

Supporting Information

Mechanism of Pd-catalyzed C(sp³)-H Activation of Aliphatic Amines: An Insight from DFT Calculations

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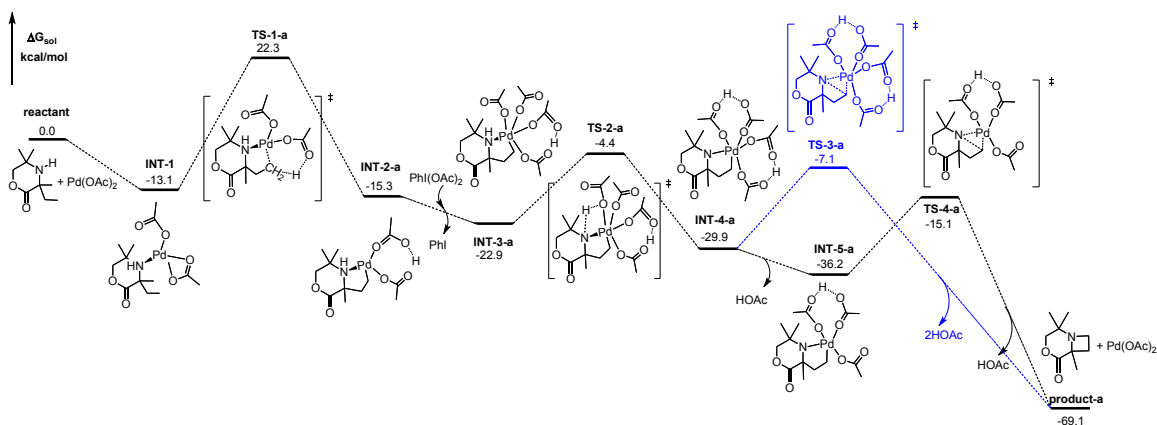


Figure S1. The total computed free energy profile for **ethyl-C-H activation** catalytic cycle. Gibbs free energies are given in kcal/mol.

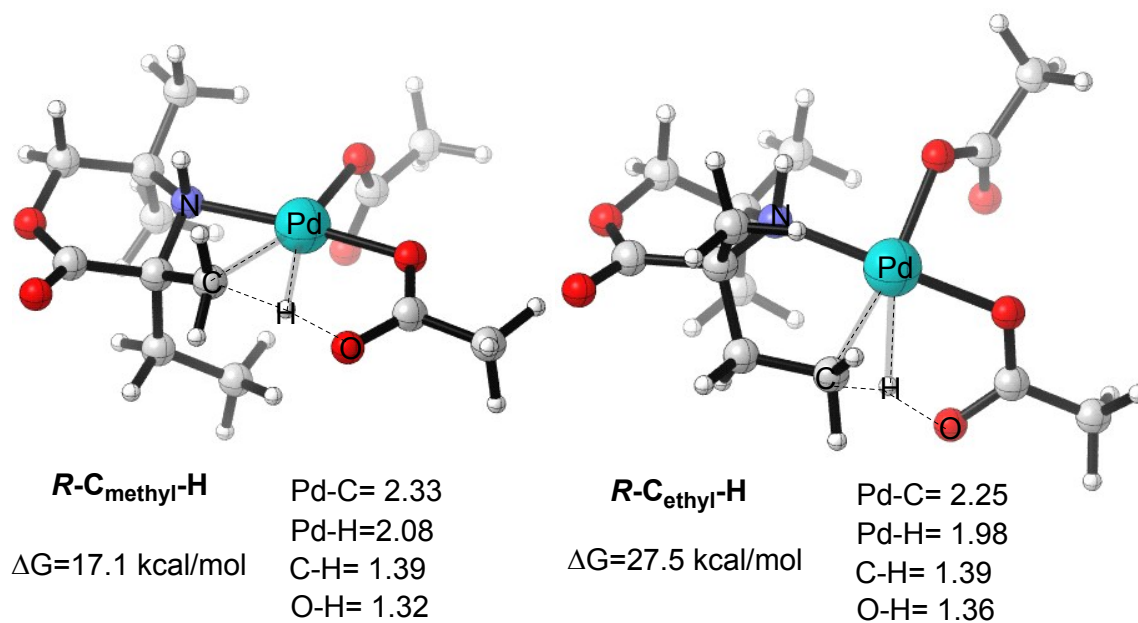


Figure S2. Optimized structures of *R*-configuration C_{methyl}-H activation and C_{ethyl}-H activation transition states. Selected distances are shown in Å. Gibbs free energies are given in kcal/mol.

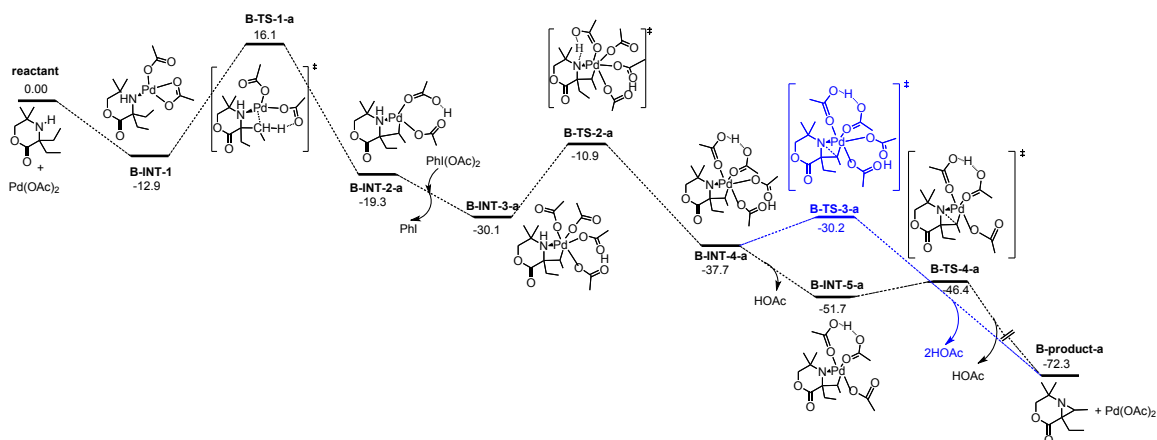


Figure S3. The total computed free energy profile for **substrate B** catalytic cycle. Gibbs free energies are given in kcal/mol.

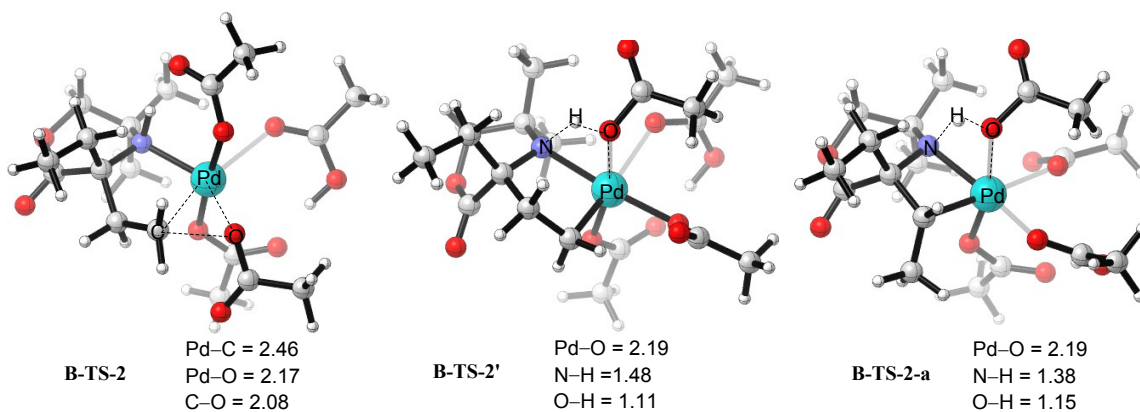


Figure S4. Optimized structures of **substrate B** transition states, selected distances are shown in Å.

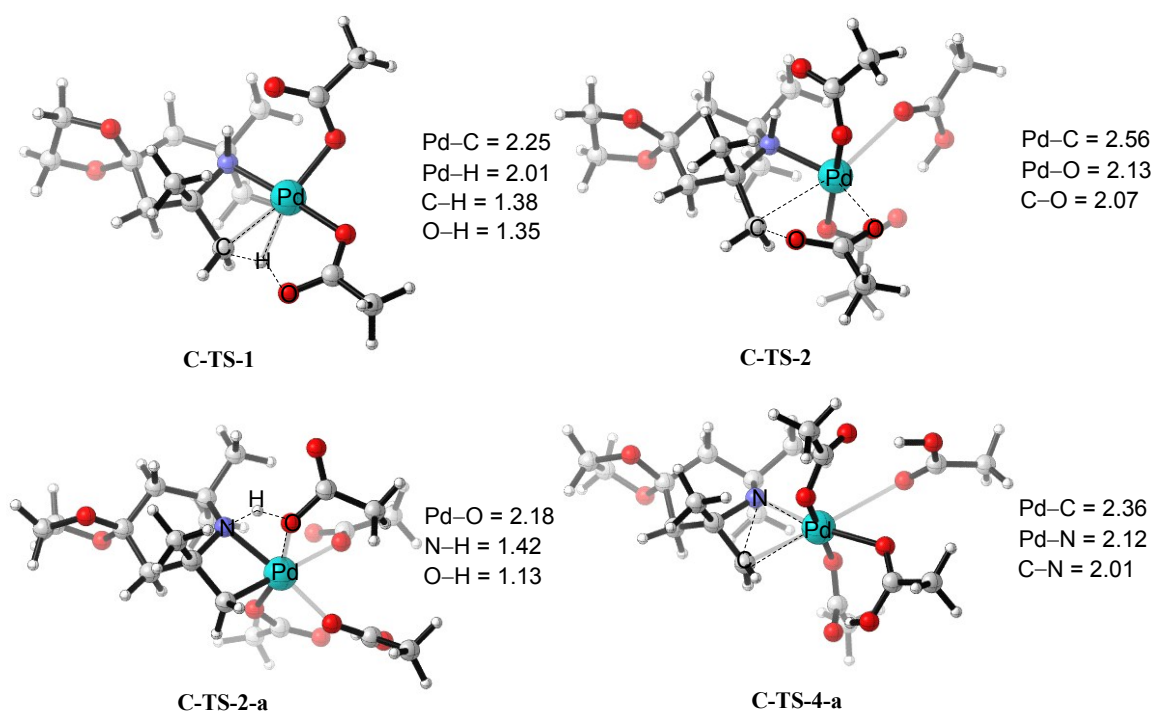


Figure S5. Optimized structures of **substrate C** transition states, selected distances are shown in Å.

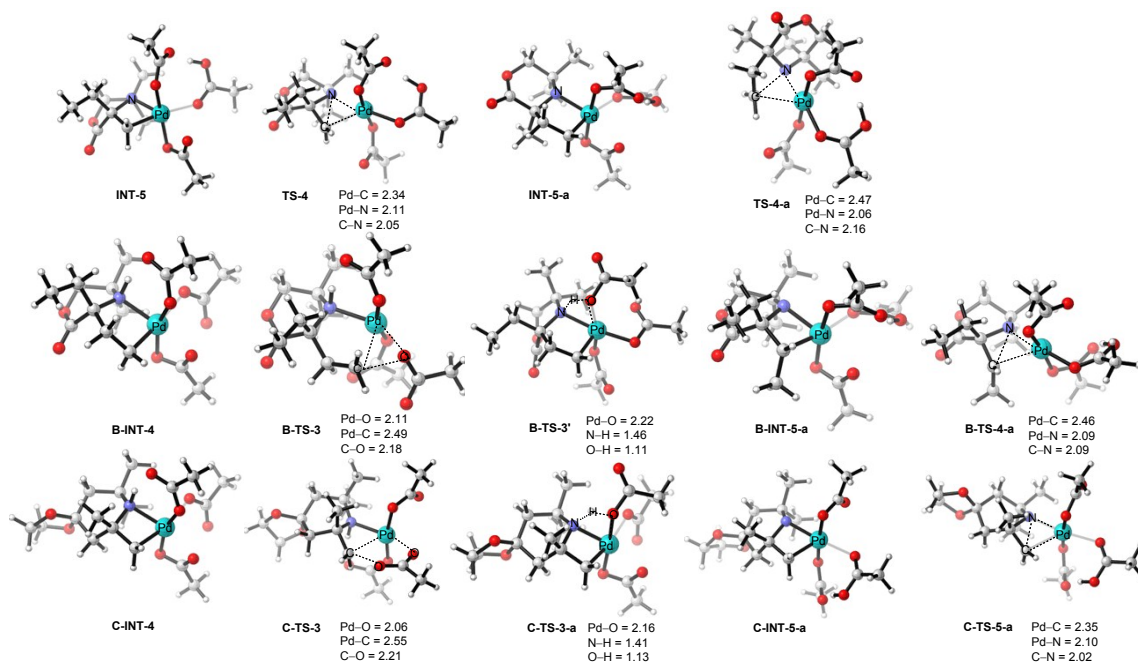


Figure S6. Optimized structures of pentacoordinated intermediates and transition states, selected distances are shown in Å.

Calculated energies and cartesian coordinates for the relevant intermediates and transition states

Table S1. Calculated energy values

Species	ZPE ^a	G ^b	H ^c	E ^d
Pd(OAc)₂	-583.634377	-583.673600	-583.622596	-583.737522
PhI(OAc)₂	-699.711750	-699.760504	-699.693705	-699.904495
PhI	-242.939149	-242.970922	-242.932309	-243.029299
CH₃COO⁻	-228.367830	-228.396041	-228.362346	-228.415657
CH₃COOH	-229.029526	-229.056772	-229.024008	-229.091479
reactant	-1141.797352	-1141.857307	-1141.771129	-1142.1576159
INT-1	-1141.823562	-1141.879631	-1141.797519	-1142.1863284
TS-1	-1141.782785	-1141.837273	-1141.757514	-1142.1400545
TS-1-a	-1141.764180	-1141.818148	-1141.738953	-1142.1217556
INT-2	-1141.824760	-1141.882737	-1141.798669	-1142.1853004
INT-2-a	-1141.820831	-1141.877077	-1141.795113	-1142.1824038
INT-3	-1598.634096	-1598.700786	-1598.598425	-1599.0999972
INT-3-a	-1598.631356	-1598.697208	-1598.595769	-1599.0978758
TS-2	-1598.603864	-1598.670918	-1598.568027	-1599.0640018
TS-2-a	-1598.601951	-1598.667522	-1598.566532	-1599.0631653
TS-2'	-1598.613829	-1598.682990	-1598.577648	-1599.0789976
INT-4	-1598.646047	-1598.715018	-1598.609726	-1599.1103108
INT-4-a	-1598.641867	-1598.710130	-1598.605603	-1599.1063299
TS-3	-1598.624438	-1598.693609	-1598.587958	-1599.0866667
TS-3-a	-1598.600158	-1598.670990	-1598.563606	-1599.0630489
INT-5	-1369.598535	-1369.660998	-1369.567541	-1369.9989061
INT-5-a	-1369.594812	-1369.657208	-1369.563995	-1369.9958099
TS-4	-1369.585197	-1369.648071	-1369.554349	-1369.9840613
TS-4-a	-1369.551771	-1369.612066	-1369.521565	-1369.9514531
Product	-556.944050	-556.981611	-556.930947	-557.1771849
Product-a	-556.950168	-556.986644	-556.937480	-557.1841521
R-C_{methyl}-H-ts	-1141.781903	-1141.835927	-1141.756763	-1142.1393539
R-C_{ethyl}-H-ts	-1141.766712	-1141.820619	-1141.741662	-1142.1246821
B-reactant	-1181.076352	-1181.138390	-1181.048121	-1181.4654874
B-INT-1	-1181.103823	-1181.160861	-1181.076181	-1181.4948618
B-TS-1	-1181.069207	-1181.124697	-1181.042948	-1181.4558601
B-TS-1-a	-1181.056999	-1181.113379	-1181.030278	-1181.4431346
B-INT-2	-1181.108433	-1181.165750	-1181.081519	-1181.4991204
B-INT-2-a	-1181.108544	-1181.167993	-1181.080923	-1181.4975691
B-INT-3	-1637.913995	-1637.981535	-1637.877331	-1638.4090537
B-TS-2	-1637.895260	-1637.965166	-1637.857905	-1638.3889911
B-TS-2'	-1637.878270	-1637.946437	-1637.867298	-1638.3906352
B-INT-4	-1408.877632	-1408.937433	-1408.846706	-1409.310236
B-TS-3	-1408.857780	-1408.919534	-1408.826324	-1409.287708
B-TS-3'	-1408.836551	-1408.897154	-1408.805504	-1409.2633302

B-INT-3-a	-1637.921430	-1637.989103	-1637.884295	-1638.4153206
B-TS-2-a	-1637.890783	-1637.958725	-1637.853589	-1638.3792972
B-product	-825.276186	-825.323396	-825.256606	-825.6042875
B-INT-4-a	-1637.933802	-1638.003875	-1637.896015	-1638.4262225
B-TS-3-a	-1637.917281	-1637.990440	-1637.878735	-1638.407332
B-INT-5-a	-1408.886570	-1408.951292	-1408.854075	-1409.315253
B-TS-4-a	-1408.877395	-1408.845035	-1408.941151	-1409.3047027
B-product-a	-596.237147	-596.276364	-596.222451	-596.4983339
C-reactant	-1220.343312	-1220.405682	-1220.314765	-1220.7615482
C-INT-1	-1220.370248	-1220.429000	-1220.342681	-1220.7913843
C-TS-1	-1220.330531	-1220.388167	-1220.303688	-1220.7462196
C-INT-2	-1220.373632	-1220.433328	1220.346026	-1220.7925741
C-INT-3	-1677.185255	-1677.254066	-1677.148006	-1677.7096406
C-TS-2	-1677.160388	-1677.232723	-1677.122563	-1677.6844025
C-TS-2-a	-1677.153811	-1677.222568	-1677.116584	-1677.6725914
C-INT-4	-1448.141676	-1448.206233	-1448.109287	-1448.6004145
C-INT-4-a	-1677.190786	-1677.262284	-1677.152727	-1677.7130262
C-TS-4-a	-1677.174929	-1677.250626	-1677.136149	-1677.6951127
C-TS-3	-1448.114908	-1448.178450	-1448.083132	-1448.5753199
C-TS-3-a	-1448.107578	-1448.168200	-1448.076214	-1448.563363
C-product	-864.551494	-864.599918	-864.531307	-864.9085231
C-INT-5-a	-1448.141676	-1448.206233	-1448.109287	-1448.6004145
C-TS-5-a	-1448.132290	-1448.197272	-1448.099849	-1448.589341
C-product-a	-635.494916	-635.534119	-635.480371	-635.7864356

^aSum of electronic and zero-point energies

^bSum of electronic and thermal free energies

^cSum of electronic and thermal enthalpies

^dElectronic energies

Cartesian coordinates

Pd(OAc)₂

NImag=0

0 1 (charge, spin multiplicity)

H	-4.32407700	0.93383400	-0.38167400
C	-3.93823300	0.00194000	0.03482900
C	-2.44321400	0.00147100	-0.00469100
H	-4.26721600	-0.07893000	1.07649200
H	-4.32592100	-0.85889400	-0.51347800
O	-1.77205600	-1.08771500	-0.01005900
O	-1.76986200	1.08908500	-0.00908700
Pd	0.00002100	-0.00084600	-0.00912400
O	1.77169300	-1.08895000	-0.00883500
C	2.44319000	-0.00021600	-0.00461400
O	1.77017300	1.08786700	-0.00996700

C	3.93819200	0.00156500	0.03459000
H	4.26708400	0.05046100	1.07829600
H	4.32562600	-0.91717400	-0.40903300
H	4.32433700	0.87878400	-0.48799300

PhI(OAc)₂

NImag=0

0 1 (charge, spin multiplicity)

C	2.47189200	-1.76379200	0.17424400
O	1.61012900	-1.48464700	-0.79484400
O	2.32640100	-1.48089800	1.35516800
C	3.69932900	-2.48514300	-0.36017100
H	4.18268600	-1.87581600	-1.12906800
H	4.39485000	-2.67971700	0.45643600
H	3.40050300	-3.42594600	-0.83105600
I	-0.35726800	-0.71841300	-0.20424600
O	-2.20066000	0.40352900	0.22646400
C	-3.20540900	-0.45046600	0.24654600
O	-3.06836700	-1.65546000	0.05555100
C	-4.54327900	0.20344700	0.53548300
H	-4.52195900	0.65911800	1.52972200
H	-4.73401900	1.00203700	-0.18662000
H	-5.33447000	-0.54465900	0.48709700
C	0.47569600	1.26037600	-0.07602700
C	-0.02468900	2.23785100	-0.93039100
C	1.47527000	1.50703400	0.85786600
C	0.51253500	3.52368800	-0.84382000
H	-0.82015500	2.01652400	-1.63153100
C	2.00179000	2.80092500	0.92167700
H	1.84185800	0.71377600	1.49920900
C	1.52428100	3.80347900	0.07700900
H	0.13767200	4.30256300	-1.50094800
H	2.78490100	3.01807800	1.64182800
H	1.93881000	4.80535300	0.13672800

PhI

NImag=0

0 1 (charge, spin multiplicity)

I	1.56673400	0.00000000	-0.00004300
C	-0.58118600	-0.00000200	0.00001800
C	-1.26366200	1.21552200	0.00003600
C	-1.26366100	-1.21552100	0.00003500
C	-2.66098000	1.20700100	0.00007900
H	-0.72204200	2.15463900	0.00002200
C	-2.66098300	-1.20699900	0.00006700
H	-0.72204700	-2.15464100	0.00002100
C	-3.36112900	0.00000000	0.00009000
H	-3.19814400	2.15114900	0.00009700
H	-3.19814600	-2.15114800	0.00007400
H	-4.44693400	0.00000200	0.00012100

CH₃COO⁻

NImag=0

0 2 (charge, spin multiplicity)

C	-0.09242000	0.12531300	-0.00035900
O	-0.78113000	-1.04498000	0.00011700
O	-0.64192600	1.20355800	-0.00008100
C	1.39678100	-0.11233300	0.00009100
H	1.68160200	-0.69665400	-0.87974600
H	1.91755700	0.84400000	-0.00182600
H	1.68152000	-0.69284100	0.88250200

H	-1.72239700	-0.80100700	0.00038900
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CH₃COOH

NImag=0

0 1 (charge, spin multiplicity)

C	-0.09242000	0.12531300	-0.00035900
O	-0.78113000	-1.04498000	0.00011700
O	-0.64192600	1.20355800	-0.00008100
C	1.39678100	-0.11233300	0.00009100
H	1.68160200	-0.69665400	-0.87974600
H	1.91755700	0.84400000	-0.00182600
H	1.68152000	-0.69284100	0.88250200
H	-1.72239700	-0.80100700	0.00038900

Reactants

NImag=0

0 1 (charge, spin multiplicity)

C	3.07082900	0.27041900	0.50226600
C	1.84202800	-1.68516400	-0.57841200
C	3.27012300	-2.21957100	-0.67711100
H	3.60286300	-2.60370200	0.29409100
H	3.33547700	-3.02824200	-1.40855000
C	0.93610800	-2.80534800	-0.03617000
H	-0.09259300	-2.44968400	0.07446000
H	0.92223900	-3.66639400	-0.71490600
H	1.28414600	-3.13386900	0.94751000
C	1.34331900	-1.23522000	-1.97045200
H	1.28865100	-2.07921400	-2.66745900
H	0.34052200	-0.80383700	-1.88415400
H	2.00056200	-0.47972100	-2.41033100
N	1.85876600	-0.57755800	0.39361900
H	1.03883500	0.00466100	0.25198700
C	2.65607700	1.74872200	0.49120200
H	1.97726200	1.94294700	1.32878900
H	3.52373400	2.40288700	0.57147500
H	2.13680800	1.98980300	-0.44080800
C	3.78824700	-0.08168300	1.84887800
H	3.02561300	0.03553700	2.62738100
H	4.03534900	-1.14931200	1.83729300
C	5.04272200	0.72679100	2.19816900
H	5.48980800	0.34294400	3.12106100
H	5.79826300	0.67142600	1.40922300
H	4.81472500	1.78430200	2.36194000
O	4.18793100	-1.21453700	-1.13998800
C	4.08298000	0.04106200	-0.63620900
O	4.81589400	0.90435100	-1.06388500
H	-1.35126200	4.67151000	-0.45208800
C	-0.71476000	3.81196100	-0.66637500
C	-1.44996600	2.54380200	-0.37671700
H	-0.43647200	3.82894200	-1.72561600
H	0.20415300	3.85309000	-0.07766700
O	-0.83657000	1.42380200	-0.24099400
O	-2.72203900	2.50861100	-0.27447000
Pd	-2.65281600	0.45113700	0.03904700
O	-2.55861400	-1.59681300	0.33959000
C	-3.83573900	-1.65188300	0.43024900
O	-4.46086500	-0.54255800	0.31490900
C	-4.55397800	-2.94739000	0.62790100
H	-4.77481000	-3.38454700	-0.35203300
H	-3.92264000	-3.64434400	1.18207600

H -5.49691500 -2.77641700 1.15023700

INT-1

NImag=0

0 1 (charge, spin multiplicity)

C	1.66005400	-0.42792600	-0.77452800
C	1.03482400	-0.76991100	1.68030300
C	2.50387200	-0.45988900	1.98853400
H	2.65023200	0.62152400	2.09511200
H	2.81817300	-0.94655900	2.91570200
C	0.16615900	-0.15180700	2.78594900
H	-0.88833800	-0.38922700	2.61829700
H	0.45499200	-0.56735700	3.75665900
H	0.27559600	0.93495200	2.81978100
C	0.78457500	-2.28211700	1.59182800
H	0.95391100	-2.72614800	2.57785800
H	-0.24494100	-2.48591200	1.29237600
H	1.45586600	-2.78520600	0.89219300
N	0.75710000	-0.05195000	0.38408400
H	0.90701000	0.95763200	0.60286200
C	0.96485600	-1.42317900	-1.71988100
H	0.15986600	-0.91776500	-2.26140600
H	0.52805800	-2.26117200	-1.17483300
C	1.99498000	0.90306400	-1.51966600
H	1.03181400	1.38004200	-1.73565900
H	2.51684500	1.56982600	-0.82308700
O	3.39324300	-0.95892100	0.97810300
C	2.99990100	-1.05346100	-0.31190300
O	3.73596300	-1.59668200	-1.10257400
H	-4.34842000	-2.65212700	-1.68420700
C	-4.32938800	-2.35952000	-0.62870300
C	-3.19746200	-1.40074000	-0.40911800
H	-5.27946300	-1.87926100	-0.38811000
H	-4.18583100	-3.25845600	-0.02621900
O	-2.02305500	-1.83091100	-0.11535500
O	-3.35614200	-0.14428800	-0.53262200
Pd	-1.28699200	0.14052700	-0.10615800
O	-1.20011500	2.15999700	-0.25939700
C	-0.37403100	2.96196200	0.33930800
O	0.64782000	2.62641600	0.96394700
C	-0.76644500	4.42562100	0.22115400
H	-1.03545800	4.66451600	-0.81058900
H	-1.64992600	4.61133300	0.84042100
H	0.05364600	5.05961300	0.55961400
H	1.68919100	-1.81222800	-2.43579500
C	2.80015900	0.77988200	-2.81645700
H	2.97413000	1.77993500	-3.22574800
H	3.76764200	0.30123600	-2.65315300
H	2.26329500	0.20345400	-3.57513400

TS-1

NImag=1

0 1 (charge, spin multiplicity)

C	-1.39012400	-0.96351400	0.39546000
C	-2.00067300	1.16863300	-0.88277700
C	-3.40677200	0.91607100	-0.32512600
H	-3.49308700	1.33059900	0.68712400
H	-4.16828900	1.38360500	-0.95425500
C	-1.70853000	2.67389500	-0.86289900
H	-0.70393700	2.86688500	-1.24613800

H	-2.42847400	3.19525200	-1.50086600
H	-1.76904400	3.08590800	0.14757900
C	-1.85926300	0.62604400	-2.31256600
H	-2.51691100	1.19067400	-2.98032500
H	-0.82961300	0.74740900	-2.65949000
H	-2.13327500	-0.42767800	-2.40086900
N	-1.07626800	0.47526100	0.07022500
H	-0.94897700	1.06293100	0.91215800
C	-0.33363200	-1.77703400	-0.39767300
H	1.00212600	-1.92350000	-0.18595800
H	-0.56867700	-1.80947800	-1.46315800
C	-1.25439800	-1.11701600	1.94090400
H	-0.32389700	-0.61491700	2.23123900
H	-2.06970900	-0.54453800	2.40281700
O	-3.74573000	-0.48132800	-0.29692300
C	-2.80317700	-1.41187900	-0.01071700
O	-3.09553500	-2.58308100	-0.06461500
H	4.56826700	-2.96749100	-1.33748400
C	4.53163700	-2.18380200	-0.57561400
C	3.10722600	-1.70044900	-0.42864800
H	4.85593700	-2.63092400	0.36848500
H	5.19594000	-1.36418300	-0.84723600
O	2.20989700	-2.54284900	-0.12799500
O	2.88384200	-0.46017600	-0.61709500
Pd	0.92017600	0.10726300	-0.32332600
O	1.60641600	2.01771700	-0.08050800
C	1.17366500	2.66416600	0.96286000
O	0.23752000	2.31905700	1.70368300
C	1.94364200	3.94909300	1.23209200
H	1.40470100	4.56456500	1.95339300
H	2.92809400	3.69595700	1.63893300
H	2.10760300	4.50020200	0.30282700
H	-0.35553800	-2.81356200	-0.04798300
C	-1.25892000	-2.54776300	2.48484100
H	-1.24891200	-2.51768700	3.57856200
H	-2.14265900	-3.10229500	2.16231000
H	-0.37125600	-3.10206000	2.16654300

TS-1-a

NImag=1

0 1 (charge, spin multiplicity)

C	2.07359000	-0.96381800	0.30467800
C	1.88352200	1.47791900	-0.52104400
C	3.27509000	1.23889800	-1.12627400
H	3.18094500	0.87684800	-2.15867100
H	3.84573900	2.16998800	-1.14722200
C	1.05931200	2.25053500	-1.56167500
H	0.02485000	2.37656000	-1.24431500
H	1.50323300	3.23697000	-1.72650900
H	1.04668700	1.72753500	-2.52580800
C	1.95610200	2.24236600	0.80485000
H	2.24221000	3.27861100	0.59976600
H	0.97833400	2.24143800	1.29024700
H	2.70749700	1.82762900	1.47952700
N	1.25741200	0.11383000	-0.36290100
H	1.13394500	-0.20672100	-1.32663800
C	1.96236100	-0.92062300	1.84685900
H	2.47814900	-0.06037700	2.27474700
C	1.48436100	-2.27754100	-0.25206200

H	1.66073400	-2.30709200	-1.33676600
O	4.09716500	0.30657200	-0.40302100
C	3.58245800	-0.87819300	0.00814000
O	4.32228100	-1.79858000	0.25665500
H	-4.87539500	-2.81294500	-0.81139800
C	-4.65855100	-1.82401600	-0.40591700
C	-3.16772400	-1.60381600	-0.32364400
H	-5.07526900	-1.06960700	-1.08176600
H	-5.11962100	-1.69332800	0.57401700
O	-2.40380600	-2.22493600	-1.12341100
O	-2.74667900	-0.77434500	0.54819200
Pd	-0.77030100	-0.27556800	0.21277200
O	-1.22079400	1.59294000	0.88515800
C	-2.06854000	2.26703500	0.14269400
O	-2.36094300	1.99630100	-1.01948600
C	-2.67229000	3.45977400	0.87495600
H	-1.90425200	4.01200600	1.42299500
H	-3.17627700	4.11526200	0.16343200
H	-3.39934100	3.09706900	1.60888100
H	2.42580800	-1.82328800	2.25108800
H	0.91669300	-0.87625600	2.15850700
H	2.05370600	-3.11227200	0.16711300
C	-0.01488400	-2.44792100	0.03880500
H	-0.33318500	-3.37524700	-0.45557400
H	-0.21007300	-2.62421000	1.10039600
H	-1.13977200	-2.02645700	-0.65816300

INT-2

NImag=0

0 1 (charge, spin multiplicity)

C	-1.93778300	-0.72503600	0.38154200
C	-1.86207300	1.76919600	-0.31642100
C	-3.36016600	1.68371800	-0.00757500
H	-3.53383000	1.75671900	1.07438900
H	-3.91266600	2.49028400	-0.49580500
C	-1.27758300	3.06925100	0.24808900
H	-0.19380000	3.07415100	0.10667200
H	-1.70243300	3.93383700	-0.27013200
H	-1.49442400	3.17853200	1.31779100
C	-1.59829000	1.68162900	-1.82670200
H	-2.11125700	2.50310800	-2.33744400
H	-0.52625100	1.76031200	-2.02104800
H	-1.95619200	0.74574100	-2.26164000
N	-1.21634700	0.62516900	0.40555500
H	-1.08460000	0.90195400	1.37730600
C	-0.86849300	-1.62439600	-0.25292700
H	3.32091900	0.03091000	0.98849400
H	-1.09672100	-1.94583000	-1.26965300
C	-2.27056600	-1.11657900	1.84731800
H	-1.31763500	-1.10016600	2.39347900
H	-2.90690900	-0.33730600	2.28935600
O	-3.93934200	0.46884200	-0.50836900
C	-3.24677600	-0.69664300	-0.41608400
O	-3.70476700	-1.69448900	-0.91680100
H	4.80104400	-2.65918300	-1.23050900
C	3.83721200	-3.04751500	-0.88512000
C	3.01091700	-1.89632200	-0.33624200
H	3.33023900	-3.54483900	-1.71233700
H	4.04463900	-3.76004300	-0.08242400

O	3.38717800	-1.36411800	0.74026700
O	1.99671000	-1.55473600	-1.03213400
Pd	0.59060400	-0.23626700	-0.28078800
O	3.53724300	1.05066000	1.18917500
C	2.84718000	1.90453100	0.49985600
O	1.86758200	1.63306400	-0.21847400
C	3.33217400	3.33092200	0.62897200
H	3.36312100	3.61559500	1.68472700
H	4.35495200	3.40125300	0.24690200
H	2.68452800	4.00921100	0.07412100
H	-0.57188600	-2.47284700	0.36506100
C	-2.93724700	-2.48359300	2.02892400
H	-3.08286600	-2.68130900	3.09510000
H	-3.90986200	-2.52984200	1.53417300
H	-2.31935100	-3.28691600	1.61970400

INT-2-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.28144400	-0.92190200	0.25226000
C	1.93099300	1.53701800	-0.43097700
C	3.33658700	1.44524300	-1.04287900
H	3.26563400	1.16680800	-2.10343100
H	3.84643300	2.40997900	-0.98289100
C	1.04775300	2.33557200	-1.40049300
H	0.04664400	2.44897300	-0.98564600
H	1.47642900	3.32915400	-1.56507300
H	0.96722800	1.84004200	-2.37512500
C	1.94407700	2.21121300	0.94594500
H	2.13749000	3.28082300	0.81701200
H	0.97303500	2.09411400	1.43179400
H	2.72839400	1.81660600	1.59377900
N	1.39895500	0.13192900	-0.37617500
H	1.33131300	-0.14358400	-1.35853300
C	2.15768300	-0.97065900	1.79185800
H	2.59334600	-0.09750400	2.27846400
C	1.74071800	-2.23220400	-0.36213800
H	1.96197900	-2.22750800	-1.43858100
O	4.21589200	0.51079300	-0.39547900
C	3.77649800	-0.72672000	-0.04021100
O	4.58002900	-1.60573700	0.15370200
H	-4.12184600	-3.32244800	0.55248600
C	-4.42772700	-2.54913200	-0.15241200
C	-3.36790300	-1.46934200	-0.29390200
H	-4.62128000	-2.99070700	-1.13423600
H	-5.36301000	-2.09090000	0.18416000
O	-3.55113500	-0.56809100	-1.15309400
O	-2.36529400	-1.55941200	0.49244000
Pd	-0.62080900	-0.49791900	0.09630200
O	-3.41956400	1.78440100	-0.42292000
C	-2.45673600	2.19964900	0.33987700
O	-1.41549500	1.57101000	0.60258200
C	-2.68825700	3.57500800	0.92312800
H	-1.79993100	3.92158200	1.45033100
H	-2.95984500	4.27579300	0.12907600
H	-3.53247100	3.53142400	1.61845100
H	2.69361900	-1.85290900	2.14925400
H	1.10697500	-1.03941600	2.08222500
H	2.29141200	-3.07871300	0.05953500

C	0.22804600	-2.34077200	-0.12234200
H	-0.28785100	-2.85971600	-0.93378100
H	-0.01483500	-2.83652900	0.82125900
H	-3.32885700	0.78389400	-0.75135700

INT-3

NImag=0

O 1 (charge, spin multiplicity)

C	2.22876600	0.45795700	-0.67594100
C	2.04304100	-1.15928800	1.35657800
C	3.56648100	-1.04314100	1.18400400
H	3.94597900	-0.09017900	1.56829600
H	4.05785000	-1.85195500	1.72793400
C	1.67897700	-0.96835100	2.83438600
H	0.59773100	-1.05813300	2.95499800
H	2.15080300	-1.76110300	3.42318400
H	2.01252400	-0.00039200	3.21920100
C	1.56729100	-2.52956700	0.86557200
H	2.11198000	-3.29628600	1.42688900
H	0.50246400	-2.62740000	1.07018600
H	1.75603300	-2.68604600	-0.19683800
N	1.47785000	0.01474600	0.57419200
H	-3.23746900	-0.85044000	-0.89238500
C	1.07834800	0.63779600	-1.66248300
H	1.37774700	0.82746400	1.23508900
H	1.00196300	-0.11850400	-2.43724100
C	2.99506100	1.78691800	-0.41713000
H	2.25754800	2.52130300	-0.08295200
H	3.69657900	1.65292300	0.41261400
O	3.96554600	-1.21365700	-0.18937600
C	3.24000200	-0.59384100	-1.14560700
O	3.45470600	-0.80802800	-2.31362300
H	-4.93733500	1.85755800	-2.35394500
C	-3.92572200	2.14877200	-2.06978700
C	-3.14554900	0.95950300	-1.57687500
H	-3.40360000	2.62112500	-2.90279500
H	-3.98186500	2.87391500	-1.25036400
O	-3.83467800	-0.01048800	-1.09754200
O	-1.89139700	0.99290900	-1.66713300
Pd	-0.43148400	0.24644200	-0.31317000
O	-1.31742000	-1.91816200	2.07845300
C	-2.11372700	-0.97600000	1.97163900
O	-2.00051500	0.03436800	1.16866900
C	-3.37767400	-0.93120200	2.82914800
H	-3.44397700	0.02424000	3.35798800
H	-4.25753800	-1.00568400	2.18202100
H	-3.37915600	-1.75536500	3.54379000
H	0.89807100	1.65478900	-2.00190600
C	3.74656800	2.32490500	-1.64119900
H	4.20233900	3.28760700	-1.39218600
H	4.53994900	1.64831300	-1.96848400
H	3.07713500	2.48410200	-2.49142000
C	-1.05038400	-3.86183500	-1.47093700
H	-1.89606600	-4.35883400	-1.94785400
H	-0.82904800	-4.37378400	-0.52847200
H	-0.16376300	-3.90751100	-2.10499100
C	-0.72484600	3.96386100	1.81881300
H	-1.70548700	3.71939100	2.24022500
H	-0.88451300	4.61854600	0.95940400

H	-0.12162800	4.46275700	2.57818600
C	-0.05562700	2.66896900	1.39673200
O	0.81667100	2.14002600	2.10136700
O	-0.48434500	2.21993800	0.25190300
C	-1.42228100	-2.42747200	-1.14352800
O	-0.39732100	-1.63583800	-1.09288100
O	-2.61303800	-2.13855100	-0.95008500

INT-3-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.45174700	-0.15458800	-1.04923400
C	2.03827000	-0.90345900	1.38346100
C	3.50060800	-0.46406900	1.62099900
H	3.52046400	0.56045000	2.00789600
H	3.95648400	-1.12842500	2.35796700
C	1.26313700	-0.47645200	2.63996500
H	0.27004300	-0.91718600	2.62724000
H	1.79318200	-0.85481500	3.52084100
H	1.19419800	0.60986700	2.72428200
C	1.89158700	-2.41324400	1.17934600
H	2.07116300	-2.90538600	2.14007000
H	0.86953500	-2.64364200	0.87732200
H	2.60626800	-2.82176200	0.46461900
N	1.59259700	-0.07124200	0.19943800
H	1.71590300	0.91828800	0.53835700
C	2.34096600	-1.46921600	-1.86052100
H	2.91920600	-2.27773800	-1.41330600
C	1.98191200	1.04168200	-1.89181600
H	2.22462200	1.97229500	-1.37194600
O	4.37278800	-0.51723100	0.47690400
C	3.95328500	-0.03951800	-0.71435300
O	4.74926200	0.31559500	-1.54840700
H	-0.39742900	-3.94981600	-1.82126700
C	-1.32763200	-3.80165700	-1.27130400
C	-1.65164600	-2.33322300	-1.08541400
H	-2.15862600	-4.30305300	-1.76953100
H	-1.21618100	-4.21831700	-0.26473800
O	-2.83607000	-1.99970500	-0.92777100
O	-0.60644100	-1.56674500	-1.11161700
Pd	-0.45410300	0.32498900	-0.36125100
O	-4.01602100	0.11193500	-0.57015400
C	-3.38866700	1.15585600	-0.97115000
O	-2.17603700	1.19706400	-1.30229400
C	-4.19435000	2.42486300	-1.05474800
H	-3.84035500	3.04115800	-1.88231100
H	-5.25727500	2.20423500	-1.15631900
H	-4.03212700	2.98199100	-0.12534100
H	2.76146000	-1.28147400	-2.85136700
H	1.30634100	-1.78945400	-1.94791300
H	2.52913500	1.05157300	-2.84098300
C	0.49148800	0.93698500	-2.13427700
H	-0.00869400	1.87751200	-2.35465000
H	0.18649500	0.14311900	-2.81525400
H	-3.41410500	-0.75466600	-0.64599300
O	-0.39725100	2.26463300	0.32141500
C	0.56691400	2.89820000	0.90783900
O	1.72353100	2.47283300	1.08308200
C	0.16195400	4.27315700	1.41065700

H	-0.42916800	4.79924700	0.65790300
H	-0.46372600	4.15298700	2.30086200
H	1.05291800	4.84634300	1.66908900
O	-1.75128500	-0.05468600	1.35934100
C	-2.00842200	-1.19796500	1.91504200
O	-1.35247300	-2.24079700	1.78157200
C	-3.24507500	-1.17189400	2.81304100
H	-3.15424300	-0.37635900	3.55885500
H	-4.12847500	-0.94826700	2.20682400
H	-3.37294500	-2.13539300	3.30851300

TS-2

NImag=1

O 1 (charge, spin multiplicity)

C	-2.31799700	-0.50846100	-0.71699000
C	-2.11303600	0.66111100	1.55693900
C	-3.63982300	0.49658800	1.43361000
H	-3.95274400	-0.53328800	1.63530500
H	-4.13863500	1.15499500	2.14726600
C	-1.64095000	0.22066100	2.94916200
H	-0.56696500	0.39702500	3.03995400
H	-2.14147800	0.81649800	3.71921800
H	-1.84469700	-0.83828600	3.13238200
C	-1.74662300	2.13718900	1.31970700
H	-2.29029500	2.74626600	2.04997300
H	-0.67608800	2.27038300	1.47412900
H	-2.01756600	2.48085400	0.32059800
N	-1.54636400	-0.28989600	0.55715200
H	3.10831200	1.07126100	-1.08025800
C	-1.18157500	-0.45922700	-1.73347900
H	-0.91903200	-1.47969100	0.84635900
H	-1.18539800	0.39698800	-2.40036400
C	-3.02431300	-1.90159500	-0.70450100
H	-2.24639700	-2.64972400	-0.52491700
H	-3.71550300	-1.95520800	0.14261700
O	-4.11400400	0.91252500	0.13688300
C	-3.39012700	0.55817800	-0.95087900
O	-3.65483200	1.00982300	-2.03843200
H	4.74795900	-1.37389100	-3.02465200
C	3.96795400	-1.80958600	-2.39697200
C	3.10454000	-0.72215000	-1.81032800
H	3.36025700	-2.51316300	-2.96511100
H	4.46005100	-2.34207100	-1.57582000
O	3.74648200	0.31404200	-1.38595400
O	1.86466500	-0.87518300	-1.76365600
Pd	0.33839500	-0.13656500	-0.36635600
O	1.32390300	1.87415800	2.13392300
C	2.12316000	0.95643700	1.92696300
O	1.97148200	-0.00500000	1.06308200
C	3.42933500	0.86664400	2.71243000
H	3.47466500	-0.08171200	3.25741300
H	4.27675600	0.88596900	2.02018000
H	3.50584900	1.69772900	3.41441100
H	-0.92535700	-1.40346100	-2.21055500
C	-3.77501800	-2.23000100	-2.00142200
H	-4.19352900	-3.23855600	-1.93489200
H	-4.59573800	-1.53332300	-2.18941800
H	-3.11270300	-2.20188900	-2.87188800
C	0.72741400	4.05873800	-1.06014500

H	1.49869100	4.65213000	-1.55292800
H	0.60630100	4.41989400	-0.03344300
H	-0.22826300	4.15325800	-1.57724600
C	2.07952400	-3.13945400	1.05898100
H	2.69039700	-2.23110900	1.04718300
H	2.06893900	-3.56570300	0.05284900
H	2.48274700	-3.85327100	1.77753900
C	0.69611200	-2.73024000	1.47716800
O	0.19014000	-2.92492400	2.55691000
O	-0.02511400	-2.10869100	0.48463400
C	1.17758100	2.61244600	-0.98064700
O	0.17404000	1.78262100	-0.95928600
O	2.38209800	2.34046700	-0.93575000

TS-2-a

NImag=1

0 1 (charge, spin multiplicity)

C	-2.54461700	0.19709300	-1.04043200
C	-2.17075700	0.33314000	1.46054300
C	-3.57906400	-0.30751900	1.58003000
H	-3.47649200	-1.38991000	1.71224700
H	-4.08172200	0.11083600	2.45464500
C	-1.35881900	-0.29230200	2.60726800
H	-0.39108500	0.19529900	2.68832900
H	-1.89643800	-0.12269600	3.54642900
H	-1.23127300	-1.36963400	2.48732600
C	-2.19773500	1.85908600	1.65700800
H	-2.40563200	2.07056700	2.71032300
H	-1.21377300	2.27053500	1.42565700
H	-2.96494600	2.35903300	1.06654500
N	-1.69187300	-0.14419200	0.13495900
H	-1.22257400	-1.51817800	0.13984700
C	-2.60402500	1.69453600	-1.46815700
H	-3.30842300	2.26823200	-0.86625100
C	-1.96990000	-0.64633300	-2.18964800
H	-2.08132500	-1.71032800	-1.96215400
O	-4.47896900	-0.08134700	0.48383900
C	-4.02454300	-0.17432700	-0.78227900
O	-4.78087600	-0.39285000	-1.69578300
H	0.22291700	4.37037900	-0.90880300
C	1.14607400	4.10159900	-0.39359500
C	1.49512600	2.63957500	-0.57995800
H	1.97610600	4.72417300	-0.73041900
H	1.00611500	4.24537700	0.68292000
O	2.67757800	2.28228600	-0.51383700
O	0.45228600	1.89227700	-0.79436300
Pd	0.36840100	-0.10499400	-0.48113800
O	3.98951600	0.20908100	-0.77329500
C	3.39834400	-0.80419800	-1.31009400
O	2.17030700	-0.89945400	-1.52066800
C	4.31259700	-1.93972600	-1.69697700
H	3.80224300	-2.62918100	-2.36893400
H	5.22132200	-1.54945100	-2.15992600
H	4.60670100	-2.47491100	-0.78759800
H	-2.95351500	1.73922600	-2.50263300
H	-1.62174800	2.15562400	-1.39027000
H	-2.53605300	-0.45619900	-3.10789200
C	-0.51171800	-0.29087900	-2.37228200
H	0.10093000	-1.06418500	-2.83292900

H	-0.32488300	0.69076900	-2.80562400
H	3.33754800	1.00518000	-0.60829900
O	-0.32287500	-2.12361300	-0.11042900
C	0.08004400	-3.06116300	0.81235900
O	-0.72946300	-3.54692100	1.56666400
C	1.54551100	-3.37453400	0.75264700
H	1.86172900	-3.52812000	-0.28170000
H	2.07927400	-2.50124000	1.14516100
H	1.75498200	-4.25543500	1.35909700
O	1.65225300	-0.18094800	1.29443800
C	1.87072800	0.82272300	2.09467300
O	1.17372900	1.84043100	2.17801800
C	3.10669300	0.64739800	2.97378800
H	3.05360700	-0.29937500	3.52016700
H	3.99867600	0.60874100	2.34021500
H	3.19287600	1.47742000	3.67610700

TS-2'

NImag=1

0 1 (charge, spin multiplicity)

C	2.02802000	0.44824500	-1.09441500
C	2.62524900	-0.07432300	1.32456200
C	4.03009700	0.06677200	0.72273900
H	4.32752700	1.11664200	0.62270700
H	4.74886700	-0.42529000	1.37857300
C	2.73650900	0.17550500	2.83121300
H	1.78638800	0.02002600	3.33962800
H	3.53355400	0.45578900	3.51313600
H	2.59312300	1.20212900	2.41185600
C	2.46375200	-1.64447500	1.69710600
H	3.04598900	-1.55647700	2.61879300
H	1.42719900	-1.84528100	1.96809700
H	2.84630900	-2.39766500	0.99535100
N	1.55197400	-0.14686500	0.24255700
H	1.21357700	0.83107300	0.25137500
C	1.08111675	0.28238239	-2.30349147
H	-2.52352000	-2.72839800	0.61733500
H	0.82572875	-0.75493261	-2.44734947
C	2.29860000	1.93245800	-0.98824700
H	1.41434500	2.41661800	-0.60127300
H	3.12443700	2.16772000	-0.31882500
H	-3.30386358	-0.28878282	-4.00500102
C	-2.98512016	0.71475102	-3.70538606
C	-1.90923273	0.58178661	-2.62762153
H	-2.55556387	1.22353729	-4.56914030
H	-3.86001264	1.25010415	-3.33290907
O	-2.46085737	0.44619437	-1.44081854
O	-0.71977008	0.57230049	-2.90211298
Pd	-0.58831500	0.16430500	-0.13953300
O	-2.38764300	-1.94497000	1.28973900
C	-2.08548600	-1.10741500	2.17624100
O	-1.41548100	-0.08763700	1.87057100
C	-2.48565400	-1.35979700	3.61387900
H	-3.54736400	-1.61515800	3.65930800
H	-1.92243900	-2.21988900	3.99096300
H	-2.27835000	-0.49102200	4.23892500
H	0.90087375	0.92314539	-3.15635647
C	-0.02254300	-4.21964500	-0.86236200
H	1.00221500	-4.00893500	-0.55373000

H	-0.01541200	-4.41873700	-1.93955800
H	-0.41537600	-5.09846400	-0.34939000
C	-1.76850500	4.03721100	1.34367900
H	-1.57450700	5.10396600	1.46445400
H	-2.06300100	3.60590600	2.30490400
H	-2.58650600	3.87072000	0.64102300
C	-0.47497000	3.34856900	0.85764000
O	0.57728800	3.95582100	0.84771800
O	-0.81562600	2.13135700	0.47497900
C	-0.91032400	-3.02190500	-0.58415100
O	-0.34978700	-1.88652600	-0.78238600
O	-2.08790200	-3.20407300	-0.19952000
C	3.31063500	-0.25494400	-1.56741000
O	4.17971400	-0.56845100	-0.56748900
O	3.55250200	-0.52679100	-2.71423800
C	2.63512851	2.49655105	-2.38113881
H	2.32921986	3.52048963	-2.43470831
H	3.69004981	2.43030446	-2.54742906
H	2.11993749	1.93079365	-3.12906714

INT-4

NImag=0

0 1 (charge, spin multiplicity)

C	2.39844000	0.76858900	-0.31493800
C	2.08858900	-0.80359100	1.66955800
C	3.62284300	-0.71754600	1.57057700
H	3.98916900	0.24224600	1.94874000
H	4.08348300	-1.51517800	2.15719700
C	1.65544600	-0.48471900	3.11343300
H	0.56535500	-0.52091500	3.17817600
H	2.06849000	-1.21347800	3.82012000
H	1.97943000	0.51805700	3.40477100
C	1.66007300	-2.24501100	1.32515500
H	2.09024500	-2.92007300	2.07353300
H	0.57442600	-2.33458800	1.36105900
H	2.01112400	-2.55122800	0.34075100
N	1.56396200	0.30351000	0.83043800
H	-2.64138500	-1.46214900	-1.21831900
C	1.32061100	0.95650300	-1.38262900
H	-3.02521800	0.73889100	1.45076900
H	1.39684800	0.32206200	-2.25923300
C	3.07115900	2.12909200	0.04357700
H	2.25795300	2.76663900	0.40365800
H	3.75531700	1.98763100	0.88673300
O	4.08476400	-0.92096200	0.22299300
C	3.46490400	-0.23256900	-0.76698700
O	3.79370400	-0.40058500	-1.91780400
H	-4.99022500	0.86110200	-2.35925000
C	-4.06611900	1.36520600	-2.07583800
C	-3.00218000	0.37747500	-1.68347600
H	-3.70175100	1.99747000	-2.88750900
H	-4.24893400	2.00280800	-1.20435200
O	-3.43028100	-0.79626700	-1.32453400
O	-1.80134800	0.71068500	-1.69316300
Pd	-0.17710800	0.18092600	-0.24188900
O	-3.40337000	-0.09497300	1.90716100
C	-2.56242200	-1.09089800	1.85175200
O	-1.44775600	-1.04252900	1.31344800
C	-3.06230900	-2.36614800	2.48160900

H	-3.83415000	-2.16342500	3.22478600
H	-3.49144900	-2.98935200	1.68943500
H	-2.22860900	-2.91333100	2.92407300
H	1.00602500	1.97955200	-1.56837300
C	3.82009100	2.79034100	-1.11991500
H	4.23243300	3.75146100	-0.79773800
H	4.64544200	2.17034500	-1.48041800
H	3.16002300	2.98393500	-1.97159400
C	0.27764900	-3.75445900	-2.02221100
H	-0.41775500	-4.35185000	-2.61313000
H	0.63523300	-4.36143400	-1.18323400
H	1.14384700	-3.46209000	-2.61821400
C	-1.48811700	4.17695100	0.88920900
H	-0.50827800	4.49539200	1.24845100
H	-2.27603600	4.51730000	1.56289900
H	-1.65407500	4.62984000	-0.09462900
C	-1.55282300	2.66355300	0.74197900
O	-2.65174800	2.09057100	0.88212300
O	-0.42107300	2.12349800	0.45284300
C	-0.43587200	-2.53230400	-1.46828600
O	0.36833200	-1.56615700	-1.16877500
O	-1.67091400	-2.56022700	-1.32688500

INT-4-a

NImag=0

0 1 (charge, spin multiplicity)

C	-2.75346200	-0.14572100	-0.76711100
C	-2.20834500	0.46964400	1.60014100
C	-3.49513800	-0.30473600	1.99218000
H	-3.22446900	-1.32214600	2.29023900
H	-3.98042600	0.20166800	2.83098400
C	-1.20403800	0.15474700	2.72213000
H	-0.31344900	0.77382700	2.62397300
H	-1.65848800	0.36171900	3.69755700
H	-0.90549200	-0.89611300	2.68698900
C	-2.46158500	1.99407700	1.56014000
H	-2.50954000	2.38654700	2.58151300
H	-1.64373700	2.49092500	1.03508300
H	-3.40114100	2.25122900	1.06813900
N	-1.80965400	-0.20559900	0.36180300
H	2.67682500	-1.25354400	1.54040600
C	-3.06407100	1.21809500	-1.46632800
H	-3.73274600	1.84153400	-0.87194300
C	-2.15496500	-1.12875900	-1.78796300
H	-2.10048900	-2.12333200	-1.34139800
O	-4.50347600	-0.39708600	0.97463000
C	-4.14508800	-0.64109100	-0.30577400
O	-4.94322600	-1.10153700	-1.08463900
H	-0.54843600	4.19994900	-1.89752000
C	0.23985100	4.19703200	-1.14078900
C	0.81378000	2.79740700	-0.97201000
H	1.03238100	4.89298200	-1.41642700
H	-0.21008500	4.51746300	-0.19541200
O	2.04639900	2.65524000	-0.94231900
O	-0.09704700	1.88506600	-0.86839600
Pd	0.15216300	-0.10317800	-0.37792100
O	3.69697700	0.79589800	-0.94112600
C	3.25618300	-0.35716700	-1.34950600
O	2.05363400	-0.62350600	-1.52800100

C	4.30579000	-1.40927700	-1.58862600
H	4.11059600	-1.91022600	-2.53968400
H	5.30814100	-0.98162600	-1.57940100
H	4.20838500	-2.15555100	-0.79361400
H	-3.56978700	1.01455100	-2.41400800
H	-2.14757100	1.77627300	-1.64419500
H	-2.78018700	-1.18696500	-2.68702600
C	-0.77136300	-0.65353700	-2.14541200
H	-0.09071400	-1.41058300	-2.52821000
H	-0.71899700	0.27849900	-2.70683500
H	2.92797100	1.49221000	-0.89033000
O	0.10741900	-2.14510300	-0.01377900
C	1.08119000	-2.87620400	0.40494800
O	2.17054600	-2.50088000	0.87784700
C	0.81370100	-4.36886200	0.26606700
H	-0.23144200	-4.59600100	0.48522800
H	1.00993800	-4.66724600	-0.76955800
H	1.47649200	-4.92917500	0.92668500
O	3.18166200	-0.51720500	2.04523900
C	2.56399400	0.63101100	1.96901100
O	1.49110700	0.81394900	1.37888600
C	3.28769900	1.76808700	2.64415100
H	3.84313200	1.41528500	3.51471800
H	4.00303900	2.18482100	1.92671700
H	2.58162900	2.55127700	2.92084800

TS-3

NImag=1

0 1 (charge, spin multiplicity)

C	-2.28036400	0.95628400	0.39750900
C	-2.90960000	-1.08393700	-0.89613500
C	-4.23995000	-0.31009800	-0.99109500
H	-4.16714100	0.49564500	-1.73009900
H	-5.05487000	-0.98023600	-1.27404600
C	-2.59396300	-1.72714200	-2.25395100
H	-1.62344500	-2.22931400	-2.21175900
H	-3.35089700	-2.47571800	-2.51028200
H	-2.55693600	-0.97337000	-3.04553500
C	-3.03831100	-2.17941000	0.18520000
H	-3.91368700	-2.79714500	-0.04096800
H	-2.15036300	-2.80671700	0.19110200
H	-3.18100300	-1.77471500	1.19011300
N	-1.92416200	0.01499000	-0.69175600
H	2.32887100	-0.16430000	1.90496500
C	-1.10933000	0.47116800	1.16135900
H	2.58273000	0.53074700	-1.28210500
H	-1.25302200	-0.38050500	1.81309700
C	-2.23984000	2.43326800	-0.06804700
H	-1.39474400	2.51818200	-0.75232400
H	-3.14639500	2.62660400	-0.65561200
O	-4.62041500	0.23444300	0.28951000
C	-3.62891300	0.71005100	1.07753900
O	-3.84260000	0.99569300	2.23151500
H	4.67880700	2.34993800	2.41873800
C	3.93171500	2.65479600	1.68383100
C	2.75144900	1.71200200	1.68088600
H	3.59037800	3.67184500	1.87930000
H	4.39650900	2.62715700	0.69216100
O	3.10278700	0.46046600	1.94944000

O	1.60923000	2.07276300	1.42358000
Pd	0.13893200	-0.43545900	-0.55429400
O	2.51241500	-2.97322900	-0.80811900
C	2.94613600	-1.84089100	-0.87573300
O	2.18756000	-0.73994100	-0.90807800
C	4.43175200	-1.51566100	-0.90981600
H	4.67321200	-0.88273300	-1.76968500
H	4.69290400	-0.96062700	-0.00300000
H	5.00841800	-2.43929900	-0.95890200
H	-0.23721900	1.10134300	1.33800200
C	-2.11798900	3.44762400	1.07467400
H	-2.12803700	4.46405400	0.66851800
H	-2.93761000	3.35941100	1.79214300
H	-1.17587200	3.32045500	1.61753400
C	0.68416200	-3.84381400	1.86430500
H	1.00705200	-3.91596100	2.90355200
H	1.39949300	-4.36522200	1.22086200
H	-0.29517500	-4.30815000	1.73089600
C	1.41879900	3.50243300	-2.12164900
H	2.29705500	3.78001100	-2.70614000
H	1.41415900	4.09105800	-1.19743000
H	0.50137500	3.71253300	-2.67211700
C	1.47664100	2.05126700	-1.73255300
O	0.40286800	1.42489400	-1.55553800
O	2.65935300	1.55013700	-1.58789800
C	0.67586400	-2.39251200	1.43018200
O	-0.07356500	-2.18439100	0.37806600
O	1.32788500	-1.53350500	2.03124500

TS-3-a

NImag=1

0 1 (charge, spin multiplicity)

C	2.29771200	0.24901100	1.47698300
C	2.58752400	1.22384400	-0.83562700
C	3.29011900	-0.11093400	-1.18947200
H	2.60811100	-0.72971400	-1.77902500
H	4.18647500	0.08373000	-1.78626100
C	1.84656700	1.66655800	-2.11073500
H	1.28427600	2.58325900	-1.93510500
H	2.58219500	1.84255900	-2.90220300
H	1.14776000	0.90662300	-2.47031200
C	3.60536800	2.34661900	-0.50661800
H	4.02356900	2.73832700	-1.43845400
H	3.10929500	3.17107600	0.01178600
H	4.44473800	2.00582900	0.09725300
N	1.66443900	0.91779900	0.30065200
H	-0.78876400	-1.67789200	-2.57200500
C	3.29007400	1.14245200	2.28377100
H	4.26258000	1.24251700	1.80674200
C	1.05887600	0.03637100	2.35945900
H	0.56031700	-0.91394500	2.18018100
O	3.75103200	-0.92756900	-0.08641500
C	3.09237300	-0.99294700	1.09870300
O	3.27658400	-1.92715300	1.84257100
H	-2.73231200	4.57812100	-0.21847800
C	-2.12302700	3.99548200	-0.91103800
C	-1.78486000	2.64415100	-0.29214400
H	-2.70173400	3.82905500	-1.82641600
H	-1.21871000	4.54323900	-1.18393300

O	-2.50198000	2.18191700	0.60820000
O	-0.72962000	2.09262600	-0.80165200
Pd	-0.12961400	0.15872800	-0.34585400
O	-3.97859100	0.10268100	1.39220200
C	-3.35994700	-0.65813800	2.29242000
O	-2.20943200	-0.48368100	2.66570700
C	-4.24443400	-1.77290400	2.80400600
H	-3.74044600	-2.30484600	3.61032600
H	-5.19796300	-1.36792400	3.15441100
H	-4.46691300	-2.46864100	1.98852600
H	3.45434000	0.66286500	3.25186200
H	2.87865100	2.14214900	2.44639000
H	1.27004400	0.11494000	3.43369300
C	0.22401500	1.18808200	1.90342800
H	-0.85958900	1.09744500	1.85318900
H	0.60528200	2.19400400	2.03345000
H	-3.35315700	0.80689600	1.06752400
O	0.50937500	-2.29956500	-2.14941800
C	0.76591200	-2.54739100	-0.94866200
O	0.53495100	-1.74446700	0.03339100
C	1.40172000	-3.86298900	-0.54992700
H	1.66616500	-4.43655000	-1.43830600
H	2.28166000	-3.67974300	0.07243900
H	0.68975600	-4.43294700	0.05572200
O	-1.75653000	-1.49729700	-2.88845400
C	-2.50115500	-0.94924200	-1.97418000
O	-2.08738900	-0.45992900	-0.90619600
C	-3.97454300	-0.91151400	-2.28006400
H	-4.30083900	-1.87103700	-2.68719900
H	-4.52898400	-0.65641700	-1.37731900
H	-4.15561500	-0.14861900	-3.04504500

INT-5

NImag=0

0 1 (charge, spin multiplicity)

C	2.14674100	0.04057600	-0.17095700
C	0.94588400	0.12919400	2.05764000
C	2.41394600	0.18669700	2.51868200
H	2.83500900	1.18297200	2.34451700
H	2.48488800	-0.03837500	3.58505000
C	0.15669100	1.21709300	2.80488300
H	-0.87466700	1.24595400	2.44960500
H	0.14404000	1.01877300	3.88231200
H	0.59182900	2.20404000	2.62728700
C	0.36296300	-1.26081700	2.38834600
H	0.44594900	-1.43577000	3.46651200
H	-0.69080400	-1.31085400	2.11084100
H	0.88201800	-2.06836300	1.87053900
N	0.97410100	0.51595500	0.62644200
C	1.42851200	-0.58773100	-1.36200300
H	-2.42961400	2.10288300	0.64966700
H	1.54432700	-1.66175200	-1.47125600
C	3.00823700	1.26800900	-0.58980200
H	2.30968900	1.96912300	-1.05606300
H	3.38893900	1.75835800	0.31309300
O	3.22246600	-0.80736500	1.86469100
C	3.04518500	-0.98155500	0.53445900
O	3.62052300	-1.87447400	-0.04280500
Pd	-0.44772700	-0.26405700	-0.63574400

O	-2.53328300	-0.28278000	0.45548300
C	-3.36529300	0.44509600	1.00944700
O	-3.25962200	1.74231300	1.13150400
C	-4.62983700	-0.12108500	1.60726300
H	-4.80126700	0.30528000	2.59869000
H	-5.47873700	0.16406300	0.97717600
H	-4.56824700	-1.20745000	1.66083000
H	1.45124700	-0.02262100	-2.29026900
C	4.16958000	0.94893100	-1.53857700
H	4.69219100	1.87211200	-1.80722200
H	4.89476900	0.26760300	-1.08607200
H	3.82015000	0.48610200	-2.46705900
C	-1.88852500	-3.94431500	-1.39379100
H	-2.24607600	-4.09129200	-2.41381000
H	-2.72536900	-4.07623200	-0.69997900
H	-1.12428000	-4.68360400	-1.14312500
C	-0.31063300	3.87019500	-1.96041600
H	0.60329000	4.29534500	-1.53060800
H	-1.08895900	4.63438200	-1.91846400
H	-0.10871500	3.58047400	-2.99223300
C	-0.72541100	2.67497800	-1.11540500
O	-0.34434900	1.54044100	-1.60648600
O	-1.34960500	2.86714300	-0.06091600
C	-1.34074100	-2.55413000	-1.23497800
O	-0.57652500	-2.30472500	-0.22094400
O	-1.61443400	-1.62342900	-2.03672400

INT-5-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.45441800	-0.26190900	-0.62141500
C	1.72363100	-0.13319400	1.77985200
C	3.11985100	0.48528900	2.05910400
H	3.03111000	1.57571800	2.07213000
H	3.47822400	0.14013900	3.03250300
C	0.75550900	0.65770900	2.68109500
H	-0.23241200	0.19822700	2.68392300
H	1.12831300	0.66746600	3.71168400
H	0.66201700	1.68572800	2.32282600
C	1.67569100	-1.63048500	2.16088800
H	1.62737700	-1.73093900	3.25038500
H	0.78385700	-2.09949700	1.73744500
H	2.55467700	-2.18025000	1.82030600
N	1.49416300	0.22662900	0.37956900
H	-3.26774400	1.09739800	0.11833800
C	2.55501800	-1.79072400	-0.92771400
H	3.05444300	-2.33691700	-0.12680600
C	2.03953300	0.50609900	-1.89037800
H	2.13175200	1.57720200	-1.69892300
O	4.15891600	0.14020800	1.13029300
C	3.89144000	0.11740600	-0.19509900
O	4.77953500	0.24640700	-1.00091100
H	-1.62299300	-4.03895400	-2.05464200
C	-2.36159000	-3.36031400	-1.62026400
C	-1.71852800	-2.04108700	-1.28306300
H	-3.19136900	-3.20728200	-2.31109400
H	-2.73534100	-3.82437000	-0.70175900
O	-2.24406600	-0.94086500	-1.57485500
O	-0.58599300	-2.06158000	-0.65280700

Pd	-0.41849700	0.00073800	-0.41721700
H	3.15270300	-1.92297300	-1.83371700
H	1.56779300	-2.22720000	-1.07150200
H	2.68818400	0.24846000	-2.73561300
C	0.60195500	0.15602600	-2.20425800
H	0.04135300	0.91754500	-2.74548800
H	0.45424200	-0.83409500	-2.63380000
O	-0.36741200	2.06159300	-0.36549600
C	-1.46287000	2.71793300	-0.57758900
O	-2.60428600	2.23346900	-0.66237700
C	-1.25439300	4.21173000	-0.76383300
H	-0.44017500	4.57259000	-0.13256200
H	-0.98009300	4.40267200	-1.80702600
H	-2.18067700	4.74414300	-0.54378200
O	-3.83340900	0.53159400	0.75390700
C	-3.10883100	-0.26259500	1.49094400
O	-1.88068400	-0.40475300	1.39374900
C	-3.90386700	-1.02228300	2.52509900
H	-4.33081300	-0.31714300	3.24495200
H	-4.73958400	-1.53657800	2.04249200
H	-3.26572400	-1.73763700	3.04250900

TS-4

NImag=1

0 1 (charge, spin multiplicity)

C	2.22688500	0.29574500	-0.56234200
C	1.68938500	-0.70090000	1.66163400
C	3.10172300	-0.16750800	1.97225100
H	3.08053100	0.91617500	2.13292200
H	3.50844400	-0.65110000	2.86325000
C	0.76459500	-0.43016500	2.85597400
H	-0.23999100	-0.79940200	2.63559300
H	1.12932800	-0.94987700	3.74822700
H	0.69927800	0.64050000	3.06711300
C	1.76686800	-2.21818900	1.38834200
H	2.24943500	-2.70906600	2.24002000
H	0.76310900	-2.61822000	1.26864600
H	2.35266400	-2.46804300	0.50039400
N	1.25292200	0.19830400	0.55314700
C	1.23931700	-0.40744700	-1.40187500
H	-2.81646400	1.42842700	1.17322600
H	1.23087000	-1.48726600	-1.45235200
C	2.54574700	1.76060500	-0.94669800
H	1.59141200	2.28938800	-0.95673900
H	3.14995200	2.19630000	-0.14089700
O	4.02518000	-0.48591600	0.91043400
C	3.54945800	-0.44780400	-0.35459500
O	4.19321700	-0.90219700	-1.26945700
Pd	-0.71077600	0.03306700	-0.19172800
O	-2.77708200	-0.01009500	-0.78980700
C	-3.75338100	0.23474300	-0.05575100
O	-3.70735200	0.91672400	1.05127600
C	-5.12358100	-0.26310700	-0.43128900
H	-5.54864800	-0.82046600	0.40824500
H	-5.77982800	0.59180000	-0.62003000
H	-5.06699700	-0.89464200	-1.31652800
H	0.72245300	0.12114600	-2.19831800
C	3.26065700	1.91815200	-2.29347300
H	3.41552800	2.98027400	-2.50631000

H	4.23194600	1.41889100	-2.30800800
H	2.66457000	1.50332500	-3.11349600
C	-1.70468100	-4.10304400	-0.26168600
H	-1.91576500	-4.73040000	-1.12821500
H	-2.60632300	-3.97805600	0.34390600
H	-0.95540000	-4.59472300	0.36758600
C	-0.67968900	4.28734100	0.15607000
H	0.34265200	4.43739000	0.52021300
H	-1.35694600	4.90833400	0.74306200
H	-0.70340900	4.57867200	-0.89620400
C	-1.04395200	2.82390800	0.31256000
O	-0.57337500	2.04564900	-0.60087100
O	-1.73345800	2.45390900	1.28860900
C	-1.18202700	-2.74998100	-0.72892500
O	-1.03490500	-1.90238400	0.27398900
O	-0.91235900	-2.51727400	-1.90030200

TS-4-a

NImag=1

0 1 (charge, spin multiplicity)

C	2.29060700	-0.78727300	-0.81467700
C	1.54966900	-0.99783600	1.59204100
C	2.26445200	0.35737700	1.81718100
H	1.51618900	1.15146400	1.88452300
H	2.83439100	0.33324700	2.75100800
C	0.32631100	-1.00342400	2.52711800
H	-0.26571400	-1.90719700	2.38442700
H	0.67415000	-0.95924400	3.56408500
H	-0.32919100	-0.14519000	2.35979100
C	2.43406400	-2.19868700	2.01709600
H	2.40459200	-2.29992500	3.10585700
H	2.05178000	-3.12592500	1.58294700
H	3.48103100	-2.08515700	1.73969800
N	1.17484400	-1.02880000	0.14603500
H	-1.61587000	2.35439900	1.08916100
C	3.35215300	-1.92796800	-0.89043000
H	4.04751900	-1.92385200	-0.05384900
C	1.50927800	-0.80600800	-2.13976400
H	1.16861800	0.18543700	-2.43336500
O	3.22320500	0.77095900	0.81157800
C	3.07679900	0.47889300	-0.50466200
O	3.67278400	1.12006200	-1.33825400
H	-3.99067300	-3.80443800	-0.30249500
C	-3.39632800	-3.23356800	0.41192400
C	-2.48525900	-2.26233300	-0.33276400
H	-4.06156200	-2.67625000	1.07921600
H	-2.80530000	-3.91011600	1.03577800
O	-2.56402400	-2.11091400	-1.55111100
O	-1.64759900	-1.65035800	0.47025900
Pd	-0.58613900	-0.02851900	-0.21359700
H	3.94006500	-1.77400100	-1.79871000
H	2.87277400	-2.90956500	-0.93730700
H	2.07826900	-1.24066900	-2.97156300
C	0.37890300	-1.70326200	-1.74344700
H	-0.64022200	-1.59994400	-2.12007700
H	0.61715300	-2.71304100	-1.43058600
O	-0.20755200	2.83759900	0.95352800
C	0.47337700	2.68976300	-0.08745300
O	0.47348900	1.62982100	-0.82151300

C	1.39729700	3.79071900	-0.56478300
H	1.37918400	4.62646600	0.13460100
H	2.41296500	3.40027200	-0.67442200
H	1.07253400	4.12886200	-1.55373800
O	-2.64674600	2.27085000	1.13141300
C	-3.14441700	1.58362400	0.14435600
O	-2.49137800	0.85296400	-0.62426800
C	-4.63076400	1.73370700	-0.04100300
H	-4.85249400	2.75818700	-0.35598100
H	-4.99058600	1.02829500	-0.78848500
H	-5.13540900	1.57115600	0.91525800

Products

NImag=0

O 1 (charge, spin multiplicity)

C	0.84190400	-0.33394100	0.06026500
C	-1.70461100	-0.26252400	-0.08067000
C	-1.34482600	0.94574400	-0.94700800
H	-0.98069000	0.61238800	-1.92649700
H	-2.20343100	1.60276100	-1.10210400
C	-2.67311900	-1.16934000	-0.85690800
H	-2.92755700	-2.04518300	-0.25359800
H	-3.60062200	-0.64186600	-1.10601200
H	-2.20919700	-1.52526500	-1.78092700
C	-2.35439700	0.18910700	1.23630400
H	-3.34127700	0.61657900	1.03352700
H	-2.48827500	-0.66140400	1.91113600
H	-1.76629800	0.95424000	1.74937200
N	-0.44605800	-1.04851200	0.10134300
C	0.34160400	-0.95554200	1.32701700
H	0.02234000	-0.29349100	2.12825200
C	1.96220100	-0.99574500	-0.73893200
H	1.69641700	-2.05509300	-0.82189400
H	1.95894300	-0.59425600	-1.76091900
O	-0.34029900	1.77473600	-0.32737200
C	0.82897000	1.17950900	0.03402400
O	1.78136500	1.86415200	0.32357800
H	0.78252800	-1.89119900	1.66626800
C	3.35617400	-0.83762400	-0.12168700
H	4.10488700	-1.35019200	-0.73400000
H	3.63221900	0.21512200	-0.03914200
H	3.39049500	-1.27252300	0.88306600

Products-a

NImag=0

O 1 (charge, spin multiplicity)

C	-1.00794000	0.46958400	0.30306000
C	1.44596300	-0.14387500	0.16701000
C	1.05567200	-1.12617900	-0.94814600
H	1.12659500	-0.64798300	-1.93252400
H	1.70531900	-2.00582200	-0.96051900
C	2.79571900	0.50385200	-0.16841500
H	3.06869700	1.21600400	0.61532600
H	3.58310400	-0.25368000	-0.23441800
H	2.76597300	1.04131800	-1.12133800
C	1.54668800	-0.88145300	1.51378200
H	2.37502100	-1.59714700	1.49529300
H	1.71995300	-0.16307100	2.31888300
H	0.63599800	-1.44098300	1.74151700
N	0.42057700	0.90565700	0.27390800

C	-1.66945800	0.51618000	1.68343300
H	-1.28215300	-0.26153000	2.34799100
C	-1.35373200	1.65808800	-0.64544200
H	-1.96981100	1.42121400	-1.51384500
O	-0.28105700	-1.64989500	-0.80032800
C	-1.30881900	-0.88639100	-0.34654200
O	-2.43543000	-1.31972300	-0.42198600
H	-2.74708700	0.36831900	1.58096900
H	-1.47161700	1.48798100	2.14279700
H	-1.80319000	2.49100200	-0.10061300
C	0.16411200	1.81210600	-0.87648000
H	0.47684300	1.41875500	-1.85478400
H	0.59496900	2.81150100	-0.75714000

R-C_{methyl}-H-ts

NImag=1

0 1 (charge, spin multiplicity)

C	1.38468300	-1.09151900	0.55933900
C	2.16359700	0.96653300	-0.76722100
C	2.60137000	-0.11734400	-1.74850100
H	1.74467700	-0.47969800	-2.32916900
H	3.34460500	0.27796500	-2.44379100
C	1.55220900	2.13443600	-1.54993600
H	1.22867900	2.91992900	-0.86592600
H	2.30670900	2.55521400	-2.22261900
H	0.68926000	1.81721200	-2.14019600
C	3.35016300	1.47085400	0.07878200
H	4.11558600	1.90880200	-0.56924400
H	3.00671500	2.24444100	0.77186300
H	3.82382200	0.67375000	0.65741600
N	1.15032700	0.34706600	0.15340600
H	0.99545300	0.98798000	0.94760600
C	1.31033500	-1.24092100	2.09415900
H	2.11677000	-0.63483900	2.52573700
C	0.27784400	-1.90442900	-0.18904200
H	-1.06047900	-1.93758100	-0.03605100
H	0.54142200	-2.09046700	-1.23342000
O	3.24459400	-1.21880300	-1.09047000
C	2.73029200	-1.67691100	0.07674000
O	3.28602000	-2.58047100	0.65265500
H	-4.97375500	-2.39879100	0.35027600
C	-4.58032700	-2.02645700	-0.59963400
C	-3.13753300	-1.61773400	-0.41242200
H	-4.62836900	-2.84988800	-1.31818700
H	-5.18063800	-1.18849300	-0.95223100
O	-2.31725300	-2.47362100	0.03561000
O	-2.81801900	-0.42403400	-0.72244700
Pd	-0.84273100	0.05445100	-0.34954200
O	-1.47294800	1.99414100	-0.30130900
C	-1.01720500	2.76263900	0.64257100
O	-0.07484000	2.50470200	1.41176300
C	-1.76794100	4.08210400	0.75370500
H	-1.94877700	4.50630600	-0.23684000
H	-2.74448800	3.89782500	1.21339400
H	-1.20615700	4.78085500	1.37478000
H	1.56840000	-2.27977400	2.31283700
C	-0.02315200	-0.87579000	2.75793100
H	-0.84953700	-1.48404700	2.37792100
H	0.05278300	-1.06107300	3.83415000

H	-0.28530100	0.17866400	2.62677300
H	0.20949000	-2.88656700	0.29474600

R-C_{ethyl}-H-ts

NImag=1

0 1 (charge, spin multiplicity)

C	-2.09452400	-1.07724100	0.17417800
C	-1.95560800	1.49422000	0.06546500
C	-3.48927700	1.28421300	0.08243400
H	-3.85458900	1.08435300	1.09404300
H	-3.98257400	2.19124100	-0.27176100
C	-1.55537400	2.15164900	1.39126900
H	-0.49285600	2.39342100	1.39336500
H	-2.13534300	3.07188500	1.52572100
H	-1.76538600	1.49838200	2.24268600
C	-1.57968500	2.36747400	-1.14323700
H	-1.91106400	3.39671100	-0.97771300
H	-0.50199900	2.37153000	-1.31962700
H	-2.07568200	1.99825200	-2.04903900
N	-1.27067600	0.14944500	-0.13790100
H	-1.10233300	0.09711700	-1.14503100
C	-1.29344600	-2.28460600	-0.34780000
H	-1.20985200	-2.20969700	-1.43930500
C	-2.37317200	-1.22954300	1.68215300
H	-1.44258700	-1.16203200	2.24969200
H	-3.05703500	-0.47739100	2.07612100
O	-3.94485700	0.24026600	-0.79109200
C	-3.42210000	-0.99995200	-0.60979800
O	-3.96664200	-1.96052300	-1.09380100
H	4.97705500	-2.74587100	-0.55079300
C	4.73723300	-1.70890700	-0.31120200
C	3.24218600	-1.53369800	-0.19268500
H	5.23641900	-1.39388400	0.60557100
H	5.08964700	-1.07663000	-1.13313200
O	2.47727200	-2.24395600	-0.90977000
O	2.81845000	-0.65132300	0.62441200
Pd	0.81175300	-0.23490100	0.36196400
O	1.38308400	1.70509400	0.67388600
C	1.91418200	2.25620200	-0.38967700
O	1.83517500	1.80365100	-1.53243900
C	2.65602100	3.55103800	-0.08236800
H	2.05158000	4.20345600	0.55387100
H	3.57229800	3.31788900	0.46938100
H	2.91239200	4.06130000	-1.01168100
H	-1.88896300	-3.18300400	-0.16013000
C	0.09762900	-2.39796100	0.27553200
H	0.08395800	-2.42742400	1.36899500
H	0.51425700	-3.37544200	-0.00123400
H	1.23693000	-2.04836300	-0.39917600
H	-2.82444600	-2.20946500	1.85899400

B-reactant

NImag=0

0 1 (charge, spin multiplicity)

C	-2.30382800	0.18257400	0.30109600
C	-1.43349800	-1.90733800	-0.88025700
C	-2.91519700	-2.04719400	-1.24986100
H	-3.18119600	-1.37226000	-2.07206200
H	-3.16015400	-3.06836200	-1.55456800
C	-0.57947300	-2.10225800	-2.14024600

H	0.48001400	-1.98596600	-1.89651300
H	-0.72138600	-3.10610200	-2.55372500
H	-0.84045100	-1.37385800	-2.91661500
C	-1.04943900	-2.96732500	0.17324100
H	-1.22668700	-3.98214900	-0.20132400
H	0.01024600	-2.85895500	0.41620800
H	-1.62414000	-2.84412900	1.09515600
N	-1.18157700	-0.56353500	-0.32317100
H	-0.71979200	0.03627300	-0.99993500
C	-1.69693500	0.89366500	1.54365900
H	-0.75206000	1.32989900	1.19694200
H	-1.41629700	0.10716800	2.25142600
C	-2.91382300	1.20383800	-0.72866200
H	-2.22966700	2.06252600	-0.75811400
H	-2.85734700	0.74950000	-1.72333400
C	-4.35404100	1.68903300	-0.50760700
H	-4.61697600	2.42271900	-1.27711500
H	-5.06799000	0.86313800	-0.58343500
H	-4.49793000	2.15685700	0.46715000
O	-3.75890600	-1.78161800	-0.11486700
C	-3.42828100	-0.77235200	0.73135000
O	-4.07122300	-0.63659500	1.74664000
H	4.03152800	-3.01833200	2.10318700
C	3.95636300	-2.96129500	1.01530000
C	3.31946300	-1.66897400	0.61677200
H	4.96951300	-3.00240900	0.60104400
H	3.38140500	-3.80102800	0.62192700
O	2.54689500	-1.57993700	-0.40044300
O	3.53657100	-0.58688000	1.26283100
Pd	2.30574400	0.45890100	-0.04018600
O	1.08923200	1.54501000	-1.35516200
C	1.33863600	2.61536000	-0.69547900
O	2.11381700	2.49804400	0.31270100
C	0.73105300	3.93011600	-1.06790000
H	0.44417400	3.92794300	-2.12068100
H	-0.16364800	4.09510600	-0.45767300
H	1.43572700	4.73787900	-0.86003800
C	-2.50760200	1.97063300	2.27329700
H	-1.93749200	2.32781400	3.13776000
H	-2.70568100	2.84234300	1.64029900
H	-3.45837900	1.57460100	2.63296300

B-INT-1

NImag=0

0 1 (charge, spin multiplicity)

C	1.68799000	-0.50741900	-0.60354700
C	0.97379800	-0.45116700	1.85809400
C	2.42721500	-0.07802400	2.16342700
H	2.56307200	1.00745400	2.09052300
H	2.70907800	-0.39704000	3.17054600
C	0.07136400	0.32960700	2.82623300
H	-0.97752800	0.05961700	2.67671100
H	0.33882400	0.07905800	3.85792400
H	0.17559900	1.40823100	2.68655500
C	0.72874400	-1.95930300	2.00520600
H	0.87275000	-2.24096300	3.05319400
H	-0.29291800	-2.21136000	1.71534400
H	1.41626700	-2.56555200	1.41105400
N	0.73690300	0.04432000	0.45046200

H	0.88726600	1.07508500	0.50978200
C	1.04924800	-1.66162200	-1.43372100
H	0.49386800	-2.30601200	-0.74680000
C	2.10759000	0.70818200	-1.49010900
H	1.18593600	1.10597600	-1.92879500
H	2.48901600	1.49787000	-0.83311400
O	3.35318200	-0.73160800	1.28453000
C	2.99696800	-1.06626000	0.02476500
O	3.75406500	-1.75474200	-0.61959800
H	-4.34347100	-2.83927400	-1.23164700
C	-4.34489100	-2.38912500	-0.23294900
C	-3.21959100	-1.40194100	-0.14133800
H	-5.30053700	-1.88479700	-0.08105900
H	-4.20715800	-3.18713300	0.49951500
O	-2.03335100	-1.79097800	0.16391000
O	-3.39537600	-0.16645000	-0.38739300
Pd	-1.31409700	0.17599000	-0.04449300
O	-1.25075500	2.16985600	-0.40919800
C	-0.38869600	3.03767900	0.02024400
O	0.66509600	2.78222900	0.63046600
C	-0.77785200	4.47391100	-0.29096000
H	-1.01160100	4.57706800	-1.35387300
H	-1.68225500	4.73470000	0.26729500
H	0.03299300	5.14824900	-0.01415100
H	1.87909900	-2.25515000	-1.82227000
C	3.13447600	0.43973300	-2.59602700
H	3.27528000	1.35479600	-3.17998800
H	4.10308500	0.14144700	-2.19087200
H	2.81327500	-0.34769600	-3.28219200
C	0.13106100	-1.27892600	-2.60163900
H	0.66951800	-0.77881500	-3.41060400
H	-0.30975400	-2.19098900	-3.01642700
H	-0.69699500	-0.62897600	-2.30103300

B-TS-1

NImag=1

0 1 (charge, spin multiplicity)

C	-1.80695500	-0.74491400	0.43878000
C	-1.44078800	0.77733000	-1.58008500
C	-2.91521600	1.16073000	-1.41186300
H	-3.00818700	1.99336400	-0.70416000
H	-3.34898800	1.46894900	-2.36656600
C	-0.67479100	2.03351700	-2.01834200
H	0.39364500	1.82734000	-2.10298600
H	-1.04518200	2.35789800	-2.99566000
H	-0.80795600	2.84986200	-1.30578500
C	-1.26174400	-0.32783700	-2.63153300
H	-1.47541400	0.08300000	-3.62277500
H	-0.23057400	-0.69186200	-2.62980600
H	-1.93457800	-1.17447200	-2.48243800
N	-0.98798800	0.35021300	-0.20723800
H	-1.00932900	1.20730400	0.38931300
C	-1.12597100	-2.10586900	0.16263900
H	-1.24387600	-2.36108800	-0.89316800
C	-1.86661400	-0.39098600	1.95809000
H	-0.84878800	-0.12362900	2.26507000
H	-2.45293200	0.53026600	2.06259400
O	-3.73269300	0.06980100	-0.96134800
C	-3.25272500	-0.84705000	-0.09075700

O	-3.97494100	-1.75531500	0.25064800
H	5.13031500	-2.79226500	-0.25923800
C	4.92674900	-1.74534200	-0.49674700
C	3.44767100	-1.47236600	-0.35536700
H	5.50778800	-1.08544500	0.14664300
H	5.21538900	-1.58257300	-1.53999000
O	2.62385300	-2.26753800	-0.90414100
O	3.09354100	-0.44434300	0.30710100
Pd	1.06016800	-0.04886100	0.10115000
O	1.59774300	1.93369400	0.22760300
C	0.85869900	2.79599800	0.85062000
O	-0.33686800	2.64661400	1.16831500
C	1.58640900	4.09031000	1.18332500
H	2.35525100	3.88784700	1.93553700
H	2.09569400	4.47517900	0.29576500
H	0.88355000	4.82959100	1.56886600
H	-1.67085000	-2.87713700	0.71377900
C	0.35980800	-2.13695800	0.52220500
H	0.54747400	-1.95826400	1.58630800
H	0.72602600	-3.15861900	0.35450400
H	1.41161700	-1.93497900	-0.36326600
C	-2.42274800	-1.46188300	2.90006800
H	-2.46868400	-1.05805100	3.91617700
H	-3.42537500	-1.77766700	2.60629700
H	-1.78363500	-2.34979600	2.93114700

B-TS-1-a

NImag=1

0 1 (charge, spin multiplicity)

C	-1.45158500	-0.75966500	0.38522000
C	-1.84184400	1.46089200	-0.87579200
C	-3.25627700	1.36779100	-0.29905300
H	-3.28045600	1.77906700	0.71786200
H	-3.96950000	1.92478100	-0.91177400
C	-1.37728800	2.92241600	-0.84116700
H	-0.36124800	3.00527800	-1.23319900
H	-2.04088400	3.53039600	-1.46352500
H	-1.38013100	3.32404500	0.17517500
C	-1.79433600	0.93407800	-2.31761300
H	-2.38860500	1.59174500	-2.95921100
H	-0.76501500	0.93515500	-2.68603400
H	-2.20172100	-0.07419700	-2.42006200
N	-0.98976500	0.65096500	0.05546900
H	-0.80506100	1.21274600	0.90419800
C	-0.48013600	-1.63779300	-0.48500800
H	-0.66734900	-1.38114100	-1.53094100
C	-1.29384800	-0.88664800	1.93462500
H	-0.25829200	-0.61212900	2.16781500
H	-1.92070200	-0.09929200	2.37489100
O	-3.74635100	0.01897900	-0.27822800
C	-2.93173400	-1.01839000	0.03914300
O	-3.40877800	-2.13015800	0.05569900
H	5.12018000	-1.69041700	-0.73054400
C	4.37644500	-2.41642500	-0.40408600
C	3.00513000	-1.78874500	-0.33469300
H	4.34946300	-3.26371200	-1.09525000
H	4.64192500	-2.80810100	0.58190200
O	2.03150700	-2.51094300	0.04909000
O	2.88507800	-0.56919600	-0.66618100

Pd	0.96313800	0.14400600	-0.36421800
O	1.80222400	1.99758300	-0.10152000
C	1.44334100	2.64981100	0.96508000
O	0.49208700	2.36502400	1.71232500
C	2.31811600	3.86321100	1.24833200
H	1.89044300	4.45335900	2.05953400
H	3.32141800	3.52771000	1.52892600
H	2.42210800	4.47380100	0.34728400
H	0.90431600	-1.84318100	-0.14295400
C	-0.62166200	-3.17785000	-0.40796200
H	-0.26177900	-3.59719900	0.53121000
H	-1.66876500	-3.45527400	-0.53916000
H	-0.02684700	-3.62729400	-1.20671600
C	-1.64292100	-2.21556600	2.61284200
H	-1.64263100	-2.06432200	3.69694000
H	-2.62864600	-2.58030100	2.31782800
H	-0.91277200	-2.99554000	2.39287500

B-INT-2

NImag=0

0 1 (charge, spin multiplicity)

C	-2.26670100	-0.69051400	-0.01025000
C	-1.63380000	1.80570900	0.19640000
C	-3.14971500	1.87407900	0.51244000
H	-3.34959300	1.59007400	1.55005300
H	-3.51171800	2.89514800	0.37548300
C	-0.84865500	2.11322200	1.47748400
H	0.21715700	2.17185200	1.25987200
H	-1.17485100	3.07666800	1.88548800
H	-1.00344100	1.35134100	2.24404900
C	-1.27771500	2.81630400	-0.90575100
H	-1.42294600	3.83731600	-0.54015800
H	-0.23177200	2.70140500	-1.20052400
H	-1.92185100	2.68127400	-1.78288000
N	-1.30610000	0.43418300	-0.34645700
H	-1.39292700	0.52986600	-1.35993400
C	-1.78199300	-1.85873700	-0.89024200
H	-1.92359800	-1.57772500	-1.94171000
C	-2.22718500	-1.05417800	1.49817100
H	-1.17548500	-1.18228600	1.77493300
H	-2.59901800	-0.21695000	2.09492400
O	-3.96129500	1.06745700	-0.35478500
C	-3.67890700	-0.26420800	-0.43754700
O	-4.50477800	-1.02079300	-0.88603700
H	5.25437600	-2.42695000	-0.17777900
C	4.25748600	-2.85501400	-0.03075100
C	3.25882600	-1.72653000	0.16617100
H	3.99761000	-3.47708300	-0.88755600
H	4.29837200	-3.46106100	0.87853200
O	3.35227600	-1.02704600	1.20844000
O	2.40015900	-1.56727900	-0.76604700
Pd	0.70398800	-0.40628000	-0.44140200
O	3.56339100	1.41956600	0.93597400
C	2.80389400	2.06228100	0.10286700
O	1.78405400	1.60941400	-0.44630800
C	3.26180200	3.47652400	-0.17193400
H	3.43350600	4.00204400	0.77135200
H	4.21797100	3.44635500	-0.70370600
H	2.52610500	4.00747700	-0.77524000

H	-2.42257500	-2.73161000	-0.73132200
C	-0.31049400	-2.15023100	-0.61377800
H	-0.15137300	-2.68464200	0.32885800
H	0.16669700	-2.70894900	-1.42164300
H	3.32889300	0.39785400	1.05021300
C	-3.03341300	-2.30595100	1.87011300
H	-3.05506800	-2.41916500	2.95800700
H	-4.06622200	-2.24484700	1.51496200
H	-2.59002300	-3.21487500	1.45516300

B-INT-2-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.08085400	-0.38544400	-0.23412100
C	1.39821000	2.00518700	0.49132100
C	2.91629100	2.18203000	0.60692700
H	3.35608900	2.37015300	-0.38157700
H	3.16874500	3.02384700	1.25639500
C	0.77986300	3.23970200	-0.17562200
H	-0.27501800	3.05403200	-0.39102900
H	0.85969600	4.10973500	0.48237300
H	1.28542900	3.48264500	-1.11820100
C	0.76213000	1.75932600	1.86647600
H	0.97756900	2.60427400	2.52847600
H	-0.32100100	1.65601500	1.76781300
H	1.14430800	0.85573500	2.34638600
N	1.17530800	0.83480200	-0.41796700
H	1.27238300	1.16577200	-1.37693900
C	1.03240600	-1.46972600	0.13747200
H	0.98346800	-1.57315400	1.22560900
C	2.83745900	-0.58572600	-1.57951800
H	2.07711400	-0.80834200	-2.33875900
H	3.27720100	0.38317800	-1.85543900
O	3.54646200	1.03849500	1.20437700
C	3.12507700	-0.21001300	0.87492400
O	3.61167600	-1.16266800	1.43469200
H	-3.42358200	-3.61171700	1.87279000
C	-3.52618700	-3.30664700	0.82700900
C	-2.82925100	-1.97002900	0.63038600
H	-3.11244400	-4.07567500	0.17426200
H	-4.59592400	-3.18737300	0.63064500
O	-3.20067900	-1.00400500	1.34590100
O	-1.91001000	-1.93844600	-0.25551400
Pd	-0.57935200	-0.33356200	-0.34573200
O	-2.01772400	1.31956800	-0.98548800
C	-3.08333600	1.75700900	-0.51844600
O	-3.74551000	1.23903300	0.47074300
C	-3.72361900	2.99979000	-1.09529600
H	-3.10753500	3.41164200	-1.89412600
H	-4.71538500	2.74948900	-1.48351900
H	-3.86588900	3.74292100	-0.30510900
H	-3.37566200	0.31228600	0.81552600
C	1.06180200	-2.83685800	-0.51893800
H	1.89477400	-3.43919900	-0.13240900
H	0.12943400	-3.35817700	-0.29144300
H	1.14595900	-2.78826800	-1.60843300
C	3.94647900	-1.64322800	-1.62401900
H	4.37921400	-1.66345600	-2.62922500
H	4.74759000	-1.42161700	-0.91513700

H	3.57372100	-2.64256400	-1.39851100
B-INT-3			
NImag=0			
O 1 (charge, spin multiplicity)			
C	2.57181600	0.42450600	-0.48476600
C	1.83758900	-1.34019800	1.29808300
C	3.36460300	-1.50551200	1.27803300
H	3.88100000	-0.70740900	1.81665600
H	3.61615500	-2.44951500	1.76369500
C	1.39970600	-1.10868300	2.75151700
H	0.31176600	-1.09196700	2.81568600
H	1.75192900	-1.94364500	3.36617500
H	1.80758700	-0.17982300	3.16049600
C	1.20860300	-2.62791500	0.75641300
H	1.61611800	-3.46940400	1.32699500
H	0.13238100	-2.59508800	0.90910000
H	1.43444300	-2.78896800	-0.29859400
N	1.47436800	-0.09766100	0.46937900
H	-3.46680400	-0.70063200	-0.68430600
C	1.91413900	1.12918100	-1.67913600
H	1.29913600	0.67420800	1.15665200
H	2.63530900	1.16427900	-2.50387800
C	3.48355800	1.45633600	0.25988700
H	2.82892100	2.25090000	0.62859100
H	3.93439300	1.01077300	1.14770600
O	3.88267200	-1.61963000	-0.05609100
C	3.44878000	-0.74152700	-0.98389400
O	3.81571900	-0.85062700	-2.12983600
H	-3.70323600	3.15463600	-0.91110500
C	-3.97983500	2.41395700	-1.66914000
C	-3.29017700	1.12269600	-1.31883200
H	-5.06251700	2.28813300	-1.67622000
H	-3.62203600	2.77813000	-2.63386300
O	-3.99947400	0.22518800	-0.74805500
O	-2.07004600	1.00792600	-1.61876300
Pd	-0.49830100	0.20541400	-0.43667000
O	-1.66391700	-1.92060000	1.99260200
C	-2.18891700	-0.79895800	2.01397100
O	-1.86165500	0.21610500	1.27860100
C	-3.34170100	-0.50648600	2.97486900
H	-3.52862800	-1.36881300	3.61637900
H	-3.11065500	0.37145000	3.58582700
H	-4.24373100	-0.27405700	2.39967800
H	1.66680700	2.15529800	-1.39872200
C	-1.63688600	-3.86550700	-1.37145700
H	-2.52526000	-4.27418500	-1.85522000
H	-1.50616800	-4.36592500	-0.40599700
H	-0.74740100	-4.03776600	-1.97835400
C	-0.58847800	3.99763500	1.53442800
H	-1.61120000	3.84111400	1.89335000
H	-0.63580800	4.63733100	0.65042500
H	-0.00249600	4.47140000	2.32303400
C	0.00259500	2.64095200	1.19698100
O	0.76072400	2.05978200	1.98442800
O	-0.35934700	2.20184200	0.02277400
C	-1.84307900	-2.38915400	-1.09000700
O	-0.74690200	-1.70535800	-1.11925900
O	-2.99534100	-1.98534700	-0.85522700

C	0.67342300	0.41831200	-2.13790000
H	0.81815700	-0.61061200	-2.46378700
H	0.04175300	0.98601100	-2.81931500
C	4.60047200	2.05261600	-0.60829300
H	5.20529800	2.73362800	-0.00219200
H	5.26483500	1.28224400	-1.01041000
H	4.20448500	2.62507500	-1.45121900

B-TS-2

Nlmag=1

0 1 (charge, spin multiplicity)

C	2.40382800	-0.39819400	-0.41546800
C	1.96948600	0.72704800	1.85672700
C	3.47198800	1.02326800	1.77036000
H	3.66276800	1.88880000	1.12476400
H	3.88794800	1.22936000	2.75940900
C	1.24336300	1.96548600	2.39842300
H	0.16135900	1.82084400	2.35961100
H	1.53678500	2.13629400	3.43878200
H	1.47909400	2.85868400	1.81355200
C	1.71196800	-0.48277200	2.76437700
H	2.16257900	-0.29314300	3.74385400
H	0.64226800	-0.64021800	2.88730100
H	2.14058800	-1.41032700	2.37747000
N	1.52976200	0.50945500	0.43530600
H	1.51750300	1.45770200	-0.00013700
C	1.61860400	-1.64938200	-0.88516000
H	1.27629600	-2.22739200	-0.02372200
C	2.93022800	0.44735200	-1.62146700
H	2.06345700	0.90768200	-2.10389800
H	3.51548100	1.28163000	-1.21895600
O	4.20693900	-0.11388900	1.28114600
C	3.65783900	-0.90132700	0.33410400
O	4.20576500	-1.93692600	0.03146300
H	-3.83538000	-1.61316900	-2.89798800
C	-3.71299500	-2.02041200	-1.89016600
C	-2.23682200	-2.20858900	-1.58736300
H	-4.13998400	-1.30305900	-1.18578800
H	-4.22641900	-2.97882500	-1.80796100
O	-1.73027800	-3.28709100	-1.32285900
O	-1.55622300	-1.06513900	-1.70970000
Pd	-0.50257000	0.03978300	-0.16527400
O	-3.93591900	0.82342900	0.87246800
C	-3.14622200	1.86903500	1.03645800
O	-1.93076000	1.79217800	1.20313500
C	-3.88951800	3.18312400	0.99194300
H	-4.36199100	3.30082100	0.01156400
H	-4.68885600	3.18543800	1.73834800
H	-3.20188200	4.00832600	1.17451700
H	2.31760400	-2.31731600	-1.41380600
C	0.47913200	-1.46041300	-1.85289700
H	0.52596800	-0.67059200	-2.59342900
H	0.09686200	-2.40966100	-2.20541700
H	-3.40821000	-0.02909300	0.98856100
C	3.76713300	-0.30292400	-2.66374900
H	4.13429500	0.40854700	-3.40940000
H	4.62955500	-0.80482200	-2.21877800
H	3.18247000	-1.05808900	-3.19798000
O	-0.57504200	1.53944800	-1.53624800

C	0.03368300	2.68549600	-1.45315700
O	1.03688000	2.92986700	-0.76457600
C	-0.59979300	3.76586100	-2.31352300
H	-1.48002300	4.15529700	-1.79115100
H	0.10849300	4.58028800	-2.47102300
H	-0.93643300	3.35531000	-3.26791500
O	-0.57592800	-1.53541500	1.12025600
C	-1.72664400	-2.00150900	1.50247900
O	-2.82982500	-1.47151100	1.29924400
C	-1.64145600	-3.33957400	2.20847500
H	-0.69287400	-3.45467300	2.73608200
H	-2.48285200	-3.45395600	2.89356900
H	-1.70428100	-4.11594400	1.43839800

B-TS-2'

NImag=1

O 1 (charge, spin multiplicity)

C	2.56936600	0.20490600	-0.40204800
C	1.68646400	-1.12576100	1.61010400
C	3.12335700	-1.67533700	1.47238800
H	3.88251300	-0.99633000	1.86426900
H	3.19744400	-2.60841800	2.03308800
C	1.47878000	-0.50725500	3.00248200
H	0.44592200	-0.15925900	3.08951000
H	1.65942200	-1.25252100	3.78421800
H	2.15267100	0.33944100	3.16974000
C	0.76311700	-2.34942300	1.43758800
H	0.95497600	-3.02463900	2.27854900
H	-0.29355500	-2.09516400	1.43998100
H	0.98763500	-2.88196100	0.51305400
N	1.46233200	-0.02566600	0.59786500
H	-3.38533200	-0.77017400	-1.03988600
C	2.00960500	1.00419500	-1.59504800
H	1.00535300	1.24763200	0.98544500
C	3.68848900	1.09483000	0.25776800
H	3.21787300	2.05038200	0.50724800
H	4.02844500	0.66833600	1.20061300
O	3.43542000	-2.02929500	0.11414100
C	3.15854100	-1.13501200	-0.86427100
O	3.40465600	-1.40825300	-2.01510500
H	-5.25930200	2.17861900	-0.97381000
C	-4.20662100	2.40031700	-0.79768300
C	-3.37045300	1.15442900	-0.93216200
H	-3.85276200	3.16829000	-1.48741300
H	-4.09026800	2.77940600	0.22344800
O	-3.99806000	0.04269000	-0.78094300
O	-2.14263700	1.25817700	-1.17567500
Pd	-0.46247200	0.17320000	-0.28880300
O	-2.48920900	-2.09342700	1.29859100
C	-2.47155900	-0.98308600	1.84084300
O	-1.69440600	0.01098600	1.52515900
C	-3.43804100	-0.66818400	2.98365800
H	-4.27541800	-0.08292300	2.58745100
H	-3.83168100	-1.59324900	3.40831100
H	-2.95205300	-0.06810500	3.75727000
H	2.69273800	0.87658000	-2.44251300
C	4.90895800	1.32975700	-0.64379600
H	5.64164700	1.93980600	-0.10683500
H	5.39814700	0.39408100	-0.93120500

H	4.64585200	1.86450000	-1.56027000
C	-1.31333300	-3.78618300	-1.73361400
H	-1.98739000	-4.14352600	-2.51353800
H	-1.53780500	-4.31715000	-0.80263700
H	-0.27209100	-3.96671100	-2.00291100
C	-0.79703900	4.06673900	0.13831100
H	-1.48389000	4.10649100	0.98980800
H	-1.31835700	3.55507900	-0.67470700
H	-0.51074200	5.07692000	-0.15351300
C	0.42735000	3.28298900	0.52999800
O	1.54867700	3.74024600	0.61921800
O	0.16267900	1.98642000	0.82337400
C	-1.58421400	-2.31675300	-1.47238000
O	-0.52162600	-1.69026800	-1.06473100
O	-2.71589000	-1.85754800	-1.66388900
C	0.63338700	0.55571400	-2.01445500
H	0.04355300	1.30946000	-2.53756200
H	0.61430700	-0.40552300	-2.52203300
H	2.00578100	2.06394900	-1.33052400

B-INT-4

NImag=0

0 1 (charge, spin multiplicity)

C	2.32089300	-0.07259200	-0.30341200
C	1.05307900	-0.56239900	1.93553800
C	2.47591000	-1.03731200	2.26097200
H	3.15449500	-0.20379400	2.45813900
H	2.44784700	-1.66324200	3.15454200
C	0.60920800	0.47226300	2.97923500
H	-0.38306500	0.84655200	2.71798300
H	0.56336300	0.00333400	3.96714200
H	1.30148300	1.31893900	3.03004100
C	0.12195300	-1.78378300	1.95879900
H	0.19008300	-2.24538600	2.94921500
H	-0.91582400	-1.50356600	1.78534100
H	0.40799100	-2.53344600	1.21903200
N	1.07657100	0.12474200	0.56829300
C	1.90882400	0.07107000	-1.77965600
H	0.98177000	1.15834800	0.71507100
C	3.38525600	1.02417400	0.03146400
H	2.88971400	1.99154700	-0.09974600
H	3.67135300	0.97351300	1.08410000
O	3.01775600	-1.87743700	1.22911100
C	2.93010700	-1.46381700	-0.05500800
O	3.37620200	-2.15649500	-0.93818400
Pd	-0.69678700	-0.03468000	-0.60596700
O	-3.56047600	-0.80068400	0.95306200
C	-3.09392600	0.27758800	1.33566600
O	-1.93041400	0.76657100	1.02122600
C	-3.90101900	1.18029200	2.26964100
H	-3.29570800	1.48958700	3.12690000
H	-4.19056700	2.09060400	1.73403400
H	-4.79826300	0.66260600	2.61235200
H	2.70431700	-0.35039500	-2.40375800
C	4.65621700	0.95955300	-0.82627200
H	5.35967400	1.72734000	-0.49089100
H	5.15554800	-0.01069300	-0.74939700
H	4.44662300	1.14468400	-1.88303100
C	-3.49806300	-2.64662200	-1.53914000

H	-3.97010300	-2.42638000	-2.49861900
H	-4.21788500	-2.48224000	-0.73144200
H	-3.14580400	-3.67950400	-1.50513300
C	-0.67714200	4.22515100	-0.96787100
H	-1.69361900	4.34503200	-0.57886000
H	-0.73008400	4.26574900	-2.05755600
H	-0.04754900	5.02621600	-0.57849100
C	-0.14881800	2.88325400	-0.49553100
O	0.59681700	2.79528300	0.48861100
O	-0.55942600	1.89155800	-1.23823300
C	-2.37255800	-1.70739300	-1.28644100
O	-1.36259000	-2.03641300	-0.56918900
O	-2.35605600	-0.52091200	-1.77088800
C	0.60639200	-0.62479500	-2.09233600
H	0.14001200	-0.30731600	-3.02479200
H	0.63731100	-1.71039500	-1.99933100
H	1.82071400	1.13487100	-2.01441800

B-TS-3

NImag=1

0 1 (charge, spin multiplicity)

C	-1.58598300	-0.42626900	0.94094300
C	-1.82346200	-1.02342300	-1.56902800
C	-3.28128600	-1.25620200	-1.15620500
H	-3.82716300	-0.30720200	-1.08933600
H	-3.79159300	-1.89796100	-1.87786600
C	-1.79043800	-0.28381900	-2.91376600
H	-0.75656500	-0.04789100	-3.18281900
H	-2.20345000	-0.92630400	-3.69708700
H	-2.35454400	0.65170900	-2.88497800
C	-1.06895300	-2.35190000	-1.68045500
H	-1.63829300	-3.03349900	-2.32039800
H	-0.09357100	-2.18057100	-2.13555800
H	-0.90164300	-2.84201500	-0.72097000
N	-1.25765000	-0.10192700	-0.52104600
H	-1.66499400	0.83281300	-0.73912400
C	-0.29947000	-0.71235600	1.76098300
H	0.23357500	-1.57912200	1.33685900
C	-2.39745600	0.77899900	1.51855600
H	-1.79024600	1.67604500	1.37274200
H	-3.29071600	0.92075400	0.90040400
O	-3.36892200	-1.95374400	0.09772500
C	-2.49347500	-1.66803200	1.08407900
O	-2.50186900	-2.32949300	2.09582300
H	4.65711200	1.98756300	0.11655500
C	4.59582500	0.89692600	0.13854000
C	3.44943600	0.43964600	1.02298400
H	4.40109800	0.55230300	-0.88233900
H	5.53257300	0.46791200	0.49647400
O	3.55032600	-0.45861200	1.84096300
O	2.33033800	1.14831000	0.83338300
Pd	0.75171100	0.59394100	-0.45840500
H	-0.59241900	-1.06155900	2.76746800
C	0.67319400	0.38195900	2.02498000
H	0.36989800	1.42012900	2.09558400
H	1.51695500	0.08231700	2.63577300
C	-2.81141100	0.67418400	2.99095300
H	-3.40572500	1.55293600	3.25852900
H	-3.41079900	-0.21653500	3.19165100

H	-1.94761000	0.65011800	3.66203300
O	0.12331000	2.52070500	-0.11666400
C	-0.89458900	3.09395300	-0.69106400
O	-1.86346100	2.50545900	-1.19702000
C	-0.81363800	4.61089900	-0.69175500
H	-0.08414700	4.92673500	-1.44490000
H	-1.78761800	5.03724600	-0.93448800
H	-0.46241500	4.97689700	0.27582300
O	1.83713600	-0.98617300	-1.11128000
C	2.05405400	-2.16522400	-0.57324200
O	1.37854900	-2.70864100	0.29695000
C	3.29182800	-2.84475100	-1.14223500
H	4.14291500	-2.57244000	-0.50869100
H	3.16516000	-3.92787800	-1.09865900
H	3.50077000	-2.52033800	-2.16337400

B-TS-3'

NImag=1

0 1 (charge, spin multiplicity)

C	2.28072600	-0.10645600	-0.28460100
C	0.98754200	-1.51352000	1.43058300
C	2.34859100	-2.23327600	1.40908500
H	3.11369800	-1.69586000	1.97391600
H	2.23792400	-3.22104000	1.86015900
C	0.63879300	-1.11115800	2.87202200
H	-0.32996400	-0.60585600	2.87837500
H	0.57455300	-1.99828300	3.51149400
H	1.39679000	-0.43972100	3.28915800
C	-0.05590500	-2.51607000	0.88806000
H	-0.04028800	-3.40776000	1.52341600
H	-1.06090000	-2.10013400	0.91197800
H	0.17401300	-2.82560800	-0.13360100
N	1.06958600	-0.25755200	0.60267900
C	1.92661800	0.83843800	-1.44865200
H	0.75049900	1.07320500	1.07641200
C	3.43667400	0.56761700	0.54104600
H	3.05646500	1.53921500	0.87269600
H	3.65001500	-0.00313500	1.44553600
O	2.80878800	-2.48036400	0.07000500
C	2.75511900	-1.46598500	-0.82368400
O	3.10574900	-1.65448300	-1.96490400
Pd	-0.72160700	0.27370900	-0.39514800
O	-3.69692600	-1.09869500	0.43484100
C	-3.18251600	-0.47242900	1.36723400
O	-1.99584800	0.06020200	1.37262200
C	-3.94761400	-0.26197300	2.67430200
H	-4.14288300	0.80582700	2.81751500
H	-4.89363500	-0.80497700	2.64928100
H	-3.34747700	-0.59666200	3.52586000
H	2.66712600	0.69732400	-2.24391500
C	4.74243000	0.75981600	-0.24309500
H	5.49499700	1.20875600	0.41213400
H	5.14403600	-0.18669100	-0.61707400
H	4.61138500	1.42859000	-1.09787900
C	-3.62988800	-1.17534300	-2.64041800
H	-4.10052300	-0.44810600	-3.30492100
H	-4.34796800	-1.49607000	-1.87997600
H	-3.28137900	-2.04592200	-3.19956100
C	-0.71426600	4.03833000	0.13416000

H	-1.54931100	4.01198400	0.84028200
H	-1.09091800	3.65281300	-0.81853000
H	-0.35686200	5.05993200	0.00862800
C	0.40343900	3.16895600	0.64651400
O	1.53145200	3.53395400	0.89378300
O	0.01609900	1.88003600	0.85757700
C	-2.50323200	-0.54126800	-1.90282200
O	-1.49042000	-1.25236500	-1.52106500
O	-2.46040300	0.69415000	-1.61697900
C	0.55158000	0.56771200	-2.00688700
H	0.11531600	1.39208600	-2.57383000
H	0.47465400	-0.37278400	-2.55129700
H	2.01098900	1.87131600	-1.10233800

B-INT-3-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.25577200	0.46975500	-0.47612600
C	1.92884000	-1.35286300	1.36667400
C	3.45723000	-1.22594000	1.33582400
H	3.79639800	-0.32196700	1.85436900
H	3.90872000	-2.09138200	1.82433700
C	1.45169000	-1.32710200	2.82508000
H	0.36681600	-1.44133300	2.85813100
H	1.89416500	-2.17526700	3.35723000
H	1.74072600	-0.40464900	3.33623800
C	1.49486200	-2.65615000	0.69164100
H	2.01345200	-3.48317300	1.18824700
H	0.42115700	-2.77992500	0.81862800
H	1.74386900	-2.68736000	-0.36975100
N	1.42962100	-0.09541900	0.67668500
H	-3.28168300	-0.62838000	-0.98156200
C	1.15316600	0.79499300	-1.51006700
H	1.31055200	0.64104100	1.41737100
C	2.98664500	1.77176700	-0.02115100
H	2.22296400	2.44029800	0.38305700
H	3.66366500	1.53713400	0.80758700
O	3.96920200	-1.23930900	-0.00788900
C	3.35529800	-0.49005000	-0.94998300
O	3.75981700	-0.51180800	-2.08747100
H	-4.79707400	2.30569500	-2.20447800
C	-3.76865300	2.50140000	-1.89966300
C	-3.07557200	1.22525000	-1.50308500
H	-3.21136200	3.00011400	-2.69377500
H	-3.77643400	3.16257300	-1.02600300
O	-3.82972300	0.26670700	-1.10977800
O	-1.82024900	1.17857200	-1.58219100
Pd	-0.43625900	0.26026500	-0.24420000
O	-1.50829200	-2.15710800	1.81244500
C	-2.23518400	-1.15333900	1.85137700
O	-2.05306900	-0.05043400	1.19901400
C	-3.48692000	-1.14368600	2.72882000
H	-3.45427300	-0.29830100	3.42299900
H	-4.37271600	-1.01232300	2.09938200
H	-3.56700900	-2.07857300	3.28531800
H	0.96263100	1.86743100	-1.55437100
C	3.76414900	2.48535800	-1.13370100
H	4.20016500	3.40609600	-0.73520900
H	4.57223700	1.86902800	-1.53369700

H	3.11360300	2.76285100	-1.96856700
C	-1.27309700	-3.74191600	-1.59466900
H	-2.09001600	-4.14859100	-2.19256700
H	-1.23019600	-4.28828800	-0.64643800
H	-0.31855600	-3.85846600	-2.10926400
C	-0.80298600	3.72046400	2.25587300
H	-1.80738400	3.43452500	2.58526800
H	-0.90993800	4.47451800	1.47302100
H	-0.24690200	4.12070400	3.10444000
C	-0.11129900	2.47983200	1.72295600
O	0.71393300	1.86139400	2.41089200
O	-0.46323200	2.17512200	0.50570800
C	-1.55820000	-2.28962800	-1.26237800
O	-0.48802500	-1.57226000	-1.13302700
O	-2.73904700	-1.92507700	-1.14099500
C	1.07662700	0.13454300	-2.86110600
H	0.12514900	0.38913300	-3.33506600
H	1.89334600	0.50924700	-3.48935100
H	1.16975900	-0.94918200	-2.81069000

B-TS-2-a

NImag=1

0 1 (charge, spin multiplicity)

C	-2.33102100	-0.48578500	-0.55067300
C	-1.97697800	0.64936100	1.73396000
C	-3.50672200	0.50328700	1.70416300
H	-3.81824200	-0.52600600	1.91129400
H	-3.95556900	1.15744400	2.45396000
C	-1.42435100	0.17472500	3.08487800
H	-0.34556000	0.34170900	3.11436800
H	-1.87213200	0.75775700	3.89619400
H	-1.62560600	-0.88633300	3.25830500
C	-1.61177100	2.12750700	1.50967500
H	-2.10388800	2.72203300	2.28711700
H	-0.53284100	2.25019500	1.60102600
H	-1.94136900	2.49755400	0.53796000
N	-1.48528900	-0.28574100	0.68034200
H	3.10919500	1.05314200	-1.12200000
C	-1.23159000	-0.51891100	-1.63432600
H	-0.86191100	-1.49073900	0.93275800
C	-3.06655300	-1.86970700	-0.48856300
H	-2.30436400	-2.62602300	-0.27999300
H	-3.75945100	-1.87781300	0.35900500
O	-4.05205700	0.93836700	0.44415000
C	-3.43309300	0.56700500	-0.70185400
O	-3.83995300	0.97780600	-1.76223500
H	3.24777400	-2.50337100	-3.06836100
C	3.88049100	-1.83565400	-2.48411500
C	3.05555000	-0.73547200	-1.86647700
H	4.35178100	-2.40769600	-1.67736000
H	4.67543500	-1.41248900	-3.10116600
O	3.72674300	0.28808800	-1.45981300
O	1.81501100	-0.86786400	-1.77856300
Pd	0.35296000	-0.13787400	-0.30415300
O	1.50304300	1.85119300	2.16457700
C	2.27047800	0.91273400	1.92541600
O	2.05930800	-0.04579300	1.07290900
C	3.60739100	0.79714600	2.65508200
H	3.72933000	1.62377600	3.35602000

H	3.66001500	-0.15434600	3.19393000
H	4.42441700	0.80510600	1.92682100
H	-0.96036800	-1.54900100	-1.87468700
C	-3.82435400	-2.23508600	-1.77124800
H	-4.29571000	-3.21468300	-1.64859300
H	-4.60436200	-1.50801100	-2.00905600
H	-3.15343800	-2.29888800	-2.63353400
C	0.80274700	4.07626800	-0.83979400
H	1.54889800	4.67681200	-1.36181700
H	0.77325500	4.38473700	0.21055600
H	-0.18769300	4.22144800	-1.27313500
C	2.12219100	-3.17902300	1.02514100
H	2.73487400	-2.27188700	1.00241500
H	2.07647400	-3.59503900	0.01559100
H	2.54651500	-3.90178100	1.72230400
C	0.75504900	-2.76894600	1.49328400
O	0.28399200	-2.97662000	2.58662300
O	0.00746600	-2.12817300	0.53403600
C	1.21771000	2.61788700	-0.86538300
O	0.20058400	1.80821000	-0.81632200
O	2.41721800	2.32143300	-0.92068800
C	-1.24033400	0.36996400	-2.84825300
H	-0.29693000	0.25721600	-3.38955400
H	-2.06039700	0.06168700	-3.50895200
H	-1.39713600	1.41892600	-2.60562300

B-product

NImag=0

0 1 (charge, spin multiplicity)

C	0.60076200	0.53979100	0.22456100
C	2.49029700	-1.14026200	0.19188500
C	3.39237200	0.02701400	-0.22071700
H	3.74533900	0.56300700	0.67013400
H	4.26632600	-0.29688900	-0.79392100
C	3.23656400	-2.03092300	1.19309500
H	2.58127100	-2.83602000	1.53640300
H	4.12274900	-2.47933400	0.73449100
H	3.56416400	-1.46004500	2.07031600
C	2.07287600	-1.97393700	-1.03200800
H	2.95058600	-2.43879200	-1.49213200
H	1.37986800	-2.76080900	-0.72430000
H	1.58420200	-1.37099900	-1.80134800
N	1.30428200	-0.59146600	0.87601100
H	1.58547000	-0.31000600	1.81124000
C	-0.76042400	0.04193700	-0.33697200
H	-0.56413500	-0.75558300	-1.05951500
C	0.42553600	1.65593700	1.30317300
H	0.00841500	1.17085500	2.19583300
H	1.42880300	2.00090700	1.58788500
H	-3.51541100	1.33005400	-0.26125600
C	-4.25153800	0.63442300	0.15134800
C	-3.94141900	-0.80684300	-0.21211600
H	-4.27195700	0.77177000	1.23753100
H	-5.23516200	0.86983000	-0.25229600
O	-4.73383000	-1.52529100	-0.77215500
O	-2.72969500	-1.32164400	0.13089100
H	-1.24439400	0.85264300	-0.88633200
C	1.37366900	1.17652600	-0.95105100
O	0.83014500	1.90097800	-1.75450100

O	2.70346700	0.95443000	-1.08027600
C	-0.43558200	2.86461100	0.92941200
H	-0.42971200	3.58887900	1.74979800
H	-0.06514100	3.35759900	0.02866000
H	-1.47710200	2.58201000	0.74913900
C	-1.68285000	-0.53797500	0.73276900
H	-2.10284100	0.23414100	1.38399700
H	-1.12359400	-1.24254100	1.35165000

B-INT-4-a

NImag=0

0 1 (charge, spin multiplicity)

C	2.40021600	0.71890800	-0.10660900
C	1.93005900	-0.94336700	1.78013900
C	3.46733200	-0.91738000	1.76299400
H	3.85399900	0.00125400	2.21599500
H	3.86607500	-1.76690500	2.32146100
C	1.43424400	-0.66920600	3.21313900
H	0.34168400	-0.67473900	3.22470600
H	1.79037600	-1.43813300	3.90839900
H	1.77263100	0.31054300	3.56120700
C	1.47517700	-2.35566900	1.35455900
H	1.84057900	-3.07162800	2.09955700
H	0.38738100	-2.41247300	1.32385700
H	1.87721700	-2.63325100	0.38131600
N	1.49004200	0.21336300	0.96017900
H	-2.63303000	-1.36051700	-1.34276900
C	1.36466600	1.11119700	-1.18420000
H	-3.14670500	0.63678900	1.45693100
C	3.12350500	2.01427300	0.39817100
H	2.33378800	2.63505700	0.83216900
H	3.80311800	1.75490300	1.21634900
C	3.47779700	-0.27433600	-0.55075400
H	-4.92011900	1.05810900	-2.42242400
C	-4.00862700	1.53271200	-2.05844000
C	-2.96579900	0.51052300	-1.69940000
H	-3.60715600	2.22690200	-2.79881800
H	-4.22953800	2.09753700	-1.14647100
O	-3.41358600	-0.68004900	-1.43617800
O	-1.76217500	0.83186400	-1.64682700
Pd	-0.20154700	0.19171300	-0.17593000
O	-3.54684000	-0.22066400	1.84234600
C	-2.70705600	-1.21660300	1.74798800
O	-1.57397700	-1.13608300	1.25700100
C	-3.23794700	-2.52911700	2.26767000
H	-4.04311300	-2.37337200	2.98647400
H	-3.63038300	-3.09730100	1.41724400
H	-2.42634100	-3.10788200	2.71126900
H	1.03616600	2.13845800	-1.03307200
C	3.89851700	2.77671200	-0.68325100
H	4.39295800	3.64729800	-0.24136700
H	4.66328700	2.15220300	-1.15260100
H	3.23775100	3.14475600	-1.47498400
C	0.27942000	-3.67338900	-2.10710200
H	-0.39114500	-4.22414300	-2.76797700
H	0.56164300	-4.32641800	-1.27391400
H	1.19243000	-3.38622400	-2.63158000
C	-1.57556200	4.09301400	1.22995800
H	-0.58252800	4.39697700	1.56347800

H	-2.33046500	4.35869500	1.97228300
H	-1.80808100	4.62787700	0.30230700
C	-1.63275100	2.59743000	0.95105200
O	-2.73978100	2.02314800	0.98934200
O	-0.49073600	2.07566000	0.67169200
C	-0.43518900	-2.45428200	-1.54717500
O	0.36745500	-1.51670100	-1.16819300
O	-1.67744900	-2.46173800	-1.47643500
O	3.98778800	-1.06091100	0.43028000
O	3.93896500	-0.34677300	-1.66629000
C	1.45376900	0.73229400	-2.63464400
H	1.67854300	-0.31939700	-2.78889000
H	0.52154000	0.99686900	-3.14075700
H	2.27034400	1.31153000	-3.08635200

B-TS-3-a

NImag=1

0 1 (charge, spin multiplicity)

C	2.71324300	0.60878000	0.01183200
C	1.90534000	-1.36618300	1.33289400
C	3.15851400	-0.99044100	2.14599700
H	2.96867900	-0.10429000	2.76108700
H	3.45667200	-1.81686700	2.79462900
C	0.76676300	-1.65382800	2.32021500
H	-0.15515900	-1.90532700	1.79544400
H	1.03974200	-2.49111700	2.97223800
H	0.56186900	-0.77592500	2.93934600
C	2.21253800	-2.63173800	0.50385100
H	2.36293100	-3.47361800	1.18805800
H	1.38335500	-2.85478800	-0.16182500
H	3.12626000	-2.53832900	-0.08754400
N	1.55946900	-0.10388100	0.61322900
H	-3.03133400	-1.12362200	-0.99176000
C	2.08061800	0.47576900	-1.31807800
H	-2.97157600	1.18103400	1.70839000
C	2.89386600	2.05125600	0.55509000
H	1.89192600	2.47154500	0.63826600
H	3.30366500	1.98158400	1.57049500
C	4.07169000	-0.08926600	0.14102300
H	-4.95072100	1.51998000	-2.25639400
C	-3.93909500	1.85660400	-2.02743700
C	-3.06638100	0.70457300	-1.61123300
H	-3.49529000	2.37303300	-2.87981600
H	-3.97321700	2.55142600	-1.18175000
O	-3.67632100	-0.30365800	-1.08398600
O	-1.82715200	0.77760600	-1.78179700
Pd	-0.24381700	0.13745400	-0.48811800
O	-3.51580000	0.60561500	2.31321700
C	-3.11959400	-0.65518400	2.19726100
O	-2.20367800	-1.02104800	1.47286700
C	-3.93247200	-1.59674800	3.05549100
H	-3.93502200	-1.25332800	4.09393100
H	-4.97117000	-1.59698100	2.71059400
H	-3.52472200	-2.60497300	2.99057100
H	1.53928400	1.35327700	-1.66331000
C	3.78627000	2.94412200	-0.31449100
H	3.84589400	3.94596100	0.12164100
H	4.80105800	2.55044900	-0.40984400
H	3.37746400	3.05419800	-1.32543300

C	-0.70428300	-3.94497800	-1.95161400
H	-1.53749000	-4.42231300	-2.46882800
H	-0.42378700	-4.57085400	-1.09715200
H	0.16264400	-3.86430100	-2.61012200
C	-0.83303700	4.27604600	0.62751200
H	-0.23675700	4.42192700	1.53486100
H	-1.76324900	4.83670900	0.72713900
H	-0.24995700	4.64724100	-0.21818200
C	-1.13988900	2.79187500	0.47063600
O	-2.25221200	2.35162900	0.79124400
O	-0.13846500	2.11409000	0.00499000
C	-1.13130700	-2.57720500	-1.43871900
O	-0.14588200	-1.76451900	-1.24558300
O	-2.33917300	-2.37088000	-1.23383000
O	4.29797300	-0.75285000	1.29172500
O	4.94469400	0.02012700	-0.68915000
C	2.42920400	-0.53907900	-2.34626500
H	2.81089200	-1.46764100	-1.92805400
H	1.58322500	-0.75666600	-2.99899200
H	3.23937700	-0.09827900	-2.94820600

B-INT-5-a

NImag=0

0 1 (charge, spin multiplicity)

C	-2.18983400	0.37340400	0.03231800
C	-1.40013700	-1.34329600	-1.66049800
C	-2.90975600	-1.34858200	-1.95328200
H	-3.19532700	-0.46236500	-2.53077900
H	-3.18310100	-2.23992200	-2.52230700
C	-0.63614000	-1.28883400	-2.99429000
H	0.43594600	-1.22076900	-2.79822700
H	-0.82469500	-2.19063300	-3.58759700
H	-0.93515400	-0.41123200	-3.57455800
C	-1.02577300	-2.63341500	-0.90071800
H	-1.34863800	-3.49992600	-1.48794900
H	0.05276100	-2.69325400	-0.75924700
H	-1.49785300	-2.69584800	0.08137700
N	-1.16886700	-0.05577700	-0.97077100
C	-1.28846100	0.66697800	1.25422200
H	3.39016400	1.06314000	-0.27125900
C	-2.85226000	1.69028200	-0.49232500
H	-2.01763000	2.33899600	-0.77028700
H	-3.39080900	1.45832400	-1.41889600
C	-3.32843900	-0.62150000	0.29217100
Pd	0.45461600	0.12407800	0.25120500
O	4.02410300	0.31833600	-0.56489900
C	3.37801200	-0.68697300	-1.08951600
O	2.14438100	-0.80019000	-1.11307500
C	4.27670300	-1.73662700	-1.69674200
H	4.81441300	-1.30603600	-2.54708900
H	5.02663000	-2.04859200	-0.96455100
H	3.68933600	-2.59292300	-2.02599200
H	-1.09384500	1.73410400	1.35134700
C	-3.79428900	2.39143400	0.49242400
H	-4.18627000	3.30680000	0.03799500
H	-4.64131900	1.76105300	0.77434800
H	-3.27777000	2.68137200	1.41360400
C	2.17986800	-2.17192800	3.09726500
H	3.10383400	-1.75227100	3.49679400

H	2.36498000	-3.15179400	2.65018400
H	1.46428100	-2.31102100	3.91451200
C	1.26633100	4.24564800	-0.72740400
H	0.71306400	4.33190400	-1.66608400
H	2.21896600	4.77095600	-0.79889900
H	0.65519100	4.70111900	0.05817000
C	1.50861100	2.78115800	-0.39530800
O	2.64609200	2.39216800	-0.09148600
O	0.43331000	2.05962700	-0.46045600
C	1.58641300	-1.24056500	2.07629300
O	0.63691600	-1.67767600	1.31869800
O	1.96994500	-0.04724300	1.95012700
O	-3.68792300	-1.41222500	-0.74614700
O	-3.96320700	-0.66995400	1.32101700
C	-1.46011600	-0.02066100	2.58168300
H	-1.53025400	-1.10495500	2.49984100
H	-0.63395900	0.24190500	3.24796000
H	-2.39656000	0.33285500	3.02956400

B-TS-4-a

NImag=1

O 1 (charge, spin multiplicity)

C	-2.26991700	-0.62873100	-0.33650200
C	-1.69292700	1.09300700	1.40212600
C	-3.03018700	0.58457300	1.97484600
H	-2.89694200	-0.38680500	2.46241400
H	-3.43672900	1.29474600	2.69831600
C	-0.67763500	1.22249400	2.54962500
H	0.28082400	1.59579600	2.17970200
H	-1.04671100	1.92379500	3.30595700
H	-0.49949900	0.25175800	3.01916500
C	-1.93235500	2.46952600	0.74265500
H	-2.12722000	3.20887500	1.52654000
H	-1.06122200	2.77860400	0.17164000
H	-2.80112700	2.47282500	0.08066400
N	-1.24122200	-0.04222400	0.55110400
H	3.21342000	1.18432900	0.66789000
C	-1.44907300	-0.27370700	-1.51995900
C	-2.47904400	-2.14667400	-0.09145600
H	-1.48157100	-2.56970700	0.03520400
H	-3.00735600	-2.26613900	0.86264100
C	-3.64740000	0.03554700	-0.26963100
H	5.80824400	-0.76921100	-0.65388100
C	4.84008900	-1.25615500	-0.78074800
C	3.71729400	-0.31400500	-0.44410200
H	4.72165500	-1.63989400	-1.79398300
H	4.78145800	-2.09245300	-0.07563400
O	3.97648800	0.51851500	0.51420600
O	2.64000500	-0.38272100	-1.07391700
Pd	0.66821700	-0.06385700	-0.29310200
H	-0.85931500	-1.08962400	-1.93313100
C	-3.23830300	-2.86638200	-1.21172900
H	-3.31816800	-3.93253400	-0.97902500
H	-4.24650400	-2.46919300	-1.35261400
H	-2.71269600	-2.78282400	-2.16982700
C	1.47649800	4.18170400	-0.65669500
H	2.48141300	4.60855000	-0.66857100
H	0.88538800	4.74712200	0.07229700
H	1.00697800	4.27511500	-1.63664600

C	1.36750400	-4.02819500	1.03351700
H	0.41383200	-4.31379500	1.49011300
H	2.18276200	-4.35596300	1.67980300
H	1.42883400	-4.52530300	0.06191600
C	1.41849000	-2.51502100	0.87228200
O	2.12422700	-1.79903800	1.57811500
O	0.62779900	-2.07822000	-0.08153200
C	1.54307500	2.73272300	-0.20735000
O	0.72553200	1.93692100	-0.80770600
O	2.32378300	2.41294200	0.71275900
O	-4.03805400	0.47780400	0.94497100
O	-4.40169200	0.08460200	-1.21349200
C	-1.66903300	0.90390600	-2.40057500
H	-2.15006400	1.73930500	-1.89659800
H	-0.74118200	1.24531100	-2.86111000
H	-2.35506000	0.56618400	-3.19333000

B-product-a

NImag=0

0 1 (charge, spin multiplicity)

C	0.77707800	0.02988000	0.15328000
C	-1.77622000	0.15988000	0.22405500
C	-1.55910400	-1.32086600	0.54305900
H	-1.21192200	-1.43658800	1.57720600
H	-2.47693500	-1.90032000	0.42026200
C	-2.67827700	0.78062200	1.30295100
H	-2.83419500	1.84221200	1.09182600
H	-3.65703500	0.28913800	1.33784200
H	-2.20830400	0.70306100	2.28733100
C	-2.42395500	0.32741000	-1.15915600
H	-3.45464400	-0.03975200	-1.13195300
H	-2.45105400	1.38276500	-1.44695700
H	-1.89667200	-0.23301200	-1.93525200
N	-0.44669100	0.82895900	0.34707900
C	0.39434100	1.12252600	-0.80990200
H	0.05083800	0.76156900	-1.77998000
C	1.87870600	0.18506600	1.20107400
H	1.72509400	1.15246000	1.68830200
H	1.72401100	-0.57261900	1.98117500
O	-0.60292400	-1.93021400	-0.34721500
C	0.63416700	-1.36526600	-0.41724800
O	1.53667400	-1.97596400	-0.93955400
C	3.30717700	0.07564000	0.65421500
H	4.03360500	0.19113600	1.46507800
H	3.47096600	-0.89035600	0.17346100
H	3.50646900	0.85580900	-0.08743700
C	1.05852000	2.47963400	-0.87330800
H	1.90316000	2.46594600	-1.56982500
H	0.34244800	3.22938000	-1.22792200
H	1.41640100	2.79872900	0.10732900

C-reactant

NImag=0

0 1 (charge, spin multiplicity)

C	1.44233500	-0.78381700	1.05650900
C	1.44877000	1.00661600	-0.80087600
C	2.73659000	0.27622200	-1.22426700
H	2.46513200	-0.64351100	-1.74941900
H	3.29860800	0.89493000	-1.93116400
C	0.55088800	1.17582400	-2.04324900

H	-0.38776100	1.67680100	-1.78315700
H	1.04884400	1.77269200	-2.81678500
H	0.29648200	0.19817100	-2.46208300
C	1.77268800	2.41005600	-0.23546900
H	2.22401500	3.04812000	-1.00342700
H	0.85101300	2.89980500	0.10283400
H	2.46671400	2.37060800	0.60653900
N	0.71139100	0.17228800	0.18233500
H	0.12590500	0.77419300	0.75235900
C	0.74152800	-0.79404100	2.42559700
H	-0.30973200	-1.07775200	2.31490600
H	1.21730700	-1.51453100	3.09875700
H	0.78710900	0.19299500	2.90023000
C	1.35094500	-2.20772400	0.46343700
H	0.29830600	-2.48144400	0.35168800
H	1.83494900	-2.28307400	-0.51239900
C	2.91393300	-0.35627200	1.24891000
H	-3.36681300	4.39638300	0.13099700
C	-2.49216500	3.89935800	0.55630100
C	-2.59827600	2.42073900	0.35199900
H	-1.60519900	4.27019900	0.03121800
H	-2.39655400	4.12743400	1.61884600
O	-2.20203200	1.58838900	1.24074900
O	-3.06603200	1.92954800	-0.73139300
Pd	-2.74348800	-0.00246300	-0.01481000
O	-2.47459000	-1.93715100	0.71287400
C	-2.92802000	-2.41280900	-0.38553400
O	-3.31037200	-1.56454500	-1.26330300
C	-2.97563000	-3.88509300	-0.64197500
H	-1.99979200	-4.21040100	-1.01866800
H	-3.17792100	-4.41978400	0.28825500
H	-3.73408400	-4.11188100	-1.39304900
H	3.46232400	-1.11089400	1.82352400
H	2.94129500	0.57164500	1.82854200
C	3.67015800	-0.10705800	-0.06569200
O	4.40974000	-1.26380300	-0.49179000
O	4.65099900	0.91268200	0.19555300
C	5.78248400	-1.03958200	-0.19456300
C	5.89363600	0.47378300	-0.33973400
H	6.38872700	-1.60833200	-0.90490700
H	6.03130600	-1.35786600	0.82913300
H	6.70132800	0.92615900	0.24226300
H	6.00339100	0.76313000	-1.39586600
H	1.83490300	-2.93472200	1.12588300

C-INT-1

Nimag=0

0 1 (charge, spin multiplicity)

C	0.73322300	-0.97500000	1.24667200
C	0.92575000	-0.48223400	-1.29534600
C	2.32348100	-1.13413200	-1.09978500
H	2.23436200	-2.22089700	-1.01796300
H	2.92742800	-0.94513700	-1.99277300
C	0.04076400	-1.44450600	-2.10698800
H	-0.89175900	-0.95897800	-2.40908800
H	0.57646600	-1.74137600	-3.01539300
H	-0.21521300	-2.34735800	-1.55038500
C	1.05811500	0.84338500	-2.06829100
H	1.44931200	0.64042200	-3.07026700

H	0.08307700	1.32687100	-2.17666300
H	1.73756400	1.52952300	-1.55943900
N	0.29744600	-0.14992700	0.05142700
H	0.56381700	0.82646400	0.29367500
C	0.03804100	-0.39509500	2.49198600
H	-1.03595900	-0.60475500	2.47834900
H	0.18474100	0.68616800	2.55494400
C	0.34553900	-2.45902000	1.11919100
H	-0.72186800	-2.57247000	0.92221000
H	0.90182700	-2.98740200	0.34282000
C	2.26922800	-0.79490400	1.42582000
H	-5.90111900	-1.56677600	-0.48006500
C	-5.03959800	-2.10841200	-0.08699600
C	-3.82289700	-1.22916400	-0.10190300
H	-5.25155200	-2.40908000	0.94473600
H	-4.85470100	-3.01385500	-0.66942000
O	-2.64929600	-1.74432400	-0.02968900
O	-3.91890900	0.03734800	-0.16373400
Pd	-1.78605900	0.18333600	-0.06707400
O	-1.61477100	2.19398000	-0.18893300
C	-0.66813800	2.93074900	0.31215300
O	0.40495600	2.52400000	0.78130500
C	-0.99428100	4.41671000	0.27795600
H	-1.33251600	4.70644900	-0.72030900
H	-1.81480900	4.62329300	0.97234900
H	-0.11667000	4.99663900	0.56541600
H	0.46179800	-0.85723500	3.38981100
H	2.66178500	-1.65677200	1.97250600
H	2.46706000	0.09753900	2.02575300
C	3.09118500	-0.65018100	0.13121500
O	3.48436400	0.71673300	-0.00030400
O	4.31051300	-1.40666800	0.21848000
C	4.80754200	0.72608200	-0.52496900
C	5.41706700	-0.51079900	0.13113600
H	4.80772100	0.64279100	-1.62192200
H	5.28187200	1.66763700	-0.23884100
H	5.80934600	-0.28019800	1.13148400
H	6.20784200	-0.97914800	-0.46265200
H	0.57176100	-2.95576600	2.06842800

C-TS-1

NImag=1

0 1 (charge, spin multiplicity)

C	0.85743700	-1.05372100	-0.36184400
C	1.26597000	0.93552900	1.26173900
C	2.78894900	0.87668200	0.94948600
H	3.07954800	1.76427500	0.38029700
H	3.35190600	0.89937900	1.88695700
C	0.84769700	2.40660200	1.41525900
H	-0.20276300	2.48718100	1.70402000
H	1.46218200	2.87500000	2.19061000
H	0.98870900	2.95757000	0.48208900
C	0.92972000	0.20411500	2.57491500
H	1.40376800	0.73572000	3.40570600
H	-0.15085800	0.20239700	2.74579900
H	1.28490700	-0.82747700	2.60587200
N	0.50914200	0.35082000	0.09772700
H	0.49489800	1.02858300	-0.67995000
C	-0.26398500	-1.93608900	0.24992400

H	-1.60498800	-2.05647000	-0.03337300
H	-0.11469000	-2.11654200	1.31647900
C	0.77109500	-1.07445300	-1.89895600
H	-0.19552300	-0.69442100	-2.24179900
H	1.56882300	-0.47408600	-2.33906300
H	-5.33408700	-2.61418400	-1.23704200
C	-5.14650700	-2.31813800	-0.20009800
C	-3.71711800	-1.84123900	-0.07912400
H	-5.84443000	-1.53181400	0.08605000
H	-5.29020900	-3.20342200	0.42438200
O	-2.78292400	-2.68516400	-0.23048600
O	-3.52126800	-0.60531700	0.15599000
Pd	-1.51877700	-0.06545700	0.21513500
O	-2.20437000	1.85852300	0.13554700
C	-1.69047700	2.62888500	-0.77852700
O	-0.69403000	2.37855600	-1.47404700
C	-2.45093900	3.93612600	-0.96480500
H	-3.14102200	3.81755200	-1.80767200
H	-3.03520100	4.18986500	-0.07913300
H	-1.75241700	4.73756000	-1.21400800
H	-0.24063400	-2.91209100	-0.25096600
H	0.87831500	-2.10405100	-2.25449100
C	2.26309800	-1.48452500	0.11609600
H	2.21475000	-1.89814000	1.12656100
H	2.63603800	-2.27784100	-0.53732300
C	3.27726000	-0.34092200	0.13895100
O	4.51125900	-0.77620100	0.70322400
O	3.57012600	0.04248900	-1.21897400
C	4.97556700	-0.08177700	-1.43549200
C	5.38390600	-1.10197600	-0.37666700
H	5.21956900	-2.13168600	-0.72566400
H	6.41465300	-1.00126600	-0.02868400
H	5.14730400	-0.41146200	-2.46389900
H	5.48082200	0.88146300	-1.27724700

C-INT-2

NImag=0

0 1 (charge, spin multiplicity)

C	1.36117000	-1.03571100	-0.91143900
C	1.30602200	1.51059600	-0.20538500
C	2.83972700	1.35192200	-0.23388500
H	3.18177100	1.40580900	-1.27242900
H	3.31351200	2.17587200	0.30787800
C	0.89767800	2.78465300	-0.96303800
H	-0.19202000	2.85542800	-1.02199100
H	1.27951200	3.67116500	-0.44826100
H	1.30522300	2.79041400	-1.98124500
C	0.76169300	1.59868700	1.23044400
H	1.19697500	2.47293300	1.72570000
H	-0.32413400	1.71127300	1.21739800
H	1.00633000	0.72735500	1.83765000
N	0.69842900	0.35353400	-0.96611200
H	0.65934800	0.62972000	-1.94560700
C	0.12512400	-1.92489200	-0.70286900
H	-3.38656200	0.45459800	1.39918900
H	0.12953300	-2.50075000	0.22561000
C	2.07152900	-1.32354300	-2.23944000
H	1.37215600	-1.22202300	-3.07777400
H	2.93142000	-0.66934000	-2.40807700

C	2.32116400	-1.10429600	0.28311300
H	-5.42399300	-2.63916300	0.96864100
C	-4.38692800	-2.98877100	0.94148300
C	-3.46475600	-1.79464600	0.75196800
H	-4.17892500	-3.45382500	1.90928100
H	-4.26785600	-3.71860300	0.14022800
O	-3.41193200	-0.94337400	1.67863800
O	-2.82013800	-1.75025300	-0.34750600
Pd	-1.22210300	-0.43578700	-0.57471200
O	-2.40362200	1.49739000	-0.61966900
C	-3.17094400	2.03040000	0.20007200
O	-3.60989700	1.48409900	1.29285200
C	-3.67987600	3.43616900	-0.02738400
H	-3.20888500	3.87539200	-0.90633600
H	-4.76502600	3.40817600	-0.16629600
H	-3.48357800	4.04953200	0.85654400
H	-0.12411300	-2.56206100	-1.55520500
C	3.36560700	0.02871500	0.35262700
H	2.84267800	-2.06516500	0.25486400
H	1.73886900	-1.07951000	1.20705500
O	4.55386000	-0.36650300	-0.35535300
O	3.76496700	0.24530900	1.70616600
C	4.97543000	-0.47745900	1.91294000
C	5.65523300	-0.35592900	0.55175200
H	6.21903000	0.58396400	0.46844800
H	6.31892700	-1.19213000	0.31303200
H	4.77630500	-1.52704300	2.17386800
H	5.52319400	-0.00331000	2.73089900
H	2.43491100	-2.35593000	-2.24032200

C-INT-3

NImag=0

0 1 (charge, spin multiplicity)

C	1.59876600	0.95238000	-0.96619000
C	1.77718200	-0.19350800	1.41750600
C	3.24845500	0.23842800	1.21029400
H	3.34787600	1.31142900	1.39914700
H	3.86526200	-0.27494500	1.95423700
C	1.29753900	0.25289700	2.80855400
H	0.26900500	-0.07398800	2.97372300
H	1.92637900	-0.22336000	3.56707400
H	1.36343600	1.33677200	2.93619200
C	1.62900900	-1.71669800	1.31878900
H	2.27740900	-2.15309000	2.08610000
H	0.59847700	-1.99557500	1.53348300
H	1.93768400	-2.12613600	0.35900400
N	0.97018600	0.61420000	0.39322700
H	-3.35317100	-1.69579700	-0.67631200
C	0.39059800	0.73997200	-1.88373400
H	0.68705900	1.50586100	0.86344700
C	2.07330200	2.41285600	-1.00399200
H	1.27241600	3.09411200	-0.71036900
H	2.93968200	2.58979300	-0.36471900
C	2.73268100	-0.03033200	-1.27365800
H	-4.49982100	1.24671600	-3.15254900
C	-4.85213800	0.79205800	-2.22579300
C	-3.76819000	-0.06152700	-1.62292200
H	-5.07396800	1.59743200	-1.51683900
H	-5.75832100	0.20909300	-2.39336100

O	-4.16275600	-1.09246100	-0.96608700
O	-2.57161800	0.27761500	-1.79745700
Pd	-0.93984200	0.20904000	-0.40825700
O	-1.37155900	-1.72527700	2.34748300
C	-2.32965100	-0.97987400	2.11027100
O	-2.40510500	-0.10226500	1.15959500
C	-3.58879400	-1.04123400	2.97583500
H	-3.45216400	-1.75213700	3.79201600
H	-3.81953000	-0.05010500	3.37817300
H	-4.43976300	-1.34720100	2.35893700
H	-0.02796200	1.63497400	-2.33938100
C	-0.42066000	-4.06668200	-0.71700200
H	-1.07183800	-4.84576100	-1.11592900
H	-0.16547700	-4.32130100	0.31703900
H	0.50223700	-3.99727500	-1.29437400
C	-2.13567800	4.13069400	0.91806100
H	-3.00563600	3.76880100	1.47577600
H	-2.48820600	4.50176600	-0.04676800
H	-1.65168300	4.92731000	1.48438600
C	-1.17151800	2.97109500	0.73423400
O	-0.16416900	2.85909600	1.44588600
O	-1.52461900	2.16574900	-0.22508200
C	-1.16448300	-2.74396300	-0.69156000
O	-0.38690600	-1.71562100	-0.81820300
O	-2.39686700	-2.75181300	-0.54892700
H	0.43981900	-0.11853700	-2.54988300
H	2.36877600	2.65036300	-2.03152000
H	3.19198200	0.24071100	-2.22937200
H	2.31954800	-1.03488300	-1.38118500
C	3.82026700	-0.06117000	-0.18701900
O	4.85473200	0.90284100	-0.43062300
O	4.44618700	-1.34559400	-0.25929100
C	5.85733600	-1.14792600	-0.22843900
H	6.33262400	-1.97679600	-0.75885200
C	6.00063000	0.20599600	-0.91323600
H	6.89265400	0.76760900	-0.62433800
H	6.23449200	-1.11347000	0.80394400
H	5.97571600	0.10345600	-2.00805500

C-TS-2

NImag=1

O 1 (charge, spin multiplicity)

C	-1.62713500	0.85781100	-0.64638000
C	-1.50068700	-1.38013900	0.71252600
C	-2.96070500	-1.57358600	0.24581200
H	-2.94847300	-1.98053200	-0.77042400
H	-3.46192600	-2.30581400	0.88587700
C	-0.74907100	-2.71272200	0.52596900
H	0.31171500	-2.58688500	0.75456200
H	-1.16722100	-3.46716300	1.19917700
H	-0.82521100	-3.07354300	-0.50136700
C	-1.39354700	-0.97852500	2.19430900
H	-1.97654200	-1.68471900	2.79608400
H	-0.35375500	-1.02789700	2.52008000
H	-1.76047400	0.02440100	2.41391300
N	-0.86283200	-0.38105300	-0.23431700
H	-0.66891300	-0.92546100	-1.11227700
C	-0.86702500	2.14144300	-0.24532400
H	3.10895900	-1.42950100	1.95588600

H	-0.60555600	2.23692600	0.80759200
C	-1.92111500	0.84476700	-2.14882100
H	-0.98724900	0.88282600	-2.70922300
H	-2.47429800	-0.04979900	-2.43599600
H	2.59414800	5.05413000	-0.76039500
C	2.97228100	4.11160800	-1.15569500
C	2.02832800	2.97738300	-0.79170900
H	3.03314700	4.20084900	-2.24261700
H	3.96307700	3.90097200	-0.75265000
O	2.52349100	1.94160500	-0.29648100
O	0.72857700	3.17454400	-1.07055200
Pd	1.03920800	0.43409100	-0.08305800
O	3.57650100	-2.28781800	1.71344900
C	3.32229300	-2.60833500	0.45966000
O	2.58807300	-1.96549700	-0.27418600
C	4.01961700	-3.88060300	0.03297600
H	5.06457400	-3.86071400	0.33747100
H	3.55420700	-4.73541600	0.53040300
H	3.93934700	-4.00909700	-1.04306100
H	-1.27015000	3.01393600	-0.70546400
C	1.72964700	1.74453700	3.94832600
H	1.99454300	1.16025300	4.83213000
H	0.76783300	2.24038100	4.08915300
H	2.49878100	2.51243000	3.80841100
C	2.01420900	-1.34682500	-3.83487800
H	1.50863200	-1.99931600	-4.54708600
H	2.85556200	-1.88483300	-3.39041500
H	2.41161000	-0.46001900	-4.33203600
C	1.07356700	-0.96685200	-2.70692700
O	0.06332300	-1.65011700	-2.46417400
O	1.43676200	0.10303200	-2.07506400
C	1.72733100	0.84766900	2.72002200
O	0.83262500	1.15495800	1.83862200
O	2.54844500	-0.07153900	2.63584500
H	-2.52809600	1.71617600	-2.41035400
C	-3.82274000	-0.29954100	0.20851700
C	-2.96629000	0.99960000	0.16961100
H	-2.76315200	1.26707400	1.21198800
H	-3.57497500	1.79632800	-0.26980900
O	-4.69184500	-0.31060900	-0.93084000
O	-4.67005700	-0.26674100	1.35863600
C	-6.03603600	-0.48907000	-0.47636100
C	-5.98504600	0.09108100	0.93517700
H	-6.31012100	-1.55464400	-0.46720900
H	-6.70768900	0.04576000	-1.15358300
H	-6.70368800	-0.35442700	1.62672900
H	-6.11676400	1.18375900	0.93248200

C-TS-2-a

NImag=1

0 1 (charge, spin multiplicity)

C	-1.68900100	-0.80532100	-1.16291000
C	-1.80101100	-0.22783200	1.37380200
C	-3.28814000	-0.58997500	1.12402200
H	-3.39946200	-1.67694800	1.07900100
H	-3.87531700	-0.24151500	1.97917900
C	-1.27889700	-0.96358400	2.61957300
H	-0.23916200	-0.68763900	2.81192800
H	-1.86851900	-0.67495500	3.49546600

H	-1.33436100	-2.04964400	2.50337400
C	-1.65153800	1.28882200	1.60651400
H	-2.24690500	1.54603000	2.48919800
H	-0.60877300	1.54023900	1.80484600
H	-2.02074200	1.88989300	0.77730800
N	-1.04498600	-0.78423300	0.20411500
H	3.35262200	1.72727800	-0.75925800
C	-0.47212100	-0.42798900	-2.01435000
H	-0.19622400	-1.91396800	0.28816100
C	-2.17008700	-2.22876800	-1.51229100
H	-1.35987700	-2.95147300	-1.39083500
H	-3.02568100	-2.54343000	-0.91297900
C	-2.82816800	0.21657100	-1.25782200
H	4.50399900	-1.47425800	-2.97273800
C	4.90343500	-0.71015000	-2.30672400
C	3.78355200	0.09257100	-1.69357200
H	5.46986600	-1.19064900	-1.50192400
H	5.58891600	-0.04981800	-2.84277700
O	4.16185100	1.16526900	-1.07767000
O	2.60311000	-0.29510100	-1.80190600
Pd	0.83310600	-0.10587200	-0.45274400
O	1.43675900	1.74857800	2.33138500
C	2.31136900	0.90800600	2.10615400
O	2.29628600	0.02319400	1.15066600
C	3.56550200	0.83823800	2.97625500
H	3.50238900	1.56379900	3.78816200
H	3.68673500	-0.16913000	3.38671200
H	4.44701600	1.04944800	2.36222600
H	-0.02310500	-1.23451500	-2.59262000
C	0.42011800	4.12756200	-0.19599100
H	1.03959600	4.95752500	-0.53869700
H	0.30444000	4.19601900	0.89074900
H	-0.56833000	4.16103700	-0.65605000
C	3.03423000	-2.96882000	0.53017700
H	3.41265600	-1.98394600	0.82360200
H	3.21199900	-3.10175900	-0.53967500
H	3.52757900	-3.75154800	1.10663600
C	1.56234500	-2.97539000	0.82757600
O	1.02033900	-3.55302900	1.73963200
O	0.81350600	-2.25764900	-0.07528100
C	1.12697100	2.81577100	-0.47325500
O	0.29702100	1.83008200	-0.66195000
O	2.36183700	2.77588100	-0.49265700
H	-0.53258700	0.51851200	-2.54587100
H	-2.48242200	-2.23936000	-2.56282300
H	-3.31496100	0.14333300	-2.23551800
H	-2.41822300	1.22398800	-1.16577500
C	-3.88747600	0.01452900	-0.15986100
O	-4.93927600	-0.86640000	-0.58421600
O	-4.50164300	1.28609800	0.06985800
C	-5.91203600	1.08900300	0.11173200
H	-6.39834400	2.01643400	-0.20077400
C	-6.09528100	-0.07684000	-0.85236900
H	-6.98197900	-0.68681600	-0.66145900
H	-6.25085100	0.82524100	1.12431300
H	-6.11089500	0.26857000	-1.89651100

C-INT-4
NImag=0

0 1 (charge, spin multiplicity)

C	1.36649200	0.74963800	-1.07442400
C	1.18504100	0.14845100	1.50427000
C	2.70766600	0.38764400	1.41687300
H	2.90525400	1.46381900	1.40581500
H	3.18411500	-0.01763600	2.31483500
C	0.58225700	0.92591700	2.68598300
H	-0.50272600	0.79298500	2.69881500
H	0.99621100	0.54179900	3.62312700
H	0.80555900	1.99527800	2.62350700
C	0.85693900	-1.34366600	1.67675900
H	1.30276400	-1.67736800	2.61904400
H	-0.22106500	-1.49672800	1.73078000
H	1.25793200	-1.97525200	0.88583300
N	0.58913700	0.76008300	0.24648200
C	0.22731100	0.39986600	-2.04721100
H	0.27066400	1.73652900	0.44809800
C	1.96178600	2.13351700	-1.36818900
H	1.19809600	2.91124400	-1.29056700
H	2.78762400	2.38104700	-0.69795800
C	2.43556800	-0.34811400	-1.02450100
Pd	-1.16349300	0.01845900	-0.57181400
O	-3.14680900	-2.19054500	1.00440500
C	-3.08340100	-1.10139800	1.58095600
O	-2.31851300	-0.09780500	1.26059100
C	-3.96454400	-0.81779400	2.79901400
H	-4.45424600	-1.73475800	3.13087200
H	-3.37269000	-0.38998600	3.61328000
H	-4.72673400	-0.07907200	2.52907700
H	-0.16116300	1.23278700	-2.63061800
C	-2.45845100	-3.52539100	-1.72192800
H	-3.08880100	-3.48983000	-2.61259700
H	-3.06470900	-3.81529600	-0.85835800
H	-1.64302500	-4.24040600	-1.84810900
C	-2.77274200	4.01109900	-0.32187100
H	-3.57397300	3.78925000	0.39053000
H	-3.20608900	4.00455200	-1.32382900
H	-2.34624500	4.98758500	-0.08881700
C	-1.70299300	2.94126700	-0.18459900
O	-0.67500400	3.14446500	0.47634100
O	-2.00533200	1.84842500	-0.82368900
C	-1.92410600	-2.17058800	-1.41139600
O	-0.79462200	-2.02334600	-0.80845300
O	-2.55252200	-1.10404300	-1.71455800
H	0.35805700	-0.51267700	-2.62568500
H	2.35521300	2.13375000	-2.39029200
H	3.02925400	-0.31121200	-1.94308500
H	1.95111600	-1.32625300	-0.99027300
C	3.38638300	-0.23534500	0.18235100
O	4.53378700	0.57188200	-0.11086600
O	3.87953200	-1.55380700	0.44208400
C	5.29663700	-1.47650100	0.57759900
H	5.72510600	-2.43166700	0.26393300
C	5.63809000	-0.30230800	-0.33229800
H	6.55540500	0.22734800	-0.06371900
H	5.58876200	-1.27232500	1.61791400
H	5.69529700	-0.61679400	-1.38463700

C-INT-4-a

NImag=0

0 1 (charge, spin multiplicity)

C	-1.58216900	-0.64436300	-1.15461700
C	-1.81469500	-0.79119600	1.40538500
C	-3.27062100	-1.13869000	0.99677300
H	-3.30471800	-2.17147600	0.63954500
H	-3.90963600	-1.08234900	1.88373700
C	-1.30522100	-1.85291700	2.40182000
H	-0.27470900	-1.62922000	2.68845000
H	-1.92364600	-1.86232600	3.30672600
H	-1.32986800	-2.84694500	1.94710900
C	-1.77986700	0.58078500	2.11521600
H	-2.41165200	0.51135900	3.00760000
H	-0.76462700	0.82534500	2.42498600
H	-2.16269300	1.39396500	1.50085400
N	-0.99337200	-0.98181400	0.17517100
H	1.83220900	2.14300000	-2.14789100
C	-0.36620800	0.03872700	-1.78978900
H	3.56202700	-1.03825600	1.21191200
H	-0.47705900	1.08169400	-2.07188900
C	-1.91456800	-1.94399700	-1.91515800
H	-1.05375900	-2.61390400	-1.87289400
H	-2.78970700	-2.45111800	-1.50398400
C	-2.79245100	0.29783300	-1.05612500
H	4.80560200	0.55822600	-3.17187000
C	4.71437700	0.62194700	-2.08637800
C	3.32412500	1.04031100	-1.68788900
H	4.95232900	-0.32977000	-1.60941500
H	5.42422800	1.37490000	-1.72664000
O	2.66561600	1.72852000	-2.58304600
O	2.87126100	0.75505400	-0.56844800
Pd	0.78672700	-0.00163900	-0.09370000
O	3.79100400	-0.51203300	2.06417300
C	2.73203700	0.02726000	2.59910900
O	1.59534900	-0.00196400	2.10718500
C	2.99805600	0.73179600	3.90811500
H	3.65044500	0.12643500	4.54153400
H	3.51907700	1.67291100	3.70163200
H	2.05864900	0.94850000	4.41593200
H	0.19292600	-0.56250000	-2.50301800
C	-0.17975500	4.21277500	0.34680800
H	-0.44432800	4.95524400	-0.40757200
H	0.64806600	4.60878100	0.94512000
H	-1.01970800	4.02125800	1.01634300
C	2.61738800	-3.79248200	-1.32699300
H	1.96027300	-4.52218500	-0.84305400
H	3.64569000	-4.15350100	-1.28668000
H	2.28742400	-3.68926200	-2.36350600
C	2.50335100	-2.46207100	-0.59157300
O	3.44266300	-2.09281400	0.13488100
O	1.38440000	-1.86093800	-0.81280800
C	0.28651200	2.93397700	-0.33231100
O	0.11578900	1.87777900	0.38771300
O	0.78030400	3.00249800	-1.47545900
H	-3.24356400	0.45661000	-2.04151100
H	-2.46223400	1.26970900	-0.68191200
C	-3.86845400	-0.23914100	-0.09732200
O	-4.56055600	0.89507400	0.44381600

O	-4.86097400	-1.01975300	-0.78160800
C	-5.95888000	0.64729800	0.34071300
C	-6.03402500	-0.22332800	-0.90817200
H	-6.90102600	-0.88813900	-0.94549900
H	-6.47481500	1.60731500	0.25523100
H	-6.00791900	0.38956900	-1.82149500
H	-6.33826500	0.10979200	1.22248600
H	-2.13331600	-1.70407500	-2.96324700

C-TS-4-a

Nimag=1

0 1 (charge, spin multiplicity)

C	-2.03315000	-0.19829600	-1.24091800
C	-1.79170600	0.22997700	1.27538100
C	-3.18784500	-0.44464200	1.32106200
H	-3.04926300	-1.52788700	1.25745000
H	-3.66022500	-0.22681700	2.28414200
C	-0.92741100	-0.35652000	2.40621400
H	0.07494300	0.07819000	2.41198900
H	-1.39761100	-0.14782700	3.37384200
H	-0.82412700	-1.43825400	2.29029100
C	-1.89551800	1.75632300	1.48288600
H	-2.38525300	1.94006600	2.44469700
H	-0.90017100	2.19548700	1.51029500
H	-2.48980400	2.26685100	0.72358500
N	-1.20679700	-0.29559300	-0.00540800
H	2.35020000	1.73695200	-2.23849200
C	-0.96884100	0.69417100	-1.73280400
H	2.71528800	-1.88692800	1.68499100
H	-1.03958600	1.75451800	-1.53107600
C	-2.16239800	-1.54152300	-1.96141800
H	-1.19083500	-2.02809400	-2.03784600
H	-2.85749500	-2.19271600	-1.42456300
C	-3.40212000	0.47709600	-1.04565000
H	4.74126400	-0.92940900	-3.05253300
C	4.86802200	-0.35768100	-2.12764200
C	3.55427600	0.28361100	-1.76778500
H	5.19583000	-1.01880500	-1.32664100
H	5.61717500	0.41457200	-2.32156700
O	3.10297300	1.13930600	-2.63741900
O	2.98129100	-0.01902000	-0.70403100
Pd	0.85077200	0.03953900	-0.38565500
O	3.53272200	-1.64706000	2.19434100
C	3.42411800	-0.40879200	2.67600100
O	2.45779100	0.31547000	2.50880600
C	4.65323000	-0.00299500	3.46139600
H	4.83492600	-0.71831100	4.26899300
H	5.53225400	-0.02092900	2.80953400
H	4.51645000	0.99736800	3.87113000
H	-0.31232000	0.38479700	-2.54194400
C	1.24302200	4.29456000	0.22139400
H	1.49743200	5.07202900	-0.49905400
H	1.96816500	4.29304200	1.04052100
H	0.26084200	4.49343300	0.65968800
C	1.11169500	-4.16463800	-1.03837500
H	0.07636600	-4.51977600	-0.98946700
H	1.74399200	-4.86633100	-0.49243100
H	1.40293300	-4.12150000	-2.08988500
C	1.18864400	-2.79212200	-0.38708000

O	1.47735000	-2.67080400	0.80796900
O	0.89104700	-1.81725000	-1.19801700
C	1.24912100	2.93313800	-0.45053200
O	0.90882100	1.96243000	0.31884700
O	1.56147100	2.84051600	-1.66050900
H	-4.02146400	0.29751100	-1.92928000
H	-3.29219100	1.55769200	-0.94759500
C	-4.15036700	-0.02979900	0.19811900
O	-5.04215900	1.01936400	0.60080200
O	-4.97539100	-1.16489300	-0.09400100
C	-6.33697400	0.45345000	0.78425000
C	-6.32000600	-0.70799200	-0.20297600
H	-6.98671900	-1.53399300	0.05708600
H	-7.08432800	1.22080000	0.56562000
H	-6.54793600	-0.36617400	-1.22368400
H	-6.47515800	0.09679200	1.81534100
H	-2.56359200	-1.37439600	-2.96856800

C-TS-3

NImag=1

O 1 (charge, spin multiplicity)

C	0.78994000	-0.33843400	1.25526700
C	1.45304100	-1.39837100	-1.00383900
C	2.78102700	-1.67734000	-0.23233800
H	2.65623100	-2.52025300	0.45242200
H	3.56211600	-1.95976500	-0.94369900
C	0.66205300	-2.69944400	-1.19211400
H	-0.23151400	-2.51766300	-1.79367000
H	1.29168400	-3.42504500	-1.71859000
H	0.35508000	-3.14412200	-0.24436900
C	1.73371700	-0.78764000	-2.38895400
H	2.26580100	-1.51475400	-3.00970200
H	0.79112800	-0.54315100	-2.88882000
H	2.34296900	0.11484200	-2.31110800
N	0.66625100	-0.36242700	-0.24374600
H	1.02924800	0.56817600	-0.53482400
C	-0.06379600	0.81849900	1.72136900
H	0.06046900	1.76834800	1.21514300
C	0.38175000	-1.63406000	1.97944900
H	-0.60620600	-1.96984500	1.66969600
H	1.10594900	-2.43318900	1.81803500
H	-5.07627400	2.23696900	1.36560500
C	-4.50526200	1.65228600	2.08859400
C	-3.18970400	1.20075300	1.47210100
H	-4.32324600	2.22751200	2.99669900
H	-5.08798300	0.76177200	2.34546000
O	-3.22287600	0.93758700	0.22775100
O	-2.19234500	1.10249700	2.24180400
Pd	-1.39378600	0.17910500	-0.35370500
H	-0.20472100	0.87092700	2.79174600
C	-0.06712400	3.97210900	-2.07211900
H	-0.91656900	4.56111700	-1.71652900
H	-0.25353100	3.73676400	-3.12466800
H	0.85680600	4.54463600	-1.98337600
C	-3.49298100	-3.44479100	-0.33258400
H	-3.84250700	-3.95005000	-1.23366000
H	-4.35332500	-3.17072600	0.28634400
H	-2.86555600	-4.11759600	0.25889000
C	-2.72401300	-2.19020800	-0.71159200

O	-2.69372200	-1.75200600	-1.86247000
O	-2.10644700	-1.62434500	0.29802600
C	0.04354800	2.67791200	-1.28080800
O	-1.06014800	2.00782200	-1.22499500
O	1.12346300	2.34015000	-0.75933600
H	0.36482400	-1.42837900	3.05451000
C	3.30280600	-0.49335000	0.58594500
C	2.26964400	0.03856400	1.63183000
H	2.40082900	1.12402400	1.68293900
H	2.51307500	-0.38416600	2.60855800
O	4.47909400	-0.86692100	1.31272200
O	3.69769900	0.52904600	-0.31596300
C	5.57531200	-0.07862000	0.84252400
C	4.87918200	1.12479900	0.21258600
H	6.16108300	-0.63716400	0.09996900
H	6.21675900	0.17258700	1.69182700
H	5.42651500	1.58654400	-0.61160300
H	4.63869200	1.89320000	0.96121600

C-TS-3-a

NImag=1

O 1 (charge, spin multiplicity)

C	1.46880200	0.42282600	-1.28234800
C	1.19379900	0.61057500	1.30680500
C	2.72064100	0.84199800	1.21167000
H	2.90867500	1.87045200	0.89008000
H	3.15881000	0.73077500	2.20828200
C	0.54413900	1.68755400	2.19277600
H	-0.53677300	1.53041300	2.23671600
H	0.94668100	1.63005000	3.20932100
H	0.73223600	2.69183900	1.80186300
C	0.88592400	-0.77746700	1.91181400
H	1.26944600	-0.79286000	2.93705300
H	-0.18940200	-0.95751300	1.94529700
H	1.35910600	-1.59992500	1.37632000
N	0.65131200	0.81541700	-0.07404000
C	0.35686700	-0.20763400	-2.13987700
H	-0.22944700	1.85940200	-0.43023400
C	2.05374200	1.67428700	-1.96343100
H	1.26875300	2.40917800	-2.16016100
H	2.84015500	2.14107200	-1.36715000
C	2.55979900	-0.58863400	-0.90787100
Pd	-1.06830300	-0.16314100	-0.64942700
O	-2.93835400	-1.88229300	1.55476200
C	-3.02394500	-0.66279300	1.71200400
O	-2.36941000	0.24601200	1.04198400
C	-3.97312800	-0.07710100	2.75765900
H	-4.31338000	-0.86131600	3.43574300
H	-3.48850700	0.72646000	3.31860800
H	-4.84406000	0.35704500	2.25379900
H	-0.03116400	0.41996100	-2.94173800
C	-2.43817900	-3.87277500	-0.85404500
H	-3.13452400	-4.08334400	-1.66763200
H	-2.96258000	-3.93789000	0.10437300
H	-1.60927300	-4.58350100	-0.85578200
C	-3.55332400	2.53635400	-0.83553300
H	-3.86465500	1.63088400	-0.30667100
H	-3.61610200	2.34360900	-1.90985900
H	-4.19574700	3.37191900	-0.55770700

C	-2.13835400	2.83239600	-0.42915400
O	-1.76339000	3.74132300	0.26950900
O	-1.21615400	1.96440000	-0.97833900
C	-1.93614500	-2.47190800	-0.95466700
O	-0.78147300	-2.17315400	-0.44152100
O	-2.58471600	-1.53548200	-1.49810400
H	0.50852600	-1.24437600	-2.43172500
H	2.49556900	1.38084800	-2.92228000
H	3.18896000	-0.79506800	-1.77958800
H	2.09561800	-1.53107400	-0.60972000
C	3.45795800	-0.10470500	0.24582900
O	4.60884900	0.60557500	-0.23258200
O	3.95529700	-1.27415500	0.90491400
C	5.36092800	-1.11645600	1.07964300
H	5.81979800	-2.10823000	1.09136900
C	5.73482900	-0.26202400	-0.12582800
H	6.62959100	0.34997400	0.01287700
H	5.59212600	-0.59875600	2.02198700
H	5.85301700	-0.87823800	-1.02918600

C-product

NImag=0

0 1 (charge, spin multiplicity)

C	0.19493300	-1.23502700	-0.68787200
C	-2.09650200	-1.27831700	0.49089300
C	-1.70107300	0.13412700	0.95613900
H	-2.58706300	0.66932400	1.30903700
H	-1.01306000	0.03623700	1.80131300
C	-3.20573800	-1.23185900	-0.58720000
H	-3.43884300	-2.24690500	-0.93068400
H	-4.12736400	-0.80191800	-0.18007100
H	-2.92484400	-0.63459900	-1.45659900
C	-2.62853400	-2.07157300	1.69964100
H	-3.53114500	-1.60855400	2.11363400
H	-2.88452100	-3.09577200	1.40495800
H	-1.86774200	-2.12854800	2.48255800
N	-0.87115900	-1.96848200	0.03098500
C	1.36360900	-1.10867300	0.31305500
C	0.65234400	-2.07073600	-1.89343000
H	0.94520000	-3.07658600	-1.57046300
H	-0.15558000	-2.16471900	-2.62667900
C	-0.27142200	0.15159700	-1.17443800
H	4.17464700	1.55352600	-0.73436700
C	4.57858400	0.61707700	-0.33784700
C	3.51332000	-0.10415200	0.45503000
H	4.89441200	0.00983600	-1.19082200
H	5.43058500	0.82750300	0.30767000
O	2.47615800	-0.45251300	-0.34002000
O	3.56289900	-0.34340200	1.64127100
H	-0.95960300	0.01790400	-2.01257200
H	0.58481300	0.72460100	-1.53910700
C	-0.99824600	0.99483500	-0.11420000
O	-0.05432600	1.87755400	0.50499200
O	-1.96867900	1.84279100	-0.75849500
C	-0.68273400	3.14773600	0.64181700
C	-1.56486500	3.20056700	-0.60124300
H	-1.28083400	3.20388400	1.56330100
H	0.09417100	3.91573000	0.67286000
H	-2.45695900	3.82301600	-0.48530100

H	-0.99805300	3.54676800	-1.47764700
H	1.51452600	-1.61162100	-2.38281900
H	1.67252500	-2.10379700	0.64593300
H	1.08318600	-0.53066600	1.19468200
H	-1.12081700	-2.81433300	-0.46975200

C-INT-5-a

NImag=0

0 1 (charge, spin multiplicity)

C	-1.07513500	0.20134000	1.33738100
C	-1.56799100	1.41031900	-0.88460800
C	-3.00465400	1.33672300	-0.30788600
H	-3.11586200	2.09871300	0.46829300
H	-3.71852700	1.58173500	-1.10078300
C	-1.26383500	2.86970100	-1.28528200
H	-0.24840300	2.94188700	-1.68291100
H	-1.96571500	3.21192300	-2.05452300
H	-1.34537900	3.53069100	-0.41766500
C	-1.45922200	0.54140500	-2.15547900
H	-2.15704400	0.93914000	-2.89999200
H	-0.45196000	0.59385800	-2.57433800
H	-1.70582400	-0.50373400	-1.98361300
N	-0.62945100	1.10882300	0.23951400
H	2.46560000	-2.53536900	0.77571900
C	0.24968900	-0.52975200	1.57053500
H	0.24219800	-1.61485800	1.51676200
C	-1.45523200	1.02201100	2.58549100
H	-0.68250500	1.76925400	2.78152300
H	-2.41854700	1.52426200	2.47495800
C	-2.19631700	-0.75785900	0.90588800
H	5.46082600	-0.92046400	2.00874000
C	5.35576800	-1.04155300	0.92639300
C	3.90572800	-1.27391000	0.58929800
H	5.72496400	-0.15550700	0.41212700
H	5.94365100	-1.91817500	0.63894500
O	3.36586200	-2.29175200	1.20663500
O	3.30645700	-0.54546800	-0.21567700
Pd	1.15646000	0.17078800	-0.12939200
H	0.87699600	-0.12174100	2.36277300
C	0.03029700	-3.62057500	-1.95146900
H	0.31696300	-4.64955700	-1.73439600
H	0.35220700	-3.34329000	-2.95894000
H	-1.05913200	-3.52294600	-1.91965100
C	3.04678000	3.79206900	-0.11276400
H	2.29254800	4.54843500	0.12938400
H	3.56243000	4.08661800	-1.02777400
H	3.74795000	3.74002800	0.72328600
C	2.35901500	2.46258200	-0.31547300
O	2.09562400	2.01054600	-1.44882500
O	2.02275700	1.81442700	0.75911500
C	0.65836800	-2.67829500	-0.93752600
O	0.40539300	-1.43426800	-1.17033300
O	1.31825600	-3.14578200	0.01114600
H	-2.54042900	-1.36384600	1.75088900
H	-1.80952900	-1.43565800	0.14239300
C	-3.40092500	-0.01608300	0.30507000
O	-4.00532400	-0.89564300	-0.65313200
O	-4.41332400	0.25600000	1.28803200
C	-5.41141300	-0.88616100	-0.42993300

C	-5.48987200	-0.65094700	1.07417000
H	-6.41537200	-0.17548200	1.40973100
H	-5.82019300	-1.84476400	-0.76001800
H	-5.34221400	-1.58841400	1.63073000
H	-5.90195500	-0.07313200	-0.98558000
H	-1.53065200	0.35183300	3.45085600

C-TS-5-a

NImag=1

O 1 (charge, spin multiplicity)

C	-1.36050600	-0.36924600	-1.17332000
C	-1.61292900	0.43647300	1.24494400
C	-3.01132800	-0.22152100	1.11974400
H	-2.89817200	-1.30157700	1.25044600
H	-3.65843800	0.14655400	1.92237100
C	-0.99980400	0.05781100	2.60602500
H	-0.03471500	0.55265800	2.74341900
H	-1.66435900	0.37900100	3.41564000
H	-0.83839900	-1.01959200	2.67667200
C	-1.71437300	1.97722200	1.17506600
H	-2.35762400	2.31559100	1.99414800
H	-0.72916700	2.42017400	1.30557900
H	-2.15831900	2.35311500	0.25300900
N	-0.81455800	-0.29940700	0.21040200
H	3.15196000	1.42773900	-1.45590600
C	-0.18003500	0.43004600	-1.55811000
H	-0.24135700	1.50986400	-1.51980900
C	-1.39487500	-1.80194600	-1.71034900
H	-0.45350300	-2.30979200	-1.50503200
H	-2.21860200	-2.35579900	-1.25171700
C	-2.71948000	0.32970600	-1.35891900
H	5.60563800	-1.26487700	-1.62497800
C	5.54553300	-0.67286700	-0.70654900
C	4.20321400	0.00636100	-0.64794300
H	5.68095600	-1.31633900	0.16140000
H	6.33758900	0.07990000	-0.75171800
O	3.94686800	0.79413400	-1.65370900
O	3.43446000	-0.19958900	0.30877100
Pd	1.27832900	-0.08622900	0.20682300
H	0.60498500	0.00141300	-2.17630700
C	1.71965300	4.21010900	0.56425400
H	2.39605600	4.86596100	0.01538200
H	1.95026300	4.22417300	1.63163200
H	0.69450400	4.57709400	0.44242600
C	1.61382400	-4.27320000	0.35940000
H	0.65657300	-4.63493800	-0.03086500
H	1.87787100	-4.84622300	1.24906700
H	2.36379100	-4.42010800	-0.42229600
C	1.49031600	-2.80016700	0.72128200
O	1.46087100	-2.40047500	1.87974400
O	1.40472200	-2.02172200	-0.34040400
C	1.80815300	2.79437200	0.02187800
O	1.32564500	1.89043100	0.79972200
O	2.29217400	2.60016200	-1.11619000
H	-3.15982400	0.01134300	-2.30812200
H	-2.59992600	1.41227400	-1.41167100
C	-3.71442300	0.02081300	-0.22600300
O	-4.63043600	1.12389600	-0.17010200
O	-4.50602300	-1.14099700	-0.50565300

C	-5.95423800	0.59680800	-0.15309400
C	-5.78962800	-0.69951400	-0.93740600
H	-6.52069600	-1.47404000	-0.69237100
H	-6.62281400	1.32553100	-0.61892700
H	-5.80778200	-0.51375100	-2.02162100
H	-6.29287800	0.39903500	0.87439700
H	-1.56552900	-1.77628300	-2.79372400

C-product-a

Nlmag=1

0 1 (charge, spin multiplicity)

C	1.24694300	1.37269900	0.17196300
C	1.20685200	-1.19820800	-0.19623300
C	-0.16015700	-0.95326300	-0.89863200
H	0.00818500	-0.71981200	-1.95631400
H	-0.76211400	-1.86794700	-0.87456200
C	2.17394500	-1.80930000	-1.22783100
H	3.12329900	-2.06872000	-0.75095400
H	1.74910000	-2.71282900	-1.68042000
H	2.38414400	-1.09065900	-2.02619500
C	1.05240800	-2.17442300	0.98231900
H	0.76688000	-3.16579700	0.61462500
H	2.00201300	-2.27115300	1.51773600
H	0.28572400	-1.84086200	1.68469700
N	1.87314700	0.04657800	0.28209100
C	1.43557900	0.73128600	1.50510400
H	0.54290900	0.38840900	2.01958900
C	2.17899500	2.48512400	-0.27134700
H	3.17532200	2.33922700	0.15276300
H	2.27396900	2.50399300	-1.36351600
C	-0.17475600	1.49936200	-0.37180900
H	2.24372600	1.05783200	2.15907700
H	-0.12755600	1.80273700	-1.42418500
H	-0.72263300	2.28155900	0.16526800
C	-0.98718000	0.20461100	-0.34117700
O	-1.46328400	-0.04796900	0.98795100
O	-2.16037600	0.34922700	-1.15979200
C	-2.81478700	-0.48676100	0.88337800
C	-3.31074900	0.30425700	-0.32131900
H	-2.87082900	-1.57008700	0.70366600
H	-3.32649800	-0.25104500	1.81979400
H	-4.12419300	-0.18265800	-0.86683500
H	-3.62893800	1.31564600	-0.03022100
H	1.80217400	3.46374300	0.04957700