2.670672 -0.701825 -1.690680
H 3.731194 0.312749 -0.676974
H 3.464557 -1.400554 -0.255002
el energy= -388.57078862500
zpe= -388.339671
th energy= -388.330009
th enthalpy= -388.329065
free energy= -388.373822

4mchm_16/coords
c5
C 0.234177 -1.265296 -0.207303
H 0.736120 -2.160885 -0.615745
C 0.953172 -0.000457 -0.705672
H 0.921725 -0.001021 -1.814715
C 0.234144 1.264915 -0.208681
H 0.327347 1.322700 0.888089
C -1.245721 1.259516 -0.625085

H -1.752057 2.164716 -0.245480
C -1.983188 -0.000086 -0.128430
H -2.994051 -0.000352 -0.576865
C -1.245805 -1.260451 -0.623301
H -1.307199 -1.299177 -1.727272
C 2.428515 -0.000337 -0.315798
O 2.508765 0.000962 1.123660
C -2.155684 0.001086 1.399061
H 0.327748 -1.322148 0.889481
H 0.736250 2.160121 -0.617771
H -1.306742 1.296398 -1.729128
H -1.752048 -2.165038 -0.242140
H 2.925732 -0.898660 -0.726992
H 2.926117 0.897011 -0.728672
H 3.442259 0.001087 1.372750
H -2.715363 0.892906 1.725407
H -2.714912 -0.890479 1.726850
H -1.188697 0.001784 1.924179
el energy= -388.57070373453
zpe= -388.339488
th energy= -388.329841
th enthalpy= -388.328897
free energy= -388.373552

4mchm_17/coords
c6
C -0.225647 1.285405 -0.111493
H -0.721914 2.210523 -0.454759
C -0.955771 0.065990 -0.695818
H -0.923156 0.139997 -1.802794
C -0.241411 -1.235528 -0.295102
H -0.306675 -1.370579 0.799973
C 1.237090 -1.212505 -0.717673
H 1.738331 -2.146540 -0.407944
C 1.985906 0.003125 -0.135721
H 2.992690 0.028538 -0.592124
C 1.253993 1.301814 -0.529464
H 1.767580 2.171100 -0.082098
C -2.437305 0.048999 -0.307741
O -2.653744 -0.025529 1.113507
C 2.173231 -0.111171 1.385721
H -0.321120 1.267584 0.987011

H -0.751222 -2.100338 -0.757881
H 1.288196 -1.170412 -1.821586
H 1.312803 1.424758 -1.627247
H -2.919741 0.988090 -0.620718
H -2.953224 -0.785252 -0.819367
H -2.396411 -0.911800 1.401470
H 2.753464 0.743647 1.769361
H 1.212238 -0.127235 1.921830
H 2.717605 -1.034633 1.642567
el energy= -388.56984559793
zpe= -388.338708
th energy= -388.329037
th enthalpy= -388.328093
free energy= -388.372825

4mchm_23/coords
c7
C 0.457159 -1.271198 -0.939436
H 1.078092 -2.162083 -0.736118
C 1.325387 0.000386 -0.830196
H 2.017647 0.000862 -1.695382
C 0.457022 1.271900 -0.938561
H 1.077892 2.162700 -0.734758
C -0.776394 1.256140 -0.020030
H -0.459546 1.284860 1.035549
C -1.631683 0.000179 -0.246809
H -1.967703 0.000800 -1.304064
C -0.776713 -1.256247 -0.021361
H -0.460730 -1.286780 1.034475
C 2.264839 0.000093 0.376018
O 1.514220 -0.001046 1.608732
C -2.866437 -0.000121 0.659928
H 0.110024 -1.358018 -1.986208
H 0.109611 1.359398 -1.985188
H -1.385297 2.158515 -0.209722
H -1.385804 -2.158115 -0.212756
H 2.911629 -0.896333 0.327387
H 2.910607 0.897292 0.328537
H 2.148698 -0.000986 2.338515
H -3.489730 0.892502 0.487133
H -3.490065 -0.892369 0.486343
H -2.558160 -0.000665 1.719085

el energy= -388.56898122507
zpe= -388.337747
th energy= -388.328132
th enthalpy= -388.327187
free energy= -388.371652

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.339899 -1.095535 0.021383
H 1.024060 -1.902290 -0.296177
C 0.947765 0.277552 -0.305617
H 1.138456 0.324038 -1.395625
C -0.040575 1.395315 0.066472
H -0.177509 1.407912 1.163700
C -1.396162 1.202192 -0.632889
H -1.245223 1.290087 -1.724665
C -2.020221 -0.173348 -0.324314
H -2.905488 -0.297080 -0.974924
C -1.016817 -1.288988 -0.677056
H -1.442952 -2.273944 -0.416947
C 2.280842 0.497352 0.410893
O 3.307380 -0.431288 0.024010
C -2.503498 -0.273349 1.131378
H 0.222695 -1.184390 1.118357
H 0.385260 2.376482 -0.208455
H -2.094925 2.005436 -0.339774
H -0.850813 -1.289539 -1.770195
H 2.684371 1.490359 0.159441
H 2.120310 0.464423 1.506410
H 3.038212 -1.308449 0.328520
H -3.245864 0.511795 1.348601
H -2.977996 -1.250762 1.316457
H -1.679036 -0.160920 1.851702
el energy= -388.57016404773
zpe= -388.339002
th energy= -388.329303
th enthalpy= -388.328359
free energy= -388.373154

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.494893 -0.810653 1.118649

H 1.231867 -1.631074 1.181562
C 1.162387 0.476509 0.596817
H 1.936355 0.787259 1.321954
C 0.112294 1.600328 0.482248
H -0.229115 1.867955 1.498974
C -1.110395 1.182299 -0.353511
H -0.818579 1.015290 -1.407037
C -1.759781 -0.101150 0.188230
H -2.105871 0.105439 1.220920
C -0.714721 -1.225730 0.265334
H -1.176293 -2.136357 0.686362
C 1.884925 0.266746 -0.740359
O 2.969606 -0.673828 -0.654752
C -2.966170 -0.516231 -0.659664
H 0.153010 -0.632895 2.154769
H 0.576544 2.507114 0.055044
H -1.853223 1.999461 -0.361510
H -0.394938 -1.483702 -0.762486
H 1.181474 -0.035551 -1.535507
H 2.351387 1.213770 -1.053180
H 2.587820 -1.548855 -0.502202
H -3.722875 0.284085 -0.695876
H -2.649551 -0.731336 -1.694445
H -3.445463 -1.422698 -0.255791
el energy= -388.57015302152
zpe= -388.339108
th energy= -388.329389
th enthalpy= -388.328445
free energy= -388.373358

MP2-SMD d-aug-cc-pVDZ

4mchm_1/coords
t1
C 0.160414 1.417751 0.182270
H 0.563607 2.349418 -0.251687
C 1.031644 0.224478 -0.242356
H 1.022852 0.164385 -1.348284
C 0.450086 -1.079549 0.324859
H 1.054536 -1.941622 -0.001791
C -1.012875 -1.269901 -0.101442
H -1.416732 -2.203151 0.329304

C -1.889883 -0.081206 0.318431
H -1.866701 -0.014768 1.424047
C -1.301120 1.220798 -0.244732
H -1.912742 2.079833 0.082923
C 2.468499 0.451289 0.205753
O 3.302935 -0.610335 -0.322991
C -3.339967 -0.272707 -0.133789
H 0.208201 1.521156 1.283181
H 0.508893 -1.036036 1.429672
H -1.061865 -1.372210 -1.202939
H -1.357130 1.183291 -1.349826
H 2.832588 1.425244 -0.164310
H 2.520496 0.452163 1.309491
H 4.212694 -0.425972 -0.042821
H -3.389880 -0.338503 -1.234390
H -3.770431 -1.198516 0.282489
H -3.972652 0.572243 0.184908
el energy= -388.57879138180
zpe= -388.349094
th energy= -388.339186
th enthalpy= -388.338241
free energy= -388.383537

4mchm_3/coords
t2
C -0.163718 1.417217 0.181180
H -0.207453 1.527600 1.281691
C -1.036339 0.220253 -0.229980
H -1.038446 0.156282 -1.337000
C -0.448665 -1.080202 0.336856
H -0.499041 -1.033092 1.441901
C 1.011513 -1.270428 -0.098341
H 1.419401 -2.201974 0.332387
C 1.888947 -0.079168 0.314222
H 1.869551 -0.009430 1.419659
C 1.296310 1.220344 -0.251011
H 1.908303 2.081409 0.070979
C -2.473589 0.447760 0.229890
O -3.386909 -0.586869 -0.211198
C 3.337709 -0.270418 -0.142388
H -0.570738 2.345590 -0.256381
H -1.056555 -1.943300 0.018990

H 1.054767 -1.375138 -1.199816
H 1.347952 1.178900 -1.356194
H -2.524451 0.434075 1.330237
H -2.832652 1.430915 -0.122112
H -3.373838 -0.570883 -1.181347
H 3.970821 0.575938 0.171816
H 3.770341 -1.194653 0.275144
H 3.384303 -0.339444 -1.242938
el energy= -388.57909591211
zpe= -388.349242
th energy= -388.339393
th enthalpy= -388.338449
free energy= -388.383539

4mchm_5/coords
t3
C 0.384957 -1.261136 0.004968
H 0.829966 -2.160457 0.466642
C 1.019087 0.000292 0.612168
H 0.801620 0.000437 1.698872
C 0.384824 1.261515 0.004684
H 0.829771 2.160957 0.466301
C -1.138707 1.257445 0.198503
H -1.370972 1.288069 1.280767
C -1.784573 -0.000155 -0.403419
H -1.577532 -0.000267 -1.491675
C -1.138502 -1.257530 0.198816
H -1.584215 -2.160076 -0.255605
C 2.538832 0.000205 0.497396
O 2.911734 -0.000408 -0.904003
C -3.300753 -0.000124 -0.189976
H 0.611814 -1.299279 -1.075503
H 0.611887 1.299461 -1.075762
H -1.584893 2.159727 -0.255943
H -1.370803 -1.288249 1.281099
H 2.954038 0.896628 0.990196
H 2.953919 -0.895882 0.990924
H 3.880363 -0.000542 -0.939427
H -3.533550 0.000142 0.888967
H -3.768152 0.892117 -0.638548
H -3.768126 -0.892596 -0.638123
el energy= -388.57808520869

zpe= -388.348255
th energy= -388.338418
th enthalpy= -388.337473
free energy= -388.382623

4mchm_6/coords
t4
C 0.158471 1.423971 0.187927
H 0.209550 1.518238 1.289442
C 1.034018 0.238976 -0.250210
H 1.021004 0.185865 -1.356309
C 0.460417 -1.070316 0.313185
H 1.064393 -1.933161 -0.018978
C -1.002039 -1.267845 -0.111458
H -1.052513 -1.363136 -1.213365
C -1.884123 -0.086353 0.318729
H -1.858504 -0.027921 1.424626
C -1.303658 1.223081 -0.236271
H -1.361914 1.193238 -1.341437
C 2.475548 0.468272 0.196275
O 3.400912 -0.523521 -0.312618
C -3.334193 -0.283696 -0.131511
H 0.556290 2.361109 -0.239402
H 0.521220 -1.032227 1.418098
H -1.399098 -2.205954 0.314714
H -1.919096 2.076313 0.099412
H 2.845758 1.430915 -0.187777
H 2.524735 0.491831 1.300275
H 3.129839 -1.381118 0.050075
H -3.972038 0.553216 0.197609
H -3.387051 -0.338699 -1.232528
H -3.756521 -1.216877 0.276492
el energy= -388.57945155478
zpe= -388.349462
th energy= -388.339664
th enthalpy= -388.338720
free energy= -388.383661

4mchm_7/coords
t5
C 0.382215 1.269427 0.008597
H 0.612629 1.292979 1.088922

C 1.024013 0.022003 -0.616825
H 0.815191 0.037410 -1.705714
C 0.392924 -1.253659 -0.036700
H 0.618520 -1.316255 1.044804
C -1.131206 -1.252096 -0.224824
H -1.365822 -1.263054 -1.306859
C -1.779994 -0.008859 0.402362
H -1.568570 -0.027097 1.489647
C -1.141893 1.261417 -0.180604
H -1.590385 2.154014 0.290456
C 2.547745 0.025378 -0.490822
O 3.019099 0.048492 0.879539
C -3.296969 -0.012797 0.194988
H 0.821251 2.177961 -0.440632
H 0.839403 -2.142087 -0.517965
H -1.571410 -2.165198 0.213364
H -1.378026 1.308834 -1.261423
H 2.971084 -0.851479 -1.011740
H 2.962350 0.934800 -0.952163
H 2.758882 -0.791527 1.288237
H -3.757178 -0.917249 0.626236
H -3.767622 0.866949 0.664272
H -3.534099 0.008185 -0.882794
el energy= -388.57857293455
zpe= -388.348746
th energy= -388.338898
th enthalpy= -388.337954
free energy= -388.383038

4mchm_19/coords
t6
C 0.252785 -1.079213 0.710748
H -0.361872 -1.174850 1.622747
C 0.921913 0.309760 0.719490
H 1.436031 0.448492 1.688606
C -0.147409 1.412146 0.575194
H -0.771823 1.416830 1.485210
C -1.037916 1.201627 -0.662899
H -1.815524 1.985192 -0.698381
C -1.704637 -0.188973 -0.672944
H -2.199564 -0.320938 -1.652568
C -0.631024 -1.287366 -0.531195

H 0.000646 -1.294919 -1.437505
C 1.986790 0.456552 -0.365245
O 3.041097 -0.506775 -0.109052
C -2.788228 -0.309784 0.409546
H 1.019093 -1.870102 0.764965
H 0.340529 2.401484 0.521340
H -0.429792 1.316263 -1.577625
H -1.118238 -2.277207 -0.477952
H 1.571608 0.283435 -1.370718
H 2.403813 1.478147 -0.332748
H 3.701282 -0.398939 -0.810911
H -3.560300 0.465930 0.274384
H -3.282218 -1.294089 0.353033
H -2.376103 -0.199026 1.424372
el energy= -388.57430583263
zpe= -388.343648
th energy= -388.333994
th enthalpy= -388.333049
free energy= -388.377791

4mchm_21/coords
t7
C 0.132527 1.400901 0.579478
H -0.363496 2.386418 0.528677
C -0.929900 0.289015 0.692619
H -1.464266 0.415244 1.654159
C -0.255031 -1.096625 0.680453
H 0.339014 -1.206150 1.604493
C 0.656115 -1.284584 -0.545284
H 0.042838 -1.289483 -1.464053
C 1.721522 -0.175013 -0.657024
H 2.235625 -0.293692 -1.628453
C 1.040347 1.208462 -0.648438
H 0.440979 1.320443 -1.569546
C -1.983702 0.437905 -0.408582
O -3.088202 -0.485888 -0.246675
C 2.785735 -0.295128 0.444670
H 0.744140 1.401533 1.498217
H -1.021135 -1.889779 0.703372
H 1.151452 -2.270384 -0.491593
H 1.809617 2.000639 -0.670954
H -2.365640 1.474265 -0.414098

H -1.572799 0.220540 -1.404115
H -3.472627 -0.308958 0.627180
H 2.352605 -0.204417 1.452736
H 3.294358 -1.271744 0.384702
H 3.549280 0.493033 0.335325
el energy= -388.57474341515
zpe= -388.343871
th energy= -388.334350
th enthalpy= -388.333406
free energy= -388.377698

4mchm_22/coords
t8
C 0.154698 1.433473 0.552765
H -0.327335 2.424465 0.475070
C -0.923658 0.342939 0.723053
H -1.429615 0.499838 1.693528
C -0.268199 -1.052366 0.730613
H 0.349130 -1.143021 1.641009
C 0.605177 -1.288986 -0.513101
H 1.076671 -2.285867 -0.451825
C 1.694242 -0.207980 -0.668552
H 2.188429 -0.360790 -1.645518
C 1.045614 1.191037 -0.679823
H 1.833394 1.963905 -0.724986
C -1.997751 0.483835 -0.359992
O -3.093797 -0.449440 -0.188190
C 2.774501 -0.328097 0.417470
H 0.778453 1.456812 1.463011
H -1.039044 -1.839324 0.807252
H -0.031033 -1.294844 -1.416551
H 0.442190 1.299400 -1.598089
H -2.454458 1.483200 -0.294932
H -1.575618 0.366622 -1.370827
H -2.742940 -1.336314 -0.364545
H 3.562099 0.428819 0.266577
H 2.364019 -0.187274 1.429207
H 3.248295 -1.323234 0.382539
el energy= -388.57484871799
zpe= -388.343915
th energy= -388.334373
th enthalpy= -388.333428

free energy= -388.377754

4mchm_24/coords
t9
C -0.090953 1.276122 0.739993
H 0.625678 1.394839 1.571661
C -0.921836 -0.000598 0.997769
H -1.192363 -0.001060 2.071491
C -0.090525 -1.276908 0.739093
H 0.626100 -1.395800 1.570741
C 0.689345 -1.258824 -0.588078
H 1.325157 -2.160647 -0.648889
C 1.566543 0.000397 -0.728071
H 2.003128 0.000878 -1.743780
C 0.688725 1.259074 -0.587232
H -0.015797 1.301640 -1.433419
C -2.284820 -0.000252 0.308364
O -2.157771 0.000542 -1.137205
C 2.732798 0.000308 0.271482
H -0.756443 2.157363 0.773285
H -0.755627 -2.158475 0.771819
H -0.015135 -1.301348 -1.434358
H 1.324128 2.161180 -0.647565
H -2.849092 -0.895916 0.624163
H -2.848810 0.895240 0.625174
H -3.059935 0.001001 -1.493669
H 2.385535 -0.000183 1.315991
H 3.365202 -0.891562 0.127108
H 3.364777 0.892595 0.127952
el energy= -388.57007152667
zpe= -388.339644
th energy= -388.329917
th enthalpy= -388.328973
free energy= -388.373790

4mchm_9/coords
c1
C -0.480833 -0.832230 1.116640
H -1.212885 -1.655668 1.156770
C -1.153986 0.455614 0.603622
H -1.927711 0.764111 1.330854
C -0.111589 1.586541 0.496790

H -0.583470 2.495396 0.083400
C 1.105552 1.181220 -0.351059
H 0.802485 1.012983 -1.401349
C 1.767422 -0.098741 0.182787
H 2.119960 0.107573 1.212923
C 0.731939 -1.231352 0.261142
H 1.202977 -2.136861 0.683255
C -1.866526 0.255595 -0.731905
O -2.934305 -0.708082 -0.541944
C 2.968206 -0.501099 -0.677280
H -0.140085 -0.655147 2.153346
H 0.234438 1.836924 1.515976
H 1.842753 2.003649 -0.359864
H 0.409534 -1.489780 -0.765042
H -2.291592 1.217165 -1.068336
H -1.177673 -0.110731 -1.509528
H -3.386934 -0.803216 -1.394054
H 2.644985 -0.705995 -1.712454
H 3.723327 0.301772 -0.708777
H 3.453220 -1.410816 -0.285988
el energy= -388.57685400913
zpe= -388.346450
th energy= -388.336785
th enthalpy= -388.335840
free energy= -388.380656

4mchm_11/coords
c2
C -0.324914 -1.106767 0.049955
H -1.010877 -1.919969 -0.238960
C -0.943694 0.256143 -0.297688
H -1.132113 0.288698 -1.388966
C 0.034987 1.388814 0.054334
H -0.400318 2.361341 -0.235137
C 1.386691 1.194629 -0.651232
H 1.226143 1.263284 -1.743084
C 2.024376 -0.170349 -0.326568
H 2.908328 -0.294963 -0.978644
C 1.027442 -1.298433 -0.656198
H 0.854429 -1.314434 -1.748367
C -2.267559 0.482675 0.417981
O -3.222282 -0.516185 -0.021381

C 2.512839 -0.244405 1.128086
H -0.197967 -1.166206 1.146900
H 0.177025 1.413223 1.150307
H 2.080784 2.007488 -0.373353
H 1.463776 -2.275516 -0.382936
H -2.120041 0.403661 1.510110
H -2.655449 1.489982 0.187431
H -4.051933 -0.346070 0.450651
H 2.997134 -1.215648 1.323513
H 3.249596 0.550704 1.330713
H 1.688724 -0.129939 1.848852
el energy= -388.57644033782
zpe= -388.346268
th energy= -388.336443
th enthalpy= -388.335498
free energy= -388.380707

4mchm_13/coords
c3
C -0.031307 1.387357 0.054070
H -0.179271 1.415226 1.149301
C 0.947688 0.251239 -0.286026
H 1.146077 0.280472 -1.376785
C 0.323789 -1.108770 0.059901
H 1.011240 -1.923752 -0.220937
C -1.023333 -1.299525 -0.656376
H -0.842497 -1.317560 -1.747326
C -2.020823 -0.169326 -0.335519
H -2.900433 -0.294178 -0.993343
C -1.379611 1.194512 -0.658351
H -2.073960 2.008609 -0.384614
C 2.268969 0.482490 0.441506
O 3.283847 -0.501329 0.124611
C -2.518905 -0.240474 1.116121
H 0.408269 2.358129 -0.235219
H 0.187831 -1.165830 1.155878
H -1.463792 -2.275269 -0.384864
H -1.213644 1.262079 -1.749441
H 2.651714 1.493227 0.214551
H 2.117318 0.405588 1.529953
H 3.442405 -0.440197 -0.830988
H -3.001740 -1.212526 1.311249

H -1.699882 -0.121477 1.841970
H -3.259214 0.553074 1.311760
el energy= -388.57677951516
zpe= -388.346531
th energy= -388.336732
th enthalpy= -388.335788
free energy= -388.380941

4mchm_15/coords
c4
C -0.486255 -0.847722 1.100763
H -0.157285 -0.681156 2.142951
C -1.158944 0.441415 0.592908
H -1.944639 0.738785 1.314053
C -0.122301 1.579558 0.508749
H -0.594861 2.489742 0.098764
C 1.102806 1.186655 -0.333784
H 0.807549 1.026933 -1.387596
C 1.766637 -0.095408 0.192488
H 2.111877 0.102970 1.226643
C 0.736224 -1.233649 0.253173
H 1.208391 -2.140240 0.671836
C -1.856660 0.252391 -0.757024
O -2.911556 -0.739220 -0.707133
C 2.974348 -0.484975 -0.663764
H -1.215799 -1.674307 1.123468
H 0.214061 1.822877 1.532869
H 1.836810 2.011875 -0.330360
H 0.423615 -1.485398 -0.777649
H -2.271587 1.219137 -1.093180
H -1.162922 -0.108033 -1.528799
H -3.542964 -0.441339 -0.032846
H 2.657782 -0.683496 -1.702236
H 3.726065 0.321413 -0.685054
H 3.461230 -1.395589 -0.276860
el energy= -388.57733454995
zpe= -388.346997
th energy= -388.337298
th enthalpy= -388.336354
free energy= -388.381156

4mchm_16/coords

c5
C -0.226475 1.263464 -0.187952
H -0.734821 2.159756 -0.585976
C -0.946128 -0.000300 -0.686715
H -0.900902 -0.000663 -1.794442
C -0.226482 -1.263723 -0.187058
H -0.295765 -1.315394 0.912755
C 1.248569 -1.260968 -0.621070
H 1.760132 -2.163840 -0.242950
C 1.992206 -0.000052 -0.137541
H 2.997172 -0.000180 -0.598109
C 1.248448 1.260331 -0.622254
H 1.291798 1.297626 -1.726680
C -2.428415 -0.000225 -0.333298
O -2.573484 0.000610 1.110313
C 2.185457 0.000738 1.386465
H -0.295403 1.315783 0.911846
H -0.734770 -2.160200 -0.584715
H 1.292219 -1.299417 -1.725476
H 1.760022 2.163581 -0.245129
H -2.918093 0.895806 -0.753253
H -2.917954 -0.896865 -0.752127
H -3.524080 0.000705 1.301314
H 2.749791 -0.891233 1.705824
H 2.749450 0.893254 1.704948
H 1.225998 0.000810 1.926208
el energy= -388.57601311705
zpe= -388.345512
th energy= -388.335852
th enthalpy= -388.334908
free energy= -388.379631

4mchm_17/coords
c6
C -0.221290 1.284345 -0.109994
H -0.721349 2.207543 -0.453218
C -0.952153 0.061629 -0.686447
H -0.916309 0.133042 -1.792650
C -0.240063 -1.239652 -0.280428
H -0.306162 -1.376091 0.814273
C 1.236769 -1.217567 -0.708525
H 1.739769 -2.148264 -0.391555

C 1.987349 0.002235 -0.138612
H 2.993829 0.025390 -0.595116
C 1.254541 1.297368 -0.540856
H 1.772519 2.170100 -0.105013
C -2.436051 0.045011 -0.319810
O -2.677897 -0.016304 1.108142
C 2.175096 -0.099997 1.382832
H -0.293072 1.270469 0.991032
H -0.753643 -2.101119 -0.743609
H 1.282804 -1.181626 -1.812780
H 1.301279 1.406884 -1.640332
H -2.920948 0.975183 -0.653639
H -2.938252 -0.804760 -0.815250
H -2.333308 -0.867511 1.419633
H 2.738911 0.768430 1.762080
H 1.213921 -0.135733 1.918325
H 2.737985 -1.011733 1.643728
el energy= -388.57635976262
zpe= -388.346080
th energy= -388.336277
th enthalpy= -388.335332
free energy= -388.380473

4mchm_23/coords
c7
C 0.434093 -1.230512 -0.980602
H 1.061436 -2.123678 -0.810070
C 1.300363 0.039841 -0.842026
H 1.961876 0.078989 -1.729137
C 0.429791 1.314096 -0.872154
H 1.054493 2.191885 -0.628018
C -0.798252 1.253740 0.051285
H -0.485442 1.238550 1.109443
C -1.652806 0.009016 -0.228484
H -1.983994 0.055202 -1.285289
C -0.796748 -1.254284 -0.058462
H -0.487841 -1.333336 0.997883
C 2.295306 -0.008350 0.315707
O 1.627228 -0.077996 1.601743
C -2.888372 -0.030156 0.674664
H 0.075862 -1.285641 -2.025260
H 0.068624 1.455656 -1.907686

H -1.410123 2.162223 -0.094410
H -1.406340 -2.147039 -0.287209
H 2.944897 -0.893595 0.195021
H 2.930713 0.894762 0.283203
H 2.325733 -0.110367 2.274412
H -3.514444 0.866490 0.533291
H -3.509550 -0.916937 0.465469
H -2.583970 -0.069544 1.734843
el energy= -388.57269471865
zpe= -388.342542
th energy= -388.332778
th enthalpy= -388.331834
free energy= -388.376717

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.337257 -1.097320 0.025991
H 1.022229 -1.907442 -0.280303
C 0.945851 0.274098 -0.305841
H 1.130080 0.323345 -1.397086
C -0.039102 1.393960 0.068698
H -0.175913 1.400257 1.165650
C -1.393270 1.202180 -0.632941
H -1.239204 1.289317 -1.724345
C -2.019574 -0.172185 -0.326209
H -2.905472 -0.293431 -0.976228
C -1.016885 -1.288693 -0.677286
H -1.445045 -2.272548 -0.415864
C 2.273835 0.501974 0.411350
O 3.310922 -0.431229 0.020349
C -2.500667 -0.272032 1.129402
H 0.215902 -1.174682 1.122586
H 0.389076 2.373834 -0.207040
H -2.091781 2.005323 -0.338344
H -0.848082 -1.287794 -1.770090
H 2.673226 1.496988 0.162437
H 2.120617 0.452248 1.504725
H 3.035388 -1.309786 0.324696
H -3.240818 0.515656 1.347871
H -2.978587 -1.248977 1.311633
H -1.673666 -0.164369 1.847926
el energy= -388.57712398894

zpe= -388.346464
th energy= -388.336848
th enthalpy= -388.335903
free energy= -388.380496

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.497514 -0.812870 1.116044
H 1.232455 -1.635580 1.166743
C 1.161876 0.476665 0.596143
H 1.935045 0.793104 1.320310
C 0.111269 1.600052 0.483611
H -0.228688 1.862002 1.502018
C -1.110624 1.181409 -0.351601
H -0.816839 1.012486 -1.404238
C -1.758261 -0.102255 0.190466
H -2.104417 0.102951 1.222999
C -0.712574 -1.225549 0.263449
H -1.172834 -2.136024 0.686439
C 1.874802 0.272173 -0.743484
O 2.970926 -0.672796 -0.654646
C -2.962267 -0.516321 -0.659539
H 0.157840 -0.635042 2.152745
H 0.576290 2.506104 0.055903
H -1.854077 1.998178 -0.355575
H -0.390270 -1.479527 -0.764036
H 1.175546 -0.052130 -1.530496
H 2.334617 1.219417 -1.064051
H 2.583755 -1.543995 -0.475940
H -3.723786 0.280568 -0.687145
H -2.645217 -0.721154 -1.696629
H -3.437245 -1.428807 -0.262404
el energy= -388.57744260757
zpe= -388.346800
th energy= -388.337242
th enthalpy= -388.336298
free energy= -388.380679

MP2 d-aug-cc-pwCVDZ gas phase

4mchm_1/coords
t1
C 0.155885 1.426433 0.180781
H 0.550363 2.362394 -0.251604
C 1.031768 0.238615 -0.242277
H 1.026613 0.173238 -1.347240
C 0.461911 -1.068567 0.324116
H 1.083020 -1.916953 -0.001187
C -0.998033 -1.267841 -0.102324
H -1.396118 -2.204203 0.325323
C -1.883190 -0.086115 0.316974
H -1.859037 -0.020169 1.422571
C -1.304200 1.220158 -0.244149
H -1.921517 2.074662 0.082900
C 2.472330 0.459183 0.196162
O 3.268967 -0.627397 -0.312151
C -3.333450 -0.287042 -0.129331
H 0.202330 1.533252 1.281291
H 0.518760 -1.026329 1.429081
H -1.046566 -1.372229 -1.203113
H -1.361567 1.185831 -1.348837
H 2.840785 1.423963 -0.197280
H 2.520052 0.490754 1.301203
H 4.185825 -0.476384 -0.046847
H -3.387761 -0.355784 -1.228565
H -3.754475 -1.214686 0.289555
H -3.970563 0.552880 0.190242
el energy= -388.60253751707
zpe= -388.371816
th energy= -388.362032
th enthalpy= -388.361087
free energy= -388.406081

4mchm_3/coords
t2
C -0.157981 1.423243 0.181776
H -0.202937 1.531651 1.282052
C -1.033352 0.231790 -0.232988
H -1.021515 0.168257 -1.341008
C -0.455931 -1.071453 0.332941

H -0.506756 -1.023962 1.437648
C 1.002195 -1.269219 -0.100269
H 1.404773 -2.203258 0.328231
C 1.885733 -0.083879 0.313157
H 1.865713 -0.016584 1.418635
C 1.301433 1.220546 -0.247140
H 1.916817 2.077363 0.077390
C -2.477940 0.451794 0.212110
O -3.369671 -0.600267 -0.195039
C 3.334710 -0.282074 -0.138726
H -0.557264 2.357175 -0.250360
H -1.078448 -1.924125 0.020480
H 1.047775 -1.376509 -1.201188
H 1.356234 1.185962 -1.352126
H -2.529805 0.462392 1.312208
H -2.842129 1.429489 -0.153880
H -3.403948 -0.589945 -1.161843
H 3.970763 0.560075 0.176711
H 3.759981 -1.207677 0.280228
H 3.384917 -0.352652 -1.238041
el energy= -388.60215512164
zpe= -388.371456
th energy= -388.361682
th enthalpy= -388.360738
free energy= -388.405699

4mchm_5/coords
t3
C 0.391779 -1.260377 0.024727
H 0.831350 -2.159894 0.490512
C 1.025576 -0.000145 0.631311
H 0.820547 -0.000212 1.720747
C 0.391921 1.260323 0.024856
H 0.832010 2.159634 0.490429
C -1.131518 1.255563 0.206827
H -1.376224 1.286806 1.286323
C -1.771843 0.000189 -0.402231
H -1.551869 0.000291 -1.487656
C -1.131579 -1.255409 0.206260
H -1.572769 -2.158812 -0.249267
C 2.542767 -0.000510 0.480613
O 2.852888 0.000552 -0.926729

C -3.290459 -0.000011 -0.209696
H 0.637327 -1.298185 -1.050063
H 0.637281 1.297988 -1.050054
H -1.573320 2.159211 -0.247795
H -1.376547 -1.287353 1.285585
H 2.967650 0.896184 0.967844
H 2.967158 -0.898197 0.966459
H 3.814411 0.000678 -1.021514
H -3.538970 0.000301 0.864758
H -3.750737 0.891405 -0.664554
H -3.750258 -0.891997 -0.663919
el energy= -388.60224485610
zpe= -388.371471
th energy= -388.361717
th enthalpy= -388.360772
free energy= -388.405674

4mchm_6/coords
t4
C 0.156578 1.421986 0.183567
H 0.210119 1.516560 1.284925
C 1.034300 0.242061 -0.258494
H 1.027914 0.190204 -1.363954
C 0.462581 -1.070757 0.293711
H 1.060372 -1.929364 -0.058024
C -1.002465 -1.265648 -0.120778
H -1.060011 -1.357774 -1.222046
C -1.881763 -0.087559 0.319732
H -1.847857 -0.033024 1.425666
C -1.306472 1.223267 -0.233645
H -1.372351 1.199859 -1.337987
C 2.478172 0.468161 0.187912
O 3.396194 -0.527405 -0.292460
C -3.335750 -0.285637 -0.116051
H 0.550532 2.362207 -0.239469
H 0.531311 -1.050927 1.399012
H -1.396588 -2.206349 0.300744
H -1.919971 2.075133 0.106904
H 2.852594 1.420153 -0.217350
H 2.516741 0.531539 1.292472
H 3.168777 -1.364835 0.133531
H -3.969617 0.551105 0.217270

H -3.399417 -0.343310 -1.215324
H -3.753172 -1.217187 0.297580
el energy= -388.60218090086
zpe= -388.371409
th energy= -388.361627
th enthalpy= -388.360683
free energy= -388.405661

4mchm_7/coords
t5
C 0.383923 1.269851 0.001654
H 0.634475 1.294018 1.076260
C 1.026319 0.025854 -0.626334
H 0.820078 0.039633 -1.716001
C 0.395501 -1.248824 -0.047130
H 0.616498 -1.305666 1.035318
C -1.128147 -1.250792 -0.232282
H -1.365623 -1.261111 -1.313185
C -1.775743 -0.011348 0.401114
H -1.560617 -0.034257 1.487433
C -1.140002 1.260668 -0.177396
H -1.585983 2.150672 0.299180
C 2.549545 0.031638 -0.478595
O 2.992157 0.039315 0.890444
C -3.293617 -0.015725 0.202769
H 0.817248 2.179241 -0.449655
H 0.841791 -2.140659 -0.522591
H -1.565862 -2.166512 0.201366
H -1.385549 1.316934 -1.255508
H 2.984331 -0.829846 -1.018382
H 2.966321 0.950922 -0.917215
H 2.786987 -0.826598 1.268194
H -3.750761 -0.919313 0.636167
H -3.759648 0.863574 0.674630
H -3.537620 0.006524 -0.872373
el energy= -388.60166187211
zpe= -388.370904
th energy= -388.361153
th enthalpy= -388.360209
free energy= -388.405109

4mchm_19/coords

t6
C 0.271784 -1.069161 0.704903
H -0.332042 -1.179995 1.621954
C 0.921888 0.326915 0.713042
H 1.436662 0.466328 1.680581
C -0.152875 1.420805 0.564054
H -0.772349 1.431089 1.476746
C -1.051182 1.197880 -0.665170
H -1.834763 1.974865 -0.699055
C -1.703172 -0.198686 -0.666782
H -2.202704 -0.337160 -1.642863
C -0.617731 -1.284290 -0.529724
H 0.008938 -1.286324 -1.439036
C 1.995369 0.468746 -0.363963
O 3.007133 -0.524568 -0.108477
C -2.781185 -0.326755 0.419733
H 1.056946 -1.839535 0.747221
H 0.324632 2.414668 0.504179
H -0.455279 1.317714 -1.586877
H -1.091573 -2.279964 -0.478891
H 1.571890 0.327707 -1.372732
H 2.428856 1.484110 -0.311068
H 3.698455 -0.425817 -0.776540
H -3.566106 0.433366 0.279038
H -3.257202 -1.319260 0.377425
H -2.368794 -0.197966 1.431182
el energy= -388.59758575420
zpe= -388.366187
th energy= -388.356569
th enthalpy= -388.355625
free energy= -388.400280

4mchm_21/coords
t7
C 0.144791 1.414506 0.566464
H -0.340883 2.404405 0.505995
C -0.924219 0.312587 0.700225
H -1.439474 0.451098 1.671409
C -0.270422 -1.081393 0.691223
H 0.320169 -1.203317 1.615503
C 0.635165 -1.284819 -0.534217
H 0.018352 -1.289989 -1.449850

C 1.713342 -0.190729 -0.656539
H 2.223524 -0.323087 -1.627801
C 1.049408 1.200018 -0.659144
H 0.455486 1.313894 -1.582842
C -1.994245 0.455914 -0.387814
O -3.052898 -0.509106 -0.264628
C 2.780996 -0.313140 0.440756
H 0.759348 1.427141 1.482513
H -1.054417 -1.854899 0.709457
H 1.115605 -2.277041 -0.479825
H 1.825747 1.984124 -0.690221
H -2.402195 1.483597 -0.367996
H -1.576048 0.283997 -1.388784
H -3.475078 -0.365606 0.594277
H 2.356774 -0.195723 1.448806
H 3.268522 -1.299975 0.397227
H 3.558855 0.456562 0.313431
el energy= -388.59750689826
zpe= -388.366083
th energy= -388.356496
th enthalpy= -388.355551
free energy= -388.400080

4mchm_22/coords
t8
C 0.149755 1.425441 0.556620
H -0.332212 2.416362 0.485952
C -0.925880 0.332530 0.715734
H -1.438317 0.477863 1.683413
C -0.265287 -1.058900 0.718600
H 0.345186 -1.158214 1.632190
C 0.616979 -1.286446 -0.519651
H 1.090556 -2.281926 -0.464450
C 1.701548 -0.200923 -0.664796
H 2.199006 -0.346822 -1.640658
C 1.047981 1.194705 -0.671560
H 1.831443 1.971352 -0.710411
C -2.004297 0.470362 -0.364984
O -3.108313 -0.432155 -0.179145
C 2.780863 -0.322332 0.421108
H 0.769702 1.448700 1.468964
H -1.032876 -1.849116 0.793126

H -0.009900 -1.290419 -1.429390
H 0.452268 1.308408 -1.593721
H -2.446072 1.476765 -0.309619
H -1.580617 0.348844 -1.376364
H -2.784919 -1.328352 -0.343091
H 3.568231 0.432808 0.269232
H 2.371980 -0.178572 1.431981
H 3.253065 -1.317057 0.389568
el energy= -388.59683043998
zpe= -388.365478
th energy= -388.355831
th enthalpy= -388.354887
free energy= -388.399572

4mchm_24/coords
t9
C -0.099153 1.273834 0.757019
H 0.617492 1.385670 1.589369
C -0.933601 -0.000310 1.006672
H -1.221273 -0.000580 2.076219
C -0.099072 -1.274338 0.756437
H 0.617574 -1.386416 1.588762
C 0.670135 -1.257922 -0.575613
H 1.302745 -2.160884 -0.642365
C 1.546053 0.000155 -0.723693
H 1.964625 0.000454 -1.746531
C 0.669920 1.257982 -0.575071
H -0.047882 1.294626 -1.408288
C -2.277218 -0.000141 0.280347
O -2.084935 0.000497 -1.149643
C 2.730397 0.000187 0.254391
H -0.759319 2.158170 0.797425
H -0.759172 -2.158745 0.796533
H -0.047635 -1.294519 -1.408928
H 1.302414 2.160990 -0.641547
H -2.849220 -0.896826 0.583498
H -2.849529 0.896085 0.584300
H -2.959204 0.000710 -1.562893
H 2.403146 -0.000354 1.304805
H 3.360272 -0.890841 0.101524
H 3.359677 0.891800 0.102327
el energy= -388.59554376140

zpe= -388.364051
th energy= -388.354501
th enthalpy= -388.353557
free energy= -388.397839

4mchm_9/coords
c1
C -0.498135 -0.817069 1.111008
H -1.244347 -1.625776 1.139721
C -1.155309 0.474629 0.592254
H -1.929752 0.786532 1.315741
C -0.107339 1.597312 0.478879
H -0.568122 2.507477 0.056316
C 1.114109 1.178746 -0.355153
H 0.822829 1.011039 -1.408503
C 1.761008 -0.103976 0.187573
H 2.107491 0.104690 1.219079
C 0.715965 -1.226524 0.265182
H 1.177099 -2.135525 0.689045
C -1.875160 0.262851 -0.737626
O -2.895897 -0.732657 -0.529871
C 2.966497 -0.519122 -0.659157
H -0.164291 -0.643760 2.150328
H 0.233191 1.858684 1.496737
H 1.857082 1.995294 -0.364008
H 0.396838 -1.489691 -0.760503
H -2.327272 1.218228 -1.061045
H -1.175060 -0.069600 -1.522531
H -3.366646 -0.856727 -1.364731
H 2.649708 -0.735849 -1.693007
H 3.723693 0.280167 -0.696907
H 3.444917 -1.425013 -0.254527
el energy= -388.60031596392
zpe= -388.369260
th energy= -388.359581
th enthalpy= -388.358637
free energy= -388.403485

4mchm_11/coords
c2
C -0.338123 -1.097051 0.053799
H -1.041067 -1.894536 -0.231527

C -0.944072 0.270635 -0.289683
H -1.138115 0.301726 -1.379307
C 0.041075 1.395586 0.060388
H -0.385427 2.373290 -0.224018
C 1.388482 1.192275 -0.649119
H 1.225230 1.266029 -1.739721
C 2.016045 -0.177956 -0.330797
H 2.893582 -0.307837 -0.989880
C 1.009537 -1.297803 -0.654890
H 0.833592 -1.315331 -1.746039
C -2.273072 0.489775 0.418661
O -3.191690 -0.527833 -0.021899
C 2.517656 -0.257055 1.118594
H -0.209543 -1.162780 1.150097
H 0.188561 1.421422 1.155410
H 2.089734 1.999365 -0.374776
H 1.439833 -2.277962 -0.385766
H -2.121546 0.427201 1.513004
H -2.665797 1.494228 0.177301
H -4.039806 -0.375939 0.415654
H 2.997090 -1.230246 1.309732
H 3.260055 0.532596 1.316380
H 1.701971 -0.138999 1.846932
el energy= -388.59998529633
zpe= -388.368908
th energy= -388.359212
th enthalpy= -388.358268
free energy= -388.403068

4mchm_13/coords
c3
C -0.037367 1.392222 0.061321
H -0.188489 1.419006 1.155750
C 0.945960 0.262506 -0.279292
H 1.136086 0.295306 -1.372642
C 0.330697 -1.100846 0.061665
H 1.032864 -1.904708 -0.208850
C -1.012342 -1.298791 -0.656180
H -0.831003 -1.318639 -1.746654
C -2.016292 -0.174391 -0.339025
H -2.890190 -0.301757 -1.003299
C -1.382138 1.193524 -0.654660

H -2.081809 2.003138 -0.384104
C 2.276318 0.479901 0.438880
O 3.269467 -0.509356 0.118342
C -2.526571 -0.250254 1.107507
H 0.395409 2.367820 -0.220780
H 0.193097 -1.160369 1.156842
H -1.448188 -2.276674 -0.388090
H -1.213757 1.266590 -1.744682
H 2.659798 1.494997 0.226346
H 2.128568 0.395834 1.527081
H 3.475116 -0.415742 -0.822376
H -3.009043 -1.222086 1.297517
H -1.715246 -0.132259 1.840683
H -3.268542 0.541160 1.299226
el energy= -388.59967143058
zpe= -388.368608
th energy= -388.358924
th enthalpy= -388.357980
free energy= -388.402744

4mchm_15/coords
c4
C -0.494543 -0.844531 1.093095
H -0.173524 -0.693097 2.139706
C -1.154974 0.451271 0.590407
H -1.929583 0.755019 1.322105
C -0.115548 1.584249 0.500062
H -0.583125 2.496084 0.088703
C 1.108064 1.184036 -0.339292
H 0.816121 1.023348 -1.393423
C 1.764699 -0.097901 0.192898
H 2.103805 0.103129 1.228492
C 0.730194 -1.230987 0.251048
H 1.196492 -2.140089 0.668735
C -1.870310 0.255323 -0.750742
O -2.899446 -0.747166 -0.696706
C 2.978335 -0.492705 -0.652016
H -1.233740 -1.661051 1.092900
H 0.222576 1.833879 1.521760
H 1.843804 2.006900 -0.341493
H 0.420087 -1.486350 -0.778956
H -2.287865 1.221909 -1.088874

H -1.178508 -0.097329 -1.527476
H -3.556096 -0.452039 -0.050016
H 2.668560 -0.701025 -1.689590
H 3.728047 0.314034 -0.676866
H 3.463007 -1.398521 -0.254833
el energy= -388.60025681521
zpe= -388.369169
th energy= -388.359518
th enthalpy= -388.358574
free energy= -388.403303

4mchm_16/coords
c5
C -0.233805 1.263928 -0.207435
H -0.735339 2.159257 -0.615420
C -0.952360 0.000365 -0.705020
H -0.920719 0.000764 -1.813428
C -0.234251 -1.263781 -0.208271
H -0.328086 -1.321474 0.887879
C 1.244396 -1.258639 -0.623760
H 1.750295 -2.163229 -0.243997
C 1.981331 -0.000115 -0.128357
H 2.991491 -0.000038 -0.576923
C 1.244725 1.258746 -0.623294
H 1.306012 1.296776 -1.726757
C -2.426453 0.000468 -0.315846
O -2.507028 -0.000558 1.123261
C 2.154669 -0.000376 1.397678
H -0.327192 1.320688 0.888782
H -0.735868 -2.158654 -0.617136
H 1.305727 -1.296239 -1.727205
H 1.750929 2.163029 -0.243126
H -2.923177 0.898235 -0.727323
H -2.923580 -0.896474 -0.728625
H -3.440711 -0.000482 1.371649
H 2.714368 -0.891505 1.723861
H 2.713900 0.890929 1.724178
H 1.188669 -0.000692 1.923323
el energy= -388.60013427148
zpe= -388.368946
th energy= -388.359310
th enthalpy= -388.358366

free energy= -388.402995

4mchm_17/coords
c6
C -0.225524 1.283989 -0.111882
H -0.721515 2.208677 -0.454893
C -0.954959 0.065744 -0.695318
H -0.922867 0.139585 -1.801789
C -0.241241 -1.234381 -0.294912
H -0.306730 -1.369309 0.799565
C 1.235966 -1.211306 -0.716723
H 1.736937 -2.144926 -0.407540
C 1.984006 0.003159 -0.135427
H 2.990180 0.028515 -0.591700
C 1.252687 1.300243 -0.529342
H 1.765889 2.169538 -0.083084
C -2.435146 0.048720 -0.307624
O -2.651881 -0.024993 1.113231
C 2.172157 -0.110653 1.384635
H -0.320853 1.266104 0.986006
H -0.750527 -2.098888 -0.757464
H 1.287115 -1.169074 -1.820059
H 1.311244 1.422304 -1.626639
H -2.917362 0.987192 -0.620711
H -2.950515 -0.785327 -0.818891
H -2.394922 -0.911277 1.401406
H 2.752159 0.744012 1.767234
H 1.212243 -0.126935 1.921363
H 2.716888 -1.033337 1.640911
el energy= -388.59930537975
zpe= -388.368190
th energy= -388.358530
th enthalpy= -388.357586
free energy= -388.402292

4mchm_23/coords
c7
C 0.456340 -1.264094 -0.946229
H 1.077095 -2.155585 -0.748216
C 1.323533 0.005669 -0.829777
H 2.015096 0.011330 -1.694809
C 0.456037 1.276682 -0.929804

H 1.076520 2.165713 -0.720249
C -0.776424 1.255118 -0.012444
H -0.459852 1.277764 1.042754
C -1.630445 0.001484 -0.246338
H -1.966738 0.008172 -1.302863
C -0.775918 -1.254682 -0.028437
H -0.459231 -1.290715 1.026402
C 2.263234 -0.002092 0.374308
O 1.514569 -0.011202 1.607793
C -2.864128 -0.004549 0.659700
H 0.109293 -1.345192 -1.992939
H 0.109089 1.371191 -1.975397
H -1.385329 2.157897 -0.196785
H -1.384432 -2.155306 -0.224229
H 2.909690 -0.897661 0.319123
H 2.908640 0.894918 0.331578
H 2.150655 -0.015737 2.336176
H -3.487491 0.888283 0.492070
H -3.486916 -0.895616 0.480935
H -2.556011 -0.011052 1.718238
el energy= -388.59839536230
zpe= -388.367193
th energy= -388.357588
th enthalpy= -388.356644
free energy= -388.401087

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.339458 -1.094440 0.021472
H 1.022988 -1.900982 -0.295952
C 0.946906 0.277235 -0.305022
H 1.138305 0.323763 -1.394342
C -0.040579 1.393920 0.066147
H -0.177698 1.406984 1.162783
C -1.394769 1.200691 -0.632761
H -1.243461 1.287873 -1.723974
C -2.018414 -0.173214 -0.324006
H -2.903158 -0.297028 -0.974302
C -1.016065 -1.287810 -0.676075
H -1.441967 -2.272258 -0.416178
C 2.278535 0.496679 0.411362
O 3.305550 -0.430402 0.023353

C -2.501901 -0.272720 1.130245
H 0.222457 -1.183305 1.117905
H 0.384802 2.374622 -0.208908
H -2.093204 2.003814 -0.340794
H -0.850195 -1.288522 -1.768644
H 2.681351 1.489682 0.161333
H 2.117862 0.462077 1.506209
H 3.037104 -1.307873 0.327502
H -3.243994 0.512065 1.346628
H -2.976269 -1.249563 1.315124
H -1.678353 -0.160164 1.850623
el energy= -388.59963424011
zpe= -388.368500
th energy= -388.358812
th enthalpy= -388.357867
free energy= -388.402642

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.493765 -0.810513 1.116984
H 1.229791 -1.630932 1.180408
C 1.161028 0.475101 0.595823
H 1.934611 0.785376 1.320670
C 0.112116 1.597921 0.482549
H -0.228442 1.864085 1.499311
C -1.109924 1.181351 -0.352296
H -0.818851 1.015300 -1.405594
C -1.758881 -0.100992 0.188052
H -2.105338 0.105021 1.220107
C -0.715058 -1.224618 0.264835
H -1.176530 -2.134731 0.685490
C 1.883329 0.266441 -0.739914
O 2.969911 -0.671443 -0.653544
C -2.963771 -0.515253 -0.659971
H 0.152331 -0.632290 2.152562
H 0.576063 2.504737 0.056621
H -1.852279 1.998169 -0.359308
H -0.395813 -1.482391 -0.762612
H 1.181274 -0.037549 -1.534803
H 2.347940 1.213733 -1.052724
H 2.589751 -1.547152 -0.501029
H -3.720138 0.284566 -0.695985

H -2.646556 -0.729460 -1.694126
H -3.442722 -1.421570 -0.257006
el energy= -388.59961374308
zpe= -388.368598
th energy= -388.358888
th enthalpy= -388.357944
free energy= -388.402839

MP2-SMD d-aug-cc-pWCVDZ

4mchm_1/coords
t1
C 0.159980 1.416350 0.182285
H 0.562732 2.347733 -0.251078
C 1.030569 0.224466 -0.242009
H 1.022092 0.164148 -1.347412
C 0.449819 -1.078058 0.325058
H 1.054060 -1.939518 -0.001618
C -1.011849 -1.268425 -0.100604
H -1.415221 -2.201155 0.330303
C -1.888399 -0.080935 0.318205
H -1.866231 -0.014334 1.423256
C -1.299982 1.219685 -0.244453
H -1.910991 2.078638 0.082789
C 2.466047 0.451160 0.205679
O 3.300414 -0.610126 -0.323661
C -3.336944 -0.273086 -0.134479
H 0.207299 1.519407 1.282583
H 0.509228 -1.034823 1.429373
H -1.061229 -1.371204 -1.201506
H -1.355497 1.182276 -1.349027
H 2.830030 1.424724 -0.163853
H 2.518067 0.451318 1.308773
H 4.209819 -0.426456 -0.041905
H -3.386042 -0.338490 -1.234525
H -3.766599 -1.198901 0.281059
H -3.970276 0.570710 0.183979
el energy= -388.60824827052
zpe= -388.378600
th energy= -388.368699
th enthalpy= -388.367754
free energy= -388.413035

4mchm_3/coords
t2
C -0.163750 1.415653 0.181406
H -0.206879 1.525660 1.281411
C -1.035202 0.219801 -0.229271
H -1.037653 0.156094 -1.335787
C -0.447730 -1.079031 0.337091
H -0.497111 -1.031075 1.441608
C 1.010940 -1.269206 -0.098257
H 1.419004 -2.200006 0.332506
C 1.887231 -0.078889 0.313403
H 1.867876 -0.009040 1.418297
C 1.294795 1.219127 -0.251185
H 1.906805 2.079757 0.069798
C -2.471189 0.447092 0.230114
O -3.384634 -0.586418 -0.211745
C 3.334918 -0.269947 -0.142438
H -0.571034 2.343518 -0.255510
H -1.055217 -1.941949 0.020023
H 1.053781 -1.374394 -1.199153
H 1.345224 1.177554 -1.355818
H -2.522342 0.432530 1.329874
H -2.829418 1.430166 -0.121270
H -3.372346 -0.568414 -1.181832
H 3.967523 0.575905 0.171999
H 3.767018 -1.193769 0.275004
H 3.381762 -0.338791 -1.242366
el energy= -388.60857400427
zpe= -388.378736
th energy= -388.368904
th enthalpy= -388.367959
free energy= -388.413007

4mchm_5/coords
t3
C 0.384325 -1.260016 0.003675
H 0.829277 -2.159361 0.463819
C 1.017741 -0.000505 0.611384
H 0.799466 -0.000907 1.697345
C 0.384562 1.259477 0.004314
H 0.830201 2.158480 0.464526

C -1.137495 1.256324 0.198356
H -1.369655 1.286683 1.280104
C -1.783332 0.000268 -0.403120
H -1.577311 0.000560 -1.490950
C -1.137772 -1.256333 0.197564
H -1.583358 -2.158186 -0.256822
C 2.536245 -0.000569 0.498098
O 2.910594 0.001098 -0.902679
C -3.298002 0.000336 -0.188810
H 0.611028 -1.296528 -1.076251
H 0.610716 1.296042 -1.075754
H -1.582949 2.158608 -0.255391
H -1.369857 -1.287358 1.279299
H 2.950750 0.894550 0.992568
H 2.950537 -0.897001 0.990315
H 3.879272 0.000823 -0.936702
H -3.529759 0.000311 0.889725
H -3.765438 0.892176 -0.636608
H -3.765314 -0.891566 -0.636555
el energy= -388.60751888022
zpe= -388.377734
th energy= -388.367903
th enthalpy= -388.366959
free energy= -388.412093

4mchm_6/coords
t4
C 0.158133 1.422628 0.187565
H 0.209846 1.517691 1.288470
C 1.032765 0.238808 -0.250146
H 1.019918 0.185623 -1.355702
C 0.460292 -1.069294 0.312964
H 1.063633 -1.931703 -0.019800
C -1.001120 -1.267014 -0.110292
H -1.052441 -1.364218 -1.211478
C -1.882465 -0.086504 0.318662
H -1.858398 -0.028152 1.424090
C -1.303033 1.222188 -0.234977
H -1.363266 1.194428 -1.339579
C 2.472965 0.468293 0.195802
O 3.398550 -0.522969 -0.312797
C -3.330763 -0.283694 -0.132758

H 0.555393 2.359098 -0.240220
H 0.522216 -1.031804 1.417356
H -1.397490 -2.204179 0.317106
H -1.917631 2.074559 0.102641
H 2.842905 1.430394 -0.188289
H 2.521778 0.491939 1.299236
H 3.128217 -1.380293 0.050962
H -3.968733 0.552599 0.195792
H -3.381886 -0.338058 -1.233293
H -3.753117 -1.216640 0.274157
el energy= -388.60892574694
zpe= -388.378979
th energy= -388.369189
th enthalpy= -388.368245
free energy= -388.413170

4mchm_7/coords
t5
C 0.381762 1.268067 0.008524
H 0.612130 1.291580 1.088251
C 1.022871 0.021887 -0.616270
H 0.814114 0.037245 -1.704580
C 0.392565 -1.252535 -0.036685
H 0.618584 -1.315518 1.044156
C -1.130233 -1.250853 -0.224176
H -1.364935 -1.262169 -1.305624
C -1.778392 -0.008743 0.402129
H -1.567578 -0.026697 1.488948
C -1.140962 1.260195 -0.180369
H -1.589119 2.152518 0.290280
C 2.545260 0.025180 -0.490909
O 3.017170 0.048883 0.878892
C -3.294073 -0.012778 0.194652
H 0.820623 2.176169 -0.440297
H 0.838590 -2.140469 -0.518008
H -1.570210 -2.163354 0.214059
H -1.377268 1.307567 -1.260574
H 2.967918 -0.851549 -1.011374
H 2.959672 0.933940 -0.952334
H 2.756619 -0.790822 1.287936
H -3.753997 -0.916780 0.625616
H -3.764474 0.866495 0.663638

H -3.530808 0.008256 -0.882597
el energy= -388.60803212873
zpe= -388.378255
th energy= -388.368410
th enthalpy= -388.367465
free energy= -388.412546

4mchm_19/coords
t6
C 0.252365 -1.079111 0.707617
H -0.360659 -1.175453 1.619933
C 0.921342 0.308263 0.717423
H 1.435361 0.445756 1.686158
C -0.146604 1.410027 0.574691
H -0.769633 1.414064 1.484936
C -1.037450 1.200931 -0.661485
H -1.813871 1.984886 -0.696659
C -1.704703 -0.187711 -0.671527
H -2.200367 -0.318614 -1.650302
C -0.632538 -1.285625 -0.531921
H -0.002688 -1.292494 -1.438785
C 1.985741 0.455555 -0.365548
O 3.041512 -0.505120 -0.106598
C -2.786603 -0.308969 0.410730
H 1.017909 -1.870042 0.759981
H 0.341279 2.398739 0.521544
H -0.429995 1.314931 -1.576043
H -1.119650 -2.274901 -0.479085
H 1.572101 0.279480 -1.370449
H 2.400176 1.477633 -0.334617
H 3.701491 -0.397786 -0.808729
H -3.557216 0.467731 0.277700
H -3.281691 -1.291922 0.352326
H -2.373943 -0.201212 1.424998
el energy= -388.60379237683
zpe= -388.373155
th energy= -388.363515
th enthalpy= -388.362571
free energy= -388.407280

4mchm_21/coords
t7

C 0.132204 1.399188 0.579065
H -0.363426 2.384241 0.528853
C -0.929198 0.288364 0.691302
H -1.463587 0.414248 1.652242
C -0.254658 -1.095699 0.679300
H 0.338423 -1.204987 1.603289
C 0.656289 -1.283299 -0.544709
H 0.043818 -1.288002 -1.463301
C 1.720426 -0.174542 -0.655974
H 2.234223 -0.292714 -1.626894
C 1.039439 1.207355 -0.647458
H 0.440421 1.318722 -1.568184
C -1.982022 0.437254 -0.408738
O -3.087127 -0.485196 -0.245777
C 2.784117 -0.294522 0.444295
H 0.743153 1.399212 1.497536
H -1.020104 -1.888650 0.701837
H 1.151275 -2.268669 -0.491087
H 1.807794 1.999603 -0.670223
H -2.362714 1.473437 -0.414912
H -1.571924 0.218277 -1.403565
H -3.471164 -0.306532 0.627866
H 2.351658 -0.204677 1.452044
H 3.292946 -1.270286 0.383401
H 3.546645 0.493756 0.334813
el energy= -388.60424231010
zpe= -388.373393
th energy= -388.363885
th enthalpy= -388.362941
free energy= -388.407199

4mchm_22/coords
t8
C 0.154556 1.431619 0.552091
H -0.327088 2.422164 0.474806
C -0.922780 0.342059 0.721720
H -1.428237 0.498384 1.691899
C -0.267953 -1.051858 0.728574
H 0.348364 -1.143108 1.638928
C 0.605486 -1.287608 -0.513384
H 1.076645 -2.284031 -0.452245
C 1.693476 -0.207502 -0.667647

H 2.188157 -0.359811 -1.643777
C 1.045254 1.189992 -0.678858
H 1.832398 1.962701 -0.723231
C -1.996129 0.483587 -0.359785
O -3.092921 -0.448281 -0.186907
C 2.772104 -0.327624 0.418065
H 0.777588 1.454711 1.462117
H -1.038328 -1.838569 0.804250
H -0.029640 -1.293386 -1.416936
H 0.442885 1.298664 -1.597112
H -2.451683 1.482837 -0.294713
H -1.574956 0.365477 -1.370256
H -2.742984 -1.335509 -0.363132
H 3.558866 0.429530 0.268315
H 2.360984 -0.187907 1.429052
H 3.246322 -1.321894 0.382629
el energy= -388.60434381834
zpe= -388.373454
th energy= -388.363917
th enthalpy= -388.362973
free energy= -388.407290

4mchm_24/coords
t9
C -0.090343 1.276367 0.737891
H 0.625853 1.395557 1.569157
C -0.921187 0.001750 0.997008
H -1.192349 0.003311 2.070050
C -0.090842 -1.273783 0.741335
H 0.625614 -1.390637 1.572684
C 0.687513 -1.258307 -0.584913
H 1.321911 -2.160386 -0.645185
C 1.564796 -0.001239 -0.727232
H 2.000104 -0.002537 -1.742910
C 0.688749 1.256988 -0.587950
H -0.015469 1.298451 -1.433648
C -2.282672 0.000951 0.308013
O -2.156071 -0.002360 -1.137373
C 2.731568 -0.000392 0.269720
H -0.754802 2.157715 0.770072
H -0.755401 -2.154906 0.776361
H -0.017346 -1.301031 -1.430063

H 1.324213 2.158243 -0.649947
H -2.847007 -0.893126 0.626256
H -2.846140 0.897055 0.622062
H -3.058636 -0.002545 -1.492811
H 2.386185 0.001285 1.314198
H 3.362905 -0.892411 0.125941
H 3.363443 0.890820 0.123535
el energy= -388.59952792783
zpe= -388.369130
th energy= -388.359417
th enthalpy= -388.358473
free energy= -388.403257

4mchm_9/coords
c1
C -0.480011 -0.832522 1.114217
H -1.211478 -1.655669 1.153645
C -1.152674 0.454348 0.602783
H -1.925945 0.762026 1.329965
C -0.111405 1.584287 0.497141
H -0.582980 2.493011 0.084739
C 1.104737 1.180102 -0.349954
H 0.801695 1.012241 -1.399687
C 1.766330 -0.098700 0.182622
H 2.118619 0.106922 1.212337
C 0.732067 -1.230471 0.259764
H 1.202660 -2.135918 0.681023
C -1.865344 0.255856 -0.731241
O -2.934109 -0.706102 -0.540348
C 2.966531 -0.499680 -0.676633
H -0.139794 -0.656192 2.150612
H 0.234105 1.833825 1.516063
H 1.841254 2.002376 -0.358633
H 0.410350 -1.487898 -0.766271
H -2.288892 1.217660 -1.067164
H -1.177954 -0.111413 -1.508847
H -3.386230 -0.801884 -1.392626
H 2.643779 -0.703795 -1.711465
H 3.720838 0.303168 -0.707194
H 3.451465 -1.408962 -0.285898
el energy= -388.60633269089
zpe= -388.375960

th energy= -388.366305
th enthalpy= -388.365361
free energy= -388.410151

4mchm_11/coords
c2
C -0.324701 -1.105551 0.050069
H -1.010212 -1.918449 -0.238539
C -0.942961 0.255969 -0.297232
H -1.131674 0.288650 -1.387897
C 0.034914 1.387457 0.054307
H -0.400032 2.359597 -0.234859
C 1.385325 1.193429 -0.650608
H 1.224751 1.261961 -1.741888
C 2.022472 -0.170184 -0.326409
H 2.905612 -0.294810 -0.978560
C 1.026413 -1.297168 -0.655289
H 0.853511 -1.313474 -1.746904
C -2.265501 0.482436 0.417994
O -3.220188 -0.515893 -0.021802
C 2.511724 -0.244248 1.126572
H -0.197823 -1.164898 1.146471
H 0.176980 1.411781 1.149702
H 2.079041 2.006007 -0.373299
H 1.462450 -2.273754 -0.382117
H -2.118027 0.402925 1.509499
H -2.652864 1.489422 0.187876
H -4.049369 -0.346103 0.451131
H 2.995956 -1.214996 1.321240
H 3.248331 0.550390 1.328430
H 1.688759 -0.129944 1.847708
el energy= -388.60591486561
zpe= -388.375779
th energy= -388.365966
th enthalpy= -388.365022
free energy= -388.410199

4mchm_13/coords
c3
C -0.031330 1.386112 0.053954
H -0.178911 1.413951 1.148693
C 0.946720 0.251212 -0.285934

H 1.145450 0.280789 -1.376070
C 0.323490 -1.107541 0.059302
H 1.010447 -1.922137 -0.221606
C -1.022441 -1.298024 -0.656126
H -0.841650 -1.315392 -1.746475
C -2.019011 -0.169170 -0.335012
H -2.898274 -0.293756 -0.992375
C -1.378595 1.193409 -0.657368
H -2.072578 2.007173 -0.384009
C 2.266698 0.482234 0.441236
O 3.281346 -0.501471 0.124871
C -2.516804 -0.240801 1.115272
H 0.407651 2.356573 -0.235185
H 0.187663 -1.164817 1.154697
H -1.462424 -2.273563 -0.385408
H -1.212786 1.260911 -1.747909
H 2.649292 1.492393 0.214346
H 2.114956 0.405207 1.529066
H 3.442538 -0.437833 -0.830083
H -2.999516 -1.212395 1.309620
H -1.698357 -0.122298 1.840881
H -3.256632 0.552375 1.310899
el energy= -388.60627095478
zpe= -388.376060
th energy= -388.366269
th enthalpy= -388.365325
free energy= -388.410462

4mchm_15/coords
c4
C -0.485355 -0.847517 1.099133
H -0.157092 -0.681145 2.140999
C -1.157676 0.440353 0.592268
H -1.943006 0.737165 1.313146
C -0.122233 1.577544 0.508826
H -0.594770 2.487595 0.100096
C 1.101750 1.185656 -0.333216
H 0.806766 1.025840 -1.386520
C 1.765553 -0.095012 0.192325
H 2.111063 0.103199 1.225793
C 0.736428 -1.232467 0.252835
H 1.208310 -2.138567 0.671296

C -1.855285 0.252408 -0.756212
O -2.910605 -0.738250 -0.706130
C 2.972113 -0.484076 -0.663594
H -1.214066 -1.674013 1.121694
H 0.213903 1.820043 1.532630
H 1.834787 2.010915 -0.330166
H 0.424700 -1.484108 -0.777685
H -2.269251 1.219195 -1.091567
H -1.162763 -0.108419 -1.528024
H -3.542768 -0.438304 -0.033535
H 2.655411 -0.680686 -1.701743
H 3.724185 0.321179 -0.683541
H 3.457660 -1.395234 -0.278024
el energy= -388.60682174599
zpe= -388.376514
th energy= -388.366828
th enthalpy= -388.365884
free energy= -388.410660

4mchm_16/coords
c5
C -0.226932 1.262102 -0.187847
H -0.734974 2.158006 -0.585559
C -0.945898 -0.000370 -0.686318
H -0.900847 -0.000725 -1.793427
C -0.226724 -1.262515 -0.187154
H -0.296303 -1.314490 0.912072
C 1.247099 -1.259845 -0.620118
H 1.758134 -2.161956 -0.241245
C 1.990274 0.000097 -0.138084
H 2.993982 0.000014 -0.599872
C 1.246786 1.259475 -0.621199
H 1.290733 1.298242 -1.725028
C -2.426751 -0.000180 -0.333167
O -2.571301 0.000497 1.110657
C 2.186364 0.000674 1.384235
H -0.296314 1.314223 0.911356
H -0.734326 -2.158678 -0.584847
H 1.291271 -1.299786 -1.723880
H 1.757710 2.162123 -0.243435
H -2.916139 0.895606 -0.752438
H -2.916269 -0.896276 -0.751610

H -3.521996 0.000665 1.301126
H 2.751278 -0.890741 1.702158
H 2.750578 0.892731 1.701631
H 1.228570 0.000443 1.925655
el energy= -388.60546356343
zpe= -388.375003
th energy= -388.365354
th enthalpy= -388.364410
free energy= -388.409104

4mchm_17/coords
c6
C -0.221251 1.282886 -0.110610
H -0.721127 2.205609 -0.453569
C -0.951318 0.061184 -0.686135
H -0.915987 0.132275 -1.791833
C -0.239843 -1.238528 -0.280006
H -0.305978 -1.374242 0.814202
C 1.235704 -1.216601 -0.707305
H 1.738342 -2.146722 -0.390018
C 1.985438 0.002289 -0.138445
H 2.991308 0.025337 -0.594841
C 1.253240 1.295940 -0.540815
H 1.770786 2.168538 -0.105603
C -2.433872 0.044473 -0.319784
O -2.675755 -0.015408 1.107809
C 2.173662 -0.099281 1.381672
H -0.292865 1.268920 0.989820
H -0.752917 -2.099953 -0.742494
H 1.281965 -1.181370 -1.811027
H 1.300128 1.405118 -1.639748
H -2.918762 0.973796 -0.654133
H -2.935410 -0.805525 -0.814275
H -2.331112 -0.866302 1.419976
H 2.736791 0.769223 1.760040
H 1.213284 -0.135528 1.917294
H 2.737033 -1.010084 1.642307
el energy= -388.60583795386
zpe= -388.375599
th energy= -388.365804
th enthalpy= -388.364860
free energy= -388.409981

4mchm_23/coords
c7
C 0.429626 -1.311255 -0.873650
H 1.054051 -2.188827 -0.630880
C 1.299056 -0.038209 -0.841308
H 1.960483 -0.075761 -1.727856
C 0.433496 1.230868 -0.978031
H 1.060386 2.123427 -0.806682
C -0.796131 1.253186 -0.056714
H -0.487130 1.330467 0.999133
C -1.651283 -0.008675 -0.228411
H -1.983100 -0.053008 -1.284475
C -0.797508 -1.252689 0.048661
H -0.485031 -1.239447 1.106335
C 2.293057 0.008141 0.315278
O 1.625404 0.074862 1.601344
C -2.885357 0.028947 0.674690
H 0.069159 -1.451317 -1.909004
H 0.075481 1.287232 -2.022083
H -1.405454 2.145848 -0.283777
H -1.408927 -2.160484 -0.098765
H 2.928627 -0.894104 0.280861
H 2.941890 0.893464 0.196268
H 2.324448 0.106440 2.273494
H -3.505879 0.915935 0.467633
H -3.511489 -0.866665 0.531779
H -2.580478 0.066014 1.734175
el energy= -388.60213143395
zpe= -388.372029
th energy= -388.362267
th enthalpy= -388.361323
free energy= -388.406211

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.336888 -1.096129 0.026575
H 1.021353 -1.906165 -0.278985
C 0.945067 0.273737 -0.305197
H 1.129485 0.322914 -1.395826
C -0.039149 1.392442 0.068723
H -0.176211 1.398424 1.165066

C -1.391852 1.200850 -0.632595
H -1.237536 1.287806 -1.723394
C -2.017716 -0.172075 -0.326222
H -2.902796 -0.293434 -0.976321
C -1.015829 -1.287524 -0.676201
H -1.443772 -2.270854 -0.414936
C 2.271665 0.501465 0.411549
O 3.309210 -0.430435 0.019555
C -2.499688 -0.271560 1.127690
H 0.215395 -1.172866 1.122632
H 0.388663 2.371973 -0.206476
H -2.090008 2.003743 -0.338725
H -0.846797 -1.286947 -1.768389
H 2.670267 1.496383 0.163636
H 2.118584 0.450435 1.504259
H 3.034552 -1.309194 0.323984
H -3.239640 0.515789 1.345058
H -2.977676 -1.247899 1.309441
H -1.673859 -0.163863 1.846601
el energy= -388.60661533939
zpe= -388.375995
th energy= -388.366386
th enthalpy= -388.365442
free energy= -388.410017

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.496455 -0.813737 1.113544
H 1.230857 -1.636210 1.162990
C 1.160391 0.474963 0.595635
H 1.932867 0.790413 1.320080
C 0.111130 1.597651 0.484229
H -0.228278 1.858992 1.502356
C -1.109804 1.180375 -0.350272
H -0.816003 1.011350 -1.402250
C -1.757511 -0.102043 0.190389
H -2.103791 0.102219 1.222430
C -0.713261 -1.224735 0.262240
H -1.173284 -2.134976 0.684551
C 1.873639 0.272435 -0.742457
O 2.971419 -0.670163 -0.653350
C -2.960498 -0.514582 -0.659523

H 0.157693 -0.637144 2.150136
H 0.576191 2.503479 0.057573
H -1.852300 1.997253 -0.354350
H -0.391965 -1.477897 -0.765147
H 1.176089 -0.052910 -1.529697
H 2.331847 1.220108 -1.062107
H 2.585572 -1.542265 -0.476449
H -3.721509 0.281994 -0.686242
H -2.643331 -0.718119 -1.696187
H -3.435245 -1.426949 -0.263584
el energy= -388.60692721499
zpe= -388.376315
th energy= -388.366769
th enthalpy= -388.365824
free energy= -388.410184

MP2 cc-pVTZ gas phase

4mchm_1/coords
t1
C 0.156107 1.418246 0.180321
H 0.547051 2.344536 -0.247026
C 1.025710 0.236889 -0.239373
H 1.019079 0.170827 -1.333025
C 0.458371 -1.061839 0.324887
H 1.077000 -1.900622 0.008324
C -0.992667 -1.261433 -0.098671
H -1.388171 -2.187792 0.323971
C -1.872738 -0.085433 0.316316
H -1.851469 -0.020576 1.410508
C -1.296139 1.214013 -0.239814
H -1.907461 2.059898 0.082654
C 2.460878 0.451520 0.192607
O 3.248615 -0.618570 -0.319041
C -3.312953 -0.284815 -0.133017
H 0.204129 1.524763 1.269405
H 0.512878 -1.017176 1.418612
H -1.041420 -1.365717 -1.188115
H -1.353923 1.180046 -1.333103
H 2.818088 1.414272 -0.187230
H 2.504957 0.482265 1.287627
H 4.151293 -0.489864 -0.016266

H -3.362660 -0.352768 -1.221160
H -3.732472 -1.203036 0.278331
H -3.945231 0.546616 0.179282
el energy= -388.89558627617
zpe= -388.662706
th energy= -388.652969
th enthalpy= -388.652025
free energy= -388.696917

4mchm_3/coords
t2
C -0.157434 1.416426 0.180346
H -0.204827 1.523318 1.269310
C -1.027323 0.232501 -0.232654
H -1.011909 0.167867 -1.329373
C -0.454821 -1.063418 0.331131
H -0.506046 -1.015041 1.424504
C 0.994805 -1.262397 -0.097261
H 1.393080 -2.187281 0.325790
C 1.874277 -0.084107 0.313320
H 1.855851 -0.018196 1.407385
C 1.294333 1.214176 -0.242427
H 1.905048 2.061075 0.078360
C -2.466717 0.448867 0.204574
O -3.345282 -0.598058 -0.190770
C 3.313439 -0.281908 -0.139916
H -0.552077 2.341535 -0.246225
H -1.074172 -1.905906 0.024410
H 1.041613 -1.368384 -1.186854
H 1.350735 1.179926 -1.335923
H -2.514451 0.473018 1.294063
H -2.823498 1.417019 -0.162666
H -3.361724 -0.606258 -1.152264
H 3.945237 0.550805 0.169727
H 3.735561 -1.198918 0.271375
H 3.360484 -0.350955 -1.228141
el energy= -388.89571694304
zpe= -388.662742
th energy= -388.653067
th enthalpy= -388.652123
free energy= -388.696862

4mchm_5/coords
t3
C 0.390043 -1.253864 0.031751
H 0.822307 -2.143663 0.496050
C 1.021276 0.000005 0.632472
H 0.823367 0.000034 1.711456
C 0.390042 1.253869 0.031716
H 0.822347 2.143656 0.496011
C -1.125103 1.248143 0.205029
H -1.371213 1.277942 1.272480
C -1.759491 -0.000012 -0.402247
H -1.539040 -0.000012 -1.475910
C -1.125123 -1.248159 0.205019
H -1.561633 -2.143064 -0.244291
C 2.529382 0.000014 0.468645
O 2.828963 -0.000001 -0.924933
C -3.269705 0.000015 -0.212321
H 0.639751 -1.295075 -1.030432
H 0.639747 1.295055 -1.030464
H -1.561672 2.143032 -0.244257
H -1.371263 -1.277986 1.272465
H 2.950055 0.887301 0.953147
H 2.950073 -0.887248 0.953169
H 3.784910 -0.000113 -1.018946
H -3.516238 0.000072 0.850955
H -3.725540 0.882667 -0.661220
H -3.725586 -0.882661 -0.661123
el energy= -388.89536040568
zpe= -388.662397
th energy= -388.652692
th enthalpy= -388.651748
free energy= -388.696544

4mchm_6/coords
t4
C 0.156191 1.414402 0.181089
H 0.212930 1.508174 1.270979
C 1.028464 0.242004 -0.258933
H 1.020760 0.189559 -1.353053
C 0.461254 -1.064523 0.288292
H 1.054722 -1.911949 -0.062075
C -0.995835 -1.258387 -0.120549

H -1.055284 -1.346811 -1.210601
C -1.870051 -0.087775 0.319986
H -1.835507 -0.035587 1.414488
C -1.299553 1.217071 -0.228786
H -1.368482 1.194970 -1.321619
C 2.466356 0.464649 0.182362
O 3.370694 -0.526809 -0.287316
C -3.315175 -0.284692 -0.114369
H 0.545756 2.345430 -0.236822
H 0.531164 -1.047327 1.382258
H -1.386021 -2.190678 0.293688
H -1.907191 2.059332 0.109330
H 2.832518 1.408138 -0.221117
H 2.499612 0.539077 1.276038
H 3.150544 -1.349065 0.158132
H -3.943903 0.542695 0.214821
H -3.377955 -0.340344 -1.202481
H -3.729120 -1.207624 0.292004
el energy= -388.89559121645
zpe= -388.662605
th energy= -388.652895
th enthalpy= -388.651951
free energy= -388.696778

4mchm_7/coords
t5
C 0.383211 1.262498 -0.004833
H 0.637567 1.286900 1.057359
C 1.022704 0.025500 -0.628573
H 0.821847 0.039448 -1.707225
C 0.394143 -1.241327 -0.052831
H 0.615259 -1.296437 1.018160
C -1.120982 -1.243264 -0.231872
H -1.359634 -1.251497 -1.300948
C -1.763135 -0.011491 0.400499
H -1.547351 -0.035122 1.475008
C -1.132437 1.253439 -0.175480
H -1.573047 2.134540 0.296258
C 2.537101 0.031754 -0.468044
O 2.963306 0.038348 0.890536
C -3.272436 -0.015514 0.204610
H 0.810506 2.162852 -0.452345

H 0.834983 -2.125288 -0.521510
H -1.554134 -2.150161 0.195961
H -1.380119 1.308889 -1.241437
H 2.969206 -0.819890 -1.004104
H 2.948744 0.941637 -0.903989
H 2.755660 -0.824064 1.259833
H -3.725737 -0.910225 0.631698
H -3.734222 0.854550 0.671404
H -3.514989 0.007523 -0.859267
el energy= -388.89536830046
zpe= -388.662314
th energy= -388.652659
th enthalpy= -388.651715
free energy= -388.696400

4mchm_19/coords
t6
C 0.271810 -1.064811 0.693220
H -0.320261 -1.182315 1.603361
C 0.917356 0.323205 0.705547
H 1.425946 0.458234 1.663610
C -0.149528 1.411143 0.557450
H -0.761276 1.424726 1.461640
C -1.047644 1.190430 -0.660723
H -1.821275 1.961171 -0.692029
C -1.698990 -0.196251 -0.661102
H -2.197456 -0.332111 -1.624609
C -0.620151 -1.275965 -0.529019
H -0.004093 -1.277020 -1.431756
C 1.990316 0.461766 -0.360814
O 2.995450 -0.513449 -0.098728
C -2.765341 -0.322347 0.423876
H 1.052292 -1.824250 0.723874
H 0.324905 2.393516 0.494496
H -0.459827 1.306565 -1.574397
H -1.089545 -2.260966 -0.477322
H 1.569413 0.320081 -1.359585
H 2.407025 1.473350 -0.314216
H 3.656183 -0.447705 -0.793241
H -3.541973 0.431332 0.290786
H -3.238773 -1.303714 0.385480
H -2.351857 -0.196326 1.423119

el energy= -388.89045394014
zpe= -388.656883
th energy= -388.647301
th enthalpy= -388.646357
free energy= -388.690942

4mchm_21/coords
t7
C 0.143166 1.407807 0.558652
H -0.337422 2.387014 0.492702
C -0.919542 0.313561 0.694271
H -1.426043 0.449085 1.657126
C -0.271884 -1.073055 0.682645
H 0.309618 -1.199274 1.598384
C 0.631751 -1.275830 -0.532718
H 0.022777 -1.277125 -1.439833
C 1.706489 -0.190982 -0.651714
H 2.214145 -0.322673 -1.610842
C 1.047740 1.191921 -0.655466
H 0.462830 1.304245 -1.571361
C -1.990447 0.454907 -0.381711
O -3.030612 -0.508775 -0.263158
C 2.763222 -0.314049 0.443027
H 0.749781 1.424497 1.466278
H -1.051506 -1.834825 0.694482
H 1.104501 -2.258996 -0.479095
H 1.816661 1.967319 -0.683448
H -2.395480 1.472231 -0.352724
H -1.573743 0.300661 -1.374798
H -3.433195 -0.386112 0.601932
H 2.339346 -0.195850 1.438941
H 3.244238 -1.291657 0.404574
H 3.535414 0.445983 0.321037
el energy= -388.89080141168
zpe= -388.657119
th energy= -388.647604
th enthalpy= -388.646659
free energy= -388.691051

4mchm_22/coords
t8
C 0.147691 1.419553 0.547630

H -0.329464 2.399569 0.471058
C -0.921019 0.334503 0.711529
H -1.424966 0.478280 1.670514
C -0.265960 -1.049048 0.715183
H 0.337510 -1.148524 1.619659
C 0.613156 -1.279323 -0.513253
H 1.080413 -2.264928 -0.455947
C 1.692909 -0.202265 -0.660477
H 2.185570 -0.349396 -1.625077
C 1.043399 1.185133 -0.670332
H 1.818843 1.953455 -0.709622
C -2.000047 0.468879 -0.357871
O -3.082428 -0.437213 -0.177480
C 2.764556 -0.320740 0.420193
H 0.761375 1.448405 1.450307
H -1.029231 -1.827264 0.788193
H -0.006773 -1.283495 -1.413956
H 0.454776 1.294616 -1.583831
H -2.439206 1.464104 -0.293446
H -1.577421 0.366268 -1.360630
H -2.755630 -1.318342 -0.377180
H 3.545345 0.425040 0.269686
H 2.359156 -0.174385 1.419963
H 3.231025 -1.305845 0.394535
el energy= -388.88997654086
zpe= -388.656412
th energy= -388.646811
th enthalpy= -388.645867
free energy= -388.690498

4mchm_24/coords
t9
C -0.098679 1.264764 0.758581
H 0.611731 1.369463 1.582064
C -0.932276 0.000244 1.002140
H -1.223040 0.000452 2.058228
C -0.098737 -1.264400 0.759060
H 0.611692 -1.368816 1.582563
C 0.664678 -1.251142 -0.565685
H 1.291795 -2.143876 -0.630947
C 1.533793 -0.000155 -0.720987
H 1.940088 -0.000353 -1.735914

C 0.664800 1.250973 -0.566128
H -0.049237 1.289188 -1.387456
C -2.262482 0.000124 0.267832
O -2.068936 -0.000334 -1.146196
C 2.718391 -0.000048 0.242405
H -0.748452 2.142354 0.802346
H -0.748546 -2.141945 0.803183
H -0.049399 -1.289553 -1.386973
H 1.292015 2.143617 -0.631666
H -2.829685 -0.885920 0.572823
H -2.829556 0.886438 0.572281
H -2.938631 -0.000481 -1.556018
H 2.401984 0.000148 1.284506
H 3.340859 -0.882169 0.088772
H 3.340942 0.881959 0.088469
el energy= -388.88861215119
zpe= -388.654933
th energy= -388.645413
th enthalpy= -388.644469
free energy= -388.688706

4mchm_9/coords
c1
C -0.494648 -0.822256 1.092913
H -1.234001 -1.622222 1.105692
C -1.148413 0.466176 0.589268
H -1.912840 0.768716 1.309598
C -0.107912 1.582807 0.479802
H -0.565462 2.483372 0.063094
C 1.109007 1.172960 -0.348192
H 0.822018 1.007336 -1.391097
C 1.754432 -0.102306 0.188513
H 2.093459 0.100487 1.211364
C 0.717706 -1.221022 0.255817
H 1.173939 -2.122896 0.670215
C -1.872982 0.260864 -0.729697
O -2.890963 -0.714016 -0.521643
C 2.955509 -0.508193 -0.652888
H -0.170199 -0.664388 2.125371
H 0.228602 1.840759 1.487482
H 1.841667 1.983314 -0.355528
H 0.407267 -1.474481 -0.762715

H -2.305907 1.214794 -1.048640
H -1.179885 -0.067860 -1.508388
H -3.325753 -0.868720 -1.364419
H 2.644779 -0.717753 -1.678066
H 3.703695 0.284175 -0.685989
H 3.430126 -1.406692 -0.258051
el energy= -388.89323943845
zpe= -388.660015
th energy= -388.650376
th enthalpy= -388.649432
free energy= -388.694200

4mchm_11/coords
c2
C -0.334889 -1.089791 0.057559
H -1.032718 -1.879980 -0.216569
C -0.939788 0.268344 -0.285477
H -1.130970 0.297718 -1.364238
C 0.038414 1.387049 0.062120
H -0.384267 2.354927 -0.217189
C 1.378069 1.186255 -0.643265
H 1.215275 1.261574 -1.722228
C 2.004932 -0.175986 -0.332119
H 2.870059 -0.303297 -0.988265
C 1.003215 -1.290103 -0.649117
H 0.826409 -1.309745 -1.728485
C -2.264729 0.481443 0.415251
O -3.174410 -0.519547 -0.029790
C 2.509728 -0.255108 1.106293
H -0.202509 -1.149789 1.142358
H 0.184392 1.411343 1.146009
H 2.072181 1.984639 -0.371282
H 1.431062 -2.259064 -0.382247
H -2.111534 0.417978 1.499045
H -2.644158 1.482521 0.185609
H -4.002185 -0.394935 0.441724
H 2.983856 -1.218493 1.295344
H 3.245355 0.525878 1.300723
H 1.705314 -0.137516 1.830534
el energy= -388.89301999047
zpe= -388.659802
th energy= -388.650140

th enthalpy= -388.649196
free energy= -388.693927

4mchm_13/coords
c3
C -0.036244 1.385138 0.062936
H -0.184976 1.408720 1.146372
C 0.941521 0.263515 -0.277479
H 1.126538 0.295149 -1.360393
C 0.330829 -1.092122 0.062253
H 1.028060 -1.886830 -0.201922
C -1.003912 -1.290616 -0.651103
H -0.823319 -1.311270 -1.730066
C -2.004464 -0.173846 -0.338932
H -2.866743 -0.299584 -0.999043
C -1.373745 1.187341 -0.647405
H -2.067311 1.986836 -0.377528
C 2.268398 0.477285 0.431716
O 3.245811 -0.508696 0.120286
C -2.515849 -0.251702 1.097194
H 0.390635 2.352097 -0.213261
H 0.193205 -1.149292 1.146199
H -1.435193 -2.258328 -0.385590
H -1.207487 1.263204 -1.725948
H 2.645658 1.482603 0.215835
H 2.118186 0.407434 1.509916
H 3.435559 -0.432432 -0.819389
H -2.992032 -1.214350 1.284565
H -1.714977 -0.134542 1.825387
H -3.251492 0.530190 1.287507
el energy= -388.89315847358
zpe= -388.659845
th energy= -388.650247
th enthalpy= -388.649303
free energy= -388.693880

4mchm_15/coords
c4
C -0.493709 -0.842635 1.077927
H -0.179787 -0.702063 2.116080
C -1.148832 0.449007 0.585616
H -1.911809 0.747309 1.314192

C -0.114984 1.574031 0.494861
H -0.577191 2.475050 0.084299
C 1.105343 1.177360 -0.334312
H 0.820397 1.018067 -1.378673
C 1.756198 -0.098075 0.194811
H 2.087828 0.097535 1.221595
C 0.726536 -1.223932 0.243827
H 1.185202 -2.127299 0.651921
C -1.869769 0.257245 -0.743776
O -2.881064 -0.742317 -0.690380
C 2.964716 -0.488706 -0.643330
H -1.227401 -1.648672 1.067697
H 0.217478 1.824618 1.505829
H 1.832915 1.992156 -0.334288
H 0.422659 -1.468779 -0.778452
H -2.285994 1.217130 -1.068122
H -1.182849 -0.076092 -1.518828
H -3.517269 -0.466449 -0.023588
H 2.661123 -0.690016 -1.672205
H 3.708122 0.308465 -0.663879
H 3.442097 -1.388181 -0.254282
el energy= -388.89355381616
zpe= -388.660218
th energy= -388.650643
th enthalpy= -388.649699
free energy= -388.694272

4mchm_16/coords
c5
C 0.234131 -1.256395 -0.211862
H 0.728018 -2.142534 -0.618331
C 0.949529 -0.000004 -0.705087
H 0.922026 -0.000009 -1.801764
C 0.234131 1.256392 -0.211873
H 0.333036 1.313876 0.872551
C -1.237343 1.250771 -0.618463
H -1.736795 2.145900 -0.240797
C -1.970825 -0.000001 -0.126645
H -2.970172 -0.000004 -0.570163
C -1.237343 -1.250778 -0.618451
H -1.301313 -1.289566 -1.710228
C 2.412760 -0.000002 -0.305747

O 2.487206 0.000009 1.118184
C -2.142443 0.000008 1.390124
H 0.333037 -1.313869 0.872563
H 0.728018 2.142527 -0.618349
H -1.301314 1.289550 -1.710240
H -1.736794 -2.145904 -0.240777
H 2.904803 -0.887412 -0.717472
H 2.904806 0.887401 -0.717486
H 3.416079 -0.000006 1.363012
H -2.695325 0.881916 1.714950
H -2.695323 -0.881898 1.714961
H -1.186019 0.000012 1.910121
el energy= -388.89310215955
zpe= -388.659774
th energy= -388.650157
th enthalpy= -388.649213
free energy= -388.693830

4mchm_17/coords
c6
C -0.226308 1.275896 -0.110555
H -0.715643 2.193361 -0.445772
C -0.952710 0.067035 -0.694319
H -0.921914 0.142518 -1.788834
C -0.241989 -1.225091 -0.296622
H -0.306754 -1.355092 0.787065
C 1.226896 -1.202460 -0.714199
H 1.722192 -2.126897 -0.408914
C 1.973204 0.003332 -0.136639
H 2.967273 0.029513 -0.590785
C 1.244073 1.293337 -0.522024
H 1.751420 2.151833 -0.076384
C -2.423077 0.049968 -0.299239
O -2.629839 -0.028644 1.107708
C 2.163841 -0.112977 1.373464
H -0.324288 1.252259 0.975862
H -0.745182 -2.082678 -0.751301
H 1.277746 -1.160453 -1.806085
H 1.302974 1.419627 -1.607273
H -2.897618 0.980682 -0.609246
H -2.934770 -0.772103 -0.810841
H -2.376046 -0.912967 1.384959

H 2.738773 0.731533 1.753863
H 1.214925 -0.129110 1.907098
H 2.702046 -1.027109 1.625727
el energy= -388.89300161253
zpe= -388.659595
th energy= -388.650022
th enthalpy= -388.649078
free energy= -388.693600

4mchm_23/coords
c7
C 0.454893 -1.260962 -0.937093
H 1.068071 -2.143498 -0.738681
C 1.318225 0.000618 -0.823616
H 2.006635 0.001234 -1.675610
C 0.454862 1.262341 -0.935295
H 1.068016 2.144607 -0.735616
C -0.771264 1.248450 -0.024724
H -0.456402 1.276796 1.018986
C -1.620665 0.000163 -0.246942
H -1.958322 0.000884 -1.290915
C -0.771210 -1.248396 -0.026471
H -0.456329 -1.278189 1.017194
C 2.243330 -0.000241 0.381853
O 1.500056 -0.001247 1.600280
C -2.841972 -0.000497 0.661077
H 0.112900 -1.344181 -1.973160
H 0.112897 1.347034 -1.971250
H -1.374046 2.140679 -0.211837
H -1.373953 -2.140391 -0.214823
H 2.885221 -0.886187 0.329009
H 2.885094 0.885875 0.330378
H 2.133184 -0.001539 2.323817
H -3.459957 0.882542 0.495890
H -3.459916 -0.883334 0.494670
H -2.530745 -0.001214 1.706978
el energy= -388.89147717935
zpe= -388.658133
th energy= -388.648554
th enthalpy= -388.647609
free energy= -388.692025

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.339219 -1.087175 0.018787
H 1.016953 -1.883529 -0.296801
C 0.942351 0.277226 -0.304109
H 1.130261 0.322657 -1.382602
C -0.039017 1.386168 0.066796
H -0.172416 1.396883 1.152497
C -1.386776 1.194903 -0.624809
H -1.238936 1.284899 -1.704689
C -2.007200 -0.171968 -0.322736
H -2.881597 -0.293360 -0.967371
C -1.009205 -1.278845 -0.672701
H -1.430772 -2.253321 -0.416490
C 2.269518 0.492916 0.405306
O 3.280628 -0.431265 0.024539
C -2.488858 -0.273841 1.122073
H 0.223778 -1.176809 1.103904
H 0.381165 2.357616 -0.203296
H -2.078104 1.988363 -0.332553
H -0.845634 -1.278657 -1.754091
H 2.664298 1.477117 0.154992
H 2.105734 0.469867 1.489574
H 3.015168 -1.295581 0.349389
H -3.223670 0.501806 1.338823
H -2.957300 -1.241207 1.304892
H -1.674139 -0.162931 1.835860
el energy= -388.89304999256
zpe= -388.659718
th energy= -388.650090
th enthalpy= -388.649146
free energy= -388.693802

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.492490 -0.805587 1.106321
H 1.224179 -1.614807 1.163306
C 1.155068 0.474086 0.591950
H 1.917421 0.779202 1.313046
C 0.112468 1.589120 0.475271
H -0.223689 1.858469 1.480204
C -1.105100 1.174154 -0.350100

H -0.819513 1.006519 -1.392664
C -1.749820 -0.100091 0.189507
H -2.090905 0.103726 1.211421
C -0.711766 -1.217321 0.263170
H -1.167290 -2.119090 0.678319
C 1.882328 0.267051 -0.732268
O 2.946531 -0.673609 -0.644928
C -2.948083 -0.511899 -0.653066
H 0.157369 -0.634186 2.132948
H 0.571392 2.484415 0.049029
H -1.838983 1.983148 -0.358350
H -0.398511 -1.470106 -0.755165
H 1.184928 -0.015376 -1.525084
H 2.347190 1.206179 -1.031267
H 2.553001 -1.542274 -0.528091
H -3.697301 0.279070 -0.689479
H -2.635097 -0.723154 -1.677114
H -3.421951 -1.409932 -0.256355
el energy= -388.89278111104
zpe= -388.659552
th energy= -388.649897
th enthalpy= -388.648953
free energy= -388.693761

MP2-SMD cc-pVTZ

4mchm_1/coords
t1
C 0.159912 1.408989 0.181076
H 0.558625 2.331261 -0.247004
C 1.024889 0.224279 -0.240413
H 1.014631 0.163337 -1.334540
C 0.447401 -1.070404 0.324364
H 1.050038 -1.921946 0.007283
C -1.005109 -1.261887 -0.098468
H -1.405066 -2.185588 0.326089
C -1.877268 -0.081227 0.317786
H -1.856037 -0.016580 1.411491
C -1.292614 1.213332 -0.239767
H -1.898730 2.062630 0.083619
C 2.455313 0.445106 0.200304
O 3.276925 -0.603443 -0.326929

C -3.316186 -0.271938 -0.136040
H 0.210036 1.511527 1.270077
H 0.503912 -1.023991 1.417430
H -1.054805 -1.362966 -1.188118
H -1.349942 1.176454 -1.332954
H 2.808539 1.414720 -0.159866
H 2.502954 0.450199 1.293458
H 4.172906 -0.447247 -0.007937
H -3.362641 -0.333844 -1.225125
H -3.742796 -1.189897 0.270129
H -3.945058 0.561974 0.178356
el energy= -388.90106558373
zpe= -388.669269
th energy= -388.659396
th enthalpy= -388.658452
free energy= -388.703673

4mchm_3/coords
t2
C -0.162521 1.409155 0.180538
H -0.207759 1.516684 1.269431
C -1.028910 0.221482 -0.229325
H -1.026801 0.156285 -1.324669
C -0.447431 -1.070456 0.335292
H -0.497513 -1.021329 1.428577
C 1.002828 -1.262359 -0.094967
H 1.406107 -2.184420 0.330042
C 1.875779 -0.079531 0.313802
H 1.858323 -0.011156 1.407361
C 1.288367 1.212917 -0.245955
H 1.895681 2.063527 0.071797
C -2.460279 0.444588 0.220703
O -3.358312 -0.585856 -0.206459
C 3.313312 -0.270817 -0.144200
H -0.564522 2.329228 -0.249456
H -1.052471 -1.922693 0.024087
H 1.047107 -1.366269 -1.184613
H 1.340967 1.172107 -1.339253
H -2.506898 0.445551 1.310439
H -2.811887 1.417764 -0.132523
H -3.341514 -0.579350 -1.170675
H 3.942512 0.564895 0.164709

H 3.742085 -1.186741 0.264271
H 3.356213 -0.337112 -1.233173
el energy= -388.90177103183
zpe= -388.669652
th energy= -388.659909
th enthalpy= -388.658964
free energy= -388.703829

4mchm_5/coords
t3
C 0.382797 -1.253269 0.011218
H 0.820661 -2.142783 0.470360
C 1.013830 -0.000004 0.612623
H 0.802677 0.000010 1.688329
C 0.382805 1.253257 0.011197
H 0.820727 2.142751 0.470345
C -1.130869 1.248741 0.197121
H -1.364862 1.277383 1.266939
C -1.770589 -0.000003 -0.403014
H -1.563260 0.000000 -1.479102
C -1.130896 -1.248756 0.197092
H -1.571460 -2.142369 -0.251010
C 2.523701 -0.000001 0.485390
O 2.884409 0.000014 -0.901027
C -3.276958 0.000023 -0.192233
H 0.613227 -1.294008 -1.056213
H 0.613224 1.293979 -1.056232
H -1.571476 2.142353 -0.250944
H -1.364928 -1.277438 1.266905
H 2.933866 0.885734 0.977705
H 2.933879 -0.885733 0.977688
H 3.847181 -0.000023 -0.938732
H -3.507689 0.000105 0.875015
H -3.739958 0.882863 -0.634668
H -3.740007 -0.882855 -0.634527
el energy= -388.90047235100
zpe= -388.668361
th energy= -388.658627
th enthalpy= -388.657682
free energy= -388.702557

4mchm_6/coords

t4
C 0.157802 1.413935 0.184953
H 0.211993 1.507345 1.274616
C 1.027069 0.237703 -0.250607
H 1.014831 0.184284 -1.344945
C 0.458202 -1.064359 0.306104
H 1.056349 -1.916081 -0.026016
C -0.995717 -1.259691 -0.111147
H -1.049547 -1.352051 -1.201249
C -1.870987 -0.086320 0.318948
H -1.844767 -0.030247 1.413007
C -1.295771 1.215540 -0.231190
H -1.358025 1.187217 -1.324331
C 2.460827 0.463077 0.191950
O 3.374704 -0.519140 -0.308483
C -3.311067 -0.281234 -0.129495
H 0.551320 2.341617 -0.236577
H 0.521809 -1.030593 1.399250
H -1.388950 -2.188575 0.308107
H -1.904574 2.059067 0.102071
H 2.821030 1.418912 -0.186884
H 2.503037 0.496104 1.285193
H 3.121537 -1.363260 0.081121
H -3.942875 0.546247 0.195661
H -3.362583 -0.333568 -1.218841
H -3.730363 -1.205205 0.270578
el energy= -388.90187543158
zpe= -388.669888
th energy= -388.660063
th enthalpy= -388.659119
free energy= -388.704214

4mchm_7/coords
t5
C 0.381575 1.259990 0.002443
H 0.616468 1.283472 1.069632
C 1.019040 0.020486 -0.618337
H 0.813411 0.035154 -1.695308
C 0.391076 -1.245656 -0.040726
H 0.617253 -1.306685 1.028745
C -1.123307 -1.243771 -0.222058
H -1.359627 -1.254609 -1.291588

C -1.766189 -0.008424 0.401746
H -1.555867 -0.026475 1.477005
C -1.132726 1.252916 -0.178467
H -1.575257 2.136588 0.287173
C 2.532637 0.024324 -0.480856
O 2.988155 0.050152 0.877542
C -3.272926 -0.011495 0.194846
H 0.814770 2.159135 -0.442383
H 0.831301 -2.126406 -0.514650
H -1.559002 -2.146892 0.211409
H -1.371345 1.299665 -1.246590
H 2.952727 -0.842794 -0.997556
H 2.941766 0.922972 -0.941579
H 2.729710 -0.787246 1.278367
H -3.730251 -0.905909 0.619785
H -3.739410 0.859307 0.657129
H -3.506965 0.009290 -0.871470
el energy= -388.90135587302
zpe= -388.669422
th energy= -388.659597
th enthalpy= -388.658653
free energy= -388.703743

4mchm_19/coords
t6
C 0.253274 -1.071304 0.701288
H -0.350980 -1.171314 1.605424
C 0.916886 0.308363 0.712370
H 1.424083 0.443563 1.671735
C -0.144403 1.402574 0.567236
H -0.760876 1.411098 1.468264
C -1.033592 1.192356 -0.658533
H -1.801480 1.968697 -0.692601
C -1.697508 -0.187752 -0.666805
H -2.189298 -0.318465 -1.634158
C -0.630169 -1.277624 -0.527949
H -0.007885 -1.283294 -1.426269
C 1.980888 0.451379 -0.360317
O 3.021759 -0.500533 -0.103388
C -2.770605 -0.307261 0.411205
H 1.014571 -1.850657 0.746865
H 0.339043 2.380514 0.509470

H -0.433819 1.303181 -1.564793
H -1.110901 -2.257240 -0.474508
H 1.566856 0.285784 -1.355936
H 2.384943 1.466738 -0.328736
H 3.658203 -0.420265 -0.822848
H -3.535090 0.460040 0.281232
H -3.259864 -1.280877 0.358820
H -2.360209 -0.197615 1.414177
el energy= -388.89638749335
zpe= -388.663431
th energy= -388.653891
th enthalpy= -388.652947
free energy= -388.697432

4mchm_21/coords
t7
C 0.131839 1.393945 0.569109
H -0.358148 2.368760 0.512189
C -0.923978 0.291684 0.685538
H -1.448233 0.415599 1.639022
C -0.257580 -1.086032 0.670484
H 0.326315 -1.201470 1.586034
C 0.651870 -1.274118 -0.542981
H 0.047762 -1.274005 -1.453564
C 1.714197 -0.176092 -0.650665
H 2.226268 -0.294955 -1.608951
C 1.039329 1.198589 -0.645195
H 0.450224 1.308060 -1.558904
C -1.979904 0.436810 -0.400906
O -3.062564 -0.487961 -0.243289
C 2.765968 -0.297225 0.448006
H 0.735024 1.399437 1.479167
H -1.020671 -1.865396 0.686181
H 1.137558 -2.251298 -0.490201
H 1.800971 1.981490 -0.665473
H -2.358868 1.462636 -0.398981
H -1.569868 0.236700 -1.388574
H -3.443323 -0.317556 0.626849
H 2.333722 -0.204667 1.443503
H 3.266815 -1.264833 0.394007
H 3.524524 0.479814 0.343672
el energy= -388.89711500683

zpe= -388.664063
th energy= -388.654591
th enthalpy= -388.653647
free energy= -388.697892

4mchm_22/coords
t8
C 0.151319 1.423892 0.545136
H -0.326194 2.403475 0.464217
C -0.918434 0.341074 0.716726
H -1.417230 0.493940 1.677605
C -0.267102 -1.044061 0.723642
H 0.342174 -1.135218 1.625138
C 0.604060 -1.280079 -0.508400
H 1.070334 -2.266065 -0.446302
C 1.685946 -0.206882 -0.663319
H 2.175927 -0.358499 -1.628499
C 1.040067 1.181710 -0.675772
H 1.818263 1.947237 -0.719643
C -1.991386 0.478572 -0.354598
O -3.071050 -0.448426 -0.183816
C 2.757035 -0.324356 0.416959
H 0.768082 1.450951 1.445696
H -1.031492 -1.820754 0.796880
H -0.023947 -1.286064 -1.403145
H 0.444785 1.286723 -1.585370
H -2.439043 1.469562 -0.285427
H -1.571081 0.374102 -1.355932
H -2.723741 -1.323378 -0.390217
H 3.537132 0.423646 0.268859
H 2.349663 -0.182517 1.417132
H 3.225741 -1.308965 0.387293
el energy= -388.89701430747
zpe= -388.663855
th energy= -388.654383
th enthalpy= -388.653439
free energy= -388.697610

4mchm_24/coords
t9
C -0.090621 1.265487 0.743251
H 0.619811 1.375327 1.565714

C -0.920964 0.000069 0.993306
H -1.196659 0.000129 2.052795
C -0.090633 -1.265383 0.743388
H 0.619805 -1.375137 1.565857
C 0.681816 -1.251141 -0.575699
H 1.312118 -2.142157 -0.634874
C 1.550964 -0.000045 -0.724848
H 1.972116 -0.000101 -1.733628
C 0.681849 1.251092 -0.575825
H -0.019517 1.296723 -1.408637
C -2.268061 0.000038 0.293016
O -2.135101 -0.000091 -1.134934
C 2.719357 -0.000013 0.255882
H -0.744475 2.140284 0.781406
H -0.744494 -2.140172 0.781651
H -0.019565 -1.296832 -1.408497
H 1.312179 2.142084 -0.635079
H -2.827857 -0.884643 0.609490
H -2.827819 0.884798 0.609338
H -3.030984 -0.000181 -1.491885
H 2.386118 0.000039 1.292780
H 3.343878 -0.882402 0.109145
H 3.343898 0.882347 0.109064
el energy= -388.89257085767
zpe= -388.659949
th energy= -388.650287
th enthalpy= -388.649343
free energy= -388.694026

4mchm_9/coords
c1
C -0.479567 -0.829225 1.101703
H -1.206165 -1.641775 1.130245
C -1.146742 0.452893 0.598353
H -1.910250 0.755263 1.320450
C -0.111241 1.574783 0.491324
H -0.577440 2.472814 0.079484
C 1.100720 1.173159 -0.346445
H 0.803689 1.004839 -1.385873
C 1.757670 -0.098035 0.184629
H 2.103912 0.104693 1.204702
C 0.728908 -1.223155 0.256734

H 1.192890 -2.121061 0.671545
C -1.863202 0.254661 -0.724481
O -2.915207 -0.700167 -0.533771
C 2.951432 -0.496102 -0.669259
H -0.147139 -0.662966 2.130163
H 0.229617 1.826217 1.499064
H 1.829017 1.987425 -0.355433
H 0.413951 -1.474388 -0.760764
H -2.279093 1.210820 -1.052854
H -1.178681 -0.097366 -1.497603
H -3.342960 -0.820600 -1.389091
H 2.632643 -0.696756 -1.694049
H 3.698790 0.297767 -0.699942
H 3.430996 -1.397453 -0.285228
el energy= -388.89898516181
zpe= -388.666467
th energy= -388.656826
th enthalpy= -388.655881
free energy= -388.700628

4mchm_11/coords
c2
C -0.323064 -1.097217 0.052933
H -1.004158 -1.902026 -0.224960
C -0.938902 0.255484 -0.293766
H -1.123758 0.286558 -1.373795
C 0.032859 1.379400 0.057006
H -0.397261 2.342777 -0.225586
C 1.375745 1.187802 -0.643239
H 1.216522 1.260131 -1.722946
C 2.010957 -0.168867 -0.327900
H 2.881262 -0.291121 -0.977802
C 1.018507 -1.288972 -0.650172
H 0.844933 -1.307071 -1.730124
C -2.258227 0.476104 0.412624
O -3.199325 -0.510940 -0.026310
C 2.503717 -0.244637 1.113941
H -0.193048 -1.151581 1.137951
H 0.172833 1.400474 1.141459
H 2.063070 1.990596 -0.366606
H 1.451322 -2.254915 -0.379698
H -2.108736 0.402721 1.494064

H -2.634189 1.477760 0.188702
H -4.012155 -0.365087 0.470669
H 2.980090 -1.206951 1.306433
H 3.235805 0.539283 1.312734
H 1.692512 -0.128611 1.831428
el energy= -388.89871826363
zpe= -388.666273
th energy= -388.656578
th enthalpy= -388.655634
free energy= -388.700504

4mchm_13/coords
c3
C -0.030887 1.379404 0.055040
H -0.173801 1.402536 1.139213
C 0.942078 0.253744 -0.287610
H 1.134969 0.283613 -1.367479
C 0.324707 -1.098346 0.054732
H 1.007029 -1.902560 -0.222559
C -1.014315 -1.288824 -0.653621
H -0.837048 -1.304837 -1.733056
C -2.007650 -0.168998 -0.333018
H -2.876959 -0.291678 -0.984163
C -1.372388 1.187842 -0.647822
H -2.060323 1.990577 -0.372344
C 2.258381 0.480340 0.431397
O 3.254723 -0.503406 0.131741
C -2.502495 -0.244981 1.108153
H 0.401130 2.342101 -0.227398
H 0.190947 -1.155518 1.139167
H -1.448446 -2.255135 -0.386589
H -1.211538 1.259934 -1.727283
H 2.637048 1.479636 0.199876
H 2.100764 0.422315 1.509184
H 3.420240 -0.447115 -0.816804
H -2.977660 -1.207991 1.300224
H -1.692631 -0.127550 1.826895
H -3.236090 0.537830 1.305683
el energy= -388.89939194246
zpe= -388.666867
th energy= -388.657193
th enthalpy= -388.656249

free energy= -388.701081

4mchm_15/coords
c4
C -0.486830 -0.842810 1.084535
H -0.165913 -0.687622 2.118357
C -1.151656 0.441675 0.586648
H -1.925199 0.734219 1.304473
C -0.120641 1.569626 0.500992
H -0.586543 2.468913 0.091178
C 1.099848 1.178202 -0.329611
H 0.812320 1.018348 -1.373095
C 1.756176 -0.096133 0.194931
H 2.093769 0.097689 1.219616
C 0.730506 -1.225187 0.247282
H 1.193600 -2.125677 0.657402
C -1.856015 0.255375 -0.749320
O -2.886885 -0.737328 -0.699470
C 2.957695 -0.482888 -0.653310
H -1.212627 -1.656833 1.096498
H 0.209820 1.815105 1.513673
H 1.826082 1.994317 -0.325651
H 0.425378 -1.467419 -0.775391
H -2.271958 1.214302 -1.070917
H -1.166681 -0.082062 -1.520256
H -3.498458 -0.463167 -0.005659
H 2.647063 -0.675817 -1.682094
H 3.702926 0.313330 -0.671761
H 3.437001 -1.386167 -0.273495
el energy= -388.89972759482
zpe= -388.667227
th energy= -388.657572
th enthalpy= -388.656628
free energy= -388.701317

4mchm_16/coords
c5
C 0.226891 -1.254790 -0.191723
H 0.727141 -2.142179 -0.587044
C 0.942945 -0.000007 -0.687021
H 0.901085 -0.000015 -1.782552
C 0.226894 1.254784 -0.191743

H 0.302003 1.306661 0.895777
C -1.239816 1.251668 -0.615952
H -1.744368 2.144798 -0.240054
C -1.979412 0.000000 -0.135970
H -2.972956 -0.000003 -0.591494
C -1.239818 -1.251677 -0.615933
H -1.286995 -1.291914 -1.708163
C 2.413372 -0.000007 -0.322711
O 2.548164 0.000014 1.105037
C -2.170984 0.000012 1.377460
H 0.301999 -1.306650 0.895797
H 0.727146 2.142167 -0.587077
H -1.286992 1.291891 -1.708182
H -1.744373 -2.144800 -0.240023
H 2.897999 -0.885869 -0.741672
H 2.898005 0.885840 -0.741698
H 3.492803 0.000012 1.296383
H -2.728291 0.882442 1.694951
H -2.728286 -0.882416 1.694967
H -1.221660 0.000020 1.911338
el energy= -388.89827741074
zpe= -388.665611
th energy= -388.656007
th enthalpy= -388.655063
free energy= -388.699664

4mchm_17/coords
c6
C -0.222444 1.274095 -0.112209
H -0.715699 2.189214 -0.448736
C -0.949193 0.060774 -0.686464
H -0.914685 0.131446 -1.780439
C -0.240556 -1.230012 -0.280466
H -0.306926 -1.358688 0.803189
C 1.226910 -1.209030 -0.702659
H 1.723975 -2.129411 -0.387749
C 1.974482 0.002277 -0.139084
H 2.968402 0.025383 -0.593146
C 1.244393 1.288073 -0.535662
H 1.755719 2.150871 -0.102432
C -2.421413 0.044750 -0.310504
O -2.650428 -0.014949 1.102873

C 2.164793 -0.098833 1.371318
H -0.298011 1.255309 0.976635
H -0.747267 -2.085601 -0.733619
H 1.273768 -1.175740 -1.794991
H 1.292522 1.399563 -1.622849
H -2.899114 0.965522 -0.644110
H -2.920688 -0.793924 -0.803351
H -2.330077 -0.872891 1.402760
H 2.724860 0.759030 1.745883
H 1.215338 -0.131236 1.903999
H 2.719471 -1.001821 1.630354
el energy= -388.89915371744
zpe= -388.666559
th energy= -388.656900
th enthalpy= -388.655956
free energy= -388.700703

4mchm_23/coords
c7
C 0.433724 -1.222180 -0.976552
H 1.052632 -2.107145 -0.809446
C 1.295701 0.037764 -0.834559
H 1.955811 0.074800 -1.707051
C 0.430156 1.302336 -0.872640
H 1.046872 2.172400 -0.634386
C -0.791438 1.246497 0.041868
H -0.480902 1.234099 1.088108
C -1.640566 0.008758 -0.230264
H -1.974202 0.052611 -1.273739
C -0.790204 -1.246506 -0.062987
H -0.482933 -1.323481 0.981313
C 2.272004 -0.009153 0.326969
O 1.603436 -0.074111 1.593800
C -2.861829 -0.028877 0.675475
H 0.081745 -1.274837 -2.010808
H 0.075832 1.438360 -1.898531
H -1.396716 2.144708 -0.104206
H -1.393343 -2.129808 -0.287608
H 2.916463 -0.884548 0.207416
H 2.904431 0.882396 0.290265
H 2.295046 -0.103691 2.265446
H -3.482110 0.858270 0.541034

H -3.478255 -0.906422 0.475817
H -2.553147 -0.066666 1.722113
el energy= -388.89519904966
zpe= -388.662911
th energy= -388.653177
th enthalpy= -388.652233
free energy= -388.697084

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.335544 -1.089423 0.026243
H 1.013795 -1.890659 -0.275384
C 0.940832 0.272415 -0.303024
H 1.122943 0.319082 -1.382768
C -0.037263 1.384144 0.068784
H -0.171517 1.388853 1.154181
C -1.382973 1.194625 -0.626413
H -1.230951 1.282999 -1.705922
C -2.006790 -0.170529 -0.325670
H -2.881012 -0.289780 -0.970856
C -1.009608 -1.279296 -0.671375
H -1.434080 -2.252092 -0.412817
C 2.262783 0.495250 0.407406
O 3.286108 -0.428125 0.018521
C -2.488080 -0.270258 1.118526
H 0.214560 -1.165331 1.111127
H 0.386133 2.354144 -0.201708
H -2.074024 1.988646 -0.334176
H -0.842196 -1.279589 -1.752348
H 2.651054 1.483702 0.163815
H 2.106396 0.452015 1.489732
H 3.016247 -1.296873 0.336209
H -3.220944 0.508268 1.334778
H -2.960212 -1.236888 1.299551
H -1.671727 -0.163066 1.831566
el energy= -388.89957401749
zpe= -388.666779
th energy= -388.657215
th enthalpy= -388.656271
free energy= -388.700778

4mchm-1000rej-h-rmsd_20/coords

c9
C 0.493976 -0.809916 1.103343
H 1.222725 -1.622384 1.147285
C 1.154263 0.472256 0.591837
H 1.917057 0.781304 1.311574
C 0.111721 1.587601 0.478874
H -0.223734 1.850128 1.485676
C -1.104515 1.173428 -0.347299
H -0.815716 1.003447 -1.388591
C -1.749068 -0.100777 0.191579
H -2.090562 0.101283 1.213380
C -0.711245 -1.217601 0.260617
H -1.165986 -2.119464 0.676810
C 1.871571 0.270570 -0.735205
O 2.951205 -0.667727 -0.644994
C -2.944823 -0.509855 -0.654279
H 0.161323 -0.639503 2.130908
H 0.571898 2.482785 0.053665
H -1.838364 1.982693 -0.352876
H -0.395619 -1.465845 -0.757623
H 1.178146 -0.036989 -1.519211
H 2.324775 1.212037 -1.044227
H 2.557462 -1.536173 -0.505480
H -3.698137 0.278436 -0.682214
H -2.630697 -0.710381 -1.680523
H -3.415496 -1.413796 -0.265398
el energy= -388.89961094942
zpe= -388.666763
th energy= -388.657265
th enthalpy= -388.656321
free energy= -388.700612

MP2 aug-cc-pVTZ gas phase

4mchm_1/coords
t1
C 0.156172 1.417684 0.179194
H 0.547873 2.344601 -0.248430
C 1.025137 0.235418 -0.242409
H 1.019719 0.170706 -1.337112
C 0.458233 -1.064291 0.321401
H 1.073998 -1.905147 0.001077

C -0.994583 -1.261663 -0.099865
H -1.390468 -2.188860 0.322896
C -1.873184 -0.085134 0.317447
H -1.850538 -0.020496 1.412629
C -1.297089 1.214316 -0.239781
H -1.908053 2.061161 0.083922
C 2.458390 0.453568 0.194305
O 3.254282 -0.618093 -0.313795
C -3.314353 -0.283839 -0.131066
H 0.205098 1.522666 1.269267
H 0.515613 -1.021078 1.415867
H -1.045113 -1.364456 -1.190281
H -1.356051 1.179798 -1.333889
H 2.819404 1.414276 -0.187884
H 2.502233 0.481180 1.289667
H 4.162316 -0.480574 -0.026471
H -3.363663 -0.351293 -1.220070
H -3.733291 -1.202933 0.281098
H -3.945676 0.548838 0.182720
el energy= -388.92733614159
zpe= -388.694845
th energy= -388.685097
th enthalpy= -388.684153
free energy= -388.729070

4mchm_3/coords
t2
C -0.158411 1.414823 0.180129
H -0.206077 1.520941 1.270050
C -1.027127 0.229331 -0.233560
H -1.014365 0.165489 -1.331108
C -0.453189 -1.066405 0.330434
H -0.505304 -1.017679 1.424587
C 0.997692 -1.262717 -0.097412
H 1.397308 -2.187924 0.326024
C 1.875455 -0.083121 0.313707
H 1.857355 -0.017119 1.408773
C 1.294173 1.214587 -0.242594
H 1.904054 2.063048 0.078785
C -2.464429 0.448157 0.209418
O -3.349807 -0.595152 -0.193205
C 3.314966 -0.279409 -0.140837

H -0.554731 2.340043 -0.247038
H -1.069524 -1.911946 0.022297
H 1.044949 -1.368032 -1.187932
H 1.350689 1.179758 -1.336941
H -2.511096 0.461637 1.299783
H -2.822348 1.418420 -0.152245
H -3.390882 -0.586770 -1.155246
H 3.945762 0.555048 0.169091
H 3.737783 -1.196847 0.270991
H 3.360091 -0.348324 -1.229950
el energy = -388.92716647283
zpe= -388.694631
th energy= -388.684911
th enthalpy= -388.683967
free energy= -388.728816

4mchm_5/coords
t3
C 0.389262 -1.254106 0.026123
H 0.823879 -2.145097 0.487980
C 1.018739 -0.000004 0.629017
H 0.816928 0.000021 1.708439
C 0.389265 1.254098 0.026097
H 0.823933 2.145079 0.487940
C -1.126162 1.248927 0.202591
H -1.370273 1.279190 1.271406
C -1.762036 -0.000007 -0.402672
H -1.545409 0.000005 -1.478098
C -1.126187 -1.248943 0.202564
H -1.563954 -2.144025 -0.247402
C 2.527853 0.000006 0.475458
O 2.840542 0.000016 -0.919089
C -3.271943 0.000021 -0.206523
H 0.635414 -1.292305 -1.038069
H 0.635403 1.292270 -1.038095
H -1.563979 2.144003 -0.247341
H -1.370325 -1.279249 1.271373
H 2.947224 0.888660 0.959492
H 2.947243 -0.888640 0.959483
H 3.798259 -0.000093 -1.010596
H -3.513312 0.000061 0.858761
H -3.729031 0.883650 -0.654278

H -3.729081 -0.883614 -0.654211
el energy= -388.92687909910
zpe= -388.694309
th energy= -388.684588
th enthalpy= -388.683644
free energy= -388.728489

4mchm_6/coords
t4
C 0.157078 1.413729 0.180905
H 0.213339 1.507972 1.271644
C 1.028552 0.239217 -0.258049
H 1.022523 0.186391 -1.353068
C 0.459651 -1.066172 0.291713
H 1.051673 -1.917326 -0.055582
C -0.997853 -1.259061 -0.118402
H -1.056526 -1.348483 -1.209290
C -1.871292 -0.086663 0.320043
H -1.838432 -0.033260 1.415514
C -1.299035 1.217241 -0.229963
H -1.367097 1.193412 -1.323695
C 2.464690 0.463944 0.187465
O 3.376230 -0.521612 -0.291473
C -3.316129 -0.282738 -0.117344
H 0.548479 2.344329 -0.238604
H 0.528555 -1.045327 1.386456
H -1.389598 -2.191110 0.297304
H -1.906547 2.061133 0.107315
H 2.830764 1.411630 -0.208136
H 2.498933 0.523353 1.282397
H 3.151396 -1.358313 0.127270
H -3.944438 0.546615 0.210475
H -3.375654 -0.339354 -1.206388
H -3.731184 -1.205749 0.289962
el energy= -388.92719116496
zpe= -388.694567
th energy= -388.684853
th enthalpy= -388.683909
free energy= -388.728740

4mchm_7/coords
t5

C 0.381803 1.264081 0.000058
H 0.632745 1.287485 1.064046
C 1.020988 0.027230 -0.625200
H 0.817474 0.041849 -1.704436
C 0.394317 -1.241333 -0.050081
H 0.614390 -1.297109 1.022059
C -1.121127 -1.243887 -0.230794
H -1.358723 -1.251694 -1.300990
C -1.764820 -0.012111 0.401017
H -1.551597 -0.036093 1.476968
C -1.134056 1.254025 -0.173365
H -1.576605 2.135046 0.298887
C 2.536175 0.032996 -0.473322
O 2.972074 0.035996 0.885689
C -3.273890 -0.016787 0.200587
H 0.810081 2.165646 -0.446287
H 0.836976 -2.124734 -0.520198
H -1.554724 -2.151593 0.197241
H -1.380222 1.309393 -1.240569
H 2.965894 -0.819981 -1.010123
H 2.947644 0.944584 -0.907596
H 2.760755 -0.823615 1.263191
H -3.727523 -0.912900 0.626558
H -3.736935 0.853713 0.667296
H -3.512560 0.006745 -0.864954
el energy= -388.92665778583
zpe= -388.693985
th energy= -388.684316
th enthalpy= -388.683372
free energy= -388.728091

4mchm_19/coords
t6
C 0.269918 -1.064824 0.697958
H -0.326339 -1.176409 1.607139
C 0.916955 0.323014 0.708352
H 1.426828 0.459340 1.666724
C -0.150283 1.411749 0.559785
H -0.763468 1.422772 1.464060
C -1.046278 1.191191 -0.660780
H -1.821508 1.961589 -0.692370
C -1.696619 -0.196433 -0.662978

H -2.192628 -0.332671 -1.628843
C -0.618366 -1.276960 -0.527449
H 0.000862 -1.278704 -1.429066
C 1.986455 0.462884 -0.361288
O 2.995531 -0.515904 -0.104590
C -2.766356 -0.322549 0.419614
H 1.048050 -1.827912 0.734733
H 0.324522 2.395052 0.498390
H -0.456329 1.308366 -1.573979
H -1.089223 -2.262230 -0.475609
H 1.566386 0.318910 -1.360454
H 2.409097 1.472243 -0.313324
H 3.673594 -0.432403 -0.782370
H -3.542482 0.432271 0.283370
H -3.239631 -1.304792 0.378600
H -2.354540 -0.196619 1.420438
el energy= -388.92232036865
zpe= -388.689140
th energy= -388.679557
th enthalpy= -388.678613
free energy= -388.723193

4mchm_21/coords
t7
C 0.141984 1.405913 0.561647
H -0.340128 2.385584 0.498439
C -0.920125 0.309830 0.695167
H -1.429361 0.444857 1.657705
C -0.269031 -1.075639 0.683998
H 0.315129 -1.196865 1.599813
C 0.634168 -1.276822 -0.532629
H 0.024335 -1.279802 -1.440244
C 1.706538 -0.189065 -0.652664
H 2.213373 -0.319285 -1.613578
C 1.045510 1.193277 -0.654316
H 0.458856 1.305665 -1.570197
C -1.986995 0.453115 -0.384577
O -3.035972 -0.505488 -0.262635
C 2.765324 -0.310822 0.440958
H 0.749395 1.419658 1.469819
H -1.045195 -1.842389 0.699381
H 1.110129 -2.259374 -0.478230

H 1.814197 1.970198 -0.681466
H -2.390073 1.471854 -0.360401
H -1.570500 0.288983 -1.376930
H -3.452451 -0.373186 0.595900
H 2.341675 -0.193817 1.437989
H 3.248013 -1.288468 0.400297
H 3.536140 0.451562 0.317277
el energy= -388.92234279469
zpe= -388.689108
th energy= -388.679559
th enthalpy= -388.678615
free energy= -388.723079

4mchm_22/coords
t8
C 0.146411 1.415989 0.552774
H -0.332438 2.396506 0.480986
C -0.921854 0.328455 0.710082
H -1.429496 0.469572 1.668695
C -0.263920 -1.054487 0.710507
H 0.339053 -1.153565 1.616471
C 0.617492 -1.278729 -0.518135
H 1.087839 -2.263944 -0.462266
C 1.695120 -0.198364 -0.660668
H 2.189317 -0.341420 -1.626261
C 1.043172 1.188342 -0.666205
H 1.818330 1.958433 -0.701283
C -1.996219 0.466229 -0.363216
O -3.092263 -0.427348 -0.175857
C 2.766008 -0.318489 0.421358
H 0.759460 1.439325 1.457102
H -1.024096 -1.837707 0.780115
H -0.001567 -1.281631 -1.420446
H 0.454317 1.300299 -1.580391
H -2.427685 1.466220 -0.309208
H -1.575279 0.344083 -1.364999
H -2.774996 -1.321384 -0.337433
H 3.545059 0.430982 0.274064
H 2.357918 -0.177522 1.421710
H 3.235104 -1.303146 0.391020
el energy= -388.92173031251
zpe= -388.688543

th energy= -388.678948
th enthalpy= -388.678004
free energy= -388.722602

4mchm_24/coords
t9
C -0.097271 1.266288 0.753188
H 0.613132 1.374627 1.577319
C -0.928266 0.000109 1.000835
H -1.213669 0.000199 2.059615
C -0.097288 -1.266119 0.753405
H 0.613125 -1.374320 1.577545
C 0.668180 -1.250636 -0.570683
H 1.294755 -2.144783 -0.636652
C 1.539121 -0.000068 -0.720998
H 1.950925 -0.000161 -1.734777
C 0.668242 1.250568 -0.570875
H -0.043937 1.285258 -1.395514
C -2.264484 0.000050 0.277427
O -2.083753 -0.000142 -1.141983
C 2.718704 -0.000029 0.249292
H -0.749914 2.143028 0.793586
H -0.749935 -2.142848 0.793972
H -0.044026 -1.285397 -1.395299
H 1.294872 2.144666 -0.636953
H -2.829914 -0.887415 0.583213
H -2.829876 0.887620 0.582982
H -2.956798 -0.000263 -1.548206
H 2.395886 0.000060 1.290248
H 3.341863 -0.883070 0.097686
H 3.341911 0.882954 0.097554
el energy= -388.91975865292
zpe= -388.686523
th energy= -388.676971
th enthalpy= -388.676026
free energy= -388.720356

4mchm_9/coords
c1
C -0.493753 -0.819742 1.098357
H -1.232488 -1.621571 1.118274
C -1.148340 0.467365 0.590970

H -1.913998 0.771955 1.310688
C -0.107712 1.584724 0.478876
H -0.566435 2.485084 0.060676
C 1.108655 1.172893 -0.349864
H 0.820345 1.005594 -1.393112
C 1.754108 -0.102278 0.188119
H 2.096129 0.102080 1.210731
C 0.717050 -1.220989 0.259423
H 1.174482 -2.122625 0.675424
C -1.869024 0.261242 -0.729980
O -2.889479 -0.717957 -0.525724
C 2.952991 -0.510497 -0.656138
H -0.166279 -0.655268 2.129763
H 0.229367 1.843189 1.487133
H 1.842586 1.983344 -0.358766
H 0.404489 -1.476485 -0.758970
H -2.307449 1.212656 -1.050068
H -1.176475 -0.070972 -1.508176
H -3.339887 -0.861293 -1.364026
H 2.638271 -0.721469 -1.680658
H 3.701643 0.282485 -0.691811
H 3.427679 -1.409354 -0.259888
el energy= -388.92508193398
zpe= -388.692263
th energy= -388.682616
th enthalpy= -388.681672
free energy= -388.726452

4mchm_11/coords
c2
C -0.334608 -1.091789 0.054224
H -1.030264 -1.884062 -0.223838
C -0.939064 0.267001 -0.289377
H -1.130939 0.297270 -1.369002
C 0.038657 1.386691 0.060330
H -0.384795 2.355126 -0.219588
C 1.379836 1.186629 -0.643405
H 1.218739 1.261111 -1.723557
C 2.006218 -0.175664 -0.330274
H 2.874042 -0.302907 -0.984569
C 1.005845 -1.290510 -0.649996
H 0.831165 -1.308953 -1.730615

C -2.261568 0.483351 0.415075
O -3.178192 -0.519824 -0.024596
C 2.506328 -0.254255 1.110400
H -0.205246 -1.152522 1.140226
H 0.183220 1.409885 1.145349
H 2.073738 1.985659 -0.369292
H 1.434117 -2.259954 -0.382080
H -2.108864 0.417811 1.499098
H -2.645278 1.482466 0.182615
H -4.014306 -0.383912 0.431965
H 2.980806 -1.218284 1.300071
H 3.241233 0.528235 1.306174
H 1.698304 -0.137102 1.831949
el energy= -388.92484149170
zpe= -388.692023
th energy= -388.682354
th enthalpy= -388.681410
free energy= -388.726159

4mchm_13/coords
c3
C -0.035008 1.383658 0.061404
H -0.183387 1.407223 1.145809
C 0.941583 0.259937 -0.279121
H 1.129187 0.291423 -1.362369
C 0.328782 -1.094957 0.061965
H 1.023294 -1.893183 -0.203242
C -1.007329 -1.291359 -0.650782
H -0.827233 -1.312506 -1.730685
C -2.005944 -0.172470 -0.338728
H -2.869655 -0.297569 -0.998743
C -1.373424 1.187859 -0.648719
H -2.066100 1.989084 -0.378078
C 2.265471 0.475922 0.435022
O 3.250572 -0.505936 0.118663
C -2.516001 -0.248283 1.098559
H 0.394009 2.350490 -0.215703
H 0.191807 -1.150559 1.146967
H -1.440374 -2.258827 -0.383639
H -1.207318 1.262215 -1.728258
H 2.642732 1.482715 0.223976
H 2.114789 0.396489 1.513159

H 3.462459 -0.414554 -0.816248
H -2.993853 -1.210980 1.286300
H -1.713059 -0.131723 1.825779
H -3.250651 0.535911 1.288071
el energy= -388.92464936014
zpe= -388.691779
th energy= -388.682140
th enthalpy= -388.681196
free energy= -388.725871

4mchm_15/coords
c4
C -0.491209 -0.846172 1.079228
H -0.175777 -0.702459 2.117425
C -1.148870 0.444962 0.587538
H -1.914018 0.741830 1.315773
C -0.116139 1.572144 0.498887
H -0.580577 2.474114 0.090464
C 1.103970 1.178382 -0.332661
H 0.817580 1.019541 -1.377687
C 1.757479 -0.097120 0.194201
H 2.091513 0.097947 1.221319
C 0.729536 -1.225058 0.243823
H 1.190752 -2.128212 0.651989
C -1.865619 0.256213 -0.744577
O -2.887499 -0.737259 -0.691678
C 2.964711 -0.485375 -0.647586
H -1.222786 -1.655613 1.072353
H 0.216553 1.819807 1.511387
H 1.831265 1.994674 -0.332178
H 0.425624 -1.470291 -0.779336
H -2.277632 1.217208 -1.072607
H -1.179664 -0.087013 -1.517125
H -3.535041 -0.453906 -0.037147
H 2.657949 -0.686157 -1.676450
H 3.707056 0.313962 -0.668510
H 3.444043 -1.385216 -0.259369
el energy= -388.92506761919
zpe= -388.692190
th energy= -388.682576
th enthalpy= -388.681632
free energy= -388.726296

4mchm_16/coords
c5
C -0.233082 1.256624 -0.206841
H -0.729309 2.143956 -0.610220
C -0.947416 0.000008 -0.701941
H -0.916715 0.000003 -1.799794
C -0.233075 -1.256612 -0.206854
H -0.327208 -1.311568 0.879187
C 1.237788 -1.251575 -0.618100
H 1.738883 -2.146717 -0.240195
C 1.972464 0.000002 -0.128909
H 2.971266 0.000007 -0.576178
C 1.237791 1.251596 -0.618064
H 1.298389 1.290490 -1.710875
C -2.413109 -0.000002 -0.311713
O -2.499455 -0.000035 1.115365
C 2.148572 -0.000021 1.387920
H -0.327229 1.311573 0.879202
H -0.729314 -2.143931 -0.610242
H 1.298371 -1.290431 -1.710914
H 1.738883 2.146723 -0.240119
H -2.904108 0.888827 -0.722597
H -2.904103 -0.888822 -0.722636
H -3.430344 0.000128 1.358643
H 2.702953 -0.882957 1.710094
H 2.702973 0.882893 1.710115
H 1.192645 -0.000017 1.910618
el energy= -388.92464644268
zpe= -388.691727
th energy= -388.682098
th enthalpy= -388.681153
free energy= -388.725807

4mchm_17/coords
c6
C -0.224584 1.277507 -0.105367
H -0.715017 2.196081 -0.438944
C -0.951057 0.069253 -0.691263
H -0.918538 0.146746 -1.786777
C -0.242192 -1.224987 -0.295740
H -0.305676 -1.357303 0.788732

C 1.226651 -1.202626 -0.715569
H 1.722491 -2.127976 -0.410804
C 1.974236 0.002811 -0.137822
H 2.968372 0.029108 -0.594227
C 1.245465 1.294435 -0.520220
H 1.754954 2.152231 -0.073535
C -2.423314 0.051584 -0.303641
O -2.637994 -0.031043 1.105223
C 2.167104 -0.115707 1.372370
H -0.318744 1.252835 0.982349
H -0.747681 -2.081326 -0.752441
H 1.275938 -1.159058 -1.808343
H 1.302205 1.421474 -1.606378
H -2.898136 0.983677 -0.611601
H -2.932559 -0.772070 -0.816121
H -2.384758 -0.915087 1.388795
H 2.743236 0.729233 1.752403
H 1.217873 -0.132646 1.907123
H 2.706136 -1.031208 1.621499
el energy= -388.92434036442
zpe= -388.691333
th energy= -388.681749
th enthalpy= -388.680804
free energy= -388.725342

4mchm_23/coords
c7
C 0.450748 -1.262990 -0.933353
H 1.065683 -2.144721 -0.731971
C 1.313630 0.000187 -0.827090
H 1.996447 0.000368 -1.685053
C 0.450741 1.263406 -0.932812
H 1.065673 2.145052 -0.731049
C -0.774875 1.247945 -0.020835
H -0.460246 1.273541 1.024264
C -1.624692 0.000049 -0.244874
H -1.960987 0.000265 -1.290349
C -0.774856 -1.247926 -0.021353
H -0.460221 -1.273963 1.023735
C 2.250878 -0.000073 0.368984
O 1.519480 -0.000397 1.598882
C -2.847353 -0.000150 0.662084

H 0.106567 -1.349864 -1.969281
H 0.106584 1.350729 -1.968710
H -1.377904 2.141591 -0.205831
H -1.377872 -2.141503 -0.206723
H 2.891364 -0.887451 0.313932
H 2.891315 0.887365 0.314360
H 2.158554 -0.000311 2.319188
H -3.464920 0.883803 0.494696
H -3.464895 -0.884054 0.494345
H -2.536304 -0.000354 1.708884
el energy= -388.92261003188
zpe= -388.689720
th energy= -388.680103
th enthalpy= -388.679159
free energy= -388.723678

4mchm-1000rej-h-rmsd_19/coords
c8
C 0.337315 -1.089156 0.022604
H 1.013416 -1.889887 -0.289360
C 0.942635 0.273992 -0.304039
H 1.132417 0.318093 -1.383211
C -0.038006 1.385342 0.065072
H -0.172450 1.397027 1.151547
C -1.385717 1.194586 -0.627852
H -1.236590 1.282019 -1.708636
C -2.007957 -0.171335 -0.323620
H -2.882588 -0.293133 -0.969559
C -1.011113 -1.280770 -0.670227
H -1.434573 -2.254627 -0.411086
C 2.267230 0.492317 0.409097
O 3.286521 -0.426185 0.023041
C -2.490830 -0.269499 1.121619
H 0.220390 -1.173967 1.108781
H 0.384357 2.356458 -0.206545
H -2.076896 1.989762 -0.336582
H -0.846458 -1.283007 -1.752314
H 2.660686 1.479393 0.164903
H 2.104693 0.456468 1.493581
H 3.021729 -1.301671 0.322055
H -3.225424 0.508418 1.335180
H -2.960791 -1.236913 1.305237

H -1.675428 -0.157825 1.835751
el energy= -388.92472520064
zpe= -388.691768
th energy= -388.682138
th enthalpy= -388.681194
free energy= -388.725847

4mchm-1000rej-h-rmsd_20/coords
c9
C 0.490235 -0.814110 1.102576
H 1.219167 -1.627588 1.156528
C 1.154657 0.467487 0.593459
H 1.919413 0.769416 1.314896
C 0.113010 1.585113 0.483318
H -0.222791 1.847769 1.491072
C -1.105068 1.176075 -0.344937
H -0.818970 1.012481 -1.389035
C -1.751931 -0.099823 0.189110
H -2.093848 0.100235 1.212569
C -0.715711 -1.219531 0.257780
H -1.173345 -2.122733 0.669952
C 1.877587 0.266933 -0.733852
O 2.958406 -0.660031 -0.647992
C -2.950269 -0.506279 -0.656808
H 0.155826 -0.644792 2.130736
H 0.574122 2.482749 0.062203
H -1.838517 1.986759 -0.349396
H -0.403343 -1.468730 -0.762660
H 1.182494 -0.033754 -1.522585
H 2.330978 1.210376 -1.039421
H 2.585736 -1.534792 -0.499700
H -3.698401 0.287042 -0.689557
H -2.635460 -0.713189 -1.682033
H -3.425371 -1.406182 -0.263513
el energy= -388.92449589996
zpe= -388.691662
th energy= -388.682004
th enthalpy= -388.681060
free energy= -388.725855