

Theoretical Study on the Rearrangement of Metallabenzenes to Cyclopentadienyl Complexes

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Tables giving Cartesian coordinates and electronic energies

Cartesian coordinates for all the species calculated in this study:

1

E = -725.79421549 a.u.

Re	0.256438	0.000016	0.000004
C	-1.324996	-0.000102	1.444926
C	-1.324997	0.000193	-1.444921
C	-2.699676	-0.000064	1.260099
H	-1.042983	-0.000051	2.504367
C	-2.699676	0.000125	-1.260094
H	-1.042983	0.000100	-2.504361
C	-3.328923	0.000025	0.000003
H	-3.358573	-0.000094	2.128334
H	-3.358573	0.000139	-2.128328
H	-4.419008	0.000019	0.000004
C	1.583079	0.000346	-1.464444
O	2.342681	0.000688	-2.362372
C	0.227145	1.990968	0.000426
O	0.191020	3.159980	0.000631
C	0.226966	-1.990936	-0.000418
O	0.190767	-3.159946	-0.000688
C	1.583087	-0.000390	1.464444
O	2.342688	-0.001010	2.362373

Re	-0.420665	-0.042207	0.010506
C	0.526715	-1.919592	1.042571
C	0.328631	-2.242388	-0.332747
C	1.187518	-1.394545	-1.127666
C	1.968717	-0.608191	-0.217389
C	1.525232	-0.870932	1.122660
H	0.055374	-2.398885	1.886296
H	-0.330444	-3.004778	-0.718012
H	1.322902	-1.422481	-2.196415
H	1.932129	-0.456830	2.030647
C	-1.494302	0.517107	1.484249
O	-2.127297	0.822913	2.435358
C	-1.957881	-0.170112	-1.111179
O	-2.890293	-0.304431	-1.825297
C	-0.140338	1.769695	-0.526392
O	0.113500	2.875613	-0.859818
O	2.964597	0.216758	-0.651311
C	3.551283	1.153299	0.308166
H	4.010991	0.615180	1.143315
H	4.311992	1.691579	-0.253303
H	2.789437	1.848886	0.674443

2

E = -612.56879021 a.u.

Re	0.074885	0.000007	-0.000247
C	-1.973279	-0.723473	-0.976874
C	-1.968692	-1.161310	0.397527
C	-1.968424	0.010781	1.224401
C	-1.969459	1.166828	0.377014
C	-1.973633	0.704973	-0.990232
H	-1.998696	-1.365219	-1.844192
H	-2.008871	-2.183250	0.740188
H	-1.981240	0.020510	2.303841
H	-2.008761	2.194837	0.701314
C	-2.001124	1.330934	-1.868862
H	1.155875	-1.348647	-0.806796
O	1.767645	-2.216572	-1.325574
C	1.171010	-0.023797	1.560970
O	1.792745	-0.039139	2.565783
C	1.154900	1.373249	-0.765376
O	1.766174	2.256964	-1.257407

5

E = -840.294113 a.u.

Re	0.761575	-0.076674	-0.131754
C	-1.210397	0.618225	0.399106
C	-0.243292	-1.921152	-0.585087
C	-2.416987	-0.034090	0.368766
H	-1.302077	1.650604	0.753268
C	-1.573676	-2.268546	-0.496114
H	0.373767	-2.749411	-0.951956
C	-2.590215	-1.383150	-0.049164
H	-1.880983	-3.272122	-0.779434
C	2.485633	-0.869103	-0.656540
O	3.499892	-1.374477	-0.977895
C	0.414640	0.522871	-1.994749
O	0.184049	0.866615	-3.089994
C	0.986652	-0.706655	1.739883
O	1.092666	-1.086576	2.842297
C	1.523154	1.681724	0.330568
O	1.944773	2.743108	0.615625
H	-3.338657	0.459195	0.672238
O	-3.890951	-1.778860	0.019408
C	-4.322202	-3.126970	-0.359351
H	-5.397658	-3.122644	-0.194401
H	-4.102105	-3.321621	-1.412287
H	-3.845433	-3.878030	0.275960

3

E = -840.274676 a.u.

Re	-0.729397	0.065620	-0.198301
C	1.200604	-0.817746	-0.027717
C	0.294114	1.907343	0.199217
C	2.438240	-0.240713	0.233426
H	1.300376	-1.901042	-0.156593
C	1.639434	2.130774	0.429627
H	-0.299975	2.827347	0.232715
C	2.638063	1.132203	0.445819
H	1.989215	3.146269	0.616816
H	3.650399	1.474795	0.642419
C	-2.440224	1.047630	-0.322055
O	-3.436096	1.669804	-0.386114
C	-0.432721	0.349719	-2.147320
O	-0.247788	0.527804	-3.288070
C	-1.014881	-0.171068	1.758669
O	-1.171400	-0.298755	2.910381
C	-1.494555	-1.722200	-0.550979
O	-1.914142	-2.801028	-0.757954
O	3.512162	-1.156679	0.271620
C	4.857287	-0.685376	0.535046
H	5.480493	-1.578644	0.509028
H	5.198136	0.019148	-0.234557
H	4.935876	-0.215037	1.523694

6

E = -840.300968 a.u.

Re	0.342666	-0.022921	0.310128
C	-1.677079	0.252973	-0.403012
C	-0.524357	-1.342929	1.769773
C	-2.870873	-0.309227	0.092469
C	-1.846937	-1.678789	1.956930
H	0.151086	-1.833639	2.478949
C	-2.921166	-1.186578	1.169231
H	-2.124269	-2.369004	2.753837
H	-3.913878	-1.544541	1.441674
C	2.120258	-0.358300	1.078109
O	3.168725	-0.578179	1.565732
C	0.531379	-1.574111	-0.918377
O	0.622339	-2.494819	-1.635765
C	0.053615	1.496959	1.558104
O	-0.137659	2.384635	2.297096
C	0.999547	1.210961	-1.091593
O	1.380941	1.943950	-1.926424
H	-3.820192	-0.064151	-0.375426
O	-1.759684	1.098222	-1.473623
C	-3.030216	1.453916	-2.138467
H	-3.703072	1.955898	-1.438341
H	-2.733042	2.135398	-2.932741

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E = -727.048043699 a.u.

Electronic Supplementary Information for Dalton Transactions
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H -3.506124 0.564089 -2.558837

7

E = -954.796525 a.u.

Re	0.868914	-0.268873	0.061469
C	-0.715010	-1.558931	-0.612073
C	-0.694361	1.214785	0.293449
C	-2.057897	-1.315775	-0.748392
H	-0.442383	-2.579872	-0.900283
C	-2.058315	1.098814	0.037090
C	-2.676337	-0.065132	-0.440798
H	-2.708938	-2.107289	-1.110253
H	-2.739807	1.927375	0.197433
C	2.215184	1.030435	0.700711
O	3.008420	1.808346	1.082607
C	0.500619	-0.861002	1.920743
O	0.255978	-1.207178	3.012805
C	1.098484	0.353749	-1.810158
O	1.205821	0.723579	-2.916491
C	2.169846	-1.713459	-0.200583
O	2.924339	-2.602552	-0.369722
O	-4.027773	0.103769	-0.602740
O	-0.226201	2.418272	0.759912
C	-1.102943	3.578692	0.996815
H	-1.855364	3.345736	1.755666
H	-0.430895	4.355146	1.356851
H	-1.585078	3.894617	0.067306
C	-4.893136	-0.968825	-1.090693
H	-5.887885	-0.527020	-1.106733
H	-4.603705	-1.276764	-2.099166
H	-4.874760	-1.825764	-0.411774

8

E = -841.52641146 a.u.

Re	-0.000030	-0.443782	0.023994
C	0.730913	1.443408	1.210045
C	1.155638	1.689350	-0.132875
C	-0.000083	1.725885	-0.990724
C	-1.155827	1.689398	-0.132824
C	-0.731139	1.443514	1.210075
H	1.351754	1.399466	2.089543
H	-1.351968	1.399164	2.089566
C	1.361433	-1.411688	-0.904192
O	2.239763	-1.954249	-1.481109
C	-1.362049	-1.412342	-0.902775
O	-2.240660	-1.955432	-1.478774
C	0.000990	-1.707700	1.451059
O	0.001580	-2.440638	2.380293
O	-2.414258	1.887373	-0.624061
C	-3.543697	1.598869	0.259351
H	-3.523706	2.250486	1.139017
H	-4.429174	1.804953	-0.338250
H	-3.528361	0.547132	0.564176
H	-0.000205	1.937685	-2.046509
O	2.414097	1.887512	-0.623989
C	3.543620	1.598897	0.259384
H	3.528103	0.547227	0.564384
H	4.429026	1.804719	-0.338404
H	3.523800	2.250717	1.138879

9

E = -954.798171 a.u.

Re	0.024828	-0.499245	0.000562
C	1.114142	0.315083	-1.724106
C	1.680340	0.240015	1.224096
C	2.257718	1.133156	-1.639464
C	2.747585	1.039831	0.844594
C	2.967376	1.446400	-0.485576
H	2.638429	1.519154	-2.582209
H	3.475912	1.378615	1.575578
C	-0.778414	-1.125489	1.689993
O	-1.267659	-1.503172	2.686464
C	-0.799228	1.298194	0.184392
O	-1.254685	2.371960	0.282263
C	1.022513	-2.196738	-0.237286

O	1.637426	-3.182326	-0.387085
C	-1.543573	-1.183930	-0.949103
O	-2.525414	-1.621277	-1.438151
O	1.561605	-0.140441	2.542241
C	2.537542	0.258836	3.567278
H	2.560670	1.347298	3.675478
H	2.175015	-0.203259	4.483581
H	3.534305	-0.118357	3.320294
H	3.840513	2.079342	-0.638501
O	0.809829	0.172535	-3.054999
C	-0.276455	-0.638566	-3.586952
H	-1.243237	-0.184944	-3.362667
H	-0.110144	-0.642603	-4.663829
H	-0.233461	-1.657156	-3.198455

10

E = -841.52261845 a.u.

Re	0.624836	-0.016373	-0.058764
C	-0.108698	-0.336345	-2.241986
C	-0.840139	-1.278171	-1.423431
C	-1.742118	-0.518312	-0.597794
C	-1.509778	0.881076	-0.836669
C	-0.501995	0.984807	-1.868729
H	0.585588	-0.597054	-3.025046
H	-0.806539	-2.351590	-1.511785
H	-0.177820	1.913214	-2.310564
C	2.340485	-0.812380	-0.298366
O	3.388313	-1.323279	-0.497605
C	0.481656	-0.763562	1.690589
O	0.309464	-1.260409	2.752207
C	1.414223	1.575733	0.641199
O	1.867800	2.592796	1.038251
O	-2.227288	1.965311	-0.401720
C	-2.628446	2.017581	1.012237
H	-1.736768	1.973886	1.648066
H	-3.128929	2.978004	1.123243
H	-3.303663	1.195108	1.252009
O	-2.724247	-0.963604	0.245167
C	-2.730979	-2.385221	0.598631
H	-1.806389	-2.652004	1.119747
H	-3.585072	-2.505635	1.261971
H	-2.860703	-3.003712	-0.294854

11

E = -1069.295904 a.u.

Re	-0.627253	0.442860	0.282374
C	1.438230	0.054216	0.793175
C	0.161530	1.584146	-1.380692
C	2.594167	0.482814	0.148219
C	1.485716	1.800706	-1.724226
C	2.587062	1.286476	-1.009538
H	1.765254	2.395032	-2.587172
C	-2.463778	0.870840	-0.290546
O	-3.556804	1.128633	-0.636010
C	-0.593178	-1.165821	-0.878240
O	-0.549981	-2.108402	-1.573257
C	-0.539303	2.091498	1.382527
O	-0.464300	3.070995	2.021533
C	-1.215447	-0.622354	1.831134
O	-1.562173	-1.258936	2.756607
O	-0.821193	2.145894	-2.166622
O	1.574622	-0.728859	1.918149
C	-0.509382	2.961719	-3.349454
H	0.040992	2.375281	-4.091421
H	-1.481373	3.251772	-3.744180
H	0.065377	3.849372	-3.068277
C	2.882128	-1.126082	2.459425
H	3.439672	-1.723588	1.731277
H	3.463958	-0.247615	2.755797
H	2.642658	-1.728826	3.333443
H	3.562433	0.196178	0.538194
O	3.775657	1.671382	-1.592368
C	5.066032	1.270887	-1.046018
H	5.176464	0.182042	-1.054400
H	5.797865	1.722343	-1.713843
H	5.200785	1.656838	-0.030768

12

E = -955.99928500 a.u.

Re	-0.299330	-0.500350	0.051051
C	1.227315	1.369814	0.169490
C	1.289620	0.854825	-1.162901
C	-0.027061	0.987810	-1.760244
C	-0.855976	1.674421	-0.818164
C	-0.134928	1.825536	0.417973
H	-0.473338	2.341621	1.300378
C	0.045869	-1.198065	1.791997
O	0.291859	-1.572340	2.890213
C	0.217989	-2.147931	-0.768263
O	0.573298	-3.133786	-1.315644
C	-2.120739	-1.067566	0.143240
O	-3.267159	-1.358049	0.182745
O	-2.113142	2.106579	-1.137382
C	-2.987040	2.545920	-0.050112
H	-2.554703	3.405167	0.473151
H	-3.916225	2.835896	-0.536252
H	-3.167999	1.723249	0.649250
H	-0.269407	0.774445	-2.787490
O	2.369105	0.456366	-1.902444
C	3.469557	-0.248772	-1.228350
H	3.084799	-1.153407	-0.745130
H	4.160013	-0.509361	-2.028430
H	3.946898	0.397653	-0.491435
O	2.345030	1.555159	0.951891
C	2.152229	1.729960	2.392127
H	3.156064	1.833544	2.800153
H	1.573809	2.636090	2.599473
H	1.656876	0.854231	2.821684

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E = -859.748974 a.u.

Re	-0.990148	-0.023164	0.177098
C	0.547750	1.132026	-0.794835
C	0.673997	-1.242019	0.800686
C	1.905670	0.968426	-0.850165
H	0.218868	2.016348	-1.352369
C	2.017410	-1.132438	0.561541
H	0.438437	-2.114776	1.420224
C	2.648111	-0.095829	-0.219111
H	2.485672	1.694332	-1.411256
H	2.675299	-1.883259	0.987713
C	-2.252928	-1.192967	1.128364
O	-2.980442	-1.913873	1.712615
C	-0.697608	1.084476	1.797371
O	-0.485369	1.735602	2.748794
C	-1.098710	-1.134636	-1.463225
O	-1.124711	-1.790825	-2.434295
C	-2.381364	1.199676	-0.484168
O	-3.188527	1.953623	-0.896956
N	4.002501	-0.123121	-0.367078
C	4.714265	0.900339	-1.160877
H	4.571326	1.900054	-0.738593
H	5.779288	0.673110	-1.152832
H	4.370317	0.904306	-2.199811
C	4.827653	-1.177439	0.258930
H	4.715313	-1.173043	1.347538
H	4.558205	-2.168694	-0.119133
H	5.874123	-0.991924	0.021287

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E = -746.502188 a.u.

Re	-0.404742	-0.091417	-0.000187
C	0.555187	-1.929513	1.069492
C	0.323557	-2.289448	-0.287389
C	1.179756	-1.471913	-1.122510
C	2.040548	-0.693501	-0.257889
C	1.557976	-0.884185	1.093117
H	0.094474	-2.373964	1.937938
H	-0.345783	-3.058112	-0.641125
H	1.265154	-1.559569	-2.192858
H	1.978408	-0.451171	1.985507

C	-1.487001	0.476104	1.465251
O	-2.128735	0.788945	2.409243
C	-1.931354	-0.214453	-1.138246
O	-2.857937	-0.344260	-1.863097
C	-0.089742	1.714583	-0.533002
O	0.191465	2.814943	-0.872907
N	3.076339	0.111216	-0.648163
C	3.662794	1.044332	0.319126
H	4.597932	1.434771	-0.086736
H	2.992295	1.889539	0.536644
H	3.890874	0.526561	1.254422
C	3.254506	0.409886	-2.072707
H	4.233988	0.869063	-2.219067
H	3.222631	-0.511676	-2.659725
H	2.482448	1.097264	-2.450458

15

E = -859.751488 a.u.

Re	0.480670	0.002706	0.279786
C	-1.702627	-0.011465	-0.150439
C	0.036965	-1.514958	1.784001
C	-2.415388	-1.273763	-0.041397
C	-1.029399	-2.360939	1.781478
C	-2.108109	-2.289255	0.828717
H	-3.325158	-1.411324	-0.618806
H	-1.107440	-3.159034	2.521296
C	2.364163	-0.199640	0.772179
O	3.487409	-0.335768	1.095919
C	0.605447	-1.509580	-1.004006
O	0.661609	-2.421998	-1.734569
C	0.202510	1.357623	1.691995
O	0.009507	2.136359	2.548855
C	0.953000	1.279738	-1.133879
O	1.277515	2.030262	-1.986860
H	-2.805856	-3.126607	0.841423
N	-2.451386	1.020325	-0.597460
C	-1.971979	2.408782	-0.728466
H	-2.024715	2.729459	-1.774836
H	-2.604860	3.067837	-0.124344
H	-0.950878	2.492612	-0.380073
C	-3.889389	0.884247	-0.959672
H	-4.014162	0.255000	-1.846505
H	-4.457070	0.452109	-0.131930
H	-4.288471	1.873807	-1.181394
H	0.770108	-1.691976	2.576426

16

E = -1163.265626 a.u.

Re	-0.951764	0.001420	0.017402
C	0.502407	0.047124	-1.563216
C	0.765303	-0.007349	1.298968
C	1.878801	0.042381	-1.513005
H	0.126766	0.074807	-2.592298
C	2.115441	-0.005879	1.004212
H	0.583805	-0.017700	2.380276
C	2.638856	0.014486	-0.311581
H	2.451567	0.062701	-2.440503
H	2.828541	-0.016765	1.824284
C	-2.141784	-0.043499	1.588596
O	-2.821118	-0.070194	2.549850
C	-0.926924	1.990279	0.048440
O	-0.889978	3.159973	0.064544
C	-0.880903	-1.985913	-0.031562
O	-0.815904	-3.154043	-0.062508
C	-2.413123	0.011536	-1.308809
O	-3.258448	0.018586	-2.127483
S	4.427658	0.014561	-0.614609
C	5.229279	-0.038084	1.091347
H	6.300864	-0.049905	0.889035
H	4.970178	0.852556	1.663852
H	4.942284	-0.946684	1.620658

17

E = -1050.027139 a.u.

Re	-0.391391	-0.073538	-0.002708
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C	0.477377	-2.004839	1.038024
C	0.185304	-2.345322	-0.315659
C	1.053299	-1.568355	-1.171076
C	1.913322	-0.787492	-0.326612
C	1.538268	-1.021756	1.038498
H	0.013666	-2.425775	1.917058
H	-0.541631	-3.070118	-0.648503
H	1.111628	-1.626934	-2.246502
H	2.020018	-0.616264	1.913366
C	-1.411499	0.513506	1.497527
O	-2.011931	0.829897	2.465617
C	-1.951683	-0.108216	-1.099132
O	-2.900410	-0.189017	-1.798912
C	-0.045316	1.734422	-0.506812
O	0.248925	2.836365	-0.818719
C	3.597289	1.425243	0.410757
H	3.878231	0.917142	1.333625
H	4.424772	2.047036	0.067251
H	2.704751	2.035872	0.548055
S	3.314807	0.173802	-0.976463

18

E = -1163.275383 a.u.

Re	-0.589678	-0.089235	0.050887
C	-0.803907	1.791719	-0.968985
C	1.545286	0.326926	-0.001974
C	0.163546	2.689304	-1.369328
H	-1.819522	2.115233	-1.222036
C	2.200485	1.440937	-0.542869
C	1.552465	2.510379	-1.163518
H	-0.127966	3.606777	-1.880832
H	3.284316	1.512221	-0.494985
C	-0.421722	-1.826030	0.995248
O	-0.394199	-2.860614	1.553262
C	-0.662816	0.879168	1.787165
O	-0.678258	1.463521	2.800478
C	-0.383680	-0.991928	-1.709886
O	-0.235324	-1.506351	-2.750035
C	-2.542989	-0.240303	-0.024565
O	-3.716647	-0.280727	-0.096916
H	2.199573	3.304972	-1.535047
S	2.550749	-0.957100	0.760094
C	4.375076	-0.447630	0.631526
H	4.550249	0.483866	1.171326
H	4.925083	-1.260912	1.106714
H	4.673837	-0.358665	-0.413738

19

E = -818.002116 a.u.

Re	0.236052	0.001238	0.006325
C	-1.333477	0.003050	1.445907
C	-1.332664	0.003362	-1.429223
C	-2.718746	-0.001601	1.270729
H	-1.052979	0.006976	2.504520
C	-2.713626	-0.001454	-1.248923
H	-1.053936	0.008338	-2.489414
C	-3.350137	-0.004313	-0.002752
H	-3.367206	-0.001663	-2.120189
H	-4.438736	-0.007217	-0.001257
C	1.564774	-0.001180	-1.461578
O	2.319689	-0.002533	-2.361119
C	0.244717	1.997036	0.002421
O	0.242599	3.164822	-0.002427
C	0.237960	-1.994614	0.002961
O	0.232301	-3.162374	-0.002479
C	1.566873	-0.000844	1.477516
O	2.326221	-0.001977	2.372586
C	-3.582485	-0.002299	2.424791
N	-4.279572	-0.002896	3.370309

20

E = -704.773857 a.u.

Re	0.089581	-0.047021	0.026136
C	-1.928843	-1.161230	-0.597122
C	-1.904675	-1.079164	0.823544

C	-1.951495	0.320463	1.197346
C	-2.003503	1.090570	-0.029459
C	-1.990057	0.182745	-1.125496
H	-1.934030	-2.070429	-1.177897
H	-1.887156	-1.906331	1.516671
H	-2.072600	2.166278	-0.084380
H	-2.048926	0.450481	-2.168961
C	1.155744	-0.583935	-1.460678
O	1.756590	-0.932380	-2.415010
C	1.254257	-0.980593	1.219807
O	1.923205	-1.581880	1.982026
C	1.139618	1.537080	0.228368
O	1.735104	2.546564	0.356284
C	-2.086192	0.831921	2.513886
N	-2.221352	1.253678	3.601504

21

E = -817.999436 a.u.

Re	0.238089	-0.000035	0.000034
C	-1.336826	-0.000294	1.434279
C	-1.336902	0.000416	-1.434122
C	-2.713171	-0.000283	1.262937
H	-1.057894	-0.000662	2.493900
C	-2.713240	0.000411	-1.262723
H	-1.058007	0.000669	-2.493753
C	-3.355403	0.000049	0.000124
H	-3.367783	-0.000528	2.132640
H	-3.367884	0.000680	-2.132399
C	1.561785	0.000155	-1.474087
O	2.312961	0.000301	-2.377006
C	0.242314	1.995351	-0.000150
O	0.236203	3.163431	-0.000572
C	0.242216	-1.995424	-0.000455
O	0.236487	-3.163505	-0.000988
C	1.561521	-0.000356	1.474380
O	2.312330	-0.000577	2.377601
C	-4.792161	0.000095	0.000165
N	-5.966590	0.000132	0.000186

22

E = -818.008467 a.u.

Re	0.244613	0.000269	0.028780
C	-1.374746	0.000705	1.484380
C	-1.309965	0.001437	-1.420917
C	-2.747245	-0.001326	1.254195
C	-2.694427	-0.000579	-1.263254
H	-1.015516	0.003440	-2.476885
C	-3.345938	-0.002225	-0.022650
H	-3.425035	-0.001681	2.105968
H	-3.333064	-0.000453	-2.145890
H	-4.434861	-0.003326	-0.039502
C	1.537264	0.000149	-1.450232
O	2.267854	0.000161	-2.370949
C	0.237329	1.994934	0.057317
O	0.221509	3.162635	0.077230
C	0.234642	-1.994398	0.055221
O	0.217719	-3.162104	0.074020
C	1.652745	-0.001639	1.439980
O	2.498887	-0.002798	2.250004
C	-0.993678	0.002587	2.857990
N	-0.614391	0.004262	3.975036

23

E = -930.213854 a.u.

C	-1.270911	0.539220	0.315439
C	-0.002934	-1.820333	-0.734388
C	-2.397628	-0.214899	0.069391
H	-1.514779	1.521413	0.726890
C	-1.320602	-2.268558	-0.839217
H	0.715912	-2.571510	-1.081992
C	-2.439326	-1.519846	-0.465015
H	-1.519039	-3.262950	-1.235599
H	-3.425397	-1.957258	-0.587702
C	2.605400	-0.597899	-0.404577
O	3.680023	-0.999680	-0.654286

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C	0.658562	0.817172	-1.843426
O	0.590179	1.277265	-2.914147
C	0.893374	-0.764631	1.816092
O	0.962924	-1.231759	2.883710
C	1.317509	1.787957	0.716312
O	1.611688	2.834651	1.156444
N	-3.734494	0.379744	0.386852
O	-4.765334	-0.319211	0.165550
O	-3.771200	1.548358	0.859874
Re	0.768017	0.024669	-0.013754

24

E = -816.976579 a.u.

C	0.394950	2.173235	-0.725831
C	0.394463	2.173871	0.724269
C	1.277051	1.152747	1.173307
C	1.811775	0.512132	0.000399
C	1.277808	1.151748	-1.173450
H	-0.153490	2.855016	-1.357036
H	-0.154335	2.856210	1.354554
H	1.535432	0.904155	2.190058
H	1.536863	0.902318	-2.189821
C	-2.347854	0.557766	-0.002414
O	-3.469622	0.922589	-0.003681
C	-0.832076	-1.230999	1.356705
O	-0.991030	-2.015657	2.220393
C	-0.829403	-1.234118	-1.354756
O	-0.986640	-2.020795	-2.216915
N	2.847528	-0.485440	0.001143
O	3.273336	-0.887114	-1.120388
O	3.273090	-0.885720	1.123265
Re	-0.501513	0.076383	-0.000198

25

E = -930.203547 a.u.

C	0.693616	1.214176	-0.758639
C	0.693243	-1.214301	0.758525
C	2.074493	1.069823	-0.668097
H	0.418238	2.117424	-1.314017
C	2.074163	-1.070810	0.667285
H	0.417581	-2.117297	1.314172
C	2.681167	-0.000684	-0.000558
H	2.739548	-1.799888	1.117782
C	-2.196677	-1.242194	0.807907
O	-2.941602	-2.000607	1.305381
C	-0.900183	1.083141	1.678475
O	-0.910603	1.716666	2.658980
C	-0.901631	-1.082266	-1.677814
O	-0.912903	-1.715771	-2.658325
C	-2.196324	1.243819	-0.806619
O	-2.941032	2.002675	-1.303745
H	2.740100	1.798505	-1.118902
N	4.185278	-0.001183	-0.000931
O	4.777436	0.990092	-0.506881
O	4.776990	-0.992849	0.504772
Re	-0.876840	0.000421	0.000328

26

E = -930.214705 a.u.

C	1.544549	0.480765	0.177159
C	-0.749905	1.899422	-0.756551
C	2.161053	1.708312	0.043918
C	0.144661	2.972238	-0.764022
H	-1.737720	2.184900	-1.136164
C	1.486791	2.875007	-0.380568
H	-0.192886	3.948168	-1.110297
H	2.089578	3.778995	-0.446722
C	-2.416535	-0.381098	-0.411212
O	-3.556983	-0.511085	-0.659197
C	-0.041290	-0.819100	-1.849500
O	0.225713	-1.249032	-2.899317
C	-0.927760	0.590514	1.782858
O	-1.169606	0.994390	2.851451
C	-0.208938	-1.905017	0.722275
O	-0.057418	-2.968733	1.185115

H	3.224239	1.789864	0.253270
N	2.544425	-0.578044	0.510759
O	2.514254	-1.640096	-0.173062
O	3.354325	-0.364046	1.455542
Re	-0.503486	-0.083894	-0.045261

27

E = -848.849927 a.u.

Re	-0.606847	0.027443	-0.000288
C	1.450416	0.628531	-0.001248
C	0.186067	-1.958312	0.017558
C	2.644363	-0.103006	0.002568
H	1.617919	1.713954	-0.006384
C	1.505918	-2.378892	0.019567
H	-0.524446	-2.793116	0.025526
C	2.625042	-1.520634	0.012077
H	1.725557	-3.447008	0.027991
H	3.593533	-2.020753	0.014938
C	-2.442501	-0.704598	0.002025
O	-3.519418	-1.177842	0.003809
C	-0.582922	0.030554	1.990412
O	-0.551359	0.024310	3.159869
C	-0.574024	-0.004036	-1.990594
O	-0.536927	-0.030741	-3.159588
C	-1.156922	1.925598	-0.017796
O	-1.444915	3.066343	-0.028082
Si	4.298385	0.841621	-0.003435
C	5.743122	-0.371825	-0.004491
H	6.693916	0.175945	-0.009283
H	5.739527	-1.013151	0.885894
H	5.733507	-1.018369	-0.891052
C	4.382144	1.929575	1.534926
H	3.533782	2.623852	1.580004
H	4.366575	1.324820	2.449837
H	5.301525	2.528863	1.542329
C	4.374719	1.922842	-1.546882
H	4.354067	1.314146	-2.459074
H	3.526686	2.617591	-1.590657
H	5.294464	2.521431	-1.561572

28

E = -735.633027 a.u.

Re	-0.372206	-0.076213	0.000377
C	0.553291	-2.148168	-0.721398
C	1.423505	-1.100869	-1.153735
C	1.995708	-0.428242	-0.000160
C	1.424041	-1.100811	1.153687
C	0.553617	-2.148142	0.721813
H	0.015999	-2.835343	-1.357034
H	1.639995	-0.860374	-2.184176
H	1.640993	-0.860257	2.184018
H	0.016651	-2.835312	1.357726
C	-2.205816	-0.602279	0.000177
O	-3.321328	-0.993291	0.000082
C	-0.705477	1.222049	-1.355461
O	-0.848950	2.009503	-2.226212
C	-0.705578	1.221174	1.357035
O	-0.849125	2.008049	2.228294
Si	3.332604	0.899650	-0.000480
C	5.004588	0.024913	-0.000655
H	5.120785	-0.611360	-0.886634
H	5.825456	0.753433	-0.000807
H	5.121025	-0.611261	0.885364
C	3.166040	1.948475	1.552210
H	3.957954	2.707448	1.585061
H	2.201787	2.467925	1.589732
H	3.257767	1.342242	2.462295
C	3.165597	1.948221	-1.553293
H	2.201337	2.467667	-1.590654
H	3.957502	2.707189	-1.586470
H	3.257093	1.341843	-2.463305

29

E = -848.849863 a.u.

Re	0.699835	0.019419	0.000186
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C	-0.888551	-0.008935	1.431637
C	-0.888127	-0.006392	-1.431739
C	-2.262557	-0.044003	1.249936
H	-0.609508	0.003425	2.492324
C	-2.262215	-0.041754	-1.250497
H	-0.608832	0.007920	-2.492336
C	-2.937387	-0.058114	-0.000402
H	-2.893521	-0.061602	2.139002
H	-2.892917	-0.057744	-2.139771
C	2.024622	0.042973	-1.465820
O	2.781406	0.056896	-2.366708
C	0.631482	2.008526	0.002134
O	0.570201	3.177027	0.003646
C	0.698223	-1.971022	-0.000664
O	0.675569	-3.140849	-0.000657
C	2.025022	0.040675	1.465920
O	2.782454	0.053162	2.366287
Si	-4.853253	-0.028127	-0.000447
C	-5.371389	1.785351	0.003754
H	-4.990084	2.308907	-0.880890
H	-6.4465316	1.873852	0.003698
H	-4.990547	2.304432	0.891237
C	-5.504795	-0.899532	1.536744
H	-5.227114	-0.376452	2.459117
H	-6.600837	-0.944790	1.502390
H	-5.130750	-1.928033	1.605469
C	-5.504896	-0.892768	-1.541391
H	-6.600954	-0.937787	-1.507301
H	-5.226981	-0.365901	-2.461533
H	-5.131218	-1.921106	-1.614420

30

E = -848.848503 a.u.

Re	-0.461967	-0.142459	0.029015
C	1.654832	0.492502	-0.039602
C	0.281411	-2.145588	0.126889
C	2.734319	-0.380460	-0.176481
C	1.574011	-2.623849	-0.028794
H	-0.447157	-2.947447	0.295218
C	2.694786	-1.792496	-0.182925
H	3.742160	0.028855	-0.253658
H	1.762335	-3.697044	-0.001920
H	3.659087	-2.292866	-0.279983
C	-2.252989	-0.941836	0.061903
O	-3.301986	-1.474963	0.082498
C	-0.377727	-0.020314	2.010748
O	-0.291705	0.055507	3.175846
C	-0.339142	-0.219522	-1.953324
O	-0.217749	-0.259799	-3.116507
C	-1.240061	1.671772	-0.074676
O	-1.782216	2.716980	-0.131875
Si	2.135519	2.342261	0.018363
C	1.523060	3.192014	-1.553921
H	1.900905	4.222594	-1.578944
H	1.897247	2.679417	-2.448521
H	0.432061	3.238591	-1.616841
C	4.013016	2.563377	0.090103
H	4.249410	3.633122	0.158927
H	4.453835	2.072243	0.966389
H	4.513161	2.175847	-0.806013
C	1.414679	3.156392	1.562064
H	1.675832	2.594425	2.467023
H	1.837398	4.164402	1.665553
H	0.326342	3.259592	1.524892

31

E = -738.765946 a.u.

Re	0.143301	-0.015489	0.168535
C	-1.097563	0.355929	-1.511503
C	-1.558464	0.543651	1.296153
C	-2.447268	0.690684	-1.580242
H	-0.652487	0.253924	-2.510293
C	-2.850531	0.870735	0.888415
H	-1.446265	0.616889	2.386112
C	-3.258799	0.931827	-0.455028
H	-2.921679	0.818463	-2.554416

H	-3.601620	1.130522	1.635729
H	-4.293552	1.218380	-0.645257
C	1.058061	-0.471517	1.845302
O	1.552851	-0.763486	2.879155
C	0.837260	1.803230	0.252140
O	1.266984	2.898334	0.299987
C	1.600055	-0.541146	-1.042828
O	2.439536	-0.871942	-1.808080
P	-0.599015	-2.408948	0.011345
C	-2.239933	-2.817047	0.762314
H	-2.207754	-2.615759	1.837134
H	-3.007826	-2.177480	0.319006
H	-2.496022	-3.869300	0.596926
C	0.536869	-3.642072	0.799748
H	1.524715	-3.574492	0.333277
H	0.648045	-3.419069	1.864999
H	0.152986	-4.661440	0.682933
C	-0.762487	-3.069229	-1.712117
H	-1.517994	-2.489841	-2.250164
H	0.191749	-2.964750	-2.237699
H	-1.052655	-4.125467	-1.700743

32

E = -751.726259 a.u.

Re	0.124840	-0.000097	0.001557
C	-1.441013	0.375155	-1.357134
C	-1.437085	-0.384610	1.362310
C	-2.829095	0.334050	-1.196661
H	-1.170570	0.695868	-2.374339
C	-2.825595	-0.350746	1.203705
H	-1.163608	-0.704657	2.378900
C	-3.473101	-0.009970	0.004009
H	-3.476241	0.580154	-2.041322
H	-3.470284	-0.600549	2.049161
H	-4.563737	-0.012861	0.004755
C	1.405766	-0.259023	1.448743
O	2.141012	-0.408480	2.374165
C	1.404786	0.266071	-1.445260
O	2.141095	0.419671	-2.369193
P	0.255382	-2.403446	-0.416473
P	0.239475	2.404930	0.415296
C	1.906682	3.052756	0.905249
H	1.874438	4.133537	1.082985
H	2.245037	2.546364	1.814144
H	2.626640	2.839796	0.108828
C	-0.192232	3.512311	-1.009219
H	-0.063254	4.567570	-0.743155
H	0.452012	3.273925	-1.861411
H	-1.230778	3.334486	-1.302177
C	-0.851087	3.058760	1.763776
H	-0.751394	4.145495	1.865362
H	-1.890115	2.802947	1.538336
H	-0.579131	2.578654	2.708750
C	1.932086	-3.041994	-0.886074
H	1.906887	-4.122206	-1.068434
H	2.280880	-2.530586	-1.788205
H	2.640074	-2.829256	-0.078923
C	-0.189928	-3.518097	0.998030
H	-0.051296	-4.571642	0.730074
H	0.441246	-3.279018	1.859742
H	-1.233331	-3.346949	1.277395
C	-0.813574	-3.057195	-1.782220
H	-0.707276	-4.143006	-1.887015
H	-1.856793	-2.807116	-1.570080
H	-0.530917	-2.571820	-2.721374

33

E = -625.522089 a.u.

Re	0.417707	0.190138	-0.000025
C	2.627131	-0.224940	0.712376
C	1.842298	-1.346860	1.165469
C	1.354607	-2.029072	0.004362
C	1.837093	-1.353349	-1.162959
C	2.623941	-0.229074	-0.719625
H	3.156399	0.473030	1.342226
H	1.689821	-1.642586	2.191642

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H	0.754514	-2.927327	0.008259
H	1.680528	-1.655236	-2.186715
H	3.150292	0.465397	-1.355775
C	-0.020395	1.434671	1.345030
O	-0.250179	2.204113	2.228565
C	-0.020500	1.434860	-1.344827
O	-0.250317	2.204416	-2.228255
P	-1.829723	-0.543614	-0.000016
C	-2.346912	-1.593235	1.443536
H	-3.394178	-1.904924	1.355726
H	-1.712493	-2.483319	1.499646
H	-2.217196	-1.021570	2.367721
C	-3.134787	0.771352	-0.002003
H	-4.139867	0.335426	-0.001567
H	-3.012892	1.402758	0.883422
H	-3.012636	1.400441	-0.889039
C	-2.345857	-1.596697	-1.441443
H	-1.712452	-2.487721	-1.494125
H	-3.393610	-1.906933	-1.354289
H	-2.214121	-1.027754	-2.367015

34

E = -764.655509 a.u.

Re	0.000388	-0.188112	0.203456
C	0.001038	-0.917215	-1.805895
C	0.001441	-2.153736	0.714369
C	0.001770	-2.217443	-2.292907
H	0.001040	-0.187264	-2.631941
C	0.002128	-3.336494	-0.067190
C	0.001360	-2.404361	1.786863
H	0.002283	-3.365279	-1.457564
H	0.002108	-2.403520	-3.370199
H	0.002560	-4.300871	0.445402
H	0.002890	-4.341024	-1.945607
C	0.000504	0.256922	2.067054
O	0.000730	0.443346	3.255850
P	2.451726	-0.226105	0.170608
P	-2.451031	-0.229697	0.171206
P	-0.002334	2.229664	-0.596967
C	-3.336751	0.261413	-1.394643
H	-4.418504	0.112526	-1.298840
H	-3.145996	1.308590	-1.645436
H	-2.955891	-0.362010	-2.209542
C	-3.389176	0.715127	1.472011
H	-3.215824	1.789066	1.374772
H	-4.465051	0.518392	1.401137
H	-3.028383	0.403392	2.457345
C	-3.186842	-1.917332	0.411701
H	-2.790987	-2.591702	-0.351493
H	-2.891066	-2.302617	1.391801
H	-4.280624	-1.880439	0.346210
C	-1.398351	3.352917	-0.061000
H	-1.246285	4.369960	-0.440700
H	-2.359553	2.984585	-0.428218
H	-1.431942	3.383007	1.032810
C	1.394518	3.354805	-0.067063
H	2.354888	2.986660	-0.436617
H	1.240432	4.371129	-0.447870
H	1.431394	3.386726	1.026591
C	-0.006533	2.583666	-2.433964
H	-0.008101	3.661199	-2.634592
H	0.877473	2.136085	-2.899587
H	-0.891575	2.134216	-2.895786
C	3.388951	0.722505	1.469341
H	4.465000	0.526523	1.398998
H	3.214732	1.796075	1.369679
H	3.028334	0.412631	2.455329
C	3.189803	-1.912274	0.414571
H	4.283544	-1.874064	0.349133
H	2.894431	-2.295908	1.395447
H	2.794936	-2.588772	-0.347249
C	3.336253	0.262938	-1.396534
H	4.418218	0.115509	-1.300897
H	2.955708	-0.362548	-2.209985
H	3.144147	1.309384	-1.649359

35

E = -638.451975 a.u.

Re	0.262689	0.030070	0.072287
C	-1.770077	1.174235	0.342064
C	-1.986205	0.238857	-0.740929
C	-1.847697	-1.078717	-0.204904
C	-1.570079	-0.982337	1.199398
C	-1.521823	0.418350	1.533885
H	-1.870981	2.247080	0.283574
H	-2.256199	0.487369	-1.755494
H	-1.971338	-1.997177	-0.759560
H	-1.462333	-1.805681	1.887591
H	-1.359833	0.825755	2.519990
C	1.612755	0.125738	1.358318
O	2.445652	0.186658	2.228121
P	1.448970	-1.706830	-0.978866
P	1.278327	1.798184	-1.074826
C	1.260169	-1.968400	-2.820322
H	1.761980	-2.885979	-3.150844
H	0.195886	-2.031930	-3.070485
H	1.685685	-1.116697	-3.361267
C	3.299794	-1.826634	-0.801641
H	3.674089	-2.762432	-1.232207
H	3.785596	-0.985226	-1.302430
H	3.558285	-1.786479	0.261016
C	0.984265	-3.412445	-0.370782
H	1.563855	-4.191718	-0.880104
H	1.172534	-3.468427	0.706138
H	-0.081350	-3.594131	-0.542159
C	1.420520	3.372395	-0.081210
H	2.062346	3.184524	0.785863
H	1.838717	4.196968	-0.671359
H	0.430136	3.657542	0.287877
C	3.022306	1.713191	-1.734063
H	3.703814	1.449004	-0.919028
H	3.093162	0.947564	-2.513304
H	3.329353	2.676637	-2.157492
C	0.390667	2.434548	-2.589293
H	-0.641047	2.690897	-2.328077
H	0.885204	3.323393	-2.999065
H	0.365337	1.651623	-3.354004

36

E = -777.563176 a.u.

Re	-0.002050	0.213357	-0.001195
C	-0.172807	1.739381	1.373704
C	0.163752	1.736207	-1.380301
C	-0.164779	3.138710	1.225521
H	-0.355299	1.478342	2.430171
C	0.173820	3.135584	-1.232350
H	0.322972	1.473152	-2.439851
C	0.008933	3.794176	-0.003550
H	-0.292991	3.771982	2.107137
H	0.301151	3.767012	-2.115436
H	0.012619	4.885420	-0.004471
P	2.456704	0.430434	0.040700
P	-2.462513	0.426202	-0.044517
P	-0.023576	-1.461402	1.823058
P	0.028904	-1.470308	-1.816129
C	-3.073931	1.737120	-1.215920
H	-4.161660	1.855731	-1.143598
H	-2.578916	2.682218	-0.981647
H	-2.804476	1.461051	-2.240130
C	-3.293808	1.030345	1.517933
H	-2.832735	1.976263	1.811926
H	-4.366644	1.182037	1.352058
H	-3.159880	0.313525	2.332770
C	-3.676971	-0.927063	-0.503505
H	-4.703789	-0.570902	-0.359854
H	-3.551998	-1.198638	-1.556171
H	-3.522456	-1.817466	0.111217
C	-1.607910	-2.357886	2.292703
H	-1.425704	-3.065509	3.110596
H	-2.374988	-1.647296	2.612796
H	-1.984594	-2.911044	1.426634
C	0.474167	-0.901543	3.547635

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H	0.425610	-1.726702	4.267722
H	1.495667	-0.506690	3.526560
H	-0.187666	-0.097839	3.885873
C	1.043320	-3.006068	1.732871
H	2.092092	-2.742293	1.590167
H	0.948796	-3.605162	2.646947
H	0.726462	-3.615530	0.879883
C	3.666847	-0.919655	0.519612
H	3.537644	-1.177274	1.575459
H	3.511626	-1.817508	-0.083944
H	4.695121	-0.568370	0.374271
C	3.288144	1.012986	-1.529903
H	4.361898	1.162722	-1.367965
H	3.149873	0.288806	-2.337640
H	2.829835	1.957613	-1.832589
C	3.070307	1.755432	1.194725
H	4.158046	1.871681	1.118885
H	2.576098	2.697992	0.949183
H	2.802353	1.492619	2.222744
C	-1.052546	-3.005272	-1.732935
H	-2.099593	-2.732190	-1.596164
H	-0.957787	-3.605052	-2.646571
H	-0.746656	-3.617969	-0.878174
C	1.611936	-2.386138	-2.252959
H	1.440447	-3.086075	-3.079764
H	2.396736	-1.684618	-2.548734
H	1.959281	-2.950465	-1.381726
C	-0.437075	-0.919271	-3.552289
H	-0.376285	-1.749112	-4.265950
H	-1.458759	-0.524309	-3.551749
H	0.231114	-0.118076	-3.883876

37

E = -651.363221 a.u.

Re	-0.041335	-0.004469	-0.512215
C	-1.420803	-0.380239	-2.370912
C	-0.915969	0.964427	-2.477715
C	0.516408	0.866991	-2.610970
C	0.888187	-0.515976	-2.608197
C	-0.323450	-1.293994	-2.458195
H	-2.461683	-0.659777	-2.305360
H	-1.503929	1.867063	-2.527513
H	1.190203	1.696037	-2.763754
H	1.881312	-0.906722	-2.767837
H	-0.397280	-2.369488	-2.473389
P	0.978827	1.779816	0.596869
P	-1.908837	-0.076868	0.889431
P	1.160691	-1.623715	0.661866
C	0.076036	3.425815	0.581372
H	0.684329	4.234723	1.005480
H	-0.187030	3.677228	-0.451665
H	-0.852639	3.338687	1.155751
C	2.615172	2.369483	-0.114090
H	2.472347	2.684825	-1.152309
H	3.023686	3.211849	0.457522
H	3.334466	1.544555	-0.104691
C	1.494173	1.771255	2.403809
H	1.933011	2.734717	2.690236
H	0.631963	1.570080	3.045051
H	2.237741	0.985163	2.571335
C	3.037498	-1.523931	0.673765
H	3.394855	-1.445472	-0.358554
H	3.361960	-0.629338	1.215804
C	3.490142	-2.405631	1.144854
C	0.912985	-2.011479	2.483516
H	-0.115008	-2.350520	2.647822
H	1.600463	-2.796470	2.821302
H	1.077453	-1.111403	3.083438
C	1.003325	-3.374723	0.005644
H	1.601366	-4.082575	0.592375
H	-0.048019	-3.678838	0.034393
H	1.340733	-3.404665	-1.035607
C	-3.357781	0.982819	0.342053
H	-3.638938	0.726507	-0.684111
H	-4.228440	0.844137	0.994757
H	-3.059781	2.035962	0.358882
C	-2.810125	-1.721295	1.015288

H	-3.068365	-2.064718	0.007574
H	-2.149348	-2.469660	1.465466
H	-3.727406	-1.647058	1.613255
C	-1.934879	0.387575	2.708810
H	-1.223714	-0.226272	3.268731
H	-1.646477	1.438446	2.816802
H	-2.935821	0.252201	3.135885

38

E = -726.735793 a.u.

C	-1.311153	-0.000405	1.448610
C	-1.311103	-0.000107	-1.448815
C	-2.684665	0.000040	1.261706
H	-1.024880	0.000362	2.507115
C	-2.684611	-0.000030	-1.261933
H	-1.024810	-0.000180	-2.507312
C	-3.311732	0.000143	-0.000121
H	-3.347178	0.000339	2.127724
H	-3.347140	-0.000061	-2.127944
H	-4.401996	0.000248	-0.000159
C	1.599179	0.000405	-1.469195
O	2.357231	0.000691	-2.364726
C	0.191033	1.991335	0.001310
O	0.117759	3.157419	0.002049
C	0.191169	-1.991571	-0.000371
O	0.117373	-3.157623	-0.000174
C	1.599658	-0.000368	1.468604
O	2.358241	-0.000520	2.363693
Tc	0.261107	-0.000110	-0.000076

39

E = -750.523634 a.u.

C	-1.206809	0.000122	1.406611
C	-1.207563	-0.000068	-1.406409
C	-2.584776	0.000028	1.254103
H	-0.890650	0.000608	2.456337
C	-2.585443	-0.000079	-1.253153
H	-0.891977	-0.000489	-2.456307
C	-3.225105	-0.000059	0.000650
H	-3.228501	0.000093	2.133468
H	-3.229674	-0.000151	-2.132149
H	-4.314855	-0.000093	0.000925
C	1.493051	0.000793	-1.334291
O	2.277994	0.001393	-2.203728
C	0.066232	1.823226	0.000525
O	-0.103957	2.980598	0.000549
C	0.065915	-1.823171	-0.000791
O	-0.104736	-2.980476	-0.000689
C	1.493951	-0.000822	1.332883
O	2.279534	-0.001462	2.201742
Mn	0.240851	0.000014	-0.000292

40

E = -714.562766 a.u.

C	-1.394677	0.659323	0.327336
C	-0.345159	-1.788219	-0.648252
C	-2.616982	0.017227	0.113849
H	-1.538472	1.710783	0.617003
C	-1.695078	-2.145158	-0.695492
H	0.304828	-2.642573	-0.888573
C	-2.759730	-1.298534	-0.351740
H	-1.968788	-3.155455	-1.017921
H	-3.772986	-1.692070	-0.454477
C	2.222052	-0.510459	-1.123712
O	3.113307	-0.815236	-1.853847
C	0.595945	1.617088	-1.262414
O	0.646289	2.566340	-1.971624
C	1.451148	-1.278929	1.331408
O	1.995957	-1.998504	2.100807
C	1.227261	1.394243	1.339446
O	1.535757	2.165251	2.194222
W	0.629569	0.016790	-0.005671
H	-3.546913	0.560455	0.313104

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E = -714.244674 a.u.

C	-1.359903	0.337373	1.388240
C	-1.359487	-0.338243	-1.388450
C	-2.744034	0.316804	1.208453
H	-1.089373	0.703414	2.391217
C	-2.743597	-0.320991	-1.208246
H	-1.088397	-0.704024	-2.391366
C	-3.385334	-0.002904	0.000211
H	-3.403295	0.569821	2.046178
H	-3.402500	-0.575399	-2.045831
H	-4.477923	-0.004116	0.000330
C	1.520767	0.201435	-1.575183
O	2.198138	0.377018	-2.538626
C	0.519896	2.013285	0.245733
O	0.732422	3.166704	0.405772
C	0.521410	-2.011624	-0.245840
O	0.734557	-3.164921	-0.405870
C	1.521031	-0.198759	1.574955
O	2.198661	-0.373843	2.538309
Mo	0.269770	0.000739	-0.000073

42

E = -613.530041 a.u.

C	-1.975825	-0.722474	-0.975746
C	-1.967804	-1.159054	0.396955
C	-1.972116	0.010959	1.223073
C	-1.968758	1.164698	0.376221
C	-1.975790	0.703716	-0.989222
H	-2.002762	-1.364740	-1.843092
H	-2.007526	-2.181402	0.739691
H	-1.986800	0.020812	2.302845
H	-2.007695	2.193205	0.700282
H	-2.004652	1.330011	-1.868025
C	1.157840	-1.354169	-0.809810
O	1.770412	-2.218436	-1.325827
C	1.172701	-0.024262	1.566808
O	1.795849	-0.039656	2.566707
C	1.156741	1.379177	-0.767905
O	1.768747	2.259307	-1.257090
Tc	0.078492	-0.000016	-0.000386

43

E = -637.328687 a.u.

C	-1.856340	-0.721396	-0.975359
C	-1.843214	-1.157405	0.395369
C	-1.850741	0.011004	1.220453
C	-1.844563	1.163182	0.374702
C	-1.855899	0.702812	-0.988796
H	-1.867276	-1.363268	-1.842969
H	-1.863197	-2.179948	0.738159
H	-1.850298	0.020867	2.299938
H	-1.863979	2.191850	0.698870
H	-1.868281	1.328790	-1.867842
C	0.961365	-1.294034	-0.772027
O	1.558620	-2.164664	-1.288438
C	0.975968	-0.023247	1.496374
O	1.584497	-0.039013	2.501694
C	0.960040	1.317857	-0.732062
O	1.556477	2.204300	-1.221849
Mn	-0.002124	-0.000009	-0.000739

44

E = -601.332335 a.u.

C	0.654451	-2.000763	1.052321
C	0.485306	-2.315485	-0.331001
C	1.321351	-1.428698	-1.094264
C	1.994019	-0.564703	-0.173641
C	1.598612	-0.923777	1.156437
H	0.171390	-2.500690	1.878683
H	-0.145662	-3.094272	-0.732456
H	1.428364	-1.424510	-2.168394
H	1.953736	-0.472709	2.070540
C	-1.670764	0.321956	1.407290

O	-2.431575	0.497990	2.326138
C	-1.828392	-0.089114	-1.288737
O	-2.692678	-0.181324	-2.124812
C	-0.196938	1.857649	-0.293174
O	0.007338	3.031338	-0.479164
W	-0.388643	-0.045526	0.004137
H	2.701028	0.208510	-0.434525

45

E = -601.040057 a.u.

C	-2.051377	-0.722154	-0.972195
C	-2.051066	-1.156162	0.395245
C	-2.042384	0.010842	1.220740
C	-2.051141	1.161859	0.374308
C	-2.052275	0.703353	-0.985649
H	-2.062279	-1.365256	-1.840349
H	-2.067668	-2.180140	0.738434
H	-2.042723	0.020697	2.301378
H	-2.067156	2.191995	0.698696
H	-2.064556	1.330466	-1.865358
C	1.248487	-1.350440	-0.809467
O	1.894765	-2.220695	-1.329490
C	1.261608	-0.024244	1.564824
O	1.916901	-0.039644	2.572552
C	1.247234	1.375439	-0.767390
O	1.892714	2.261881	-1.260402
Mo	0.121972	-0.000122	-0.000398

46

E = -829.046603 a.u.

C	1.382101	0.711938	0.279471
C	0.416537	-1.793412	-0.616373
C	2.618636	0.081818	0.145545
H	1.512965	1.709582	0.716572
C	1.777535	-2.084571	-0.692839
H	-0.195775	-2.611587	-1.020937
C	2.822240	-1.223299	-0.316798
H	2.091163	-3.065842	-1.065081
H	3.834865	-1.610839	-0.392230
C	-2.190238	-1.153694	0.431291
O	-3.074567	-1.878043	0.764394
C	-0.772829	0.543152	1.919325
O	-0.937281	0.873376	3.046065
C	-1.349448	-0.216939	-1.916789
O	-1.842338	-0.321111	-2.989989
C	-1.181498	1.914381	-0.324022
O	-1.481023	3.040251	-0.568817
O	3.737027	0.894973	0.533437
C	5.069465	0.368286	0.401855
H	5.735095	1.166363	0.738842
H	5.227894	-0.521692	1.028507
H	5.313484	0.110604	-0.639207
W	-0.604809	0.002625	-0.034909

47

E = -829.053298 a.u.

C	0.800348	0.015443	-1.557324
C	1.059503	-0.014483	1.273227
C	2.186130	0.019409	-1.516674
H	0.441513	0.025575	-2.597859
C	2.424174	-0.007767	0.987664
H	0.897956	-0.028243	2.362597
C	2.939036	0.008496	-0.322822
H	3.142707	-0.015699	1.807376
C	-1.862573	-0.018232	1.662171
O	-2.511462	-0.026410	2.665748
C	-0.912071	2.020187	0.058982
O	-1.096876	3.191468	0.096389
C	-0.908400	-2.028544	0.026474
O	-1.091457	-3.200574	0.045548
C	-2.141724	0.006019	-1.395893
O	-2.955728	0.011961	-2.269558
H	2.788899	0.031059	-2.426875
O	4.317105	0.015486	-0.563181
C	5.252703	0.005450	0.541906

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H	6.239990	0.013108	0.077416
H	5.136014	0.891299	1.177067
H	5.140341	-0.894994	1.156976
W	-0.704001	-0.003760	0.016444

48

E = -829.058450 a.u.

C	-1.700385	-0.006425	0.004809
C	0.226762	2.142968	0.018008
C	-2.613653	1.067372	-0.004591
C	-0.922919	2.928928	0.008019
H	1.136008	2.763627	0.034261
C	-2.233051	2.410569	-0.004418
H	-0.844884	4.020716	0.013019
H	-3.047175	3.139169	-0.010815
C	2.473495	0.281242	-0.007398
O	3.646565	0.510531	-0.010444
C	0.612756	-0.168900	2.023453
O	0.724748	-0.302976	3.196765
C	0.590598	-0.132286	-2.029960
O	0.686904	-0.248621	-3.206492
C	0.506345	-2.032547	-0.019977
O	0.510675	-3.223478	-0.030844
H	-3.685937	0.877643	-0.009744
O	-2.261475	-1.292460	0.011856
C	-3.704723	-1.529603	0.015653
H	-4.182136	-1.126435	-0.885536
H	-3.805539	-2.615357	0.031934
H	-4.182398	-1.099347	0.904065
W	0.491508	-0.009770	-0.001284

49

E = -943.549327 a.u.

C	1.704918	-0.020256	-0.003686
C	-0.197877	2.134422	-0.011871
C	2.619635	1.039187	-0.019124
C	0.945479	2.925351	-0.026103
H	-1.102045	2.761994	-0.011961
C	2.252219	2.390082	-0.029229
H	0.852053	4.010937	-0.035426
C	-2.473844	0.281607	0.018658
O	-3.647885	0.512828	0.023313
C	-0.607982	-0.152503	-2.015698
O	-0.716319	-0.271163	-3.191776
C	-0.583997	-0.113586	2.038791
O	-0.678646	-0.209586	3.218115
C	-0.542126	-0.032564	0.029526
O	-0.561043	-3.223818	0.041242
H	3.693448	0.874426	-0.024265
O	2.261058	-1.307292	0.004562
C	3.704732	-1.541013	-0.002685
H	4.186118	-1.113856	0.885157
H	3.808553	-2.626538	0.006361
H	4.174536	-1.129862	-0.904179
W	-0.496180	-0.012870	0.009805
O	3.376076	3.229917	-0.043819
C	3.213935	4.668023	-0.056001
H	2.687256	5.023173	0.837288
H	4.229945	5.066399	-0.065882
H	2.676294	5.006814	-0.949112

50

E = -943.554191 a.u.

C	1.740076	-0.062841	-0.005188
C	-0.128117	2.196427	-0.039392
C	2.683063	0.979327	-0.022890
C	1.072726	2.926774	-0.052464
C	2.341362	2.336220	-0.044315
H	1.061749	4.015248	-0.069897
H	3.183176	3.032067	-0.056393
C	-2.442270	0.312474	-0.006505
O	-3.622317	0.484002	-0.007550
C	-0.558450	-0.089042	-2.030492
O	-0.661032	-0.188706	-3.209116
C	-0.553621	-0.025744	2.024464

O	-0.653549	-0.088732	3.205844
C	-0.544516	-1.981542	0.026944
O	-0.597676	-3.172684	0.045428
H	3.750261	0.764212	-0.020487
O	2.256898	-1.366338	0.015277
C	3.691768	-1.645926	0.018312
H	4.182638	-1.228912	0.906069
H	3.760853	-2.734185	0.035679
H	4.180821	-1.257557	-0.883328
W	-0.453073	0.025804	-0.004436
O	-1.311564	2.948623	-0.050254
C	-1.316851	4.410300	-0.073958
H	-0.830105	4.801405	-0.975683
H	-2.372955	4.682463	-0.077428
H	-0.828517	4.830441	0.813741

51

E = -848.482142 a.u.

C	-1.298047	0.478273	0.082138
C	0.020903	-1.954521	-0.495698
C	-2.484465	-0.272063	-0.053230
H	-1.490477	1.495870	0.432029
C	-1.296432	-2.399628	-0.609928
H	0.741178	-2.734275	-0.779857
C	-2.456837	-1.645472	-0.393800
H	-1.472890	-3.444842	-0.888873
H	-3.398726	-2.176236	-0.499805
C	2.465275	-0.878209	0.603335
O	3.414479	-1.434116	1.061110
C	1.642160	-0.362015	-1.880122
O	2.195697	-0.544646	-2.913477
C	0.770000	0.787344	1.803489
O	0.824537	1.270398	2.886360
C	1.125319	1.916947	-0.585676
O	1.287894	3.035273	-0.964376
W	0.779823	-0.002558	-0.072248
N	-3.758285	0.336654	0.154461
C	-4.976056	-0.456578	0.116241
H	-4.952301	-1.287810	0.839099
H	-5.829565	0.178514	0.368394
H	-5.168794	-0.896364	-0.877403
C	-3.855649	1.767330	0.409578
H	-3.412557	2.060577	1.374862
H	-3.350217	2.354959	-0.370499
H	-4.910312	2.057778	0.421058

52

E = -848.495319 a.u.

C	0.706182	-1.406035	-0.061064
C	0.707150	1.406007	0.064640
C	2.083105	-1.253404	-0.055335
H	0.443574	-2.474821	-0.108294
C	2.083886	1.252460	0.057601
H	0.445157	2.474922	0.112086
C	2.768732	-0.000704	0.000587
H	2.705220	-2.146236	-0.095235
H	2.706702	2.144802	0.097633
C	-2.261370	1.524063	0.069205
O	-3.001165	2.463115	0.112751
C	-1.115956	0.092884	-2.024224
O	-1.272336	0.147108	-3.200419
C	-1.122614	-0.090166	2.024806
O	-1.281485	-0.141914	3.200806
C	-2.263443	-1.521109	-0.072023
O	-3.005513	-2.458258	-0.117835
N	4.161207	-0.001113	-0.000341
C	4.917480	-1.254674	-0.064004
H	4.689473	-1.820697	-0.976337
H	5.985334	-1.026141	-0.061683
H	4.703706	-1.904087	0.794919
C	4.918472	1.251895	0.062415
H	4.702635	1.902163	-0.795311
H	4.693525	1.817318	0.975907
H	5.986164	1.022661	0.056776
W	-0.950590	0.000508	0.000575

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53

E = -848.503762 a.u.

C	1.649215	0.280429	-0.085873
C	-0.608542	1.851820	1.090034
C	2.155049	1.635630	-0.189251
C	0.289890	2.886984	0.976782
C	1.537752	2.773263	0.286870
H	3.144850	1.790212	-0.620106
H	0.090531	3.864928	1.428650
C	-2.544332	-0.072797	0.336519
O	-3.718377	-0.023491	0.550205
C	-0.728007	0.945167	-1.702684
O	-0.800398	1.533644	-2.729789
C	-0.295586	-1.203526	1.703052
O	-0.114913	-1.897797	2.654451
C	-0.776288	-1.761531	-1.050895
O	-0.971106	-2.754041	-1.698841
H	2.107746	3.699290	0.174753
N	2.638349	-0.671221	-0.093729
C	2.363930	-2.113442	-0.065131
H	3.101764	-2.639745	-0.683207
H	2.412663	-2.508752	0.958663
H	1.368404	-2.297986	-0.457362
C	4.081123	-0.352443	-0.017185
H	4.498096	-0.082168	-0.997571
H	4.253883	0.476860	0.673203
H	4.618234	-1.229494	0.353042
H	-1.497526	2.112048	1.682273
W	-0.570049	-0.090520	0.038159

54

E = -763.990581 a.u.

C	1.484192	0.183378	0.454585
C	0.013373	-2.174764	-0.101105
C	2.542598	-0.715088	0.607709
H	1.769868	1.200253	0.753559
C	1.258375	-2.781651	0.092049
H	-0.739651	-2.904526	-0.433109
C	2.440571	-2.108115	0.424918
H	1.347952	-3.866258	-0.026636
H	3.346310	-2.697637	0.556499
C	-2.488062	-0.725037	0.149762
O	-3.591986	-1.125464	0.348210
C	-0.898797	0.709135	1.765499
O	-1.150600	1.221906	2.803060
C	-0.941920	-0.494761	-2.036567
O	-1.218244	-0.682091	-3.173517
C	-0.622554	1.810008	-0.681817
O	-0.582474	2.924629	-1.098576
C	4.700749	0.803396	-0.399820
H	5.684815	1.247004	-0.214092
H	4.763482	0.122353	-1.253329
H	3.983838	1.598046	-0.622322
S	4.198243	-0.106599	1.125265
W	-0.578390	-0.113372	-0.070590

55

E = -763.990644 a.u.

C	0.603448	-1.246832	-0.901809
C	0.842215	1.060923	0.697743
C	1.992968	-1.222460	-0.856205
H	0.248713	-2.152144	-1.417255
C	2.210668	0.861899	0.504032
H	0.665991	2.011389	1.224887
C	2.756856	-0.224326	-0.206717
H	2.563051	-2.021759	-1.340321
H	2.908259	1.592859	0.912539
C	-2.004217	1.009801	1.364596
O	-2.605212	1.586610	2.218445
C	-1.209200	1.645608	-1.159218
O	-1.467951	2.598903	-1.815703
C	-1.240013	-1.597306	1.217053
O	-1.516709	-2.518851	1.909573
C	-2.281481	-0.849178	-1.190223
O	-3.050867	-1.343346	-1.955519

S	4.531245	-0.453804	-0.393386
C	5.280935	0.787159	0.730592
H	6.359009	0.601478	0.711042
H	5.088830	1.808600	0.392445
H	4.912120	0.664361	1.751917
W	-0.901744	0.006663	0.007508

56

E = -764.003383 a.u.

C	0.739879	2.115709	0.004283
C	-1.579548	0.352608	-0.000533
C	-0.246903	3.098679	0.005811
H	1.747203	2.559511	0.005707
C	-2.258558	1.584067	0.001762
C	-1.630061	2.833058	0.004643
H	0.032432	4.157094	0.008093
H	-3.348484	1.609965	0.001375
C	0.470829	-2.072155	-0.004508
O	0.465777	-3.266033	-0.007118
C	0.617159	-0.172213	-2.032586
O	0.633737	-0.281239	-3.212342
C	0.615228	-0.180639	2.031708
O	0.630716	-0.294491	3.211026
C	2.598744	-0.051451	0.000798
O	3.791448	0.012738	0.001505
H	-2.294188	3.700867	0.006134
S	-2.525922	-1.125404	-0.003749
C	-4.333163	-0.681077	-0.003427
H	-4.603591	-0.110318	-0.896675
H	-4.878924	-1.629849	-0.004912
H	-4.603942	-0.112915	0.891370
W	0.602507	-0.051037	-0.000186

57

E = -806.790036 a.u.

C	1.538461	0.596578	0.259793
C	0.397862	-1.883761	-0.473066
C	2.744245	-0.125511	0.174855
H	1.713226	1.611914	0.639161
C	1.738369	-2.290023	-0.526483
H	-0.270910	-2.680198	-0.830755
C	2.832681	-1.484583	-0.212521
H	1.973224	-3.313720	-0.831624
H	3.827294	-1.925452	-0.264370
C	-2.230425	-0.982085	0.298959
O	-3.206031	-1.616948	0.543687
C	-0.680883	0.462906	1.949146
O	-0.858913	0.756264	3.081426
C	-1.098825	-0.102010	-1.972270
O	-1.516127	-0.138517	-3.079206
C	-0.959685	1.963587	-0.263122
O	-1.179208	3.114688	-0.462838
C	3.985003	0.532946	0.498402
N	4.994806	1.079685	0.761185
W	-0.499815	0.007107	-0.029236

58

E = -806.790155 a.u.

C	-1.056178	-0.507055	1.316437
C	-1.052750	0.499434	-1.321418
C	-2.437712	-0.467692	1.152305
H	-0.784002	-0.954735	2.281257
C	-2.434797	0.453207	-1.163474
H	-0.778516	0.948504	-2.285012
C	-3.104664	-0.008900	-0.007085
H	-3.082397	-0.807344	1.966499
H	-3.077503	0.789721	-1.980532
C	1.650617	-0.403813	-1.643159
O	2.247011	-0.701733	-2.626223
C	1.122733	1.893735	-0.475087
O	1.508927	2.980411	-0.741346
C	1.129102	-1.890912	0.479721
O	1.519083	-2.975818	0.747660
C	1.641841	0.409064	1.649982
O	2.233003	0.709683	2.635387

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C	-4.536729	-0.012450	-0.010292
N	-5.715171	-0.015386	-0.012927
W	0.548007	0.000112	0.001077

59

E = -806.793895 a.u.

C	-1.827822	0.323698	-0.054634
C	-0.323406	-2.111532	-0.039517
C	-2.907038	-0.575882	-0.087148
C	-1.598019	-2.688584	-0.021903
H	0.460681	-2.875575	0.061987
C	-2.799883	-1.971942	-0.055826
H	-3.919818	-0.171550	-0.150293
H	-1.688394	-3.778588	0.014732
H	-3.729975	-2.540990	-0.062468
C	2.102806	-0.739231	-0.640999
O	3.119797	-1.182080	-1.072496
C	0.358703	0.930834	-1.791336
O	0.463851	1.526368	-2.806150
C	1.024289	-0.642190	1.807694
O	1.503628	-0.940736	2.848322
C	0.670564	1.781004	0.746115
O	0.875395	2.827306	1.264652
C	-2.236293	1.693543	-0.158279
N	-2.535712	2.834459	-0.234034
W	0.318461	-0.069771	-0.009728

60

E = -919.005587 a.u.

C	1.331266	0.555869	0.117484
C	0.096224	-1.955289	-0.307937
C	2.485997	-0.217861	0.049429
H	1.571208	1.597534	0.348184
C	1.426855	-2.411079	-0.361100
H	-0.603784	-2.774426	-0.531959
C	2.548667	-1.608572	-0.182475
H	1.624294	-3.468940	-0.552141
H	3.535171	-2.057720	-0.218717
C	-2.548009	-0.878400	0.157028
O	-3.583058	-1.448979	0.294419
C	-0.884959	0.266536	1.991932
O	-1.039544	0.456162	3.148118
C	-1.164624	0.008614	-2.018994
O	-1.483094	0.039268	-3.157197
C	-1.204046	1.967786	-0.122169
O	-1.440999	3.128173	-0.219015
W	-0.734290	-0.004164	-0.026041
N	3.799509	0.440972	0.235858
O	4.862580	-0.258338	0.137133
O	3.841480	1.685703	0.483827

61

E = -919.004822 a.u.

C	0.798988	-1.400676	0.198325
C	0.799892	1.400606	-0.198166
C	2.178425	-1.236446	0.170255
H	0.526441	-2.455885	0.319889
C	2.179217	1.235200	-0.171800
H	0.528168	2.456095	-0.319158
C	2.827012	-0.000906	-0.001224
H	2.833309	2.095510	-0.292511
C	-1.776940	1.149643	-1.344925
O	-2.319486	1.797743	-2.175579
C	-1.548348	-1.447278	-1.210276
O	-2.000007	-2.270665	-1.929625
C	-1.549427	1.448806	1.210885
O	-2.002601	2.271849	1.929694
C	-1.777456	-1.148173	1.346178
O	-2.319664	-1.796109	2.177154
H	2.831889	-2.097266	0.290685
W	-0.793429	0.000659	0.000641
N	4.278046	-0.001469	-0.001802
O	4.903317	-1.110192	0.116292
O	4.904124	1.106723	-0.120317

62

E = -919.005594 a.u.

C	1.612860	0.497061	-0.008043
C	-0.720803	2.056465	-0.381054
C	2.251147	1.725583	-0.199477
C	0.205200	3.101173	-0.479492
H	-1.752474	2.434864	-0.398222
C	1.593550	2.942055	-0.413025
H	-0.157722	4.122673	-0.627320
H	2.217100	3.827571	-0.532390
C	-2.313418	-0.257259	-0.799443
O	-3.375880	-0.336599	-1.327747
C	0.009549	-1.265474	-1.581885
O	0.184060	-2.002643	-2.483564
C	-1.550149	0.438538	1.642262
O	-2.221101	0.657765	2.592832
C	-0.077327	-1.712891	1.058212
O	0.147067	-2.646426	1.751085
H	3.338954	1.743137	-0.175816
W	-0.478977	-0.036199	-0.014934
N	2.649871	-0.563528	0.178398
O	2.503065	-1.698265	-0.371293
O	3.659975	-0.304762	0.913867