

Supporting Information

Catalysis by the Non-Heme Iron(II) Histone Demethylase PHF8 Involves Iron Center Rearrangement and Conformational Modulation of Substrate Orientation

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Table S1. Spin densities of intermediates and transition states in the ‘off-line’ O₂ activation process of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Od	CO ₂ leaving from 2OG	C2 of 2OG	Substrate	Other
RC1	4.19	-0.20	-0.47	0.14	0.00	0.00	0.28
TS1	4.25	-0.15	-0.27	-0.14	-0.02	0.00	0.31
IM1	3.78	0.06	0.00	0.00	0.00	0.00	0.10
TS2	3.98	0.04	-0.24	0.00	0.00	0.00	0.17
IM2	3.01	0.75	0.18	0.00	-0.01	0.00	0.02
IM3	3.19	0.64	0.00	0.00	0.00	0.00	0.13

Table S2. Mulliken charges of intermediates and transition states in the ‘off-line’ O₂ activation process of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Od	CO ₂ leaving from 2OG	C2 of 2OG	Substrate	Other
RC1	0.76	-0.15	-0.25	-0.52	0.35	0.93	-1.12
TS1	0.76	-0.15	-0.25	-0.52	0.35	0.93	-1.12
IM1	0.77	-0.54	-0.12	0.00	0.46	0.95	-1.52
TS2	0.86	-0.58	-0.25	0.00	0.50	0.94	-1.46
IM2	0.75	-0.52	-0.39	0.00	0.49	0.93	-1.27
IM3	0.70	-0.50	-0.48	-0.03	0.45	0.92	-1.06

Table S3. Spin densities of intermediates and transition states in the proposed ferryl-flip mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Ow	Os	Oa	Others
IM4	3.19	0.60	0.05	0.00	0.00	0.10
TS3	3.23	0.57	0.04	0.00	0.00	0.10
IM5	3.24	0.44	0.17	0.01	0.00	0.08
TS4	3.34	0.27	0.18	0.02	0.00	0.13
IM6	3.39	0.21	0.18	0.02	0.00	0.17
TS5	3.44	0.03	0.25	0.01	0.01	0.17
IM7	3.23	0.04	0.52	0.00	0.00	0.14
IM8	3.18	0.00	0.58	0.02	0.00	0.18

Table S4. Mulliken charges of intermediates and transition states in the proposed ferryl-flip mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Ow	Os	Oa	Others
IM4	0.69	-0.49	-0.60	-0.47	-0.71	1.60
TS3	0.71	-0.50	-0.69	-0.40	-0.71	1.61
IM5	0.80	-0.64	-0.66	-0.38	-0.71	1.61
TS4	0.74	-0.60	-0.62	-0.44	-0.71	1.65
IM6	0.72	-0.58	-0.61	-0.47	-0.71	1.67
TS5	0.65	-0.62	-0.51	-0.49	-0.69	1.66
IM7	0.68	-0.57	-0.53	-0.49	-0.79	1.70
IM8	0.68	-0.70	-0.51	-0.43	-0.79	1.77

Table S5. Spin densities of intermediates and transition states in 2OG rearrangement process of PHF8 at the QM(B2)/MM level of theory.

	Fe	O1	O2	Others
ES1	3.79	0.03	0.01	0.10
ES-TS	3.79	0.03	0.01	0.10
ES1'	3.79	0.03	0.01	0.10

Table S6. Mulliken charges of intermediates and transition states in 2OG rearrangement process of PHF8 at the QM(B2)/MM level of theory.

	Fe	O1	O2	Others
ES1	0.77	-0.61	-0.35	0.19
ES-TS	0.77	-0.61	-0.35	0.19
ES1'	0.76	-0.51	-0.34	0.09

Table S7. Spin densities of intermediates and transition states in 'in-line' O₂ activation process of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Od	CO ₂ leaving from 2OG	C2 of 2OG	Substrate	Other
RC1'	4.20	-0.22	-0.46	0.13	0.00	0.00	-1.18
TS1'	4.25	-0.36	-0.31	-0.03	0.00	0.00	0.41
IM1'	3.78	0.06	0.00	0.00	0.00	0.00	0.09
TS2'	3.98	0.03	-0.24	0.00	0.01	0.00	0.17
IM2'	2.97	0.70	0.24	0.00	-0.02	0.06	0.06
IM3'	3.15	0.62	0.01	0.00	0.00	0.00	0.17

Table S8. Mulliken charges of intermediates and transition states in 'in-line' O₂ activation process of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Od	CO ₂ leaving from 2OG	C2 of 2OG	Substrate	Other
RC1'	0.73	-0.14	-0.21	-0.49	0.35	0.93	-1.18
TS1'	0.70	-0.25	-0.02	-0.50	0.42	0.94	-1.30
IM1'	0.80	-0.55	-0.11	-0.07	0.47	0.93	-1.48
TS2'	0.86	-0.58	-0.24	-0.07	0.51	0.93	-1.42
IM2'	0.79	-0.52	-0.34	-0.08	0.48	0.93	-1.26
IM3'	0.70	-0.49	-0.47	-0.01	0.46	0.92	-1.11

Table S9. Spin densities of five snapshot intermediates and transition states in the hydrogen abstraction step from the N^ε-methyl group of the substrate during PHF8 catalysis at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
#1-RC	3.19	0.64	0.00	0.13
#1-TS	4.04	0.03	-0.47	0.34
#1-IM	4.24	0.29	-0.97	0.38
#2-RC	3.24	0.45	0.00	0.27
#2-TS	4.11	-0.21	-0.43	0.47
#2-IM	4.24	0.14	-0.95	0.53
#3-RC (RC2)	3.19	0.55	0.00	0.22
#3-TS (TS6)	4.07	-0.06	-0.46	0.39
#3-IM (IM9)	4.22	0.22	-0.96	0.45
#4-RC	3.12	0.60	0.00	0.23
#4-TS	4.01	0.04	-0.48	0.37
#4-IM	4.20	0.28	-0.94	0.41
#5-RC	3.20	0.60	0.00	0.14
#5-TS	4.10	0.07	-0.51	0.29
#5-IM	4.28	0.29	-0.96	0.33

Table S10. Mulliken charges of intermediates and transition states in the hydrogen abstraction step from the N^ε-methyl group of the substrate during PHF8 catalysis at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
#1-RC	0.70	-0.50	0.64	-0.85
#1-TS	0.79	-0.66	0.84	-0.97
#1-IM	0.79	-0.77	0.98	-1.00
#2-RC	0.63	-0.64	0.57	-0.56
#2-TS	0.78	-0.81	0.76	-0.73
#2-IM	0.76	-0.86	0.87	-0.77
#3-RC (RC2)	0.60	-0.56	0.62	-0.67
#3-TS (TS6)	0.73	-0.71	0.81	-0.83
#3-IM (IM9)	0.74	-0.78	0.93	-0.89
#4-RC	0.65	-0.48	0.57	-0.74
#4-TS	0.76	-0.64	0.76	-0.89
#4-IM	0.78	-0.69	0.83	-0.93
#5-RC	0.78	-0.55	0.69	-0.92
#5-TS	0.87	-0.62	0.76	-1.02
#5-IM	0.883	-0.821	0.90	-0.96

Table S11. Spin densities of intermediates and transition states in potential hydrogen abstraction from N^εH group of the substrate in PHF8 catalysis at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
RC3	3.17	0.52	0.00	0.26
TS7	3.69	0.30	-0.31	0.30
IM10	4.23	0.13	-0.92	0.58

Table S12. Mulliken charges of intermediates and transition states in potential hydrogen abstraction from N^εH group of the substrate in PHF8 catalysis at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
RC3	0.58	-0.52	0.55	-0.62
TS7	0.63	-0.52	0.44	-0.56
IM10	0.71	-0.79	0.92	-0.84

Table S13. Spin densities of intermediates and transition states for the rebound mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
TS8	4.28	0.18	-0.90	0.38
PD1	3.83	0.00	0.00	0.11

Table S14. Mulliken charges of intermediates and transition states for the rebound mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
TS8	0.91	-0.83	0.83	-0.91
PD1	0.83	-0.53	1.08	-1.38

Table S15. Spin densities of intermediates and transition states in the desaturation mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
TS8	4.31	0.09	-0.96	0.51
PD1	3.83	0.00	0.00	0.11

Table S16. Mulliken charges of intermediates and transition states in the desaturation mechanism of PHF8 at the QM(B2)/MM level of theory.

	Fe	Op	Substrate	Others
TS8	0.92	-0.82	0.71	-0.81
PD1	0.86	-0.82	1.40	-1.45

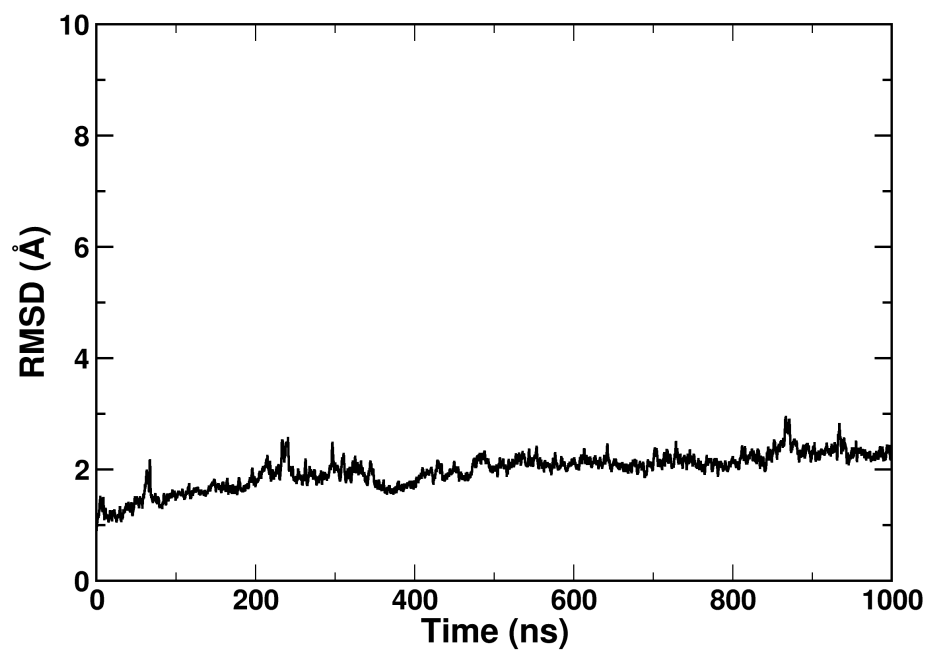


Figure S1. RMSD of the alpha-carbon atoms of PHF8 ferric-superoxo intermediate dynamics showing evidence for an equilibrated system.

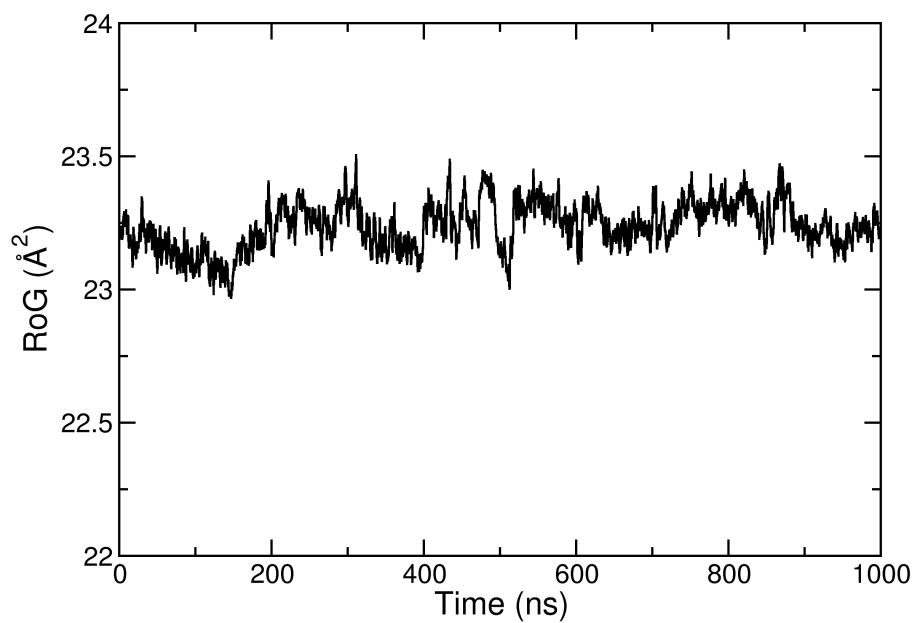


Figure S2. The radius of gyration of the alpha-carbon atoms of PHF8 ferric-superoxo intermediate dynamics showing evidence for an equilibrated system.

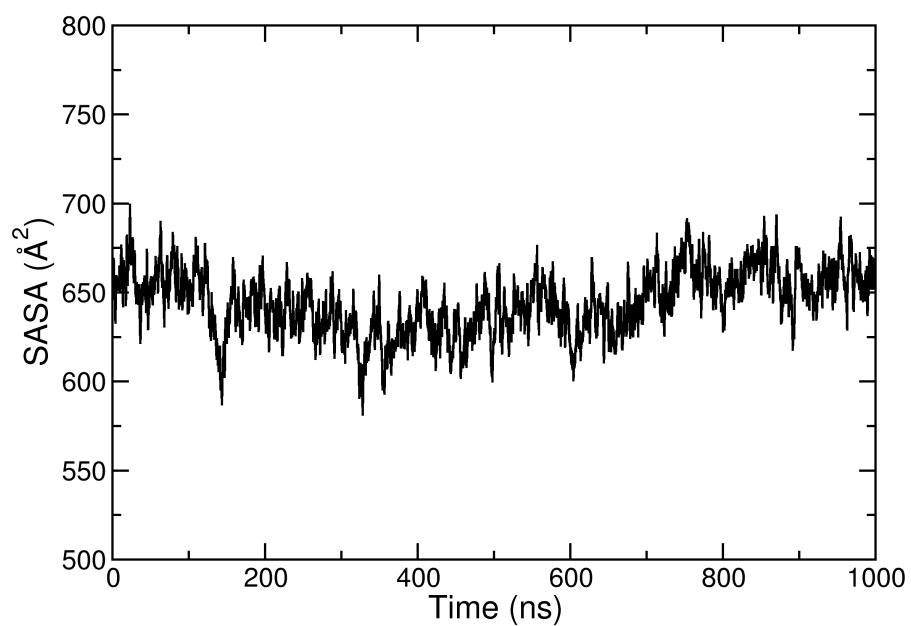


Figure S3. Solvent Accessible Surface Area (SASA) of the alpha-carbon atoms of PHF8 ferric-superoxo intermediate dynamics showing evidence for an equilibrated system.

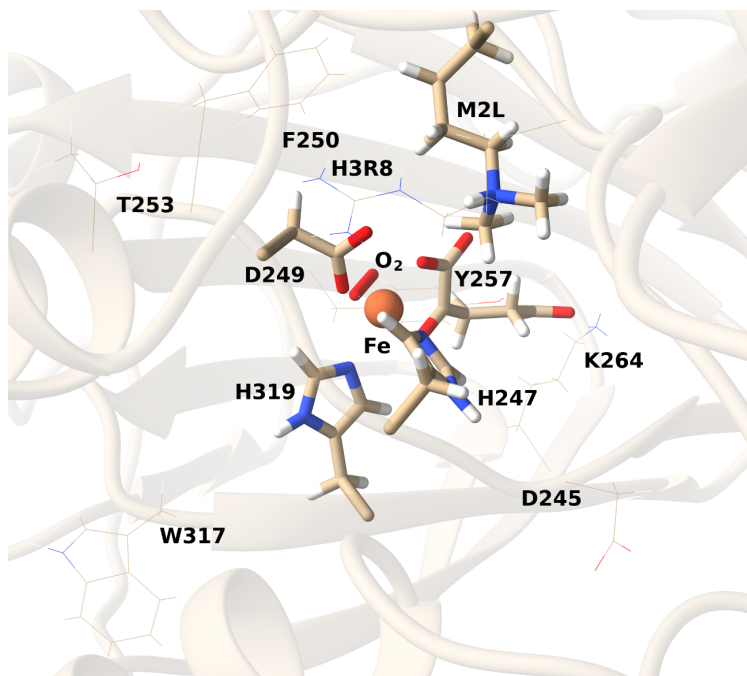


Figure S4. The interactions stabilizing the Fe-center and the substrate in the PHF8 ferric-superoxo intermediate dynamics.

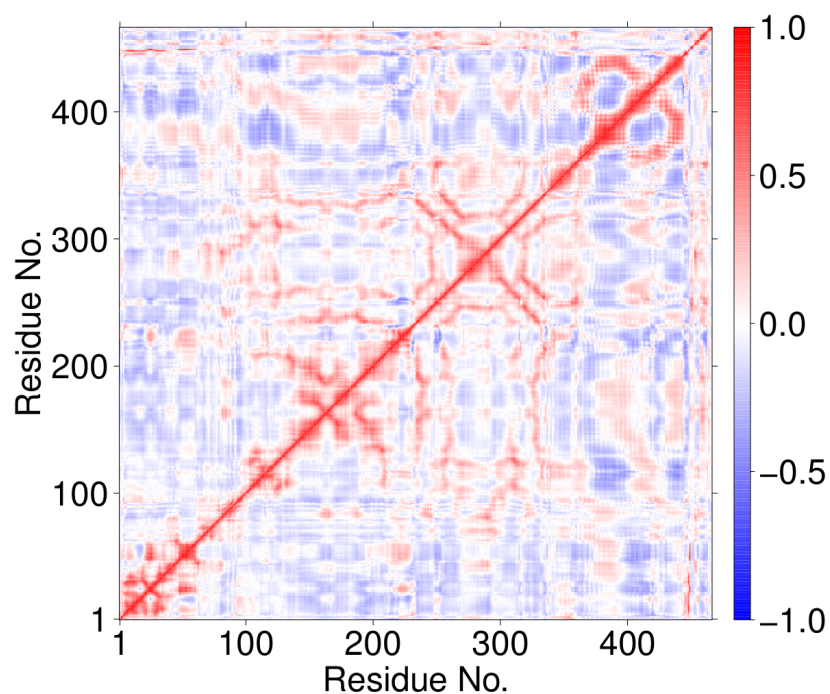


Figure S5. DCCM showing correlated motions in PHF8 ferric-superoxo intermediate dynamics. Red indicates a positive correlation in the motion of two parts of the protein and blue indicates a negative correlation in the motion of two parts of the protein.

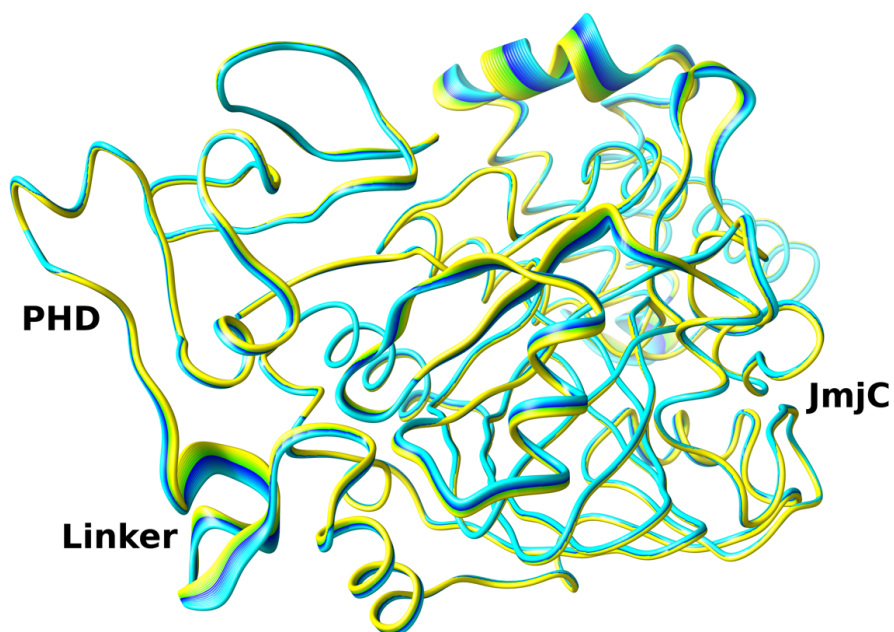


Figure S6. PCA showing the motions of most flexible regions of protein in the PHF8 ferric-superoxo intermediate dynamics. The color gradient of blue to yellow indicates the direction of motion in the flexible regions.

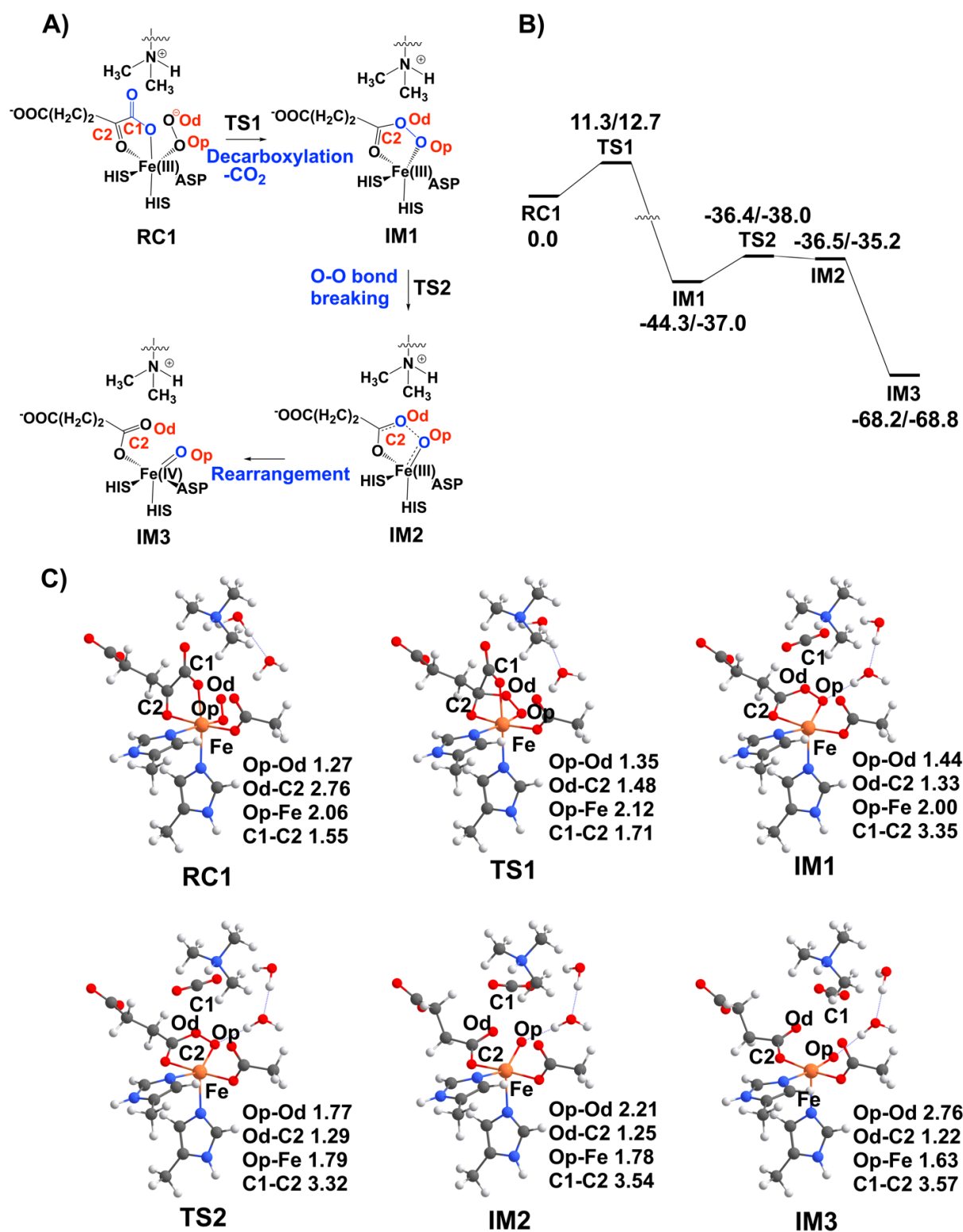


Figure S7. The O_2 activation mechanism proceeding from the PHF8-ferric-superoxo-offline complex to form the 'off-line' ferryl-oxo intermediate. (A) Proposed pathway for O_2 activation in PHF8. (B) Potential energy surface for O_2 activation in PHF8. Energies are in kcal/mol as calculated at the QM(B2)/MM and QM(B2+ZPE)/MM levels of theory. (C) QM active site geometries of transition states and intermediates in the O_2 activation mechanism of PHF8 from QM/MM calculations. Distances are in angstroms.

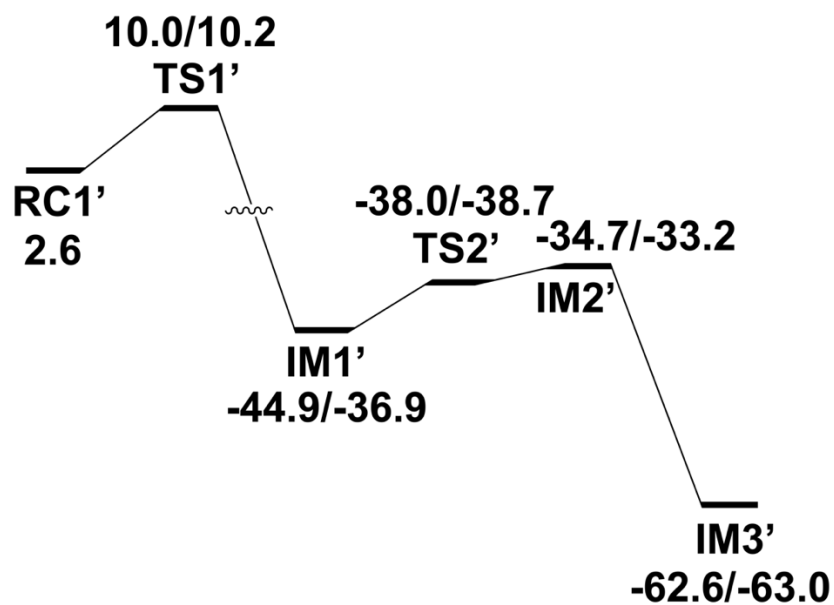


Figure S8. The potential energy profile for the O₂ activation mechanism from the 'in-line' PHF8 ferric-superoxo intermediate at the QM(B2)/MM level of theory.

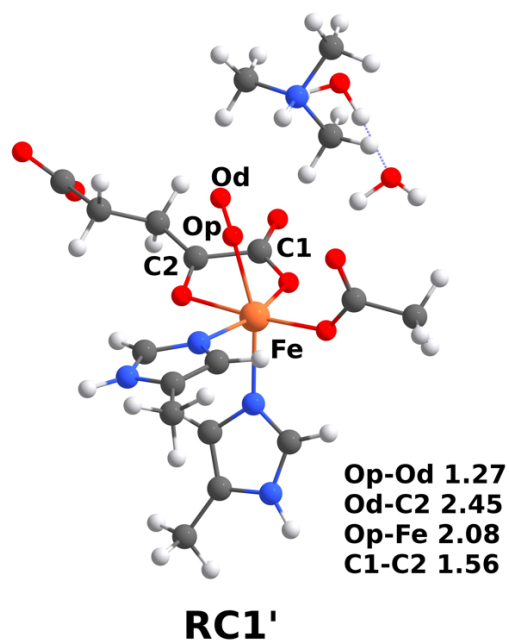
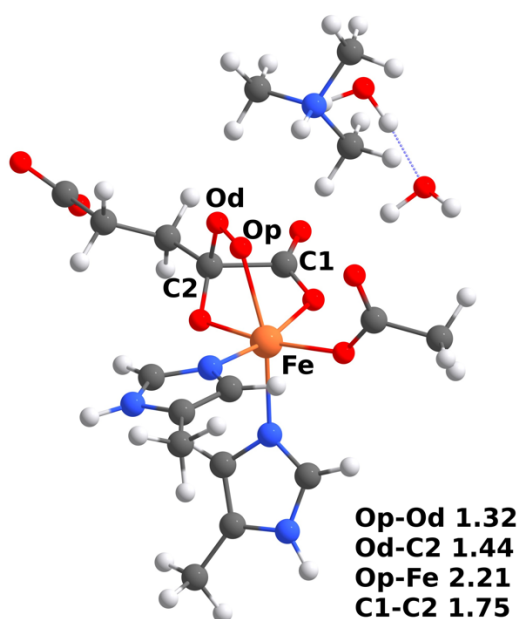


Figure S9. QM geometry of QM/MM optimized **RC1'** in the PHF8 O₂ activation mechanism with the 'in-line' geometry.



TS1'

Figure S10. QM geometry of QM/MM optimized **TS1'** in the PHF8 O₂ activation mechanism with the 'in-line' geometry.

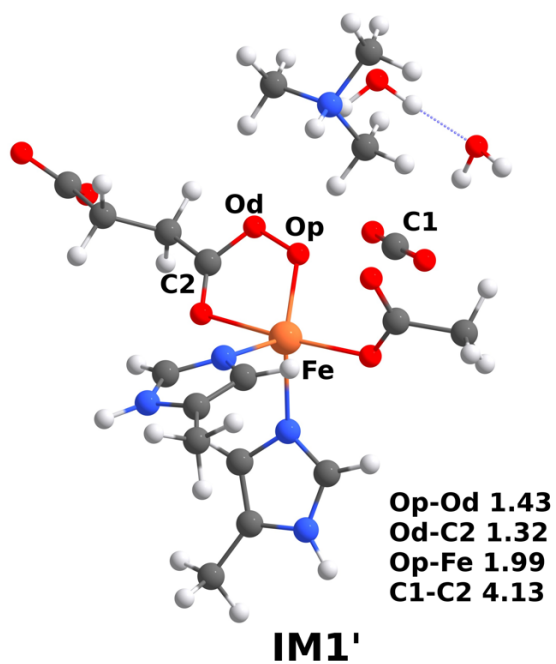


Figure S11. QM geometry of QM/MM optimized **IM1'** in the PHF8 O₂ activation mechanism with the 'in-line' geometry.

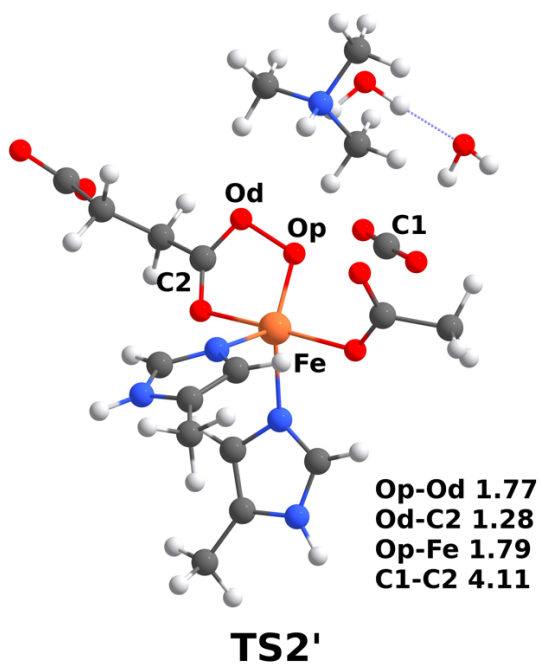


Figure S12. QM geometry of QM/MM optimized **TS2'** in the PHF8 O₂ activation mechanism with the 'in-line' geometry.

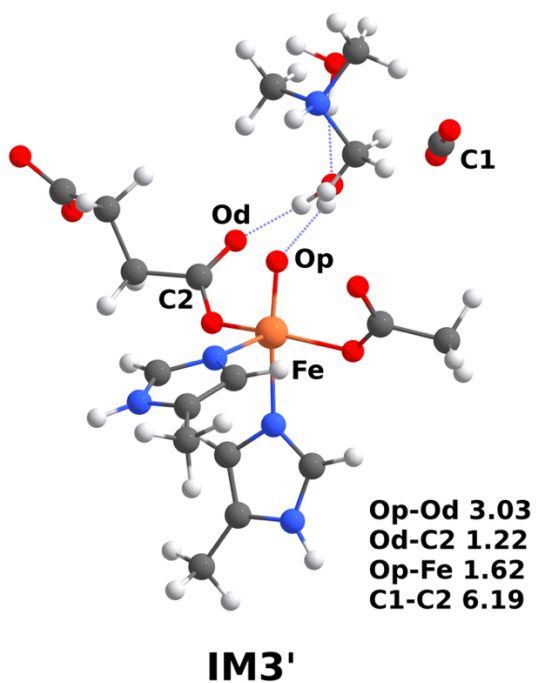


Figure S13. QM geometry of QM/MM optimized **IM3'** in the PHF8 O₂ activation mechanism with the 'in-line' geometry. (Equivalent to **IM8**).

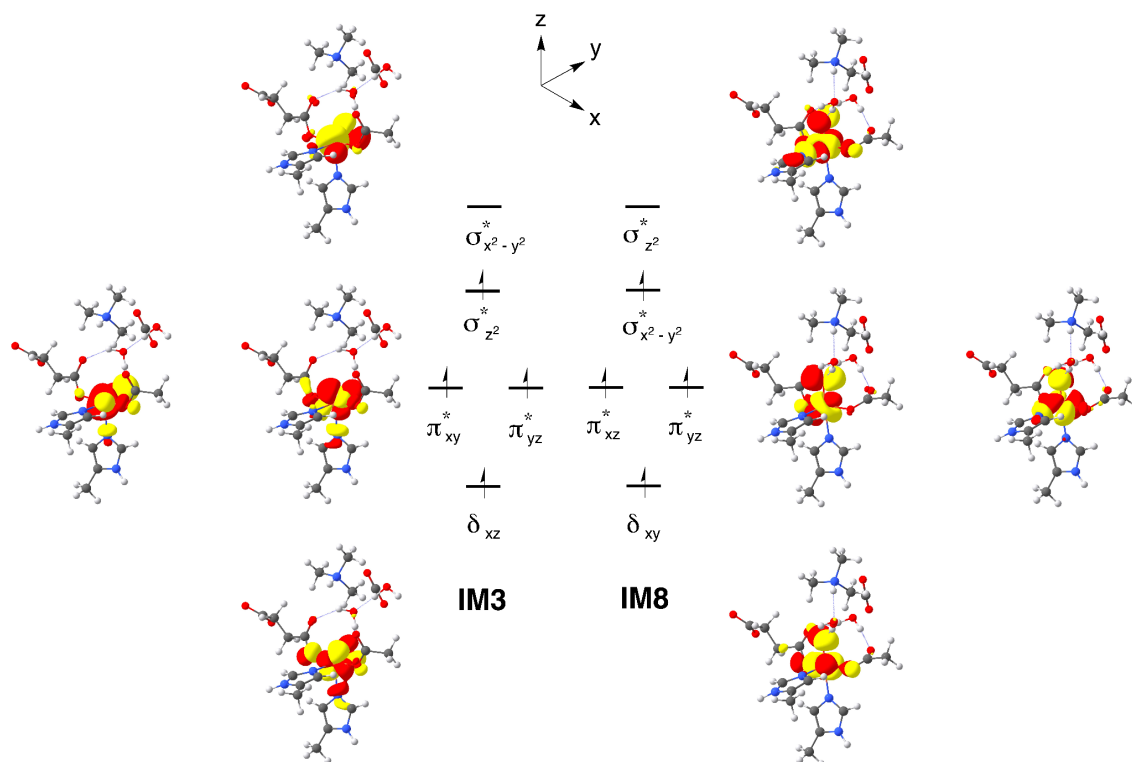


Figure S14. Orbital rearrangements in the 'off-line' (IM3) and 'in-line' (IM3' or IM8) possible PHF8 ferryl-oxo intermediates. Note the orbitals in IM3' are equivalent to RC2.

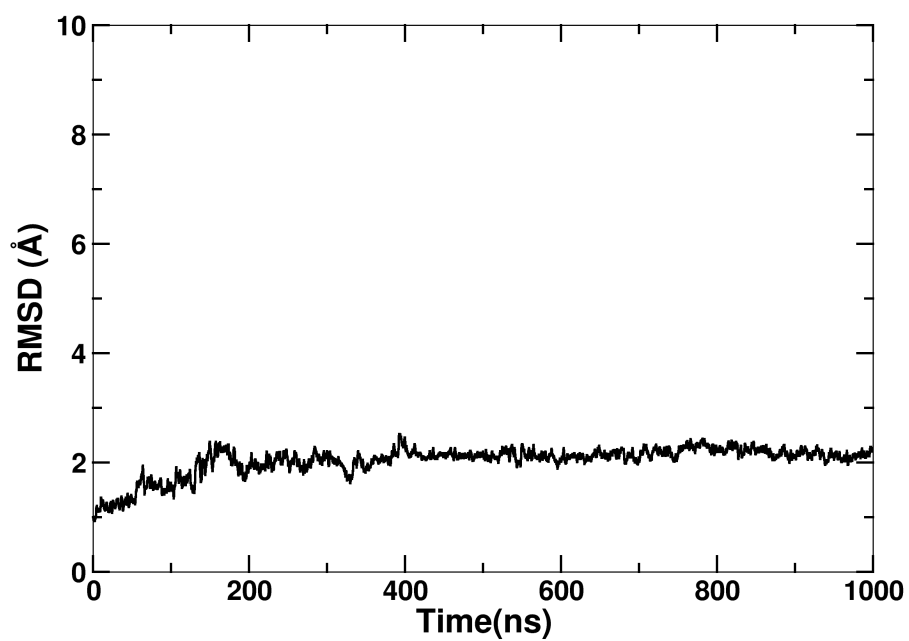


Figure S15. RMSD of the alpha-carbon atoms for the PHF8 ferryl-oxo intermediate dynamics showing evidence for an equilibrated system.

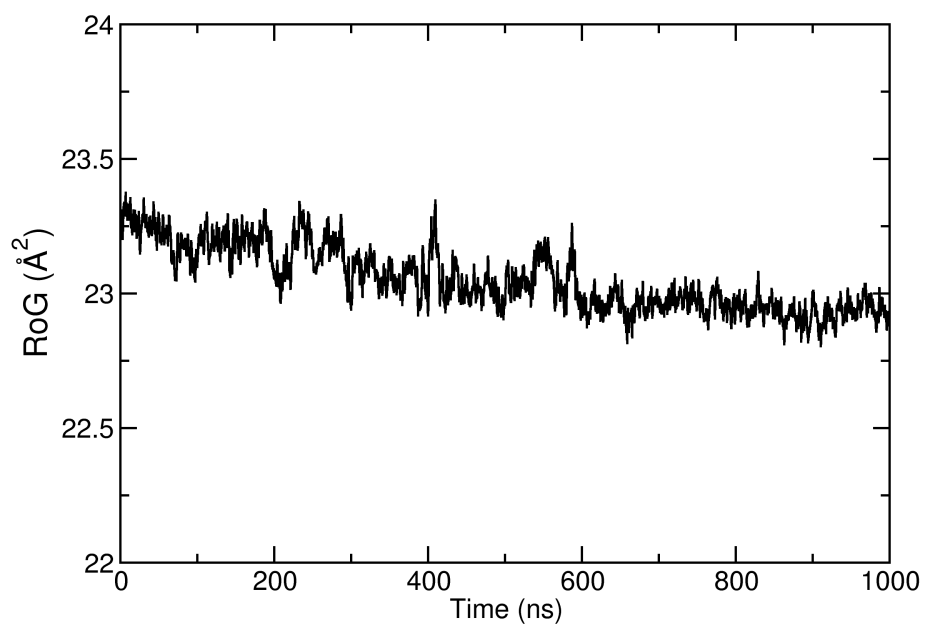


Figure S16. The radius of gyration of the alpha-carbon atoms for the PHF8 ferryl-oxo intermediate dynamics showing the volume of the protein reduces with time implying progressively stronger interactions.

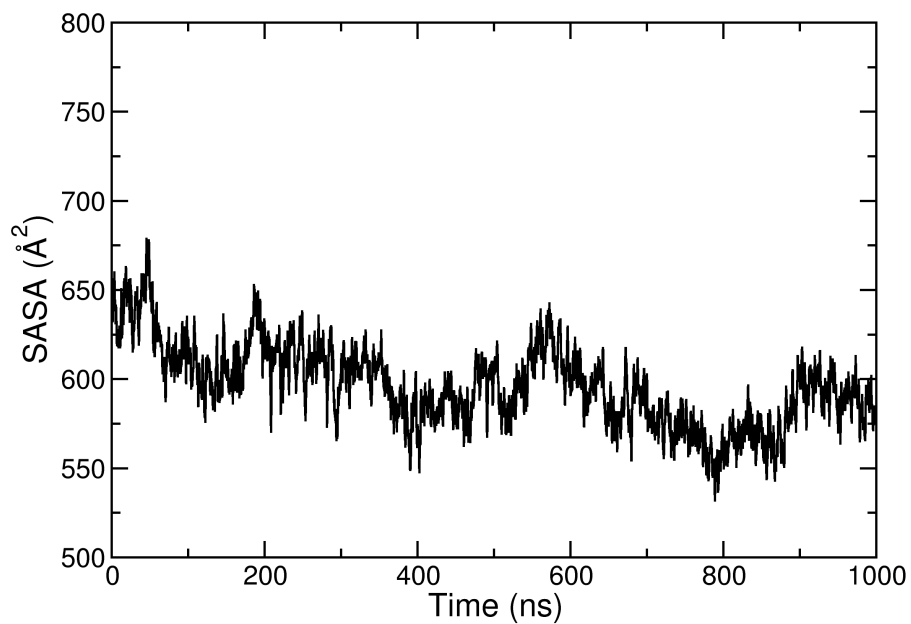


Figure S17. Solvent Accessible Surface Area of the alpha-carbon atoms for the PHF8 ferryl intermediate dynamics showing the surface area of the protein reduces implying progressively stronger interactions during catalysis.

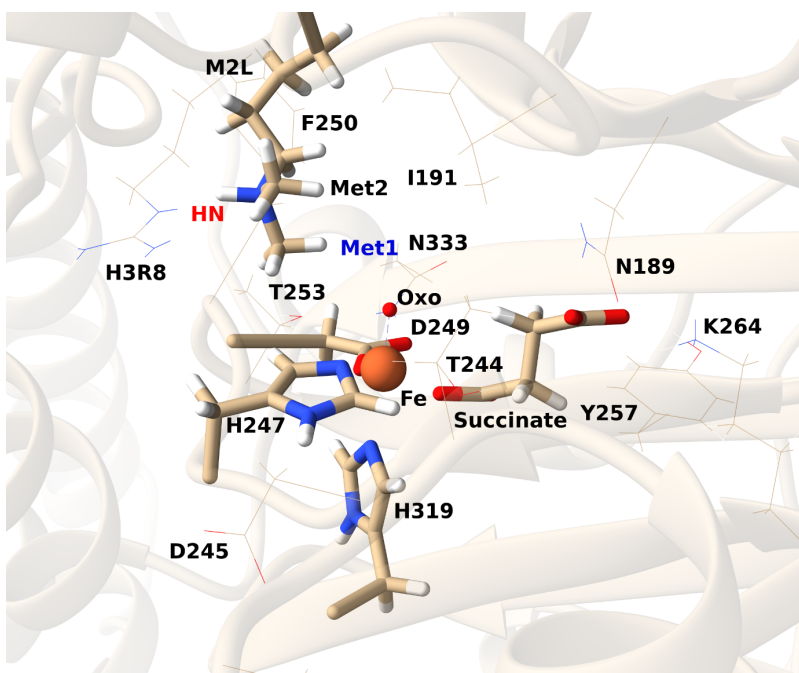


Figure S18. The interactions stabilizing the Fe-center and the substrate in the PHF8 ferryl-oxo intermediate dynamics.

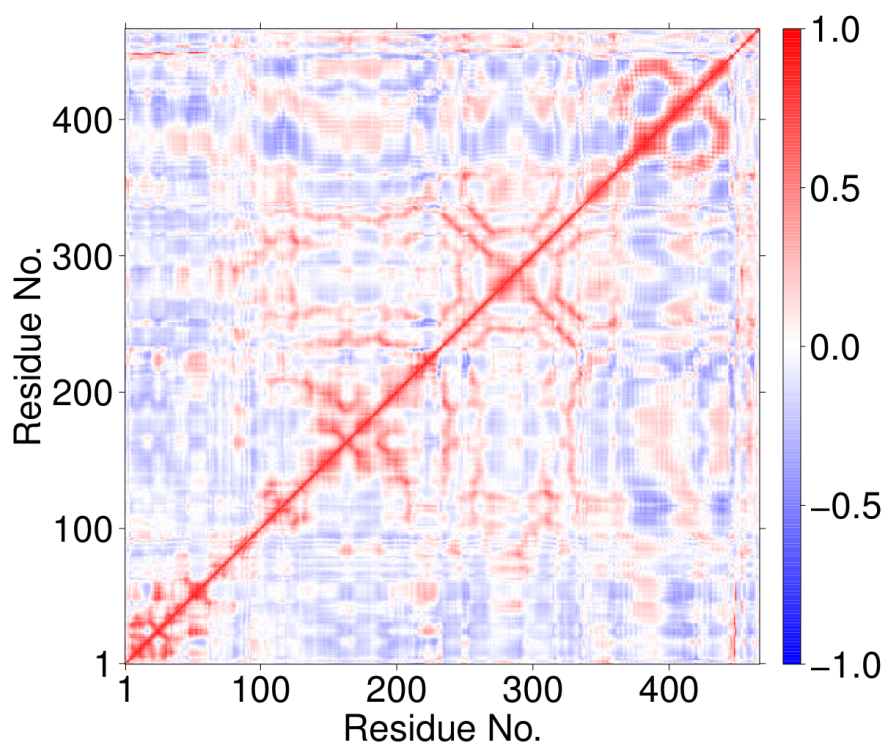


Figure S19. DCCM showing correlated motions in PHF8 ferryl-oxo intermediate dynamics. Red indicates a positive correlation in the motion of two parts of the protein and blue indicates a negative correlation in the motion of two parts of the protein.

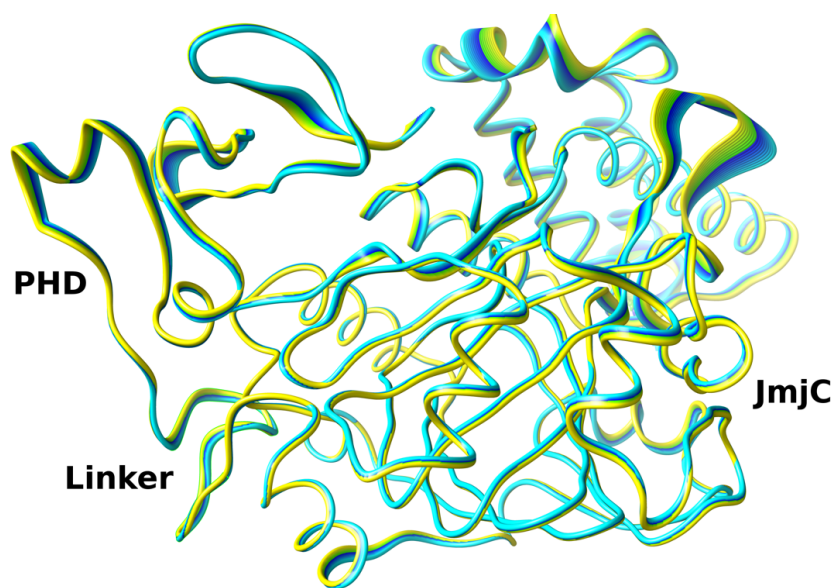


Figure S20. PCA showing the motions of most flexible regions of protein in the PHF8 ferryl-oxo intermediate dynamics. The color gradient of blue to yellow indicates the direction of motion in the flexible regions.

RC1**QM(B1)/MM = -3195.355496 (a.u.)****QM(B2+ZPE)/MM = -3197.096041 (a.u.)****QM(B2+D3+ZPE)/MM = -3197.1749 (a.u.)**

1	6	38.846644928	40.407065972	46.306936195
2	1	38.178266159	41.199482708	45.944005065
3	1	38.408228081	39.453053787	45.976461304
4	6	40.209252981	40.614556446	45.729743117
5	7	41.155815325	39.621352901	45.560673907
6	1	41.015206521	38.620151192	45.749737895
7	6	42.287944963	40.188672902	45.101245765
8	1	43.199108015	39.637355994	44.883947865
9	7	42.128645519	41.500538043	44.963347641
10	6	40.831225197	41.775277785	45.339527803
11	1	40.413488385	42.776664606	45.291594166
12	6	41.078729329	46.658911346	44.880100302
13	1	41.729414331	47.037065647	45.680267548
14	1	41.144701581	47.323161496	44.004998525
15	6	41.484787559	45.252665231	44.408676590
16	8	42.408414164	44.662933827	45.099344860
17	8	40.935930567	44.779441052	43.414500788
18	6	44.884965954	40.836209179	49.862018488
19	1	45.757934940	40.270509857	49.499552779
20	1	45.208780160	41.373219066	50.770130416
21	6	44.436193293	41.793817457	48.799883236
22	7	43.687748229	42.937426177	49.036666903
23	1	43.382873631	43.284108360	49.950148376
24	6	43.411205268	43.519794768	47.846973268
25	1	42.827198609	44.431695821	47.730468542
26	7	43.950524035	42.823582561	46.856859923
27	6	44.597465188	41.753510883	47.434026860
28	1	45.122896126	41.016384486	46.830311079
29	26	43.535116031	43.078354720	44.721253420
30	8	45.292417021	44.159546280	44.714231021
31	8	46.092189792	44.167624706	43.720723067
32	6	44.599790879	42.522450803	42.108327361
33	8	44.875159792	42.640962498	40.921447436
34	8	43.641211926	43.098467816	42.746729123
35	6	45.443421247	41.577636919	43.008806859
36	8	48.716642152	39.423543995	41.312742203
37	6	46.646572489	40.898316829	42.421376202
38	6	46.337893350	39.628018598	41.598786033
39	6	47.597380130	38.977713565	40.981436599
40	8	47.419511560	38.008935975	40.182413561
41	8	45.066041222	41.435427445	44.173453228
42	1	47.350538750	40.660117353	43.229428009
43	1	47.122813608	41.622907234	41.747158036
44	1	45.850631596	38.857715824	42.219972590
45	1	45.633461704	39.859311713	40.785977849
46	6	40.981452950	45.264655060	38.305349589
47	1	41.928453611	45.605428634	37.850336399
48	1	40.501034289	46.123920635	38.795029276
49	7	41.353214515	44.290969218	39.380963341
50	1	40.502861670	43.823371272	39.751568319
51	6	42.231313139	43.197859983	38.870170678
52	6	42.027043423	44.986064077	40.521507892
53	1	43.156670815	43.620445000	38.446748946
54	1	41.677560052	42.641963622	38.101150005
55	1	42.483747980	42.531466676	39.702518721
56	1	42.179648035	44.274817643	41.340814394

57	1	41.378441379	45.801840062	40.862416936
58	1	42.996876236	45.366293245	40.170894277
59	8	45.367433346	45.381583361	39.722318613
60	1	45.545852827	45.856688765	40.563542759
61	1	45.267689944	44.445830966	39.971498554
62	8	45.970708597	46.725027614	42.091995925
63	1	45.342412910	47.396219802	42.441393199
64	1	46.036988910	46.043624952	42.783965458
65	1	38.828508860	40.399616035	47.396744846
66	1	44.125283144	40.130368635	50.197783977
67	1	40.062466822	46.663271365	45.274129269
68	1	40.269223967	44.887981455	37.571241836

TS1**QM(B1)/MM = -3195.340857 (a.u.)****QM(B2+ZPE)/MM = -3197.075824 (a.u.)****QM(B2+D3+ZPE)/MM = -3197.158645 (a.u.)**

1	6	38.827734197	40.382987751	46.305631615
2	1	38.154434387	41.173874578	45.948344260
3	1	38.386408441	39.427880677	45.982627564
4	6	40.182646060	40.590247562	45.711627957
5	7	41.124321970	39.594086461	45.522763739
6	1	40.984351826	38.592963081	45.713538228
7	6	42.248318170	40.156930142	45.042890146
8	1	43.158732183	39.616542040	44.797089896
9	7	42.086964756	41.470325901	44.915731504
10	6	40.798880058	41.751571882	45.315645431
11	1	40.382073989	42.753679067	45.271965950
12	6	41.211437293	46.581828674	44.859894954
13	1	41.865075084	46.932965703	45.670228367
14	1	41.307550762	47.254394335	43.993675878
15	6	41.596134358	45.172703194	44.367518152
16	8	42.562435097	44.583282692	45.001417694
17	8	40.981633945	44.693724694	43.416350061
18	6	44.902159293	40.811328704	49.829071124
19	1	45.771857519	40.233359053	49.478295613
20	1	45.226817473	41.361213362	50.729099531
21	6	44.463910656	41.753977220	48.749630013
22	7	43.722974314	42.906899175	48.966417094
23	1	43.415237445	43.266188243	49.873379971
24	6	43.454999501	43.473354209	47.767201629
25	1	42.878543545	44.387421958	47.633960010
26	7	43.993352768	42.757812634	46.790235783
27	6	44.630582142	41.691639251	47.385303447
28	1	45.149960749	40.943209946	46.790249128
29	26	43.586718264	42.910766381	44.651752794
30	8	45.422532202	43.912575454	44.331047007
31	8	46.181808425	43.245976826	43.432291642
32	6	44.521460550	42.514850113	41.975936744
33	8	44.817797364	42.463014905	40.801647253
34	8	43.524507297	42.986702305	42.587311370
35	6	45.617889065	41.906065424	43.134742853
36	8	48.718142168	39.447409783	41.428528407
37	6	46.748129075	41.091904038	42.499105408
38	6	46.362363469	39.788100743	41.786803091
39	6	47.562367959	39.076637087	41.115795538
40	8	47.316467673	38.140336496	40.296364838
41	8	44.915396530	41.445762673	44.131646929
42	1	47.494474682	40.884536137	43.280763912
43	1	47.226632596	41.757863286	41.769647640

44	1	45.912609587	39.068549772	42.492781284
45	1	45.601872738	39.972087809	41.014194454
46	6	40.952372925	45.272126386	38.257388577
47	1	41.913125130	45.601256193	37.823778591
48	1	40.475147774	46.139138540	38.736742905
49	7	41.290684216	44.296452489	39.341133794
50	1	40.429814969	43.837342536	39.697547831
51	6	42.165938079	43.194202315	38.847527506
52	6	41.952870024	44.986316579	40.491628073
53	1	43.103251721	43.607867192	38.442367247
54	1	41.622305295	42.642986431	38.067848098
55	1	42.394830787	42.523688331	39.683580193
56	1	42.090408949	44.276307727	41.313905546
57	1	41.309644738	45.809981443	40.822873811
58	1	42.924498240	45.362893228	40.150854557
59	8	45.334077077	45.382903817	39.932927608
60	1	45.084731794	45.644871188	40.847197968
61	1	45.295864341	44.411328900	39.948742355
62	8	44.407548844	46.113303197	42.476403545
63	1	44.520321612	47.050598863	42.751596765
64	1	44.763344904	45.570302213	43.203377380
65	1	38.823092302	40.378614186	47.395597966
66	1	44.136960800	40.115856557	50.173827678
67	1	40.191925078	46.605546694	45.244732097
68	1	40.244630666	44.901315912	37.515992730

IM1

QM(B1)/MM = -3195.423219 (a.u.)

QM(B2+ZPE)/MM = -3197.154955 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.232622 (a.u.)

1	6	38.810068123	40.363062476	46.300574993
2	1	38.131787093	41.148032794	45.941080154
3	1	38.372999349	39.402822817	45.986174496
4	6	40.163181852	40.574958350	45.703085628
5	7	41.133163723	39.596751985	45.585112996
6	1	41.008366101	38.598686334	45.799049541
7	6	42.255816421	40.170360015	45.106756977
8	1	43.181283860	39.634578454	44.911133928
9	7	42.069088805	41.469319120	44.905083463
10	6	40.761971844	41.732068208	45.260106675
11	1	40.332249565	42.727095948	45.171596706
12	6	41.141022037	46.653371003	44.865639269
13	1	41.765831844	47.077466769	45.663451644
14	1	41.218218144	47.280020225	43.964398507
15	6	41.609790322	45.231694842	44.484041363
16	8	42.487444892	44.701738258	45.245567678
17	8	41.106569942	44.702370915	43.477854475
18	6	44.918845564	40.746219624	49.944047016
19	1	45.783909473	40.155330105	49.602817507
20	1	45.233862786	41.267455489	50.864491953
21	6	44.528989594	41.722828075	48.876124061
22	7	43.814869214	42.891329277	49.098672898
23	1	43.492987781	43.243017995	50.004394849
24	6	43.588056161	43.484335584	47.901522177
25	1	43.027707637	44.408993895	47.765407311
26	7	44.125183463	42.773530596	46.921473746
27	6	44.717209744	41.680477829	47.513357139
28	1	45.220069701	40.918072582	46.920978193
29	26	43.565274504	42.972964118	44.840397313
30	8	44.909703948	43.843498576	43.648563696

31	8	45.915085962	43.028096751	43.025507207
32	6	44.897070571	43.289232441	40.530738749
33	8	45.469059472	44.274772933	40.308918515
34	8	44.316695614	42.302499115	40.734853775
35	6	45.859431152	41.734713666	43.333970049
36	8	48.802576414	39.384353986	41.357506158
37	6	46.920697094	40.959084549	42.577709703
38	6	46.470249502	39.693753297	41.829913547
39	6	47.639623223	38.996021886	41.097120572
40	8	47.364880031	38.064077631	40.285497051
41	8	45.065118480	41.286746524	44.152359842
42	1	47.707527459	40.686748007	43.299366043
43	1	47.398521294	41.649568544	41.871612386
44	1	46.024067915	38.959843763	42.521943750
45	1	45.683224034	39.921954255	41.094370046
46	6	40.889951134	45.381244433	38.134799233
47	1	41.863450378	45.670551732	37.703219509
48	1	40.443046892	46.269399531	38.603165073
49	7	41.182704525	44.398083647	39.226438763
50	1	40.294956465	43.978446263	39.572059194
51	6	41.999780296	43.252953838	38.730715258
52	6	41.855481746	45.072429879	40.381121581
53	1	42.973408876	43.618774266	38.366473080
54	1	41.454003069	42.765902511	37.911052424
55	1	42.132582232	42.534798540	39.547623249
56	1	42.042169262	44.349492475	41.183488808
57	1	41.181180494	45.841090901	40.774702642
58	1	42.783928299	45.537959794	40.025572738
59	8	45.109818162	47.063436788	40.033814890
60	1	44.712156297	46.814676649	40.904319958
61	1	45.722898062	46.327799220	39.901138565
62	8	44.031344371	46.265919598	42.417701039
63	1	44.265447470	47.077160534	42.920022501
64	1	44.457326040	45.505772323	42.874415920
65	1	38.805421989	40.366981743	47.390543058
66	1	44.128985151	40.062210970	50.254401661
67	1	40.121395048	46.657232325	45.250883618
68	1	40.172415990	45.020392853	37.397916083

TS2

QM(B1)/MM = -3195.410279 (a.u.)

QM(B2+ZPE)/MM = -3197.156624 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2367 (a.u.)

1	6	38.843679154	40.372846630	46.279415798
2	1	38.162309460	41.156196491	45.922053332
3	1	38.407183877	39.411847405	45.965920395
4	6	40.191877975	40.588809067	45.672033073
5	7	41.168861205	39.616702518	45.548142165
6	1	41.053922002	38.619524392	45.772237918
7	6	42.277065957	40.191990558	45.042263135
8	1	43.205603708	39.665921818	44.835070927
9	7	42.074667672	41.489037132	44.829738408
10	6	40.771091579	41.745200467	45.205555682
11	1	40.330821622	42.734093889	45.110630316
12	6	41.124437982	46.620585160	44.889094129
13	1	41.762377571	47.030682918	45.683859455
14	1	41.223932645	47.236313904	43.983333823
15	6	41.544861109	45.185860990	44.511249424
16	8	42.379784870	44.606839256	45.293471618
17	8	41.053056453	44.679301476	43.491318449

18	6	44.934546492	40.784256366	49.853560902	5	7	41.046366303	39.645721455	45.486725536
19	1	45.795054179	40.196795852	49.495697914	6	1	40.932944219	38.645799757	45.698076061
20	1	45.266214460	41.308657071	50.766420915	7	6	42.151863038	40.222140077	44.982995489
21	6	44.524797181	41.760653987	48.792662665	8	1	43.075431455	39.700056206	44.752302059
22	7	43.798465397	42.919524788	49.028360402	9	7	41.963763789	41.530833737	44.827612486
23	1	43.474198739	43.258121735	49.938031239	10	6	40.672132724	41.791658853	45.235690717
24	6	43.562903737	43.525038676	47.841762386	11	1	40.238537412	42.785332571	45.179977026
25	1	42.986244752	44.440319685	47.715498551	12	6	41.113401239	46.602476249	44.900121183
26	7	44.110518770	42.831586510	46.852754418	13	1	41.761010081	46.988952465	45.699081688
27	6	44.716383889	41.735712445	47.430369134	14	1	41.224797759	47.226963168	44.002029290
28	1	45.228702440	40.990213437	46.825285091	15	6	41.496962392	45.166550752	44.496658610
29	26	43.561116589	42.991857698	44.769096621	16	8	42.329568257	44.551857824	45.266613941
30	8	44.511339188	43.879177712	43.536699515	17	8	40.986896782	44.682515635	43.480758277
31	8	45.946624386	43.010600622	42.974255940	18	6	44.928717683	40.838479497	49.824057307
32	6	44.927463687	43.291002756	40.548286526	19	1	45.799078794	40.266703866	49.464751152
33	8	45.446575958	44.315233212	40.372290084	20	1	45.253045667	41.371431563	50.734496350
34	8	44.394341755	42.266848857	40.680877569	21	6	44.497239938	41.802819032	48.760695612
35	6	45.871633816	41.778202172	43.345184580	22	7	43.762995820	42.957925266	48.994335972
36	8	48.807174377	39.363720804	41.395555325	23	1	43.449031868	43.301885683	49.905822744
37	6	46.943584036	40.909649868	42.684021423	24	6	43.504234284	43.548831755	47.806524674
38	6	46.477217433	39.677544270	41.890308726	25	1	42.920956398	44.459199258	47.679340891
39	6	47.640469949	38.980475442	41.144543600	26	7	44.045790296	42.848116547	46.817631193
40	8	47.356974509	38.056426458	40.325691656	27	6	44.670472756	41.763314188	47.397234859
41	8	45.043548411	41.348595046	44.173641260	28	1	45.172160322	41.015915878	46.787108927
42	1	47.644810578	40.600992786	43.473991810	29	26	43.504977064	42.962230525	44.732105660
43	1	47.523348540	41.558186623	42.017126843	30	8	44.328873380	43.888222082	43.456386210
44	1	46.000517448	38.930006014	42.545888883	31	8	46.007392863	42.549160638	42.918851135
45	1	45.712075069	39.949726927	41.146090401	32	6	45.219252329	43.688628134	40.723083773
46	6	40.879364462	45.354998687	38.158202086	33	8	45.911755802	44.616599687	40.857505340
47	1	41.846927014	45.660917001	37.724241843	34	8	44.524489518	42.783018807	40.514301863
48	1	40.421931874	46.231668521	38.638127909	35	6	45.681891444	41.460455195	43.435392573
49	7	41.189398532	44.364025772	39.237937203	36	8	48.696400630	39.210071231	41.534219159
50	1	40.309826901	43.923723520	39.578125205	37	6	46.455194573	40.207290453	43.007403815
51	6	42.032454462	43.243829891	38.729872739	38	6	46.378977381	39.827072081	41.517236136
52	6	41.844230898	45.038667762	40.401870441	39	6	47.569924033	38.965550368	41.040641352
53	1	42.997010170	43.634961888	38.367863091	40	8	47.363802578	38.089535083	40.148061946
54	1	41.497387930	42.752371687	37.905769568	41	8	44.772031713	41.334271620	44.330694623
55	1	42.185947540	42.521341488	39.539311822	42	1	46.112853031	39.369324129	43.630616443
56	1	42.062216771	44.306894849	41.188062767	43	1	47.517952318	40.396696479	43.232696732
57	1	41.146458582	45.775368521	40.814244470	44	1	45.440491282	39.310235176	41.271929656
58	1	42.755373656	45.541722356	40.053439307	45	1	46.405620175	40.745753033	40.906474678
59	8	44.924243818	47.086723328	40.083075212	46	6	40.829826544	45.339332611	38.283202235
60	1	44.486387459	46.886384145	40.945769692	47	1	41.774313708	45.734250131	37.869890567
61	1	45.532325972	46.337057975	40.018342774	48	1	40.324393214	46.138930103	38.844120488
62	8	43.802134389	46.378997437	42.482215255	49	7	41.215121653	44.277746676	39.266040663
63	1	44.166898574	47.149714233	42.970467629	50	1	40.373321228	43.769259363	39.602421691
64	1	44.209378092	45.568719989	42.868891199	51	6	42.101001050	43.252109022	38.646169895
65	1	38.838743449	40.376795875	47.369382482	52	6	41.867068616	44.894370630	40.463782243
66	1	44.156504723	40.096420067	50.184619137	53	1	43.042288031	43.717492996	38.315172563
67	1	40.104119416	46.648311333	45.271518769	54	1	41.572414093	42.812265471	37.788930423
68	1	40.164893354	44.993934308	37.418451541	55	1	42.311380540	42.473966948	39.387352711
IM2					56	1	42.182147910	44.113067812	41.163660420
QM(B1)/MM = -3195.420696 (a.u.)					57	1	41.135124584	45.528513366	40.972965000
QM(B2+ZPE)/MM = -3197.152129 (a.u.)					58	1	42.721576878	45.493866978	40.125438428
QM(B2+D3+ZPE)/MM = -3197.2337 (a.u.)					59	8	44.755189848	47.125146915	40.136984726
1	6	38.755037896	40.403618795	46.304433684	60	1	44.304138106	46.935967593	40.994290452
2	1	38.062136778	41.188187685	45.973528112	61	1	45.480314146	46.484063055	40.172819937
3	1	38.313939284	39.444859340	45.992144160	62	8	43.665350198	46.428667643	42.558382843
4	6	40.086845711	40.627385676	45.667763618	63	1	44.103624273	47.181274724	43.014461759
					64	1	44.081918412	45.600955430	42.896977451
					65	1	38.783681085	40.394781858	47.394006444

66	1	44.163524894	40.137158868	50.156768443
67	1	40.093706018	46.639734762	45.283397555
68	1	40.141293203	45.010805357	37.504704321

IM3

QM(B1)/MM = -3195.455710 (a.u.)

QM(B2+ZPE)/MM = -3197.205695 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2819 (a.u.)

1	6	38.741543564	40.412995107	46.400328249
2	1	38.052081373	41.199400024	46.065679954
3	1	38.317254024	39.458030831	46.056560351
4	6	40.091482489	40.656396628	45.810868466
5	7	41.025999155	39.672499380	45.544599238
6	1	40.892227559	38.662253788	45.682705414
7	6	42.146373173	40.263292964	45.093687654
8	1	43.046087296	39.735201206	44.794605579
9	7	41.993562336	41.585682297	45.065392297
10	6	40.711937246	41.840511819	45.500585021
11	1	40.315104851	42.846734076	45.573214789
12	6	41.056472853	46.521612383	44.900140503
13	1	41.708090076	46.904705193	45.698830212
14	1	41.121908949	47.178262599	44.019271748
15	6	41.477650868	45.115838643	44.432530794
16	8	42.207317702	44.433004720	45.246457072
17	8	41.116021693	44.732154212	43.317735246
18	6	44.890140853	40.790596471	49.877479989
19	1	45.758869457	40.210972569	49.526750056
20	1	45.213235996	41.330484389	50.783846124
21	6	44.460644177	41.747281091	48.806330096
22	7	43.750900596	42.915506364	49.039413195
23	1	43.457970164	43.274333202	49.952579284
24	6	43.478171400	43.496484340	47.847966640
25	1	42.910798640	44.417515437	47.725365929
26	7	43.985263807	42.772811253	46.860904282
27	6	44.603516711	41.686871126	47.438401595
28	1	45.089483748	40.922345820	46.835832991
29	26	43.489909154	42.979078946	44.773953505
30	8	44.588990107	44.090702194	44.317395880
31	8	44.560452716	42.136532143	41.823021596
32	6	47.566470516	46.358183070	40.591736566
33	8	47.923806413	46.691923958	41.648877353
34	8	47.302189111	46.040093593	39.505999061
35	6	44.928315488	41.420857253	42.751530136
36	8	48.485438785	39.420491468	41.414525684
37	6	46.009030122	40.347288835	42.581277538
38	6	46.099353513	39.701871712	41.196240244
39	6	47.435367477	38.992511224	40.887795372
40	8	47.401604969	38.020292717	40.067116115
41	8	44.466864814	41.518185305	43.975618551
42	1	45.877934708	39.590487088	43.368594572
43	1	46.973996604	40.843305784	42.794839595
44	1	45.284277788	38.982782893	41.033267600
45	1	45.975999857	40.491679874	40.434352071
46	6	41.059667205	45.175600757	38.405156773
47	1	41.983605872	45.564526508	37.945266628
48	1	40.556939558	46.015610451	38.905772956
49	7	41.502244846	44.229209232	39.479606573
50	1	40.680894211	43.727200160	39.872487946
51	6	42.428976150	43.176269889	38.974939587
52	6	42.164196234	45.000526121	40.575499079

53	1	43.324916795	43.636862386	38.527645902
54	1	41.898433306	42.577491560	38.221987588
55	1	42.725923027	42.535779148	39.815690605
56	1	42.621270675	44.307846268	41.288512362
57	1	41.402939745	45.587016478	41.097229333
58	1	42.921959607	45.654341154	40.123107137
59	8	44.898142267	47.139930920	40.661800935
60	1	45.053724654	46.275261381	41.111844003
61	1	44.602080042	47.744479255	41.380352746
62	8	45.576157274	44.746408353	41.795687072
63	1	45.343780219	44.662758363	42.743063099
64	1	45.278579512	43.882897172	41.450946906
65	1	38.747853574	40.384137103	47.489912904
66	1	44.118136314	40.097432875	50.211546665
67	1	40.040297581	46.540281804	45.293976242
68	1	40.346511622	44.778599554	37.682753505

RC1'

QM(B1)/MM = -3195.351035 (a.u.)

QM(B2+ZPE)/MM = -3197.616922 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.1686 (a.u.)

1	6	38.757710262	40.365450669	46.359517194
2	1	38.080678302	41.155510503	46.008080852
3	1	38.314503556	39.410174406	46.041514836
4	6	40.108020596	40.569367032	45.755978334
5	7	41.035581528	39.570068418	45.529914030
6	1	40.890988422	38.565891352	45.700089734
7	6	42.161412698	40.134361991	45.054541830
8	1	43.056790472	39.584479624	44.776367506
9	7	42.015467787	41.451167690	44.969534776
10	6	40.735857910	41.734336278	45.392090397
11	1	40.340264086	42.745687300	45.409110929
12	6	41.083464925	46.624309362	44.863478918
13	1	41.737908150	46.964622446	45.677786542
14	1	41.152533812	47.322574596	44.016098420
15	6	41.481137479	45.240205885	44.327650938
16	8	42.323880617	44.563558547	45.040301554
17	8	40.997740396	44.861555624	43.260790143
18	6	44.898062403	40.837070743	49.774871467
19	1	45.768537789	40.257419816	49.428473850
20	1	45.225804596	41.400629500	50.665261720
21	6	44.454148489	41.765339667	48.684777590
22	7	43.722385996	42.924717176	48.893180418
23	1	43.413190778	43.288628042	49.796953023
24	6	43.459176021	43.485315504	47.689652322
25	1	42.882517926	44.398480466	47.550244513
26	7	43.991153094	42.760673478	46.714842963
27	6	44.617530758	41.692627617	47.319718536
28	1	45.127103382	40.927467081	46.737495401
29	26	43.420643948	42.968616022	44.591195464
30	8	43.006645165	42.613586254	42.574978360
31	8	43.907503835	42.491041741	41.688013562
32	6	45.863540214	43.449368240	43.196888683
33	8	46.712722042	44.037135248	42.533050313
34	8	44.994166463	43.996692591	43.969813651
35	6	45.755609577	41.889496556	43.181642758
36	8	48.687637592	39.378401874	41.443846581
37	6	46.703058958	41.133653815	42.296094965
38	6	46.338991166	39.731153720	41.798815462
39	6	47.532250772	39.023393289	41.108349448

40	8	47.287771994	38.107684508	40.268897464
41	8	44.971293004	41.390501254	43.997165691
42	1	47.656951232	41.064510436	42.856004754
43	1	46.930505584	41.801385501	41.454638653
44	1	46.022851654	39.087013480	42.637947669
45	1	45.485463564	39.760260786	41.105293931
46	6	40.947427732	45.296487257	38.191329418
47	1	41.876787539	45.632432438	37.699017318
48	1	40.463938207	46.169647895	38.652331476
49	7	41.366093488	44.381994499	39.301333230
50	1	40.533167186	43.920680094	39.719438338
51	6	42.244686813	43.274274622	38.821364295
52	6	42.071622251	45.144029455	40.378829238
53	1	43.136466812	43.694064430	38.327965810
54	1	41.670952834	42.656375933	38.117266416
55	1	42.552825323	42.671531316	39.684460707
56	1	42.199188989	44.489925845	41.246695125
57	1	41.450230437	46.000246636	40.668081989
58	1	43.040780765	45.483425020	39.984978694
59	8	45.596375941	45.789018320	39.365211152
60	1	45.771492250	46.217198381	40.239403702
61	1	45.698280694	44.842144264	39.533094820
62	8	46.177745418	46.827531708	41.808416076
63	1	45.503624023	47.339490778	42.300121077
64	1	46.317649971	45.990774083	42.296973494
65	1	38.768890931	40.363356011	47.449442846
66	1	44.139626170	40.142705222	50.136393711
67	1	40.067416259	46.621079565	45.258069846
68	1	40.223333017	44.876817228	37.493023443

TS1'

QM(B1)/MM = -3195.337741 (a.u.)

QM(B2+ZPE)/MM = -3197.605129 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.1549 (a.u.)

1	6	38.757521002	40.367968944	46.354429621
2	1	38.076349299	41.156429181	46.007288287
3	1	38.316593600	39.411754223	46.036199230
4	6	40.104500599	40.577901597	45.746191359
5	7	41.031234411	39.579144613	45.509227570
6	1	40.888864617	38.574466955	45.677913365
7	6	42.154077761	40.146305966	45.031975521
8	1	43.051632005	39.602849700	44.748103937
9	7	42.006470816	41.464195520	44.958410692
10	6	40.730427991	41.745703725	45.388394073
11	1	40.338346359	42.758057045	45.414823344
12	6	41.114093800	46.574405592	44.821104505
13	1	41.775193175	46.908700746	45.632845625
14	1	41.183501709	47.275828686	43.976080793
15	6	41.506882952	45.188440862	44.276907200
16	8	42.340388471	44.501850421	44.983827149
17	8	41.024847220	44.822737678	43.202884261
18	6	44.895334531	40.852783804	49.777359759
19	1	45.767615984	40.278319169	49.427459803
20	1	45.221240093	41.413405384	50.670453732
21	6	44.449207932	41.785245643	48.691242088
22	7	43.697670630	42.932819785	48.904056153
23	1	43.382190871	43.286276828	49.810242177
24	6	43.434045193	43.500574934	47.705380015
25	1	42.846178488	44.407053344	47.568907679
26	7	43.987752109	42.792323368	46.729789082

27	6	44.628090162	41.727742756	47.327887599
28	1	45.157588241	40.984629331	46.735055163
29	26	43.489942360	42.899739163	44.619624808
30	8	43.210520151	42.529420416	42.450827720
31	8	44.367213801	42.160600543	41.912923741
32	6	45.791378069	43.661517098	43.098780084
33	8	46.691877163	44.177434271	42.461437132
34	8	44.954125769	44.166686115	43.902771111
35	6	45.394552765	41.961567227	42.913771732
36	8	48.610274011	39.445531522	41.454098712
37	6	46.538636396	41.179433415	42.267738552
38	6	46.240428929	39.769809033	41.730591915
39	6	47.469742969	39.072610387	41.094413761
40	8	47.259154724	38.137786343	40.263009203
41	8	44.877486288	41.579946079	44.068590734
42	1	47.350219223	41.126675968	43.008700844
43	1	46.912791455	41.811859432	41.450977128
44	1	45.888868425	39.111898517	42.545241477
45	1	45.427248526	39.787114727	40.989419264
46	6	40.994035812	45.255027272	38.225739111
47	1	41.928064608	45.566458222	37.725663732
48	1	40.531399019	46.147074172	38.671588236
49	7	41.400606534	44.357696548	39.354353213
50	1	40.560445844	43.934456134	39.796877761
51	6	42.232507000	43.204212528	38.903992973
52	6	42.154052572	45.128416609	40.392360840
53	1	43.158460810	43.568739588	38.428453923
54	1	41.646165807	42.609054644	38.190913749
55	1	42.468005391	42.589823195	39.782101169
56	1	42.346351097	44.469743972	41.246141076
57	1	41.536029718	45.971303387	40.723334978
58	1	43.091129752	45.486527893	39.941136417
59	8	45.666505388	45.845671560	39.365045043
60	1	45.824970426	46.329905272	40.211395652
61	1	45.801078401	44.915911102	39.593554252
62	8	46.213651936	47.014815321	41.759583499
63	1	45.512768280	47.504523858	42.242636733
64	1	46.373925558	46.191581852	42.259936580
65	1	38.772873619	40.363633760	47.444297883
66	1	44.139734355	40.153785373	50.135880182
67	1	40.100573902	46.580747295	45.222108902
68	1	40.261105758	44.838870086	37.534584966

IM1'

QM(B1)/MM = -3195.422545 (a.u.)

QM(B2+ZPE)/MM = -3197.692687 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2297 (a.u.)

1	6	38.673852125	40.317788161	46.344469066
2	1	37.992744067	41.109427155	46.006589773
3	1	38.210534928	39.362652443	46.055152353
4	6	40.002846268	40.501297660	45.691436304
5	7	40.957150485	39.509873459	45.558187520
6	1	40.835637979	38.517652977	45.795951473
7	6	42.071488047	40.064012909	45.041501432
8	1	42.988091417	39.516246012	44.837116562
9	7	41.889733939	41.358486882	44.824458896
10	6	40.598228496	41.641452870	45.209468397
11	1	40.170178274	42.635975722	45.110875124
12	6	41.024115162	46.607581005	44.817459516
13	1	41.678436353	47.044298119	45.586079384

14	1	41.053945624	47.224667264	43.905656239
15	6	41.459013414	45.181605135	44.421600231
16	8	42.310751153	44.603618926	45.176558007
17	8	40.960784176	44.695755792	43.391890954
18	6	44.888968773	40.805067823	49.772177161
19	1	45.754623772	40.222824917	49.417630246
20	1	45.225471395	41.361714895	50.664069399
21	6	44.444069128	41.742357647	48.689982943
22	7	43.717158000	42.902408910	48.910967870
23	1	43.408345864	43.257709432	49.817982554
24	6	43.452658664	43.473960953	47.711132124
25	1	42.873380209	44.386302515	47.575424704
26	7	43.978889925	42.757330713	46.727554748
27	6	44.601591548	41.680977351	47.323344189
28	1	45.103417948	40.919153733	46.729514260
29	26	43.313621289	42.868860427	44.638652323
30	8	44.098159550	43.405737353	42.888972512
31	8	45.091501977	42.590100039	42.253362404
32	6	45.145867991	45.635173730	43.029401575
33	8	46.213496670	45.262264755	42.734137371
34	8	44.158895742	46.166829528	43.340240318
35	6	45.448018617	41.513775248	42.942177872
36	8	48.701917154	39.276417057	41.368169572
37	6	46.595153251	40.801742415	42.256364813
38	6	46.332215231	39.391336151	41.709469927
39	6	47.592647317	38.795186357	41.044546838
40	8	47.443404595	37.843349048	40.221727504
41	8	44.929725417	41.209287209	44.012285661
42	1	47.421179468	40.743858737	42.983075700
43	1	46.936044313	41.446633191	41.435854041
44	1	46.026429686	38.706282949	42.518240282
45	1	45.507586004	39.381589426	40.980907162
46	6	41.031374024	45.182505139	38.456958707
47	1	41.955316993	45.536198105	37.966151137
48	1	40.547808795	46.036155350	38.952842610
49	7	41.463282853	44.234919880	39.534734338
50	1	40.631057044	43.783861311	39.965336788
51	6	42.306324464	43.120048982	39.015194825
52	6	42.217418913	44.969905179	40.597911482
53	1	43.213941399	43.521518806	38.534118068
54	1	41.717427609	42.543396744	38.289270290
55	1	42.576303811	42.470867176	39.857798244
56	1	42.512732865	44.272756858	41.391769729
57	1	41.565018645	45.738017582	41.025997207
58	1	43.103959639	45.417802818	40.126773912
59	8	45.671273762	45.670807859	39.383208719
60	1	45.832667309	46.394321447	40.025669979
61	1	45.695078176	44.853714005	39.898315939
62	8	46.193727322	47.740863498	41.111063223
63	1	45.442904886	48.183274422	41.587997834
64	1	46.744604003	47.376344053	41.817313345
65	1	38.717356046	40.328173572	47.433536037
66	1	44.130103144	40.112479761	50.136199212
67	1	40.013105046	46.609405449	45.224795418
68	1	40.314917406	44.790561617	37.735060157

TS2'

QM(B1)/MM = -3195.409386 (a.u.)

QM(B2+ZPE)/MM = -3197.681702 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2349 (a.u.)

1	6	38.662789284	40.318074393	46.340749108
2	1	37.973344497	41.106514759	46.012868080
3	1	38.201108100	39.360919779	46.056092315
4	6	39.979752518	40.510173762	45.666694802
5	7	40.938236658	39.524210606	45.510985159
6	1	40.830691072	38.531870007	45.757685867
7	6	42.033883473	40.081716396	44.964967076
8	1	42.951910256	39.544517931	44.741061657
9	7	41.835692184	41.377055918	44.753764806
10	6	40.553119951	41.655040760	45.172861958
11	1	40.118587450	42.646846467	45.085111574
12	6	40.998273828	46.550980302	44.796494117
13	1	41.675648949	46.961263763	45.559405216
14	1	41.036886686	47.173640887	43.889391796
15	6	41.378076966	45.114822078	44.381145228
16	8	42.196662692	44.486286847	45.140035013
17	8	40.865653146	44.662596133	43.346859029
18	6	44.898380502	40.843158567	49.664811580
19	1	45.760176276	40.261034219	49.300941334
20	1	45.248965256	41.411783329	50.543825087
21	6	44.435815080	41.767405368	48.578860028
22	7	43.680974903	42.911317757	48.795833225
23	1	43.358207912	43.257847410	49.700315552
24	6	43.413030331	43.480933679	47.597968877
25	1	42.809896582	44.376256852	47.457858733
26	7	43.965842975	42.780161621	46.616668645
27	6	44.609923645	41.715435310	47.213994351
28	1	45.136813223	40.973660561	46.617168083
29	26	43.292110504	42.834691452	44.528614544
30	8	43.833035938	43.490315039	42.948599019
31	8	45.040053888	42.482066980	42.126832361
32	6	45.022885897	45.661410613	43.088880685
33	8	46.064423401	45.263031030	42.743474307
34	8	44.063214457	46.208375292	43.455047582
35	6	45.422764569	41.565304211	42.936403664
36	8	48.707880215	39.353439789	41.315401160
37	6	46.631108935	40.778710160	42.432445129
38	6	46.332214252	39.496945574	41.639893628
39	6	47.594729137	38.875074637	41.004354159
40	8	47.436074178	37.902782807	40.204977568
41	8	44.904542602	41.351026378	44.057782696
42	1	47.261480855	40.548165212	43.302523183
43	1	47.207881407	41.451325501	41.785153254
44	1	45.869499305	38.725219832	42.277269934
45	1	45.606521200	39.693023758	40.834557458
46	6	41.014956458	45.149583996	38.408514371
47	1	41.938421046	45.487948120	37.906145279
48	1	40.534137797	46.021632166	38.874068391
49	7	41.447839207	44.242146192	39.519932441
50	1	40.617934904	43.790227779	39.953564287
51	6	42.315823693	43.125024301	39.045654839
52	6	42.177901824	45.020599010	40.568159894
53	1	43.209983603	43.527256966	38.540725084
54	1	41.736339796	42.502676687	38.350524853
55	1	42.611116266	42.523923265	39.915093318
56	1	42.465623294	44.352909208	41.390657012
57	1	41.512703511	45.801846269	40.952137674
58	1	43.068714016	45.457748885	40.094740109
59	8	45.629663476	45.617759644	39.425053653
60	1	45.806199006	46.352688464	40.049538461
61	1	45.620658096	44.814155254	39.962707973

62	8	46.201753068	47.724967337	41.109913866
63	1	45.447315362	48.176766833	41.571110301
64	1	46.710909959	47.321980801	41.826619757
65	1	38.720177821	40.328184144	47.429175342
66	1	44.152434736	40.149968672	50.053553151
67	1	39.991789628	46.576165080	45.214133444
68	1	40.291259415	44.734874548	37.706840669

IM2'

QM(B1)/MM = -3195.418376 (a.u.)

QM(B2+ZPE)/MM = -3197.676438 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2269 (a.u.)

1	6	38.617757522	40.327934674	46.358367382
2	1	37.918587077	41.113154923	46.044664177
3	1	38.159273517	39.369133684	46.075487333
4	6	39.924212513	40.529217788	45.668490084
5	7	40.879501582	39.542724015	45.494084444
6	1	40.775195037	38.548093549	45.734309906
7	6	41.970888679	40.101114854	44.945913415
8	1	42.889894450	39.571027446	44.714822467
9	7	41.773840608	41.401031844	44.751295638
10	6	40.494718924	41.678786811	45.183109920
11	1	40.060543972	42.671671341	45.111370582
12	6	41.007554507	46.525924399	44.785368705
13	1	41.691122843	46.926819299	45.547484048
14	1	41.050760575	47.151287329	43.880530998
15	6	41.368494804	45.088484397	44.362568011
16	8	42.190060729	44.448150868	45.118573367
17	8	40.845306148	44.639598249	43.336464173
18	6	44.899220793	40.868962721	49.659320847
19	1	45.769284358	40.296902667	49.299368429
20	1	45.239419411	41.444342256	50.537816798
21	6	44.426431846	41.784342485	48.570309211
22	7	43.676675565	42.932227524	48.785915734
23	1	43.368533981	43.288687098	49.692036913
24	6	43.390852677	43.489211254	47.587423200
25	1	42.791478441	44.386825549	47.447916366
26	7	43.927821103	42.774391366	46.606146030
27	6	44.579862853	41.714671062	47.204490428
28	1	45.089657768	40.964769923	46.603912129
29	26	43.272115420	42.808493929	44.514914971
30	8	43.790559589	43.498996514	42.974210584
31	8	45.028510892	42.061499323	42.098909827
32	6	45.064529850	45.543120225	42.924889989
33	8	46.079472747	45.099578037	42.556474571
34	8	44.150857222	46.157481316	43.308199075
35	6	45.209496671	41.216541716	43.002707129
36	8	48.621841307	39.251681105	41.423508468
37	6	46.193050737	40.080544755	42.716370266
38	6	46.248884017	39.581665528	41.269736058
39	6	47.554543025	38.853094075	40.904176286
40	8	47.490697351	37.909262196	40.056025872
41	8	44.666166354	41.257172162	44.162620012
42	1	45.965488693	39.262112432	43.413609167
43	1	47.195194229	40.461683986	42.982868268
44	1	45.399145632	38.925637910	41.036299405
45	1	46.178514831	40.451358489	40.593390599
46	6	41.013313395	45.137618091	38.445197282
47	1	41.929425048	45.488067280	37.937743167
48	1	40.526306953	46.003991497	38.915314720

49	7	41.463011782	44.234113811	39.552786998
50	1	40.639046832	43.784436590	39.999749581
51	6	42.326112189	43.115132804	39.074249000
52	6	42.209987677	45.019115160	40.583999735
53	1	43.209148307	43.515105231	38.548285625
54	1	41.735811703	42.483824827	38.396394641
55	1	42.643032263	42.524457570	39.943535611
56	1	42.515425657	44.353782764	41.402697821
57	1	41.550897709	45.801665672	40.975994857
58	1	43.090158643	45.457514449	40.091965845
59	8	45.638017549	45.696011280	39.334801140
60	1	45.847529130	46.390980735	39.993679087
61	1	45.693512489	44.856923190	39.811375731
62	8	46.259589294	47.704379622	41.119532117
63	1	45.499772935	48.150571644	41.577159400
64	1	46.768147242	47.301329913	41.836401244
65	1	38.693606233	40.332984565	47.445698420
66	1	44.159185128	40.168164733	50.045710183
67	1	40.002315064	46.556677853	45.205624829
68	1	40.291699077	44.720343886	37.742899384

IM3'

QM(B1)/MM = -3195.448511 (a.u.)

QM(B2+ZPE)/MM = -3197.720927 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2752 (a.u.)

1	6	38.740663669	40.371749810	46.297236625
2	1	38.052707972	41.160217413	45.965083285
3	1	38.286678141	39.414490455	45.999485230
4	6	40.067347963	40.574661519	45.643520569
5	7	41.028127469	39.592347701	45.491539562
6	1	40.917365516	38.597632514	45.729389257
7	6	42.129424113	40.155582570	44.959308944
8	1	43.048915569	39.620037377	44.739716753
9	7	41.928977814	41.450675719	44.756133636
10	6	40.643197397	41.726247100	45.161712542
11	1	40.199962857	42.713677987	45.062366631
12	6	41.193758984	46.601218130	44.897040969
13	1	41.852599116	46.942117813	45.707321581
14	1	41.296354663	47.277881799	44.033924174
15	6	41.551616951	45.188693380	44.391179201
16	8	42.535663639	44.592511644	44.991818980
17	8	40.897553205	44.722996445	43.458549613
18	6	44.895660483	40.893453383	49.581586096
19	1	45.765270004	40.328165401	49.210324170
20	1	45.245878734	41.485349592	50.444929639
21	6	44.389483834	41.787880294	48.490099974
22	7	43.626461957	42.926724658	48.703765676
23	1	43.326478434	43.289645194	49.609193971
24	6	43.320208927	43.469066725	47.504417769
25	1	42.724481416	44.368367084	47.368156146
26	7	43.854162339	42.751885447	46.524172934
27	6	44.527970086	41.708074650	47.123580571
28	1	45.056569151	40.969318509	46.527078614
29	26	43.403633329	42.893924579	44.432030997
30	8	43.197537602	43.167708871	42.848330594
31	8	46.146456876	42.531100925	42.474550795
32	6	45.561288118	47.307243548	40.786412504
33	8	46.679610697	47.258263261	41.103006340
34	8	44.459616319	47.435429164	40.435071350
35	6	45.758536451	41.596481387	43.167332927

36	8	48.653978569	39.152274233	41.568837337
37	6	46.348827052	40.205672854	42.928692361
38	6	46.330644823	39.745246911	41.459180888
39	6	47.548396330	38.895510727	41.037767750
40	8	47.381658590	38.018299004	40.136632045
41	8	44.915284736	41.709740749	44.167487262
42	1	45.870415380	39.466555819	43.587225025
43	1	47.411928810	40.286602121	43.214102327
44	1	45.410137839	39.199799160	41.206791255
45	1	46.365933881	40.643686801	40.818611818
46	6	40.862316969	45.240231445	38.207841241
47	1	41.790518682	45.624383678	37.750747125
48	1	40.334134822	46.081634055	38.677809641
49	7	41.267658264	44.297147881	39.302436046
50	1	40.477050965	43.666212085	39.543647556
51	6	42.415008173	43.434562321	38.894259583
52	6	41.612813622	45.041880783	40.548828472
53	1	43.286372254	44.073915390	38.696569398
54	1	42.138035277	42.883708183	37.985715169
55	1	42.633996096	42.732396839	39.708802304
56	1	41.897670021	44.329240115	41.332083314
57	1	40.718384562	45.582158795	40.878882196
58	1	42.429423273	45.741807750	40.324267799
59	8	45.540372805	45.130314371	38.732707542
60	1	45.506249615	44.286779362	38.229538788
61	1	45.391261489	44.861999587	39.669995107
62	8	45.085057921	44.734683642	41.397591234
63	1	44.218200938	44.482000718	41.758332545
64	1	45.647334884	44.040174371	41.808370958
65	1	38.782280946	40.373430858	47.386425541
66	1	44.173288791	40.187955872	49.992097643
67	1	40.172470114	46.633104303	45.276540164
68	1	40.167686426	44.813547166	37.484310830

IM4

QM(B1)/MM = -3195.463449 (a.u.)

QM(B2+ZPE)/MM = -3197.206036 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2859 (a.u.)

1	6	38.788029938	40.371647282	46.390473693
2	1	38.112112775	41.155815102	46.023846635
3	1	38.365267260	39.411784158	46.058637668
4	6	40.154648340	40.594234150	45.830723673
5	7	41.100674251	39.609457367	45.627546259
6	1	40.959009575	38.600347506	45.765224526
7	6	42.238466562	40.195396560	45.204975444
8	1	43.146891868	39.662679200	44.940134942
9	7	42.080086770	41.510886575	45.137146515
10	6	40.783974241	41.773618597	45.513339061
11	1	40.390185287	42.784017598	45.554677488
12	6	41.029305433	46.648406257	44.875378739
13	1	41.671520885	46.982808670	45.703402362
14	1	41.095452970	47.357538892	44.038004987
15	6	41.474691545	45.281082108	44.336067301
16	8	42.082727523	44.492194301	45.121738699
17	8	41.212361576	45.049746680	43.129998869
18	6	44.902303367	40.899339442	49.748256619
19	1	45.775524744	40.334414116	49.384627530
20	1	45.236166278	41.456706974	50.640702043
21	6	44.440485678	41.837852238	48.673936309
22	7	43.689515220	42.981333681	48.901556982

23	1	43.375283002	43.325839627	49.811091396
24	6	43.419364736	43.560029347	47.706205765
25	1	42.818886939	44.458734064	47.578781942
26	7	43.966812169	42.861705924	46.724131305
27	6	44.610353771	41.793428654	47.308227272
28	1	45.132875176	41.053224647	46.705873758
29	26	43.473755580	42.957816747	44.601036843
30	8	44.524234407	44.115718635	44.159378637
31	8	44.791180712	42.014816291	41.824529364
32	6	46.967169090	46.425501570	40.735784635
33	8	47.628188083	46.382892610	41.690573245
34	8	46.431119628	46.504380704	39.703013375
35	6	45.132582504	41.323425672	42.794237566
36	8	48.628071919	39.292729575	41.405078553
37	6	46.199013348	40.239651579	42.626105365
38	6	46.247732337	39.596544056	41.239230312
39	6	47.563184395	38.881644579	40.892365812
40	8	47.508128275	37.924270811	40.055289273
41	8	44.653357534	41.449440476	43.995958214
42	1	46.052524443	39.486607953	43.413644172
43	1	47.178280676	40.710524232	42.827525561
44	1	45.419945912	38.888307609	41.092512533
45	1	46.111549752	40.393341311	40.486707397
46	6	41.124808940	45.284404785	37.929034761
47	1	42.085836561	45.332029960	37.396058432
48	1	40.823681643	46.313942042	38.163053292
49	7	41.385981160	44.572522736	39.223298726
50	1	40.485298002	44.273062854	39.648481998
51	6	42.152890293	43.302075626	39.032092756
52	6	42.125103582	45.481020063	40.156091110
53	1	43.139380065	43.532445401	38.604905061
54	1	41.582715529	42.649106567	38.358306277
55	1	42.256104982	42.809205921	40.006059274
56	1	42.396283167	44.953575562	41.070929071
57	1	41.478715467	46.331252546	40.407787961
58	1	43.034058896	45.810761117	39.632245173
59	8	44.671131497	46.132213192	41.986179335
60	1	44.512302984	47.014633252	42.385280794
61	1	44.695110212	45.506807304	42.736323053
62	8	42.517788471	42.826623727	42.724477251
63	1	42.023769864	43.689376856	42.662363124
64	1	43.346248237	42.754467303	42.165855236
65	1	38.773321636	40.368699071	47.480355471
66	1	44.158458377	40.191935598	50.114783229
67	1	40.014148261	46.637261266	45.272114199
68	1	40.320101110	44.846962497	37.338139781

TS3

QM(B1)/MM = -3195.456415 (a.u.)

QM(B2+ZPE)/MM = -3197.201549 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2807 (a.u.)

1	6	38.768536472	40.373435086	46.390967135
2	1	38.087538418	41.155281252	46.029573962
3	1	38.346099550	39.412135987	46.062921019
4	6	40.130671059	40.600214721	45.822683819
5	7	41.082771327	39.619288845	45.631753334
6	1	40.946977603	38.610379934	45.776193534
7	6	42.220748311	40.210514508	45.214304537
8	1	43.133208885	39.677104704	44.965135201
9	7	42.055271701	41.524002424	45.134471376

10	6	40.755342963	41.781021184	45.498757084
11	1	40.357155810	42.790451710	45.530480842
12	6	40.995632244	46.686128933	44.870608423
13	1	41.636373329	47.032655579	45.694792643
14	1	41.051421565	47.389167663	44.027779770
15	6	41.448451005	45.316744871	44.345968705
16	8	42.041738924	44.539808395	45.156559806
17	8	41.207106666	45.071871898	43.141450736
18	6	44.900466170	40.910377720	49.729296490
19	1	45.773853100	40.347571548	49.362739150
20	1	45.236472196	41.471697163	50.618487277
21	6	44.427884157	41.843109386	48.654554573
22	7	43.675517254	42.985450357	48.883536919
23	1	43.369027026	43.333307551	49.794376263
24	6	43.389732118	43.556418908	47.688454688
25	1	42.785710049	44.452564868	47.558719387
26	7	43.927976046	42.852451588	46.705189447
27	6	44.582876671	41.790376683	47.287374799
28	1	45.102698748	41.049861376	46.683391070
29	26	43.432618552	43.014741593	44.609363489
30	8	44.543898644	44.146788092	44.248561662
31	8	44.621418396	41.857315790	41.832336507
32	6	46.958959524	46.428831492	40.748398384
33	8	47.638434389	46.365242183	41.688987692
34	8	46.406546309	46.528464826	39.725873642
35	6	45.108066352	41.223823571	42.830291709
36	8	48.626399322	39.312153465	41.345944725
37	6	46.229036028	40.237491446	42.563640658
38	6	46.245248167	39.582853050	41.184293448
39	6	47.567325270	38.879073778	40.840504135
40	8	47.519567468	37.907112419	40.022649515
41	8	44.724427399	41.390644629	44.020048464
42	1	46.187591284	39.484433971	43.362677079
43	1	47.181181673	40.778664476	42.708791009
44	1	45.424992141	38.860530682	41.069185643
45	1	46.085793050	40.360120510	40.416731061
46	6	41.131733542	45.281145477	37.958413089
47	1	42.091214531	45.339739368	37.423183169
48	1	40.824861232	46.306667495	38.202563952
49	7	41.402607480	44.560310261	39.245919122
50	1	40.504762819	44.259337203	39.676073554
51	6	42.166475760	43.291050858	39.040528985
52	6	42.152127875	45.458431402	40.182075829
53	1	43.144508597	43.523804799	38.595395275
54	1	41.585537192	42.637618235	38.376224648
55	1	42.289137422	42.799399172	40.013291370
56	1	42.443144305	44.914376594	41.082245415
57	1	41.504947979	46.299851443	40.459382435
58	1	43.049348398	45.802368594	39.647581434
59	8	44.692381467	46.107793303	42.026187627
60	1	44.517187152	46.996826136	42.402512081
61	1	44.677896325	45.494449904	42.787790483
62	8	42.685204653	42.864701015	42.806201914
63	1	42.127083239	43.670012334	42.686445060
64	1	43.694000061	42.458632101	42.173872769
65	1	38.762619302	40.371370654	47.480934126
66	1	44.161036126	40.201201438	50.101290495
67	1	39.982623902	46.662810430	45.272277038
68	1	40.329083111	44.845388602	37.363488255

IM5

QM(B1)/MM = -3195.459072 (a.u.)

QM(B2+ZPE)/MM = -3197.206879 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2881 (a.u.)

1	6	38.713312291	40.395843239	46.391881643
2	1	38.027108874	41.181044141	46.048833204
3	1	38.277305200	39.437010826	46.074818824
4	6	40.058229488	40.616149317	45.784102697
5	7	41.017384895	39.635404610	45.607973241
6	1	40.903896309	38.634807856	45.816035041
7	6	42.139725617	40.219188517	45.141770524
8	1	43.063131984	39.696311187	44.910016152
9	7	41.952066035	41.526278754	45.006459203
10	6	40.658332951	41.787623501	45.391634517
11	1	40.234934281	42.785962906	45.354088242
12	6	40.887554781	46.602590446	44.826953745
13	1	41.581638013	46.967528772	45.597737149
14	1	40.934793090	47.259204117	43.944508237
15	6	41.228057068	45.171728952	44.355835246
16	8	42.091485083	44.538850293	45.058211119
17	8	40.654379759	44.749487365	43.343833611
18	6	44.881123646	40.968042175	49.603134236
19	1	45.759782351	40.413013581	49.236837469
20	1	45.220776645	41.558546813	50.472068351
21	6	44.379043346	41.864513198	48.510493883
22	7	43.610432813	42.999725527	48.717510246
23	1	43.298806877	43.359032312	49.620217638
24	6	43.314731080	43.542111575	47.511373708
25	1	42.700315971	44.427187818	47.361692876
26	7	43.860246232	42.827383149	46.539295592
27	6	44.531819168	41.786994584	47.144222236
28	1	45.058382731	41.039064176	46.556676948
29	26	43.334729990	42.974489149	44.432074585
30	8	44.599827604	43.942922573	43.959957693
31	8	45.952105953	42.236895043	42.591841837
32	6	47.063856669	46.414872394	40.754401805
33	8	47.766640590	46.380755940	41.679458115
34	8	46.488664362	46.482265996	39.741710901
35	6	45.643404473	41.126989844	43.212892114
36	8	48.734721677	39.152841553	41.333626511
37	6	46.426703475	39.918472972	42.761913615
38	6	46.385484716	39.574034316	41.266869288
39	6	47.644139121	38.802221202	40.827784635
40	8	47.525744718	37.881678377	39.965981511
41	8	44.821546268	41.076411368	44.135964205
42	1	46.099363292	39.060368607	43.363832061
43	1	47.483824767	40.130403761	42.997476291
44	1	45.489326574	38.995051793	41.006744453
45	1	46.367196969	40.506182067	40.675949510
46	6	41.194207272	45.242919728	38.439567222
47	1	42.181192142	45.421844891	37.981366840
48	1	40.809427762	46.203371996	38.807938645
49	7	41.447373187	44.377455095	39.638243625
50	1	40.548812025	44.023714868	40.018255433
51	6	42.249196340	43.159808201	39.310012911
52	6	42.156230729	45.158349420	40.704331668
53	1	43.184739519	43.473108100	38.825734076
54	1	41.663122503	42.521194875	38.635035911
55	1	42.466523022	42.627797552	40.245604214
56	1	42.351289088	44.493828850	41.554565379
57	1	41.507303167	45.985139113	41.016271199

58	1	43.095559114	45.534672656	40.280750061
59	8	44.834154185	46.154912155	42.053770557
60	1	44.634255331	47.037479734	42.433377492
61	1	44.723883802	45.512551968	42.784269645
62	8	42.844233259	42.659197671	42.707744095
63	1	42.044781154	42.075161600	42.680007407
64	1	45.424687907	43.001399452	43.023203343
65	1	38.734547528	40.391318255	47.481650383
66	1	44.165693616	40.252412313	50.008228162
67	1	39.890506685	46.640100466	45.265765115
68	1	40.453193051	44.859037042	37.738425772

TS4

QM(B1)/MM = -3195.455138 (a.u.)

QM(B2+ZPE)/MM = -3197.207076 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2879 (a.u.)

1	6	38.715489231	40.384090070	46.379983844
2	1	38.032341850	41.172286046	46.037411400
3	1	38.273947883	39.426648938	46.066342791
4	6	40.058398126	40.596216109	45.764993260
5	7	41.012177050	39.610583287	45.581863646
6	1	40.895599101	38.610766736	45.793794753
7	6	42.131709349	40.184684620	45.100730336
8	1	43.054334693	39.665514695	44.858022498
9	7	41.944870949	41.492244036	44.963716869
10	6	40.657113494	41.764126337	45.362300327
11	1	40.237324839	42.763457389	45.322838770
12	6	40.900308202	46.562920647	44.803803817
13	1	41.602857629	46.919342559	45.570621921
14	1	40.952860371	47.218361027	43.920873694
15	6	41.220354676	45.126626239	44.330444819
16	8	42.088645767	44.483723655	45.019674696
17	8	40.624869613	44.708977392	43.329255461
18	6	44.882022559	40.966774140	49.557082379
19	1	45.759996699	40.409930901	49.192161870
20	1	45.224602131	41.569945153	50.415938610
21	6	44.371521642	41.848120562	48.456178199
22	7	43.600925937	42.983722762	48.655762024
23	1	43.290054846	43.348775778	49.555753044
24	6	43.297208926	43.514708528	47.447646252
25	1	42.679458989	44.396242533	47.291910065
26	7	43.840883949	42.791624669	46.480076927
27	6	44.518166130	41.757322536	47.090189360
28	1	45.042306824	41.008842731	46.501417936
29	26	43.326026051	42.899541595	44.375857710
30	8	44.606967608	43.918077008	43.868509118
31	8	45.968280145	42.319410530	42.670258840
32	6	47.054098101	46.406188723	40.746841365
33	8	47.733138807	46.390678479	41.689710903
34	8	46.502308976	46.454989173	39.720072436
35	6	45.623553267	41.230310299	43.225308163
36	8	48.725307572	39.154946044	41.404622116
37	6	46.394903975	39.983293529	42.824162127
38	6	46.386725806	39.645094237	41.325432963
39	6	47.627552885	38.842878451	40.888315918
40	8	47.491869383	37.938507103	40.009333410
41	8	44.719942548	41.149830568	44.109501835
42	1	46.028769899	39.131368996	43.414470053
43	1	47.447444202	40.172729638	43.093632538
44	1	45.478457173	39.098286665	41.036906127

45	1	46.408288445	40.587458856	40.749883954
46	6	41.171509441	45.268208675	38.385809079
47	1	42.162643749	45.432771459	37.931901664
48	1	40.796382801	46.235403227	38.746097568
49	7	41.405704495	44.405032675	39.590096708
50	1	40.500296055	44.060051094	39.962231883
51	6	42.200150272	43.180109092	39.270695714
52	6	42.110261927	45.183198118	40.660479850
53	1	43.148427345	43.485023631	38.806199689
54	1	41.619800985	42.551741727	38.581328648
55	1	42.394076048	42.639445405	40.206116151
56	1	42.286679716	44.522453911	41.516921164
57	1	41.468164969	46.020869796	40.958382558
58	1	43.059675838	45.546050560	40.247277256
59	8	44.785495586	46.182227978	41.995233462
60	1	44.607687453	47.063529431	42.390908144
61	1	44.686581319	45.534566980	42.721286439
62	8	42.747169197	42.669613345	42.681733901
63	1	41.938593224	42.092309859	42.652152152
64	1	45.292948357	43.243530641	43.229486218
65	1	38.739529711	40.381883496	47.469701471
66	1	44.171399607	40.254133663	49.975682295
67	1	39.905704259	46.614176967	45.246752025
68	1	40.428113177	44.887013621	37.685723624

IM6

QM(B1)/MM = -3195.455369 (a.u.)

QM(B2+ZPE)/MM = -3197.203112 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2844 (a.u.)

1	6	38.725209947	40.375429179	46.376985573
2	1	38.041724924	41.162319368	46.032223960
3	1	38.284622129	39.417057515	46.065235006
4	6	40.067235677	40.587716502	45.760603586
5	7	41.023854172	39.604402311	45.577537527
6	1	40.911314750	38.604992798	45.794131204
7	6	42.139896266	40.179115776	45.090505864
8	1	43.064601324	39.664290830	44.845903614
9	7	41.946737855	41.485590088	44.950481008
10	6	40.659691296	41.756464242	45.352204916
11	1	40.236659410	42.754251160	45.309674375
12	6	40.904413342	46.557463543	44.797901088
13	1	41.610975022	46.909254667	45.563047304
14	1	40.956733409	47.213856860	43.915536057
15	6	41.215556033	45.120387154	44.321954377
16	8	42.079114179	44.469968777	45.010606090
17	8	40.616219909	44.708288715	43.321039629
18	6	44.886999286	40.972151972	49.529459179
19	1	45.761898160	40.413040193	49.160817707
20	1	45.235940986	41.577683307	50.384047463
21	6	44.372186109	41.850887519	48.428637106
22	7	43.599905165	42.985342923	48.629453532
23	1	43.289492236	43.349784199	49.529622710
24	6	43.293532361	43.516442509	47.422662599
25	1	42.673307182	44.396228155	47.268180323
26	7	43.837592884	42.794272862	46.454248383
27	6	44.518133903	41.760937415	47.062639455
28	1	45.044619905	41.016542371	46.470811896
29	26	43.315615605	42.885193901	44.353580295
30	8	44.569790059	43.970740643	43.831394202
31	8	45.955288923	42.313911574	42.610740397

32	6	47.054866900	46.398713168	40.732071091
33	8	47.718591507	46.400687724	41.685898816
34	8	46.518194697	46.427694872	39.696657745
35	6	45.607896854	41.256903224	43.193047571
36	8	48.706314522	39.125395119	41.443279054
37	6	46.360111608	39.981276236	42.834198889
38	6	46.370963589	39.627984032	41.339699270
39	6	47.611356013	38.821750938	40.915281674
40	8	47.480510043	37.923952686	40.028226921
41	8	44.699892890	41.199326860	44.093537155
42	1	45.973449275	39.143751579	43.432099863
43	1	47.410848002	40.158433486	43.118720482
44	1	45.463434466	39.085702349	41.039351588
45	1	46.405854473	40.568953030	40.762724551
46	6	41.168625563	45.269819332	38.366838043
47	1	42.160957362	45.429704152	37.914126743
48	1	40.796206104	46.239483099	38.723235904
49	7	41.397578613	44.409741458	39.574233038
50	1	40.490908805	44.065323107	39.943648336
51	6	42.193435113	43.184028718	39.261059216
52	6	42.096564926	45.191429306	40.645209959
53	1	43.144284543	43.487318938	38.800817755
54	1	41.616065803	42.554488770	38.570322677
55	1	42.382471122	42.644872541	40.198186022
56	1	42.266470686	44.534216092	41.505350466
57	1	41.453428393	46.030879332	40.936086442
58	1	43.048697844	45.552739545	40.236875515
59	8	44.761606884	46.228243924	41.949375565
60	1	44.593017215	47.110096463	42.349774393
61	1	44.656255716	45.581455582	42.674840431
62	8	42.703931659	42.672661062	42.673530077
63	1	41.902150009	42.083624679	42.642166180
64	1	45.214863158	43.368521132	43.234148455
65	1	38.749056002	40.376203270	47.466709434
66	1	44.178491308	40.261689785	49.955284544
67	1	39.911081313	46.610830624	45.243446540
68	1	40.424275668	44.888432869	37.667871004

TS5

QM(B1)/MM = -3195.425650 (a.u.)

QM(B2+ZPE)/MM = -3197.174195 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2551 (a.u.)

1	6	38.903356664	40.483112071	46.240116143
2	1	38.209126528	41.263334262	45.901695349
3	1	38.480819415	39.521849353	45.908162868
4	6	40.246447585	40.733733613	45.632516948
5	7	41.226283663	39.771179935	45.463628499
6	1	41.123275041	38.770301812	45.671344556
7	6	42.326304773	40.369646256	44.961800961
8	1	43.258855032	39.866025501	44.725823898
9	7	42.113000854	41.670736618	44.798449231
10	6	40.815457980	41.910281448	45.198550825
11	1	40.365471307	42.897024076	45.141160277
12	6	41.050313209	46.729076524	44.939681490
13	1	41.689773949	47.119618219	45.743103356
14	1	41.123280158	47.384217988	44.057740764
15	6	41.462709892	45.313652068	44.485679870
16	8	42.389723232	44.740353999	45.163174786
17	8	40.880423917	44.843543361	43.499409548
18	6	44.935493475	40.925264741	49.624798043

19	1	45.805123702	40.364683367	49.246554438
20	1	45.282894677	41.495935011	50.503534050
21	6	44.438896220	41.846481050	48.551353955
22	7	43.682078253	42.986098139	48.783367645
23	1	43.378435945	43.334022237	49.694131476
24	6	43.381019891	43.551719142	47.592257451
25	1	42.787425997	44.453646141	47.461312027
26	7	43.913387783	42.844201074	46.606721732
27	6	44.580619931	41.786842027	47.184180627
28	1	45.098603276	41.052470739	46.573028519
29	26	43.636168941	43.164783558	44.534671206
30	8	45.192835044	44.332403664	44.534496619
31	8	46.488951843	42.583740673	43.066451386
32	6	46.873367115	46.427363464	40.929526200
33	8	47.634129834	46.307421477	41.796782828
34	8	46.176398619	46.589808317	40.008650501
35	6	45.909963336	41.536586926	43.406320041
36	8	48.712247827	39.172552781	41.472108223
37	6	46.486353276	40.198802762	42.943818993
38	6	46.446653706	39.931365831	41.427777463
39	6	47.581990126	38.995707613	40.956459306
40	8	47.341853851	38.133503691	40.060416964
41	8	44.877166506	41.504760380	44.183099351
42	1	46.000880247	39.375675373	43.488462595
43	1	47.552575163	40.227540400	43.217551493
44	1	45.475404423	39.531995523	41.102975061
45	1	46.604573479	40.889657182	40.901702600
46	6	41.027558529	45.183013292	38.128304302
47	1	42.039089693	45.216709553	37.698793259
48	1	40.736630805	46.210872056	38.380934743
49	7	41.122875517	44.401971300	39.406884845
50	1	40.177883343	44.065302712	39.683737718
51	6	41.950544803	43.165916976	39.255687670
52	6	41.674898073	45.240868722	40.511405957
53	1	42.964603419	43.462548722	38.954921912
54	1	41.490688652	42.526304166	38.490716183
55	1	41.965969013	42.634710941	40.215781811
56	1	41.680832838	44.661803611	41.443003030
57	1	41.031197676	46.122542383	40.629349077
58	1	42.690186714	45.542598287	40.213318809
59	8	44.593543381	45.578790328	42.578902061
60	1	44.168318505	46.445340399	42.716694477
61	1	44.973903420	45.159721841	43.596781024
62	8	43.372521411	43.521358079	42.902667112
63	1	43.857861754	44.555370307	42.605230889
64	1	45.850098138	43.751000304	44.034967923
65	1	38.896957281	40.463499397	47.329905897
66	1	44.207053480	40.214135134	50.014332602
67	1	40.029590759	46.734465427	45.321995447
68	1	40.263687042	44.802208178	37.450399342

IM7

QM(B1)/MM = -3195.472853 (a.u.)

QM(B2+ZPE)/MM = -3197.213638 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2941 (a.u.)

1	6	38.656023228	40.349328644	46.372741948
2	1	37.965667152	41.136526163	46.040418185
3	1	38.212925809	39.391583997	46.063013641
4	6	39.995865542	40.562500301	45.747785495
5	7	40.940974913	39.570766604	45.558965898

6	1	40.812085650	38.568258711	45.754279855
7	6	42.078494237	40.146150002	45.115212827
8	1	42.997883477	39.616210706	44.880748348
9	7	41.912111760	41.454003074	45.003063706
10	6	40.621651892	41.735518629	45.383340695
11	1	40.240507703	42.754436208	45.398668880
12	6	41.237370582	46.801568293	44.889560779
13	1	41.692083316	47.460195580	45.650593404
14	1	41.207498135	47.378922262	43.954003015
15	6	42.263652086	45.684474401	44.642034501
16	8	42.149317050	44.528219106	45.170976552
17	8	43.224456542	46.050057144	43.930559283
18	6	44.862748109	40.844035525	49.690724649
19	1	45.734572913	40.278775277	49.324307319
20	1	45.203993371	41.421813624	50.566950869
21	6	44.370185173	41.754671766	48.606283945
22	7	43.630225593	42.905566664	48.832148046
23	1	43.357392873	43.278213346	49.743439503
24	6	43.307862021	43.448813233	47.635381777
25	1	42.713602352	44.351295752	47.508926158
26	7	43.809786572	42.718297599	46.649859373
27	6	44.480100220	41.667652901	47.236860560
28	1	44.981986047	40.917448814	46.630398133
29	26	43.369542746	42.894805046	44.567055964
30	8	44.969876995	44.185808919	44.330453895
31	8	45.938646695	42.475576441	42.633009858
32	6	47.199178203	46.503423550	40.782293283
33	8	47.995255803	46.392549131	41.622858587
34	8	46.426732960	46.625451173	39.921590594
35	6	45.594474041	41.433396790	43.216569849
36	8	48.636026242	39.147939795	41.504652439
37	6	46.301515272	40.125574569	42.860425379
38	6	46.329318599	39.775761827	41.364807423
39	6	47.535643957	38.907428661	40.953387008
40	8	47.374159281	38.028443898	40.053865464
41	8	44.712102236	41.384971727	44.163990581
42	1	45.878552237	39.299465705	43.450385340
43	1	47.352640875	40.262450741	43.166642139
44	1	45.401190341	39.282936160	41.042008105
45	1	46.420667727	40.717399578	40.794777119
46	6	41.191484475	45.382329083	38.478211825
47	1	42.138449310	45.577199160	37.946511480
48	1	40.787964147	46.346863804	38.816835157
49	7	41.579253169	44.612120053	39.704696064
50	1	40.769097772	44.384114875	40.326112934
51	6	42.205637009	43.290965460	39.405157060
52	6	42.513592206	45.450840116	40.524531431
53	1	43.090595347	43.439998088	38.767961796
54	1	41.450221335	42.662700655	38.914061247
55	1	42.492620811	42.828146096	40.357943020
56	1	42.839646456	44.887409552	41.406394511
57	1	41.987953756	46.359907679	40.844794958
58	1	43.367757281	45.717850097	39.882682863
59	8	40.328689599	43.984494764	42.130365572
60	1	41.182532965	43.769320542	42.561530664
61	1	44.469325938	44.994482308	44.017419426
62	8	42.866562867	43.072185535	43.033188235
63	1	39.856814340	43.107067597	42.170827761
64	1	45.404997179	43.723923939	43.548240389
65	1	38.698507795	40.344560090	47.461888243
66	1	44.127612259	40.139134181	50.078998655

67	1	40.217706207	46.619339556	45.228890372
68	1	40.450011061	44.940776157	37.812392401

IM8
QM(B1)/MM = -3195.461430 (a.u.)
QM(B2+ZPE)/MM = -3197.208547 (a.u.)
QM(B2+D3+ZPE)/MM = -3197.2884 (a.u.)

1	6	38.661561296	40.306698876	46.370410726
2	1	37.967747189	41.087584295	46.030917766
3	1	38.218928943	39.344670190	46.073848133
4	6	39.996004546	40.517667822	45.736405766
5	7	40.951327207	39.534206997	45.562657862
6	1	40.837184304	38.535726571	45.783884628
7	6	42.070491294	40.109937800	45.078592571
8	1	42.991412200	39.575574862	44.860027746
9	7	41.879155009	41.412279221	44.924726639
10	6	40.592910255	41.683913258	45.321147229
11	1	40.181470599	42.689451967	45.284476404
12	6	41.359969187	46.778164699	44.898587802
13	1	41.787050931	47.476593454	45.637844932
14	1	41.364823600	47.307941845	43.933437282
15	6	42.397208121	45.651732956	44.742281215
16	8	42.132031766	44.453262694	45.145791271
17	8	43.474080288	45.979705775	44.238984887
18	6	44.862666039	40.877722652	49.626476022
19	1	45.729539252	40.315123124	49.244784473
20	1	45.217922522	41.454612215	50.497836753
21	6	44.354898301	41.792988188	48.552797011
22	7	43.596478679	42.929021472	48.795954063
23	1	43.318769221	43.284350601	49.712954295
24	6	43.270875865	43.489659362	47.610976879
25	1	42.662809072	44.384854776	47.505006357
26	7	43.790794396	42.788702012	46.610387073
27	6	44.475493896	41.736348919	47.182954639
28	1	44.998964191	41.009130683	46.567297974
29	26	43.261398554	42.929539526	44.542395331
30	8	45.187555342	45.350895811	41.968436487
31	8	45.556566053	42.571793401	42.156105960
32	6	47.108211528	46.472618036	40.722997210
33	8	47.845746027	46.508680756	41.621382817
34	8	46.498873985	46.502758681	39.729187022
35	6	45.454468129	41.703774625	43.009203054
36	8	48.534146953	39.229641047	41.595547527
37	6	46.183344399	40.364358728	42.838639268
38	6	46.211437990	39.826973723	41.398789535
39	6	47.444232122	38.971784812	41.032348414
40	8	47.302678288	38.085217664	40.135919699
41	8	44.800084214	41.852568832	44.148813111
42	1	45.772590679	39.624667329	43.541885028
43	1	47.231289075	40.546325945	43.139581824
44	1	45.304163729	39.254348873	41.156968465
45	1	46.232213150	40.694538327	40.715929143
46	6	41.220127537	45.380195609	38.305349600
47	1	42.182958414	45.503483383	37.782366212
48	1	40.865700163	46.380775324	38.587315442
49	7	41.540465419	44.649166715	39.574055436
50	1	40.697806214	44.427835489	40.144876516
51	6	42.193201709	43.326917381	39.338743426
52	6	42.421458267	45.518089633	40.420014760
53	1	43.111861086	43.471723735	38.750618954

54	1	41.474673886	42.681876832	38.815271687
55	1	42.432040674	42.886875097	40.314672281
56	1	42.786837456	44.963370210	41.288570122
57	1	41.848170744	46.400349532	40.734868365
58	1	43.280396113	45.818986352	39.804267161
59	8	40.286473028	44.049395872	42.050315527
60	1	41.145063210	43.846802590	42.473679885
61	1	45.246648110	44.379695589	42.071414518
62	8	42.830221974	43.182006615	42.998394710
63	1	39.793665851	43.187614841	42.148926856
64	1	44.713860862	45.647963097	42.763583281
65	1	38.706884153	40.317110867	47.459403269
66	1	44.137469667	40.170434015	50.028844421
67	1	40.329579685	46.608647625	45.211043811
68	1	40.456298385	44.941649315	37.663236300

ES1

QM(B1)/MM = -3045.298115 (a.u.)

QM(B2+ZPE)/MM = -3047.382065 (a.u.)

QM(B2+D3+ZPE)/MM = -3046.925 (a.u.)

1	6	38.833947146	40.461838331	46.362141331
2	1	38.174695546	41.267016965	46.014421961
3	1	38.379842273	39.520933321	46.030074194
4	6	40.186173646	40.653857085	45.763034145
5	7	41.129960126	39.657085775	45.596897879
6	1	40.996063709	38.657311082	45.801812735
7	6	42.253935170	40.218029762	45.109946741
8	1	43.164483535	39.665100228	44.892714495
9	7	42.090615910	41.526897875	44.946238054
10	6	40.798467606	41.806332118	45.336200607
11	1	40.378033012	42.806639401	45.267835007
12	6	41.108018538	46.771186407	44.973143706
13	1	41.711997812	47.206061651	45.781700005
14	1	41.159158561	47.418210440	44.083559687
15	6	41.622728758	45.380061167	44.554544960
16	8	42.572901106	44.885172635	45.254148970
17	8	41.109947220	44.848484951	43.556438964
18	6	44.927152859	40.814806420	49.889518528
19	1	45.789916979	40.232292052	49.528907940
20	1	45.256772446	41.336096562	50.804914676
21	6	44.515026188	41.795782260	48.833638849
22	7	43.798682058	42.958733626	49.077189476
23	1	43.479613270	43.294635452	49.990052558
24	6	43.563810324	43.570501701	47.892872986
25	1	43.002091124	44.496794137	47.775629618
26	7	44.101698513	42.878270067	46.897716910
27	6	44.700859707	41.776009822	47.470088109
28	1	45.204808277	41.026305464	46.862837652
29	26	43.483407238	43.078416766	44.836359648
30	6	45.054203802	42.888159352	42.348290257
31	8	45.300938971	43.028789333	41.155027713
32	8	44.373316887	43.673132014	43.105625584
33	6	45.616782079	41.633523620	43.078019698
34	8	48.767251166	39.411110203	41.281651939
35	6	46.765296585	40.895586650	42.438259517
36	6	46.396870250	39.673983891	41.570720779
37	6	47.637207708	38.986053738	40.956434524
38	8	47.439364232	38.017851500	40.162301317
39	8	45.127040860	41.339382282	44.161967166
40	1	47.445325032	40.572291868	43.238895260

41	1	47.305545137	41.605539795	41.800089165
42	1	45.851891996	38.913481724	42.154420747
43	1	45.725081971	39.972604328	40.750902213
44	6	41.045053658	45.256812526	38.430564626
45	1	41.984007554	45.621880559	37.977554573
46	1	40.548096414	46.094820173	38.939593240
47	7	41.440234364	44.269804525	39.487626969
48	1	40.595005897	43.784097901	39.847661547
49	6	42.338122624	43.202863433	38.956337514
50	6	42.106338724	44.957130004	40.637814828
51	1	43.250867244	43.650152572	38.530578608
52	1	41.793619777	42.643130204	38.183828325
53	1	42.603508337	42.527262373	39.778391880
54	1	42.255401329	44.243779265	41.455339617
55	1	41.449199261	45.757394486	40.995658920
56	1	43.073395589	45.351619789	40.296517797
57	8	45.479014418	45.578469223	39.751228164
58	1	45.439378333	45.983078338	40.647885542
59	1	45.473324953	44.628046494	39.967645895
60	8	45.260253019	46.364717371	42.371381562
61	1	44.759656750	47.176735997	42.605995566
62	1	44.756721832	45.603065376	42.717120116
63	1	38.825918553	40.442064258	47.451917385
64	1	44.151407005	40.122416217	50.216445899
65	1	40.083162500	46.736306223	45.342630915
66	1	40.342095140	44.883712667	37.685773959

ES-TS

QM(B1)/MM = -3045.296195 (a.u.)

QM(B2+ZPE)/MM = -3047.380859 (a.u.)

QM(B2+D3+ZPE)/MM = -3046.9215 (a.u.)

1	6	38.803945611	40.448841902	46.397724808
2	1	38.145849147	41.253850998	46.047952966
3	1	38.350506141	39.508436361	46.064834974
4	6	40.159949643	40.640618372	45.808700559
5	7	41.097400221	39.641661523	45.623995056
6	1	40.959093957	38.638771352	45.812065349
7	6	42.228836737	40.204122274	45.158019901
8	1	43.135790788	39.653379878	44.923532815
9	7	42.075214000	41.517941212	45.030643789
10	6	40.784437879	41.799162581	45.419468610
11	1	40.376541399	42.805979136	45.384632745
12	6	41.092663333	46.756365904	44.955244212
13	1	41.700741524	47.186672655	45.763023265
14	1	41.140846953	47.405428825	44.067320560
15	6	41.607706644	45.367710794	44.533155229
16	8	42.518583136	44.848699262	45.263514323
17	8	41.132375678	44.858160750	43.504116362
18	6	44.926253882	40.818594239	49.868463703
19	1	45.788683610	40.233511223	49.511179105
20	1	45.257652330	41.345561786	50.779943415
21	6	44.514915754	41.793478815	48.806743146
22	7	43.802199658	42.959496388	49.044403019
23	1	43.480510612	43.297291387	49.955191129
24	6	43.571514901	43.567007517	47.856164580
25	1	43.011190353	44.493557811	47.734334832
26	7	44.107307606	42.869034675	46.864491347
27	6	44.701394631	41.767918744	47.443063572
28	1	45.201051621	41.009117242	46.843160440
29	26	43.446455595	43.059622909	44.799959191

30	6	45.217372855	43.008296563	42.472140361
31	8	45.492485746	43.245920723	41.302101295
32	8	44.618987943	43.780326957	43.310935487
33	6	45.605583133	41.616794861	43.045587806
34	8	48.767954194	39.383298240	41.290302928
35	6	46.753497335	40.882714545	42.398235842
36	6	46.396332606	39.641609251	41.558436273
37	6	47.641454165	38.958551502	40.952118983
38	8	47.452524589	37.994171120	40.150718527
39	8	44.974500919	41.204844560	44.010648910
40	1	47.437150905	40.573817307	43.204043646
41	1	47.292921471	41.588939029	41.757315228
42	1	45.861397935	38.887779527	42.159448058
43	1	45.716851285	39.913032279	40.735215865
44	6	41.053833878	45.261232457	38.417399675
45	1	41.992362554	45.619622650	37.958189417
46	1	40.561288850	46.105110887	38.920794827
47	7	41.450198369	44.283400443	39.482857071
48	1	40.603634846	43.808569941	39.854286873
49	6	42.334486896	43.201807920	38.959078403
50	6	42.132534929	44.979385892	40.618782603
51	1	43.250677158	43.634593104	38.524595476
52	1	41.781814050	42.638347997	38.195223914
53	1	42.591590991	42.530523349	39.787887897
54	1	42.262363270	44.278186026	41.449986217
55	1	41.491413588	45.797400339	40.964906922
56	1	43.106385043	45.352519507	40.271055682
57	8	45.501918289	45.670410441	39.731383388
58	1	45.466296563	46.089455925	40.622625732
59	1	45.550132802	44.729823583	39.978482027
60	8	45.349090941	46.463147933	42.339656497
61	1	44.814265016	47.247270514	42.595276345
62	1	44.937614000	45.683576482	42.760724903
63	1	38.798695638	40.430408171	47.487541285
64	1	44.151948750	40.127838416	50.202193055
65	1	40.070589799	46.721903960	45.332398537
66	1	40.347087271	44.883601709	37.678500783

ES1'

QM(B1)/MM = -3045.296587 (a.u.)

QM(B2+ZPE)/MM = -3047.383852 (a.u.)

QM(B2+D3+ZPE)/MM = -3046.9215 (a.u.)

1	6	38.812103026	40.458141515	46.403517759
2	1	38.150326802	41.264933848	46.065014773
3	1	38.353858580	39.519942103	46.070877199
4	6	40.158524579	40.652416580	45.792286957
5	7	41.086024836	39.651624517	45.567140083
6	1	40.949495783	38.648133365	45.751674673
7	6	42.204105284	40.216594268	45.070008120
8	1	43.100180281	39.665471943	44.796109887
9	7	42.052424198	41.532605449	44.960775839
10	6	40.775502102	41.812639895	45.396132142
11	1	40.372429824	42.821794662	45.392986003
12	6	41.080719337	46.741849593	44.957939259
13	1	41.679930612	47.193677866	45.761295565
14	1	41.122501040	47.376609027	44.059771641
15	6	41.612327107	45.349985806	44.564872997
16	8	42.440047750	44.804995741	45.369303374
17	8	41.218826492	44.863323192	43.490142998
18	6	44.911202414	40.793468030	49.958933306

19	1	45.779747854	40.212045645	49.610542939
20	1	45.226550006	41.316164916	50.878335743
21	6	44.504561623	41.768856976	48.896070594
22	7	43.782596959	42.930012785	49.129019070
23	1	43.465422202	43.274973427	50.039395342
24	6	43.536371488	43.524847701	47.938476116
25	1	42.966660887	44.444833255	47.810182358
26	7	44.071760358	42.823029661	46.949085400
27	6	44.681306168	41.733376689	47.531643377
28	1	45.184586245	40.973793745	46.935810184
29	26	43.462431149	43.064116206	44.894501554
30	6	45.551543938	43.346897802	42.796219975
31	8	46.257608822	43.918901678	41.961904122
32	8	44.737508851	43.905158092	43.602489889
33	6	45.627153815	41.780867542	42.929555968
34	8	48.703620682	39.360099713	41.375074261
35	6	46.576907764	41.060139464	42.012121143
36	6	46.338564538	39.583195448	41.689356577
37	6	47.577440430	38.928664994	41.035342848
38	8	47.402584619	37.978202292	40.215336070
39	8	44.949770773	41.255657006	43.800093680
40	1	47.573673841	41.141190749	42.491010652
41	1	46.663479009	41.665210822	41.100103226
42	1	46.120781212	39.018964075	42.612657251
43	1	45.466096275	39.440341452	41.035287840
44	6	41.061425037	45.261521484	38.364357409
45	1	42.006939905	45.577509131	37.888507293
46	1	40.596642653	46.137426710	38.838109463
47	7	41.435000261	44.312935249	39.464569906
48	1	40.576726363	43.886830446	39.867077643
49	6	42.260777955	43.170303215	38.975823895
50	6	42.164852932	45.027984943	40.559670054
51	1	43.197498888	43.541224578	38.526005929
52	1	41.678672335	42.612804172	38.229710935
53	1	42.471465633	42.508282754	39.825665279
54	1	42.280814553	44.359317815	41.420416543
55	1	41.563174939	45.885495010	40.881252720
56	1	43.141252088	45.358288566	40.174694431
57	8	45.647183233	45.762432724	39.532535056
58	1	45.770521802	46.346270268	40.317119879
59	1	45.823589437	44.885963739	39.906553096
60	8	46.051220048	46.983245511	41.920581766
61	1	45.332485984	47.525545700	42.316542956
62	1	45.969395005	46.092672523	42.309478826
63	1	38.812568316	40.433123390	47.493215515
64	1	44.129745283	40.101099359	50.272011082
65	1	40.058495119	46.703456259	45.334304676
66	1	40.340844562	44.877292953	37.642415900

RC2

QM(B1)/MM = -3008.486083 (a.u.)

QM(B2+ZPE)/MM = -3010.028721 (a.u.)

QM(B2+D3+ZPE)/MM = -3010.1017 (a.u.)

1	6	41.971194215	43.370105515	45.319032393
2	1	41.532533348	44.074381859	44.599431404
3	1	41.339369947	42.470647636	45.305634747
4	6	43.374958425	43.067150244	44.913229062
5	7	44.060285075	41.912053652	45.225390245
6	1	43.704268862	41.135884673	45.794528092
7	6	45.322842189	42.016607984	44.767503247

8	1	46.093277939	41.261136695	44.900891035
9	7	45.478317528	43.181988459	44.161133235
10	6	44.283554529	43.850692349	44.245836045
11	1	44.154734218	44.842559383	43.823538720
12	6	46.743795822	48.262077582	42.772691183
13	1	47.059026704	49.122442646	43.378712700
14	1	47.126491019	48.431078978	41.751574211
15	6	47.456388615	46.993028342	43.255304628
16	8	46.829341521	45.869626286	42.960380288
17	8	48.553991544	47.051459231	43.779138203
18	6	47.734017956	43.859842110	49.041599819
19	1	48.516661846	43.087091082	49.076714725
20	1	48.046762631	44.670067380	49.721076943
21	6	47.584448552	44.350224147	47.635976488
22	7	46.893872818	45.500611401	47.301175541
23	1	46.455545259	46.168746346	47.943057331
24	6	46.850488825	45.604856144	45.965849671
25	1	46.333478530	46.407733714	45.454014777
26	7	47.496834680	44.592893604	45.400885159
27	6	47.967525476	43.803456067	46.431047951
28	1	48.536856446	42.899102499	46.232066701
29	26	47.222250908	44.015517870	43.421288550
30	8	46.856021828	43.600908009	41.891551319
31	8	49.798017844	43.030341225	41.935468708
32	6	49.284789437	42.220333235	42.705096965
33	8	50.874131134	38.439910251	40.681832676
34	6	49.591006991	40.729837207	42.613102522
35	6	49.283967312	40.142525069	41.222120927
36	6	49.717937509	38.663102847	41.131121739
37	8	48.903624408	37.791525603	41.527945657
38	8	48.452872916	42.566877572	43.654732558
39	1	49.023965771	40.186795175	43.381360237
40	1	50.666745464	40.601679986	42.825097940
41	1	48.200367117	40.213569126	41.028527299
42	1	49.817572404	40.726871983	40.457648417
43	6	45.576165042	44.795098830	36.739499917
44	1	45.250172023	43.860151906	36.258406581
45	1	46.659286665	44.900186801	36.588913725
46	7	45.336691424	44.636180356	38.206441906
47	1	45.802301007	45.414170816	38.739702360
48	6	43.889955687	44.625083954	38.586722388
49	6	46.034538000	43.403770163	38.699497711
50	1	43.417827350	45.602494256	38.396255282
51	1	43.819230000	44.377989850	39.655823502
52	1	43.386952349	43.839839247	38.003863351
53	1	47.072060530	43.429185711	38.329434208
54	1	45.499069643	42.515804231	38.338559102
55	1	46.023204669	43.403282791	39.794594409
56	8	44.319845854	41.187109639	40.355201585
57	1	43.425844242	40.760122719	40.435420009
58	1	44.920292377	40.546566536	40.758993963
59	8	46.789269193	46.252060118	40.029798588
60	1	47.691784214	45.822135613	40.027017989
61	1	46.515148493	46.034787507	40.945313520
62	1	45.058708265	45.619266566	36.248528074
63	1	45.655271918	48.222250422	42.732730898
64	1	41.901522363	43.788053252	46.323289752
65	1	46.819501105	43.451787834	49.471969389

TS6

QM(B1)/MM = -3008.453232 (a.u.)

QM(B2+ZPE)/MM = -3010.000582 (a.u.)

QM(B2+D3+ZPE)/MM = -3010.0762 (a.u.)

1	6	41.897838252	43.378869913	45.313550799
2	1	41.436509586	44.076200858	44.602071009
3	1	41.279430564	42.470349080	45.316549594
4	6	43.288658342	43.091025637	44.866424557
5	7	44.018884030	41.966684328	45.186035090
6	1	43.709575398	41.196122094	45.790637782
7	6	45.243447466	42.073470466	44.639859043
8	1	46.039314692	41.342132427	44.756322176
9	7	45.332819101	43.214011150	43.971546559
10	6	44.132559114	43.863631606	44.110366494
11	1	43.945056051	44.833848850	43.660693962
12	6	46.772308104	48.358263898	42.771639999
13	1	47.070594344	49.183746581	43.431178079
14	1	47.139086840	48.607934957	41.760868241
15	6	47.514049610	47.073452796	43.156056118
16	8	46.968225265	45.965978065	42.675879915
17	8	48.563623708	47.107774592	43.768354449
18	6	47.736761988	43.901024276	48.839950669
19	1	48.532573434	43.140460899	48.839343083
20	1	48.075648898	44.722536289	49.493323082
21	6	47.513865133	44.379620150	47.439359480
22	7	46.814189319	45.530912349	47.133007922
23	1	46.403068895	46.195301783	47.796107751
24	6	46.733834807	45.638328515	45.796451561
25	1	46.215450831	46.454441401	45.306784125
26	7	47.356954855	44.630968161	45.203298524
27	6	47.854137339	43.838243465	46.217443348
28	1	48.424458516	42.937266096	46.003367734
29	26	46.994742977	44.049247448	43.093973964
30	8	46.295806746	43.681772553	41.464883779
31	8	49.717234482	43.046408501	41.621266604
32	6	49.168613641	42.251755282	42.384431835
33	8	50.901810295	38.393209057	40.633615907
34	6	49.524835725	40.772096614	42.389136306
35	6	49.272997081	40.095723130	41.029173731
36	6	49.735527864	38.623499397	41.051026302
37	8	48.931021227	37.771426123	41.504517234
38	8	48.250918197	42.605552809	43.242176296
39	1	48.953056940	40.256185510	43.172570390
40	1	50.596849447	40.690059725	42.638369646
41	1	48.193531099	40.128481165	40.801879895
42	1	49.818951080	40.640607238	40.244506468
43	6	45.800341485	44.646879193	36.890554626
44	1	45.466990172	43.694047380	36.453114799
45	1	46.882505033	44.750527860	36.728837958
46	7	45.571089804	44.560578544	38.378041556
47	1	45.981979782	45.421716820	38.847868577
48	6	44.124172469	44.482067627	38.734875629
49	6	46.331737109	43.434146403	38.967960337
50	1	43.593572332	45.406459957	38.445652105
51	1	44.039874634	44.319118426	39.817021777
52	1	43.689076638	43.612669603	38.221505666
53	1	47.378038748	43.448221793	38.625141302
54	1	45.798147564	42.479227145	38.877691911
55	1	46.411449131	43.600290634	40.298926416
56	8	44.467256897	41.063903682	40.107707148
57	1	43.690434708	40.449873448	40.193482494
58	1	45.138685093	40.673818117	40.684573634

59	8	46.856633573	46.427928250	39.927681720
60	1	47.772524999	46.021127828	39.921447123
61	1	46.620538984	46.232458419	40.864781252
62	1	45.270404951	45.463832979	36.400839305
63	1	45.685002515	48.289732062	42.737916702
64	1	41.860966282	43.800862601	46.317856504
65	1	46.855196132	43.485476067	49.328037395

IM9

QM(B1)/MM = -3008.479307 (a.u.)

QM(B2+ZPE)/MM = -3010.019478 (a.u.)

QM(B2+D3+ZPE)/MM = -3010.0934 (a.u.)

1	6	42.033986160	43.370927582	45.265621088
2	1	41.608485450	44.069291179	44.531879171
3	1	41.410411860	42.466288486	45.239339342
4	6	43.445447227	43.069042068	44.891200964
5	7	44.135412337	41.931544509	45.250178691
6	1	43.771322493	41.161039855	45.822331499
7	6	45.397567546	42.025825866	44.793381941
8	1	46.164068350	41.274025404	44.966355003
9	7	45.554153057	43.167185869	44.140284070
10	6	44.350710953	43.828882542	44.193635249
11	1	44.205363161	44.802476376	43.733694006
12	6	46.813544225	48.401276393	42.777528694
13	1	47.096620398	49.265963554	43.391349908
14	1	47.177571303	48.596755596	41.754193358
15	6	47.563469505	47.150293989	43.243356759
16	8	47.056488738	46.012893549	42.805903384
17	8	48.589113107	47.235573776	43.895578164
18	6	47.726854150	43.881310402	49.025333630
19	1	48.510079104	43.108442357	49.041106637
20	1	48.047840893	44.681644932	49.712738613
21	6	47.571753531	44.392584659	47.627874715
22	7	46.901613279	45.557730909	47.306792329
23	1	46.459204160	46.218073365	47.953857696
24	6	46.890208557	45.692086139	45.971027199
25	1	46.408584975	46.525345474	45.471695801
26	7	47.529814874	44.686231353	45.391464942
27	6	47.966239173	43.869614077	46.415545577
28	1	48.533817397	42.962340514	46.218837322
29	26	47.212051302	44.114415446	43.285821920
30	8	46.467450588	43.632997635	41.609791237
31	8	49.486336308	42.922505236	41.115728878
32	6	49.234194292	42.363380958	42.174032877
33	8	50.886474087	38.414450131	40.745288399
34	6	49.460961163	40.863723374	42.343326754
35	6	49.193348111	40.067595867	41.055860627
36	6	49.703671303	38.614461510	41.133862814
37	8	48.918965151	37.739068299	41.577843330
38	8	48.776783696	42.997860489	43.238004808
39	1	48.851361434	40.492707796	43.180387973
40	1	50.517858524	40.736530891	42.643444471
41	1	48.108548578	40.059094809	40.854437287
42	1	49.698170019	40.577460491	40.222970541
43	6	45.710797101	44.833059164	36.687864304
44	1	45.479836526	43.908584436	36.139535003
45	1	46.783688950	45.044133718	36.579117225
46	7	45.450495934	44.541400938	38.142645947
47	1	45.788269788	45.357517179	38.734837189
48	6	44.004767613	44.324655964	38.459654124

49	6	46.263105508	43.400562211	38.550071201
50	1	43.425480845	45.242476796	38.254181187
51	1	43.923844431	44.058267465	39.522307584
52	1	43.642191666	43.485779884	37.848754625
53	1	47.325015394	43.465720833	38.288175284
54	1	45.750730705	42.525724801	38.956296392
55	1	47.076147811	43.809601493	40.874955770
56	8	44.566910964	41.132396231	40.159083004
57	1	43.805806461	40.497902348	40.209600185
58	1	45.218739577	40.785210753	40.783969399
59	8	46.592525584	46.382585724	39.934619482
60	1	47.528313371	46.014258832	39.887465710
61	1	46.404387753	46.177900472	40.875897467
62	1	45.125688642	45.641022228	36.248647848
63	1	45.727342261	48.316788742	42.744446284
64	1	41.944410311	43.790625218	46.267567885
65	1	46.818538590	43.466906015	49.462711237

RC3

QM(B1)/MM = -3007.544150 (a.u.)

QM(B2+ZPE)/MM = -3009.083005 (a.u.)

QM(B2+D3+ZPE)/MM = -3009.1581 (a.u.)

1	6	42.147435322	43.150545123	44.780324857
2	1	41.699121050	43.949230228	44.172940286
3	1	41.517382607	42.257540931	44.652040365
4	6	43.550677065	42.915252063	44.325566345
5	7	44.297321948	41.793065036	44.621657886
6	1	43.975123633	40.967178696	45.139981291
7	6	45.558174847	41.980463189	44.185011242
8	1	46.363442049	41.262961605	44.324802488
9	7	45.655738732	43.161399929	43.596994727
10	6	44.417150268	43.755033867	43.665140120
11	1	44.236790008	44.751923957	43.272702008
12	6	46.699929007	48.479279543	42.833745225
13	1	46.981393745	49.279120324	43.532332051
14	1	47.054287737	48.805936050	41.842433209
15	6	47.483587442	47.194883988	43.147217884
16	8	46.878905553	46.084884563	42.797176955
17	8	48.608884010	47.243637268	43.621619694
18	6	47.988518858	43.526850965	48.568897583
19	1	48.784956950	42.767663576	48.547129533
20	1	48.297749849	44.290685732	49.300990690
21	6	47.804660711	44.121521080	47.205815605
22	7	47.113742309	45.299278338	46.988966859
23	1	46.722198987	45.927214477	47.699469460
24	6	47.011800085	45.507861002	45.670289524
25	1	46.478674586	46.351447876	45.249415750
26	7	47.625180552	44.540066411	44.997654630
27	6	48.131208821	43.668871534	45.945123486
28	1	48.695148083	42.783999960	45.660045907
29	26	47.320420934	44.216192842	42.948014495
30	8	46.845328738	43.981063240	41.403045919
31	8	49.417925056	43.026178844	40.672028540
32	6	49.295505773	42.479828528	41.756784119
33	8	51.431906365	38.787562071	40.981637570
34	6	49.692516326	41.028123738	41.996186320
35	6	49.431364290	40.065708705	40.830570393
36	6	50.182643538	38.726936293	41.034514241
37	8	49.494601167	37.692428966	41.257626757
38	8	48.852515649	43.102981127	42.845993630

39	1	49.196000495	40.675036579	42.910873926
40	1	50.777895404	41.028894559	42.205645608
41	1	48.352420400	39.876144560	40.714623017
42	1	49.807712334	40.524808852	39.902024625
43	6	44.895599242	43.996348832	37.142283693
44	1	44.571009342	43.202709522	36.451584095
45	1	45.992962501	44.030315344	37.144893865
46	7	44.469540218	43.623109212	38.528831492
47	1	44.743418258	44.427487544	39.170331375
48	6	42.998853141	43.450838368	38.696748641
49	6	45.214559929	42.419588599	39.011868179
50	1	42.792862049	43.188840072	39.742822988
51	1	42.656760915	42.626006949	38.055025699
52	1	42.475907023	44.391011902	38.447694422
53	1	45.053070728	42.319664858	40.092600984
54	1	46.285824674	42.566647089	38.812210454
55	1	44.839937410	41.531748044	38.481088454
56	8	48.164826472	43.331492425	38.064651677
57	1	48.418638878	43.120986287	37.139784283
58	1	48.771832571	42.855528172	38.658876870
59	8	45.055118538	45.616907584	40.289171695
60	1	45.619638763	46.279191633	39.797834884
61	1	45.732299679	45.122988055	40.827819544
62	1	44.516932655	44.956268874	36.791238878
63	1	45.613874012	48.388702099	42.815101162
64	1	42.087756061	43.433394681	45.831277679
65	1	47.079830196	43.082112011	48.974556925

TS7

QM(B1)/MM = -3007.499752 (a.u.)

QM(B2+ZPE)/MM = -3009.045569 (a.u.)

QM(B2+D3+ZPE)/MM = -3009.1268 (a.u.)

1	6	42.030348664	43.227288916	44.808210937
2	1	41.566366608	44.039144290	44.232866789
3	1	41.382140021	42.345599851	44.697479730
4	6	43.397104006	42.977755410	44.266707912
5	7	44.167858321	41.862749054	44.528430047
6	1	43.894368655	41.047960566	45.091874745
7	6	45.376291520	42.023904809	43.959593323
8	1	46.193114789	41.311793552	44.051601869
9	7	45.415847397	43.182902888	43.316955233
10	6	44.193639340	43.789887232	43.494577344
11	1	43.966840416	44.771498615	43.088409818
12	6	46.604563531	48.553384932	42.835088658
13	1	46.953204431	49.297197601	43.563257577
14	1	46.916681284	48.923313173	41.843346066
15	6	47.356991707	47.230847435	43.025768456
16	8	46.744508476	46.163371567	42.530980971
17	8	48.463528117	47.196451660	43.532513543
18	6	47.956341426	43.620577622	48.293694976
19	1	48.775780942	42.888427454	48.230100010
20	1	48.287528627	44.411414442	48.986540863
21	6	47.662133105	44.181639018	46.934823655
22	7	46.930123942	45.339238455	46.744445615
23	1	46.574295280	45.966280003	47.475566729
24	6	46.739749675	45.523661854	45.432668995
25	1	46.163885625	46.348779410	45.032793587
26	7	47.336578393	44.559405109	44.737850271
27	6	47.920897663	43.713485351	45.664148862
28	1	48.490862609	42.839584262	45.359507525

29	26	47.069771881	44.251138321	42.649374754
30	8	46.590471413	44.021003147	40.996363213
31	8	49.478417482	43.096292051	40.596821425
32	6	49.221261819	42.530579738	41.642610440
33	8	51.405475443	38.834562224	40.947544346
34	6	49.637793218	41.088700102	41.929379820
35	6	49.398041496	40.106619742	40.774973264
36	6	50.158041913	38.769260212	41.005248797
37	8	49.467748094	37.742100871	41.242688406
38	8	48.598298761	43.124517741	42.660446624
39	1	49.135123553	40.745466277	42.844002670
40	1	50.721199639	41.114396203	42.143453052
41	1	48.323319551	39.901727899	40.649412192
42	1	49.782113660	40.550904101	39.842888458
43	6	45.266274109	43.788401218	37.651204381
44	1	45.066039037	42.977550275	36.921717890
45	1	46.334071574	44.030670030	37.564172266
46	7	45.049201183	43.235492819	39.012521654
47	1	45.929970596	43.913259770	40.194955691
48	6	43.682092361	43.289825713	39.535627473
49	6	45.666035860	41.912484635	39.158370477
50	1	43.654523449	42.878176990	40.555099381
51	1	43.002620280	42.685161922	38.902557447
52	1	43.333263529	44.330536060	39.552361497
53	1	45.663092513	41.618038189	40.216913404
54	1	46.703223834	41.966469292	38.798587665
55	1	45.106229006	41.160348178	38.568592458
56	8	48.437027407	43.170375252	37.969218836
57	1	48.601505877	43.023828259	37.010147626
58	1	49.178443008	42.794832758	38.469072474
59	8	44.771242445	46.332504506	40.427719744
60	1	45.360699233	46.659095701	39.697840429
61	1	45.434737977	46.157232454	41.125753982
62	1	44.669037453	44.643465561	37.334596315
63	1	45.516303866	48.503274022	42.870403243
64	1	42.027485768	43.497399695	45.864193557
65	1	47.096491633	43.152259477	48.772656114

IM10

QM(B1)/MM = -3007.558106 (a.u.)

QM(B2+ZPE)/MM = -3009.073818 (a.u.)

QM(B2+D3+ZPE)/MM = -3009.1488 (a.u.)

1	6	42.147074370	43.177521907	44.762145571
2	1	41.693415879	43.985599173	44.171411551
3	1	41.515299284	42.286981072	44.625047726
4	6	43.541017993	42.943748242	44.279617974
5	7	44.285944092	41.811358407	44.546367864
6	1	43.964924641	40.976594108	45.050391022
7	6	45.531624759	41.991114431	44.071666778
8	1	46.330528775	41.260618371	44.176775530
9	7	45.628926395	43.178759377	43.491315369
10	6	44.396067307	43.782073422	43.603884895
11	1	44.204457596	44.776705470	43.209006043
12	6	46.777236983	48.521528441	42.876696627
13	1	47.027941287	49.338361944	43.566631172
14	1	47.109599830	48.849865450	41.877714742
15	6	47.615635745	47.277250141	43.191944569
16	8	47.139433610	46.147041316	42.725508226
17	8	48.690668619	47.363315370	43.767934960
18	6	47.966256917	43.527142870	48.614860612

19	1	48.765314711	42.770621835	48.596395771
20	1	48.266832912	44.289264568	49.352235199
21	6	47.789405996	44.123027817	47.251922342
22	7	47.118053140	45.310476719	47.027641381
23	1	46.730873753	45.946097918	47.733310594
24	6	47.026151218	45.511226664	45.705167634
25	1	46.520196325	46.369231888	45.277695834
26	7	47.620174890	44.528991874	45.038855186
27	6	48.107523572	43.657817445	45.994034265
28	1	48.655369580	42.758567723	45.721461298
29	26	47.328125109	44.250725367	42.884509008
30	8	46.705816586	44.000189150	41.060433454
31	8	49.451653814	43.015619292	40.536476358
32	6	49.347244370	42.511855531	41.650531715
33	8	51.469066160	38.802798831	40.978777065
34	6	49.746455686	41.070345388	41.932128292
35	6	49.464094004	40.070270895	40.804110393
36	6	50.219320565	38.737266494	41.026891448
37	8	49.535102542	37.701036346	41.251167826
38	8	48.912740285	43.180241132	42.703711484
39	1	49.261528800	40.753849090	42.866253510
40	1	50.834315584	41.073995796	42.128362065
41	1	48.383343163	39.878259475	40.713418805
42	1	49.824208414	40.499005831	39.854613619
43	6	44.816709408	43.725632620	37.345818598
44	1	44.591932634	43.034809158	36.506941243
45	1	45.912190939	43.786552405	37.421790502
46	7	44.321863078	43.100795360	38.564941494
47	1	47.413211440	44.216698005	40.425619345
48	6	43.002975554	43.374547874	39.097371464
49	6	45.199886161	42.261429145	39.305222312
50	1	42.733487732	42.610600863	39.843752076
51	1	42.266794590	43.422172662	38.278774413
52	1	43.030590954	44.373863834	39.571756917
53	1	45.756682907	42.909589300	40.071392989
54	1	45.988842570	41.848872206	38.662280749
55	1	44.636565576	41.500271994	39.863007904
56	8	48.089754139	43.246913015	38.005960337
57	1	48.323432499	43.101944807	37.061076422
58	1	48.707897863	42.721343014	38.542324189
59	8	44.823776750	45.855896386	40.383433234
60	1	45.403604231	46.427099384	39.822020661
61	1	45.476262834	45.193945554	40.725237704
62	1	44.414556993	44.700423892	37.069915127
63	1	45.695694192	48.387644390	42.856508086
64	1	42.100195219	43.445699237	45.817584144
65	1	47.055037195	43.077278125	49.009027642

HAT-snapshot#1-RC = IM8 geometry

HAT-snapshot#1-TS

QM(B1)/MM = -3195.419177 (a.u.)

QM(B2+ZPE)/MM = -3197.169388 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2538 (a.u.)

1	6	38.620665917	40.301394144	46.362279388
2	1	37.918609334	41.079982754	46.034236511
3	1	38.168856097	39.337796394	46.085713334
4	6	39.935105055	40.504450530	45.686562497
5	7	40.889315434	39.520803265	45.498891019
6	1	40.789984498	38.527011011	45.747807382

7	6	41.980131585	40.085522477	44.947858739
8	1	42.896540324	39.553266385	44.707649813
9	7	41.772603932	41.382674479	44.762647003
10	6	40.505186531	41.661220408	45.215525058
11	1	40.084995750	42.662544764	45.165744503
12	6	41.314366094	46.800687208	44.810669400
13	1	41.774546769	47.457283882	45.568188425
14	1	41.308206064	47.374115724	43.870098883
15	6	42.312765657	45.651491423	44.583038832
16	8	41.993507424	44.438856166	44.876442777
17	8	43.408659835	45.973492885	44.108978489
18	6	44.862394793	40.950587438	49.451720733
19	1	45.727444075	40.389003385	49.063898740
20	1	45.233045678	41.556816234	50.296861796
21	6	44.320879549	41.830871707	48.364483455
22	7	43.533444958	42.947844286	48.595536530
23	1	43.239462887	43.297763355	49.506941623
24	6	43.202341077	43.492157380	47.401869452
25	1	42.572746396	44.371936231	47.293345321
26	7	43.742616331	42.802711260	46.407246876
27	6	44.448691238	41.771946879	46.993483964
28	1	44.996126208	41.052625872	46.388310199
29	26	43.096081931	42.873873355	44.225660712
30	8	45.196217069	45.290338048	41.833849573
31	8	45.501342692	42.511488245	41.857691955
32	6	47.204335887	46.451082157	40.773752351
33	8	47.896405313	46.457554990	41.707790418
34	8	46.641207399	46.514237319	39.754282295
35	6	45.400385150	41.672614594	42.745973267
36	8	48.565436293	39.219455465	41.504220127
37	6	46.181395603	40.357576633	42.655517417
38	6	46.230802147	39.741370830	41.251195386
39	6	47.493342126	38.915777052	40.932357626
40	8	47.389815461	37.999615147	40.059768388
41	8	44.695420156	41.842473813	43.842418970
42	1	45.798542298	39.644620089	43.401108100
43	1	47.221432990	40.594596256	42.945258334
44	1	45.347529127	39.118782869	41.048406213
45	1	46.216181583	40.567039043	40.518040553
46	6	41.306224358	45.281692572	38.593521077
47	1	42.314687396	45.269564057	38.149305035
48	1	41.011021967	46.335146799	38.693704448
49	7	41.486414630	44.759979987	40.003034221
50	1	40.583231460	44.564223358	40.491942082
51	6	42.220830571	43.477026662	40.076971464
52	6	42.214955212	45.812072022	40.790871955
53	1	43.224284142	43.561728355	39.639946613
54	1	41.584102523	42.642134181	39.757917658
55	1	42.480087497	43.214512656	41.377680670
56	1	42.432562496	45.431056026	41.790050831
57	1	41.590455555	46.714688629	40.828503712
58	1	43.166236260	46.011140459	40.278574153
59	8	39.977617780	44.114298382	42.243722139
60	1	40.857509034	43.870916689	42.603991270
61	1	45.230485920	44.312559141	41.892963778
62	8	42.547649250	43.146535415	42.558067601
63	1	39.497929039	43.241290485	42.281020948
64	1	44.731250415	45.574216379	42.639147785
65	1	38.695845425	40.321895275	47.449475354
66	1	44.162992743	40.243607856	49.897908988
67	1	40.289571822	46.637317343	45.144097528

68 1 40.552175132 44.810307098 37.963225258

HAT-snapshot#1-IM

QM(B1)/MM = -3195.455879 (a.u.)

QM(B2+ZPE)/MM = -3197.725527 (a.u.)

QM(B2+D3+ZPE)/MM = -3197.2807 (a.u.)

1	6	38.541577160	40.294965572	46.423101878
2	1	37.842565913	41.082854895	46.116648645
3	1	38.075099530	39.338031222	46.149138953
4	6	39.844866338	40.492108878	45.726575589
5	7	40.800082592	39.507499326	45.548555722
6	1	40.694317041	38.511356715	45.784695518
7	6	41.902650309	40.071354523	45.023668137
8	1	42.822181332	39.537347135	44.799429352
9	7	41.702409686	41.370651096	44.842546037
10	6	40.422487377	41.649150716	45.264866159
11	1	40.011182429	42.655282309	45.229984181
12	6	41.247201516	46.787237565	44.841210018
13	1	41.709137783	47.465228235	45.579258983
14	1	41.225601659	47.336277027	43.886984013
15	6	42.256965112	45.646144632	44.634299046
16	8	41.990150011	44.450930975	45.040240688
17	8	43.320089153	45.965874870	44.092617826
18	6	44.854015478	40.891598246	49.559472186
19	1	45.717695074	40.326937440	49.173276148
20	1	45.218792389	41.479465988	50.419520262
21	6	44.331821770	41.794049268	48.481978358
22	7	43.576563130	42.931658495	48.723638145
23	1	43.302819845	43.289167633	49.639973704
24	6	43.243797960	43.485067971	47.535525946
25	1	42.634978032	44.380500949	47.430658842
26	7	43.753947614	42.779572038	46.534237319
27	6	44.440214961	41.730164773	47.110522180
28	1	44.958534578	40.995708800	46.497896918
29	26	43.051407110	42.864274498	44.407238974
30	8	45.315640504	45.047419073	42.160437599
31	8	44.852548921	42.137524901	41.707631877
32	6	47.030098214	46.448909218	40.693837733
33	8	47.801094596	46.528709078	41.558977108
34	8	46.352299883	46.427867516	39.745768854
35	6	45.127914240	41.482317163	42.722335020
36	8	48.560840045	39.294256521	41.477396127
37	6	46.131892146	40.33332991	42.636563505
38	6	46.185297015	39.631792267	41.275435953
39	6	47.499109481	38.898927185	40.946569501
40	8	47.438087258	37.951209505	40.101219573
41	8	44.624068796	41.734052496	43.900273448
42	1	45.930836261	39.627031470	43.455586141
43	1	47.129762160	40.762778570	42.841735119
44	1	45.356114388	38.920344703	41.151429096
45	1	46.053676944	40.397825458	40.491539590
46	6	41.211346635	45.553811389	38.148501119
47	1	42.179389399	45.668803579	37.632701624
48	1	40.873214597	46.550479716	38.462104273
49	7	41.518188634	44.779747959	39.411826217
50	1	40.684553028	44.619615119	40.029523130
51	6	42.039161307	43.448107602	39.148077894
52	6	42.478680256	45.587952312	40.247254972
53	1	43.055048130	43.377055761	38.745851612
54	1	41.293729034	42.650104379	39.105747530

55	1	43.239163045	42.851819745	42.027468252
56	1	42.762419413	45.020105377	41.138478293
57	1	41.977260306	46.521775322	40.534260016
58	1	43.358337323	45.805735262	39.625726869
59	8	40.210102480	44.155147484	41.725486751
60	1	41.077006751	43.850843948	42.109760394
61	1	45.088152618	44.121748340	41.969904144
62	8	42.590119132	43.267123649	42.641468307
63	1	39.589042365	43.417316344	41.957792653
64	1	44.651875854	45.343219804	42.810795649
65	1	38.642565426	40.310569464	47.508286293
66	1	44.137270681	40.186596384	49.980561950
67	1	40.227272112	46.622681485	45.188676028
68	1	40.448307883	45.132706538	37.493894458

HAT-snapshot#2-RC

QM(B1)/MM = -3007.284108 (a.u.)

QM(B2+ZPE)/MM = -3008.821440 (a.u.)

QM(B2+D3+ZPE)/MM = -3008.8971 (a.u.)

1	6	42.072920514	43.580379668	45.504293368
2	1	41.621923287	44.317858100	44.824979099
3	1	41.404222936	42.711016554	45.522814307
4	6	43.442095566	43.226036988	45.020519845
5	7	44.140822889	42.105949636	45.417038131
6	1	43.775414012	41.333802933	45.991096294
7	6	45.404128206	42.195317354	44.967399927
8	1	46.182627094	41.468401828	45.185568324
9	7	45.550046483	43.312470842	44.268261799
10	6	44.337823381	43.961234238	44.277879823
11	1	44.196721855	44.920103604	43.788891384
12	6	46.843869315	48.365368282	42.727470992
13	1	47.230899157	49.240229611	43.266109666
14	1	47.157720531	48.485303522	41.675876379
15	6	47.554016256	47.100258290	43.237781670
16	8	46.812633633	46.006837005	43.184835428
17	8	48.713262413	47.124055926	43.591652514
18	6	48.098160924	43.875685841	49.062557704
19	1	48.798133818	43.025609190	49.071534233
20	1	48.530252261	44.657223682	49.709781009
21	6	47.922305354	44.379365663	47.662887156
22	7	47.371785651	45.616388445	47.369869617
23	1	47.071232341	46.334602185	48.037088567
24	6	47.240844413	45.726245753	46.039287170
25	1	46.791870168	46.585729927	45.557667307
26	7	47.707893872	44.640594621	45.435353876
27	6	48.143187107	43.792505586	46.436031054
28	1	48.570533905	42.818646142	46.208521673
29	26	47.250185635	44.173132314	43.447351434
30	8	46.686959307	43.828744215	41.942157053
31	8	49.305593077	42.911045088	41.285708230
32	6	49.100088288	42.291220639	42.320723170
33	8	50.857809191	38.273108317	40.689849949
34	6	49.467718487	40.812161200	42.428022425
35	6	49.302255630	40.054422635	41.102789097
36	6	49.760040613	38.589789663	41.220229796
37	8	49.000001677	37.810102989	41.847828499
38	8	48.579853669	42.807443751	43.412305311
39	1	48.869910436	40.337560245	43.219725195
40	1	50.522602074	40.764639871	42.757338804
41	1	48.233643079	40.058982047	40.826123605

42	1	49.860238283	40.565732494	40.307150984
43	6	45.288353770	43.938181531	37.172642989
44	1	45.058065357	43.058168312	36.551961315
45	1	46.367189370	44.148726759	37.085408569
46	7	45.011545263	43.563342859	38.597263842
47	1	45.094677792	44.412099483	39.233513995
48	6	43.640743800	43.037605252	38.839062162
49	6	46.043680590	42.601033645	39.086750538
50	1	43.525151581	42.070076911	38.327997978
51	1	42.906114442	43.760565992	38.456335484
52	1	43.478018759	42.889482290	39.916506195
53	1	45.754027897	42.240121929	40.082271222
54	1	47.004996448	43.122307235	39.139737643
55	1	46.093833766	41.754768266	38.389582510
56	8	48.776506137	44.846942807	39.389319557
57	1	48.945740393	44.200847427	40.110967526
58	1	48.755788377	44.344907186	38.543027164
59	8	45.187493857	45.527880687	40.469397522
60	1	45.762414669	45.040543700	41.118816569
61	1	45.828626665	46.106368943	39.972248245
62	1	44.730467915	44.790623959	36.785121891
63	1	45.755102746	48.363794467	42.778970543
64	1	42.088832434	43.977785093	46.519124911
65	1	47.169027774	43.578984682	49.549124585

HAT-snapshot#2-TS

QM(B1)/MM = -3007.248447 (a.u.)

QM(B2+ZPE)/MM = -3008.787288 (a.u.)

QM(B2+D3+ZPE)/MM = -3008.8651 (a.u.)

1	6	42.002263402	43.493754945	45.508806779
2	1	41.516212374	44.214029349	44.835445896
3	1	41.352389782	42.610635948	45.552915195
4	6	43.359794523	43.158068362	44.983255363
5	7	44.099573750	42.066419127	45.384682440
6	1	43.776826090	41.307466263	46.001186159
7	6	45.335253993	42.159238271	44.869051938
8	1	46.136396439	41.453789080	45.075073214
9	7	45.427447434	43.253530419	44.122763715
10	6	44.204028407	43.881742364	44.172877547
11	1	44.010793672	44.814196578	43.652428076
12	6	46.864223557	48.297532082	42.643015044
13	1	47.244987056	49.168781411	43.190995781
14	1	47.147101590	48.433249086	41.584664033
15	6	47.592255789	47.037010221	43.125070244
16	8	46.982110717	45.900827403	42.803357994
17	8	48.661032550	47.097601656	43.689216738
18	6	48.067536976	43.889108469	48.974320742
19	1	48.782429171	43.051330337	48.976709295
20	1	48.502330943	44.687136961	49.599400588
21	6	47.847510732	44.365820032	47.571316801
22	7	47.279362505	45.590856394	47.264731236
23	1	46.993097844	46.319676249	47.925981829
24	6	47.126728504	45.668755625	45.931181354
25	1	46.682476943	46.527458775	45.442512094
26	7	47.587687862	44.576169280	45.339430059
27	6	48.047365639	43.756499487	46.351523766
28	1	48.483297940	42.781728742	46.142918099
29	26	47.122448359	44.060357583	43.246455837
30	8	46.293643094	43.537113416	41.633052678
31	8	49.303465753	42.849657304	41.085080683

32	6	49.103526861	42.248837986	42.137585127
33	8	50.909169753	38.200878120	40.672559104
34	6	49.505888020	40.787502165	42.288197142
35	6	49.345016480	39.987503187	40.990118693
36	6	49.801651297	38.531809411	41.171764806
37	8	49.032798168	37.779347753	41.821284973
38	8	48.545179462	42.777933938	43.194343409
39	1	48.918826406	40.326450734	43.095335981
40	1	50.562266253	40.770167027	42.615490588
41	1	48.275836662	39.981535554	40.716619640
42	1	49.905320771	40.468214298	40.177075787
43	6	45.526828286	43.789366527	37.189453505
44	1	45.323217052	42.878472122	36.607975991
45	1	46.582857982	44.068701851	37.048096821
46	7	45.324413342	43.467003373	38.649280928
47	1	45.195751456	44.381368647	39.194297966
48	6	44.077045706	42.694088660	38.931287078
49	6	46.508967782	42.822619930	39.254971048
50	1	44.084281744	41.762852655	38.346692250
51	1	43.208427462	43.309441715	38.658801240
52	1	44.047508572	42.440906600	40.003225699
53	1	46.525441171	43.114746732	40.540862137
54	1	47.435035900	43.288674445	38.911886805
55	1	46.479419895	41.728186000	39.189702961
56	8	48.957319029	44.987124104	39.418603036
57	1	49.117121906	44.301578602	40.106752438
58	1	48.974533451	44.513782119	38.552627857
59	8	45.041360882	45.518098597	40.350275326
60	1	45.534360352	44.946339487	41.006808939
61	1	45.745732520	46.104146382	39.960692559
62	1	44.903671772	44.608044875	36.829579865
63	1	45.776798088	48.275921039	42.714472229
64	1	42.042473475	43.904187719	46.517764370
65	1	47.157298676	43.581256916	49.488870040

HAT-snapshot#2-IM

QM(B1)/MM = -3007.276591 (a.u.)

QM(B2+ZPE)/MM = -3008.810566 (a.u.)

QM(B2+D3+ZPE)/MM = -3008.8857 (a.u.)

1	6	42.047241981	43.507051904	45.504221252
2	1	41.577632913	44.226847408	44.818661024
3	1	41.399453637	42.621899951	45.529928709
4	6	43.421695265	43.176933208	45.019505338
5	7	44.140185272	42.070810970	45.419734971
6	1	43.790354909	41.300729477	46.007095095
7	6	45.397042168	42.172336509	44.957228907
8	1	46.185178792	41.456682267	45.179264071
9	7	45.525456526	43.286441015	44.244862914
10	6	44.302179002	43.917548852	44.264373034
11	1	44.135557300	44.865525093	43.762781075
12	6	46.907102080	48.400396583	42.738648623
13	1	47.236074775	49.319975268	43.239163590
14	1	47.217248008	48.481132224	41.682150130
15	6	47.664776986	47.203083849	43.325917199
16	8	47.091768753	46.030734326	43.097165807
17	8	48.728393432	47.335577867	43.890002430
18	6	48.052759923	43.861212912	49.183369569
19	1	48.753648548	43.012242559	49.210448341
20	1	48.465606952	44.643921780	49.840851689
21	6	47.905914004	44.361440720	47.780087873

22	7	47.394418525	45.610111170	47.468533244
23	1	47.104334945	46.343767530	48.123792386
24	6	47.284300242	45.707140703	46.133822103
25	1	46.891181941	46.586420736	45.638266437
26	7	47.718821498	44.600539856	45.545764751
27	6	48.116260992	43.754146358	46.562002148
28	1	48.514891336	42.762362347	46.359054730
29	26	47.242439089	44.178030389	43.462259532
30	8	46.496023562	43.772102479	41.683120662
31	8	49.055023511	42.829404326	41.058775097
32	6	49.042607494	42.270048617	42.161043078
33	8	50.910390311	38.221514636	40.674057151
34	6	49.489848520	40.822155369	42.297261017
35	6	49.351498648	40.014082490	41.002026462
36	6	49.810931357	38.558158151	41.188545975
37	8	49.048930014	37.808200767	41.848505608
38	8	48.640183040	42.843305431	43.258699068
39	1	48.914967476	40.346818089	43.106199916
40	1	50.542735908	40.834639697	42.636441541
41	1	48.287439905	40.002435928	40.711973601
42	1	49.917123514	40.490768584	40.190379684
43	6	45.342853375	43.822477359	37.124942597
44	1	45.111715479	42.945891659	36.501428444
45	1	46.413351851	44.058403855	37.009027633
46	7	45.115923100	43.429581546	38.557634387
47	1	45.147756027	44.319902947	39.198151053
48	6	43.769103320	42.856462011	38.846289231
49	6	46.157143251	42.530379513	39.013663142
50	1	43.634440362	41.927690538	38.272936234
51	1	43.001545156	43.595990243	38.581140144
52	1	43.719268925	42.625192121	39.920211087
53	1	47.291236804	43.657802030	41.130054606
54	1	47.178893871	42.835866093	38.793596766
55	1	45.889600643	41.861110345	39.833802369
56	8	48.836951377	44.867350178	39.219894465
57	1	49.053757561	44.168948162	39.871296387
58	1	48.775012635	44.429589341	38.333948069
59	8	45.096001804	45.419423963	40.303245931
60	1	45.659497870	44.869672462	40.959179303
61	1	45.749667413	46.038594477	39.879019676
62	1	44.763500487	44.675977777	36.772870744
63	1	45.819476270	48.339834617	42.776984858
64	1	42.058901185	43.916063483	46.514488995
65	1	47.108851891	43.562701057	49.639434938

HAT-snapshot#3-RC = RC2

HAT-snapshot#3-TS = TS6

HAT-snapshot#3-IM = IM9

HAT-snapshot#4-RC

QM(B1)/MM = -3007.981695 (a.u.)

QM(B2+ZPE)/MM = -3009.521771 (a.u.)

QM(B2+D3+ZPE)/MM = -3009.5933 (a.u.)

1	6	50.137418728	46.288608152	42.724442823
2	1	49.351013207	45.703362060	42.229030427
3	1	51.096014556	45.852828581	42.410972540
4	6	50.030792904	47.713823520	42.292128972
5	7	51.039541623	48.641938199	42.430003119
6	1	51.995154993	48.442970575	42.746177815

7	6	50.558561674	49.856535746	42.108376696
8	1	51.138489460	50.774470780	42.136414857
9	7	49.286552237	49.756923590	41.756823416
10	6	48.944561322	48.431061515	41.846461401
11	1	47.948335556	48.074465340	41.605247298
12	6	44.034074322	50.028046273	41.278057391
13	1	43.435907431	50.200634903	42.187867962
14	1	43.388532504	50.185840658	40.405596077
15	6	45.125587109	51.078571419	41.165197489
16	8	46.108904384	51.015387973	42.008584901
17	8	45.011718754	51.940224833	40.291381946
18	6	50.064138823	51.798182288	46.843456139
19	1	50.712840406	52.670426491	46.666503161
20	1	49.483802348	52.010755064	47.756497807
21	6	49.149021097	51.611182695	45.672779859
22	7	47.922047258	50.973668533	45.750832090
23	1	47.518992422	50.548210362	46.590324493
24	6	47.362228832	50.966959613	44.521876388
25	1	46.389530255	50.538748568	44.290141823
26	7	48.158096317	51.572027976	43.646623176
27	6	49.267529395	51.986791219	44.352484009
28	1	50.073841410	52.531302871	43.867943115
29	26	47.946365927	51.328976395	41.516919423
30	8	47.672107869	50.910916149	39.977969916
31	8	48.655305645	53.487568399	39.146776605
32	6	49.518653014	53.156769583	39.952673645
33	8	53.558889316	54.365017273	38.572016515
34	6	50.992490749	53.351469498	39.613526158
35	6	51.237295706	54.792011411	39.176300478
36	6	52.651779200	55.223884892	38.743508812
37	8	52.753210551	56.464283370	38.597265160
38	8	49.264438804	52.664011106	41.143365636
39	1	51.239981360	52.668189728	38.782693990
40	1	51.624589337	53.067751862	40.465948710
41	1	50.563645072	55.017380074	38.332735946
42	1	50.942424125	55.485212117	39.983120662
43	6	46.698864398	48.559634489	35.494518409
44	1	47.587882150	48.289721548	34.903429512
45	1	46.363338960	49.571339451	35.204791923
46	7	47.105754532	48.651112037	36.935471000
47	1	46.294388212	49.147912624	37.420634022
48	6	47.362365936	47.343107128	37.598674723
49	6	48.298880976	49.543436390	37.115764055
50	1	46.477969823	46.697812886	37.485563832
51	1	47.555333071	47.516436448	38.665769800
52	1	48.252749690	46.885033764	37.141677494
53	1	48.085201494	50.538912767	36.696461936
54	1	49.169427706	49.063150002	36.648436566
55	1	48.462156410	49.675223751	38.193273541
56	8	45.048379588	50.006927984	38.059402482
57	1	45.312683890	50.753216106	38.632001148
58	1	44.356725354	50.413975601	37.459395837
59	8	50.413787235	47.220276140	36.365347889
60	1	50.710337890	46.915769977	37.262891375
61	1	51.010554272	46.742547863	35.756929633
62	1	45.884240373	47.865255263	35.288866991
63	1	44.362724499	48.988996870	41.298859222
64	1	50.063714169	46.170946834	43.805549096
65	1	50.692180342	50.944812593	47.099173424

HAT-snapshot#4-TS

QM(B1)/MM = -3007.944322 (a.u.)
 QM(B2+ZPE)/MM = -3009.487529 (a.u.)
 QM(B2+D3+ZPE)/MM = -3009.561 (a.u.)

1	6	50.196042761	46.209340152	42.757220459
2	1	49.412927321	45.623812828	42.257001376
3	1	51.155805585	45.765729319	42.459681740
4	6	50.102881948	47.628287934	42.307332615
5	7	51.099730862	48.563447820	42.475976615
6	1	52.046676859	48.371842163	42.820222952
7	6	50.628406869	49.770699048	42.121754303
8	1	51.204091897	50.690850509	42.164872162
9	7	49.373719970	49.659089867	41.719145208
10	6	49.033757920	48.333241450	41.810181766
11	1	48.050407577	47.967043020	41.533047449
12	6	44.051359876	50.012773953	41.217327089
13	1	43.489977603	50.208820741	42.145850923
14	1	43.371037577	50.148222664	40.367600182
15	6	45.140555983	51.057390359	41.040299821
16	8	46.130701783	51.042260599	41.864306909
17	8	45.009868205	51.881217252	40.124784867
18	6	50.047340748	51.763445246	46.820833060
19	1	50.684495656	52.643098206	46.637730720
20	1	49.456579247	51.980238693	47.726286099
21	6	49.146402992	51.548666991	45.643628701
22	7	47.919068567	50.913277968	45.714694264
23	1	47.504846789	50.502137081	46.555412214
24	6	47.379541908	50.889221210	44.472902330
25	1	46.405412398	50.464466836	44.239094713
26	7	48.186636502	51.475713716	43.599209699
27	6	49.282774414	51.899730825	44.317696373
28	1	50.099785885	52.438043504	43.842861600
29	26	48.000895669	51.169023940	41.332320793
30	8	47.673480756	50.434660520	39.748638958
31	8	48.658794564	53.469424102	38.957523988
32	6	49.514044526	53.112563518	39.763291416
33	8	53.578068462	54.370445875	38.551662363
34	6	50.992664843	53.328392639	39.467370979
35	6	51.241918572	54.785749355	39.095312641
36	6	52.668197533	55.227902961	38.715767388
37	8	52.775585732	56.471143989	38.604514978
38	8	49.236678202	52.571692404	40.922467658
39	1	51.269517086	52.679903130	38.618229442
40	1	51.601864281	53.016562176	40.326698135
41	1	50.589814644	55.047986877	38.245946051
42	1	50.928440034	55.444219682	39.924080039
43	6	46.682266759	48.640259215	35.658216449
44	1	47.626962572	48.351173981	35.173660140
45	1	46.356054327	49.630514888	35.294492325
46	7	46.943450959	48.801480906	37.136945993
47	1	46.062982679	49.314161420	37.511385893
48	6	47.139957109	47.527172701	37.883176483
49	6	48.077780239	49.710052218	37.396066428
50	1	46.249419767	46.893293279	37.757546904
51	1	47.283236871	47.770768040	38.943695925
52	1	48.035104485	47.022800812	37.491002748
53	1	47.960070385	50.688619556	36.905177942
54	1	49.043785538	49.202103020	37.264893829
55	1	47.994045586	50.104019759	38.683119728
56	8	44.814330830	50.111775909	37.982134830
57	1	44.986148825	50.842387087	38.616859291

58	1	44.144484393	50.496566485	37.342055719
59	8	50.165301553	47.341792324	36.582285669
60	1	50.535099606	46.964722969	37.426275453
61	1	50.826078675	47.075362528	35.921329219
62	1	45.894047922	47.926604734	35.418475607
63	1	44.379961612	48.974128921	41.253447913
64	1	50.107010436	46.108063569	43.838832043
65	1	50.685984428	50.922986868	47.092552189

HAT-snapshot#4-IM

QM(B1)/MM = -3007.962539 (a.u.)
 QM(B2+ZPE)/MM = -3009.501116 (a.u.)
 QM(B2+D3+ZPE)/MM = -3009.5733 (a.u.)

1	6	50.207054813	46.269024006	42.742330522
2	1	49.421135506	45.696974330	42.230656954
3	1	51.164737684	45.824991302	42.437851130
4	6	50.119186799	47.698397749	42.320620684
5	7	51.123084433	48.625387720	42.499513583
6	1	52.070558115	48.420375807	42.833574767
7	6	50.657030690	49.841066175	42.166735009
8	1	51.241302419	50.755238775	42.222155689
9	7	49.399291482	49.746320667	41.766387168
10	6	49.052920900	48.418729907	41.839239307
11	1	48.067007952	48.067664677	41.552068154
12	6	44.037236363	50.108474071	41.260115525
13	1	43.461430115	50.266895827	42.186584797
14	1	43.362372505	50.239256884	40.405404731
15	6	45.092490147	51.192749480	41.110756649
16	8	46.040709767	51.241807344	41.987028066
17	8	44.975081157	51.986251718	40.169637783
18	6	50.061571895	51.720371779	46.922171265
19	1	50.693267526	52.603772711	46.738682023
20	1	49.488476226	51.922514800	47.841947746
21	6	49.138365870	51.518606993	45.759909427
22	7	47.899717555	50.906545024	45.847332292
23	1	47.489588571	50.501102947	46.694298128
24	6	47.341625887	50.893249821	44.614651743
25	1	46.352249977	50.496661424	44.393699783
26	7	48.150802772	51.462407686	43.730716580
27	6	49.265412257	51.865111668	44.433021140
28	1	50.087049372	52.386515632	43.948119617
29	26	47.934303152	51.247154622	41.501004021
30	8	47.486954375	50.332569798	39.910482004
31	8	48.606770042	53.450984016	39.001749992
32	6	49.463409333	53.115392267	39.815175250
33	8	53.531699575	54.349224772	38.554316658
34	6	50.942494336	53.318465243	39.506133408
35	6	51.197222563	54.770610700	39.112658024
36	6	52.622033999	55.207253660	38.715669241
37	8	52.727743388	56.449122209	38.587939188
38	8	49.185533549	52.604975648	40.988138555
39	1	51.210465864	52.658364769	38.662953328
40	1	51.556765038	53.014673347	40.365115229
41	1	50.539006823	55.023001350	38.264697171
42	1	50.892399592	55.441449180	39.934619265
43	6	46.600320265	48.549917086	35.491151117
44	1	47.489554974	48.233445008	34.924633655
45	1	46.281429513	49.548510020	35.143936466
46	7	47.008550010	48.732116448	36.933642365
47	1	46.198680924	49.301944130	37.387360383

48	6	47.204790477	47.475765858	37.713503831
49	6	48.208318407	49.553873073	37.005260087
50	1	46.297915078	46.857887924	37.631176869
51	1	47.370846345	47.756483895	38.761952073
52	1	48.084801473	46.943845788	37.321512196
53	1	48.066396625	50.640195371	36.939655046
54	1	49.150958574	49.025104491	36.827933193
55	1	48.266118496	50.149659693	39.362954592
56	8	44.995836166	50.083531285	37.980697362
57	1	45.239362064	50.782234345	38.623048617
58	1	44.311520922	50.515134939	37.389328060
59	8	50.315612774	47.249527280	36.482460318
60	1	50.642096599	46.912244011	37.359667035
61	1	50.929950565	46.840532799	35.845346055
62	1	45.777816944	47.856810890	35.314630816
63	1	44.394080235	49.078648714	41.273881368
64	1	50.116597143	46.144631755	43.821409437
65	1	50.706949605	50.876981161	47.167624306

HAT-snapshot#5-RC

QM(B1)/MM = -3003.221918 (a.u.)

QM(B2+ZPE)/MM = -3004.759203 (a.u.)

QM(B2+D3+ZPE)/MM = -3004.82 (a.u.)

1	6	40.644057686	44.181055907	39.583196840
2	1	40.625976884	45.269475859	39.733932694
3	1	39.950188782	43.954467897	38.759030840
4	6	42.042798400	43.777437523	39.235027828
5	7	42.376200711	42.651149086	38.515767407
6	1	41.703369217	41.957492424	38.157425296
7	6	43.716555828	42.582680746	38.410066094
8	1	44.248493695	41.778341329	37.907857850
9	7	44.276663424	43.626090755	39.013560678
10	6	43.245643963	44.381607925	39.528761895
11	1	43.433081169	45.285063267	40.100726782
12	6	46.043717521	47.589032719	41.780839782
13	1	46.251396646	47.399977458	42.847584136
14	1	46.634010361	48.465134339	41.481648955
15	6	46.583288271	46.435717131	40.942045687
16	8	45.948426055	45.317256426	40.964933942
17	8	47.626183285	46.660858438	40.303688519
18	6	44.207712925	39.369621125	42.532315789
19	1	44.683202840	38.617308277	41.883259996
20	1	44.449668279	39.096825014	43.571438191
21	6	44.753011236	40.726233536	42.201993957
22	7	44.667128282	41.830503156	43.038134783
23	1	44.226190334	41.862838342	43.959072978
24	6	45.208600017	42.892675531	42.404115631
25	1	45.252168165	43.899621348	42.812541754
26	7	45.659062108	42.532330415	41.210660705
27	6	45.395792844	41.187157789	41.076080728
28	1	45.679887821	40.645350106	40.178320227
29	26	46.311822613	43.846375369	39.680145467
30	8	46.695617647	44.894096537	38.494457323
31	8	49.166858667	43.151040877	38.468100269
32	6	48.175089622	42.617045612	37.959477032
33	8	49.695109586	40.988925087	34.386100997
34	6	48.205787633	42.216077750	36.504858343
35	6	48.255916514	40.708700624	36.255673825
36	6	48.672213440	40.387252676	34.806649799
37	8	47.985567621	39.546046211	34.177722019

38	8	47.072199831	42.384161563	38.633796747
39	1	49.098119389	42.666976740	36.055723148
40	1	47.319612727	42.642080364	36.007696053
41	1	49.011243429	40.251376766	36.920966458
42	1	47.286514653	40.251635724	36.470905801
43	6	45.306655038	49.664988420	35.892373090
44	1	44.815464894	49.435725838	34.934645250
45	1	46.386861132	49.473998731	35.786615276
46	7	44.812733911	48.694276279	36.926477189
47	1	45.490178713	48.787004861	37.737157371
48	6	43.415935705	48.914156607	37.388106645
49	6	44.997052622	47.279315795	36.479505704
50	1	43.304964511	49.936283551	37.778154178
51	1	43.177014865	48.173263616	38.163517476
52	1	42.728099263	48.762756964	36.544775485
53	1	44.913155110	46.626444772	37.358240992
54	1	46.003657131	47.156467413	36.055793386
55	1	44.215722552	47.008543200	35.754356477
56	8	42.771271305	45.773523020	34.738413033
57	1	42.129041063	45.304789619	35.323974975
58	1	43.548960927	45.183145517	34.795303614
59	8	46.954574529	48.725386245	38.532169129
60	1	47.262134071	47.996057412	39.118309923
61	1	47.484284850	48.618657956	37.703065905
62	1	45.165356092	50.713757089	36.153497969
63	1	44.981792542	47.821248078	41.700473860
64	1	40.221105081	43.710544878	40.470776569
65	1	43.125904328	39.261278465	42.454731276

HAT-snapshot#5-TS

QM(B1)/MM = -3003.181427 (a.u.)

QM(B2+ZPE)/MM = -3004.731082 (a.u.)

QM(B2+D3+ZPE)/MM = -3004.8038 (a.u.)

1	6	40.557187721	44.194481721	39.617185911
2	1	40.542114245	45.282788101	39.767127316
3	1	39.862367298	43.969959720	38.793411533
4	6	41.952981606	43.783397313	39.268149276
5	7	42.276562143	42.663297789	38.537943765
6	1	41.601612369	41.983489670	38.164397889
7	6	43.614389424	42.573226503	38.441620663
8	1	44.137669495	41.776891447	37.919549270
9	7	44.179986112	43.591301156	39.073692592
10	6	43.160490739	44.361212137	39.587589175
11	1	43.361694878	45.253549042	40.171170460
12	6	46.023340551	47.642470381	41.833014044
13	1	46.222556295	47.447786654	42.900842884
14	1	46.614083397	48.524163241	41.546113561
15	6	46.563904392	46.497218359	40.987882724
16	8	45.928211902	45.392456154	40.967854947
17	8	47.629332154	46.720145901	40.369677975
18	6	44.225611123	39.384715445	42.514697695
19	1	44.691592559	38.631540303	41.859160057
20	1	44.478198960	39.107774390	43.550662978
21	6	44.772434195	40.740048174	42.180517023
22	7	44.684817635	41.848168024	43.009668646
23	1	44.235943706	41.889765801	43.924238203
24	6	45.240736280	42.903612174	42.371267662
25	1	45.277219283	43.913378115	42.774325928
26	7	45.701998820	42.539858358	41.184583564
27	6	45.427227338	41.196262855	41.058043139

28	1	45.711029648	40.641710261	40.167858652
29	26	46.210599652	43.981322018	39.511673661
30	8	46.202209007	45.209868085	38.231072461
31	8	48.935270224	43.669251081	37.913576420
32	6	48.030881736	42.899345402	37.531869884
33	8	49.782667994	40.854219621	34.301995110
34	6	48.171174197	42.259718712	36.170226331
35	6	48.322044541	40.740236561	36.161866367
36	6	48.753627339	40.285498300	34.756656228
37	8	48.063912948	39.416082670	34.173836324
38	8	46.980446936	42.624048823	38.234663870
39	1	49.059643605	42.686677416	35.693846006
40	1	47.299078613	42.536572808	35.553011763
41	1	49.111099943	40.443777427	36.876431563
42	1	47.387669811	40.251762372	36.452610773
43	6	45.553244730	49.373118121	35.899477395
44	1	45.085079887	49.054970186	34.955750839
45	1	46.649569251	49.363777401	35.781342935
46	7	45.255538748	48.330528273	36.954954561
47	1	45.862068095	48.604736472	37.791328881
48	6	43.821284874	48.203518632	37.342663670
49	6	45.806843311	47.026886198	36.558358427
50	1	43.437984865	49.188261363	37.646339316
51	1	43.741381877	47.483495931	38.167757313
52	1	43.249625154	47.804363662	36.490899049
53	1	46.001857293	46.154030906	37.587732666
54	1	46.837012596	47.112111898	36.192934374
55	1	45.112322736	46.455910915	35.933396048
56	8	43.095801811	45.846661338	34.889791773
57	1	42.416309526	45.358603162	35.417954960
58	1	43.847336291	45.220216045	34.905724184
59	8	47.112358182	48.835110078	38.789960551
60	1	47.375661594	48.067530192	39.358640104
61	1	47.910780038	49.020848017	38.261815738
62	1	45.245568663	50.383758114	36.167823358
63	1	44.960875039	47.869427466	41.745122984
64	1	40.141780289	43.718802784	40.505574079
65	1	43.142822045	39.277091451	42.451040725

HAT-snapshot#5-IM

QM(B1)/MM = -3003.224705 (a.u.)

QM(B2+ZPE)/MM = -3004.763374 (a.u.)

QM(B2+D3+ZPE)/MM = -3004.8319 (a.u.)

1	6	40.696033623	44.149010208	39.625378765
2	1	40.706791977	45.238106925	39.774633595
3	1	40.021254995	43.940348602	38.780892517
4	6	42.091061964	43.697327347	39.320184756
5	7	42.402089771	42.590952808	38.558165650
6	1	41.714097571	41.949325129	38.138632403
7	6	43.738186822	42.461955974	38.502183883
8	1	44.256001720	41.675233159	37.959526775
9	7	44.321517731	43.446221418	39.180159831
10	6	43.305478183	44.226859426	39.692661118
11	1	43.512776295	45.093317330	40.313168735
12	6	46.019175137	47.486583278	42.006426847
13	1	46.155481105	47.186538995	43.057554477
14	1	46.652649698	48.359499220	41.817398548
15	6	46.507194403	46.405295106	41.054065028
16	8	45.953257136	45.263635287	41.082671980
17	8	47.442222064	46.735558845	40.270939004

18	6	44.095655314	39.233729852	42.664263828
19	1	44.562140728	38.468154552	42.024221575
20	1	44.279471651	38.934768308	43.707590783
21	6	44.714034839	40.567904862	42.376477761
22	7	44.634157142	41.671760306	43.213337771
23	1	44.161426056	41.720207541	44.119369001
24	6	45.246938237	42.712261930	42.605238456
25	1	45.302290103	43.716864503	43.019133558
26	7	45.739671313	42.340497714	41.433529249
27	6	45.425670213	41.007322151	41.283655795
28	1	45.715524659	40.454402433	40.393247313
29	26	46.356115484	43.662631820	39.752554515
30	8	46.815170207	44.906509199	38.427196916
31	8	49.255461322	43.050287048	38.529668497
32	6	48.275258514	42.516914714	37.991077269
33	8	49.764522396	40.958305827	34.356121746
34	6	48.324297799	42.162927732	36.525904267
35	6	48.350561718	40.661570346	36.240445321
36	6	48.733781023	40.369899092	34.778657095
37	8	48.017084010	39.563421989	34.136057375
38	8	47.172485841	42.241590597	38.642007715
39	1	49.226698491	42.613355035	36.098288605
40	1	47.448158380	42.609211323	36.030825655
41	1	49.110081150	40.177789780	36.882093516
42	1	47.378435477	40.214577261	36.463241436
43	6	45.308110582	49.444095940	35.597392721
44	1	44.871641869	49.351325025	34.592416115
45	1	46.392242082	49.254501252	35.535627512
46	7	44.746650240	48.336615045	36.464054030
47	1	45.357378005	48.364116968	37.331890203
48	6	43.314322592	48.491626148	36.866844331
49	6	44.974101533	47.039908663	35.841438616
50	1	43.148876855	49.516007916	37.230313122
51	1	43.103820883	47.761973628	37.661335770
52	1	42.667301089	48.241213298	36.013089332
53	1	47.089214065	45.725255393	38.888127217
54	1	45.989274114	46.628658992	35.896988294
55	1	44.159606776	46.651789541	35.221409809
56	8	42.108632554	46.544972976	34.767458413
57	1	41.917353653	45.773328907	35.348166329
58	1	41.490243286	46.356690917	34.021260394
59	8	46.659581327	48.582413278	38.324890205
60	1	47.011531638	47.994331733	39.028046297
61	1	47.314430939	48.532320439	37.584251727
62	1	45.156821087	50.449147187	35.991157618
63	1	44.972368933	47.760450682	41.875046752
64	1	40.229944791	43.695004773	40.499854372
65	1	43.013820629	39.179762573	42.542655584

TS8

QM(B1)/MM = -3003.203973 (a.u.)

QM(B2+ZPE)/MM = -3004.743572 (a.u.)

QM(B2+D3+ZPE)/MM = -3004.816 (a.u.)

1	6	40.472151858	44.170496471	39.650060021
2	1	40.462840773	45.257505975	39.809909095
3	1	39.764784860	43.954156556	38.835271211
4	6	41.861632781	43.757073189	39.284344730
5	7	42.173689271	42.670801109	38.500035656
6	1	41.493386382	42.017421827	38.091336080
7	6	43.508650586	42.575802019	38.391040203

8	1	44.023688669	41.812614706	37.813515579
9	7	44.082055887	43.556860163	39.072353646
10	6	43.073870536	44.308011810	39.629092399
11	1	43.288346017	45.172921903	40.247945310
12	6	45.966739324	47.677447347	41.607496269
13	1	46.235173093	47.445210746	42.652106531
14	1	46.534489022	48.572112113	41.315106281
15	6	46.455977422	46.555776558	40.701564118
16	8	45.784503983	45.467442142	40.670315307
17	8	47.499116376	46.772010384	40.051058014
18	6	44.158715530	39.391852861	42.560075220
19	1	44.639885909	38.635443922	41.919777898
20	1	44.403542517	39.132366368	43.602099229
21	6	44.693814188	40.747971709	42.210151261
22	7	44.605922080	41.866238708	43.025541571
23	1	44.165546859	41.913275982	43.945337886
24	6	45.148216861	42.918003922	42.366978141
25	1	45.189406086	43.930769218	42.764909901
26	7	45.598167449	42.539615979	41.180932442
27	6	45.333604072	41.192920699	41.075315368
28	1	45.606318948	40.629165056	40.186729292
29	26	46.117917538	43.899286098	39.442164647
30	8	46.100714033	44.991593805	37.856153407
31	8	49.062122715	43.412446956	38.181156266
32	6	48.118942296	42.770795368	37.691866911
33	8	49.753754660	40.883469819	34.315874599
34	6	48.225851066	42.243218881	36.286633181
35	6	48.302100342	40.721069729	36.180530719
36	6	48.721039995	40.312781980	34.758493039
37	8	48.025763549	39.457153387	34.160257186
38	8	47.017094424	42.527859164	38.346294171
39	1	49.128967158	42.665660486	35.833576015
40	1	47.356474225	42.601774700	35.714546282
41	1	49.067306245	40.337251962	36.879964869
42	1	47.341136657	40.267133452	36.437696161
43	6	45.381846029	49.445670507	35.762375121
44	1	44.840918563	49.199182200	34.837690347
45	1	46.462834030	49.306552057	35.601796513
46	7	44.991978643	48.440457333	36.828162252
47	1	45.663912467	48.666403969	37.629566016
48	6	43.567755562	48.512585583	37.276300922
49	6	45.350759284	47.085664333	36.422408760
50	1	43.319437693	49.554297071	37.525097516
51	1	43.452111151	47.870290088	38.161057447
52	1	42.920276993	48.118109916	36.475318981
53	1	45.486643561	45.749327914	37.780765773
54	1	46.411226067	46.929176704	36.200444849
55	1	44.569564534	46.549684214	35.868959537
56	8	42.404073609	46.638461149	35.035848578
57	1	42.149412180	45.840852263	35.554414008
58	1	41.791187763	46.525452992	34.273015639
59	8	47.079562427	48.903464184	38.411580625
60	1	47.340418527	48.162507856	39.012994008
61	1	47.612735277	48.750500145	37.587689061
62	1	45.208348002	50.478093177	36.065804171
63	1	44.898052195	47.891650148	41.597889268
64	1	40.069875944	43.691038113	40.542450685
65	1	43.077873074	39.272981627	42.484467486

PD1

QM(B1)/MM = -3003.328041 (a.u.)

QM(B2+ZPE)/MM = -3004.846059 (a.u.)

QM(B2+D3+ZPE)/MM = -3004.9152 (a.u.)

1	6	40.719305077	44.107224949	39.643328585
2	1	40.736056505	45.199983726	39.768885089
3	1	40.068237293	43.889195810	38.783153326
4	6	42.117918662	43.628641696	39.395578507
5	7	42.448537373	42.591011356	38.552776852
6	1	41.767212578	41.996995310	38.061190874
7	6	43.788052649	42.429447208	38.575262567
8	1	44.320453476	41.688204526	37.984282475
9	7	44.350826155	43.312644523	39.390909984
10	6	43.320674354	44.068862265	39.900969080
11	1	43.502379751	44.861246505	40.620088200
12	6	46.027526184	47.354612410	41.647746930
13	1	46.301450543	47.216040023	42.704135043
14	1	46.652653286	48.136452443	41.195144190
15	6	46.227578262	46.061807334	40.861795232
16	8	45.987453554	44.962030307	41.415149600
17	8	46.641394754	46.151967601	39.658950008
18	6	43.861615309	38.950783344	42.852476179
19	1	44.286763486	38.150736814	42.226148194
20	1	43.951229629	38.625354459	43.898205111
21	6	44.614665591	40.223700277	42.630710652
22	7	44.634721520	41.293564073	43.510979580
23	1	44.147786274	41.367925251	44.409086157
24	6	45.340566197	42.297531231	42.943258790
25	1	45.479038157	43.277655012	43.396903480
26	7	45.795400853	41.930382102	41.755213781
27	6	45.357152454	40.641682421	41.552232728
28	1	45.571680408	40.099432800	40.634587847
29	26	46.352377768	43.286351637	40.204833965
30	8	44.923148617	46.141956600	37.370332105
31	8	49.156962089	43.474302971	38.438700187
32	6	48.217788468	42.838634775	37.917886965
33	8	49.778120584	41.021770018	34.400698870
34	6	48.340630304	42.357639506	36.486038858
35	6	48.405146129	40.835244266	36.332942895
36	6	48.781143371	40.428158358	34.895400015
37	8	48.093585329	39.538075918	34.339205082
38	8	47.122882359	42.544938460	38.526319075
39	1	49.248734574	42.782232482	36.041847502
40	1	47.465323143	42.715338963	35.920643421
41	1	49.180414003	40.427872973	37.008269830
42	1	47.445775166	40.385804948	36.607161492
43	6	45.171222000	49.476010594	35.790205706
44	1	44.588105910	49.254296106	34.883788887
45	1	46.244646726	49.319707520	35.582594274
46	7	44.806273355	48.483359378	36.846409057
47	1	45.452145004	48.681884414	37.657614125
48	6	43.382187944	48.511930742	37.283124022
49	6	45.222461244	47.083463967	36.401305960
50	1	43.116198942	49.537306110	37.579161793
51	1	43.265253928	47.814778945	38.122301691
52	1	42.752511120	48.150560049	36.453960710
53	1	45.611450052	46.079913340	38.065888602
54	1	46.296631135	47.155646061	36.162824575
55	1	44.619487402	46.860984627	35.508129510
56	8	42.397408007	46.661459589	34.931378374
57	1	42.238619537	45.873639260	35.496100099
58	1	41.716815632	46.499714790	34.235198987

59	8	46.726144628	48.657940599	38.764687612
60	1	46.756592646	47.723601239	39.101699440
61	1	47.643964667	48.809534222	38.435037063
62	1	45.038862398	50.512662189	36.099885747
63	1	44.990980694	47.691396067	41.632997766
64	1	40.225251274	43.674734532	40.513345936
65	1	42.790056394	39.019928014	42.665265524

TS9

QM(B1)/MM = -3003.185674 (a.u.)

QM(B2+ZPE)/MM = -3004.728025 (a.u.)

QM(B2+D3+ZPE)/MM = -3197. -3004.8029 (a.u.)

1	6	40.504325713	44.218838596	39.660314788
2	1	40.452748447	45.300033040	39.844321211
3	1	39.773728442	43.986552284	38.870293309
4	6	41.895739572	43.899266323	39.215883296
5	7	42.252934924	42.816976222	38.436957511
6	1	41.603510326	42.092565573	38.094877302
7	6	43.570005592	42.871907081	38.188453562
8	1	44.116006016	42.149910665	37.586003124
9	7	44.096642954	43.947415325	38.774079032
10	6	43.063698992	44.595533521	39.418369552
11	1	43.225645646	45.502917476	39.991008695
12	6	46.061441212	47.756331662	41.731033143
13	1	46.312713954	47.564689565	42.787858461
14	1	46.617040847	48.652697997	41.421025997
15	6	46.586842088	46.629388897	40.869350984
16	8	45.847107165	45.593998453	40.697825132
17	8	47.710681366	46.766234382	40.345993599
18	6	44.305440914	39.564839110	42.402330197
19	1	44.797461236	38.821146523	41.755373111
20	1	44.612162435	39.343490839	43.437104224
21	6	44.750041282	40.941124088	42.003486087
22	7	44.667554619	42.052947496	42.826315772
23	1	44.266231742	42.080872661	43.762948105
24	6	45.114764281	43.129846815	42.143095947
25	1	45.145291479	44.140219965	42.545237080
26	7	45.501034880	42.775126578	40.925823123
27	6	45.290530636	41.416752928	40.829092279
28	1	45.528919769	40.866850923	39.922741480
29	26	46.085457477	44.225403357	39.290908830
30	8	46.353081600	45.886009090	37.982445166
31	8	49.088997437	43.449130475	38.064859940
32	6	48.092865383	42.983385957	37.501881505
33	8	49.785487774	40.846198473	34.339491763
34	6	48.210313903	42.328267772	36.156212976
35	6	48.339222497	40.803866336	36.214393983
36	6	48.770841904	40.283295753	34.830863219
37	8	48.097583321	39.364622178	34.308665532
38	8	46.900268201	43.011232645	38.054838037
39	1	49.110699742	42.724022937	35.676381146
40	1	47.345526177	42.583670546	35.532117866
41	1	49.117917074	40.520681312	36.945414924
42	1	47.392519128	40.341622733	36.514323271
43	6	45.712139348	48.671239913	35.883477329
44	1	45.567508411	48.611174660	34.794579461
45	1	46.786194657	48.551134595	36.084310526
46	7	44.976229715	47.469505787	36.498511783
47	1	45.698451872	46.745248472	37.268265042
48	6	43.787123419	47.780571419	37.333127864

49	6	44.634879385	46.575968639	35.429474910
50	1	44.093023869	48.488226803	38.117178234
51	1	43.424289286	46.850436690	37.789939235
52	1	42.975942497	48.201878156	36.720401936
53	1	46.973785113	46.455706134	38.472441803
54	1	45.495928944	46.179380015	34.879775506
55	1	43.595744281	46.539933748	35.067769894
56	8	41.638706747	46.675223859	34.947751764
57	1	41.537691027	45.815833567	35.421612771
58	1	41.141969338	46.460016950	34.123087622
59	8	47.369461494	48.895033946	38.594051985
60	1	47.769221356	48.327406413	39.275819441
61	1	47.791665123	48.586785949	37.758270792
62	1	45.397120709	49.674725874	36.169565605
63	1	44.989381875	47.945947750	41.678100680
64	1	40.146670569	43.716653425	40.559180835
65	1	43.230895047	39.383628843	42.378219210

PD2

QM(B1)/MM = -3003.323972 (a.u.)

QM(B2+ZPE)/MM = -3004.860403 (a.u.)

QM(B2+D3+ZPE)/MM = -3197. -3004.9267 (a.u.)

1	6	40.655335638	44.175248599	39.526784471
2	1	40.676947999	45.266816188	39.656794553
3	1	39.990710937	43.972348088	38.672801994
4	6	42.050984561	43.686570672	39.284219108
5	7	42.360539244	42.521954673	38.614146311
6	1	41.677395054	41.875679632	38.206091135
7	6	43.694897450	42.335101487	38.672756586
8	1	44.200759769	41.489835296	38.211330620
9	7	44.278555455	43.323384678	39.335090828
10	6	43.265302088	44.175736707	39.713512056
11	1	43.458870316	45.068281219	40.300702255
12	6	46.098625884	47.362625693	41.501857637
13	1	46.429925603	47.311752138	42.550583172
14	1	46.695789529	48.103096200	40.950764427
15	6	46.269728658	46.003912470	40.831207919
16	8	45.943688543	44.959291217	41.448396965
17	8	46.740854263	45.963305762	39.649423669
18	6	43.847515677	38.988685717	42.873267696
19	1	44.284121045	38.170727855	42.278732860
20	1	43.935873741	38.704912385	43.933930338
21	6	44.583802022	40.263090702	42.604989610
22	7	44.586928316	41.362067788	43.448192630
23	1	44.115962242	41.447635564	44.354045855
24	6	45.263593768	42.362593156	42.840821960
25	1	45.387125133	43.361027279	43.257555701
26	7	45.714812630	41.966619917	41.660013270
27	6	45.307084179	40.661586010	41.505429842
28	1	45.529477771	40.089748724	40.607505730
29	26	46.304604963	43.355010174	40.124135773
30	8	43.313263428	38.969578261	38.336497523
31	8	49.164061182	43.463234568	38.493625287
32	6	48.232092108	42.939800442	37.856654236
33	8	49.813960960	40.960035528	34.434980808
34	6	48.472793640	42.433252903	36.451361751
35	6	48.363530465	40.911427893	36.320341322
36	6	48.781778537	40.422949550	34.920272938
37	8	48.090534268	39.522639844	34.384229535
38	8	47.036316025	42.780973511	38.333461596

39	1	49.472283127	42.741036837	36.139607484
40	1	47.755092784	42.909071611	35.763931865
41	1	49.043736494	40.433690181	37.050760122
42	1	47.347562864	40.567057332	36.547397981
43	6	45.188838988	49.105093390	35.251567181
44	1	45.175914517	49.260392344	34.159117142
45	1	46.173642077	48.701803175	35.534761762
46	7	44.145942192	48.101082299	35.556449970
47	1	42.747160556	48.172039603	38.316898168
48	6	42.742832447	48.461167504	35.307666600
49	6	44.408148619	46.908392537	35.948159241
50	1	42.624325604	49.533505046	35.510977192
51	1	42.087928467	47.872998846	35.961647387
52	1	42.491037063	48.244853895	34.257111037
53	1	44.244765387	48.661801571	38.286583286
54	1	45.444245504	46.594483736	36.128389101
55	1	43.562666269	46.206778193	36.064198144
56	8	41.646256137	45.566329151	35.745678071
57	1	41.336323595	44.624019355	35.814006665
58	1	41.175650819	45.878247134	34.914140758
59	8	45.972654541	48.186799123	38.278655687
60	1	46.259188712	47.365993483	38.750318106
61	1	46.665018465	48.329466971	37.601680370
62	1	45.052513018	50.081217135	35.717040046
63	1	45.059936501	47.692339707	41.523774481
64	1	40.178799407	43.731394620	40.400840646
65	1	42.777604848	39.042934937	42.672232486