Supporting Information

Pt(II)-Chiral Diene-Catalyzed Enantioselective Formal [4+2] Cycloaddition Initiated by C-C Bond Cleavage and Elucidation of a Pt(II)/(IV) Cycle by DFT Calculations

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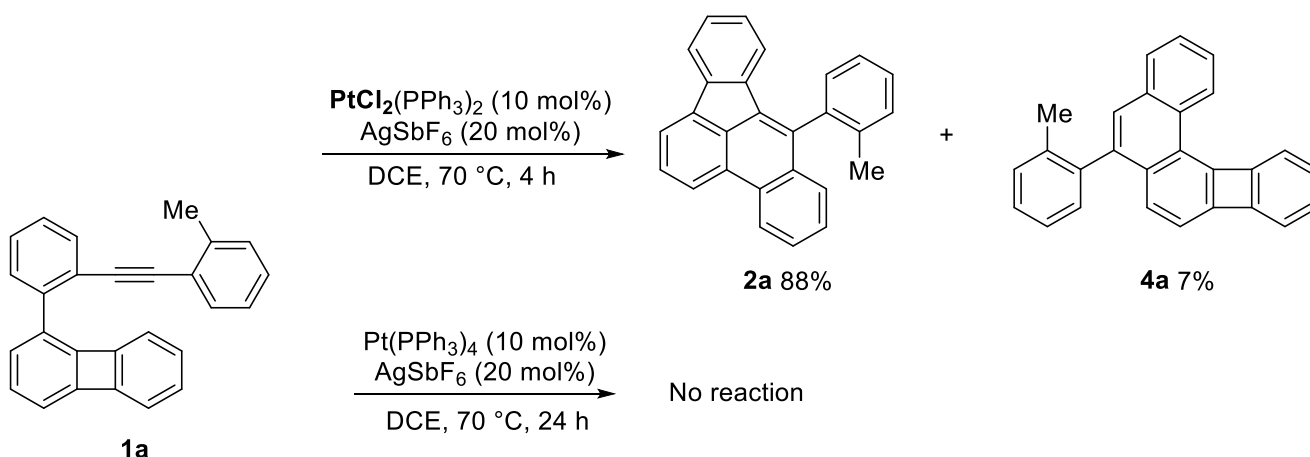
1) Experimental details

General information: Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded with JEOL ECX-500 (500 MHz) spectrometer. Chemical shift values for protons are reported in parts per million (δ) relative to internal standard TMS (0.00 ppm). ^{195}Pt NMR spectra were obtained by BRUKER AVANCE600 (129 MHz) spectrometers and referenced to the external standard K_2PtCl_6 dissolved in 1.5 mM HCl in D_2O (0.00 ppm). Data are presented as follows: chemical shift, multiplicity (m = multiplet), and area integration. High-resolution mass spectra (HRMS) were measured with a direct analysis in real time (DART)-orbitrap mass spectrometer[S1]. Optical rotations were measured with a JASCO DIP-1000 polarimeter. X-ray structures were obtained by a Rigaku R-AXIS RAPID diffractometer. Preparative thin-layer chromatography (PTLC) was performed with silica gel-precoated glass plates (Merck 60 GF254) prepared in our laboratory. All reagents expect for metal reagents were weighed and handled in air and backfilled under argon at room temperature. All reactions were performed under an argon atmosphere. Unless otherwise noted, organic compounds and solvents were purchased from Tokyo Kasei Co., Aldrich Inc., and other commercial suppliers and were used without further purification. The spectral data of compounds **1** and **2** were accorded in those in the literature.[S2]

General procedure for a Pt-catalyzed enantioselective reaction
[PtCl$_2$(R,R)-Ph-bod] (0.005 mmol, 10 mol%), AgSbF$_6$ (0.01 mmol, 20 mol%) and substrates **1** (0.05 mmol, 1.0 eq.) were placed in a Schlenk tube, which was then evacuated and backfilled with argon (×3). To the reaction vessel was added dehydrated DCE (1.0 mL, prepared by argon bubbling for 30 sec). The solution was then stirred at room temperature for 1-24 h. The solvent of the reaction mixture was evaporated to dryness. The obtained crude products were purified by PTLC to give products **2**.

The comparison of the reactivity between Pt(II) and Pt(0) species
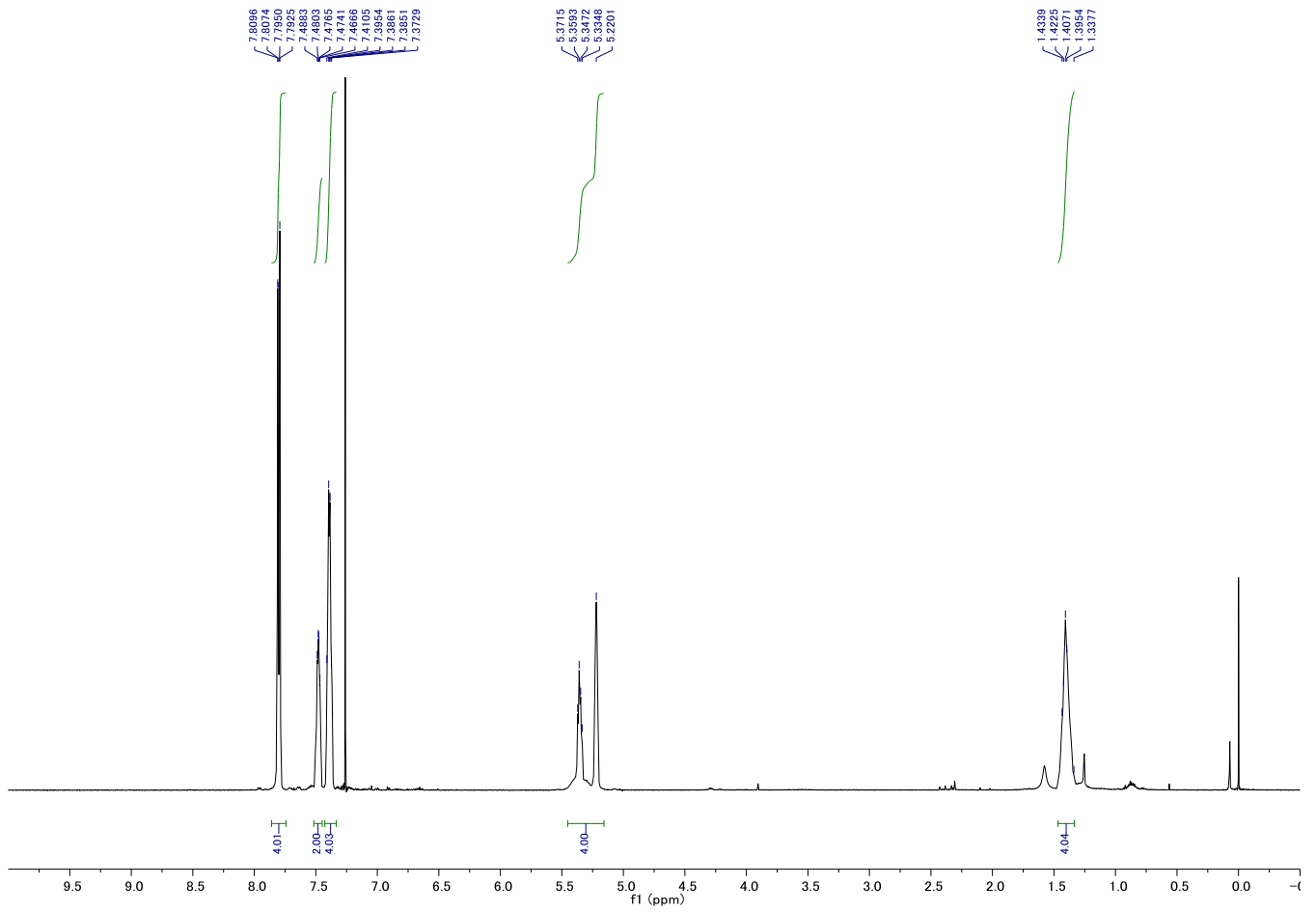In the presence of the dicationic Pt(II) catalyst bearing two phosphine ligands, the desired reaction proceeded in a high yield with a slight amount of cycloisomerized product **4a**. In contrast, tetrakis(triphenylphosphine)platinum(0) was inactive for [4+2] cycloaddition via C-C bond activation. These results supported that platinum-catalyzed reaction of **1a** to synthesize **2a** consist of the redox mechanism between Pt(II) and Pt(IV).
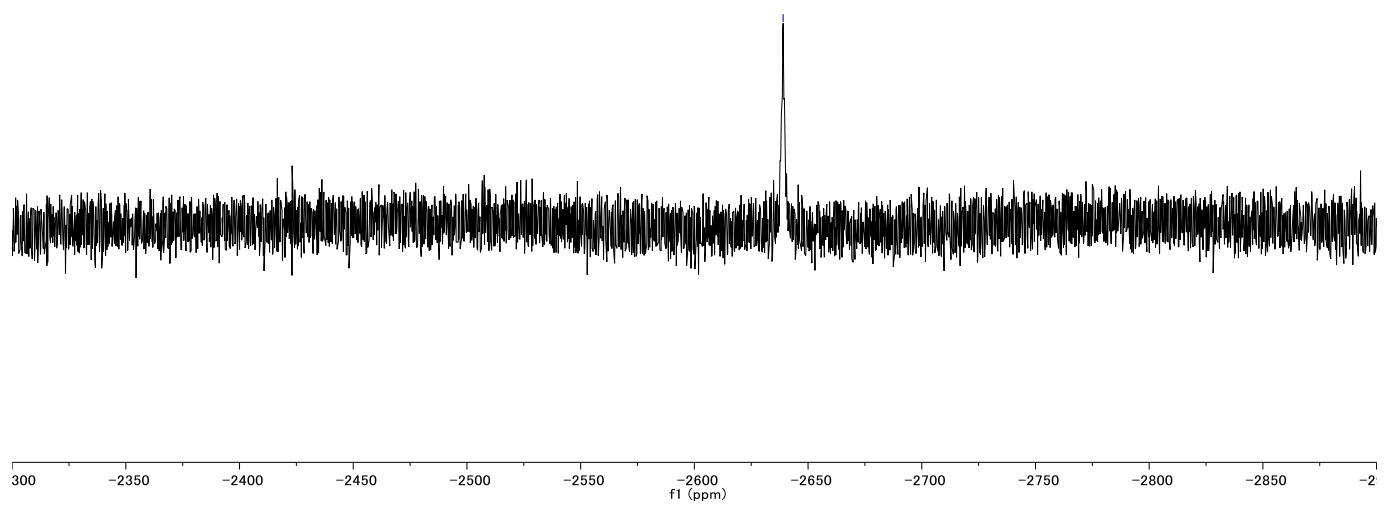

Scheme S1. The comparison of a Pt(II) catalyst and a Pt(0) catalyst

Synthesis of PtCl$_2$[(R,R)-Ph-bod]
To a round-bottom flask, [PtCl$_2$(C$_2$H$_4$)]$_2$ (1.0 eq.) and (R,R)-Ph-bod (2.1 eq.) were added. Dehydrated DCE (1.0 mL / 0.05 mmol) was added to the reaction vessel, then the reaction mixture was stirred at 80 °C for 24 h. The solution of reaction mixture was evaporated to dryness. The obtained crude products were purified by flash chromatography (silica gel) to give PtCl$_2$[(R,R)-Ph-bod] as a yellow solid. mp 252-253 °C (decomp.); ^{1}H NMR (CDCl$_3$) δ 7.81-7.79 (m, 4H), 7.49-7.47 (m, 2H), 7.41-7.37 (m, 4H), 5.37-5.22 (m, 4H), 1.43-1.34 (m, 4H); ^{195}Pt NMR (CDCl$_3$) δ -2639.03; HRMS (DART, positive): m/z calcd. for C$_{20}$H$_{22}$Cl$_2$NPt$^+$ [M + NH$_4$]$^+$ 541.07716, found 541.0778; [α]$^{21}_D$ = - 633 (c 0.45, CHCl$_3$, >99% ee). The crystal data of [PtCl$_2$(R,R)-Ph-bod]: C$_{20}$H$_{18}$Cl$_2$Pt, M = 524.36, monoclinic, space group P2$_1$ (#4), a = 10.4227(4) Å, b = 10.1502(4) Å, c = 16.9847(6) Å, β = 103.762(7) °, T =123 K. V =1745.27(12) Å^3, Z = 4, μ(CuKα) = 172.326 cm^{-1}; Number of Reflections Measured, Total 19584 and Unique 6275 (Rint =0.2229), $R1$ = 0.0979, $wR2$ = 0.2579, Flack parameter (Parsons' quotients = 2092) 0.04(2). CCDC 2048739.

7.8096
7.8074
7.7950
7.7925
7.4883
7.4803
7.4765
7.4741
7.4666
7.4105
7.3954
7.3861
7.3851
7.3729

5.3715
5.3593
5.3472
5.3348
5.2201

1.4339
1.4225
1.4071
1.3954
1.3377

4.01
2.00
4.03
4.00
4.04

−2639.0301

f1 (ppm)

f1 (ppm)

S3

2) Computational details

Reaction paths were explored by the SC-AFIR method[S3] implemented in the GRRM17 program[S4]. In the initial search, electronic structure calculations were carried out by the GFN2-xTB method[S5] in the Orca program[S6]. During the SC-AFIR search for [4+2] cycloaddition paths, $C(sp^2)$ atoms at the four-membered-ring of the biphenylene moiety, C(sp) atoms at the alkyne of the substrate, and the Pt of the catalyst were regarded as active atoms and chosen as the target atoms of the SC-AFIR method. In the SC-AFIR search for cycloisomerization paths, $C(sp^2)$ atom at the C8b-position of the biphenylene moiety, C(sp) atoms at the alkyne of the substrate, and the Pt of the catalyst were chosen as the target atoms. The collision energy parameter γ of the AFIR method was set as $\gamma = 200.0$ kJ/mol. All important paths were reoptimized by the locally updated planes (LUP) method[S7] using the GRRM17 and Gaussian16[S8] programs, at the ωB97X-D[S9]/Def2-SVPP[S10] level with consideration of solvation effects of 1,2-dichloroethane (DCE) for platinum catalyzed reaction or phenylchloride (PhCl) for rhodium catalyzed reaction modeled by the CPCM method[S11]. Vibrational frequencies of all obtained structures were calculated at the same level of theory to confirm whether these structures corresponded to local minima (having no imaginary frequency) or transition states (having only one imaginary frequency). The intrinsic reaction coordinate (IRC)[S12] was computed for determining the pathway from transition states to local minima. Single point energies were calculated at the level of ωB97X-D/Def2-TZVP[S10] with solvation effects of DCM or PhCl modeled by the SMD method[S13]. Natural bond orbital (NBO) version 3 analysis[S14] was conducted by the Gaussian16 program.

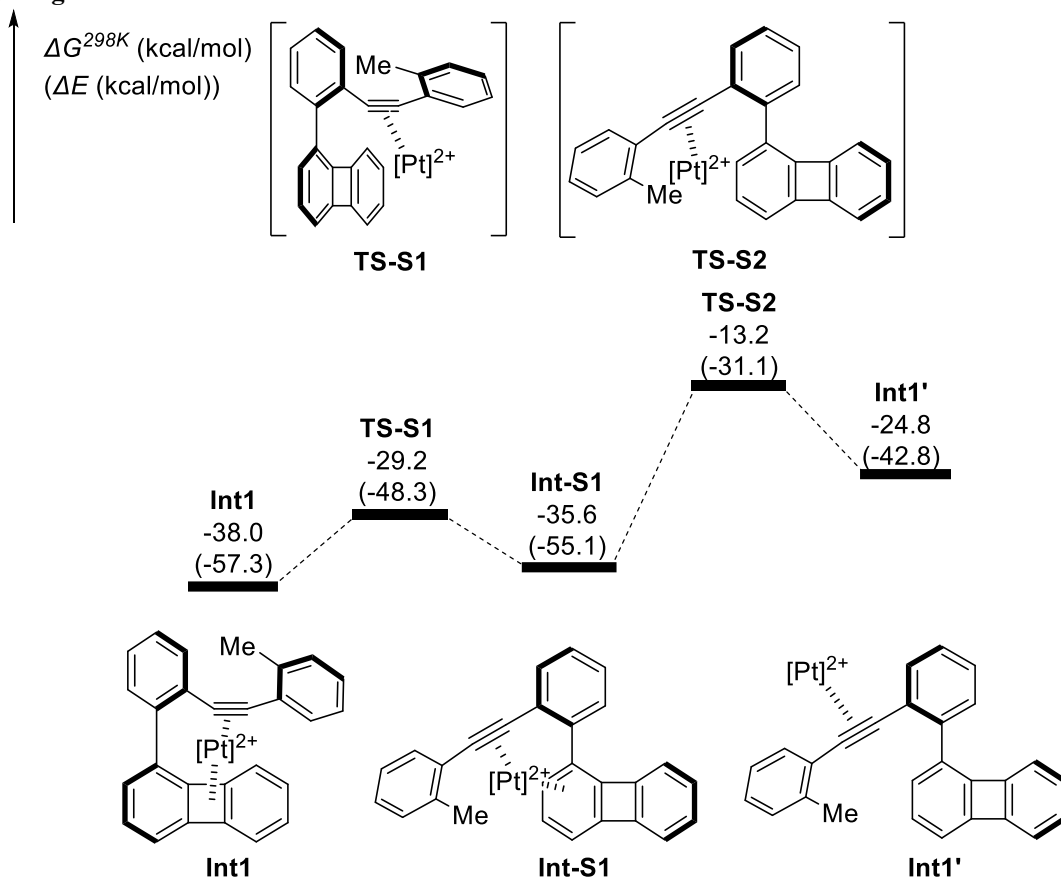**2-1) The energy diagram of isomerization between Int1 and Int1'.**

Figure S1. Free energy diagram of isomerization between Int1 and Int1" ([Pt] = Pt[(*R,R*)-Ph-bod])

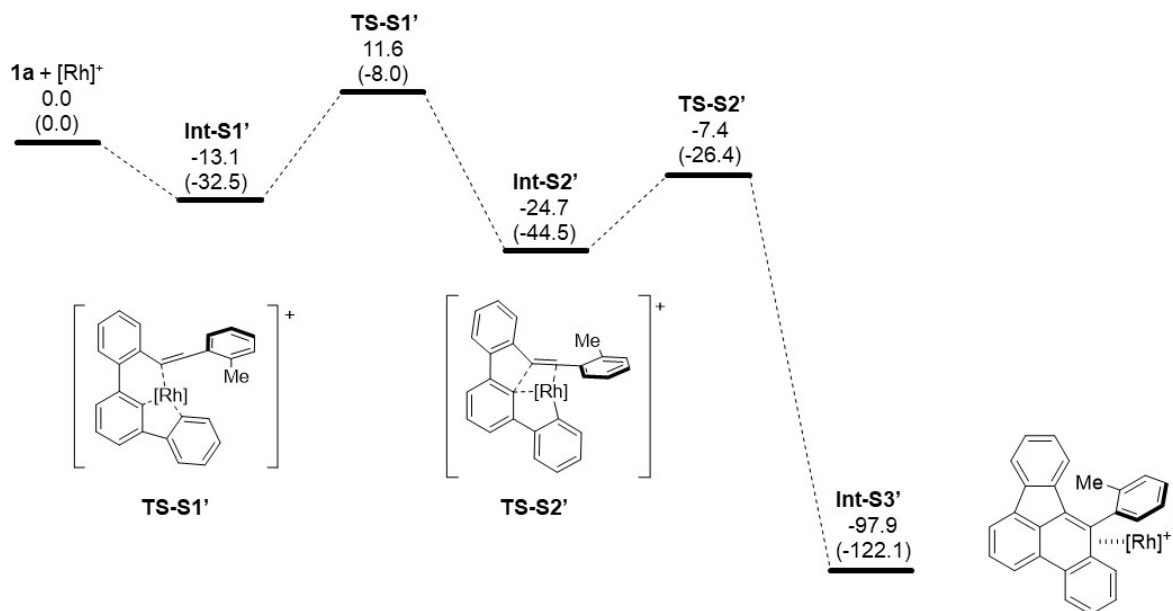**2-2) The energy diagram of [4+2] cycloaddition catalyzed by [Rh{(*R,R*)-Ph-bod}]$^+$**

Figure S2. Free energy diagram of [4+2] cycloaddition catalyzed by [Rh{(*R,R*)-Ph-bod}]$^+$ ([Rh] = Rh[(*R,R*)-Ph-bod])

2-3) Energy of each structure (in Hartree).

	Thermal correction to Gibbs Free Energy[*]	E[**]	G
[4+2] Cycloaddition catalyzed by [Pt{(R,R)-Ph-bod}]²⁺			
1a	0.308920331	-1039.633504	-1039.324583
[Pt{(R,R)-Ph-bod}]²⁺	0.281123348	-892.0272773	-891.7461539
Int1	0.62075532	-1931.752049	-1931.131294
TS1 (TS1_(R))	0.617020618	-1931.713251	-1931.09623
TS1_(S)	0.618777492	-1931.711597	-1931.092819
Int2	0.620921314	-1931.743916	-1931.122995
TS2	0.619083986	-1931.729142	-1931.110058
Int3	0.62193861	-1931.785959	-1931.164021
TS3	0.624550928	-1931.786642	-1931.162091
Int4	0.627096892	-1931.883671	-1931.256574
Cycloisomerization			
Int1'	0.618791602	-1931.729060	-1931.110268
TS1'	0.617342948	-1931.705814	-1931.088471
Int2'	0.621993810	-1931.741144	-1931.119150
TS2'	0.619080680	-1931.717773	-1931.098692
Int3'	0.626372296	-1931.755765	-1931.129392
TS3'	0.619367318	-1931.742653	-1931.123285
Int4'	0.625417455	-1931.787053	-1931.161635
Oxidative addition of 1-phenylbiphenylene			
1-Phenylbiphenylene	0.202483855	-693.101159	-692.8986751
Int1"	0.509089748	-1585.184429	-1584.6753392
TS1"	0.509112251	-1585.145340	-1584.636278
Int2"	0.508915161	-1585.177566	-1584.6686506
Isomerization between Int1 and Int1'			
TS-S1	0.620535428	-1931.737812	-1931.117277
Int-S1	0.621053738	-1931.748593	-1931.127540
TS-S2	0.618569079	-1931.710420	-1931.091851
[4+2] cycloaddition catalyzed by [Rh{(R,R)-Ph-bod}]⁺			
1a	0.308693539	-1039.635884	-1039.327191
[Rh{(R,R)-Ph-bod}]⁺	0.280978531	-883.4613647	-883.1803861
Int-S1'	0.620562606	-1923.149013	-1922.52845
TS-S1'	0.620880166	-1923.109939	-1922.489058
Int-S2'	0.621201607	-1923.168189	-1922.546988
TS-S2'	0.61993405	-1923.139297	-1922.519363
Int-S3'	0.628310049	-1923.291835	-1922.663525

[*]ωB97X-D/Def2-SVPP, CPCM = DCE (for Pt-catalyzed reaction) or PhCl (for Rh-catalyzed reaction)
[**]ωB97X-D/Def2-TZVP, SMD = DCE (for Pt-catalyzed reaction) or PhCl (for Rh-catalyzed reaction)

2-4) Cartesian coordinates of stationary points optimized at ωB97X-D/Def2-SVPP
2-4-1) [4+2] Cycloaddition catalyzed by [Pt{(R,R)-Ph-bod}]²⁺

1a (NIMGA = 0)

C	1.023672525568	0.221551730054	0.955213849681
C	0.172831554282	-0.552665435428	1.799421372350
C	0.414578347365	-1.891623142058	2.069382393887
C	1.526594018258	-2.585497901844	1.520761444333
C	2.349739601323	-1.836619278447	0.720233305883
C	2.103955591782	-0.465583543115	0.450530300094
C	3.577854703103	-1.785463193407	-0.156688825316
C	3.329256781541	-0.413658538763	-0.425639582285
C	4.647453070496	-2.456633705491	-0.693670640036
C	5.493943976203	-1.690092098206	-1.537788124915
C	5.250061772282	-0.347242113429	-1.800343643678
C	4.140082809591	0.337394303914	-1.239195216024
C	0.792228860467	1.657275670817	0.657211593809
C	1.861265296089	2.556052329385	0.764780113593
C	1.702668871657	3.910550521746	0.480255154259
C	0.457299661096	4.394576886020	0.076759093169
C	-0.616164815458	3.518830085821	-0.046328391160
C	-0.466150849858	2.149393582225	0.235224534453
C	-1.583931586779	1.271248989163	0.050330560556
C	-2.520532484276	0.514291000323	-0.108716697654
C	-3.596603477742	-0.419708420224	-0.262437676052
C	-4.856865918361	0.006088316084	-0.740687454602
C	-5.870169895895	-0.948355277453	-0.866661796712
C	-5.656359392137	-2.286564278260	-0.532707764299
C	-4.409645139339	-2.698973079931	-0.060913841257
C	-3.383902885673	-1.767989648555	0.072963882221
C	-5.090867039612	1.448872566338	-1.100473793570
H	-0.694213089085	-0.070361830497	2.257594716885
H	-0.273254815306	-2.427346041428	2.730010472245
H	1.694500431019	-3.642634849588	1.739012281830
H	4.854477145124	-3.511791881088	-0.499406330465
H	6.363822384864	-2.171206507026	-1.994456580377
H	5.933256065336	0.198577900414	-2.457586946876
H	3.962114626770	1.393929645645	-1.453893094401
H	2.835702255850	2.181230109248	1.091623760064
H	2.553378041964	4.590269237255	0.578825567161
H	0.322466147023	5.456312853692	-0.146372044420
H	-1.591718324271	3.886579531105	-0.374442439257
H	-6.851649799825	-0.635039884555	-1.235841132947
H	-6.469266800365	-3.010044053902	-0.642477835903
H	-4.235406624909	-3.745796407940	0.202385153602
H	-2.400812856671	-2.074629523317	0.441531376244
H	-4.922762842364	2.107169515472	-0.230120265883
H	-4.394226997136	1.778825294161	-1.890923521531
H	-6.120113348911	1.607522899685	-1.459069120636

[Pt{(R,R)-Ph-bod}]²⁺ (NIMGA = 0)

C	-1.409872307030	-0.771806574957	0.154025957005
C	-0.750228903069	-1.722030413849	-0.837718464998
C	0.527066256302	-0.933985721836	-1.072207580091
C	-0.558720980783	-0.560137811363	1.290186645391
C	1.383016736981	-0.830847816878	0.074840776786
C	0.699722289365	-1.413955181510	1.303526570693
C	-0.452830322840	-3.092143629097	-0.19544910241
C	0.367947031945	-2.905669396201	1.094064427185

C	-2.822220669591	-0.370234351616	0.085816726570
C	-3.702298699386	-1.030227691298	-0.788156248293
C	-5.048167146882	-0.678036494118	-0.830941816361
C	-5.528725928174	0.350064960494	-0.019862832903
C	-4.661529872399	1.021868202061	0.845667248025
C	-3.321039695059	0.661693239524	0.905401927651
C	2.804187371558	-0.453502469578	0.026247575949
C	3.453727287169	0.006411167180	1.185730335273
C	4.788700776712	0.392290240156	1.136759118454
C	5.496449960023	0.310110950574	-0.064309208037
C	4.864017557193	-0.153640373134	-1.219251482287
C	3.524121733672	-0.525306980197	-1.179191140563
H	-1.316151989643	-1.817297020405	-1.769388313215
H	0.887560427050	-0.774550505634	-2.092971991859
H	-0.931171170664	-0.125576221733	2.223510280620
H	1.275410177240	-1.257299646232	2.221159731814
H	0.091738963080	-3.699333224329	-0.934843907938
H	-1.407051328667	-3.603063092068	0.004290094569
H	1.311418315247	-3.471761053867	1.059453256655
H	-0.187020154199	-3.253162286194	1.979046909923
H	-3.350810205761	-1.842605841165	-1.427024791240
H	-5.724318287855	-1.210127505251	-1.504462328653
H	-6.584663161970	0.629975658920	-0.061067069637
H	-5.034411677643	1.829963697832	1.479512928140
H	-2.659019185081	1.202110412677	1.587495142960
H	2.909716768004	0.089175986578	2.129724843563
H	5.280553348400	0.759152536843	2.040878482314
H	6.547633881260	0.608176134229	-0.099957091674
H	5.418166249931	-0.227311532541	-2.158145332493
H	3.049124640018	-0.896748331559	-2.089795328545
Pt	0.023511600003	0.869280990928	-0.129943077449

Int1 (NIMGA = 0)

C	2.352724882250	2.100478448757	-1.039706140282
C	2.975391083020	3.186199179079	-0.351585375320
C	2.287102807656	4.307470006341	0.086097347443
C	0.894101410532	4.461345813614	-0.117722039510
C	0.291501929638	3.424453624650	-0.778911891253
C	1.001579303773	2.285927474764	-1.241434410987
C	-0.994548441112	2.856548170566	-1.294375125453
C	-0.297582342689	1.673614196070	-1.726615725981
C	-2.310699002270	3.077799860745	-1.572439099216
C	-2.966722408331	2.056251461552	-2.320079144128
C	-2.305739744708	0.936336159517	-2.793613966540
C	-0.922521984252	0.732945035642	-2.545308118215
C	3.151682798473	0.916043034233	-1.438106456157
C	4.479717914917	1.137978536877	-1.839577350256
C	5.340140968012	0.098747329856	-2.170348132476
C	4.888171517234	-1.218938553522	-2.114535355136
C	3.575223785233	-1.469121477016	-1.746505756521
C	2.693424042402	-0.422442649145	-1.408498005366
C	1.365964783634	-0.893883435664	-1.051892927647
C	0.506484765715	-1.801279632251	-1.082583596504
C	-0.360112919753	-2.939067518047	-1.112180883093
C	0.108242374432	-4.186786991077	-0.635834830082
C	-0.788939907097	-5.259984554947	-0.647035928997
C	-2.096143380538	-5.113275887096	-1.104476084896
C	-2.546559669998	-3.877907295380	-1.579490153451
C	-1.680191248008	-2.796689519202	-1.586486592643

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C	1.525807607815	-4.389289072860	-0.177066626506
H	4.040564524693	3.118640091735	-0.119042031078
H	2.838615007419	5.085647586464	0.619788214667
H	0.357889876508	5.341881989450	0.240655118386
H	-2.843205753164	3.983266111091	-1.275941764278
H	-4.028339264659	2.176199209592	-2.550588635041
H	-2.849607491404	0.204552250836	-3.394993454878
H	-0.388510809025	-0.096016013261	-3.013536961179
H	4.846526366642	2.163807415482	-1.911641609375
H	6.365232754925	0.321103514318	-2.476902944236
H	5.551231826355	-2.050216800138	-2.365361782075
H	3.211936029603	-2.497894671060	-1.710501986905
H	-0.451384553196	-6.234161888680	-0.282395999574
H	-2.772288372626	-5.972192933911	-1.091329269990
H	-3.571324414641	-3.760267322672	-1.939710206912
H	-2.021650716400	-1.822738823775	-1.943056228761
H	2.149109899750	-4.746999909573	-1.016260707245
H	1.577791678682	-5.148031097300	0.619266444456
H	1.982008129840	-3.459872232079	0.196336415849
C	-0.363537664472	-1.190527376336	1.828886585823
C	-1.783001787489	-0.914589917316	2.291128960116
C	-2.172635582584	0.323419893340	1.502766352174
C	0.568282514576	-0.168229514971	2.134466005020
C	-1.221415701814	1.337724567341	1.646575683151
C	-0.147529693821	1.055167175360	2.690250018554
C	-1.766678402322	-0.541085658826	3.797783392851
C	-0.823073819819	0.653115998816	4.027942859958
H	-2.441678048780	-1.766444263544	2.093161172537
H	0.517396019887	1.914988176086	2.818096268339
H	-2.796171200502	-0.312386100591	4.113024591871
H	-1.440634449793	-1.429478553043	4.360279919319
H	-1.368088069172	1.532035127516	4.404931589654
H	-0.036686203024	0.413935970754	4.760218865671
Pt	-0.289620728342	0.061514992981	0.067449491246
H	-1.400916226581	2.359600932119	1.303079986392
H	-0.060215874619	-2.219829344792	1.622927913903
C	2.028541597522	-0.338232250112	2.145079492462
C	2.598349179811	-1.621936342343	2.185223042048
C	2.871732095391	0.779278204357	2.048844571177
C	3.975392906493	-1.783768129262	2.088435657927
H	1.966114865478	-2.502896391294	2.313385320981
C	4.249518593783	0.614401135255	1.948057608607
H	2.452158407397	1.786742892141	2.009492178298
C	4.803046018474	-0.666032209007	1.956699032686
H	4.406386970300	-2.787451747672	2.119579251294
H	4.894852859071	1.491464514554	1.855822375891
H	5.885145545464	-0.794597344768	1.870976757592
C	-3.464631355663	0.465521876713	0.821967797174
C	-4.127263948975	1.702889018074	0.814421265277
C	-4.051003534066	-0.633594274885	0.173200978582
C	-5.355771564986	1.834983822942	0.172409958484
H	-3.696586705805	2.560505596680	1.336747636610
C	-5.263418463827	-0.490168900972	-0.491646531200
H	-3.541186032864	-1.600477447789	0.161505316180
C	-5.920081076460	0.743208411904	-0.488133522497
H	-5.872155016554	2.798009345980	0.184175661219
H	-5.701762648615	-1.346032903025	-1.010990521030
H	-6.879299468931	0.852177082928	-1.001193426019

TS1 (TS1_(*R*)) (NIMGA = 1, 265.26*i* cm⁻¹)

C	1.420105043969	1.715432585947	-1.945046681956
C	1.553600351048	3.079062261289	-2.337614831408
C	0.479134809794	3.915983811207	-2.598152530114
C	-0.842444486172	3.446336387334	-2.525914035442
C	-1.008301489564	2.159541847222	-2.063499109682
C	0.098049379393	1.367011996517	-1.689410527038
C	-2.073737003958	1.156509490411	-2.055911826349
C	-1.371406037031	0.018647756606	-1.611329223263
C	-3.348318409039	1.046405317683	-2.574657602573
C	-3.912519304210	-0.238054506818	-2.642575206350
C	-3.183866977757	-1.366674816858	-2.275830171411
C	-1.871036939858	-1.262143299902	-1.785483450725
C	2.628056678270	0.853936355506	-1.807310239725
C	3.828615722689	1.268755955769	-2.403928604334
C	5.002878069412	0.530987915798	-2.294843969906
C	5.010642774730	-0.668229395690	-1.587985290012
C	3.827516296084	-1.124681048224	-1.022639605290
C	2.640852515147	-0.386124094424	-1.130769056712
C	1.440625856905	-0.990697917893	-0.547473368653
C	1.082449947800	-2.169362262191	-0.256953577594
C	0.625174989970	-3.467907469193	-0.031080054801
C	0.221367546998	-4.280361267407	-1.134507647884
C	-0.272600658232	-5.553268061878	-0.845227722626
C	-0.357740146011	-6.016798460951	0.466057322916
C	0.071392652613	-5.230255563841	1.544739241686
C	0.571660571908	-3.968144827573	1.297604744082
C	0.380686926035	-3.845592252131	-2.563338768388
H	2.554392815807	3.506086647609	-2.411661241382
H	0.675793665321	4.947385694168	-2.900207320769
H	-1.688631673623	4.055844675246	-2.849443583751
H	-3.886735449196	1.918657184659	-2.951325356422
H	-4.931308040923	-0.357455895713	-3.019580004546
H	-3.638440183235	-2.357350226372	-2.353033502900
H	-1.334925067705	-2.160844681958	-1.484858817073
H	3.859907995398	2.186881003147	-2.990552682432
H	5.914853325381	0.900039665198	-2.770456328799
H	5.928300953990	-1.251933899101	-1.484021175494
H	3.814641701669	-2.068673323978	-0.472647042540
H	-0.589775328020	-6.200389355096	-1.667315147743
H	-0.754080988821	-7.018446144985	0.653784409328
H	0.016026900057	-5.613536257189	2.565629212780
H	0.924826252918	-3.342141609262	2.119061809819
H	-0.524644298973	-4.080223195860	-3.146175468626
H	0.604728827667	-2.773106532149	-2.664863432433
H	1.217844144929	-4.402418547773	-3.020426877977
C	-1.915285882385	0.911208455893	1.609536023601
C	-1.310022200641	0.146546045777	2.778672555119
C	0.103495953406	-0.185572858674	2.325357528282
C	-1.086611908139	1.956938491651	1.214675070187
C	0.916800569168	0.932985960644	2.077972838897
C	0.098952129636	2.213244137637	2.135213833389
C	-1.237656235148	1.121492305006	3.985432975444
C	-0.426642317338	2.369019162013	3.590166375356
C	-3.299657170953	0.700089439038	1.156215249702
C	-3.848446455442	-0.590723268247	1.112279326053
C	-5.165032120596	-0.779985565424	0.704237780056
C	-5.951807965637	0.317493145604	0.350760766349
C	-5.416189579466	1.605254635146	0.397122944690

C	-4.095315473031	1.797184938309	0.791453893815
C	2.383013671222	0.913520191903	1.980773018202
C	3.063385876695	1.940227894592	1.305257643737
C	4.444808212825	1.890392639790	1.153569931210
C	5.166544426617	0.820934232008	1.684027185936
C	4.503299431024	-0.197807758237	2.371367553336
C	3.121344953489	-0.155756784186	2.516498761607
H	-1.873915020457	-0.759285999960	3.025236406768
H	0.519803654782	-1.172628090310	2.532932607662
H	-1.405361268010	2.727198718157	0.508026723518
H	0.663907523213	3.095443793122	1.819144785833
H	-0.770278080405	0.584617163410	4.825439124207
H	-2.262662462533	1.383343143472	4.290553213711
H	0.433585311751	2.524303944418	4.259464146860
H	-1.042365936242	3.280819116984	3.628514922772
H	-3.233600388333	-1.457310084181	1.371121059890
H	-5.578686633442	-1.790581910046	0.659092763807
H	-6.988706545657	0.167870314408	0.037839077611
H	-6.031808704687	2.467187560024	0.127626438389
H	-3.689310695266	2.810608470248	0.840720700504
H	2.509275805846	2.768625138169	0.857139245391
H	4.958880215421	2.686100383002	0.609226092706
H	6.252202302375	0.780591866564	1.562231850339
H	5.067762163384	-1.030637382367	2.797977461264
H	2.619149777252	-0.951712687953	3.070490031627
Pt	-0.156728519416	0.171413217379	0.164895379766

TS1_(_S_) (NIMGA = 1, 278.16i cm^{-1})

C	2.124565711132	1.122612884209	-1.714861759796
C	2.831348975953	2.339508322291	-1.940589694549
C	2.216243200930	3.561837128782	-2.163646718775
C	0.817357346798	3.670083047135	-2.221810240335
C	0.103531539789	2.530721697395	-1.922385702827
C	0.755557239828	1.328868122505	-1.575118392472
C	-1.271356784239	2.055389026871	-2.083522219097
C	-1.138538403111	0.698532913759	-1.715360544847
C	-2.424189394486	2.523389010971	-2.680046026663
C	-3.464394930510	1.602440185680	-2.893178473116
C	-3.305401452633	0.252636853146	-2.592535627407
C	-2.110924015836	-0.235971203987	-2.034248504490
C	2.869064118307	-0.164038059336	-1.618448480499
C	4.180460941261	-0.230390663243	-2.116750956203
C	4.934999357409	-1.396799429031	-2.060887677015
C	4.391367493157	-2.555669678136	-1.511074375806
C	3.086182901141	-2.529116895686	-1.041470255324
C	2.321439442646	-1.353918029190	-1.092864872632
C	0.942295209596	-1.441876840634	-0.607114280965
C	0.122685111239	-2.399392564927	-0.466625143785
C	-0.815131194051	-3.430656682196	-0.427857746492
C	-1.096574613670	-4.145714242291	0.774755658892
C	-2.031195604362	-5.177056470418	0.707109855533
C	-2.656558514954	-5.510789737223	-0.494840338612
C	-2.362343102043	-4.827007700024	-1.681453306619
C	-1.450245040590	-3.790810310852	-1.649528796136
C	-0.445824360266	-3.789359545122	2.076602258088
H	3.921300433455	2.322189459755	-1.905298063683
H	2.839806799243	4.442538332732	-2.334222741790
H	0.323852690532	4.596650061569	-2.522036793816
H	-2.517143147187	3.562667608909	-3.002800760091

H	-4.405046384802	1.946234408020	-3.330730338592
H	-4.122594216000	-0.447459313838	-2.782383202802
H	-2.018322934443	-1.294753613757	-1.796684204536
H	4.633040655851	0.643512406611	-2.585321844050
H	5.953685789366	-1.396269805235	-2.456377426228
H	4.976076681398	-3.476913349950	-1.454978526838
H	2.643090851380	-3.429918057499	-0.609331847617
H	-2.272677109651	-5.739522614668	1.612571972763
H	-3.382521064703	-6.328283607099	-0.509391223972
H	-2.844077358215	-5.111249133684	-2.619198899756
H	-1.186810194176	-3.253798046508	-2.563736973816
H	0.597789650531	-3.466205696617	1.934814583791
H	-0.454690919602	-4.646465377580	2.766375942323
H	-1.003761180152	-2.970429912854	2.564505517527
C	0.161676807471	-0.207622881840	2.268496060669
C	-1.161810533957	0.347964267348	2.780963061248
C	-1.660481729059	1.202968129428	1.625311699573
C	1.144747093303	0.772705024751	2.018123868167
C	-0.684187989964	2.114208168658	1.223869957106
C	0.544543158672	2.166096172734	2.121597715919
C	-0.901134008716	1.278205425449	3.993790631088
C	0.095219571015	2.380125145567	3.592360073716
H	-1.858050160640	-0.456184198630	3.040472724283
H	1.227533357461	2.955263564495	1.796449340775
H	-1.860616138631	1.701030753664	4.329564190957
H	-0.508816973155	0.657804243789	4.814557727763
H	-0.358971948052	3.380612322543	3.659924947385
H	0.986444566791	2.379155481215	4.238638945445
Pt	-0.111987717347	0.216275505386	0.136581811175
H	-0.892731568465	2.937628395789	0.537333454402
H	0.426152057226	-1.244822295319	2.470762138830
C	2.579623221317	0.523048230044	1.847786737966
C	3.120837927641	-0.752178211482	2.095649131336
C	3.431724926911	1.538098209236	1.376904754248
C	4.465263184046	-1.007776663628	1.861281520215
H	2.489708974686	-1.558155460011	2.474961476186
C	4.777407406040	1.278970486020	1.142196156873
H	3.045683376824	2.535516694005	1.161321307820
C	5.295500406345	0.005248006070	1.376593685571
H	4.868573023005	-2.004868782521	2.052876455279
H	5.423177231690	2.075146934031	0.763819450496
H	6.351673419232	-0.199913238093	1.183313748519
C	-3.049565236066	1.153154754422	1.141532530253
C	-3.682118821938	2.312206190504	0.667588204666
C	-3.755575746551	-0.061413187963	1.142446075726
C	-4.998749512588	2.259006379731	0.218272138685
H	-3.153191038038	3.268340441016	0.671668171568
C	-5.065433400496	-0.113530034008	0.678469793245
H	-3.268883898903	-0.981601156253	1.476836891588
C	-5.691504065027	1.048160767735	0.222101796204
H	-5.486199171951	3.170268301400	-0.137274347079
H	-5.601017636482	-1.066167291073	0.672434943928
H	-6.724161267028	1.008344645918	-0.134832068303

Int2 (NIMGA = 0)
C	-1.218770030395	1.352524733263	-2.269715571209
C	-1.134022135118	1.768932625200	-3.610024178947
C	0.068161077708	1.704380327733	-4.312268593688
C	1.238975420778	1.284120617318	-3.682845149304

C	1.188250858740	0.857715830067	-2.353967165802
C	-0.054500057139	0.828938891579	-1.712937414414
C	2.314859726265	0.552300869525	-1.467034945151
C	1.940735108971	0.220060621565	-0.162704140775
C	3.679585085152	0.676550859064	-1.744428787581
C	4.614400919046	0.477489365732	-0.730125469142
C	4.204050218619	0.158037985125	0.566084834790
C	2.845570897419	0.025637232341	0.866256150745
C	-2.438807191492	1.594677648835	-1.458502778200
C	-3.717923627946	1.501069949390	-2.008844253318
C	-4.844336129128	1.828426461226	-1.257271195105
C	-4.714341149819	2.242526675198	0.067634065370
C	-3.454367649813	2.320399283938	0.648856533721
C	-2.315902188760	2.013008307393	-0.108139852622
C	-1.007725652543	2.135915366498	0.494732271437
C	0.054141127506	2.424579104628	1.058751287272
C	1.292952227535	2.813022647946	1.651606504856
C	2.278124056279	3.458287673618	0.869025019096
C	3.507260577872	3.726293115047	1.478352924388
C	3.753783351424	3.378399019631	2.804755798597
C	2.768117107106	2.748746932227	3.569941455508
C	1.539821026947	2.462515443931	2.992457301040
C	2.033223241895	3.870519049378	-0.556609710544
H	-2.017755734595	2.192238671238	-4.094269194103
H	0.101214025738	2.036318355310	-5.352665575040
H	2.191466111201	1.309678015770	-4.218053293598
H	4.011947158790	0.946852399757	-2.749992947547
H	5.679794355486	0.577238470818	-0.951764390793
H	4.943714333683	0.006841497961	1.356352029731
H	2.519362499401	-0.225965793221	1.879049808213
H	-3.836996328425	1.162093002331	-3.040821727371
H	-5.835965278932	1.747078165951	-1.709357596591
H	-5.599545764729	2.490865543007	0.656897618312
H	-3.340300218524	2.632383829154	1.688807099009
H	4.291741286289	4.215704767168	0.894036573698
H	4.728642364875	3.599487907627	3.247918962026
H	2.962722925882	2.477267574797	4.610172929353
H	0.759623932127	1.953356098234	3.563758407308
H	2.945909265861	3.742833102481	-1.159948297096
H	1.222543321154	3.295910770232	-1.029110570056
H	1.750576917827	4.937745705797	-0.599528204625
C	0.659630703262	-2.779298226470	0.086850676537
C	-0.207025875757	-3.619243348613	0.957585732876
C	-1.362895073244	-2.849527968543	1.534053592835
C	-0.099938381049	-1.893183979378	-0.764146577358
C	-2.126768917852	-2.191984576406	0.644452237110
C	-1.585206815512	-2.302213620467	-0.770882965332
C	-0.810631758651	-4.607993706147	-0.129045655321
C	-1.608327647076	-3.805604900144	-1.171415881671
C	2.076976772131	-2.983622801908	0.006294691842
C	2.792058298253	-3.449684594807	1.135404348103
C	4.169010714716	-3.600016646204	1.080642599586
C	4.850980360284	-3.324028991237	-0.107379247326
C	4.158926760241	-2.885882897316	-1.241033322602
C	2.787698965076	-2.702706366763	-1.185002353782
C	-3.389967541658	-1.501211479345	0.980181309586
C	-4.472463827050	-1.523142793875	0.089436692863
C	-5.707436650625	-0.994013720355	0.461358219092
C	-5.874289733598	-0.416219024391	1.719174439628

C	-4.792459894201	-0.352754764944	2.598809601443
C	-3.560507663462	-0.888261704690	2.231816311572
H	0.341626356685	-4.196637983960	1.707449145370
H	-1.590577880241	-2.935683771945	2.598980606606
H	0.324362667349	-1.739847389838	-1.764722189054
H	-2.144833339405	-1.690623742695	-1.491562224294
H	-1.449255628916	-5.306773465478	0.431780575414
H	0.001698111589	-5.193101290174	-0.586831242569
H	-2.653986841000	-4.144698018449	-1.221651516109
H	-1.174575753168	-3.916411944217	-2.177754123063
H	2.273312264727	-3.644379569832	2.075651015720
H	4.716681810199	-3.933168093202	1.964976032078
H	5.935682023525	-3.453255173888	-0.151724915616
H	4.697650131863	-2.682549039622	-2.168894239336
H	2.257419294202	-2.374201853457	-2.079952888613
H	-4.364702209559	-1.987268551610	-0.895246023433
H	-6.545136813226	-1.032648727149	-0.240425542293
H	-6.842770027149	0.001795726854	2.007598793357
H	-4.907412564367	0.122192665469	3.577157564175
H	-2.714692774590	-0.826793487082	2.923062807856
Pt	-0.038402989836	0.065916873345	0.148848298830

TS2 (NIMGA = 1, 334.81*i* cm⁻¹)

TS2 (NIMGA = 1, 334.81i cm^{-1})

C	2.010619188643	-1.818601742617	-0.905882784767
C	2.635840291790	-2.277543736520	-2.068467012689
C	1.965574015540	-2.241670535398	-3.290302984248
C	0.645631226693	-1.798192235689	-3.368953646269
C	-0.011417964771	-1.328673700188	-2.226932273071
C	0.721393503922	-1.289254094773	-1.032209771133
C	-1.396400606961	-0.858620887495	-2.147854551564
C	-1.720840762194	-0.118389750877	-1.003378862461
C	-2.417258302244	-1.184998172622	-3.049627185785
C	-3.728289786169	-0.801715743634	-2.782456144886
C	-4.032481619738	-0.093088179849	-1.617571410778
C	-3.024813309159	0.261552156135	-0.718480081971
C	2.474186943765	-2.062989610383	0.465390418563
C	3.770741079163	-2.315469193207	0.901959264512
C	3.993246512854	-2.581930571181	2.253344800132
C	2.933141080909	-2.608543511406	3.164265727878
C	1.627752365337	-2.367447050180	2.736145490531
C	1.412046743150	-2.104059468670	1.384409895741
C	0.106750304462	-1.785527338254	0.788170731631
C	-1.127186046894	-2.042580094249	1.046005801011
C	-2.464855764839	-2.318725008591	1.167477110751
C	-3.070230306013	-3.307268121276	0.319062945646
C	-4.448953141166	-3.455831310988	0.410101370963
C	-5.201810206505	-2.677257506684	1.293927409101
C	-4.608126603496	-1.717214663914	2.129210428792
C	-3.244884751568	-1.535108885591	2.070797850969
C	-2.243183932745	-4.133291582394	-0.616707514309
H	3.635504136377	-2.714067805380	-2.002744307031
H	2.467521937212	-2.601522710931	-4.191442715663
H	0.126086619649	-1.796463861997	-4.330238720397
H	-2.189689455212	-1.770235406444	-3.944362126289
H	-4.524706998450	-1.071763352531	-3.480174750674
H	-5.065418132617	0.190428303970	-1.399466906042
H	-3.274909421815	0.809242879902	0.192450196607
H	4.607832719179	-2.282923489583	0.201358254406
H	5.012248239163	-2.765703226177	2.603303039974

H	3.125110180013	-2.820509223151	4.218927171105
H	0.793262375584	-2.383099441145	3.440891168465
H	-4.953406747155	-4.189747132407	-0.222672771200
H	-6.285122913260	-2.820974104963	1.332409125355
H	-5.220623458356	-1.121627859726	2.808611558589
H	-2.742967275425	-0.786884144703	2.688668260180
H	-2.881897257630	-4.763268843155	-1.252369821276
H	-1.622091659478	-3.495854479936	-1.267780411056
H	-1.559881635563	-4.789842012880	-0.050528016858
C	-0.344903638732	2.612734436089	0.154937291661
C	0.702185475650	3.163879187025	1.110281385923
C	1.862423313958	2.211318356977	1.243366771414
C	0.234438169347	2.144773333756	-1.022794297263
C	2.446840620539	1.846301959382	0.078559700830
C	1.720458086162	2.423473575678	-1.123119755791
C	1.242554195055	4.425904022621	0.351619285469
C	1.837522090062	3.980394519350	-0.998521039894
C	-1.765563229040	2.979092526249	0.330058916290
C	-2.369872728683	2.859892994576	1.592313257864
C	-3.720417381163	3.153758017158	1.756341314087
C	-4.476079622960	3.593938315620	0.666730726906
C	-3.876266436190	3.741047072179	-0.584852176728
C	-2.529181100277	3.430972726264	-0.755362596695
C	3.746598853392	1.151495460260	-0.054033374981
C	4.156727602134	0.589423109494	-1.271871502864
C	5.406689183366	-0.015762587064	-1.398873192072
C	6.274580250508	-0.069139386353	-0.309527972346
C	5.880135125182	0.483826848824	0.910933907752
C	4.633771885921	1.088600898684	1.035073230763
H	0.275251716550	3.441314905734	2.080691246692
H	2.242437974031	1.948072544716	2.232684265301
H	-0.342747290132	2.015582638011	-1.943199857340
H	2.118438432294	2.081985137774	-2.083472487775
H	1.998952767378	4.906314927615	0.990204175795
H	0.418672953125	5.144432151200	0.214740564603
H	2.900205278292	4.254517369946	-1.084753293171
H	1.307481552708	4.444444195481	-1.845005325590
H	-1.787161629290	2.498484165170	2.444645879720
H	-4.186419877670	3.039187757254	2.738330007893
H	-5.535921393686	3.829136420467	0.796084777578
H	-4.462316437432	4.096611712466	-1.436129518858
H	-2.067332330747	3.548275032828	-1.738736818121
H	3.494247024724	0.603600282425	-2.139826255581
H	5.700417788270	-0.449064437074	-2.358873336927
H	7.257396463442	-0.537698286456	-0.410144414277
H	6.553959821975	0.453176535721	1.771405840672
H	4.359550417365	1.540043338630	1.991312944866
Pt	-0.159498085376	0.263835614443	0.206667128794

Int3 (NIMGA = 0)

C	2.487999973762	1.279602763804	1.655835396433
C	3.050957029108	1.068488119190	2.905736815014
C	2.190775256674	0.810927497272	3.981086279218
C	0.806096771193	0.757018745280	3.815180556254
C	0.216540602200	0.970351603891	2.558383286841
C	1.090889085976	1.248375660322	1.509075620731
C	-1.243521498978	0.875753635753	2.322391479547
C	-1.790385877704	0.419418726541	1.108263036739
C	-2.143731447599	1.270927691328	3.326347713380

C	-3.519915953082	1.226965883996	3.128717645219
C	-4.033071026488	0.791877998442	1.908955511965
C	-3.164750108909	0.395633541037	0.891511860440
C	3.092351294426	1.512377842939	0.330985008284
C	4.405914042702	1.725081168341	-0.056769369945
C	4.674712470250	1.946419700346	-1.413054852132
C	3.654073866679	1.953778816221	-2.366224195849
C	2.325704064905	1.753144139836	-1.982674175008
C	2.065560322243	1.542574857154	-0.633973855789
C	0.769781895287	1.432901071281	0.076816814546
C	-0.434069187711	1.801611956230	-0.530100486807
C	-1.161232531389	2.889391379470	-0.956169719251
C	-0.738460589971	4.233178967441	-0.633058130482
C	-1.529391413704	5.275016407498	-1.100912038877
C	-2.684164495840	5.026973965914	-1.848238756208
C	-3.104627168188	3.722139988540	-2.163742646137
C	-2.353166746337	2.662667420688	-1.719835356608
C	0.489664811940	4.502189676359	0.176895892909
H	4.133624533715	1.085465784633	3.049280106348
H	2.612392132268	0.627421436848	4.972548221935
H	0.177789511899	0.511649470420	4.674468899015
H	-1.750672014979	1.648156950595	4.273724632451
H	-4.192634620107	1.547100958021	3.928039110565
H	-5.111938303164	0.754532331637	1.738460881898
H	-3.578439930961	0.050498941599	-0.060127291700
H	5.216368454391	1.721453570870	0.675129994303
H	5.707381794237	2.108884704620	-1.732331514174
H	3.894629584250	2.118575341677	-3.419106120093
H	1.520864643678	1.763418527073	-2.722707922810
H	-1.248143536472	6.306468685385	-0.877448831651
H	-3.278970881778	5.876573381378	-2.195318464399
H	-4.010813388027	3.560812046240	-2.750021725332
H	-2.640189437245	1.633092574399	-1.946157343683
H	0.601117904601	5.578942784995	0.368798432513
H	0.450666267637	3.980125355716	1.148082519772
H	1.393659722128	4.153659739886	-0.352985130908
C	-1.105823172394	-2.525034514684	-0.364963110754
C	-0.266632925549	-3.327902225999	-1.354822942190
C	1.087112883569	-2.700321670387	-1.571136960690
C	-0.385887109212	-2.223994977189	0.773444033118
C	1.783141758514	-2.428317415326	-0.446865401623
C	1.006807280539	-2.805589221415	0.801829572457
C	-0.007403849826	-4.669077348803	-0.581545642613
C	0.761373444726	-4.353265223139	0.717273580145
C	-2.587064742091	-2.528757925819	-0.460521640017
C	-3.214572976787	-2.216542743437	-1.677612987759
C	-4.603834720123	-2.159601217245	-1.760385941393
C	-5.382148881467	-2.438668624959	-0.634981371958
C	-4.766731656789	-2.779134609693	0.570499155642
C	-3.377316220138	-2.821451735927	0.659554153652
C	3.187630515259	-1.961394088547	-0.385428658447
C	3.883016794857	-1.880447340127	0.831378279011
C	5.233150269054	-1.531078507652	0.869800926602
C	5.919531005922	-1.249698459617	-0.308162120005
C	5.237145369476	-1.302221580230	-1.525733279808
C	3.891263738496	-1.646695685791	-1.562348472082
H	-0.798616982794	-3.513149211171	-2.295547584850
H	1.468641473404	-2.575056489440	-2.586048928568
H	-0.863268825855	-1.948478876475	1.718290492656

H	1.511117558738	-2.541503069969	1.735666479018
H	0.567779957579	-5.337318879635	-1.239836559784
H	-0.972094096684	-5.158998202740	-0.372183882176
H	1.738524461261	-4.859627478125	0.745378649170
H	0.197090534602	-4.674712446318	1.606813919365
H	-2.608776447262	-1.989038673572	-2.560092106614
H	-5.081418947817	-1.898498551219	-2.708312934831
H	-6.472780236262	-2.398519246732	-0.700557557354
H	-5.372983991553	-3.011527573929	1.449892704777
H	-2.903422076600	-3.089433496921	1.607201299063
H	3.383624999138	-2.103951451477	1.775563270973
H	5.748357829236	-1.483143046357	1.833230007806
H	6.978698645203	-0.979280719219	-0.280502396472
H	5.758493224563	-1.066085165673	-2.457464607169
H	3.384195487986	-1.675502710254	-2.529491423157
Pt	-0.626206372724	-0.190834942738	-0.441400797032

TS3 (NIMGA = 1, 21.66i cm^{-1})

C	2.545170864479	-1.392940305296	-1.559093661008
C	3.147497277463	-1.247918141713	-2.799818730151
C	2.323763416832	-1.016036256930	-3.908972004270
C	0.936941917438	-0.921988872645	-3.784950925904
C	0.306399496532	-1.073739324122	-2.538887352240
C	1.144932112957	-1.331923717110	-1.455506704648
C	-1.158360776185	-0.938537658996	-2.352189050753
C	-1.737000595543	-0.434284698007	-1.171094964639
C	-2.031911152143	-1.348244882183	-3.373821897010
C	-3.413019964819	-1.274540258018	-3.225769848875
C	-3.958668818200	-0.797159474899	-2.036688867365
C	-3.117669534080	-0.386523687493	-1.001909476736
C	3.107930901828	-1.561398269303	-0.206217462561
C	4.410071603982	-1.737045283492	0.235045365641
C	4.638093653290	-1.865282668112	1.610775447864
C	3.588060221851	-1.821924095171	2.530554797931
C	2.270486014235	-1.662246655696	2.093834389893
C	2.052169164405	-1.539708401468	0.727015483379
C	0.780331764037	-1.459026879699	-0.028369130972
C	-0.447042629633	-1.786922316890	0.551458195095
C	-1.205162325460	-2.846176014443	0.994242179991
C	-0.788095625635	-4.206623321967	0.740313120072
C	-1.609084231378	-5.219867457061	1.218971200691
C	-2.787211395589	-4.928951393894	1.912452535711
C	-3.201771114447	-3.607673772685	2.160766271478
C	-2.420931006123	-2.575303740054	1.704083553302
C	0.465713415022	-4.521389287616	-0.011636910864
H	4.233132688994	-1.292717209155	-2.911193600927
H	2.776933105067	-0.882328334529	-4.894473196915
H	0.340121539795	-0.693803940926	-4.670960173197
H	-1.614788028917	-1.761988658985	-4.295237258602
H	-4.063719579420	-1.606824502259	-4.038257774874
H	-5.041769701236	-0.739696511261	-1.902371188609
H	-3.559282997239	-0.016460286357	-0.072892283084
H	5.243474423970	-1.770881486605	-0.469742795807
H	5.661711723532	-1.994372278308	1.971738173789
H	3.796913247964	-1.914611810339	3.598906588384
H	1.442741660726	-1.630990613775	2.807570434887
H	-1.333017743759	-6.262527509785	1.046982469493
H	-3.405438268563	-5.757130991571	2.270198702112
H	-4.126632911601	-3.412746638167	2.706237349533

H	-2.702377525712	-1.534413919299	1.879523975710
H	0.569547601793	-5.605937503083	-0.158466869482
H	0.470798805168	-4.036322393825	-1.002570995188
H	1.353640699054	-4.164136561517	0.539197610909
C	-1.131609873079	2.547742384270	0.345245216038
C	-0.301286473500	3.339454124796	1.350973181109
C	1.059810499909	2.721079142548	1.549862464455
C	-0.412397423425	2.275040687120	-0.799518992974
C	1.754168810282	2.478106787116	0.418068715072
C	0.971200940413	2.878430667369	-0.819395008419
C	-0.061908462033	4.700091394101	0.607232218343
C	0.709163111172	4.420931429253	-0.697878007131
C	-2.611159632730	2.517673093514	0.445106284424
C	-3.231106043548	2.167559285504	1.655583587003
C	-4.618854759471	2.079220123566	1.737096678006
C	-5.403653678591	2.366730534014	0.618306746739
C	-4.796562054087	2.747255770433	-0.579448956835
C	-3.408401635386	2.819496708555	-0.668007854431
C	3.155698333225	2.003921459903	0.336464233338
C	3.785812169154	1.776862887779	-0.897293475686
C	5.130403045239	1.411589272693	-0.965706364634
C	5.876123467940	1.255650774209	0.199258568639
C	5.258927674658	1.451899702743	1.436799400062
C	3.919674234690	1.817703302668	1.503345322496
H	-0.833747661399	3.496144903819	2.296640260647
H	1.437229753216	2.558604068751	2.561113232324
H	-0.888513899115	1.998502665322	-1.744787579175
H	1.477854261627	2.649617158605	-1.760801262079
H	0.505062764941	5.361433709935	1.279403828785
H	-1.033334860829	5.181325999149	0.409415506009
H	1.680969294688	4.937833040315	-0.714971285474
H	0.141302258848	4.756085177378	-1.580008521347
H	-2.620450577416	1.934139916995	2.533147588019
H	-5.090249135146	1.787422822653	2.679124686095
H	-6.493143032555	2.302269206230	0.683341109795
H	-5.408184566765	2.987311359305	-1.453014808667
H	-2.940634630587	3.118799579280	-1.609250156243
H	3.235299286478	1.885430267439	-1.833247317131
H	5.593466212327	1.248188680148	-1.942890036641
H	6.931184183783	0.972997916839	0.147500159312
H	5.828111560877	1.320090060903	2.361140381770
H	3.469668368076	1.976915896557	2.485810828466
Pt	-0.609488053615	0.201378937147	0.395787894864

Int4 (NIMGA = 0)

C	-2.956123974342	0.996840819534	-1.575361600257
C	-3.594154669094	0.811331824033	-2.789233884755
C	-2.806906799654	0.771126189010	-3.960556377628
C	-1.425634961834	0.935326574096	-3.939001745928
C	-0.760581641998	1.132136522933	-2.709338712225
C	-1.559943461792	1.127010408124	-1.572040426513
C	0.672566328272	1.345414332826	-2.493178826472
C	1.149320414645	1.687887677004	-1.175018520301
C	1.611603691691	1.238331048548	-3.535651604751
C	2.956291960770	1.472298417536	-3.313290420402
C	3.423031447588	1.832803568542	-2.035524049408
C	2.536993125039	1.941507709532	-0.988966442089
C	-3.405378521497	1.155895461600	-0.177310149798
C	-4.681167285001	1.194316293187	0.367599565047

C	-4.816904782028	1.410963863366	1.743012318134
C	-3.696114499293	1.578656072912	2.558255427393
C	-2.406679190507	1.547364103042	2.017334392956
C	-2.269168562849	1.344316402294	0.648133552711
C	-1.069669207353	1.315681908688	-0.219378115041
C	0.249255622651	1.739070615151	-0.015647570230
C	0.659450492414	2.418482155069	1.249584195803
C	0.277798224979	3.769641948056	1.383435254890
C	0.624052538226	4.437952416235	2.561852075097
C	1.325317554947	3.798075170998	3.583236904831
C	1.705562912868	2.465946516851	3.436917081605
C	1.373981341681	1.783387998866	2.268726968303
C	-0.489262034541	4.475418276417	0.293810495540
H	-4.679864295359	0.709121370176	-2.856530944619
H	-3.303192729689	0.623622496079	-4.923119589449
H	-0.874738867634	0.922281911840	-4.881367758406
H	1.274786556045	0.964049670173	-4.536688511181
H	3.662797374784	1.377489944635	-4.141660343710
H	4.486666670508	2.018120136326	-1.872276320666
H	2.894308676564	2.209182951242	0.007220807900
H	-5.563936222568	1.060279032995	-0.262106294213
H	-5.815743833049	1.445132749996	2.185949657323
H	-3.825327112660	1.744291143127	3.630755574905
H	-1.535588385827	1.692878257571	2.660119871228
H	0.336053122518	5.486684727791	2.679557806762
H	1.579326097677	4.346069275633	4.494509460379
H	2.261537830509	1.954476713433	4.226477524833
H	1.681098287235	0.741560428256	2.157886150183
H	-0.567804224401	5.553059290032	0.504106002972
H	-0.003773134110	4.356368463854	-0.690276463323
H	-1.515558362459	4.075933823206	0.205260996307
C	2.010936916214	-2.039205410486	0.555865667247
C	1.305522747538	-2.193626825542	1.897904078064
C	-0.044180247349	-1.544751157823	1.615632758757
C	1.222457883796	-2.578745247331	-0.482271754331
C	-0.820345354920	-2.223259602693	0.630233357752
C	-0.012489300935	-3.334828698209	-0.020076178695
C	1.107249998690	-3.697182337566	2.212455048530
C	0.357153220106	-4.382473999639	1.056324250808
C	3.365117489559	-1.495730806361	0.391315952332
C	4.030083624759	-0.876188597679	1.463985209230
C	5.289419627358	-0.312598295218	1.285672772193
C	5.910074364810	-0.367680725989	0.037426976946
C	5.267119553466	-0.991466906106	-1.034341567555
C	4.006448257779	-1.547091541383	-0.862068511308
C	-2.280281843166	-2.138843114633	0.493749026156
C	-2.888686065519	-2.354397330290	-0.753764903993
C	-4.274495143490	-2.346722474551	-0.865083124232
C	-5.063859890919	-2.149932896167	0.269511493512
C	-4.466239830471	-1.935673872832	1.512081405710
C	-3.080310461772	-1.913869064498	1.625062489659
H	1.817609916891	-1.686085259492	2.720124443142
H	-0.504715031033	-0.888005443759	2.359937260496
H	1.597226603229	-2.727127377149	-1.497443950136
H	-0.541791216053	-3.790421455579	-0.863652024746
H	0.547803983939	-3.770862192142	3.157876031039
H	2.095587187777	-4.150879379916	2.382223816826
H	-0.565805287384	-4.870634471857	1.405589663002
H	0.976205093303	-5.155123668163	0.575001470161

H	3.571975546373	-0.822465414907	2.452685862049
H	5.789640792618	0.169415347443	2.128943726172
H	6.900350227712	0.074144880928	-0.100999237000
H	5.750747479344	-1.040809481292	-2.012877454751
H	3.521997591822	-2.022507577275	-1.716622343168
H	-2.273944993176	-2.503596849921	-1.646052348974
H	-4.741472008745	-2.498372544126	-1.841308831197
H	-6.153684271846	-2.156551996568	0.183358910520
H	-5.083580290547	-1.776255438903	2.399265301578
H	-2.621529250775	-1.756784910796	2.604016438114
Pt	0.392667067426	-0.571763657772	-0.220778254324

2-4-2) Cycloisomerization

Int1' (NIMGA = 0)

C	-3.125241896942	1.095604905960	-1.346361421879
C	-2.487456276424	2.269577176796	-1.846939907906
C	-2.741141779529	3.530834763733	-1.330493420744
C	-3.660149360138	3.737549842367	-0.268302127875
C	-4.297417589816	2.612424939198	0.186332786285
C	-4.050662681369	1.323515721108	-0.354012780301
C	-5.296869504848	2.016162673168	1.145413432307
C	-5.067434495918	0.730597393661	0.588721605773
C	-6.200664039259	2.231246959633	2.155057659344
C	-6.904328923846	1.083406515109	2.604660143918
C	-6.699225093852	-0.171101942523	2.042911677975
C	-5.763857348401	-0.380076725991	0.995924417000
C	-2.811097323646	-0.263266456958	-1.853674403087
C	-3.844729505892	-1.095424367538	-2.292939409023
C	-3.586471815495	-2.380537357630	-2.766970477211
C	-2.278057589457	-2.860021199891	-2.815212700283
C	-1.234796437247	-2.059148117635	-2.365641785336
C	-1.487947988831	-0.770707386178	-1.875488737718
C	-0.418631852994	0.034620534004	-1.322114202255
C	0.052788378500	1.111020149404	-0.895620336911
C	0.586321643657	2.369515982708	-0.483942040769
C	1.559891954836	2.976754474888	-1.304231494601
C	2.132549660345	4.180918659666	-0.928076861907
C	1.732815257767	4.782436934500	0.268960164439
C	0.760318299317	4.189527409518	1.072700279725
C	0.161490773339	2.976500383652	0.720742336164
H	-1.778273717595	2.171632501868	-2.673903539545
H	-2.214758205507	4.389891270685	-1.755703585652
H	-3.835977794241	4.735900317895	0.138181284557
H	-6.389108534233	3.213823833318	2.593929187595
H	-7.637803516644	1.192005059057	3.408702574106
H	-7.278987111113	-1.021312311445	2.413225487289
H	-5.639525159791	-1.368177661248	0.546682883673
H	-4.870882198679	-0.718188063742	-2.272732017658
H	-4.414153772265	-3.008259276859	-3.107246457333
H	-2.069898616865	-3.864751877419	-3.190271705246
H	-0.210125694368	-2.440028101251	-2.379107178254
H	2.890062872485	4.650474362697	-1.559611561234
H	2.180413705160	5.731144747253	0.577344911163
H	0.450684081262	4.683821862159	1.997821272261
C	-0.888495945044	2.367724792394	1.608599185978
H	-1.466806378863	1.582937317591	1.096097374251
H	-1.599657310725	3.138773548351	1.945553112912
H	-0.428581478833	1.936859113730	2.515998893312

H	1.859280975133	2.481698242368	-2.231196442501
Pt	1.536105736636	-0.635795979100	-0.528295244728
C	0.932605243797	-2.091037070013	1.031980607057
C	1.085305569063	-0.743704404732	1.506328931637
C	2.271427840906	-2.813923005860	1.088811335475
C	-0.348701620045	-2.771388404332	0.834273160382
C	2.438737957808	-0.449929927659	2.136289062340
H	0.226616369996	-0.138381660370	1.803192416661
C	3.188485462589	-1.860342512297	0.335133845194
C	2.712686222284	-2.924840637447	2.569057109446
H	2.249355292694	-3.793646278654	0.604118282012
C	-1.559173728975	-2.128967241304	1.157282499838
C	-0.394844545702	-4.075981919261	0.309968544477
C	3.369305595714	-0.613826057318	0.945738548738
C	2.763472427421	-1.523624928676	3.203370940648
H	2.465659387596	0.557159315936	2.563833541597
H	3.847966030463	-2.235255333804	-0.452370069696
H	3.699884978549	-3.411856801460	2.585575191879
H	2.010786044904	-3.586312331461	3.099983276554
C	-2.772436563343	-2.774046050105	0.966238740415
H	-1.565605636777	-1.117211099318	1.567194409202
C	-1.612835421689	-4.717079497136	0.116059912162
H	0.522107284746	-4.599279218353	0.034687329657
C	4.372431921742	0.386268095644	0.557543343720
H	3.754755744383	-1.305565007280	3.628883448793
H	2.028518200749	-1.420696285372	4.016715735799
C	-2.803770653792	-4.067588725804	0.441579418588
H	-3.698743867870	-2.262451213313	1.232635529017
H	-1.632419273932	-5.728127822653	-0.297477752284
C	4.165686711063	1.749048077630	0.834024282282
C	5.544626975425	-0.006952233643	-0.111753888875
H	-3.761899345765	-4.570308735419	0.286270192991
C	5.107088650393	2.695003063554	0.443876642617
H	3.247022424245	2.084614043704	1.323129100858
C	6.489115252932	0.941659024532	-0.489053299892
H	5.735579326317	-1.063209358221	-0.315195352961
C	6.271035994674	2.293492869064	-0.214360600628
H	4.928209591751	3.752915882757	0.651223695585
H	7.403353415920	0.624232151684	-0.996613965625
H	7.013466231750	3.037917987666	-0.514068079775

TS1' (NIMGA = 1, 465.49i cm^{-1})

C	-3.034171785570	0.981140563521	-1.337293027783
C	-2.221228049721	2.098883524072	-1.736112478640
C	-2.444182221696	3.389769676214	-1.217648303358
C	-3.420251872115	3.652484901673	-0.244370934473
C	-4.187368658188	2.565902256138	0.125760462391
C	-4.008998582783	1.266137470088	-0.419030782641
C	-5.285200518235	2.048616998876	1.006271751032
C	-5.121588111308	0.751474579503	0.457293932213
C	-6.222955017995	2.334762783285	1.969457277243
C	-7.028253419798	1.243194119767	2.375187711915
C	-6.878425968999	-0.027203724220	1.824984269137
C	-5.907394051247	-0.310370185332	0.831912952987
C	-2.721370158725	-0.360911309181	-1.845492380827
C	-3.726648244534	-1.212331058412	-2.308699155930
C	-3.413474532319	-2.483276168413	-2.785819676100
C	-2.086971775079	-2.911324145813	-2.802045202671
C	-1.079261169436	-2.079890539011	-2.321043451514

C	-1.378498534730	-0.803696355346	-1.829495317959
C	-0.348044628838	0.052173909466	-1.223374993618
C	-0.353198124853	1.318554343311	-0.933167655345
C	0.380240367071	2.471719332823	-0.483964514034
C	1.325174675375	3.034384601228	-1.365728960544
C	2.088875410335	4.122401613833	-0.970385257962
C	1.914046666989	4.648706200583	0.312233699734
C	0.979650953962	4.093137232224	1.186044949239
C	0.183143892020	3.008710501482	0.808644620363
H	-1.651478965542	2.023532768228	-2.669414548417
H	-1.819111895006	4.208827201910	-1.584239895403
H	-3.555300815009	4.653057890359	0.169442910255
H	-6.357414347894	3.328516859339	2.401979737806
H	-7.795462189046	1.403470990611	3.137511142003
H	-7.534867438764	-0.832270740679	2.166690165337
H	-5.819393250199	-1.310269022779	0.401130967873
H	-4.763151599300	-0.864049160190	-2.311682084751
H	-4.208281261356	-3.139064918722	-3.150335126369
H	-1.833671832538	-3.906100300732	-3.176582152122
H	-0.046947309817	-2.438430236396	-2.320328245101
H	2.822694814575	4.556560301084	-1.653346578699
H	2.512368965706	5.504497258413	0.636657662040
H	0.854702979384	4.520783852022	2.184981803094
C	-0.843653676083	2.462759868447	1.763672140400
H	-1.469669798568	1.682262590307	1.302937194785
H	-1.512007121947	3.268420025592	2.109552832645
H	-0.357962481791	2.043580480979	2.662303794107
H	1.447665234920	2.598516519769	-2.360409457840
Pt	1.501981852979	-0.657180960146	-0.529987667214
C	0.890851382409	-2.008933055472	1.064878532701
C	1.057099338118	-0.649786167539	1.500417407525
C	2.205935028729	-2.770462011414	1.204901446195
C	-0.409883304714	-2.686584188628	0.917989655926
C	2.419136093865	-0.354030754277	2.105661945623
H	0.205464070260	-0.029199440616	1.785282979865
C	3.182280946670	-1.903965234203	0.428266188341
C	2.596357959814	-2.802533602577	2.703380456957
H	2.160290359282	-3.779172328257	0.784920235353
C	-1.607705569705	-2.015479902942	1.218310572271
C	-0.479628068841	-4.007533819242	0.447438584184
C	3.357049181627	-0.624500857373	0.934029968673
C	2.709131943720	-1.363985244958	3.242835335204
H	2.480398472676	0.678472750610	2.465717487642
H	3.832208460302	-2.338993614944	-0.335779081506
H	3.551495761094	-3.342289189466	2.793400942209
H	1.838556297449	-3.382896180278	3.252822408233
C	-2.833949474835	-2.645067682447	1.049365619561
H	-1.595494036950	-0.986986923500	1.584751709712
C	-1.708974882479	-4.637134732311	0.279326215698
H	0.428209006140	-4.554518666695	0.187493062015
C	4.392038743513	0.334278383048	0.502900651452
H	3.713741076687	-1.159019969963	3.643850744276
H	1.989146515947	-1.179895193889	4.055371183614
C	-2.889488085495	-3.956960987470	0.575835697013
H	-3.751801205375	-2.105225210551	1.291834433388
H	-1.743886890021	-5.663555887104	-0.094184056756
C	4.166538196431	1.715359284564	0.614707867984
C	5.605966255165	-0.118591135450	-0.037053199504
H	-3.856055666552	-4.448793858185	0.438188739221

C	5.131616141142	2.623127747054	0.188663027711
H	3.218041662854	2.090050278661	1.010741295612
C	6.573318598873	0.792120140151	-0.453236591600
H	5.808452472885	-1.190019169810	-0.110520975629
C	6.337681834959	2.163994788761	-0.343087706414
H	4.938566076227	3.695898407557	0.270989462627
H	7.519970882947	0.428343329477	-0.861043779770
H	7.098419325899	2.877760495957	-0.670572544030

Int2' (NIMGA = 0)

C	-3.140080766648	0.750565991050	-0.908637031857
C	-2.138377515024	1.865260054963	-0.955065105077
C	-2.528273799973	3.161594120601	-0.340201037400
C	-3.766300982444	3.431610053458	0.180390211024
C	-4.653384906662	2.346213524159	0.173330503133
C	-4.342616587449	1.056163388389	-0.358862764368
C	-5.991409929790	1.891909295707	0.570318117878
C	-5.714139507712	0.594670890688	0.066265328803
C	-7.188287657148	2.231518899913	1.173464048863
C	-8.125693144654	1.186870114246	1.259092096654
C	-7.848758350030	-0.094550215331	0.769530427055
C	-6.622886228973	-0.432834064649	0.152152591835
C	-2.742241189920	-0.529434042642	-1.464881575461
C	-3.699701238361	-1.438730545486	-1.937514698005
C	-3.310235512196	-2.655403936485	-2.479703434351
C	-1.951319037876	-2.969102928915	-2.550071972003
C	-0.995200355926	-2.076511976948	-2.076454653550
C	-1.362307805134	-0.843574048779	-1.519070234393
C	-0.371965210093	0.103207909623	-0.963457318455
C	-0.706357382692	1.382462347658	-0.689061244435
C	0.280740441901	2.405794494144	-0.234483621435
C	1.163283122377	2.955992824983	-1.177591440578
C	2.068125509015	3.950733584133	-0.817914811607
C	2.105153319707	4.397311907972	0.502632162381
C	1.238545913737	3.848672525826	1.445866057461
C	0.306313628466	2.863088341413	1.097595832903
H	-2.107040511478	2.175458140229	-2.035908012233
H	-1.773850391299	3.953797726706	-0.365323890831
H	-4.024354941860	4.410461467074	0.585149464295
H	-7.404636320365	3.229398603152	1.559434761393
H	-9.097360272009	1.376015929743	1.721840257694
H	-8.615350555516	-0.867785917277	0.869819668761
H	-6.439412731332	-1.444685155151	-0.213370182692
H	-4.758002573857	-1.168978247590	-1.913276521118
H	-4.060793830681	-3.354870088429	-2.855582870005
H	-1.631175292456	-3.924042623365	-2.974776830715
H	0.058366254376	-2.359983066813	-2.135540200612
H	2.747225043054	4.369553511426	-1.565086942570
H	2.815522200275	5.172838714228	0.802463370040
H	1.274604840067	4.201081292606	2.481458927161
C	-0.657255363212	2.353293779740	2.141134256810
H	-1.261714741920	1.506745550142	1.776825903156
H	-1.354101987787	3.151419639568	2.453025470444
H	-0.123219431071	2.025936052618	3.049608312632
H	1.123269754602	2.597978066631	-2.210663501278
Pt	1.528321851827	-0.500453403822	-0.577197253722
C	1.136515176769	-1.903686760594	1.020927777596
C	1.367070903023	-0.565063544750	1.488444551808
C	2.447424110292	-2.689340687062	1.002221426979

C	-0.178693471837	-2.585406782269	1.070335846670
C	2.793599468394	-0.312702178441	1.947664333376
H	0.567238085506	0.036217204162	1.923699819378
C	3.401281168549	-1.832880413716	0.191954745748
C	2.956175239875	-2.781244936445	2.465533066388
H	2.341084715376	-3.682299627303	0.555808733498
C	-1.326853074802	-1.906901380544	1.511599647128
C	-0.314942420592	-3.913680968933	0.642218681228
C	3.636964905009	-0.584073844462	0.705323380200
C	3.151697765008	-1.361210160111	3.033519153746
H	2.914136803747	0.708077443530	2.327250332195
H	3.957822683840	-2.254339782404	-0.649348627996
H	3.899962049587	-3.347885126901	2.465875230605
H	2.227529697648	-3.356826631464	3.058430924945
C	-2.570952828438	-2.526257097696	1.501452120067
H	-1.262899933290	-0.870962013940	1.849459854223
C	-1.558966050016	-4.539921191566	0.643618383734
H	0.548954705356	-4.473293715148	0.279672373639
C	4.661221631858	0.363105580219	0.216884398139
H	4.191873947711	-1.193353463197	3.353338138376
H	2.507841144337	-1.185888311322	3.909681419732
C	-2.692164725707	-3.846565528856	1.064505340758
H	-3.452994760080	-1.972182677915	1.833574698697
H	-1.642689823262	-5.574125171137	0.299948874041
C	4.468122021733	1.744663768152	0.354433977489
C	5.832332616298	-0.101729335954	-0.400544232354
H	-3.671086217357	-4.333345187946	1.052703952600
C	5.416564931292	2.643500830013	-0.127278410173
H	3.554721681324	2.128358259454	0.816329182033
C	6.784400226411	0.798010558657	-0.874076144576
H	6.012931936048	-1.175928329669	-0.492620121690
C	6.578084163390	2.172697175352	-0.740961727905
H	5.244383382577	3.718329524478	-0.023363540156
H	7.697294812550	0.422862501278	-1.344421665602
H	7.326826512863	2.877528567309	-1.112810546127

TS2' (NIMGA = 1, 997.36*i* cm^{-1})

C	3.230948983686	0.669224151838	0.584603065898
C	2.260811606228	1.725398075938	0.369230446968
C	2.647916888836	3.032193855627	-0.051633087042
C	3.966114016448	3.335399796078	-0.362317009263
C	4.874120733176	2.294411970976	-0.224639848714
C	4.528226123602	1.011779132756	0.239234439810
C	6.305549417055	1.877315472114	-0.370148980094
C	5.974169028515	0.577069356954	0.088024378513
C	7.575613395889	2.241540970785	-0.737163157837
C	8.553130620434	1.219623064392	-0.633546507178
C	8.231551380148	-0.058858713367	-0.194185588369
C	6.911567811547	-0.420636247573	0.183570773537
C	2.795293265367	-0.589716209672	1.146431142756
C	3.735277742084	-1.542779333394	1.587422817987
C	3.328333004339	-2.739167567662	2.142222390852
C	1.958497243055	-3.019060940924	2.285001626053
C	1.021408197156	-2.100193939628	1.864669809380
C	1.405688011798	-0.869056999812	1.281237151717
C	0.413358935674	0.066816586632	0.804694108121
C	0.780910707785	1.352844796735	0.430232795162
C	-0.201690803905	2.397719210164	0.004900654362
C	-0.328909703706	2.748841173988	-1.352300141323

C	-1.247263883029	3.750955810935	-1.689013596414
C	-1.996491772050	4.408583408082	-0.715631236683
C	-1.860703815555	4.057456686383	0.627244162029
C	-0.970136229785	3.048871166177	0.980842225357
C	0.518271239528	2.125660373643	-2.432561396706
H	1.541904307798	1.846632950984	1.412144253460
H	1.877892707652	3.800487666049	-0.141838469655
H	4.248473722279	4.333303317283	-0.700455572998
H	7.836233407482	3.241501067288	-1.090158228547
H	9.587069718411	1.442433191706	-0.910374604513
H	9.019621678177	-0.814653538747	-0.137489101403
H	6.696162603702	-1.438520361276	0.515150937783
H	4.798991711450	-1.319672065011	1.516959260252
H	4.073623507246	-3.463488231545	2.479741111229
H	1.634919427361	-3.963981421450	2.727546531979
H	-0.039844390572	-2.328408292072	1.980135739327
H	-1.363448650888	4.030432729824	-2.740541509357
H	-2.695828609957	5.196112986119	-1.009710165794
H	-2.449693051967	4.562894832935	1.396437862608
H	-0.853457233025	2.763725767605	2.030774670322
H	-0.098506598940	1.833389274165	-3.298697784092
H	1.068928594402	1.238180602485	-2.083107291282
H	1.267872501046	2.849066649401	-2.799642534429
C	-3.510091222911	-1.685759594164	0.085436333839
C	-2.710234450477	-2.660980167907	-0.755360924869
C	-1.361927553692	-1.974662027386	-0.950273325207
C	-3.726710569067	-0.458653549580	-0.494610428648
C	-1.550702723960	-0.648554556179	-1.469174577537
C	-2.993237503054	-0.326881633890	-1.824415723719
C	-3.371639771214	-2.804606325030	-2.151394590372
C	-3.517271787961	-1.413625544465	-2.798940175210
H	-2.626655258880	-3.628236060375	-0.252257600057
H	-3.079855298949	0.673497161111	-2.262040619406
H	-2.754942769527	-3.476404403957	-2.769141401443
H	-4.350293963650	-3.289838314513	-2.015351666022
H	-2.942190686007	-1.342545582764	-3.735353974301
H	-4.567139920903	-1.188231998956	-3.041928577449
Pt	-1.548749875263	-0.443493481322	0.601292997653
H	-0.756094055117	-0.127907593266	-2.005864159254
H	-4.009709822722	-2.016372701698	0.999688700846
C	-4.647784656487	0.575425210519	0.020022125972
C	-5.742746217796	0.221868927369	0.824438358968
C	-4.433525695114	1.927894141644	-0.279103422195
C	-6.598139990142	1.201710168010	1.320764254723
H	-5.943548204499	-0.829141094545	1.047142500994
C	-5.285345943060	2.907735562113	0.224717085185
H	-3.577726486828	2.227841862302	-0.888667018578
C	-6.370379124336	2.547380328291	1.024207880669
H	-7.452883309337	0.912392677924	1.937848121698
H	-5.097863387190	3.959338754048	-0.008409342590
H	-7.043676250282	3.315641696913	1.414114268215
C	-0.106009773914	-2.746389686891	-1.067121771834
C	1.051765868859	-2.162643721564	-1.609020682314
C	-0.034542428465	-4.073064149706	-0.616107228719
C	2.244955581774	-2.871073781483	-1.674468644276
H	1.037028168292	-1.132885611316	-1.971832568458
C	1.157291827382	-4.788688567127	-0.693550431561
H	-0.906958140605	-4.562015128157	-0.180093965708
C	2.302265790101	-4.188034112192	-1.213571787476

H	3.136470315426	-2.391451126705	-2.086252334042
H	1.192009193333	-5.819651064509	-0.332624021952
H	3.241564472568	-4.745295098372	-1.262284349764

Int3' (NIMGA = 0)

C	-3.204814588329	-0.774535792463	0.603799418826
C	-2.220884032333	-1.810749003161	0.584082860403
C	-2.561137896191	-3.130876879742	0.315870520878
C	-3.878270709979	-3.515865946977	-0.017000932520
C	-4.803619625090	-2.502822172215	-0.068317858663
C	-4.485130877262	-1.161008112984	0.237893042516
C	-6.226734793314	-2.108759437404	-0.358268151407
C	-5.914847466102	-0.757221726301	-0.059987239167
C	-7.473469653747	-2.513190602327	-0.759299511823
C	-8.446020089687	-1.485028979463	-0.863981483710
C	-8.143360507483	-0.158774317267	-0.583263912409
C	-6.847640356913	0.245754695456	-0.169256006330
C	-2.832566670658	0.568849735277	1.034958687050
C	-3.805627609302	1.536961168738	1.305685326220
C	-3.453662341372	2.799464437753	1.762532259540
C	-2.109680353471	3.148284829792	1.977293234171
C	-1.128050349568	2.229476777488	1.693553652607
C	-1.453000214932	0.924841307920	1.214322464275
C	-0.438035703455	-0.003181060979	0.908357319613
C	-0.769454881491	-1.455647927665	0.828787096088
C	0.225246426990	-2.283550523127	0.022069206804
C	1.220627606819	-3.003363416134	0.694289711868
C	2.182031584119	-3.727415016412	-0.006021150361
C	2.143254697883	-3.743087133141	-1.397313236175
C	1.142458476324	-3.044403931551	-2.071490933879
C	0.166934043443	-2.312224582474	-1.385385372740
H	-0.577500653145	-1.700478982838	1.904809410568
H	-1.775625038549	-3.890748765972	0.323708798361
H	-4.116440782298	-4.557557535014	-0.240627579753
H	-7.722066157437	-3.550676742708	-0.993273076853
H	-9.460570868369	-1.743520173017	-1.179870541243
H	-8.924628817176	0.599347181913	-0.685785128404
H	-6.643496677287	1.300031937642	0.030844822290
H	-4.859814645411	1.289715957814	1.194575633545
H	-4.241285242399	3.527816664725	1.972886685669
H	-1.849284588165	4.137347359701	2.358359105844
H	-0.083555516449	2.491909003134	1.866528652418
H	2.963988491459	-4.265857062007	0.535437439708
H	2.895372694955	-4.298958325708	-1.963503848953
H	1.115707712599	-3.064741190572	-3.165342071586
C	-0.915979968739	-1.613071807927	-2.170188909882
H	-1.302333784877	-0.712784697502	-1.663881732208
H	-1.785094539250	-2.278415111202	-2.316738328290
H	-0.552357708284	-1.317795335624	-3.167959426270
H	1.251394813024	-2.985000480855	1.788283696825
Pt	1.507649798077	0.453415482481	0.710169092192
C	1.476401281444	2.056830226303	-0.824877289142
C	1.500234179983	0.728495450765	-1.366055698905
C	2.899372084840	2.562034314065	-0.626546932310
C	0.327989750153	2.977768001518	-0.926122564266
C	2.883707008226	0.245139606631	-1.770184333090
H	0.642949590003	0.322048047659	-1.901375487814
C	3.594217690264	1.470403436294	0.164587102000
C	3.550834294782	2.666058859083	-2.033388654713

H	2.946392083580	3.517081273897	-0.095899741147
C	-0.864153185706	2.580070019791	-1.557468726887
C	0.403271283755	4.276466016090	-0.396548169768
C	3.647373193614	0.243214939527	-0.453974560293
C	3.498909775916	1.293145576156	-2.732251871226
H	2.820887613364	-0.751679269373	-2.220765291223
H	4.178283281716	1.714793967429	1.056101716199
H	4.587737345191	3.009676920433	-1.897224345343
H	3.021955146197	3.437564852886	-2.614686802489
C	-1.947722937422	3.445469085260	-1.644095789247
H	-0.959050223290	1.583711932190	-1.992540021944
C	-0.679343198579	5.145992722231	-0.490215240384
H	1.305900662561	4.619336449885	0.111842941394
C	4.421596734610	-0.925216296194	0.010425419341
H	4.502900404329	0.954166643797	-3.030312108381
H	2.881794274393	1.327609968110	-3.643645140790
C	-1.858534713573	4.732180430979	-1.108832050456
H	-2.865881644540	3.114533810211	-2.135425163063
H	-0.601996898173	6.151573368274	-0.069637630578
C	4.951202637885	-1.827250612425	-0.922085028108
C	4.645638966339	-1.152185353583	1.378428407629
H	-2.710569907419	5.413687715834	-1.176568952170
C	5.695962012950	-2.926004500686	-0.498397137927
H	4.796937180984	-1.671728939672	-1.992557883131
C	5.371714198561	-2.261219048406	1.800540480774
H	4.228980097397	-0.469398333394	2.125052252644
C	5.900822324259	-3.150592614306	0.862327609084
H	6.109669719885	-3.616103177575	-1.238234476189
H	5.523989167029	-2.434229269386	2.869075277537
H	6.472158963880	-4.021483516665	1.194819780895

TS3' (NIMGA = 1, 718.31*i* cm^{-1})

C	3.275473710543	-0.628495109143	-0.483391494762
C	2.315731796857	-1.671349709246	-0.244099308517
C	2.703081337593	-2.961476439403	0.143915740695
C	4.044198078042	-3.301446350560	0.372535928675
C	4.951681688578	-2.281542540111	0.191586239975
C	4.590359200691	-0.982084140702	-0.228329764969
C	6.396529528257	-1.881214012206	0.244098263930
C	6.051802550766	-0.571205005772	-0.174586731811
C	7.683706218501	-2.268175151763	0.515214737245
C	8.669191508282	-1.262030598667	0.352428249701
C	8.338211482013	0.025300672776	-0.052211553659
C	7.000827193704	0.410235775786	-0.329715291244
C	2.830797943832	0.661700360444	-1.005664622321
C	3.755137004947	1.651707886020	-1.374063641435
C	3.338361526619	2.854182365192	-1.921496652387
C	1.976323610325	3.097577244094	-2.133051840025
C	1.048415865828	2.136541331686	-1.775610280222
C	1.450269200271	0.918417362117	-1.195200925728
C	0.447402266249	-0.057419041412	-0.759452139848
C	0.890042214148	-1.352052213643	-0.348431924319
C	-0.111044161418	-2.354930638774	0.150280921672
C	-0.243486053820	-2.576342585437	1.533311755002
C	-1.170839326236	-3.536205009357	1.956494771298
C	-1.921411489655	-4.277523963509	1.046816743767
C	-1.773147834424	-4.057470917758	-0.321466668900
C	-0.872696678766	-3.094217144426	-0.764561756190
C	0.611725477227	-1.873916907618	2.558244321965

S27

H	0.541839169108	-1.107777185234	-1.585700408925
H	1.934508137023	-3.723523236314	0.287506762590
H	4.326251985608	-4.309638039833	0.680049393159
H	7.952095355069	-3.276410855455	0.838077607320
H	9.716398371456	-1.504376015348	0.552973688414
H	9.132228701922	0.769319313219	-0.160270096964
H	6.784460148550	1.435071727663	-0.639176060467
H	4.819693209887	1.467344576283	-1.246390385110
H	4.079670923876	3.608114237441	-2.197859238808
H	1.644720968851	4.040479616574	-2.573425047229
H	-0.012779038551	2.335722686291	-1.938424977886
H	-1.292091390152	-3.714609614347	3.029110007967
H	-2.628746395237	-5.028060082523	1.409850971771
H	-2.357463884749	-4.631242817871	-1.044700801983
H	-0.745823029439	-2.928293245855	-1.838929511177
H	0.021595178037	-1.610196194463	3.451026975454
H	1.088429641655	-0.959699236245	2.171428442691
H	1.431571276580	-2.535303599793	2.890739620162
C	-3.542170058689	1.587667110618	-0.212108813923
C	-2.846715661029	2.608039655181	0.666794273361
C	-1.487048341329	1.978936478812	0.939632807934
C	-3.753438038724	0.354218281829	0.371899762781
C	-1.651902320980	0.647809134319	1.454822691179
C	-3.097118393493	0.273962752552	1.746088234067
C	-3.596635395458	2.736019242953	2.017719680898
C	-3.719433474574	1.347726519892	2.674017736226
H	-2.776488967723	3.572280704422	0.156441789593
H	-3.159794572556	-0.722155648288	2.195365707592
H	-3.049647939308	3.442439596735	2.661703307857
H	-4.585539375728	3.174897280707	1.814530280792
H	-3.194309567560	1.310643407179	3.641139203065
H	-4.770589078759	1.080031401126	2.862119010136
Pt	-1.566995521564	0.413955132469	-0.613081248088
H	-0.864862736484	0.156600727788	2.028422969729
H	-4.001749406248	1.895312957635	-1.154512603193
C	-4.607130493719	-0.715726733694	-0.182503580467
C	-5.564046299029	-0.430687625282	-1.171754950003
C	-4.469899026998	-2.037672925949	0.263348300422
C	-6.354841473207	-1.444860813583	-1.701894000445
H	-5.711509864164	0.594362227830	-1.519465046212
C	-5.257903631015	-3.053305659958	-0.272620517429
H	-3.724169327738	-2.290792932961	1.019164682522
C	-6.202332099177	-2.760021899194	-1.255649993023
H	-7.100919978603	-1.206600860514	-2.464405243985
H	-5.130187536795	-4.079927649351	0.080838895461
H	-6.825626726067	-3.555543362477	-1.672902605461
C	-0.264139666026	2.790652065166	1.084442008924
C	0.893798998548	2.250935356206	1.670487310364
C	-0.222205236225	4.114890688988	0.620416207332
C	2.059285428009	2.999528488810	1.769388037971
H	0.899572877334	1.226448486667	2.046939653938
C	0.941436313811	4.870520581761	0.731391975274
H	-1.094763727672	4.570449224108	0.150249927245
C	2.086870692396	4.313607801519	1.297534342749
H	2.951446991269	2.554756127234	2.216801270198
H	0.954618425874	5.898467009095	0.360905241142
H	3.004450353907	4.903073670426	1.372657428385

Int4' (NIMGA = 0)

C	-2.505845148471	-1.058669103427	0.564107858732
C	-1.429486473045	-1.969173946983	0.214058831010
C	-1.665243442764	-3.063611041749	-0.649237791181
C	-2.881364825258	-3.271804805780	-1.301167145842
C	-3.859127848102	-2.333231599485	-1.035603160072
C	-3.688924091548	-1.272323354306	-0.120808922572
C	-5.270211836663	-1.906837122335	-1.299369734117
C	-5.121105963458	-0.838609941084	-0.379300611451
C	-6.428800227507	-2.143906741743	-1.995067731563
C	-7.488478632899	-1.238976865270	-1.738267888287
C	-7.348684441492	-0.187746923473	-0.839532128498
C	-6.144625510932	0.042123189465	-0.125516807937
C	-2.330003685389	-0.068470179247	1.620423768262
C	-3.401516938604	0.679207202974	2.139654781497
C	-3.208179884082	1.574028863362	3.178838739971
C	-1.930524053645	1.753689857962	3.726639810967
C	-0.864086657223	1.015889325310	3.240210043573
C	-1.055120143662	0.093927378032	2.195619180131
C	0.054960008010	-0.724736433224	1.720885531955
C	-0.137400150306	-1.795677494663	0.821580361217
C	0.984326200504	-2.772147658823	0.667906690578
C	1.485254276594	-3.314748521943	1.867298266999
C	2.558445816254	-4.196468381518	1.875175855087
C	3.168660484958	-4.539156251577	0.669378534345
C	2.679834186098	-4.012792136966	-0.521447234767
C	1.585321471958	-3.138093065833	-0.558056041380
H	0.893704466450	-0.836227700482	2.427220532996
H	-0.865967569224	-3.788308697358	-0.800736472324
H	-3.029410896684	-4.124984383289	-1.964750791327
H	-6.545509850171	-2.966086899740	-2.704382554241
H	-8.439556712289	-1.369457028330	-2.261397132967
H	-8.193281904689	0.487267931343	-0.676157532273
H	-6.073721062589	0.885562232690	0.564645897959
H	-4.403106800292	0.541019186159	1.736784240255
H	-4.056403436247	2.142136371803	3.568742761352
H	-1.778094567456	2.462246601472	4.544786120041
H	0.133059039831	1.132338679489	3.675273922491
H	2.917740934916	-4.609979539027	2.820752806223
H	4.023556210079	-5.220428202475	0.654872674744
H	3.161168916358	-4.285361788440	-1.465887058603
C	1.139461698404	-2.656863252688	-1.917315092131
H	0.379940535337	-1.869109516898	-1.871223268816
H	0.707645156061	-3.489287192725	-2.498625445524
H	1.994468792780	-2.284985224009	-2.505073071364
H	1.004587426605	-3.054791666656	2.814096814790
Pt	1.380553729134	0.591590168145	0.462630477984
C	0.224831712890	1.969134311995	-0.837912874247
C	0.688166758146	0.792683282842	-1.507563933369
C	1.279668102954	3.064099582070	-0.876923882883
C	-1.185621094886	2.279565926177	-0.572643643209
C	2.016686919124	0.970821465440	-2.228673269973
H	-0.016271964954	0.023858691067	-1.832514203714
C	2.481173280972	2.347169318989	-0.297333871396
C	1.536820803979	3.451005381720	-2.354129268359
H	0.999953304566	3.935615395704	-0.276041749206
C	-2.193719806035	1.702566320418	-1.362016295983
C	-1.532130295648	3.241488678823	0.390989502636
C	2.943413205606	1.258815277898	-1.053850181604
C	1.947558500428	2.204295277152	-3.160023017953

H	2.301494868064	0.069320451462	-2.780190276249
H	3.068414877421	2.803825746728	0.504157312465
H	2.326602254331	4.217739350376	-2.367494367975
H	0.623867867433	3.913463812905	-2.760090930122
C	-3.517365829136	2.104897124736	-1.210901879721
H	-1.947683711458	0.965040849609	-2.128965124415
C	-2.857570451557	3.622969251600	0.553346946073
H	-0.762595841876	3.680855172223	1.030688787700
C	4.233168551422	0.580308389475	-0.829817185198
H	2.931129616516	2.335990673446	-3.636362837579
H	1.223737305100	1.984673003501	-3.960034279208
C	-3.850321016924	3.063429870162	-0.254535019256
H	-4.291373184091	1.668483969170	-1.846586172359
H	-3.120347562929	4.361223216802	1.314601220748
C	4.412031792917	-0.758231685437	-1.214408965424
C	5.291215450263	1.253643447438	-0.196295319440
H	-4.891121948876	3.376776381145	-0.135358938839
C	5.611551011690	-1.414120940479	-0.958454842579
H	3.598430782617	-1.305513766584	-1.691630345917
C	6.496395423624	0.600671188271	0.043417673822
H	5.185447610837	2.302427660008	0.090637940805
C	6.657274958438	-0.734848667443	-0.331289221398
H	5.728808445531	-2.460896047185	-1.249761422267
H	7.316852139332	1.138790569926	0.524725830430
H	7.603122406619	-1.247084172831	-0.135816289847

2-4-3) oxidative addition of non-substituted biphenylene

1-Phenylbiphenylene (NIMGA = 0)
C	-0.754441450655	1.027411915203	0.071609770680
C	-0.856699031418	2.449844661234	0.124711094418
C	0.255240937379	3.278888641963	0.146422346954
C	1.578862975861	2.766073787073	0.112707969857
C	1.676921091003	1.399178498160	0.066549732957
C	0.539227078701	0.551818827681	0.048659815995
C	2.577842975547	0.191712512978	-0.016992798039
C	1.439485112957	-0.656660536994	-0.041238159305
C	3.859345760810	-0.294024275861	-0.078908793111
C	3.978782929340	-1.706273356714	-0.169966933271
C	2.865234071265	-2.536790596980	-0.197613701527
C	1.543223383610	-2.022469403163	-0.132888070764
C	-1.946352903897	0.145747218693	0.042736687041
C	-3.116366004544	0.525488518707	-0.631721958563
C	-4.227075555945	-0.317115250611	-0.661173052291
C	-4.188506775746	-1.554057416823	-0.015799743691
C	-3.030760728568	-1.942260458191	0.660746815947
C	-1.920914589293	-1.099475640122	0.689377038728
H	-1.850355461761	2.905014603083	0.169971468843
H	0.104813351814	4.361209222733	0.195464958501
H	2.443524921794	3.433548607256	0.122095162068
H	4.745700918086	0.344804468145	-0.062580331138
H	4.976307024067	-2.152379402139	-0.220930279261
H	3.010052246023	-3.618639943479	-0.270361748838
H	0.679561544274	-2.691396139570	-0.157935403099
H	-3.154757969819	1.483197108680	-1.158725571923
H	-5.127842972389	-0.006457389582	-1.198298284588
H	-5.059910727498	-2.214578221111	-0.039553515894
H	-2.992641041337	-2.906366515702	1.175906407934
H	-1.025602789649	-1.403118183100	1.239934622705

Int1" (NIMGA = 0)

C	-0.067016111239	-1.498041985937	-1.624943104789
C	-0.518961711614	-0.924486418868	-2.862466069062
C	-1.846894028301	-0.643378119686	-3.100630677112
C	-2.883688001870	-0.910816072450	-2.151861607693
C	-2.469678485271	-1.390538794095	-0.951330287930
C	-1.075633138564	-1.635983498432	-0.640960070398
C	-2.874294486962	-2.055766101882	0.320977876120
C	-1.528264675146	-2.370632937962	0.613747208929
C	-3.913158762114	-2.431957956594	1.140224627615
C	-3.542346731381	-3.137847923127	2.306281199919
C	-2.211944333781	-3.434940337420	2.600838430109
C	-1.151153806639	-3.054338312568	1.748240489309
C	1.331896965279	-1.943578014378	-1.427878161088
C	2.400362601483	-1.250262430377	-2.027849475055
C	3.712951120304	-1.622444414229	-1.767410740963
C	3.980805872478	-2.699933968300	-0.919169561616
C	2.930600790011	-3.412234499810	-0.340607018725
C	1.613378575064	-3.035978873385	-0.590102064222
H	0.210264225112	-0.747322610157	-3.655071860961
H	-2.123744305996	-0.235557312892	-4.076598684578
H	-3.932804625208	-0.763718795783	-2.411691858139
H	-4.958890098886	-2.206123024987	0.922041708036
H	-4.321758285322	-3.460885433918	3.001561664044
H	-1.981437173573	-3.979038992963	3.520551115780
H	-0.115309965669	-3.292267488322	1.998746626346
H	2.204883354123	-0.383671090696	-2.664826774070
H	4.534803938151	-1.060850226285	-2.217967278632
H	5.015308307759	-2.985058407192	-0.710347368830
H	3.136235684010	-4.266950090400	0.308570032441
C	-1.080382665378	1.916839287707	0.130909165529
C	-0.487678831708	2.573977894492	1.367767896218
C	0.753822086314	1.729549615524	1.597750339360
C	-0.110537480125	1.843002044638	-0.916533001236
C	1.705348391646	1.784767038717	0.564646802392
C	1.184368643000	2.584427894821	-0.620312207222
C	-0.093505379964	4.029443893089	1.017499609016
C	0.863297375874	4.036316360738	-0.190116956645
C	-2.532330629514	1.789482568980	-0.064871246651
C	-3.338682082712	1.258106440182	0.952571426707
C	-4.709581999118	1.128808759570	0.758731355237
C	-5.289559384211	1.556141509081	-0.438267599704
C	-4.495614759167	2.109911117408	-1.443304708363
C	-3.118824116960	2.216977267313	-1.264435117098
C	3.073686306859	1.248718623449	0.642863221446
C	4.081396834710	1.762388148687	-0.188338309489
C	5.382851748566	1.274340255289	-0.102485818376
C	5.690262453979	0.252222302681	0.794608064977
C	4.692722666545	-0.278401838866	1.615735379714
C	3.397483551691	0.219462134185	1.548399018100
H	-1.169483149418	2.531425216998	2.224527029113
H	0.997433842850	1.366289547142	2.600207851426
H	-0.396542613811	1.633904230937	-1.952499168615
H	1.854783296619	2.546890995474	-1.484452635193
H	0.377145471959	4.473852025699	1.907943509623
H	-1.010738598205	4.602331229172	0.810443137546
H	1.807917279376	4.549457693785	0.046393285892
H	0.418378576129	4.554227179287	-1.053910048987

H	-2.885702261350	0.908074450906	1.884752916423
H	-5.330158270649	0.692531197680	1.545406166748
H	-6.368667484333	1.461168632331	-0.585439470216
H	-4.949512162206	2.454968938010	-2.375568862789
H	-2.503456711431	2.653631477897	-2.055055176100
H	3.865765929750	2.566557042326	-0.894894781168
H	6.160125570755	1.694181008635	-0.745684594559
H	6.709783298004	-0.138296389467	0.850991626378
H	4.925156559445	-1.088489464587	2.311273001445
H	2.627595896710	-0.217313331682	2.190867087190
Pt	0.137963029311	0.095685417304	0.245353965748
H	0.794088955741	-3.610721879325	-0.152780498611
H	0.969565455659	2.806476831746	-1.887769034211

TS1" (NIMGA =1, 226.94i cm^{-1})

C	0.724648913028	2.294613474225	1.164804386498
C	0.543566773132	2.895682661802	2.436340999290
C	-0.705776372606	3.024139965271	3.030218838063
C	-1.873973237973	2.611115470834	2.364962221575
C	-1.717577243760	1.978822655264	1.147168295084
C	-0.431113494338	1.754541514657	0.621341470844
C	-2.561665810114	1.689280575759	-0.015337685217
C	-1.606242888128	1.286773063972	-0.963352142423
C	-3.852120900997	1.981099809464	-0.413467497062
C	-4.156393383741	1.863346929075	-1.780535486459
C	-3.174739189853	1.552226884763	-2.718026145673
C	-1.846655174540	1.298253814576	-2.326069760555
C	2.049794127921	2.255324676549	0.503553251870
C	3.204755514076	1.899168970202	1.211917209387
C	4.440696350546	1.882204820272	0.571685298728
C	4.537670853394	2.217706803299	-0.780239632039
C	3.393524314677	2.573217359698	-1.492963476422
C	2.154262085300	2.596231030043	-0.853936868659
H	1.426973623488	3.281866882546	2.952554613874
H	-0.783210747345	3.508055101894	4.006916173984
H	-2.864301700235	2.831301607384	2.769759396560
H	-4.600027091787	2.333295568323	0.300058809864
H	-5.175823157621	2.061915887408	-2.121044918431
H	-3.429892802888	1.501604983606	-3.779505076547
H	-1.080241614115	1.068706441640	-3.072142953880
H	3.133071209015	1.615483252715	2.265742033563
H	5.335157766068	1.593288844194	1.129414559000
H	5.510268756193	2.197833412163	-1.279269509796
H	3.464717669605	2.843788102736	-2.549849039912
C	-1.352945747504	-1.673092877317	0.390820851836
C	-0.697898471112	-2.835111957468	-0.330373734064
C	0.610593761066	-2.228790397492	-0.825146798696
C	-0.433595670271	-1.097000736478	1.323275221172
C	1.501874540494	-1.847957931373	0.188708772758
C	0.832450085626	-1.908902418741	1.548665838118
C	-0.407684156752	-3.945790413277	0.713053434362
C	0.431089341496	-3.371644400037	1.869171411705
C	-2.801452899397	-1.450074571534	0.402057722783
C	-3.557377806436	-1.653593411013	-0.764296400355
C	-4.929245944146	-1.434075809449	-0.753505262496
C	-5.562947590699	-1.032546072567	0.424931113656
C	-4.821873277423	-0.843452914930	1.591892305013
C	-3.444767151974	-1.041028548105	1.581592171337
C	2.925062123901	-1.568556527590	-0.001934376935

C	3.814408614307	-1.691971401198	1.079608377439
C	5.185168443805	-1.557767016322	0.881597309184
C	5.682483703126	-1.270258053871	-0.388765147204
C	4.805851350905	-1.111978080950	-1.465273733771
C	3.439127689023	-1.265659236626	-1.277581827894
H	-1.304470153679	-3.210663020435	-1.161071403166
H	0.940813943390	-2.418304389722	-1.850006675699
H	-0.763476330526	-0.406259101907	2.103122044697
H	1.435018036390	-1.458134081625	2.343271205816
H	0.124009338228	-4.756489045992	0.191663452966
H	-1.364852879784	-4.355062440846	1.071216905134
H	1.345847395505	-3.959820527531	2.037256725400
H	-0.132571719162	-3.366333292335	2.815242381825
H	-3.065367079728	-1.949056598374	-1.694643560719
H	-5.508612373680	-1.574433014860	-1.669172432710
H	-6.643382379119	-0.865970684101	0.432382793240
H	-5.318507281775	-0.537868866657	2.515925374485
H	-2.877027582995	-0.897929038207	2.503855177640
H	3.447643433186	-1.928747663957	2.080292015689
H	5.867480023981	-1.675736324234	1.726847473494
H	6.759138898969	-1.157251690384	-0.540930842038
H	5.192630951282	-0.865842931115	-2.456967763402
H	2.765013978485	-1.132569588371	-2.127723584989
Pt	-0.036968126396	-0.128398375498	-0.524669336316
H	1.259858402979	2.902507396804	-1.406303274168

Int2" (NIMGA = 0)

C	-0.262959680476	2.863085531649	-0.536831018727
C	0.279970757453	4.096071425413	-0.941627530681
C	1.604144708242	4.430257627281	-0.674279799441
C	2.438974507006	3.533870812290	-0.007176611720
C	1.937871205892	2.297885076703	0.399258709305
C	0.588575967571	1.992766556580	0.145280076759
C	2.695624114718	1.218842608026	1.045634816130
C	1.956554598883	0.051817535264	1.268043141130
C	4.044034631962	1.222618994734	1.407637636689
C	4.617085931487	0.080052559071	1.967692779938
C	3.853650788650	-1.068654513797	2.181540716012
C	2.497344512705	-1.089948389211	1.836763654971
C	-1.672867640962	2.530127622532	-0.891057757888
C	-2.025461508614	2.423331726535	-2.243396380221
C	-3.331978856124	2.103248768195	-2.610746186038
C	-4.303586461457	1.895839282371	-1.630357656244
C	-3.965924176672	2.014844220317	-0.282165682792
C	-2.659909372047	2.334382253027	0.087593816372
H	-0.364960021468	4.800248503442	-1.474642849783
H	1.994239770703	5.398645826197	-0.997019732923
H	3.481485048020	3.797000475112	0.188345890356
H	4.654527942980	2.115235477157	1.248790683561
H	5.674863428180	0.086485730741	2.242162070741
H	4.310024485865	-1.959213326729	2.621460659240
H	1.895473613260	-1.988562529111	2.003461746593
H	-1.262732863145	2.575437804160	-3.012893066526
H	-3.590783106599	2.012473187904	-3.669179623900
H	-5.326982094186	1.639360608044	-1.917716356751
H	-4.724167926700	1.857482372157	0.489112747847
C	0.942977319909	-1.741097638100	-1.162335789423
C	0.178313883584	-3.012884526122	-1.245333638054
C	-0.979392314545	-3.035076177142	-0.280090290650

C	0.044652253446	-0.555812315043	-1.064557156392
C	-1.843171677872	-2.014012700583	-0.393016269295
C	-1.397132140493	-0.986540224447	-1.412955130513
C	-0.418804675743	-2.902264466183	-2.709736772088
C	-1.311909929955	-1.654148542216	-2.809813672636
C	2.344504394559	-1.667893494590	-1.342952287698
C	3.157602505208	-2.829360505646	-1.202670604825
C	4.531959366697	-2.742780093593	-1.312401524132
C	5.130461135956	-1.506501419009	-1.583108490883
C	4.355288263497	-0.352183412031	-1.750178713189
C	2.982571167786	-0.426094202436	-1.626381159213
C	-3.088820066001	-1.839983108105	0.380736698568
C	-4.243883206492	-1.357747621862	-0.250756356594
C	-5.431344951835	-1.207921209377	0.461994515601
C	-5.476986470248	-1.523857186397	1.820689798045
C	-4.329736639325	-1.995687535643	2.461569893346
C	-3.143445102728	-2.154943131320	1.746487044912
H	0.798333490692	-3.910063346188	-1.177928497158
H	-1.106316244220	-3.885284657612	0.394166220223
H	0.383489635358	0.265207542572	-1.712584823936
H	-2.055957125787	-0.109373213115	-1.442509354454
H	-0.988547323050	-3.831398916425	-2.860868064699
H	0.400738800793	-2.889258392278	-3.444339451691
H	-2.328749473533	-1.913684982733	-3.139736328396
H	-0.907431942227	-0.928362829959	-3.533745380211
H	2.711283876754	-3.793854779758	-0.960904983420
H	5.148444107569	-3.633841346618	-1.178995625021
H	6.218736147366	-1.441080365595	-1.664878171317
H	4.833393371971	0.604708707288	-1.968281596049
H	2.392036940321	0.480937154210	-1.763898294041
H	-4.220474023466	-1.105777349165	-1.314825008046
H	-6.325271930605	-0.837024858823	-0.047272193533
H	-6.407219027812	-1.399133661902	2.381812530584
H	-4.357457106793	-2.237285991879	3.527638775729
H	-2.242402482224	-2.511558573899	2.254803299339
Pt	0.001054018111	0.211692044420	0.881502558375
H	-2.402337957567	2.440607785176	1.146443427849

2-4-4) Isomerization between Int1 and Int1'

TS-S1 (NIMGA =1, 16.55i cm^{-1})

C	-1.247920593608	1.572923538042	1.181540549379
C	-0.789939030286	1.025389144911	2.446571347618
C	-1.577679606422	0.168735759066	3.201511693068
C	-2.890344566447	-0.204889518016	2.800643067362
C	-3.318305808150	0.277020994905	1.589250501022
C	-2.516234494695	1.135275084253	0.797767165260
C	-4.470351381100	0.515455612273	0.642560724334
C	-3.653973075985	1.367344311964	-0.141067060723
C	-5.799825349289	0.320609375053	0.367157577245
C	-6.287364786580	1.000324481565	-0.775315578635
C	-5.479266565391	1.828739015301	-1.551240051793
C	-4.117166368370	2.047233480241	-1.241359660353
C	-0.705732686472	2.853062807680	0.632829626647
C	-1.389229045915	4.047659640049	0.878590008687
C	-0.890259035146	5.250677588713	0.384931179958
C	0.296084531545	5.268524745025	-0.354085085035
C	0.979283040565	4.083669521615	-0.603742349555
C	0.473758550834	2.871753133543	-0.113176813078
C	1.151247653618	1.586180369452	-0.349728222727

C	2.269805887860	1.356769070014	-0.909384771052
C	3.519277490329	1.096991668253	-1.433022155517
C	4.679526950929	1.368710317296	-0.638312382084
C	5.921751701516	1.116141414173	-1.215357589133
C	6.023247912390	0.594156847946	-2.504600573066
C	4.886134618951	0.326330158608	-3.283802640241
C	3.639187900359	0.595920452314	-2.761608678011
C	4.558908960396	1.955088404129	0.733655648580
H	0.171753545350	1.362951120323	2.842147672565
H	-1.188644411043	-0.196344987817	4.154944393251
H	-3.516023658287	-0.817331744569	3.453236184369
H	-6.452890479763	-0.317174684756	0.966025559398
H	-7.335674886949	0.871275234227	-1.058649802002
H	-5.913860736406	2.328416048171	-2.421227120456
H	-3.494938000791	2.712769237747	-1.843218595722
H	-2.313868802046	4.032559653219	1.462053755007
H	-1.428683351077	6.181799579075	0.579163702118
H	0.688095496352	6.212539823179	-0.740773854556
H	1.902616679245	4.093629024592	-1.189382310403
H	6.830233468291	1.316429698240	-0.642145412666
H	7.014918323899	0.393459814952	-2.919535927340
H	4.991158301361	-0.075162071014	-4.293589737609
H	2.733581033918	0.423300546531	-3.348362634658
H	4.357367010372	3.039281138363	0.661297859259
H	5.490421089334	1.818784152830	1.302413127196
H	3.727198657024	1.502191765125	1.296525997729
C	-0.724937694617	-2.146676811753	0.933655677309
C	0.649851202007	-2.754805428724	1.130711877201
C	1.562486498156	-1.819402111031	0.355828233348
C	-1.150139365503	-2.117721991259	-0.391324397257
C	1.116100305245	-1.643506145429	-0.975787506872
C	-0.050893423369	-2.536156616680	-1.353155605866
C	0.704590502961	-4.146674963205	0.445385240648
C	0.316873094568	-4.011753363428	-1.039684691274
H	0.924063028721	-2.811578772189	2.190011974755
H	-0.343044968468	-2.403794887292	-2.400684332319
H	1.719294401422	-4.557987158086	0.563538516331
H	0.014166230846	-4.814365681280	0.983685248828
H	1.147066179431	-4.302500292069	-1.702258117627
H	-0.544228677888	-4.649277091785	-1.293511474744
Pt	0.073023948580	-0.161893156286	0.197146595818
H	1.767712775087	-1.243092482297	-1.756588094447
H	-1.419967965319	-2.051407496896	1.770483865128
C	-2.546736784110	-2.026659070221	-0.844996190020
C	-3.543578116172	-2.718857491189	-0.140915146800
C	-2.876186470539	-1.360460620031	-2.034523704783
C	-4.842340036743	-2.769703640743	-0.640047230474
H	-3.292112620903	-3.254603876808	0.778192212833
C	-4.181364097198	-1.391685117884	-2.514576108785
H	-2.108085399707	-0.802640317360	-2.578708527746
C	-5.161485803221	-2.108288184754	-1.825921881861
H	-5.609872040712	-3.327977354015	-0.098050878488
H	-4.435434373576	-0.856381512553	-3.432665371545
H	-6.183558019665	-2.142732760855	-2.212393121448
C	2.923428086533	-1.548691066305	0.855455108400
C	4.029735932797	-1.821774911010	0.040461009983
C	3.124073973383	-1.139167309303	2.182993697914
C	5.320810362012	-1.692495023330	0.551025257544
H	3.884267043375	-2.164906994410	-0.987508264547

C	4.413553469771	-0.993625738345	2.681498703755
H	2.262763027340	-0.918055630397	2.820485225425
C	5.514014991793	-1.275926234085	1.867072107857
H	6.178920367767	-1.917936858599	-0.086957275049
H	4.563744932930	-0.659879204053	3.711228422883
H	6.527442371619	-1.170947767457	2.263409256691

Int-S1 (NIMGA = 0)

C	-1.934668340963	-1.430775315532	-0.950874808274
C	-0.800757333691	-0.871637099686	-1.681897366480
C	-0.954423347200	0.258578865255	-2.525876950352
C	-2.171800109832	0.954403280162	-2.655898261228
C	-3.229377114595	0.379315202018	-1.992422398724
C	-3.117116289007	-0.785330535541	-1.163591375984
C	-4.685506989778	0.455974006037	-1.692766022527
C	-4.588020079179	-0.685654626890	-0.863092156144
C	-5.862649142767	1.143131677557	-1.889850717458
C	-6.981323140354	0.624129575203	-1.206274397572
C	-6.888259121573	-0.503557113033	-0.387834210863
C	-5.674202953787	-1.196193592980	-0.189044046190
C	-1.759333410877	-2.563398444195	-0.025682363988
C	-2.829820447179	-3.423367903968	0.246510677739
C	-2.702378322625	-4.469855920565	1.155341036483
C	-1.490410602336	-4.677893977564	1.814324632428
C	-0.407718704543	-3.846118073894	1.548179958517
C	-0.530026765582	-2.793373719522	0.628896629252
C	0.663325886684	-2.005746217195	0.383151776475
C	1.881380776460	-1.825378605097	0.242084776503
C	3.304624905007	-1.858292172266	0.136106229959
C	3.929491194646	-1.764081820636	-1.129100794621
C	5.313349784184	-1.934366775512	-1.177176208734
C	6.053874977570	-2.192912519180	-0.023290650638
C	5.427309091929	-2.273720314283	1.220584013298
C	4.051583255222	-2.100736878813	1.302639713590
C	3.124870891424	-1.511044667211	-2.372899387361
H	0.000444757987	-1.562338137626	-1.966370995391
H	-0.096613557646	0.562785931264	-3.132915272814
H	-2.259768677343	1.842078547877	-3.283485508743
H	-5.942622037811	2.030334394868	-2.521106832922
H	-7.950730304123	1.116808601887	-1.318302976266
H	-7.788455256125	-0.861504335732	0.119234315059
H	-5.629029609618	-2.065395439122	0.469825145601
H	-3.773503225446	-3.285189136561	-0.285177280688
H	-3.553748198579	-5.127665143263	1.346734985904
H	-1.383599646402	-5.493887426752	2.533161700365
H	0.547224602006	-4.004205826771	2.054537143034
H	5.823969859878	-1.867327058066	-2.141761911417
H	7.136581090862	-2.325771737274	-0.097857725924
H	6.009687476298	-2.471318157782	2.123608666781
H	3.537927640303	-2.167578730474	2.264930062604
H	2.361893822393	-2.296269687853	-2.516943462372
H	3.769655070842	-1.492253850486	-3.264382344230
H	2.598898126816	-0.541531539876	-2.317718382536
C	-0.103050452004	2.325228611428	-0.207597871806
C	1.268049836636	2.950799967317	-0.014716408514
C	2.116579990910	1.790657152856	0.469061256966
C	-0.667839689083	1.832981045794	0.986687769561
C	1.531764975759	1.143563252172	1.574003350826
C	0.321394046467	1.871493834804	2.138548215746

C	1.207250652637	4.007051484149	1.120859629559
C	0.677473769579	3.356643822740	2.411358588349
H	1.646712569619	3.387735930960	-0.943973708047
H	-0.068083810290	1.377127256609	3.035048207611
H	2.214018684536	4.429564350496	1.262805027234
H	0.552374773354	4.824735651290	0.781576235031
H	1.429388941092	3.379277528590	3.215284256595
H	-0.220645386148	3.871211602552	2.786461323842
Pt	0.483205001028	0.209527149547	-0.111473683368
H	2.079114069534	0.421042723967	2.185769647539
H	-0.716488606239	2.599254979625	-1.068418544646
C	-2.096529272128	1.594659611773	1.224569493943
C	-3.051631712941	2.449903680640	0.656457413876
C	-2.510222942212	0.573091226965	2.097687921523
C	-4.397817385475	2.309666105444	0.989661968036
H	-2.739444193315	3.257341927613	-0.010646118929
C	-3.856466043558	0.416475407416	2.397720558443
H	-1.773278841961	-0.113724297029	2.524261313216
C	-4.799736125366	1.296827400703	1.857652732995
H	-5.135375844195	2.994763889154	0.565195492169
H	-4.175582541644	-0.390738554268	3.061554830138
H	-5.857279904962	1.183381494922	2.109232742808
C	3.477552562955	1.587625574641	-0.035620873925
C	4.508744303505	1.220313354584	0.843801634910
C	3.779935384363	1.840029016425	-1.384780831807
C	5.818137827485	1.128833909321	0.384476789947
H	4.293418532739	1.041118842936	1.899671531033
C	5.085274951894	1.717012744826	-1.845715006069
H	2.985062868307	2.109552250931	-2.085258853183
C	6.107031620630	1.372560506354	-0.958668659272
H	6.617564383465	0.859525472763	1.078670500590
H	5.308914120386	1.897703152149	-2.899917318955
H	7.136199370418	1.289993936887	-1.318152466831

TS-S2 (NIMGA = 1, 54.82i cm^{-1})

C	1.771892606462	-2.668949903528	-1.079612323055
C	0.847572069662	-3.639427879705	-1.569462659542
C	0.405075930830	-4.697702466921	-0.791453779721
C	0.830843023250	-4.875864552309	0.552569736811
C	1.725802289518	-3.947107227885	1.015748299511
C	2.202579069255	-2.881619428959	0.207940996843
C	2.574220300550	-3.450815810245	2.161795832108
C	3.066891652893	-2.400907203284	1.343348436218
C	2.985661194419	-3.624338427492	3.459362809609
C	3.944720336898	-2.689706625659	3.931332837972
C	4.446672038539	-1.677612143578	3.121697492555
C	4.017463501691	-1.512348763834	1.778954812991
C	2.214564487723	-1.508014341273	-1.890005071854
C	3.574524189109	-1.247377973450	-2.078125911915
C	3.999050556241	-0.145870221048	-2.819843370010
C	3.066934231374	0.716057914271	-3.399352907379
C	1.708525941239	0.484929059440	-3.217992750110
C	1.274902815133	-0.615442756742	-2.459580219506
C	-0.122677666454	-0.788034184257	-2.148735588485
C	-1.264902207189	-1.091638570772	-1.818873337551
C	-2.562204181652	-1.607756732005	-1.489239401402
C	-2.780860420445	-2.212991895711	-0.230162918445
C	-4.041435301897	-2.766041974428	0.009862875296
C	-5.053236619063	-2.717968109537	-0.947684421830

C	-4.829317689529	-2.103105228182	-2.179941588488
C	-3.584304099317	-1.548194457961	-2.450662132237
C	-1.716286505449	-2.237504358938	0.831866917990
H	0.481708968728	-3.546601225912	-2.595932733268
H	-0.299930818281	-5.412096760602	-1.225320822728
H	0.454998728677	-5.704854478920	1.156205890362
H	2.619164547863	-4.426565413848	4.104072100099
H	4.308735162646	-2.777219705398	4.959040332848
H	5.198277014040	-0.994323194794	3.527168998700
H	4.445267112671	-0.735557632743	1.142091424880
H	4.310692441161	-1.925988720974	-1.638527106784
H	5.068620358675	0.040564207557	-2.946962324171
H	3.399450906038	1.578466332288	-3.981787174351
H	0.967797334438	1.169282786555	-3.639382375801
H	-4.234256564072	-3.245157159437	0.974084902506
H	-6.028124033905	-3.161168855628	-0.726662489996
H	-5.621762145349	-2.061212300362	-2.931357157314
H	-3.386433854563	-1.072111626857	-3.414102594029
H	-0.711518369074	-2.393813739512	0.410013634689
H	-1.911600937172	-3.031198711021	1.569335791029
H	-1.700753148404	-1.275952776283	1.376905085028
C	0.376524045827	1.289867349445	1.530956344172
C	-0.883068873743	1.502149161249	2.353704165506
C	-1.873876917560	1.725387447344	1.220947041271
C	0.800315465447	2.437427613990	0.783903158021
C	-1.422289041263	2.785488383365	0.367106122005
C	-0.223320755364	3.552445700490	0.893666869512
C	-0.759180144837	2.762798578746	3.235825112827
C	-0.424211202309	3.984069675083	2.361132344816
H	-1.107695353319	0.608831941651	2.944797682748
H	0.011990225865	4.408581038971	0.254267404236
H	-1.702071450519	2.904686232533	3.785593020510
H	0.026960059217	2.572470148289	3.982610483004
H	-1.234804474911	4.728822877541	2.382332895900
H	0.491201711730	4.489152785558	2.705353455387
Pt	-0.457480307696	1.055812056865	-0.390781161857
H	-2.077238329082	3.247947902297	-0.377388942445
H	1.049061399531	0.460674755118	1.772589761818
C	2.126407019973	2.610091335567	0.177133601440
C	3.219290519437	1.852877967659	0.631350671682
C	2.320177824929	3.542275686561	-0.858050731003
C	4.480954140478	2.041065451523	0.077142742882
H	3.092009882548	1.138361663915	1.447292638396
C	3.579253922680	3.712695639186	-1.420978117895
H	1.480142315224	4.123076333638	-1.246071688399
C	4.662460817202	2.968698623811	-0.949407475201
H	5.331588825360	1.465294284769	0.450784979161
H	3.717386823899	4.432009979322	-2.231725200444
H	5.654128923655	3.110564941211	-1.386928289913
C	-3.209044234918	1.129083324193	1.165308432297
C	-3.997020830665	1.233867223300	0.001279286247
C	-3.733403222780	0.458945546905	2.284589255805
C	-5.272414559353	0.689426765205	-0.035910351149
H	-3.606038218898	1.726462075071	-0.892436974315
C	-5.016967403737	-0.074821841167	2.245915034186
H	-3.152132575676	0.366609800676	3.203929127926
C	-5.785826747852	0.037215399976	1.087505668555
H	-5.868075733045	0.765222198896	-0.948219273817
H	-5.417575393029	-0.584398838530	3.125342570848

| H | -6.789813765976 | -0.393964751097 | 1.055337376331 |

2-4-5) [4+2] Cycloaddition catalyzed by [Pt{(*R,R*)-Ph-bod}]$^{2+}$
1a (NIMGA = 0)

C	-1.021669559439	0.224572034045	-0.954601007797
C	-0.169828798626	-0.547173905196	-1.799882531521
C	-0.410508625762	-1.885685616350	-2.072710567347
C	-1.522237546754	-2.581444297374	-1.526085625304
C	-2.346283411443	-1.834971078247	-0.724324286566
C	-2.101471988935	-0.464440184946	-0.451668363494
C	-3.574698593817	-1.786426354640	0.152283393131
C	-3.326888950091	-0.415159883035	0.424312819908
C	-4.643969445552	-2.459214505279	0.687738790203
C	-5.490899932461	-1.695099428292	1.533470568942
C	-5.247635965260	-0.352843793609	1.799165902281
C	-4.137977282374	0.333497784897	1.239684626106
C	-0.791810138299	1.659964883793	-0.654037479043
C	-1.861523347443	2.557897426867	-0.761370589589
C	-1.704408538733	3.912074849044	-0.474801246934
C	-0.459868637165	4.396581628304	-0.069481372486
C	0.614195225482	3.521629377866	0.053318469092
C	0.465710764718	2.152518796520	-0.230229189215
C	1.583659813160	1.274689854709	-0.045798804821
C	2.519217021767	0.516420937355	0.112560351651
C	3.592994049860	-0.420187203707	0.265437817877
C	4.857990879865	0.004114901590	0.732067997600
C	5.868666964838	-0.953029873311	0.857618919756
C	5.647742303747	-2.292641868660	0.534380870752
C	4.396350343817	-2.703603914306	0.074099056181
C	3.373096712045	-1.769872707873	-0.059104323384
C	5.099308451857	1.448503318060	1.080330158893
H	0.697075372317	-0.063132518151	-2.256479745302
H	0.277965344578	-2.419454195173	-2.734282205237
H	-1.689369202203	-3.638234607730	-1.746677980800
H	-4.850361704808	-3.514082360234	0.491185716259
H	-6.360554513672	-2.177677286626	1.989041710459
H	-5.931035686528	0.191049900273	2.457805277730
H	-3.959939694282	1.389472836092	1.457071470595
H	-2.835156322550	2.182376811022	-1.089840368859
H	-2.555580985595	4.591261539935	-0.573354934845
H	-0.326166592204	5.458148082082	0.155248897957
H	1.589208218035	3.889507924727	0.382856040289
H	6.853784434814	-0.640740672585	1.217941522112
H	6.458743072779	-3.018364698171	0.643585326653
H	4.216447525510	-3.751613832155	-0.180579037951
H	2.386144632394	-2.075092133918	-0.418397234124
H	4.928690251828	2.101172221919	0.206229413060
H	4.408110461232	1.786515452483	1.872140018115
H	6.131112764179	1.605988521446	1.432147108594

[Rh{(*R,R*)-Ph-bod}]$^{+}$ (NIMGA = 0)

C	1.374458698952	0.526042946318	0.160299780583
C	0.739577911680	1.584498093156	-0.740750335119
C	-0.547914688294	0.844159330416	-1.057071130611
C	0.553555702583	0.253263225448	1.292231209740
C	-1.366875319265	0.585229009618	0.076678348433
C	-0.710209969868	1.092034712135	1.358638645635
C	0.469407280452	2.893094470574	0.028213667918
C	-0.401980730943	2.601475495407	1.268740506795

C	2.797362740436	0.119712222966	0.063937316486
C	3.703183012559	0.835169678258	-0.733516598609
C	5.042876060108	0.455711106828	-0.806781507511
C	5.500565427802	-0.651506431644	-0.093278456652
C	4.610033728179	-1.375451765521	0.701962057960
C	3.274673704930	-0.991382303139	0.783123163712
C	-2.793647512275	0.187006847672	0.007447172790
C	-3.384600006442	-0.511163585314	1.073672974992
C	-4.716693946212	-0.912162946176	1.009690951663
C	-5.484080459953	-0.615701410426	-0.118374266737
C	-4.909804490743	0.081472499132	-1.181745330229
C	-3.574532143579	0.476981132520	-1.121651029806
H	1.318601669808	1.760727448160	-1.654350173316
H	-0.922567321283	0.797756256746	-2.085002632545
H	0.935950331394	-0.240803290250	2.191872232147
H	-1.302909118024	0.861271794235	2.251777388215
H	-0.029288787401	3.602201331468	-0.651787831948
H	1.434658228333	3.342151761831	0.313367417127
H	-1.355794472197	3.152006922388	1.226387040764
H	0.107990451636	2.908555613459	2.195768350320
H	3.373150605288	1.712222740674	-1.294699572267
H	5.733685813602	1.032942687880	-1.427247656608
H	6.550585284725	-0.950121852847	-0.154616084293
H	4.958266541606	-2.245157662891	1.265636585222
H	2.593367264957	-1.572592969051	1.411874841779
H	-2.792939016490	-0.758809282591	1.959834519366
H	-5.158836805579	-1.459357776904	1.846637197889
H	-6.531375872450	-0.926220997539	-0.167105249733
H	-5.506609532259	0.324378232193	-2.065126893203
H	-3.144612779154	1.036159627852	-1.956552760892
Rh	-0.023007781437	-0.993299166736	-0.261301520715

Int-S1' (NIMGA = 0)

C	-0.745263455295	-2.305014474693	-1.092357928410
C	-0.719900060992	-3.481624143429	-0.276360230390
C	0.457333483512	-4.106325282968	0.094352335798
C	1.734235002993	-3.614628062003	-0.293602954465
C	1.723092522133	-2.460095481980	-1.025004153932
C	0.513312477159	-1.810701962141	-1.430963639365
C	2.519653530690	-1.503198973615	-1.867175857254
C	1.324117654789	-0.899565942809	-2.329535059506
C	3.760665389671	-1.098965089455	-2.290174467103
C	3.769775474615	-0.034430451603	-3.225683614000
C	2.594552416447	0.541746832745	-3.697638691651
C	1.318030750590	0.113156784567	-3.257182151065
C	-2.031631280480	-1.792583540406	-1.640411850211
C	-3.003315888906	-2.686508444794	-2.097337622703
C	-4.215105501818	-2.224499778197	-2.611799045849
C	-4.470507513643	-0.855944280483	-2.684841961176
C	-3.512526746254	0.050925264021	-2.240506648919
C	-2.300004799242	-0.410337794487	-1.715659804753
C	-1.342231035057	0.535771965421	-1.204234001440
C	-0.613626802660	1.520048998960	-1.019354528371
C	0.076673915362	2.779135882269	-0.973987972035
C	-0.666385522313	3.980109622776	-0.937166779774
C	0.044748746547	5.182760835661	-0.876160812934
C	1.439261224837	5.204804290355	-0.856337869080
C	2.162783165405	4.011653037753	-0.906291245258
C	1.481007761844	2.802535119957	-0.966179892306

C	-2.170429505370	3.964058438184	-0.991037355242
H	-1.671389451918	-3.906496919335	0.053915643100
H	0.400484380821	-5.010758810346	0.706180479029
H	2.649333085553	-4.145076495305	-0.023692571671
H	4.690037942419	-1.551880176267	-1.939726417158
H	4.728979121130	0.340214058657	-3.593827317243
H	2.656915717167	1.355086101272	-4.425905005668
H	0.405174315446	0.579347848107	-3.633086598523
H	-2.807174571498	-3.761204232443	-2.062949652288
H	-4.961968538935	-2.942180167108	-2.961036031500
H	-5.420667373211	-0.491988027464	-3.083772991259
H	-3.706842310035	1.125249419861	-2.273759654334
H	-0.509733509250	6.125214147351	-0.842518880855
H	1.964456846284	6.162533021648	-0.804811158346
H	3.255840995289	4.022987065939	-0.899166665649
H	2.028636797682	1.857686165210	-1.012894342905
H	-2.585969993274	4.959125641701	-0.769252411146
H	-2.519620856875	3.667333103382	-1.996354841656
H	-2.596015200625	3.239174840987	-0.277342419628
C	1.467348161351	-0.239202471336	2.129738384096
C	0.879730987595	1.012212736009	2.772599928462
C	-0.386376548560	1.197802807762	1.953952511765
C	0.576509473046	-1.305489466081	2.178628651979
C	-1.300585048613	0.113491760137	2.050082238526
C	-0.723216930571	-1.011530407799	2.907479070452
C	0.531762255627	0.719182483903	4.251176008984
C	-0.435106544817	-0.479969238509	4.331765073022
C	2.875503702142	-0.325732507972	1.682344231116
C	3.543828247916	0.811532019025	1.203380577321
C	4.856791691788	0.727716310817	0.746761538748
C	5.530465881846	-0.493304261967	0.776372146490
C	4.883412598719	-1.628512430304	1.267887117816
C	3.568125323145	-1.545617751133	1.716478273612
C	-2.745124177921	0.185502673561	1.722906605129
C	-3.445768040445	-0.979092310026	1.373255956606
C	-4.784890304681	-0.920230942402	0.999788738858
C	-5.450909155298	0.306240702707	0.976952774291
C	-4.770126193213	1.469323298554	1.337950158566
C	-3.427675651301	1.409058405283	1.709861659386
H	1.542335937547	1.880598231551	2.688085588223
H	-0.690452804494	2.203517160349	1.652554761478
H	0.857236746863	-2.329733687212	1.924817152048
H	-1.374934796122	-1.892613113874	2.934799302530
H	0.081411096678	1.626484746065	4.684674570020
H	1.464528142779	0.522047688153	4.803981305838
H	-1.390491452551	-0.196447194494	4.802188707243
H	-0.006983869811	-1.300123745533	4.929741424138
H	3.030007545969	1.774978689575	1.168431436908
H	5.355269645797	1.623204211123	0.365999553278
H	6.562250572024	-0.560430260279	0.420524772216
H	5.409190968275	-2.586387832571	1.307711012906
H	3.080943441248	-2.438444074527	2.114726905746
H	-2.928434920772	-1.942274075590	1.359854945659
H	-5.308273245906	-1.836362813860	0.713702774121
H	-6.502138172761	0.355070000069	0.679884846471
H	-5.287787021116	2.432559209466	1.334698515850
H	-2.910813805398	2.325044772208	2.007297256933
Rh	-0.013837136855	-0.160159924661	0.405682105776

TS-S1' (NIMGA = 1, 291.25*i* cm^{-1})

C	-0.851773217307	-2.690825154725	-0.792268853107
C	-0.656138702687	-4.041246567725	-0.383269796397
C	0.597068887306	-4.611407196942	-0.214484693246
C	1.766173622802	-3.885159620696	-0.505584169160
C	1.601309971792	-2.551572083400	-0.809098424046
C	0.321303891743	-1.940953856968	-0.818364428342
C	2.397228315722	-1.497312611032	-1.445423029979
C	1.413683413577	-0.497701582611	-1.610234564787
C	3.617985964369	-1.419271187672	-2.085632124719
C	3.839698612591	-0.313525693174	-2.924577516249
C	2.828125905717	0.609041643959	-3.178976752111
C	1.568755726070	0.503183043003	-2.558182430014
C	-2.197126843674	-2.197074532762	-1.191923796710
C	-3.217358525129	-3.121836627997	-1.459809434457
C	-4.479937887395	-2.727174314812	-1.891224127414
C	-4.753878011469	-1.377766187485	-2.100058785380
C	-3.755221738685	-0.441613231795	-1.867660178755
C	-2.489342385065	-0.828875058222	-1.400952872226
C	-1.560182272908	0.235033875440	-1.106945939658
C	-1.081651965448	1.388202834127	-1.044919779092
C	-0.866206642049	2.815913168174	-1.057706950656
C	-1.974483996944	3.693484109387	-1.135795551865
C	-1.726704172093	5.069332967025	-1.110782909692
C	-0.433801527695	5.581117015906	-1.011275882628
C	0.654132772616	4.712030494460	-0.936298138758
C	0.435447167665	3.340106299083	-0.960201324524
C	-3.381375260429	3.178548470918	-1.260128057615
H	-1.528671829411	-4.663521807062	-0.176613558445
H	0.665908345289	-5.657038977762	0.096068207909
H	2.748086373192	-4.363571156218	-0.523755812843
H	4.370140060102	-2.204270138334	-1.979130986044
H	4.805430560453	-0.203346314213	-3.425204695328
H	3.007539797759	1.432727111815	-3.875316710201
H	0.777801977182	1.213771259223	-2.802657096484
H	-3.027451759966	-4.190159383216	-1.353003776083
H	-5.245783538050	-3.484065680541	-2.079071720543
H	-5.738185317811	-1.052942231604	-2.446124847946
H	-3.957173305252	0.616983573663	-2.028343853328
H	-2.574889801158	5.757939048577	-1.166865791616
H	-0.277589204395	6.663054640300	-0.990115424320
H	1.672838352560	5.099748453216	-0.857452192854
H	1.283278020177	2.655035348634	-0.899661073109
H	-4.112564858467	3.984075217815	-1.091401580191
H	-3.557824434702	2.775120494468	-2.273338780908
H	-3.582350770778	2.370876629677	-0.537321731855
C	1.957568597994	0.137242807547	1.675068768310
C	1.273772055145	1.341556177870	2.316464204687
C	-0.151952271220	1.319004814393	1.792788422306
C	1.232334105136	-1.012730773993	1.890695972712
C	-0.864681139065	0.158621613440	2.083633331457
C	0.019354428709	-0.858132238067	2.785969099118
C	1.238164074206	1.087412503467	3.850508732034
C	0.487847295532	-0.229285202656	4.130709816239
C	3.345199752100	0.179385485665	1.165783810348
C	3.816493475384	1.288015977446	0.448660130216
C	5.115322061030	1.308971267244	-0.050923974713
C	5.969314016427	0.227921394397	0.173738971545
C	5.517110678578	-0.872107914065	0.902290200867

C	4.214089840229	-0.897352562330	1.394356402921
C	-2.330984956317	0.002182910103	1.980670916831
C	-2.906690305244	-1.273658612968	1.878902946516
C	-4.280239763567	-1.425111754497	1.711569963435
C	-5.104811624809	-0.302201460807	1.648948597690
C	-4.547509755518	0.972461317096	1.766144229623
C	-3.173287202290	1.123669098437	1.931648108993
H	1.774673284598	2.287445942911	2.078923312952
H	-0.635445061000	2.254263053557	1.505508286230
H	1.614596566334	-2.007779849646	1.657613607237
H	-0.479940377124	-1.818504518129	2.951218472923
H	0.738808271996	1.944547477247	4.329091589725
H	2.272000101530	1.052752420440	4.229727112688
H	-0.395100447881	-0.064785484780	4.768575191022
H	1.133540064505	-0.959126726984	4.643884343684
H	3.155763102812	2.137710397733	0.258463462654
H	5.461906919799	2.174216067329	-0.622177836976
H	6.990869638384	0.246012031043	-0.215943431872
H	6.184643111520	-1.716796633540	1.093216448455
H	3.875166867946	-1.758331985315	1.976208063547
H	-2.272909115922	-2.163973898625	1.888891624815
H	-4.705818219683	-2.427129001301	1.613980199715
H	-6.183251550918	-0.419247586908	1.512001385092
H	-5.188350989325	1.857598931079	1.730456832457
H	-2.755358938474	2.128453117206	2.031547918686
Rh	0.217760703938	-0.006555325698	0.073051007107

Int-S2' (NIMGA = 0)

C	0.016218723133	0.614645220752	2.838505240998
C	0.716006081924	0.823347555043	4.036168422944
C	2.106366662694	0.690198195279	4.067912381959
C	2.816715852342	0.308121809137	2.927284563319
C	2.131644197085	0.105361652454	1.725987082593
C	0.751864895807	0.321693888962	1.691272122722
C	2.634346492574	-0.433415883531	0.456687305478
C	1.641969102908	-0.564285905856	-0.531139713052
C	3.924893241719	-0.889040100198	0.181749038343
C	4.211483148535	-1.471375511207	-1.053653791558
C	3.209121640664	-1.612981115562	-2.013221753624
C	1.910545336617	-1.157537613920	-1.754353652437
C	-1.463326871460	0.629848940811	2.729250558702
C	-2.254997502701	1.554550263685	3.414211108353
C	-3.642206950139	1.555974563097	3.274019068948
C	-4.272108762301	0.629615205337	2.440388016805
C	-3.511848636489	-0.303520864036	1.747179826790
C	-2.113780024802	-0.317855774131	1.886496819164
C	-1.340207291730	-1.294493576720	1.156861780605
C	-0.725807735568	-2.162417099385	0.533078365825
C	-0.003017665423	-3.268838911077	-0.024718968801
C	1.023785303823	-3.874434571652	0.735282749211
C	1.756683964483	-4.899822675356	0.132162899232
C	1.484667071831	-5.322916686855	-1.168965351304
C	0.456677731722	-4.729733583955	-1.902255159518
C	-0.282482631446	-3.701711704202	-1.329816544922
C	1.312160777721	-3.435610932021	2.144726776405
H	0.171411302715	1.060461118467	4.954868498774
H	2.639917891320	0.851370686029	5.008322823897
H	3.898008110318	0.154090229089	2.984406560085
H	4.708872096543	-0.800001576767	0.939203120392

H	5.223725958256	-1.826010582398	-1.265346622987
H	3.431409211930	-2.081718526004	-2.976071394345
H	1.130930615196	-1.277979963248	-2.511100397477
H	-1.773488718230	2.298342143255	4.054278329018
H	-4.237617926358	2.295548811836	3.815957318724
H	-5.358638653081	0.636732398858	2.326005837063
H	-3.991545858579	-1.032122029324	1.089505787124
H	2.559819048599	-5.380498550048	0.698153179827
H	2.079257572605	-6.126924698101	-1.611435281462
H	0.235666659199	-5.062434390168	-2.919377623035
H	-1.079117897015	-3.218150432247	-1.899024729641
H	2.121217221402	-4.037538884054	2.585941171080
H	1.612959453979	-2.375507167959	2.180370308919
H	0.417111250749	-3.539569592589	2.782265628582
C	0.753696829575	2.013269475462	-1.199813046578
C	0.212722760078	1.711308807766	-2.592805889153
C	-0.907400317980	0.702974868732	-2.472447061560
C	-0.279499644846	2.324473902219	-0.326296758763
C	-1.927368341776	1.066929737603	-1.650431495801
C	-1.652157575976	2.407028266469	-0.975946433141
C	-0.424781072078	3.048457969907	-3.089496575258
C	-1.532277994713	3.477457656703	-2.107172842336
C	2.180981477528	2.329406934253	-0.958245318156
C	3.161177120687	2.028140652750	-1.915496086048
C	4.505189299947	2.295874766416	-1.670927526390
C	4.897380185623	2.869865662246	-0.462383829212
C	3.932859727187	3.184604516278	0.495626335201
C	2.589865639108	2.920779348477	0.248346656796
C	-3.228666334775	0.370969645778	-1.533649206642
C	-4.391117183427	1.076864671369	-1.194355542951
C	-5.617887350895	0.421228563582	-1.097732090920
C	-5.700977936891	-0.951992181146	-1.325173149420
C	-4.549521330258	-1.665901874941	-1.665715641539
C	-3.328185670324	-1.008021026968	-1.772047415020
H	0.982873425072	1.361245309529	-3.286037617970
H	-0.957847066025	-0.153777567693	-3.148859510507
H	-0.118790163476	2.829342616066	0.628844807800
H	-2.415201997924	2.677353463331	-0.236891221287
H	-0.824830952014	2.885050577797	-4.101846700454
H	0.366519928154	3.811252802379	-3.164511908483
H	-2.507758355875	3.567199116270	-2.610317899595
H	-1.307285719157	4.450818791281	-1.644452786941
H	2.889726604818	1.554871720496	-2.859982783084
H	5.251453752858	2.043642228620	-2.428808921423
H	5.953727584154	3.074156393879	-0.267027545705
H	4.227294966564	3.636792930717	1.446345619695
H	1.860304760510	3.166435381759	1.022004987782
H	-4.352163656745	2.153300784771	-1.010864220011
H	-6.514200875718	0.990060924035	-0.836429052519
H	-6.661269821611	-1.467234241298	-1.237340729332
H	-4.601270648157	-2.743478288903	-1.842540406528
H	-2.431156790956	-1.578348711118	-2.022598269981
Rh	-0.164455572705	0.157195869320	-0.053225695981

TS-S2' (NIMGA = 1, 346.38*i* cm^{-1})

C	2.397041886783	1.413156333502	1.092525239917
C	3.108900859054	1.687235344218	2.262122854890
C	2.480605426423	1.620362067020	3.503425896863
C	1.116727847745	1.356814437190	3.581105694055

C	0.371246341618	1.090039654143	2.424249027335
C	1.048072810475	1.018766109867	1.188957920979
C	-1.085634613501	0.909257710145	2.403418436179
C	-1.608386341022	0.416066901099	1.199385472334
C	-1.951083259590	1.276916021172	3.443072466337
C	-3.328357852786	1.175186636034	3.267251104239
C	-3.844997001603	0.716431968097	2.052795021384
C	-2.987478117895	0.338153721658	1.018842882616
C	2.906736466258	1.720955124123	-0.250314229738
C	4.226274728337	1.950513728116	-0.632857927555
C	4.504215225199	2.302121498115	-1.953552850473
C	3.475730361241	2.431899337519	-2.891777453606
C	2.150408589839	2.214893751774	-2.516115025899
C	1.877583063862	1.871725384769	-1.191274963506
C	0.552321918920	1.577386388635	-0.672644878930
C	-0.710610578624	1.558157852967	-0.935892119656
C	-1.976038037438	2.087322526433	-1.344986792189
C	-2.481820631217	3.272979739245	-0.760901861143
C	-3.741387620471	3.709544140081	-1.176146842885
C	-4.478068679324	3.006078344255	-2.131044168876
C	-3.968723304403	1.838723116522	-2.703104443966
C	-2.720074987721	1.379996457872	-2.304939508269
C	-1.714052165956	3.997673625955	0.308499147053
H	4.153851879611	2.000223421124	2.195679286783
H	3.048694218576	1.825783618349	4.414231173045
H	0.621181130986	1.354332317983	4.555010778749
H	-1.554249109332	1.668417031866	4.383697960322
H	-4.003646996235	1.471562324930	4.074493446236
H	-4.926942730826	0.654191294847	1.904836987473
H	-3.410254689334	-0.003413720656	0.071590896861
H	5.041811579673	1.838215714156	0.084725648327
H	5.540286992873	2.471778071942	-2.258508016159
H	3.708859204315	2.708898541702	-3.923152419265
H	1.337406850457	2.315046291345	-3.239340650794
H	-4.160665717923	4.619056589341	-0.736354539253
H	-5.462620002748	3.375799906034	-2.430988780757
H	-4.543861553224	1.289974302368	-3.452928126224
H	-2.296326145196	0.469329634287	-2.734837081137
H	-2.212438518544	4.939851480469	0.583159860637
H	-1.634690935349	3.370645268223	1.215018449947
H	-0.685932142658	4.228786541075	-0.017485904922
C	-1.041945669733	-2.458597042042	-0.227043968240
C	-0.171901912225	-2.805537503827	-1.427927863104
C	1.024285311274	-1.876655896085	-1.445516271848
C	-0.301353170681	-2.375158101599	0.931121308910
C	1.789365598251	-1.919890905021	-0.315576902351
C	1.149273320308	-2.783593908473	0.765025004928
C	0.373785206065	-4.245408673132	-1.144593311321
C	1.144790481146	-4.236578449125	0.188076450312
C	-2.516575766071	-2.509025643538	-0.305043326791
C	-3.183709768434	-2.166120455086	-1.491039118616
C	-4.574835186213	-2.153798098395	-1.548682914318
C	-5.323531933714	-2.503958156223	-0.423907088542
C	-4.671779917720	-2.874308023234	0.753403156173
C	-3.281003748746	-2.876904254126	0.812580546265
C	3.215385742186	-1.532733006662	-0.228105123540
C	3.844562748385	-1.340563820360	1.010269217295
C	5.207365808353	-1.062572609812	1.082514199869
C	5.969183642593	-0.981423644500	-0.083064179005

C	5.357279004500	-1.173976333387	-1.322188481572
C	3.994942426462	-1.448006180399	-1.393317952579
H	-0.721591690948	-2.777209021800	-2.374538834454
H	1.355439956204	-1.418332256148	-2.380914889958
H	-0.742678147849	-2.304184948029	1.927647762914
H	1.685596223516	-2.740148728134	1.718366777208
H	1.019533538722	-4.542844722841	-1.985110216251
H	-0.478003123701	-4.943329082988	-1.116917055298
H	2.188477469027	-4.563189204562	0.054759970377
H	0.679669548057	-4.904625033991	0.929655729332
H	-2.614246742944	-1.877250435507	-2.377448423142
H	-5.076398669098	-1.866869362679	-2.476727309145
H	-6.416039958000	-2.496113280847	-0.467540889777
H	-5.251368791131	-3.162480527465	1.634367270985
H	-2.786058887802	-3.172725004726	1.740332457236
H	3.264548487089	-1.382453962206	1.935152861694
H	5.675506688166	-0.906844806422	2.058244460165
H	7.040584452830	-0.770109994283	-0.025750452658
H	5.946260510577	-1.117123130910	-2.241464760367
H	3.540359663279	-1.624875508611	-2.370729915621
Rh	-0.158576323714	-0.246280347735	-0.043402642556

Int-S3' (NIMGA = 0)

C	2.647105742766	0.038002164219	1.914052289865
C	3.063073136373	-0.843918290943	2.888252959394
C	2.082242195287	-1.482856982601	3.687963696832
C	0.724784765815	-1.249321804195	3.536157802058
C	0.273020126618	-0.327716337815	2.555677307678
C	1.263722330796	0.275439740792	1.776267322190
C	-1.103767754921	0.077405324978	2.262320836377
C	-1.352239767702	1.154207443973	1.329215129515
C	-2.211174265467	-0.488221677995	2.956512310411
C	-3.478827112413	0.002826500858	2.782844015740
C	-3.714914066864	1.091145907893	1.907154066048
C	-2.684850745162	1.642857563732	1.193874169144
C	3.315208219896	0.844583807949	0.877665800373
C	4.662639815787	1.003445475426	0.579046422949
C	5.019823337919	1.828964330297	-0.490412646111
C	4.044582731172	2.478299054075	-1.251376397201
C	2.686040193217	2.331093839948	-0.954132662772
C	2.326391016286	1.520372984620	0.117768419429
C	1.002949698131	1.187294322855	0.690306457604
C	-0.283699353863	1.690865669992	0.495053783751
C	-0.538167169561	2.804242591582	-0.461771228817
C	-0.250392479607	4.121218919620	-0.054823561931
C	-0.460212498152	5.155118045895	-0.973441508754
C	-0.938804895092	4.900230381233	-2.258751001127
C	-1.225667181885	3.593370048964	-2.649212415707
C	-1.025273372603	2.551602397793	-1.745950433947
C	0.285694185514	4.404492137487	1.325272720240
H	4.121250086836	-1.065366148279	3.046550637142
H	2.411042116822	-2.186721120570	4.456926575745
H	0.017454666999	-1.765987087676	4.187219207742
H	-2.040689316509	-1.317420529790	3.645136320259
H	-4.314427896480	-0.442877102856	3.327672281178
H	-4.729239619145	1.477433169057	1.785786086417
H	-2.871609929722	2.464687463952	0.500138812573
H	5.429486113695	0.486817067479	1.161247312554
H	6.076068271253	1.961205661561	-0.740158430361

H	4.345805878302	3.112964490221	-2.089054688186
H	1.930280108884	2.844251986214	-1.552702553141
H	-0.241237887410	6.184319452396	-0.673493649541
H	-1.089837482337	5.728568178421	-2.956468608685
H	-1.603380845572	3.382274145463	-3.652910519473
H	-1.240805562916	1.521484666349	-2.037246810430
H	0.341742739115	5.487979950635	1.513245741200
H	-0.349621579418	3.953530162458	2.107099816950
H	1.301066957936	3.986887549541	1.448867730542
C	-1.925534223536	-1.623702238242	-0.995060385667
C	-1.289549404807	-1.426437199744	-2.370337696907
C	0.086466575697	-0.938280055362	-1.956946263236
C	-1.179821369173	-2.533541481813	-0.211077651118
C	0.827587581293	-1.879638877618	-1.210802828311
C	0.007996549445	-3.140036701162	-0.936239235332
C	-1.200549990602	-2.773176269704	-3.120483552985
C	-0.421341444962	-3.795284657925	-2.266350364871
C	-3.332165021951	-1.229119683580	-0.725488635425
C	-3.912279782097	-0.130824948217	-1.379472850812
C	-5.241897879901	0.216167133844	-1.157820505901
C	-6.024583441682	-0.531086001177	-0.276481584036
C	-5.461607848689	-1.621599796450	0.384451285066
C	-4.128607631265	-1.965859598680	0.163120299219
C	2.304442989520	-1.879175433340	-1.075581576403
C	2.922955163329	-2.580931732635	-0.030949985481
C	4.311242030339	-2.642252753198	0.061591524693
C	5.104956695855	-2.004823759432	-0.891762012848
C	4.501480074226	-1.294388606267	-1.929623252683
C	3.113773682280	-1.228546957288	-2.019124120956
H	-1.817610496183	-0.678923916994	-2.973623634196
H	0.557387865973	-0.089162184169	-2.460086514075
H	-1.575279059719	-3.002913118241	0.693423795924
H	0.545741157226	-3.851207031641	-0.298649923773
H	-0.705881655693	-2.601293484408	-4.090023652912
H	-2.222931122371	-3.124674475363	-3.335181640728
H	0.479091769645	-4.153555087946	-2.791600582082
H	-1.038472538639	-4.679321183349	-2.038355168911
H	-3.319120812358	0.479047829427	-2.064440720043
H	-5.668715753180	1.078474475195	-1.677184492798
H	-7.070905257948	-0.263172080899	-0.105745360709
H	-6.064502698907	-2.216993498949	1.075609717131
H	-3.715719422525	-2.835846784631	0.678292435805
H	2.312693072780	-3.070667720684	0.733310281722
H	4.774979920114	-3.190027596201	0.886619383142
H	6.195107155110	-2.056517834549	-0.822804020820
H	5.115837718018	-0.786854914014	-2.678014212324
H	2.658376988890	-0.686037588949	-2.850887235828
Rh	-0.342221046014	-0.619161181030	0.093596792875

2-5) Electronic state of Pt center analyzed by natural bond orbital (NBO) analysis

Int1 (d^8 electron configuration)

165. (1.98264) LP (1)Pt   84   s(0.16%)p 0.08(0.01%)d99.99(99.82%)
                                                     f 0.00(0.00%)
                                    -0.0001   0.0402 -0.0052   0.0001 -0.0010
                                    -0.0001 -0.0005 -0.0028 -0.0001   0.0007
                                    -0.0003   0.0100 -0.0001 -0.0007 -0.0003
                                     0.0045 -0.0007   0.0002   0.6343 -0.0204
                                    -0.0048   0.6838 -0.0083 -0.0033 -0.3264
                                    -0.0050   0.0007 -0.1354   0.0024   0.0011
                                    -0.0530   0.0112   0.0015 -0.0006   0.0001
                                    -0.0005 -0.0010 -0.0010   0.0006 -0.0009

166. (1.97600) LP (2)Pt   84   s(0.91%)p 0.02(0.02%)d99.99(99.07%)
                                                     f 0.00(0.00%)
                                     0.0001   0.0951   0.0042 -0.0029 -0.0022
                                    -0.0002 -0.0003   0.0015 -0.0004 -0.0001
                                    -0.0005   0.0046   0.0009   0.0004   0.0003
                                    -0.0129 -0.0004 -0.0005   0.4665 -0.0030
                                    -0.0016 -0.0789 -0.0065 -0.0007   0.7375
                                     0.0123 -0.0007   0.2038   0.0017 -0.0001
                                    -0.4257 -0.0017   0.0009 -0.0005 -0.0007
                                     0.0015   0.0019   0.0003   0.0007 -0.0017

167. (1.82955) LP (3)Pt   84   s(0.11%)p 0.24(0.03%)d99.99(99.86%)
                                                     f 0.02(0.00%)
                                     0.0006   0.0337   0.0006 -0.0014 -0.0016
                                    -0.0001   0.0038 -0.0101   0.0021 -0.0018
                                     0.0028 -0.0075   0.0012 -0.0011   0.0013
                                     0.0090 -0.0000   0.0003   0.2975 -0.0089
                                    -0.0014 -0.4664   0.0069   0.0016 -0.5647
                                     0.0032   0.0017   0.5293 -0.0108 -0.0012
                                    -0.3052   0.0030   0.0007 -0.0030 -0.0012
                                    -0.0002   0.0014   0.0036   0.0003 -0.0009

168. (1.81286) LP (4)Pt   84   s(0.00%)p 1.00(0.03%)d99.99(99.96%)
                                                     f 0.06(0.00%)
                                     0.0002   0.0048   0.0028 -0.0003 -0.0006
                                    -0.0000 -0.0001   0.0160   0.0007 -0.0015
                                     0.0010   0.0010   0.0012 -0.0010 -0.0002
                                     0.0066   0.0000   0.0002   0.2791 -0.0013
                                     0.0005 -0.4842 -0.0071 -0.0023 -0.1094
                                    -0.0027 -0.0002 -0.8024 -0.0018 -0.0020
                                    -0.1772 -0.0024   0.0001 -0.0020 -0.0016
                                    -0.0010 -0.0011   0.0007   0.0006 -0.0032

169. (0.30478) LP*(5)Pt   84   s(95.46%)p 0.00(0.26%)d 0.04(4.28%)
                                                     f 0.00(0.00%)
                                     0.0000   0.9770   0.0036   0.0016   0.0015
                                     0.0002   0.0000   0.0068   0.0005   0.0021
                                     0.0000   0.0172   0.0027 -0.0012   0.0000
                                     0.0469 -0.0034   0.0039 -0.1591   0.0079
                                    -0.0104   0.0450   0.0064 -0.0011 -0.0584
                                    -0.0328 -0.0015 -0.0481   0.0065 -0.0012
                                    -0.0910   0.0106   0.0040   0.0030   0.0007
                                    -0.0009 -0.0001   0.0042 -0.0008   0.0009

170. (0.13776) LP*(6)Pt   84   s(0.13%)p99.99(99.23%)d 4.44(0.58%)
                                                     f 0.43(0.06%)
                                    -0.0000   0.0358   0.0006   0.0021   0.0041
                                    -0.0003 -0.0000 -0.2241 -0.0021   0.0049
                                    -0.0000   0.5311   0.0014 -0.0039 -0.0000
                                    -0.8124 -0.0004   0.0048   0.0148 -0.0023

```
                                    0.0038 -0.0213 -0.0121 -0.0007 -0.0096
                                   -0.0544 -0.0021   0.0005 -0.0075   0.0007
                                    0.0397   0.0147   0.0067 -0.0115   0.0139
                                   -0.0116 -0.0013   0.0022   0.0089   0.0039
```
171. (0.11394) LP*(7)Pt   84   s(0.18%)p99.99(99.20%)d 2.68(0.49%)
                                               f 0.74(0.14%)
```
                                   -0.0000   0.0415 -0.0005   0.0089   0.0044
                                   -0.0005 -0.0000   0.5347 -0.0049 -0.0011
                                   -0.0000 -0.6309   0.0046   0.0006 -0.0000
                                   -0.5550   0.0058 -0.0000   0.0197 -0.0180
                                   -0.0046 -0.0049 -0.0465 -0.0013 -0.0062
                                   -0.0050 -0.0037   0.0084   0.0074 -0.0002
                                    0.0378 -0.0168   0.0065 -0.0266 -0.0038
                                    0.0138   0.0053 -0.0149 -0.0139 -0.0013
```
172. (0.07248) LP*(8)Pt   84   s(0.09%)p99.99(99.50%)d 4.04(0.36%)
                                               f 0.59(0.05%)
```
                                    0.0000   0.0277   0.0014 -0.0103   0.0023
                                    0.0003 -0.0000 -0.8120 -0.0053 -0.0122
                                   -0.0000 -0.5617 -0.0034 -0.0064   0.0000
                                   -0.1413 -0.0014 -0.0018   0.0141 -0.0201
                                    0.0019 -0.0063   0.0110   0.0085   0.0078
                                    0.0125   0.0047 -0.0156 -0.0398   0.0002
                                    0.0242 -0.0072   0.0044   0.0031 -0.0120
                                   -0.0125 -0.0029   0.0131 -0.0002   0.0055
```

Int2 (d^6 electron configuration)
166. (1.97794) LP (1)Pt   84   s(0.09%)p 0.01(0.00%)d99.99(99.90%)
                                               f 0.04(0.00%)
```
                                   -0.0000   0.0301 -0.0017 -0.0009   0.0025
                                    0.0002   0.0004 -0.0011   0.0012   0.0002
                                    0.0001 -0.0003 -0.0001 -0.0001   0.0006
                                   -0.0023   0.0013 -0.0014   0.0950 -0.0015
                                    0.0013 -0.9696   0.0036   0.0027 -0.0885
                                   -0.0034   0.0001   0.1130 -0.0002 -0.0007
                                   -0.1710 -0.0004   0.0010   0.0007 -0.0028
                                    0.0011 -0.0025   0.0043 -0.0006   0.0005
```
167. (1.95979) LP (2)Pt   84   s(0.00%)p 0.00(0.01%)d 1.00(99.99%)
                                               f 0.00(0.00%)
```
                                   -0.0003   0.0042 -0.0008 -0.0017 -0.0031
                                    0.0000   0.0000 -0.0023 -0.0000   0.0005
                                   -0.0012 -0.0062   0.0012   0.0016 -0.0008
                                   -0.0041   0.0004   0.0011   0.2633   0.0030
                                   -0.0005 -0.0910   0.0022   0.0000   0.6784
                                    0.0044 -0.0034   0.3807   0.0030 -0.0017
                                    0.5631   0.0008 -0.0038   0.0009 -0.0010
                                    0.0022 -0.0004 -0.0004 -0.0020   0.0007
```
168. (1.91556) LP (3)Pt   84   s(0.00%)p 1.00(0.01%)d99.99(99.98%)
                                               f 0.10(0.00%)
```
                                    0.0002 -0.0002   0.0017   0.0009   0.0007
                                    0.0000   0.0011   0.0019   0.0009 -0.0001
                                    0.0007   0.0078   0.0014   0.0002   0.0004
                                    0.0089   0.0004 -0.0005   0.9450   0.0178
                                    0.0016   0.1484   0.0022 -0.0016 -0.2343
                                   -0.0006   0.0001   0.0449   0.0017   0.0005
                                   -0.1659 -0.0034   0.0001   0.0001 -0.0001
                                    0.0015   0.0004   0.0004   0.0035   0.0003
```
169. (0.10234) LP*(4)Pt   84   s(1.60%)p60.11(96.37%)d 1.19(1.91%)
                                               f 0.07(0.11%)
```
                                   -0.0000   0.1251 -0.0175 -0.0079   0.0031
```

```
                             -0.0002 -0.0000 -0.1827   0.0084 -0.0017
                             -0.0000 -0.9474   0.0132   0.0023 -0.0000
                             -0.1799   0.0103 -0.0000   0.0143 -0.0382
                             -0.0019   0.0049   0.0208   0.0010   0.0387
                              0.1035   0.0143 -0.0399   0.0194 -0.0068
                             -0.0399   0.0310 -0.0048   0.0181   0.0035
                              0.0072   0.0206 -0.0003   0.0081   0.0138
170. (0.06806) LP*( 5)Pt  84          s(   0.78%)p99.99( 97.54%)d 2.13(   1.67%)
                                        f 0.02(   0.02%)
                             -0.0000   0.0863 -0.0097 -0.0159   0.0041
                             -0.0004 -0.0000 -0.9496 -0.0164 -0.0014
                             -0.0000   0.2229   0.0029   0.0014 -0.0000
                             -0.1538   0.0006 -0.0040 -0.0079 -0.0240
                             -0.0021   0.0128   0.0620   0.0068 -0.0097
                             -0.0294 -0.0025   0.0455   0.0923   0.0073
                             -0.0169 -0.0070 -0.0035   0.0059   0.0076
                             -0.0027 -0.0050 -0.0006 -0.0012 -0.0058
171. (0.06213) LP*( 6)Pt  84          s(   1.30%)p74.83( 96.94%)d 1.34(   1.74%)
                                        f 0.02(   0.02%)
                             -0.0000   0.1099 -0.0152 -0.0231   0.0105
                             -0.0002 -0.0000   0.1967   0.0106 -0.0001
                             -0.0000   0.1576   0.0090   0.0057 -0.0000
                             -0.9516 -0.0121 -0.0087   0.0085   0.0092
                             -0.0025 -0.0009 -0.0038   0.0061 -0.0314
                             -0.0117   0.0041 -0.0214 -0.0240 -0.0012
                              0.0430   0.1144   0.0074   0.0000 -0.0005
                             -0.0079   0.0118   0.0008   0.0052   0.0023
```

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