

Electronic Supplementary Information

**A DFT-Based Mechanistic Proposal for the Light-Driven Insertion Of
Dioxygen Into A Pt(II)-C Bond**

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Contents

<i>S.1 Dinuclear mechanism.....</i>	<i>S2</i>
<i>S.2 High energy points with different basis sets.....</i>	<i>S3</i>
<i>S.3 Oxygen coordination.....</i>	<i>S3</i>
<i>S.4 Synthesis of palladium complexes analogous to 4.....</i>	<i>S4</i>
<i>S.5 UV-VIS experimental spectra for all complexes.....</i>	<i>S7</i>
<i>S.5 Computed Excitations of all complexes.....</i>	<i>S8</i>
<i>S.6 Cartesian coordinates of intermediates and transition states.....</i>	<i>S12</i>

S.1 Dinuclear Mechanism

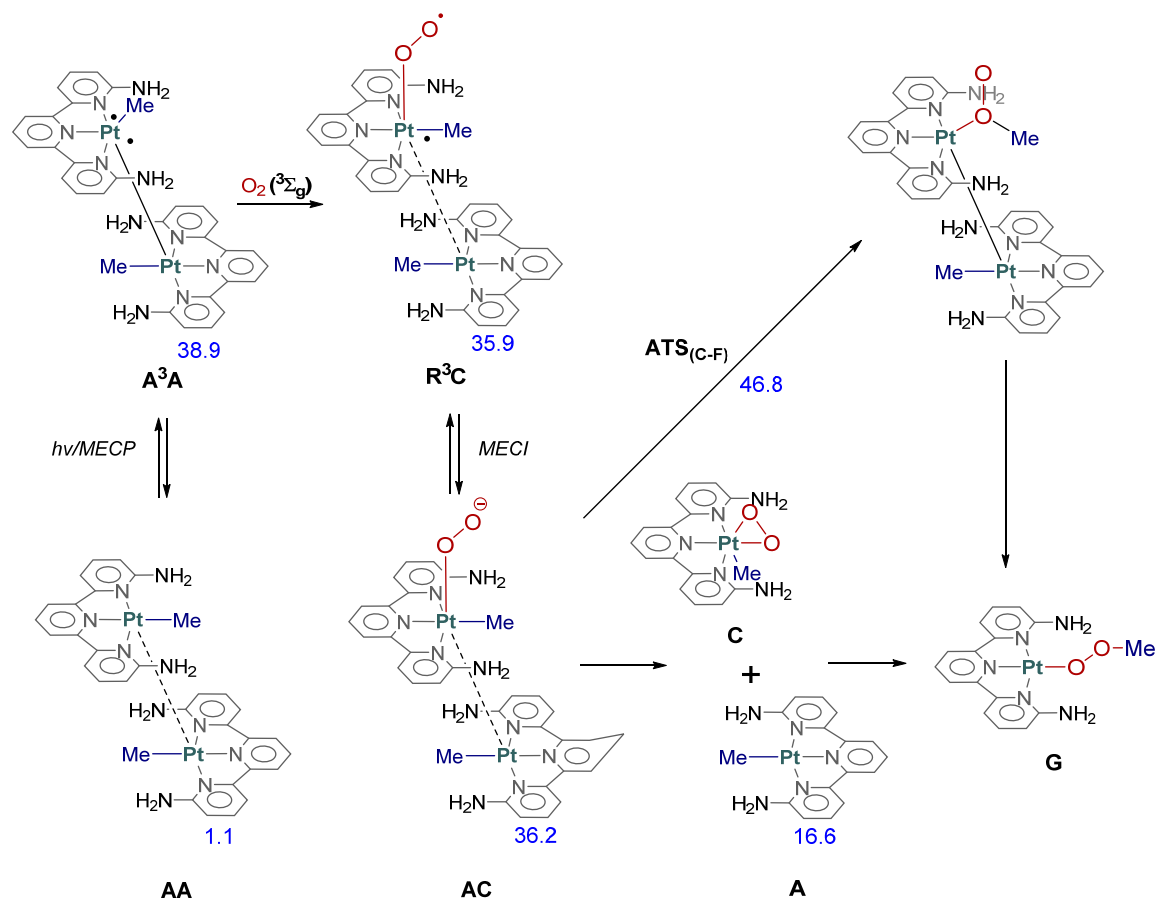


Figure S1. Free energy profile for the dinuclear methyl exchange M06/6-31G(d)/Lan12dz(f). All energies in kcal/mol.

The mechanism originally proposed by some of us consisted in the formation of bimolecular adducts which can show a CT band to create a vacancy for dioxygen to occupy. However, TD-DFT calculations found that the vertical spectrum of the dimer is very similar to that of the monomer. In addition, the complex RInt_{1b} can dissociate singlet oxygen without a significant barrier to return to reactants, showing no competitive formation of the methylperoxy product. Therefore, the mechanism involving the monomer remains a more plausible explanation for the insertion reaction.

S.2 High energy points with different basis sets

Table S1. Energy difference between the lowest migration transition state and the MECF. Relative free energies in kcal mol⁻¹. BS1 corresponds to 6-31+G* for light atoms and LANL2DZ(f) for Pt, and BS2 corresponds to 6-311++G** for light atoms and LANL2TZ(f) for Pt.

Complex/TS	BS1	BS2	ω B97-xD/BS2	Inserts O ₂
1/TS _(C-F)	0.5	1.5	-0.3	Yes
2/TS _(C-F)	3.0	4.1	8.1	No
4/TS _(C-G)	-1.6	-0.9	-3.5	Yes

Table S1 shows that the energy difference between the lowest energy productive pathway and unproductive one is not an artifact of the method. The trend is kept for all complexes when the basis set is increased, and when the functional is replaced. Thus, the results are robust within the dispersion-corrected DFT framework.

S.3 Coordination of oxygen

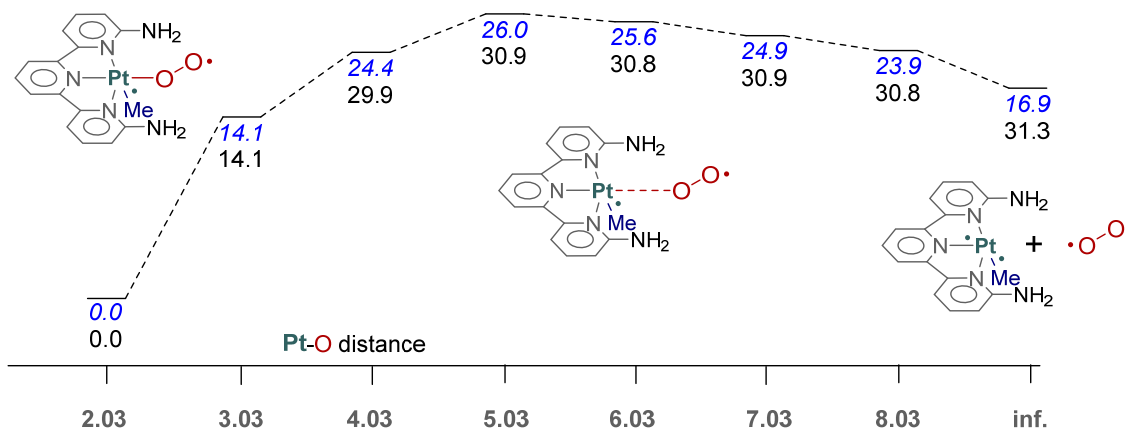


Figure S2. Gibbs free energies (blue) and potential energies (black) for the coordination of dioxygen to the excited triplet complex. All energies in kcal/mol, and distances in Å.

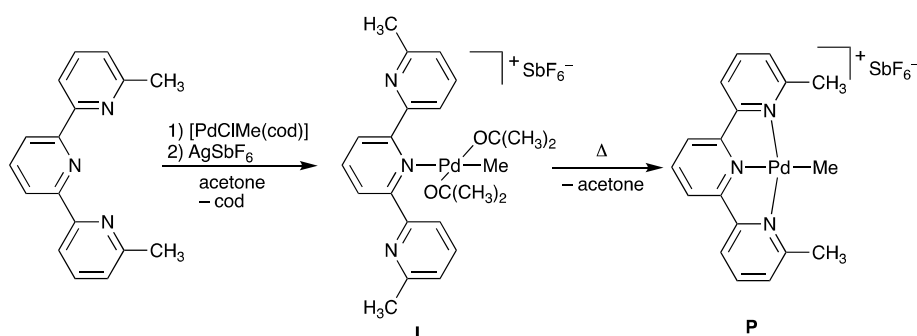
Coordination of dioxygen shows no barrier in the potential energy surface, evidencing the lack of a transition state. But the Gibbs energies show a maximum around 5 Å which indicates the entropic penalty of bringing both fragments together.

S.4 Synthesis of palladium complexes analogous to 4

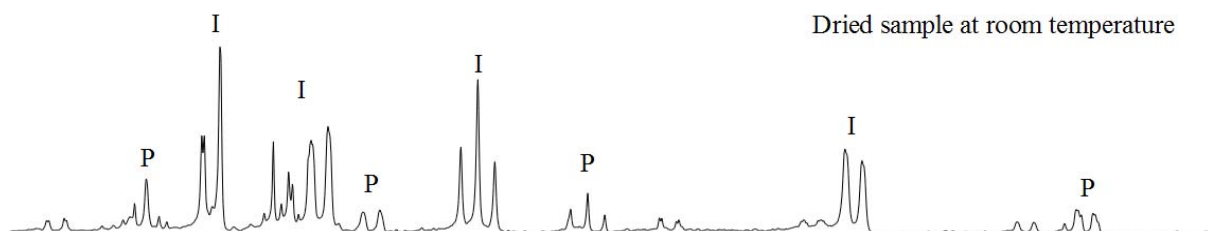
Synthesis of palladium complexes analogous to complex 4.

Reaction with [PdClMe(cod)]:

In acetone:



Chloro(1,5-cyclooctadiene)methylpalladium(II) (37.53 mg, 0.14 mmol) and AgSbF₆ (48.65g, 0.14 mmol) were dissolved in dry acetone (10 mL) and stirred for 20 minutes in the dark. A white precipitate was formed. The white solid was filtered and the remaining solution was transferred to a solution of 6,6''-dimethylterpyridine (37.00 mg, 0.14 mmol) in dry acetone (5 mL). The mixture was stirred for another 15 minutes. The solvent was removed under vacuum. The yellow solid was washed with dry dichloromethane (2 x 10 mL) and dried under vacuum. The ¹H NMR spectrum of the initial product in d₆-acetone at room temperature showed a mixture of the intermediate [PdMe(dimethylterpy)(acetone)₂]⁺ (I) and the product [PdMe(dimethylterpy)]⁺ (P), which upon heating is slowly converted over several days to the final product P, as shown in the series of ¹H NMR spectra shown below.



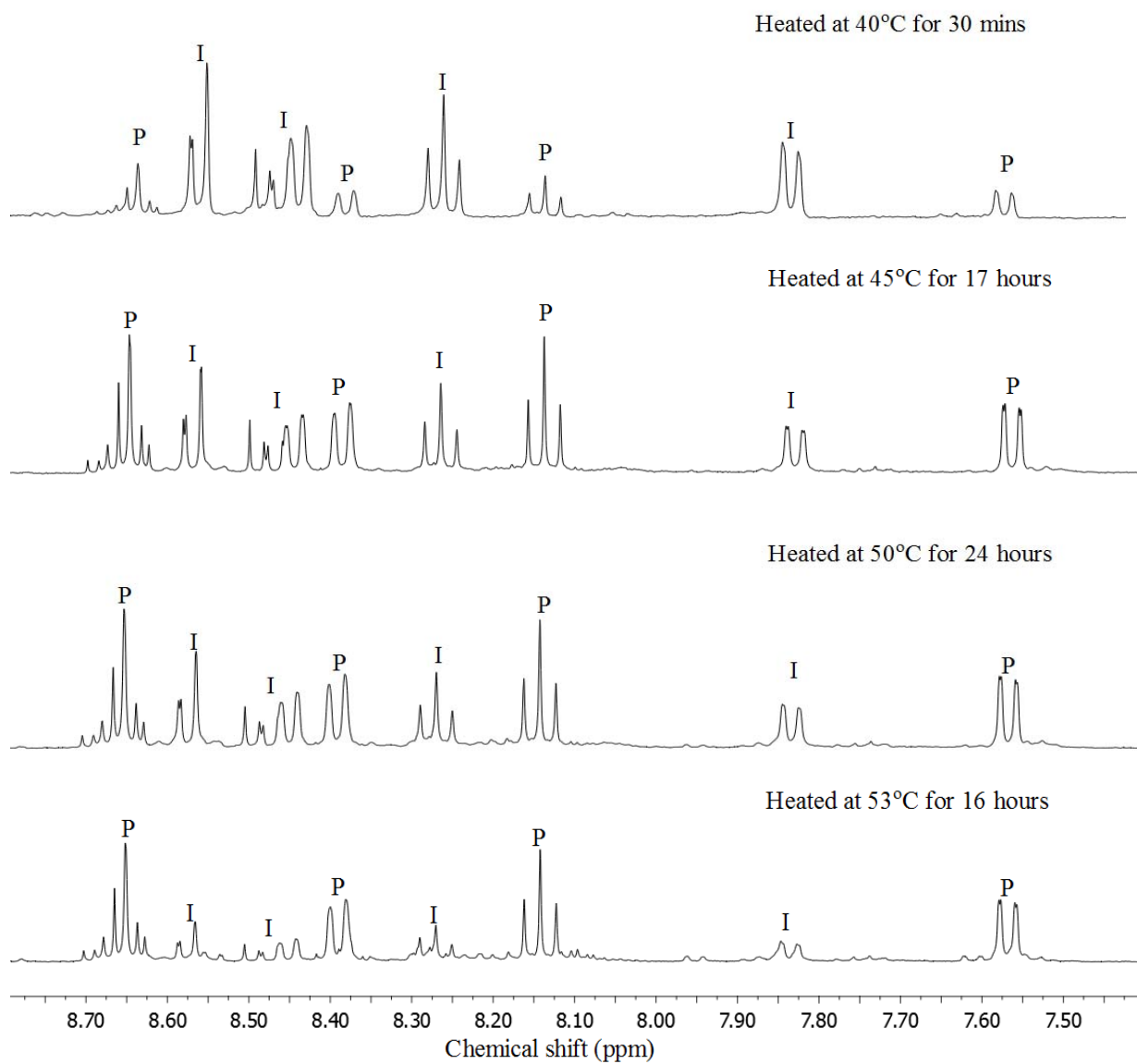
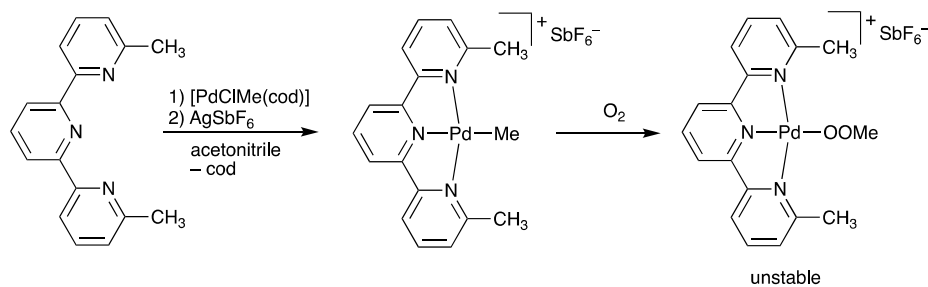


Figure S3. ^1H NMR spectra showing the conversion of intermediate complex $[\text{PdMe}(\text{dimethylterpy})(\text{acetone})_2]^+$ (I) to the product complex $[\text{PdMe}(\text{dimethylterpy})]^+$ (P) upon heating over time in d_6 -acetone at 298K.

In acetonitrile:



Chloro(1,5-cyclooctadiene)methylpalladium(II) (37.5 mg, 0.14 mmol) and AgSbF_6 (48.65 g, 0.14 mmol) were dissolved in dry acetonitrile (10 mL) and stirred for 20 minutes in the dark. A white precipitate was formed. The white solid was filtered and the remaining solution was transferred to a solution of 6,6''-dimethylterpyridine (37.00 mg, 0.14 mmol) in dry acetonitrile (10 mL). The mixture was stirred for another 15 minutes. The solvent was removed under vacuum. The yellow complex $[\text{PdMe}(6,6''\text{-dimethylterpyridine})]\text{SbF}_6$ was washed with dry dichloromethane (2 x 10 mL) and dried under vacuum (38.7 mg, 0.10 mmol, 72%). ^1H NMR (400 MHz, CD_3CN , 298K) δ 8.42 (t, $^3J_{\text{HH}} = 7.9$ Hz, 1H, H^1), 8.27 (d, $^3J_{\text{HH}} = 7.9$ Hz, 2H, H^2), 8.01 (d, $^3J_{\text{HH}} = 7.8$ Hz, 2H, H^3), 7.91 (dd, $^3J_{\text{HH}} = 7.8, 7.6$ Hz, 2H, H^4), 7.32 (d, $^3J_{\text{HH}} = 7.6$ Hz, 2H, H^5), 2.13 (s, 6H), 0.14 (s, 3H, H^7). ^{13}C NMR (100 MHz, CD_3CN , 298K) δ 162.93 (C), 156.95 (C), 156.75 (C), 142.05 (CH), 141.09 (CH), 128.73 (CH), 128.22 (CH), 124.98 (CH), 27.49 (CH₃), -3.27 (Pd-CH₃). HRMS (ESI+, TOF) m/z $[\text{M}+\text{H}]^+$ 382.0547, calcd: $[\text{C}_{18}\text{H}_{18}\text{N}_3\text{Pd}]^+$ 382.0535. Elem. Anal. Calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{PdSbF}_6$: C, 34.95; H, 2.933; N, 6.794. Found: C, 34.05; H, 3.05; N, 6.72.

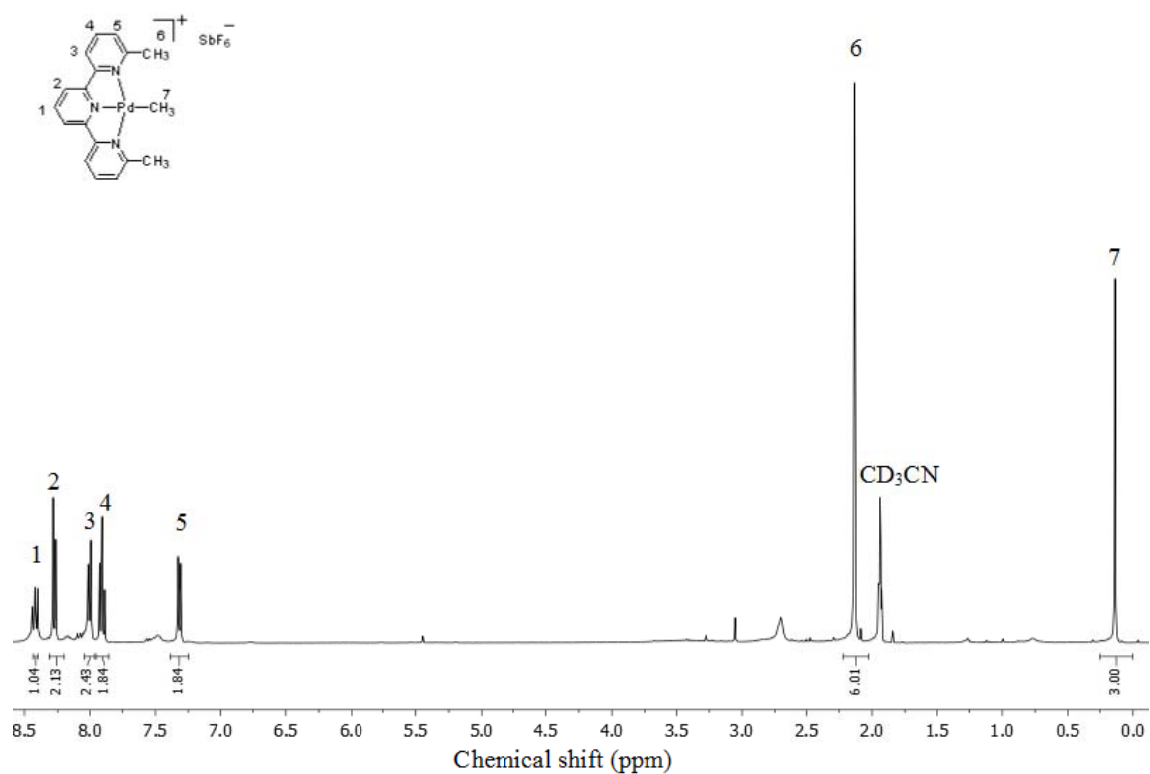


Figure S4. ^1H NMR spectrum of $[\text{PdMe}(6,6''\text{-dimethylterpyridine})]\text{SbF}_6$ in CD_3CN at 298K.

S.5 UV-VIS Experimental Spectra for all Complexes

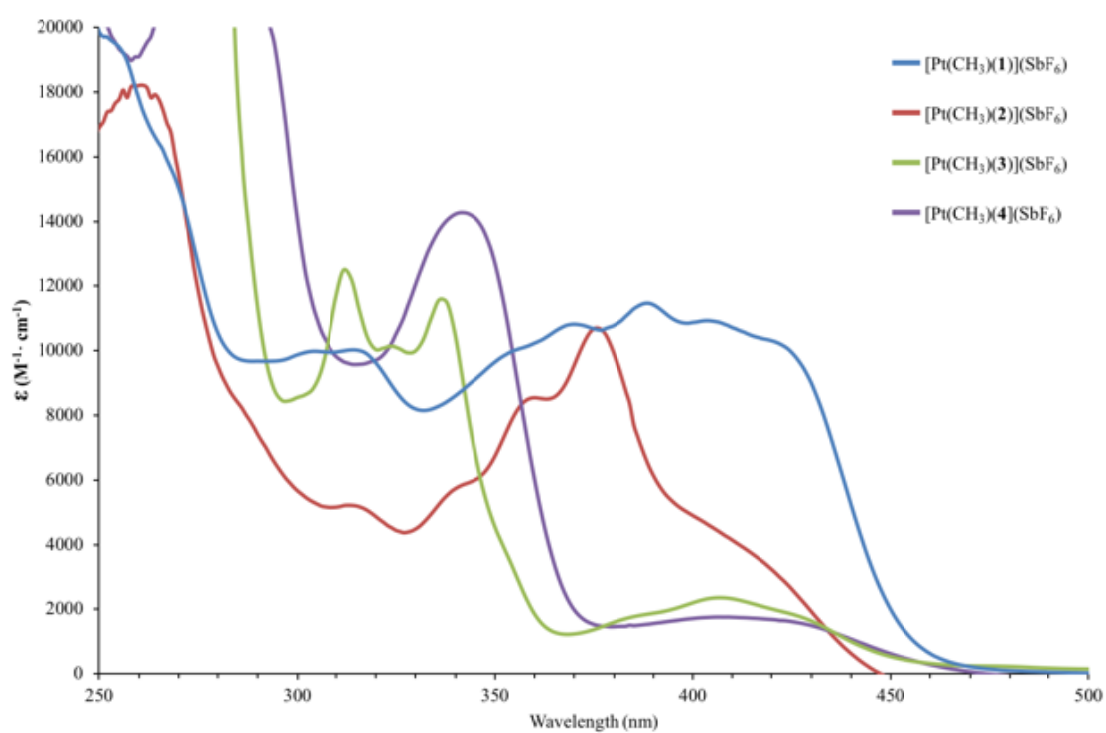


Figure S5. Absorption spectra for complexes 1-4 measured in acetonitrile at room temperature.

S.6 Computed Excitations for all Complexes

Complex 1

Excited State 1: Energy = 404 nm, $f = 0.1343$

HOMO-3 – LUMO 0.32

HOMO – LUMO 0.62

Excited State 2: Energy = 402 nm, $f = 0.0039$

HOMO-2 – LUMO 0.44

HOMO-1 – LUMO 0.54

Excited State 3: Energy = 384 nm, $f = 0.0066$

HOMO-2 – LUMO 0.52

HOMO-1 – LUMO 0.42

Excited State 4: Energy = 384 nm, $f = 0.0066$

HOMO-2 – LUMO 0.52

HOMO-1 – LUMO 0.42

Excited State 5: Energy = 364 nm, $f = 0.2789$

HOMO-3 – LUMO 0.59

HOMO – LUMO 0.30

Excited State 6: Energy = 363 nm, $f = 0.0034$

HOMO-3 – LUMO+1 0.59

HOMO – LUMO+1 0.30

Excited State 7: Energy = 351 nm, $f = 0.0262$

HOMO-2 – LUMO+1 0.70

Excited State 8: Energy = 337 nm, $f = 0.0048$

HOMO-4 – LUMO+2 0.15

Complex 2

Excited State 1: Energy = 416 nm, $f = 0.0080$

HOMO-1 – LUMO 0.59

HOMO – LUMO 0.59

Excited State 2: Energy = 401 nm, $f = 0.0372$

HOMO-3 – LUMO 0.40

HOMO-1 – LUMO 0.44

Excited State 3: Energy = 379 nm, $f = 0.0104$

HOMO-2 – LUMO 0.58

HOMO – LUMO 0.24

Excited State 4: Energy = 366 nm, $f = 0.0481$

HOMO-1 – LUMO+1 0.39

HOMO-1 – LUMO+1 0.56

Excited State 5: Energy = 358 nm, f = 0.2245
HOMO-3 – LUMO 0.48
HOMO – LUMO 0.24

Excited State 6: Energy = 354 nm, f = 0.0343
HOMO-1 – LUMO+1 0.50
HOMO – LUMO+1 0.34

Excited State 7: Energy = 350 nm, f = 0.0100
HOMO-4 – LUMO 0.67
HOMO-1 – LUMO+1 0.13

Excited State 8: Energy = 338 nm, f = 0.0312
HOMO-2 – LUMO 0.17
HOMO-2 – LUMO+1 0.62

Complex 3

Excited State 1: Energy = 432 nm, f = 0.0032
HOMO – LUMO 0.70

Excited State 2: Energy = 400 nm, f = 0.0102
HOMO-3 – LUMO 0.63
HOMO-1 – LUMO 0.31

Excited State 3: Energy = 389 nm, f = 0.0175
HOMO-2 – LUMO 0.31
HOMO-1 – LUMO 0.60

Excited State 4: Energy = 373 nm, f = 0.0000
HOMO-3 – LUMO 0.26
HOMO – LUMO+1 0.65

Excited State 5: Energy = 364 nm, f = 0.0000
HOMO-3 – LUMO 0.65
HOMO – LUMO+1 0.26

Excited State 6: Energy = 359 nm, f = 0.0227
HOMO-1 – LUMO+1 0.69

Excited State 7: Energy = 332 nm, f = 0.0725
HOMO-2 – LUMO+1 0.65
HOMO-1 – LUMO 0.16

Excited State 8: Energy = 320 nm, f = 0.0000
HOMO-5 – LUMO 0.41
HOMO-3 – LUMO+1 0.57

Complex 4

Excited State 1: Energy = 500 nm, f = 0.0000
HOMO-1 – LUMO+1 0.27
HOMO – LUMO 0.59

Excited State 2: Energy = 449 nm, f = 0.0000
HOMO-3 – LUMO 0.23
HOMO-2 – LUMO 0.61

Excited State 3: Energy = 439 nm, f = 0.0000
HOMO-3 – LUMO+1 0.35
HOMO – LUMO 0.36

Excited State 4: Energy = 428 nm, f = 0.0087
HOMO-1 – LUMO 0.32
HOMO – LUMO 0.62

Excited State 5: Energy = 427 nm, f = 0.0000
HOMO-3 – LUMO+1 0.20
HOMO-1 – LUMO 0.62

Excited State 6: Energy = 408 nm, f = 0.0000
HOMO-3 – LUMO 0.38
HOMO – LUMO+1 0.50

Excited State 7: Energy = 403 nm, f = 0.075
HOMO-2 – LUMO 0.70

Excited State 8: Energy = 400 nm, f = 0.0122
HOMO-2 – LUMO 0.62
HOMO-1 – LUMO+1 0.30

Excited State 9: Energy = 393 nm, f = 0.0000
HOMO – LUMO+2 0.28
HOMO – LUMO+4 0.56

Excited State 10: Energy = 385 nm, f = 0.0236
HOMO – LUMO+1 0.70

Excited State 11: Energy = 382 nm, f = 0.0000
HOMO-3 – LUMO 0.43
HOMO – LUMO+1 0.48

Excited State 12: Energy = 378 nm, f = 0.0000
HOMO-1 – LUMO+2 0.28
HOMO-1 – LUMO+4 0.57

Excited State 13: Energy = 369 nm, f = 0.0000
HOMO-2 – LUMO+4 0.50
HOMO-1 – LUMO+1 0.26

Excited State 14: Energy = 363 nm, f = 0.0000

HOMO-4 – LUMO 0.30
HOMO-1 – LUMO+1 0.56

Excited State 15: Energy = 359 nm, $f = 0.0048$
HOMO-3 – LUMO 0.14
HOMO-1 – LUMO+1 0.68

Excited State 16: Energy = 356 nm, $f = 0.0000$
HOMO-3 – LUMO+1 0.37
HOMO-2 – LUMO+1 0.53

Excited State 17: Energy = 355 nm, $f = 0.0000$
HOMO-4 – LUMO 0.62
HOMO-1 – LUMO+1 0.30

Excited State 18: Energy = 353 nm, $f = 0.0105$
HOMO-4 – LUMO 0.53
HOMO-3 – LUMO 0.26

Excited State 19: Energy = 363 nm, $f = 0.0003$
HOMO-2 – LUMO+1 0.39
HOMO-1 – LUMO+4 0.45

Excited State 20: Energy = 344 nm, $f = 0.0506$
HOMO-3 – LUMO+1 0.50
HOMO – LUMO+4 0.35

Excited State 21: Energy = 334 nm, $f = 0.0029$
HOMO-2 – LUMO+2 0.29
HOMO-2 – LUMO+4 0.55

S.7 Cartesian Coordinates Of Intermediates and Transition States

Complex 1 a

E = -1011.536139

Number of negative frequencies = 0

N	-1.491187	-1.927513	0.044681
C	-0.627875	-2.967015	0.059675
C	-2.833958	-2.188658	0.239653
C	-1.092606	-4.302830	0.132409
C	-3.325376	-3.470614	0.344380
C	-2.433423	-4.549197	0.264469
H	-0.364645	-5.109774	0.093590
H	-4.386225	-3.642227	0.498961
H	-2.801638	-5.570313	0.329116
N	-3.066269	0.158160	0.338599
C	-3.715408	-1.015024	0.356276
C	-3.683940	1.348442	0.346474
C	-5.103923	-1.024901	0.467100
C	-5.071667	1.395887	0.457137
C	-5.771872	0.194942	0.529969
H	-5.663815	-1.955678	0.489692
H	-5.606238	2.341628	0.472374
H	-6.855495	0.210095	0.616620
N	-1.435607	2.199060	0.031524
C	-0.544726	3.215055	0.040397
C	-2.771458	2.496998	0.220305
C	-0.974020	4.563492	0.095982
C	-3.228922	3.792591	0.310021
C	-2.308505	4.846258	0.220004
H	-0.224729	5.350421	0.049596
H	-4.285151	3.993821	0.460296
H	-2.649339	5.877624	0.270450
C	0.766984	0.103764	-1.086241
H	0.857145	0.985499	-1.737295
H	1.657971	0.094244	-0.432113
H	0.834590	-0.783878	-1.732111
Pt	-1.093612	0.130135	-0.149013
N	0.773398	2.938127	-0.025127
H	1.436598	3.680222	0.154299
H	1.085045	1.990471	0.149590
N	0.697175	-2.728098	-0.015877
H	1.037443	-1.788578	0.148617
H	1.339083	-3.487662	0.168321

Dioxygen

E = -150.251917

Number of negative frequencies = 0

O	0.896263	1.251748	0.000000
O	-0.309611	1.251748	0.000000

Complex 1 ³a

Number of negative frequencies = 0

E = -1011.464600

N	-1.545966	-2.068375	-0.470338
C	-0.736613	-3.129659	-0.618629
C	-2.770538	-2.231010	0.099882
C	-1.137585	-4.417986	-0.209173
C	-3.215252	-3.468161	0.537065
C	-2.376807	-4.575422	0.371200
H	-0.465729	-5.260545	-0.358332
H	-4.182293	-3.579344	1.018857
H	-2.701189	-5.557899	0.707387
N	-2.940626	0.158756	0.124621
C	-3.589845	-1.013338	0.252205
C	-3.557003	1.348698	0.248397
C	-4.958129	-1.019003	0.516415
C	-4.925063	1.391705	0.511568
C	-5.623127	0.195969	0.640175
H	-5.504931	-1.954579	0.597564
H	-5.446821	2.341519	0.590890
H	-6.694304	0.211244	0.826197
N	-1.471799	2.347440	-0.445992
C	-0.632080	3.387097	-0.577889
C	-2.703834	2.544108	0.098478
C	-1.012859	4.688836	-0.191592
C	-3.128010	3.795410	0.515215
C	-2.261381	4.881580	0.356621
H	-0.316797	5.513381	-0.330294
H	-4.101734	3.933711	0.975900
H	-2.570182	5.874926	0.675032
C	0.619551	0.070808	0.883986
H	1.583191	0.055856	0.349455
H	0.560587	0.965088	1.516414
H	0.517611	-0.838625	1.488725
Pt	-0.920336	0.129010	-0.569230
N	0.586140	3.162261	-1.148854
H	1.297810	3.870869	-1.018888
H	0.935721	2.209482	-1.141651
N	0.466954	-2.935192	-1.229062
H	0.822037	-1.984704	-1.260754
H	1.175037	-3.648934	-1.108771

Complex 1 c

E = -1161.78191466

Number of negative frequencies = 0

N	-1.477591	-1.887543	0.136851
C	-0.575020	-2.896332	0.103117
C	-2.828881	-2.164749	0.236839
C	-1.025951	-4.240654	0.192594
C	-3.291999	-3.454709	0.320457
C	-2.362596	-4.509839	0.300770
H	-0.283673	-5.035052	0.171134
H	-4.355389	-3.655466	0.407553
H	-2.708528	-5.538182	0.371173

N	-3.088931	0.183874	0.240588
C	-3.725449	-0.999949	0.227916
C	-3.694349	1.377682	0.131051
C	-5.115334	-1.007221	0.163123
C	-5.083758	1.415671	0.058406
C	-5.783523	0.212559	0.088539
H	-5.673458	-1.938923	0.153207
H	-5.615427	2.359136	-0.026465
H	-6.868968	0.224289	0.033453
N	-1.425356	2.207706	0.216403
C	-0.518048	3.201256	0.371395
C	-2.768332	2.518071	0.104442
C	-0.928113	4.553481	0.217086
C	-3.202539	3.816727	0.005502
C	-2.249553	4.850769	0.027025
H	-0.172153	5.332580	0.283688
H	-4.261426	4.040566	-0.079631
H	-2.568014	5.885299	-0.075275
C	-1.335961	0.136690	-1.932185
H	-1.685496	1.126218	-2.242942
H	-0.335974	-0.074596	-2.326487
H	-2.047415	-0.644748	-2.216801
Pt	-1.098701	0.146727	0.133611
O	0.657699	0.216007	1.639547
O	0.878718	0.099227	0.239030
N	0.723409	-2.609173	-0.039820
H	1.043999	-1.631204	0.049633
H	1.397828	-3.359246	0.033363
N	0.751519	2.891152	0.662044
H	0.951394	1.967485	1.071650
H	1.381959	3.650668	0.884828

Complex 1 e

E = -1161.774290

Number of negative frequencies = 0

N	-1.488852	-1.887913	0.204179
C	-0.595882	-2.913122	0.220976
C	-2.846794	-2.161179	0.151277
C	-1.076978	-4.256146	0.191855
C	-3.329633	-3.444755	0.124625
C	-2.415741	-4.515307	0.147204
H	-0.343947	-5.059651	0.199826
H	-4.398542	-3.630887	0.092282
H	-2.776790	-5.540684	0.124247
N	-3.132997	0.184576	0.192923
C	-3.754003	-1.001542	0.148929
C	-3.745684	1.378386	0.210263
C	-5.146783	-1.018630	0.123538
C	-5.136333	1.409141	0.191696
C	-5.823832	0.197560	0.149483
H	-5.700758	-1.952331	0.091623
H	-5.681847	2.348298	0.210825

H	-6.910756	0.202428	0.136692
N	-1.478041	2.237944	0.257407
C	-0.564228	3.235681	0.187267
C	-2.828734	2.530748	0.227561
C	-1.002450	4.587284	0.138788
C	-3.280659	3.826290	0.185236
C	-2.339740	4.872090	0.148275
H	-0.251043	5.372048	0.091208
H	-4.344937	4.039649	0.167461
H	-2.678288	5.904834	0.116290
C	-0.945773	0.225570	-1.753052
H	-1.312646	1.194024	-2.106865
H	0.137189	0.081923	-1.871845
H	-1.543215	-0.600972	-2.150588
Pt	-1.116446	0.179657	0.292815
O	1.672089	-0.319576	-0.394291
O	0.859055	0.256902	0.595349
N	0.713070	-2.670957	0.292105
H	1.158267	-1.742782	-0.000622
H	1.312353	-3.485924	0.235705
N	0.735590	2.927700	0.147485
H	1.038507	1.949618	0.296487
H	1.417350	3.674322	0.157115

Complex 1 TS₁

E = -1161.741991

Number of negative frequencies = 1

N	-1.705954	-1.918540	0.406641
C	-0.843030	-2.960866	0.489616
C	-3.046437	-2.181506	0.196175
C	-1.310002	-4.294074	0.350255
C	-3.531633	-3.460036	0.057033
C	-2.637301	-4.538454	0.133520
H	-0.584972	-5.101549	0.419622
H	-4.589580	-3.634326	-0.110711
H	-2.999562	-5.557753	0.024840
N	-3.296372	0.173326	0.217411
C	-3.930546	-1.013510	0.139976
C	-3.935549	1.357287	0.216930
C	-5.317439	-1.036416	0.043338
C	-5.324835	1.377607	0.130806
C	-6.008756	0.170795	0.042391
H	-5.858165	-1.976323	-0.014118
H	-5.872250	2.315292	0.138459
H	-7.093753	0.169935	-0.021230
N	-1.699640	2.253496	0.413520
C	-0.830819	3.294747	0.366377
C	-3.048880	2.521433	0.285402
C	-1.309604	4.628743	0.261315
C	-3.545808	3.799184	0.172506
C	-2.650243	4.878455	0.171380
H	-0.580146	5.435596	0.255658

H	-4.612590	3.969906	0.070061
H	-3.019818	5.897991	0.092539
C	0.448504	0.224787	-1.136257
H	1.331058	0.824172	-0.936071
H	0.633261	-0.828997	-1.335126
H	-0.291445	0.702587	-1.782389
Pt	-1.338491	0.146271	0.513400
O	1.231207	0.900886	1.709590
O	0.629172	-0.076261	0.983901
N	0.492951	3.065115	0.371928
H	0.862001	2.224812	0.879404
H	1.076555	3.890128	0.446743
N	0.468725	-2.743009	0.674538
H	0.813760	-1.819766	0.944573
H	1.067193	-3.539430	0.849762

Complex 1 TS₃

E = -1161.774290

Number of negative frequencies = 1

N	-1.488852	-1.887913	0.204179
C	-0.595882	-2.913122	0.220976
C	-2.846794	-2.161179	0.151277
C	-1.076978	-4.256146	0.191855
C	-3.329633	-3.444755	0.124625
C	-2.415741	-4.515307	0.147204
H	-0.343947	-5.059651	0.199826
H	-4.398542	-3.630887	0.092282
H	-2.776790	-5.540684	0.124247
N	-3.132997	0.184576	0.192923
C	-3.754003	-1.001542	0.148929
C	-3.745684	1.378386	0.210263
C	-5.146783	-1.018630	0.123538
C	-5.136333	1.409141	0.191696
C	-5.823832	0.197560	0.149483
H	-5.700758	-1.952331	0.091623
H	-5.681847	2.348298	0.210825
H	-6.910756	0.202428	0.136692
N	-1.478041	2.237944	0.257407
C	-0.564228	3.235681	0.187267
C	-2.828734	2.530748	0.227561
C	-1.002450	4.587284	0.138788
C	-3.280659	3.826290	0.185236
C	-2.339740	4.872090	0.148275
H	-0.251043	5.372048	0.091208
H	-4.344937	4.039649	0.167461
H	-2.678288	5.904834	0.116290
C	-0.945773	0.225570	-1.753052
H	-1.312646	1.194024	-2.106865
H	0.137189	0.081923	-1.871845
H	-1.543215	-0.600972	-2.150588
Pt	-1.116446	0.179657	0.292815
O	1.672089	-0.319576	-0.394291

O	0.859055	0.256902	0.595349
N	0.713070	-2.670957	0.292105
H	1.158267	-1.742782	-0.000622
H	1.312353	-3.485924	0.235705
N	0.735590	2.927700	0.147485
H	1.038507	1.949618	0.296487
H	1.417350	3.674322	0.157115

Complex 1 f

scf done: -1161.824387

Number of negative frequencies = 0

N	-1.875130	-1.930435	0.269194
C	-1.011434	-2.972660	0.287301
C	-3.228601	-2.192691	0.312886
C	-1.494175	-4.307826	0.311304
C	-3.735088	-3.469987	0.345853
C	-2.839358	-4.550981	0.337821
H	-0.768632	-5.117821	0.311089
H	-4.806231	-3.640919	0.382175
H	-3.213565	-5.571542	0.358958
N	-3.442313	0.165410	0.329144
C	-4.098508	-1.013527	0.332353
C	-4.064945	1.361328	0.322101
C	-5.488509	-1.013969	0.352984
C	-5.455115	1.400479	0.342441
C	-6.160928	0.203308	0.362425
H	-6.044130	-1.946845	0.359685
H	-5.983844	2.348934	0.343285
H	-7.247457	0.218728	0.381401
N	-1.813200	2.207285	0.312019
C	-0.915581	3.223099	0.359812
C	-3.158982	2.511600	0.296854
C	-1.364468	4.572519	0.298358
C	-3.628533	3.802196	0.264695
C	-2.699889	4.856397	0.248476
H	-0.616614	5.362268	0.312543
H	-4.694700	4.004891	0.251592
H	-3.042749	5.887647	0.213077
C	1.191911	0.271515	-1.204750
H	1.135766	1.345588	-1.415615
H	2.234831	-0.060900	-1.163552
H	0.630083	-0.302015	-1.952593
Pt	-1.500661	0.133373	0.247081
O	1.355637	0.548314	1.141299
O	0.593024	-0.026237	0.059433
N	0.311357	-2.750412	0.269965
H	0.683286	-1.804601	0.339911
H	0.944447	-3.532527	0.365479
N	0.393618	2.960449	0.442757
H	0.774382	2.044155	0.792365
H	1.009742	3.758856	0.532316

Complex 1 TS₄

E = -1161.813915

Number of negative frequencies = 1

N	-1.711847	-1.957075	0.415359
C	-0.829544	-2.971135	0.583409
C	-3.063564	-2.226305	0.400852
C	-1.299147	-4.313263	0.592218
C	-3.555718	-3.508876	0.437791
C	-2.640376	-4.573132	0.511043
H	-0.570193	-5.114997	0.686941
H	-4.625265	-3.695163	0.423344
H	-2.999646	-5.599364	0.527038
N	-3.258100	0.133409	0.404728
C	-3.927240	-1.043105	0.377939
C	-3.867657	1.340395	0.346561
C	-5.316378	-1.024032	0.336545
C	-5.255938	1.391119	0.303723
C	-5.975726	0.200826	0.306404
H	-5.880340	-1.952220	0.319376
H	-5.770598	2.346977	0.260528
H	-7.061615	0.227872	0.273347
N	-1.608198	2.126546	0.367472
C	-0.669876	3.088937	0.526393
C	-2.941331	2.473437	0.346601
C	-1.055496	4.456168	0.519166
C	-3.355734	3.783952	0.363178
C	-2.379544	4.792777	0.427100
H	-0.281014	5.214521	0.608527
H	-4.412042	4.034234	0.343014
H	-2.677686	5.838555	0.428449
C	1.465223	0.561898	-1.582434
H	1.306344	1.640309	-1.453593
H	2.527246	0.316944	-1.446059
H	1.130549	0.248080	-2.577485
Pt	-1.338784	0.074397	0.282373
O	1.190379	0.008330	0.704663
O	0.709543	-0.200559	-0.662339
N	0.470888	-2.704668	0.748670
H	0.837700	-1.740924	0.835529
H	1.110115	-3.476871	0.879602
N	0.609669	2.731894	0.688448
H	0.896048	1.739517	0.798070
H	1.306754	3.454063	0.811532

Complex 1 g

E = -1161.857978

Number of negative frequencies = 0

N	-2.235106	-1.879437	0.223160
C	-1.352633	-2.891237	0.061125
C	-3.564525	-2.168647	0.440404
C	-1.791815	-4.239954	0.135191
C	-4.029187	-3.460183	0.519144

C	-3.113057	-4.514421	0.364641
H	-1.059697	-5.033348	0.002175
H	-5.081546	-3.663031	0.693045
H	-3.455550	-5.544963	0.421508
N	-3.819244	0.181886	0.447642
C	-4.448882	-1.002867	0.571868
C	-4.442073	1.373348	0.538699
C	-5.821155	-1.017378	0.799338
C	-5.814306	1.401968	0.765198
C	-6.496278	0.195777	0.892856
H	-6.359616	-1.954856	0.903465
H	-6.348021	2.344757	0.842612
H	-7.568781	0.201460	1.069770
N	-2.223434	2.225494	0.162394
C	-1.335226	3.226722	-0.032230
C	-3.550658	2.529449	0.374387
C	-1.765217	4.579777	0.006900
C	-4.006330	3.825840	0.418790
C	-3.083650	4.869344	0.233283
H	-1.027891	5.364097	-0.149157
H	-5.056571	4.041132	0.590181
H	-3.418635	5.903459	0.263672
C	2.129681	0.181928	1.007546
H	2.454929	1.070718	0.445063
H	2.568728	0.200656	2.011274
H	2.455304	-0.726687	0.477976
Pt	-1.887483	0.172738	0.163870
O	0.737174	0.185725	1.206832
O	0.152462	0.163113	-0.124460
N	-0.051395	2.918629	-0.258799
H	0.617326	3.655700	-0.433204
H	0.237646	1.934653	-0.331399
N	-0.065433	-2.597080	-0.165621
H	0.598622	-3.342364	-0.322030
H	0.228603	-1.617517	-0.270256

Complex 1 CP1

E = -1161.73962631

Number of negative frequencies = 3

N	-1.852010	-1.942952	0.404516
C	-0.994302	-2.991675	0.396900
C	-3.207546	-2.200235	0.366754
C	-1.483540	-4.325351	0.373768
C	-3.718175	-3.476214	0.331844
C	-2.829092	-4.562660	0.339230
H	-0.761427	-5.139115	0.375867
H	-4.790250	-3.640783	0.301029
H	-3.208643	-5.581444	0.317142
N	-3.430372	0.157714	0.402007
C	-4.081261	-1.021288	0.360952
C	-4.056734	1.349640	0.392657
C	-5.471218	-1.027635	0.313307

C	-5.446591	1.387205	0.350653
C	-6.147463	0.187559	0.312086
H	-6.026331	-1.960207	0.277418
H	-5.981513	2.332718	0.346284
H	-7.233449	0.199506	0.277292
N	-1.806980	2.214864	0.448789
C	-0.925663	3.242351	0.416888
C	-3.154385	2.505046	0.402196
C	-1.380358	4.583805	0.327062
C	-3.635098	3.791877	0.334348
C	-2.720620	4.854724	0.293519
H	-0.637702	5.378593	0.300080
H	-4.703283	3.980760	0.302103
H	-3.074309	5.881260	0.239494
C	1.077531	0.346800	-1.745247
H	0.541971	1.283361	-1.865363
H	2.137816	0.360503	-1.515258
H	0.608245	-0.579958	-2.062276
Pt	-1.467730	0.125379	0.471165
O	1.217094	0.595396	1.497563
O	0.573408	-0.079177	0.557098
N	0.396980	2.992043	0.435432
H	1.002533	3.796703	0.541165
H	0.743616	2.129637	0.879037
N	0.331008	-2.782900	0.387994
H	0.722092	-1.845375	0.487364
H	0.950512	-3.575906	0.479444

Complex 1 TS₅

E = -1161.749414

Number of negative frequencies = 1

N	0.371805	-2.107823	-0.616427
C	0.464087	-3.219224	0.145345
C	-0.275298	-2.189142	-1.837848
C	0.021796	-4.474324	-0.344772
C	-0.735460	-3.384310	-2.337737
C	-0.562883	-4.552807	-1.579101
H	0.145616	-5.351987	0.285044
H	-1.243674	-3.420486	-3.296477
H	-0.914531	-5.508380	-1.960842
N	-0.123190	0.166402	-1.865161
C	-0.471241	-0.921743	-2.563767
C	-0.121689	1.411229	-2.360904
C	-0.949947	-0.767180	-3.862792
C	-0.590906	1.622750	-3.655108
C	-1.016683	0.519740	-4.391358
H	-1.245937	-1.622805	-4.463214
H	-0.611746	2.615166	-4.096501
H	-1.385801	0.663141	-5.404026
N	0.920250	1.965146	-0.238442
C	1.259606	2.856403	0.716278
C	0.405456	2.429127	-1.434224

C	1.269205	4.244635	0.435890
C	0.359763	3.772014	-1.729816
C	0.833591	4.692473	-0.782787
H	1.603545	4.932017	1.209279
H	-0.050030	4.115997	-2.674521
H	0.825302	5.756876	-1.004919
C	2.393058	-0.446737	1.315997
H	2.956939	-1.355056	1.063070
H	3.084788	0.404657	1.282410
H	2.020186	-0.536184	2.349377
Pt	0.929540	-0.142753	-0.132956
O	-0.666319	-0.109377	1.512993
O	-1.485541	0.843590	1.381465
N	1.613828	2.413520	1.941067
H	1.702524	3.095135	2.683959
H	1.315061	1.487368	2.227522
N	0.996440	-3.139757	1.377650
H	1.164264	-2.238817	1.806896
H	0.960818	-3.945589	1.987416

Complex 1 ³c

E = -1161.767180

Number of negative frequencies = 0

N	-0.074132	-2.273398	-0.304592
C	0.085079	-3.437914	0.341122
C	-0.252861	-2.251659	-1.646489
C	0.053445	-4.662992	-0.365241
C	-0.282886	-3.414859	-2.395918
C	-0.126595	-4.637324	-1.727639
H	0.176913	-5.598937	0.175461
H	-0.397436	-3.393473	-3.475137
H	-0.140126	-5.567162	-2.292111
N	-0.019612	0.159745	-1.549779
C	-0.391411	-0.917965	-2.274784
C	-0.064485	1.409683	-2.056405
C	-0.879921	-0.748951	-3.568374
C	-0.550659	1.619267	-3.345160
C	-0.967959	0.530895	-4.097793
H	-1.213797	-1.604233	-4.147784
H	-0.626300	2.623402	-3.751108
H	-1.369805	0.680547	-5.096890
N	0.593251	2.224961	0.113348
C	1.065566	3.159221	0.951696
C	0.426615	2.510244	-1.199250
C	1.382264	4.456499	0.484222
C	0.724245	3.757474	-1.721372
C	1.209099	4.741435	-0.849149
H	1.756438	5.202557	1.182145
H	0.613678	3.972720	-2.779593
H	1.452317	5.730719	-1.230869
C	2.388727	-0.443158	0.073985
H	2.692658	-1.312953	0.669223

H	2.506013	-0.638679	-0.997439
H	2.936341	0.457350	0.375823
Pt	0.414108	-0.113479	0.476835
O	0.844284	-0.573250	2.436863
O	0.289132	0.215849	3.306157
N	0.238806	-3.413479	1.688050
H	0.446048	-2.535233	2.157668
H	0.537182	-4.257108	2.159659
N	1.261975	2.813277	2.248355
H	0.789794	1.986491	2.618079
H	1.440425	3.552279	2.916177

Complex 1 h

E = -1161.749920

Number of negative frequencies = 0

N	0.371646	-2.107500	-0.593037
C	0.440145	-3.215705	0.175061
C	-0.272644	-2.184818	-1.815745
C	0.016812	-4.472076	-0.325029
C	-0.730321	-3.379559	-2.319899
C	-0.553811	-4.549896	-1.566483
H	0.134000	-5.350306	0.305459
H	-1.237570	-3.415597	-3.279200
H	-0.895486	-5.505975	-1.955755
N	-0.086478	0.167340	-1.851468
C	-0.476844	-0.915104	-2.534739
C	-0.115166	1.414174	-2.334778
C	-1.018102	-0.752382	-3.807882
C	-0.647594	1.635619	-3.602754
C	-1.107304	0.537680	-4.325531
H	-1.349989	-1.602995	-4.396565
H	-0.694086	2.631886	-4.033412
H	-1.526611	0.687931	-5.317441
N	0.998208	1.959042	-0.242851
C	1.377397	2.852008	0.695901
C	0.441384	2.427039	-1.421110
C	1.361769	4.243734	0.417840
C	0.379646	3.768536	-1.713020
C	0.878684	4.691676	-0.781064
H	1.727455	4.928842	1.178690
H	-0.062948	4.111545	-2.643261
H	0.857499	5.756106	-1.002131
C	2.435917	-0.500992	1.325191
H	2.929782	-1.458417	1.112642
H	3.187057	0.297535	1.268772
H	2.056162	-0.538558	2.360099
Pt	1.001716	-0.151421	-0.138449
O	-0.617820	-0.022035	1.424103
O	-1.755441	0.185784	0.908204
N	0.941837	-3.130514	1.423568
H	0.977020	-2.223709	1.873423
H	0.837625	-3.928580	2.036767

N	1.815546	2.422867	1.895434
H	1.937176	3.101875	2.637033
H	1.578537	1.489999	2.211369

Complex 1 TS₆

E = -1161.754157

Number of negative frequencies = 1

N	0.149267	-2.116159	-0.342000
C	0.279346	-3.257164	0.371871
C	-0.395196	-2.177843	-1.610613
C	-0.147127	-4.498063	-0.163446
C	-0.834794	-3.363348	-2.156689
C	-0.707341	-4.544597	-1.412597
H	-0.023054	-5.395678	0.438182
H	-1.283308	-3.376804	-3.145601
H	-1.053380	-5.490074	-1.823813
N	-0.292085	0.193461	-1.652697
C	-0.437849	-0.921300	-2.381814
C	-0.066287	1.402642	-2.185423
C	-0.524306	-0.822132	-3.769020
C	-0.137889	1.561287	-3.568176
C	-0.399670	0.438095	-4.350201
H	-0.642110	-1.704134	-4.393037
H	0.039084	2.524683	-4.038777
H	-0.451691	0.537892	-5.431617
N	0.672268	2.011394	0.052423
C	1.038198	2.922554	0.980275
C	0.322022	2.440430	-1.211969
C	1.141076	4.293698	0.644634
C	0.368680	3.772275	-1.562290
C	0.803972	4.710629	-0.616664
H	1.471860	4.995212	1.406849
H	0.065645	4.091097	-2.555128
H	0.858353	5.764587	-0.878916
C	2.559986	-0.312370	0.136811
H	2.816789	-1.349013	0.379860
H	2.826399	-0.069790	-0.898372
H	3.019726	0.388162	0.841903
Pt	0.518499	-0.105176	0.295607
O	0.973644	-0.592589	2.591830
O	0.309971	0.104558	3.449260
N	0.861451	-3.223304	1.588401
H	0.943652	-2.350118	2.109447
H	0.823365	-4.064985	2.148723
N	1.345935	2.502312	2.227215
H	0.908269	1.652594	2.591864
H	1.482650	3.224888	2.923900

Complex 1 TS₂

E = -1161.727339

Number of negative frequencies = 1

N	1.646633	-1.624496	-1.505280
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C	2.707476	-2.435459	-1.314320
C	1.279137	-1.255515	-2.765604
C	3.476062	-2.865125	-2.417334
C	1.996064	-1.653007	-3.873960
C	3.120718	-2.466807	-3.683127
H	4.334605	-3.508972	-2.242257
H	1.696815	-1.352693	-4.873100
H	3.705756	-2.792350	-4.539996
N	-0.531634	-0.213369	-1.625732
C	0.059396	-0.443926	-2.822322
C	-1.686622	0.480372	-1.558639
C	-0.484448	0.055436	-4.000100
C	-2.260601	1.014037	-2.709842
C	-1.651200	0.804495	-3.939345
H	-0.001897	-0.131651	-4.954767
H	-3.194859	1.564482	-2.630689
H	-2.089908	1.207372	-4.848940
N	-2.549469	-0.500211	0.444144
C	-3.136536	-0.416775	1.641565
C	-2.348986	0.634603	-0.242059
C	-3.550236	0.815832	2.191766
C	-2.734177	1.891102	0.203140
C	-3.346532	1.966728	1.460112
H	-4.018904	0.844598	3.174029
H	-2.543312	2.781333	-0.392126
H	-3.657692	2.929740	1.860752
C	2.526684	0.382377	0.930437
H	2.685649	0.603631	-0.126690
H	2.119669	1.196160	1.524649
H	3.308660	-0.214982	1.391255
Pt	0.565029	-0.783215	0.052236
O	0.049035	-0.146553	1.911885
O	1.239838	-0.864798	1.922638
N	-3.283771	-1.584790	2.344600
H	-3.987811	-1.612472	3.071554
H	-3.204566	-2.437662	1.802916
N	3.047103	-2.785538	-0.050247
H	2.348722	-2.729449	0.683454
H	3.736495	-3.517495	0.067575

Complex 2 a

E = -956.199443

Number of negative frequencies = 0

N	-1.610005	-1.843017	-0.070998
C	-0.744644	-2.862426	-0.146981
C	-2.936391	-2.114758	0.145091
C	-1.140192	-4.189263	-0.036301
C	-3.386631	-3.422388	0.258922
C	-2.483203	-4.474969	0.164002
H	-0.394121	-4.975502	-0.109313
H	-4.441899	-3.617829	0.429759
H	-2.828305	-5.502078	0.252309

N	-3.191264	0.224877	0.212377
C	-3.834286	-0.951481	0.257283
C	-3.804095	1.413237	0.248646
C	-5.219131	-0.967940	0.386200
C	-5.192391	1.456185	0.375775
C	-5.888452	0.253575	0.449436
H	-5.776678	-1.899794	0.426414
H	-5.729696	2.399880	0.410058
H	-6.971068	0.266638	0.547657
N	-1.542031	2.259544	-0.003204
C	-0.656081	3.278450	-0.019081
C	-2.884008	2.559424	0.142814
C	-1.088008	4.627454	0.017781
C	-3.344780	3.854793	0.203844
C	-2.423749	4.909466	0.121963
H	-0.339911	5.415188	-0.033040
H	-4.405430	4.056284	0.318970
H	-2.767182	5.940641	0.155136
C	0.790976	-0.003444	-0.713123
H	1.094148	0.750986	-1.454923
H	1.487098	0.052564	0.141912
H	0.956841	-0.980677	-1.190941
Pt	-1.196851	0.179575	-0.150946
N	0.661869	3.004517	-0.096781
H	0.982399	2.060360	0.080064
H	1.325288	3.751116	0.062041
H	0.297735	-2.599125	-0.301652

Complex 2³a

E = -956.115027

Number of negative frequencies = 0

N	-1.608334	-1.855579	-0.067203
C	-0.744722	-2.876595	-0.147207
C	-2.936071	-2.124105	0.148237
C	-1.143015	-4.202519	-0.039162
C	-3.388481	-3.431506	0.259428
C	-2.487212	-4.485610	0.161804
H	-0.399013	-4.990569	-0.114653
H	-4.444571	-3.623810	0.429442
H	-2.834141	-5.512359	0.247938
N	-3.169313	0.208141	0.207567
C	-3.825531	-0.954043	0.261604
C	-3.781121	1.436206	0.242485
C	-5.210656	-0.969234	0.404831
C	-5.196262	1.461556	0.394589
C	-5.881942	0.269785	0.477475
H	-5.769538	-1.899672	0.452612
H	-5.735803	2.404128	0.440965
H	-6.963192	0.280940	0.592985
N	-1.533155	2.230395	-0.029067
C	-0.668815	3.256362	0.014202
C	-2.898965	2.519941	0.113280

C	-1.083886	4.637491	0.080477
C	-3.354334	3.907579	0.131610
C	-2.455654	4.935860	0.113784
H	-0.319747	5.409503	0.108278
H	-4.422780	4.104434	0.162160
H	-2.789819	5.969621	0.132692
C	0.805207	0.003942	-0.724054
H	1.105373	0.743843	-1.483713
H	1.508631	0.070543	0.124707
H	0.981135	-0.976367	-1.192193
Pt	-1.192415	0.169450	-0.153317
N	0.633651	3.004908	0.007641
H	0.970085	2.044900	-0.013421
H	1.312298	3.756814	0.037530
H	0.297980	-2.614311	-0.303163

Complex 2 c

E = -1106.439182

Number of negative frequencies = 0

N	-1.509891	-1.849531	0.206615
C	-0.583216	-2.807259	0.275684
C	-2.844954	-2.149711	0.179614
C	-0.943439	-4.148899	0.305796
C	-3.251564	-3.474660	0.205946
C	-2.291479	-4.482004	0.266499
H	-0.171713	-4.910903	0.361688
H	-4.309427	-3.722677	0.188672
H	-2.601867	-5.523568	0.287886
N	-3.136616	0.192090	0.181570
C	-3.763962	-0.996864	0.140103
C	-3.736959	1.390703	0.143227
C	-5.151602	-1.008093	0.069669
C	-5.128478	1.424030	0.074008
C	-5.820774	0.216313	0.041519
H	-5.708990	-1.940069	0.034841
H	-5.669374	2.365693	0.042479
H	-6.906208	0.227377	-0.012821
N	-1.456288	2.193432	0.194630
C	-0.505713	3.151895	0.220770
C	-2.798303	2.525546	0.174485
C	-0.895231	4.517491	0.231688
C	-3.204450	3.837163	0.183999
C	-2.224141	4.846295	0.214008
H	-0.119879	5.279549	0.255524
H	-4.259907	4.091767	0.174108
H	-2.525254	5.891014	0.225091
C	-1.278034	0.169044	-1.890561
H	-1.758474	1.097037	-2.217979
H	-0.245042	0.118836	-2.252162
H	-1.849716	-0.702726	-2.227045
Pt	-1.148698	0.156645	0.197175
O	0.187238	0.088221	1.942267

O	0.781532	0.023759	0.651218
N	0.781908	2.783532	0.210159
H	1.036054	1.796155	0.369793
H	1.493928	3.492791	0.322604
H	0.448120	-2.460132	0.309234

Complex 2 e

E = -1106.428156

Number of negative frequencies = 0

N	-1.540991	-1.902461	0.260964
C	-0.639537	-2.886862	0.267946
C	-2.881279	-2.167853	0.248604
C	-1.030934	-4.218793	0.285048
C	-3.321653	-3.483489	0.259964
C	-2.388725	-4.516511	0.280523
H	-0.277584	-5.000911	0.298646
H	-4.385540	-3.704511	0.252949
H	-2.726158	-5.549884	0.288753
N	-3.129278	0.184511	0.213358
C	-3.775844	-0.995681	0.203974
C	-3.719772	1.381222	0.114430
C	-5.162301	-0.996026	0.124837
C	-5.111279	1.430455	0.027417
C	-5.819194	0.233278	0.041616
H	-5.730456	-1.922071	0.117061
H	-5.638258	2.377083	-0.052788
H	-6.904004	0.254214	-0.023007
N	-1.432830	2.189669	0.207413
C	-0.509336	3.177959	0.323483
C	-2.777667	2.511523	0.128754
C	-0.932576	4.536866	0.294467
C	-3.211371	3.814079	0.115145
C	-2.259649	4.846949	0.191428
H	-0.172370	5.311912	0.362289
H	-4.271737	4.041830	0.064957
H	-2.580839	5.885652	0.175300
C	-1.123071	0.086043	-1.844794
H	-1.732904	0.928582	-2.184834
H	-0.055302	0.212149	-2.060597
H	-1.530604	-0.871628	-2.183499
Pt	-1.111779	0.114145	0.216844
O	1.614973	0.575969	-0.544029
O	0.820778	-0.235262	0.250234
N	0.778515	2.862904	0.511033
H	1.179102	1.953997	0.127544
H	1.419959	3.647689	0.499897
H	0.401712	-2.563692	0.258127

Complex 2 TS₁

E = -1106.400540

Number of negative frequencies = 1

N	-1.563284	-1.889507	0.240213
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C	-0.663510	-2.878324	0.270260
C	-2.899386	-2.169260	0.177993
C	-1.049287	-4.211432	0.235034
C	-3.336652	-3.485273	0.143011
C	-2.403387	-4.516697	0.171504
H	-0.291593	-4.989059	0.260877
H	-4.399375	-3.706230	0.094157
H	-2.736296	-5.551193	0.145091
N	-3.143720	0.181482	0.187106
C	-3.793088	-1.002569	0.158591
C	-3.759818	1.373794	0.178662
C	-5.180244	-1.011678	0.121828
C	-5.152926	1.409826	0.147752
C	-5.853583	0.209834	0.118788
H	-5.736658	-1.944548	0.098727
H	-5.687687	2.355292	0.143317
H	-6.939980	0.223258	0.092234
N	-1.493393	2.214054	0.209668
C	-0.595698	3.227293	0.166852
C	-2.841152	2.518013	0.182534
C	-1.038890	4.577431	0.126341
C	-3.305329	3.811119	0.134117
C	-2.375877	4.863320	0.110307
H	-0.288639	5.364645	0.107375
H	-4.371385	4.014345	0.109727
H	-2.717899	5.894984	0.079241
C	0.401288	0.047679	-1.560626
H	1.308507	0.633894	-1.432738
H	0.557638	-0.999564	-1.813096
H	-0.384397	0.542239	-2.138835
Pt	-1.167202	0.117019	0.264296
O	1.688397	0.576435	0.977095
O	0.811003	-0.330700	0.498226
N	0.715679	2.949987	0.119979
H	1.092460	2.041265	0.471575
H	1.346532	3.738055	0.201441
H	0.378355	-2.566275	0.327392

Complex 2 f

E = -1106.478201

Number of negative frequencies = 0

N	-2.112420	-2.313276	-3.247284
C	-1.300204	-3.306285	-2.827237
C	-3.123429	-2.600634	-4.139631
C	-1.462997	-4.625397	-3.324154
C	-3.320662	-3.865857	-4.638400
C	-2.461295	-4.895844	-4.220529
H	-0.783906	-5.400216	-2.975952
H	-4.124515	-4.068745	-5.339102
H	-2.593526	-5.903894	-4.606035
N	-3.644758	-0.304496	-3.916604
C	-3.976131	-1.464204	-4.514461

C	-4.287397	0.863400	-4.133034
C	-5.053375	-1.480156	-5.396599
C	-5.369561	0.887193	-5.002422
C	-5.747234	-0.298149	-5.630043
H	-5.350242	-2.397321	-5.896990
H	-5.913827	1.807743	-5.192981
H	-6.594066	-0.298247	-6.311437
N	-2.658402	1.681087	-2.582512
C	-2.089359	2.618121	-1.817538
C	-3.725392	1.990983	-3.377132
C	-2.541200	3.933906	-1.831913
C	-4.217495	3.285783	-3.423850
C	-3.612510	4.271313	-2.646879
H	-2.054329	4.672908	-1.201842
H	-5.067662	3.529484	-4.055421
H	-3.987565	5.291372	-2.676597
C	0.788242	0.199328	-2.056791
H	0.703641	1.257450	-2.333458
H	1.592833	0.061765	-1.326643
H	0.955718	-0.420811	-2.946659
Pt	-2.112449	-0.290145	-2.715651
O	-0.647407	0.518798	-0.250924
O	-0.425638	-0.252050	-1.451421
N	-0.316885	-3.028119	-1.952815
H	0.205443	-3.792733	-1.546403
H	-0.292482	-2.129577	-1.471030
H	-1.290287	2.247081	-1.166232

Complex 2 TS₄

E = -1106.465844

Number of negative frequencies = 1

N	-1.725208	-1.973554	0.396822
C	-0.834962	-2.976426	0.581882
C	-3.076606	-2.246007	0.390244
C	-1.296212	-4.321070	0.608954
C	-3.560526	-3.530919	0.446110
C	-2.636839	-4.587997	0.531504
H	-0.563575	-5.118177	0.713539
H	-4.628767	-3.725480	0.437858
H	-2.990143	-5.616026	0.560936
N	-3.271298	0.111494	0.367989
C	-3.942688	-1.063020	0.360499
C	-3.879154	1.322814	0.324768
C	-5.333386	-1.037372	0.338725
C	-5.265831	1.380409	0.304451
C	-5.988568	0.189342	0.315011
H	-5.901995	-1.963033	0.333297
H	-5.781022	2.336562	0.270890
H	-7.074629	0.219439	0.296098
N	-1.617168	2.076695	0.275105
C	-0.660146	3.006004	0.369441
C	-2.933754	2.442121	0.312610

C	-0.961579	4.359192	0.443171
C	-3.291706	3.781153	0.376041
C	-2.294896	4.750467	0.430138
H	-0.157117	5.085410	0.514221
H	-4.339648	4.067886	0.397190
H	-2.562834	5.802861	0.478822
C	1.401556	0.718965	-1.479849
H	1.170323	1.771679	-1.269442
H	2.477654	0.546036	-1.346532
H	1.099401	0.469225	-2.503133
Pt	-1.356911	0.050051	0.221423
O	1.113001	0.055953	0.758581
O	0.699521	-0.159900	-0.630280
N	0.462184	-2.688549	0.740125
H	0.806644	-1.715456	0.848005
H	1.108935	-3.448835	0.901631
H	0.360506	2.629520	0.405089

Complex 2 g

E = -1106.511188

Number of negative frequencies = 0

N	-2.295090	-1.945761	0.239862
C	-1.402091	-2.953020	0.134906
C	-3.632595	-2.224372	0.418220
C	-1.846435	-4.300732	0.188420
C	-4.101612	-3.514989	0.479235
C	-3.178945	-4.569587	0.356435
H	-1.112241	-5.097294	0.091270
H	-5.159197	-3.718313	0.618537
H	-3.525699	-5.599567	0.395755
N	-3.854256	0.125980	0.454660
C	-4.508104	-1.046130	0.541158
C	-4.448244	1.334832	0.538577
C	-5.887668	-1.029326	0.732942
C	-5.822234	1.395637	0.732478
C	-6.533254	0.199643	0.828020
H	-6.453980	-1.953337	0.808013
H	-6.338400	2.348781	0.807982
H	-7.609379	0.228710	0.978575
N	-2.199192	2.106793	0.215143
C	-1.254008	3.040645	0.079030
C	-3.506475	2.460728	0.401249
C	-1.562885	4.395174	0.117851
C	-3.868817	3.798329	0.446978
C	-2.885929	4.775135	0.302871
H	-0.772886	5.131809	0.003030
H	-4.907843	4.081058	0.593988
H	-3.158714	5.827035	0.335686
C	2.066460	0.619637	0.829845
H	2.217667	1.460704	0.135351
H	2.542104	0.841730	1.792067
H	2.510107	-0.292551	0.400447

Pt	-1.923048	0.089299	0.178474
O	0.702887	0.434688	1.112213
O	0.083849	0.147911	-0.169351
N	-0.104441	-2.645640	-0.009065
H	0.570205	-3.385294	-0.147487
H	0.187255	-1.662941	-0.121139
H	-0.242708	2.662947	-0.063481

Complex 2 CP1

E = -1106.39879482

Number of negative frequencies = 2

N	-1.875810	-1.858004	0.393147
C	-0.969974	-2.840924	0.380375
C	-3.209127	-2.148175	0.343513
C	-1.347456	-4.177019	0.321002
C	-3.640508	-3.464763	0.285743
C	-2.699658	-4.490815	0.275528
H	-0.584758	-4.950384	0.309194
H	-4.702422	-3.691537	0.243427
H	-3.026638	-5.526566	0.228765
N	-3.462060	0.201308	0.382651
C	-4.107694	-0.983783	0.342319
C	-4.084932	1.390593	0.369607
C	-5.495079	-0.998435	0.298544
C	-5.477634	1.421855	0.329352
C	-6.173852	0.219582	0.297395
H	-6.046224	-1.934212	0.266531
H	-6.014823	2.366001	0.323047
H	-7.260363	0.228093	0.269270
N	-1.826738	2.239204	0.430114
C	-0.929589	3.250337	0.403203
C	-3.171519	2.541185	0.377659
C	-1.367050	4.598774	0.316594
C	-3.635669	3.832971	0.302730
C	-2.704296	4.883545	0.270432
H	-0.617345	5.386528	0.295089
H	-4.700918	4.036959	0.257653
H	-3.045404	5.914413	0.211482
C	0.999724	-0.007292	-1.752843
H	0.546453	0.966670	-1.909074
H	2.054723	-0.073304	-1.509957
H	0.465067	-0.898310	-2.068628
Pt	-1.498202	0.150681	0.456930
O	1.263418	0.501520	1.331750
O	0.500936	-0.243512	0.551743
H	0.071340	-2.523013	0.418371
N	0.383531	2.966174	0.426970
H	1.021497	3.747144	0.515362
H	0.719931	2.066085	0.807379

Complex 2 TS₅

E = -1106.411924

Number of negative frequencies = 1

N	0.361105	-2.037975	-0.600150
C	0.539722	-3.120703	0.164108
C	-0.292371	-2.148651	-1.801654
C	0.099313	-4.378930	-0.228098
C	-0.745334	-3.383016	-2.240572
C	-0.546303	-4.511133	-1.449173
H	0.265954	-5.231359	0.423813
H	-1.264064	-3.464157	-3.192346
H	-0.903947	-5.480769	-1.786561
N	-0.130238	0.203854	-1.889871
C	-0.479621	-0.899001	-2.568694
C	-0.105085	1.441933	-2.397921
C	-0.932878	-0.764493	-3.875820
C	-0.546173	1.631812	-3.706915
C	-0.970251	0.517938	-4.427131
H	-1.233112	-1.624581	-4.467880
H	-0.552001	2.615399	-4.168304
H	-1.319253	0.646620	-5.448765
N	0.850527	1.998050	-0.236813
C	1.179421	2.878364	0.730599
C	0.403086	2.462472	-1.459480
C	1.240004	4.264895	0.443392
C	0.409848	3.803188	-1.763020
C	0.868635	4.714136	-0.796366
H	1.559705	4.950274	1.224652
H	0.055517	4.156221	-2.726918
H	0.898550	5.777001	-1.023749
C	2.351498	-0.550722	1.238182
H	2.881989	-1.429861	0.845691
H	3.053570	0.289642	1.305177
H	1.949524	-0.778613	2.234466
Pt	0.840174	-0.095498	-0.114371
O	-0.262670	-0.056959	1.855265
O	-1.404581	0.478966	1.678407
N	1.470968	2.407069	1.960382
H	1.574055	3.077503	2.711622
H	1.088479	1.496608	2.219297
H	1.048833	-2.962866	1.112404

Complex 2 h

E = -1106.412392

Number of negative frequencies = 0

N	0.379725	-2.113262	-0.595059
C	0.476609	-3.224428	0.163562
C	-0.248589	-2.198359	-1.826680
C	0.066214	-4.485269	-0.337571
C	-0.683036	-3.398858	-2.336353
C	-0.499026	-4.567963	-1.580967
H	0.195766	-5.363548	0.290315
H	-1.174151	-3.442275	-3.303643
H	-0.827865	-5.527532	-1.972593

N	-0.056237	0.150300	-1.879554
C	-0.461319	-0.930141	-2.550774
C	-0.127409	1.406058	-2.337905
C	-1.030267	-0.759913	-3.813298
C	-0.691070	1.635499	-3.588557
C	-1.142060	0.533303	-4.315780
H	-1.369763	-1.606581	-4.403304
H	-0.771148	2.635536	-4.005694
H	-1.580380	0.686910	-5.298899
N	1.062341	1.923550	-0.289704
C	1.545417	2.777427	0.618672
C	0.434661	2.407117	-1.408587
C	1.464272	4.154623	0.457165
C	0.330168	3.774191	-1.619240
C	0.854304	4.659194	-0.682053
H	1.874062	4.808372	1.221506
H	-0.171106	4.151134	-2.506590
H	0.773370	5.731619	-0.840317
C	2.243217	-0.321855	1.498071
H	2.841504	-1.241761	1.458471
H	2.947524	0.522197	1.490056
H	1.682547	-0.286756	2.445389
Pt	0.983416	-0.143585	-0.134375
O	-0.721232	0.073993	1.326553
O	-1.829834	0.287768	0.751324
N	0.996281	-3.135349	1.404434
H	1.039089	-2.229549	1.855801
H	0.913763	-3.935582	2.018127
H	2.007247	2.338014	1.498954

Complex 2 ³c

E = -1106.423019

Number of negative frequencies = 0

N	-0.099398	-2.249122	-0.308358
C	0.049058	-3.402971	0.342056
C	-0.258246	-2.236636	-1.646157
C	0.030567	-4.627779	-0.315761
C	-0.277125	-3.425670	-2.372921
C	-0.133520	-4.632285	-1.696340
H	0.147927	-5.550837	0.245477
H	-0.378744	-3.417473	-3.454765
H	-0.139877	-5.568387	-2.249835
N	-0.014754	0.167455	-1.561528
C	-0.385297	-0.909300	-2.289262
C	-0.058763	1.415921	-2.066881
C	-0.861318	-0.745759	-3.586138
C	-0.537690	1.623855	-3.360277
C	-0.946158	0.535608	-4.116545
H	-1.188010	-1.602705	-4.167882
H	-0.611967	2.627491	-3.767764
H	-1.339087	0.685005	-5.119148
N	0.605680	2.216708	0.105122

C	1.067807	3.148363	0.951593
C	0.424443	2.514784	-1.202710
C	1.358504	4.456805	0.497989
C	0.697576	3.772902	-1.711791
C	1.171074	4.754678	-0.830543
H	1.723489	5.201012	1.202779
H	0.574658	4.000424	-2.766059
H	1.392899	5.752993	-1.201598
C	2.402313	-0.467295	0.049563
H	2.700670	-1.342746	0.638735
H	2.514173	-0.655661	-1.023906
H	2.957415	0.427592	0.354370
Pt	0.430128	-0.126645	0.466274
O	0.859813	-0.635512	2.403706
O	0.334529	0.162476	3.280721
N	1.278366	2.790811	2.242692
H	0.828447	1.948489	2.605883
H	1.449496	3.524395	2.918262
H	0.182830	-3.335206	1.421544

Complex 2 TS₆

E = -1106.416976

Number of negative frequencies = 0

N	0.150875	-1.987637	-0.343757
C	0.284038	-3.044488	0.472937
C	-0.302486	-2.156499	-1.628396
C	-0.028383	-4.327316	0.057508
C	-0.624063	-3.428763	-2.090110
C	-0.488579	-4.520631	-1.243955
H	0.089720	-5.157073	0.748184
H	-0.989583	-3.558922	-3.105655
H	-0.743060	-5.516797	-1.597096
N	-0.156400	0.195227	-1.708634
C	-0.397002	-0.935692	-2.425718
C	-0.053605	1.429759	-2.260978
C	-0.656560	-0.822983	-3.784600
C	-0.311049	1.573636	-3.619019
C	-0.628979	0.442860	-4.371765
H	-0.862227	-1.702992	-4.388402
H	-0.250960	2.548478	-4.095731
H	-0.827591	0.545322	-5.435392
N	0.701580	2.014293	-0.048300
C	1.084621	2.899484	0.899921
C	0.363456	2.463922	-1.313802
C	1.168191	4.276775	0.594135
C	0.431629	3.800918	-1.642190
C	0.846138	4.716174	-0.666860
H	1.486731	4.966704	1.371740
H	0.159195	4.137148	-2.638403
H	0.903687	5.775453	-0.905546
C	2.646872	-0.366631	0.395697
H	3.098256	-0.293954	-0.597435

H	3.016280	0.411479	1.070225
H	2.765492	-1.365472	0.827976
Pt	0.534315	-0.044177	0.121256
O	0.665046	-0.384163	2.277342
O	-0.507386	-0.669347	2.730005
H	0.648313	-2.829545	1.475105
N	1.416959	2.447469	2.126741
H	1.565614	3.123125	2.864903
H	1.164595	1.506963	2.420801

Complex 2 TS₂ Conformation 1

E = -1106.384169

Number of negative frequencies = 1

N	1.669373	-1.578024	-1.472601
C	2.742539	-2.356547	-1.272867
C	1.287725	-1.252297	-2.729893
C	3.499404	-2.837956	-2.330062
C	2.010083	-1.699656	-3.829928
C	3.129741	-2.497247	-3.626794
H	4.363509	-3.464559	-2.129772
H	1.701552	-1.433573	-4.837069
H	3.706250	-2.851525	-4.477647
N	-0.517253	-0.193276	-1.609487
C	0.069027	-0.440847	-2.805226
C	-1.676134	0.492249	-1.550624
C	-0.473991	0.039861	-3.989301
C	-2.251164	1.011334	-2.709460
C	-1.641827	0.790523	-3.936124
H	0.008486	-0.160360	-4.941576
H	-3.187980	1.558364	-2.636896
H	-2.081452	1.183118	-4.849678
N	-2.525677	-0.494182	0.451071
C	-3.119531	-0.420394	1.645588
C	-2.345849	0.642819	-0.237467
C	-3.562106	0.804726	2.190148
C	-2.759336	1.892008	0.202056
C	-3.379215	1.957616	1.456225
H	-4.036038	0.825811	3.170070
H	-2.585165	2.784803	-0.394436
H	-3.712546	2.914775	1.853016
C	2.554766	0.395123	0.948758
H	2.708990	0.635865	-0.105134
H	2.198189	1.217338	1.563294
H	3.323242	-0.237306	1.386728
Pt	0.587233	-0.739339	0.076938
O	0.057365	-0.077430	1.915727
O	1.244129	-0.798945	1.955343
N	-3.243719	-1.589135	2.351085
H	-3.947885	-1.631430	3.077131
H	-3.139882	-2.442261	1.813980
H	2.986129	-2.587410	-0.237919

Complex 2 TS₂ Conformation 2

E = -1106.385459

Number of negative frequencies = 1

N	1.666862	-1.613167	-1.521572
C	2.745887	-2.401129	-1.334626
C	1.279375	-1.260571	-2.780235
C	3.514866	-2.818470	-2.442218
C	1.994514	-1.649607	-3.892641
C	3.139042	-2.436608	-3.707003
H	4.388107	-3.443234	-2.271161
H	1.678674	-1.364700	-4.891139
H	3.722595	-2.755780	-4.567257
N	-0.546861	-0.254767	-1.629863
C	0.043504	-0.473688	-2.829399
C	-1.702695	0.437029	-1.559567
C	-0.510753	0.020730	-4.004618
C	-2.286852	0.966592	-2.706858
C	-1.684744	0.757153	-3.940150
H	-0.028943	-0.159212	-4.960972
H	-3.221855	1.515233	-2.622733
H	-2.131730	1.154682	-4.847980
N	-2.596674	-0.519065	0.450407
C	-3.183357	-0.396995	1.641240
C	-2.354052	0.603475	-0.238534
C	-3.549034	0.828734	2.195528
C	-2.694517	1.875541	0.219255
C	-3.299014	1.985860	1.467987
H	-4.019168	0.868720	3.175319
H	-2.470163	2.757046	-0.379014
H	-3.566643	2.962857	1.865282
C	2.428185	0.338505	1.030065
H	2.605540	0.619914	-0.009655
H	1.958646	1.096464	1.651359
H	3.228667	-0.237866	1.485534
Pt	0.540534	-0.859352	0.043873
O	-0.032665	-0.391632	1.944380
O	1.195354	-1.043282	1.909593
N	3.101570	-2.742811	-0.072479
H	2.406804	-2.708523	0.666770
H	3.811431	-3.456039	0.039049
H	-3.370154	-1.324800	2.182829

Complex 3 a

E = -900.860845

Number of negative frequencies = 0

N	-1.639166	-1.862202	-0.085025
C	-0.775085	-2.873909	-0.227948
C	-2.967653	-2.140917	0.115610
C	-1.170389	-4.205305	-0.181367
C	-3.416308	-3.452521	0.171119
C	-2.511226	-4.498657	0.021596
H	-0.427409	-4.988196	-0.304611

H	-4.471187	-3.659694	0.330876
H	-2.855661	-5.528966	0.063059
N	-3.232229	0.194608	0.174210
C	-3.868700	-0.979284	0.262565
C	-3.828023	1.390197	0.269267
C	-5.246036	-0.986297	0.471113
C	-5.203944	1.442993	0.478247
C	-5.900999	0.239588	0.577633
H	-5.806892	-1.913662	0.550323
H	-5.732733	2.388521	0.563841
H	-6.975663	0.257916	0.740980
N	-1.569063	2.199070	-0.063952
C	-0.664628	3.176187	-0.196964
C	-2.888255	2.522311	0.129652
C	-1.012166	4.520678	-0.151591
C	-3.288577	3.849586	0.183503
C	-2.343872	4.861291	0.040170
H	-0.241871	5.277797	-0.267938
H	-4.335982	4.095910	0.336482
H	-2.650798	5.903530	0.078332
C	0.809966	0.205288	-0.424080
H	1.050912	0.768785	-1.340783
H	1.306426	0.712619	0.419771
H	1.266760	-0.790883	-0.523366
Pt	-1.231980	0.168503	-0.125872
H	0.264163	-2.597893	-0.385399
H	0.364143	2.856117	-0.344924

Complex 3³a

E = -900.782549

Number of negative frequencies = 0

N	-1.563569	-1.853893	0.287402
C	-0.665843	-2.858304	0.263621
C	-2.911275	-2.140227	0.204779
C	-1.042944	-4.183333	0.176543
C	-3.335615	-3.467931	0.100376
C	-2.406676	-4.492278	0.091508
H	-0.283352	-4.959908	0.179949
H	-4.397856	-3.686678	0.019415
H	-2.734651	-5.526064	0.013637
N	-3.165627	0.204276	0.181486
C	-3.809479	-0.998940	0.246112
C	-3.776226	1.424882	0.243457
C	-5.193214	-0.988275	0.347373
C	-5.159848	1.451312	0.345966
C	-5.863705	0.240936	0.388806
H	-5.755971	-1.917746	0.398004
H	-5.697718	2.395408	0.396881
H	-6.947521	0.255991	0.469884
N	-1.506503	2.217298	0.278558
C	-0.581721	3.196050	0.249064
C	-2.846521	2.540517	0.197589

C	-0.921898	4.530947	0.158238
C	-3.233775	3.879296	0.090148
C	-2.276652	4.877380	0.075850
H	-0.141191	5.286263	0.156870
H	-4.289768	4.127372	0.011275
H	-2.576208	5.919615	-0.004029
C	0.360076	0.151251	-1.136107
H	0.309009	1.053636	-1.752829
H	1.267001	0.146411	-0.509494
H	0.291387	-0.756881	-1.742492
Pt	-1.170633	0.175800	0.281257
H	0.379372	-2.562880	0.330516
H	0.454991	2.871800	0.314916

Complex 3 c

E = -1051.088663

Number of negative frequencies = 0

N	-1.504523	-1.836777	0.201024
C	-0.572698	-2.789335	0.274398
C	-2.839072	-2.146703	0.182431
C	-0.924469	-4.133117	0.317505
C	-3.236805	-3.473687	0.221496
C	-2.270258	-4.474906	0.286701
H	-0.147676	-4.889703	0.376671
H	-4.293341	-3.727998	0.210773
H	-2.574123	-5.518105	0.318348
N	-3.147585	0.188629	0.171968
C	-3.768512	-1.000629	0.136432
C	-3.750652	1.386622	0.122824
C	-5.157964	-1.014433	0.063547
C	-5.139887	1.420009	0.050144
C	-5.829128	0.207660	0.025707
H	-5.714132	-1.947473	0.034872
H	-5.682493	2.360690	0.011572
H	-6.914473	0.215498	-0.029817
N	-1.473663	2.186553	0.183074
C	-0.526595	3.124476	0.248143
C	-2.803194	2.518155	0.157679
C	-0.856042	4.474279	0.275996
C	-3.178681	3.852002	0.180836
C	-2.195799	4.837783	0.237778
H	-0.067103	5.218672	0.328346
H	-4.230690	4.123886	0.163700
H	-2.482594	5.886119	0.256935
C	-1.318671	0.156497	-1.913009
H	-1.752699	1.103164	-2.252780
H	-0.296547	0.043140	-2.289957
H	-1.942524	-0.686332	-2.230705
Pt	-1.158057	0.172211	0.178651
O	0.174784	0.169113	1.899960
O	0.770622	0.156490	0.610437
H	0.457403	-2.438323	0.300301

H 0.497690 2.757530 0.279675

Complex 3 TS₁

E = -1051.057777

Number of negative frequencies = 1

N	-1.589943	-1.915237	0.256780
C	-0.690492	-2.902631	0.310349
C	-2.926836	-2.196629	0.185421
C	-1.073421	-4.237181	0.292338
C	-3.361625	-3.513934	0.163732
C	-2.426843	-4.543592	0.217723
H	-0.316054	-5.014082	0.340802
H	-4.423442	-3.738507	0.109508
H	-2.758434	-5.578768	0.203726
N	-3.178732	0.150858	0.190442
C	-3.825915	-1.030507	0.142939
C	-3.786721	1.351363	0.147574
C	-5.213409	-1.030655	0.059227
C	-5.174843	1.395880	0.065657
C	-5.878614	0.194206	0.023504
H	-5.775336	-1.959831	0.019391
H	-5.706738	2.342903	0.031358
H	-6.963287	0.211849	-0.042168
N	-1.519172	2.143085	0.282474
C	-0.580112	3.091388	0.350898
C	-2.843984	2.479986	0.193816
C	-0.912007	4.441878	0.321027
C	-3.224815	3.812493	0.164132
C	-2.248598	4.804469	0.226815
H	-0.125384	5.188810	0.380137
H	-4.276011	4.080043	0.097980
H	-2.538331	5.852222	0.206860
C	0.313151	-0.002228	-1.589068
H	0.917480	0.903344	-1.538356
H	0.875013	-0.928508	-1.690918
H	-0.569251	0.052216	-2.233654
Pt	-1.205688	0.103846	0.275654
O	1.545012	0.987693	0.724295
O	0.814831	-0.104861	0.481607
H	0.351722	-2.592514	0.374810
H	0.441688	2.711022	0.451865

Complex 3 f

E = -1051.134375

Number of negative frequencies = 0

N	-1.899349	-1.866963	0.272803
C	-0.991598	-2.847180	0.268030
C	-3.232881	-2.163711	0.301762
C	-1.363783	-4.186297	0.278092
C	-3.660169	-3.482086	0.315142
C	-2.714977	-4.505063	0.300009
H	-0.597921	-4.956325	0.269419

H	-4.721171	-3.715439	0.338350
H	-3.037975	-5.542967	0.308288
N	-3.493034	0.183522	0.326021
C	-4.136957	-1.001367	0.319002
C	-4.114851	1.378956	0.324399
C	-5.526596	-1.010900	0.325581
C	-5.504933	1.413031	0.331303
C	-6.201975	0.207535	0.334399
H	-6.081173	-1.945137	0.322059
H	-6.042494	2.357261	0.332694
H	-7.288669	0.217160	0.340194
N	-1.858713	2.188428	0.304984
C	-0.920303	3.138649	0.316869
C	-3.184434	2.519345	0.314976
C	-1.261298	4.488364	0.317470
C	-3.577267	3.847789	0.323739
C	-2.602572	4.844338	0.319692
H	-0.476714	5.239758	0.322207
H	-4.631680	4.110315	0.335959
H	-2.897927	5.890736	0.324289
C	1.061391	0.066948	-1.138329
H	0.867074	1.052922	-1.581148
H	2.139837	-0.112245	-1.072918
H	0.571443	-0.722828	-1.722086
Pt	-1.547151	0.153580	0.272542
O	1.166195	1.049372	0.958721
O	0.529501	0.011643	0.185559
H	0.105825	2.754864	0.360980
H	0.050393	-2.531832	0.259703

Complex 3 TS₄

E = -1051.119763

Number of negative frequencies = 1

N	-1.744030	-1.930179	0.328366
C	-0.841474	-2.917452	0.318336
C	-3.079141	-2.213081	0.404855
C	-1.226703	-4.250479	0.377796
C	-3.516889	-3.527805	0.468187
C	-2.580434	-4.557005	0.453386
H	-0.468686	-5.028270	0.367609
H	-4.578786	-3.750104	0.530956
H	-2.910200	-5.591657	0.502979
N	-3.285214	0.135745	0.364795
C	-3.958554	-1.039929	0.407893
C	-3.894103	1.345820	0.334095
C	-5.346983	-1.019065	0.430887
C	-5.282621	1.399019	0.349408
C	-6.003746	0.208875	0.400202
H	-5.914655	-1.944957	0.464737
H	-5.801122	2.353708	0.322962
H	-7.089809	0.238592	0.413783
N	-1.629822	2.102940	0.309138

C	-0.672837	3.034867	0.366134
C	-2.948221	2.465709	0.313261
C	-0.979088	4.389679	0.385271
C	-3.309045	3.805187	0.331737
C	-2.313187	4.777231	0.358517
H	-0.176936	5.121017	0.423972
H	-4.357258	4.091670	0.332473
H	-2.583487	5.830202	0.369664
C	1.418068	0.473123	-1.306564
H	1.011588	1.490537	-1.391328
H	2.485431	0.519338	-1.053324
H	1.273744	-0.064792	-2.250651
Pt	-1.370708	0.070673	0.285670
O	0.947689	0.375964	0.991561
O	0.747282	-0.270692	-0.310931
H	0.344691	2.647664	0.418131
H	0.199752	-2.606159	0.259769

Complex 3 g

E = -1051.168171

Number of negative frequencies = 0

N	-2.244760	-2.001172	0.688743
C	-1.384337	-3.018253	0.793652
C	-3.576310	-2.239475	0.495134
C	-1.806636	-4.339546	0.715414
C	-4.051244	-3.539912	0.409747
C	-3.156997	-4.601007	0.521050
H	-1.079704	-5.141423	0.807059
H	-5.110787	-3.727498	0.256851
H	-3.518545	-5.624157	0.455032
N	-3.736261	0.115536	0.486119
C	-4.423769	-1.040185	0.385224
C	-4.307253	1.332389	0.418111
C	-5.800041	-0.994422	0.195700
C	-5.682304	1.425401	0.226207
C	-6.421272	0.250262	0.116348
H	-6.384601	-1.906425	0.112290
H	-6.177788	2.390489	0.165372
H	-7.496778	0.305061	-0.030593
N	-2.039943	2.055400	0.760883
C	-1.099365	2.990049	0.937821
C	-3.343333	2.432194	0.578815
C	-1.400428	4.346943	0.937192
C	-3.698306	3.773086	0.566370
C	-2.716672	4.743235	0.746529
H	-0.605417	5.072227	1.085332
H	-4.735579	4.062190	0.419507
H	-2.984771	5.796838	0.740045
C	1.379179	0.820441	-0.425076
H	0.498196	0.928097	-1.079175
H	2.021913	1.704216	-0.518804
H	1.939662	-0.081270	-0.708314

Pt	-1.798687	-0.005970	0.770669
O	0.990245	0.769004	0.929677
O	0.147892	-0.366467	1.091430
H	-0.089427	2.609186	1.084663
H	-0.341548	-2.740651	0.941468

Complex 3 CP1

E = -1051.05517118

Number of negative frequencies = 2

N	-1.900417	-1.879759	0.391259
C	-0.993516	-2.860916	0.379468
C	-3.234513	-2.172904	0.348579
C	-1.367012	-4.198644	0.326994
C	-3.662666	-3.490950	0.299636
C	-2.719135	-4.514843	0.288527
H	-0.603144	-4.970646	0.316051
H	-4.724010	-3.721855	0.265801
H	-3.043681	-5.551591	0.247399
N	-3.500470	0.173173	0.378036
C	-4.141637	-1.011040	0.345487
C	-4.122057	1.366156	0.363533
C	-5.530954	-1.023724	0.305917
C	-5.512358	1.401225	0.325706
C	-6.207370	0.194687	0.299749
H	-6.085650	-1.957443	0.280374
H	-6.052685	2.343797	0.316517
H	-7.293888	0.202953	0.271150
N	-1.863954	2.184255	0.431865
C	-0.936361	3.144608	0.421390
C	-3.191042	2.507665	0.375891
C	-1.280941	4.490544	0.349532
C	-3.590592	3.833629	0.319332
C	-2.624093	4.836937	0.301873
H	-0.499764	5.245017	0.333470
H	-4.646209	4.088682	0.282453
H	-2.927024	5.879819	0.250015
C	1.028323	-0.000809	-1.703607
H	0.595765	0.983817	-1.855436
H	2.073765	-0.081325	-1.426897
H	0.501189	-0.876044	-2.071973
Pt	-1.535276	0.141771	0.448071
O	1.106122	0.982703	1.122603
O	0.484928	-0.033837	0.557981
H	0.047942	-2.542794	0.413496
H	0.092717	2.786977	0.495335

Complex 3 TS₅

E = -1051.065791

Number of negative frequencies = 1

N	0.224377	-2.033891	-0.538170
C	0.355398	-3.105145	0.249597
C	-0.320278	-2.162050	-1.791136

C	-0.038271	-4.372413	-0.164606
C	-0.722405	-3.404842	-2.253125
C	-0.581296	-4.522086	-1.432432
H	0.082773	-5.217216	0.506929
H	-1.155813	-3.503488	-3.245115
H	-0.901512	-5.498648	-1.786804
N	-0.134155	0.187311	-1.892685
C	-0.447270	-0.918605	-2.582361
C	-0.095978	1.431688	-2.390438
C	-0.820869	-0.781670	-3.915521
C	-0.464299	1.621594	-3.718776
C	-0.830958	0.501168	-4.465033
H	-1.086166	-1.640514	-4.525638
H	-0.458116	2.606705	-4.176981
H	-1.115601	0.628542	-5.506493
N	0.794050	1.970876	-0.202434
C	1.178365	2.818184	0.755238
C	0.361340	2.445289	-1.414478
C	1.181152	4.194107	0.556442
C	0.353815	3.807921	-1.665680
C	0.771283	4.691602	-0.672380
H	1.501246	4.851935	1.359081
H	0.011537	4.185080	-2.625899
H	0.765113	5.761954	-0.861994
C	2.348999	-0.480753	1.110629
H	2.886422	-1.295962	0.610153
H	2.973245	0.421199	1.123498
H	2.065269	-0.768403	2.128949
Pt	0.652730	-0.083659	-0.036828
O	-0.083308	-0.021823	2.011127
O	-1.320824	0.302145	1.809318
H	1.482891	2.364887	1.696513
H	0.786113	-2.925433	1.232260

Complex 3 ³c

E = -1051.077817

Number of negative frequencies = 0

N	-0.131186	-2.244571	-0.300339
C	-0.018784	-3.394501	0.364435
C	-0.279295	-2.249049	-1.640323
C	-0.065077	-4.627904	-0.276423
C	-0.322847	-3.446656	-2.351664
C	-0.216477	-4.647518	-1.658227
H	0.021308	-5.545674	0.298968
H	-0.417519	-3.451198	-3.434069
H	-0.242438	-5.590681	-2.199062
N	-0.012934	0.145904	-1.569675
C	-0.368743	-0.928184	-2.302529
C	-0.031523	1.395930	-2.076955
C	-0.790297	-0.763520	-3.620084
C	-0.449023	1.605230	-3.389113
C	-0.833791	0.515291	-4.158894

H	-1.099222	-1.618542	-4.214428
H	-0.488957	2.606619	-3.807242
H	-1.173850	0.663935	-5.180671
N	0.611461	2.170950	0.110730
C	1.024746	3.090618	0.981025
C	0.412943	2.490164	-1.183564
C	1.255074	4.409130	0.603785
C	0.630036	3.791296	-1.633221
C	1.053082	4.757794	-0.726490
H	1.585246	5.138094	1.338890
H	0.486572	4.056767	-2.676829
H	1.227154	5.776930	-1.063809
C	2.446325	-0.505409	-0.078680
H	2.752821	-1.383865	0.501881
H	2.504017	-0.703224	-1.154676
H	3.039347	0.375691	0.192110
Pt	0.503473	-0.114541	0.446252
O	1.141318	-0.349465	2.372979
O	0.607475	0.540030	3.148625
H	0.109997	-3.314939	1.443639
H	1.159107	2.747404	2.007684

Complex 3 TS₂

E = -1051.042519

Number of negative frequencies = 1

N	1.725300	-1.526520	-1.506435
C	2.844510	-2.238400	-1.309729
C	1.302282	-1.255847	-2.762450
C	3.603147	-2.711098	-2.369132
C	2.021351	-1.701186	-3.865610
C	3.184109	-2.435431	-3.666038
H	4.503115	-3.285428	-2.169843
H	1.675143	-1.486675	-4.872659
H	3.755475	-2.791739	-4.519447
N	-0.526350	-0.247857	-1.629190
C	0.052409	-0.494489	-2.829944
C	-1.681826	0.442891	-1.570594
C	-0.511184	-0.039308	-4.014470
C	-2.276708	0.939218	-2.728752
C	-1.688064	0.695559	-3.961103
H	-0.033608	-0.243908	-4.968192
H	-3.210246	1.491247	-2.650550
H	-2.144117	1.066823	-4.875405
N	-2.599014	-0.457135	0.453744
C	-3.186345	-0.299210	1.640279
C	-2.325350	0.647748	-0.251074
C	-3.519745	0.944928	2.173684
C	-2.631779	1.936187	0.183951
C	-3.235641	2.083318	1.429067
H	-3.991851	1.013541	3.150955
H	-2.383854	2.800997	-0.429412
H	-3.477040	3.073662	1.809877

C	2.405907	0.324611	1.123486
H	2.567497	0.692416	0.108084
H	1.965194	1.041548	1.810995
H	3.210939	-0.290072	1.518965
Pt	0.561109	-0.847505	0.055252
O	-0.070688	-0.449063	1.945285
O	1.169355	-1.077560	1.936896
H	3.121885	-2.428300	-0.275241
H	-3.401129	-1.212226	2.196318

Complex 4 a

E = -979.424294

Number of negative frequencies = 0

N	-1.501721	-1.937326	0.036197
C	-0.642127	-2.979542	0.061002
C	-2.840609	-2.184007	0.240013
C	-1.111679	-4.293029	0.183204
C	-3.337154	-3.470033	0.369240
C	-2.462228	-4.548537	0.315779
H	-0.387373	-5.104205	0.181880
H	-4.399566	-3.629993	0.528894
H	-2.833159	-5.566366	0.407978
N	-3.079125	0.158318	0.353853
C	-3.728310	-1.013198	0.352039
C	-3.696686	1.346815	0.341871
C	-5.118776	-1.024841	0.435187
C	-5.086342	1.396008	0.424948
C	-5.787944	0.195067	0.487315
H	-5.680745	-1.954585	0.441110
H	-5.622920	2.340686	0.423458
H	-6.872989	0.210234	0.552132
N	-1.445301	2.208711	0.023086
C	-0.558299	3.227740	0.041489
C	-2.777877	2.492258	0.219953
C	-0.993641	4.554443	0.146161
C	-3.240814	3.792292	0.332897
C	-2.337651	4.846773	0.269274
H	-0.247726	5.345776	0.138791
H	-4.299119	3.981628	0.487447
H	-2.681320	5.875328	0.346728
C	0.688268	0.103781	-1.195216
H	0.746631	0.989329	-1.843992
H	1.587916	0.089598	-0.561714
H	0.719799	-0.782288	-1.845248
Pt	-1.114402	0.130130	-0.180693
C	0.906206	2.958395	-0.011728
H	1.153758	2.016809	0.486189
H	1.267099	2.899066	-1.045913
H	1.447174	3.775685	0.477121
C	0.828623	-2.751116	-0.004593
H	1.182021	-2.703557	-1.041970
H	1.106585	-1.815846	0.489035

H 1.350782 -3.581957 0.481687

Complex 4 ³a

E = -979.361994

Number of negative frequencies = 0

N	-1.424421	-1.949587	0.336991
C	-0.544632	-2.976030	0.295529
C	-2.771854	-2.195788	0.240039
C	-0.989887	-4.286521	0.160665
C	-3.250914	-3.494304	0.085216
C	-2.353033	-4.549580	0.045592
H	-0.261930	-5.094648	0.150564
H	-4.318646	-3.673895	-0.011777
H	-2.710805	-5.569569	-0.074048
N	-3.015564	0.157000	0.223586
C	-3.654662	-1.029595	0.320480
C	-3.620849	1.361421	0.313059
C	-5.035181	-1.028886	0.495326
C	-5.000667	1.399902	0.489416
C	-5.701081	0.195330	0.576322
H	-5.590871	-1.959207	0.585456
H	-5.530741	2.345421	0.575838
H	-6.777676	0.211297	0.726835
N	-1.364482	2.221425	0.303538
C	-0.459356	3.225248	0.253834
C	-2.706136	2.502356	0.222714
C	-0.873345	4.547436	0.130156
C	-3.153835	3.813099	0.078225
C	-2.230338	4.845693	0.033886
H	-0.125332	5.336892	0.115262
H	-4.217690	4.020278	-0.004293
H	-2.563131	5.875359	-0.074184
C	-0.000762	0.096736	-1.679040
H	-0.281715	0.997986	-2.235230
H	1.079720	0.085916	-1.472246
H	-0.302668	-0.808995	-2.216839
Pt	-0.958702	0.127434	0.200336
C	0.982850	2.860020	0.347105
H	1.150623	2.129600	1.150528
H	1.327982	2.399719	-0.588849
H	1.600825	3.743583	0.537924
C	0.903471	-2.643174	0.408420
H	1.271623	-2.193670	-0.524197
H	1.073596	-1.912293	1.211036
H	1.499479	-3.538962	0.611719

Complex 4 c

E = -1129.660962

Number of negative frequencies = 0

N	-1.469369	-1.900699	0.196932
C	-0.584426	-2.918045	0.155464
C	-2.819358	-2.161527	0.182861

C	-1.045485	-4.240287	0.159096
C	-3.300814	-3.458059	0.178350
C	-2.398895	-4.516687	0.179419
H	-0.312777	-5.042900	0.135846
H	-4.371241	-3.641488	0.172270
H	-2.756055	-5.543341	0.182072
N	-3.093441	0.179751	0.189704
C	-3.723571	-1.001083	0.153335
C	-3.699548	1.373437	0.170877
C	-5.113830	-1.012452	0.083953
C	-5.089316	1.413699	0.101457
C	-5.784662	0.207810	0.058471
H	-5.671987	-1.943481	0.049070
H	-5.628584	2.356261	0.079940
H	-6.869965	0.219467	0.002568
N	-1.427035	2.222494	0.231607
C	-0.519106	3.220332	0.214728
C	-2.770743	2.513125	0.220386
C	-0.950183	4.552259	0.244544
C	-3.222752	3.820107	0.240201
C	-2.297321	4.857949	0.265570
H	-0.199483	5.338408	0.242086
H	-4.288493	4.028907	0.235980
H	-2.631446	5.892089	0.288512
C	-1.106536	0.172121	-1.817291
H	-1.604823	1.081357	-2.170692
H	-0.056417	0.161216	-2.131320
H	-1.628175	-0.718285	-2.184631
Pt	-1.088575	0.156399	0.277293
O	0.077048	0.133235	2.126445
O	0.790484	0.125903	0.910735
C	0.931600	2.906176	0.139502
H	1.248926	2.306446	0.998509
H	1.150726	2.304132	-0.752061
H	1.514069	3.830800	0.092935
C	0.873275	-2.637788	0.080608
H	1.102757	-2.004360	-0.785860
H	1.213260	-2.085737	0.962526
H	1.429637	-3.575198	-0.009703

Complex 4 TS₁

E = -1129.613881

Number of negative frequencies = 1

N	-1.531649	-1.946823	0.181149
C	-0.706763	-3.018633	0.263268
C	-2.872261	-2.158845	-0.038405
C	-1.201153	-4.308829	0.039561
C	-3.388650	-3.423880	-0.263055
C	-2.536262	-4.519251	-0.245203
H	-0.508428	-5.144161	0.101873
H	-4.450348	-3.553561	-0.450252
H	-2.918095	-5.520306	-0.428990

N	-3.085611	0.186036	0.151312
C	-3.743939	-0.982378	0.026223
C	-3.707296	1.369064	0.299510
C	-5.134123	-0.985803	0.025023
C	-5.098638	1.410634	0.319558
C	-5.806842	0.223423	0.173970
H	-5.692796	-1.911848	-0.072881
H	-5.628537	2.351004	0.438355
H	-6.893415	0.238849	0.181915
N	-1.460661	2.250995	0.195493
C	-0.616249	3.298675	0.046046
C	-2.798783	2.514812	0.370981
C	-1.069108	4.610514	0.242824
C	-3.282733	3.799880	0.546841
C	-2.396335	4.869036	0.520197
H	-0.350481	5.421130	0.151139
H	-4.344035	3.967433	0.703752
H	-2.748865	5.885219	0.677980
C	0.623533	0.056139	-1.449283
H	-0.073905	0.612922	-2.081392
H	1.596017	0.526614	-1.333116
H	0.663683	-1.010433	-1.663599
Pt	-1.110945	0.124975	0.243921
O	1.487409	0.861779	1.314042
O	0.876770	-0.126023	0.676663
C	0.778537	3.090517	-0.413195
H	1.281685	2.288895	0.149283
H	0.775328	2.826213	-1.479205
H	1.353708	4.015568	-0.305433
C	0.725670	-2.866171	0.639207
H	1.306827	-2.329206	-0.116676
H	0.823433	-2.296462	1.569565
H	1.174270	-3.854250	0.776438

Complex 4 e

E = -1129.644287

Number of negative frequencies = 0

N	-1.422421	-1.962798	0.171463
C	-0.577150	-3.015228	0.176423
C	-2.773283	-2.178685	0.233449
C	-1.075941	-4.320402	0.240133
C	-3.300188	-3.459677	0.298481
C	-2.438060	-4.548778	0.300787
H	-0.370036	-5.147239	0.248658
H	-4.374309	-3.609385	0.351453
H	-2.831588	-5.560940	0.353469
N	-3.007975	0.184354	0.209209
C	-3.649367	-0.995217	0.222137
C	-3.630887	1.369165	0.097369
C	-5.040944	-1.007438	0.180211
C	-5.021651	1.407077	0.044966
C	-5.719137	0.205733	0.098935

H	-5.598428	-1.939199	0.192063
H	-5.556723	2.348825	-0.038057
H	-6.805333	0.212208	0.061103
N	-1.386428	2.243633	0.205952
C	-0.506019	3.251917	0.408681
C	-2.723976	2.521094	0.067942
C	-0.942049	4.579223	0.309828
C	-3.183743	3.822330	-0.022441
C	-2.270788	4.869760	0.065478
H	-0.211274	5.372677	0.447876
H	-4.244615	4.021605	-0.144016
H	-2.607487	5.900223	-0.016662
C	-1.330783	0.173941	-2.025441
H	-1.866599	1.097578	-2.267977
H	-0.310370	0.171751	-2.424358
H	-1.913868	-0.713716	-2.291060
Pt	-0.978520	0.174734	0.012738
O	1.482406	0.876944	-1.169956
O	0.943044	0.003018	-0.295212
C	0.891709	2.937425	0.774527
H	0.913950	2.242503	1.625487
H	1.410159	2.418710	-0.055343
H	1.431997	3.849779	1.042884
C	0.891148	-2.787246	0.126452
H	1.179388	-2.269743	-0.795400
H	1.219832	-2.149167	0.955449
H	1.420391	-3.743031	0.183886

Complex 4 TS₃

E = -1129.607589

Number of negative frequencies = 0

N	-1.717303	-1.974971	0.512157
C	-0.872880	-3.024157	0.589114
C	-3.067370	-2.188164	0.447480
C	-1.372582	-4.330248	0.545500
C	-3.596996	-3.467433	0.409392
C	-2.733150	-4.556950	0.445130
H	-0.670390	-5.158613	0.598267
H	-4.671220	-3.616556	0.352148
H	-3.126281	-5.569827	0.406683
N	-3.239072	0.175839	0.442839
C	-3.917429	-0.986598	0.446288
C	-3.834780	1.381307	0.444249
C	-5.307977	-0.967614	0.456805
C	-5.226089	1.447095	0.452420
C	-5.955811	0.263601	0.458010
H	-5.883977	-1.888165	0.466196
H	-5.741256	2.402948	0.461141
H	-7.041976	0.301353	0.467220
N	-1.588152	2.260029	0.587037
C	-0.706848	3.262908	0.757910
C	-2.917956	2.536244	0.474266

C	-1.141518	4.593401	0.740366
C	-3.390610	3.840182	0.442220
C	-2.481749	4.885888	0.560065
H	-0.409022	5.385638	0.876385
H	-4.451563	4.044136	0.331800
H	-2.825415	5.917214	0.532781
C	-1.281776	-0.027664	-1.980832
H	-2.338116	-0.287064	-1.858492
H	-1.145449	0.876821	-2.567040
H	-0.650249	-0.865201	-2.268548
Pt	-1.236810	0.078947	0.356341
O	0.560580	0.811188	-1.180366
O	0.720699	0.042390	-0.023343
C	0.725281	2.934651	0.990226
H	0.823942	2.219444	1.816325
H	1.142345	2.447257	0.100169
H	1.294078	3.838701	1.229133
C	0.582134	-2.771582	0.748808
H	0.967645	-2.158320	-0.074624
H	0.768961	-2.196105	1.665542
H	1.132647	-3.715135	0.805900

Complex 4 f

E = -1129.696646

Number of negative frequencies = 1

N	-1.534149	-1.946823	0.186149
C	-0.709263	-3.018633	0.265768
C	-2.872261	-2.158845	-0.038405
C	-1.201153	-4.308829	0.039561
C	-3.388650	-3.423880	-0.263055
C	-2.536262	-4.519251	-0.245203
H	-0.508428	-5.144161	0.099373
H	-4.450348	-3.553561	-0.452752
H	-2.918095	-5.520306	-0.428990
N	-3.083111	0.186036	0.146312
C	-3.743939	-0.982378	0.026223
C	-3.707296	1.369064	0.299510
C	-5.134123	-0.985803	0.025023
C	-5.098638	1.410634	0.319558
C	-5.806842	0.223423	0.173970
H	-5.692796	-1.911848	-0.070381
H	-5.626037	2.351004	0.438355
H	-6.893415	0.238849	0.181915
N	-1.460661	2.253495	0.197993
C	-0.618749	3.301175	0.046046
C	-2.798783	2.517312	0.373481
C	-1.069108	4.613014	0.242824
C	-3.285233	3.799880	0.546841
C	-2.396335	4.869036	0.520197
H	-0.352981	5.423630	0.148639
H	-4.346535	3.969933	0.703752
H	-2.748865	5.885219	0.677980

C	0.741033	0.053639	-1.429283
H	-0.016405	0.630422	-1.978892
H	1.726017	0.514114	-1.393116
H	0.736183	-1.012933	-1.648599
Pt	-1.118445	0.124975	0.248921
O	1.482409	0.849279	1.294042
O	0.876770	-0.113523	0.594163
C	0.778537	3.093017	-0.413195
H	1.281685	2.288895	0.144283
H	0.772828	2.836213	-1.481705
H	1.353708	4.015568	-0.302933
C	0.725670	-2.866171	0.644207
H	1.309327	-2.339206	-0.116676
H	0.823433	-2.291462	1.569565
H	1.169270	-3.854250	0.786438

Complex 4 TS₄

E = -1129.678548

Number of negative frequencies = 1

N	-1.698871	-2.033150	0.378659
C	-0.868422	-3.102264	0.379193
C	-3.049821	-2.246344	0.507399
C	-1.386326	-4.396432	0.528290
C	-3.590836	-3.511826	0.651659
C	-2.742398	-4.611338	0.667202
H	-0.688882	-5.230284	0.531274
H	-4.663494	-3.639564	0.760746
H	-3.141666	-5.615491	0.786386
N	-3.201944	0.108218	0.430752
C	-3.891852	-1.053897	0.473433
C	-3.809481	1.309976	0.310765
C	-5.281135	-1.026206	0.444649
C	-5.197542	1.373956	0.271059
C	-5.932834	0.197662	0.348142
H	-5.853949	-1.947928	0.481280
H	-5.702930	2.330838	0.180712
H	-7.018417	0.234152	0.321799
N	-1.557373	2.133586	0.436861
C	-0.680914	3.147588	0.606825
C	-2.887411	2.440572	0.269686
C	-1.097519	4.477994	0.448678
C	-3.334619	3.741008	0.125446
C	-2.415080	4.783175	0.180163
H	-0.350695	5.260487	0.565802
H	-4.390554	3.944520	-0.025072
H	-2.737252	5.813265	0.050353
C	1.470930	0.702261	-1.371478
H	1.187881	1.747384	-1.193413
H	2.546735	0.572899	-1.190453
H	1.226654	0.425048	-2.403670
Pt	-1.280092	0.033054	0.334289
O	1.191290	-0.069895	0.851133

O	0.767221	-0.198790	-0.544342
C	0.717169	2.905230	1.053789
H	0.823568	3.324339	2.065039
H	0.981411	1.841580	1.085123
H	1.427159	3.448753	0.416641
C	0.596552	-2.938740	0.204732
H	0.827549	-2.733741	-0.848522
H	0.985701	-2.086703	0.777554
H	1.107841	-3.862436	0.493028

Complex 4 g

E = -1129.731870

Number of negative frequencies = 0

N	-2.219629	-1.905824	0.263727
C	-1.356870	-2.943126	0.193964
C	-3.556351	-2.164677	0.436944
C	-1.825187	-4.261531	0.273805
C	-4.051678	-3.453884	0.524573
C	-3.170495	-4.525285	0.435985
H	-1.102651	-5.071300	0.208821
H	-5.114951	-3.624820	0.663599
H	-3.535799	-5.547296	0.499539
N	-3.804439	0.182886	0.453974
C	-4.443063	-0.997434	0.532731
C	-4.438250	1.367762	0.497554
C	-5.826210	-1.017397	0.682783
C	-5.821297	1.397859	0.646219
C	-6.509132	0.192773	0.740570
H	-6.370709	-1.954568	0.748748
H	-6.362198	2.338704	0.683346
H	-7.589957	0.196853	0.854891
N	-2.210111	2.257750	0.209961
C	-1.342016	3.288375	0.113611
C	-3.546392	2.527660	0.368714
C	-1.804722	4.610618	0.148176
C	-4.036241	3.821185	0.413485
C	-3.149797	4.885283	0.294108
H	-1.077978	5.414555	0.060707
H	-5.099372	4.000648	0.542927
H	-3.510358	5.910559	0.321905
C	2.206049	0.167863	0.546008
H	2.456314	1.059373	-0.050777
H	2.785660	0.173163	1.476814
H	2.450694	-0.734246	-0.037019
Pt	-1.862075	0.174514	0.163791
O	0.856957	0.174798	0.934520
O	0.102381	0.163746	-0.301510
C	0.114920	3.029598	-0.014640
H	0.467429	2.385768	0.800212
H	0.337855	2.489894	-0.941490
H	0.666505	3.974531	-0.002422
C	0.100371	-2.696390	0.046297

H	0.318254	-2.183512	-0.896872
H	0.463953	-2.033144	0.840318
H	0.646376	-3.644098	0.079230

Complex 4 CP1

E = -1129.61656439

Number of negative frequencies = 1

N	-1.859877	-1.938486	0.373345
C	-1.008855	-2.988297	0.400477
C	-3.210127	-2.180198	0.337203
C	-1.500309	-4.298915	0.343158
C	-3.728043	-3.463014	0.290575
C	-2.857096	-4.545628	0.280211
H	-0.786499	-5.118922	0.353201
H	-4.802064	-3.620788	0.261439
H	-3.238439	-5.562275	0.233019
N	-3.441601	0.173958	0.380735
C	-4.090762	-1.003494	0.354257
C	-4.068816	1.362108	0.373451
C	-5.481824	-1.014553	0.344891
C	-5.459901	1.400306	0.364481
C	-6.160368	0.199451	0.354965
H	-6.036944	-1.947498	0.330336
H	-5.996443	2.344266	0.362213
H	-7.247133	0.209371	0.349128
N	-1.818319	2.240925	0.358678
C	-0.943267	3.270651	0.358552
C	-3.162397	2.517205	0.362460
C	-1.400669	4.594608	0.337619
C	-3.649460	3.812352	0.347155
C	-2.752474	4.874123	0.328134
H	-0.665501	5.395417	0.331281
H	-4.719694	3.995599	0.347140
H	-3.110382	5.900436	0.308551
C	1.185045	0.344124	-1.870183
H	0.732683	1.283718	-2.175269
H	2.239492	0.326174	-1.612664
H	0.708459	-0.576697	-2.194857
Pt	-1.471779	0.144176	0.355819
O	1.250380	0.326867	1.285677
O	0.554333	-0.037353	0.224479
C	0.516135	3.008604	0.403177
H	0.792138	2.487055	1.328173
H	0.828732	2.345544	-0.409511
H	1.073474	3.946840	0.335639
C	0.462241	-2.784664	0.508314
H	0.867100	-2.282312	-0.377370
H	0.716743	-2.155937	1.368390
H	0.958312	-3.753745	0.618091

Complex 4 ³c

E = -1129.658810

Number of negative frequencies = 0

N	-0.102542	-2.264013	-0.303658
C	0.021629	-3.426622	0.353401
C	-0.260739	-2.245312	-1.643148
C	-0.015594	-4.640196	-0.339532
C	-0.290471	-3.421928	-2.385957
C	-0.164842	-4.634990	-1.717846
H	0.078735	-5.573750	0.210880
H	-0.386405	-3.401899	-3.467699
H	-0.178408	-5.568469	-2.275937
N	-0.011431	0.156836	-1.562401
C	-0.383053	-0.918001	-2.286781
C	-0.042877	1.404683	-2.072960
C	-0.854072	-0.753957	-3.587667
C	-0.512606	1.612929	-3.368127
C	-0.926364	0.524232	-4.122929
H	-1.183681	-1.609333	-4.169567
H	-0.576063	2.614011	-3.783111
H	-1.311028	0.673142	-5.128766
N	0.645973	2.221591	0.092434
C	1.085289	3.163891	0.938782
C	0.441744	2.506023	-1.210172
C	1.337861	4.462088	0.485724
C	0.687991	3.778855	-1.718044
C	1.141225	4.767436	-0.851841
H	1.687238	5.214877	1.188921
H	0.548942	4.003368	-2.771363
H	1.341070	5.769141	-1.225531
C	2.467153	-0.424703	-0.061288
H	2.806254	-1.287785	0.524340
H	2.538351	-0.627508	-1.135757
H	3.028177	0.479240	0.205191
Pt	0.510014	-0.108985	0.452596
O	1.115504	-0.379423	2.379414
O	0.101916	-0.278367	3.175728
C	1.280505	2.783087	2.367336
H	0.350250	2.385910	2.793331
H	2.035288	1.991109	2.461995
H	1.600050	3.643911	2.963168
C	0.195633	-3.374799	1.833479
H	1.142333	-2.884193	2.097566
H	-0.604892	-2.786435	2.299327
H	0.194271	-4.380673	2.265209

Complex 4 TS₅

E = -1129.637802

Number of negative frequencies = 1

N	0.292968	-2.105451	-0.534372
C	0.376599	-3.220998	0.221850
C	-0.301624	-2.178848	-1.775125
C	-0.081712	-4.448714	-0.273299
C	-0.762174	-3.377299	-2.289860

C	-0.640273	-4.537254	-1.532462
H	0.005291	-5.327581	0.360523
H	-1.231875	-3.404556	-3.268922
H	-0.998600	-5.488324	-1.918643
N	-0.162408	0.176621	-1.821218
C	-0.448971	-0.920998	-2.531539
C	-0.103634	1.412816	-2.332351
C	-0.815690	-0.783809	-3.867930
C	-0.462687	1.609163	-3.663362
C	-0.833973	0.497154	-4.416089
H	-1.060313	-1.645110	-4.483088
H	-0.434640	2.593626	-4.121570
H	-1.113186	0.627583	-5.458671
N	0.855525	1.991099	-0.169364
C	1.202752	2.891769	0.773276
C	0.375716	2.434194	-1.381378
C	1.161473	4.263027	0.489799
C	0.319484	3.781761	-1.688475
C	0.738593	4.713972	-0.744430
H	1.462072	4.960849	1.267697
H	-0.066355	4.106723	-2.650586
H	0.707743	5.777242	-0.968955
C	2.455467	-0.442592	1.193165
H	2.955801	-1.355798	0.846085
H	3.138341	0.404614	1.050684
H	2.197063	-0.537044	2.254011
Pt	0.824488	-0.122178	-0.044374
O	-0.283813	-0.183245	1.939640
O	-1.349798	0.503011	1.863326
C	1.611492	2.444329	2.134220
H	1.062390	1.547233	2.437376
H	2.685165	2.219835	2.171617
H	1.421838	3.246066	2.855411
C	0.945087	-3.164273	1.597215
H	2.040993	-3.134236	1.572813
H	0.592195	-2.279540	2.135977
H	0.652532	-4.058919	2.155779

Complex 4 h

E = -1129.638306

Number of negative frequencies = 0

N	0.337361	-2.114186	-0.537349
C	0.403021	-3.225071	0.226852
C	-0.286019	-2.181205	-1.763865
C	-0.078393	-4.448284	-0.256700
C	-0.770841	-3.375046	-2.267473
C	-0.649937	-4.534933	-1.510249
H	-0.000652	-5.324491	0.382083
H	-1.262403	-3.397261	-3.235888
H	-1.024488	-5.482760	-1.888999
N	-0.140947	0.172429	-1.802933
C	-0.453155	-0.919423	-2.509552

C	-0.107532	1.410338	-2.309470
C	-0.869677	-0.776496	-3.831022
C	-0.517725	1.614734	-3.624777
C	-0.911865	0.506844	-4.371263
H	-1.134622	-1.635655	-4.440797
H	-0.513457	2.602781	-4.076034
H	-1.231021	0.642782	-5.401609
N	0.902619	1.985619	-0.169491
C	1.227726	2.885060	0.782174
C	0.391805	2.430118	-1.367307
C	1.159276	4.257581	0.511743
C	0.309432	3.779318	-1.663156
C	0.724898	4.711114	-0.717773
H	1.446347	4.954358	1.295562
H	-0.095535	4.105212	-2.616967
H	0.676415	5.775387	-0.934292
C	2.458718	-0.452005	1.283327
H	2.970314	-1.384402	1.012821
H	3.171276	0.375528	1.170432
H	2.128871	-0.506125	2.328051
Pt	0.924367	-0.136267	-0.068239
O	-0.502478	-0.109083	1.677010
O	-1.540549	0.572043	1.418401
C	1.626633	2.432643	2.144031
H	1.041773	1.558364	2.448574
H	2.689815	2.166796	2.185897
H	1.462799	3.242321	2.862342
C	0.970828	-3.170001	1.602600
H	2.066719	-3.202706	1.582517
H	0.666716	-2.258676	2.125629
H	0.627911	-4.036373	2.177061

Complex 4 TS₆

E = -1129.643564

Number of negative frequencies = 1

N	0.157109	-2.135091	-0.345675
C	0.242084	-3.269826	0.379975
C	-0.386827	-2.177846	-1.602963
C	-0.228831	-4.480463	-0.134523
C	-0.878600	-3.359226	-2.139939
C	-0.802011	-4.528362	-1.394034
H	-0.139047	-5.377455	0.473422
H	-1.332541	-3.357589	-3.127526
H	-1.185621	-5.463965	-1.794339
N	-0.311972	0.190972	-1.638686
C	-0.386832	-0.925972	-2.379310
C	-0.065857	1.394245	-2.180459
C	-0.360137	-0.845046	-3.769555
C	-0.031809	1.541653	-3.565069
C	-0.207981	0.408966	-4.357543
H	-0.406715	-1.739251	-4.386345
H	0.173690	2.505571	-4.023968

H	-0.165411	0.496140	-5.440397
N	0.730930	2.051139	0.014833
C	1.116523	2.978678	0.916080
C	0.256992	2.451324	-1.206158
C	1.020993	4.340617	0.620562
C	0.132904	3.795826	-1.528797
C	0.518158	4.755213	-0.601224
H	1.351010	5.062209	1.364001
H	-0.274191	4.088986	-2.492989
H	0.428876	5.813634	-0.834239
C	2.574344	-0.357443	0.065698
H	2.728198	-1.249529	-0.551232
H	2.968043	0.535021	-0.433199
H	3.019562	-0.483009	1.060609
Pt	0.557924	-0.102268	0.315252
O	1.007664	-0.355815	2.551575
O	-0.101802	-0.328639	3.178069
C	0.837810	-3.218441	1.743131
H	1.746065	-2.606072	1.763365
H	0.132128	-2.770420	2.454759
H	1.078094	-4.227561	2.092235
C	1.649190	2.530226	2.231644
H	0.844796	2.124594	2.857566
H	2.393906	1.735305	2.109829
H	2.108731	3.368538	2.764420

Complex 4 TS₂

E = -1129.622686

Number of negative frequencies = 1

N	1.694184	-1.684460	-1.512053
C	2.797557	-2.440215	-1.332206
C	1.301948	-1.312320	-2.754640
C	3.541513	-2.853462	-2.437834
C	2.016887	-1.697919	-3.879648
C	3.152492	-2.481570	-3.714878
H	4.426408	-3.464112	-2.277442
H	1.698715	-1.398073	-4.873314
H	3.729086	-2.796173	-4.581386
N	-0.501458	-0.260189	-1.600696
C	0.082422	-0.498289	-2.800929
C	-1.651351	0.446731	-1.544922
C	-0.455479	-0.000060	-3.981598
C	-2.219798	0.978482	-2.701105
C	-1.615969	0.758442	-3.929251
H	0.025404	-0.195752	-4.935003
H	-3.149098	1.537440	-2.624640
H	-2.051224	1.159569	-4.841105
N	-2.490766	-0.456214	0.508736
C	-3.084954	-0.337516	1.702973
C	-2.328474	0.637960	-0.240946
C	-3.541145	0.898961	2.174013
C	-2.769972	1.905144	0.140342

C	-3.386703	2.029086	1.381393
H	-4.014032	0.965646	3.152293
H	-2.607966	2.770524	-0.499595
H	-3.734739	2.999714	1.729296
C	0.681652	1.193410	1.153672
H	0.950212	1.523056	0.146677
H	-0.253387	1.599434	1.534779
H	1.507053	1.137817	1.858366
Pt	0.550497	-0.975131	0.066689
O	0.023523	-0.578541	1.959605
O	1.172774	-1.358227	1.946567
C	-3.225847	-1.590564	2.504848
H	-2.236024	-2.036454	2.669938
H	-3.695777	-1.403849	3.476638
H	-3.829420	-2.329561	1.962137
C	3.198610	-2.804148	0.055035
H	3.429799	-1.904438	0.640152
H	2.390908	-3.331866	0.576851
H	4.084209	-3.446691	0.042500