Substitution and Isomerisation of Asymmetric β-Diketonato Rhodium (I) Complexes: A Crystallographic and Computational Study

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Supporting information

Table S1. Crystal data and structure refinement for [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)$_2$] and [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)].

	[Rh(PhCOCHCO-CH$_2$CH$_3$)(CO)$_2$]	[Rh(PhCOCHCO-CH$_2$CH$_3$)(CO)(PPh$_3$)]
Empirical formula	$C_{13}H_{11}O_4Rh$	$C_{30}H_{26}O_3PRh$
Formula weight	334.13	568.39

Temperature	100(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	monoclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$
Unit cell dimensions	a = 10.4080(4) Å	a = 8.9967(3) Å
	b = 7.8360(3) Å	b = 15.7725(5) Å
	c = 15.9878(6) Å	c = 19.3044(7) Å
	α = 90°.	α = 90.051(2)°
	β = 103.2130(10)°	β = 94.536(2)°
	γ = 90°.	γ = 104.963(2)°
Volume	1269.40(8) $Å^3$	2637.48(15) $Å^3$
Z	4	4
Density (calculated)	1.748 Mg/m^3	1.431 Mg/m^3
Absorption coefficient	1.348 mm^{-1}	0.737 mm^{-1}
F(000)	664	1160
Crystal size	0.25 x 0.21 x 0.12 mm^3	0.23 x 0.12 x 0.05 mm^3
Theta range for data collection	2.13 to 28.30°	1.06 to 28.37°
Index ranges	-13<=h<=13, -10<=k<=10, -21<=l<=21	-12<=h<=12, -21<=k<=21, -25<=l<=25
Reflections collected	14494	64974
Independent reflections	3154 [R(int) = 0.0342]	13157 [R(int) = 0.0408]
Completeness to theta = 28.35°	100.0 %	99.8 %
Max. and min. transmission	0.8550 and 0.7293	0.9641 and 0.8488
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3154 / 0 / 164	13157 / 79 / 651
Goodness-of-fit on F2	1.105	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0219, wR2 = 0.0543	R1 = 0.0436, wR2 = 0.1055
R indices (all data)	R1 = 0.0273, wR2 = 0.0572	R1 = 0.0676, wR2 = 0.1192
Largest diff. peak and hole	0.531 and -0.598 $e.Å^{-3}$	1.880 and -0.788 $e.Å^{-3}$

Table S2. Computed Relative Energies for the formation of isomer A (isomer B in brackets) of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)] from [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)$_2$] and PPh$_3$. Results for the substitution reaction via the *A* path in Scheme 3 is presented here.

	Electronic Energy /kJ mol^{-1}	ΔH^{298K} /kJ mol^{-1}	ΔS^{298K} /J K^{-1} mol^{-1}	ΔG^{298K} /kJ mol^{-1}	ΔG^{342K} /kJ mol^{-1}
Reactant	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
TS1_A (TS1_B)	29.4 (24.7)	26.5 (21.8)	-102.0 (-92.1)	56.9 (49.2)	61.4 (53.3)
Inter_A (Inter_B)	22.9 (17.0)	22.2 (16.7)	-73.5 (-76.0)	44.1 (39.4)	47.4 (42.7)
TS2_A (TS2_B)	55.9 (54.5)	51.3 (49.4)	-82.5 (-73.8)	75.9 (71.4)	79.5 (74.6)
Prod_A (Prod_B)	21.4 (12.8)	20.3 (12.0)	-21.4 (-19.0)	26.7 (17.7)	27.6 (18.5)
Prod_A, separated (Prod_B, separated)	21.7 (16.8)	17.0 (12.1)	49.1 (57.8)	2.4 (-5.1)	0.3 (-7.6)

Table S3. Computed Relative Energies for the formation of isomer A (isomer B in brackets) of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PH$_3$)] from [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)$_2$] and PH$_3$.

	Electronic Energy /kJ mol^{-1}	ΔH^{298K} /kJ mol^{-1}	ΔS^{298K} /J K^{-1} mol^{-1}	ΔG^{298K} /kJ mol^{-1}
Reactant A (reactant B)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
TS1_A (TS1_B)	42.3 (43.0)	40.3 (40.6)	-76.9 (-76.3)	63.3 (63.3)
Inter_A (Inter_B)	41.9 (41.4)	42.9 (42.2)	-51.8 (-56.3)	58.4 (58.9)
TS2_A (TS2_B)	69.5 (70.3)	66.9 (66.9)	-65.1 (-60.6)	86.3 (84.9)
Prod_A (Prod_B)	35.9 (38.1)	36.7 (38.8)	2.0 (13.5)	36.1 (34.7)
Prod_A, separated (Prod_B, separated)	41.2 (41.5)	38.4 (38.4)	74.8 (72.4)	16.1 (16.8)

Table S4. Computed relative energies for PPh_3-assisted isomerisation of product isomer A into isomer B according to Scheme 5V.

	Electronic Energy (gas phase) /kJ mol^{-1}	ΔH^{298K} (gas phase) /kJ mol^{-1}	ΔS^{298K} (gas phase) /J K^{-1} mol^{-1}	ΔG^{298K} (gas phase) /kJ mol^{-1}	ΔG^{298K} (+ solvent effect) /kJ mol^{-1}
Prod_A + PPh_3	0.0	0.0	0.0	0.0	0.0
TS1_PPh_3_A	37.3	34.8	-89.2	61.3	74.2
Inter_PPh_3_A	13.6	14.0	-85.6	39.5	45.3
TSi_PPh_3	26.1	23.0	-90.5	50.0	61.6
Inter_PPh_3_B	20.4	20.4	-62.3	38.9	44.7
TS2_PPh_3_B	42.3	39.0	-77.8	62.2	80.4
Prod B + PPh_3	2.4	2.4	-22.9	9.2	36.0

Table S5. Computed relative energies for CH_3CN-assisted isomerisation of isomer A into B according to Scheme 5V.

	Electronic Energy (gas phase) /kJ mol^{-1}	Electronic Energy (in CH_3CN)[a] /kJ mol^{-1}	ΔH^{298K} (gas phase) /kJ mol^{-1}	ΔS^{298K} (gas phase) /J K^{-1} mol^{-1}	ΔG^{298K} (gas phase) /kJ mol^{-1}	ΔG^{298K} (+ solvent effect)[b] /kJ mol^{-1}
Prod_A + CH_3CN	0.0	0.0	0.0	0.0	0.0	0.0
TS1_CH_3CN_A	69.5	66.4	65.8	-24.3	73.0	69.8
Inter_CH_3CN_A	62.2	58.7	60.6	-7.5	62.8	59.3
TSi_CH_3CN	66.5	63.7	62.5	-39.3	74.3	71.5
Inter_CH_3CN_B	58.9	62.2	57.1	4.5	55.7	59.0
TS2_CH_3CN_B	75.4	78.2	70.6	-24.1	77.8	80.6
Prod B + CH_3CN	2.8	5.1	2.9	10.3	-0.2	2.1

[a]Single point calculations on gas phase-optimized geometries
[b]Effect of CH_3CN solvent added to the Free Energy

Table S6. Computed relative electronic energies for the formation of isomer A of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)] using different basis sets for Rh (Pathway A_(*C*)).

	B3LYP/ 6-311G(d,p), LANL2DZ ΔE *(kJ/mol)*	***B3LYP/ 6-311G(d,p),*** LANL2DZ ***+f135*** ΔE *(kJ/mol)*	***B3LYP/ 6-311G(d,p),*** LANL2DZ ***+f040*** ΔE *(kJ/mol)*
Reactant	0.0	0.0	0.0
TS1_A	30.3	32.1	31.5
Inter_A	24.1	26.3	27.6
TS2_A	50.8	54.5	52.6
Prod_A	15.0	18.1	18.3
Prod_A, separated	19.7	22.8	23.0

Table S7. Comparison of Rh-ligand bond length (Å) at TS1_A optimized with LANL2DZ, LANL2DZ +f135, LANL2DZ+f040

	Rh-P (forming)	*Rh-O_{eq} (breaking)*	*Rh-CO_{eq}*	*Rh-CO_{ax}*	*Rh-O_{ax}*
B3LYP/6-311G(d,p), LANL2DZ	2.642	2.291	1.887	1.866	2.087
B3LYP/6-311G(d,p), LANL2DZ ***+f135***	2.636	2.297	1.880	1.857	2.082
B3LYP/6-311G(d,p), LANL2DZ ***+f040***	2.630	2.294	1.880	1.859	2.079

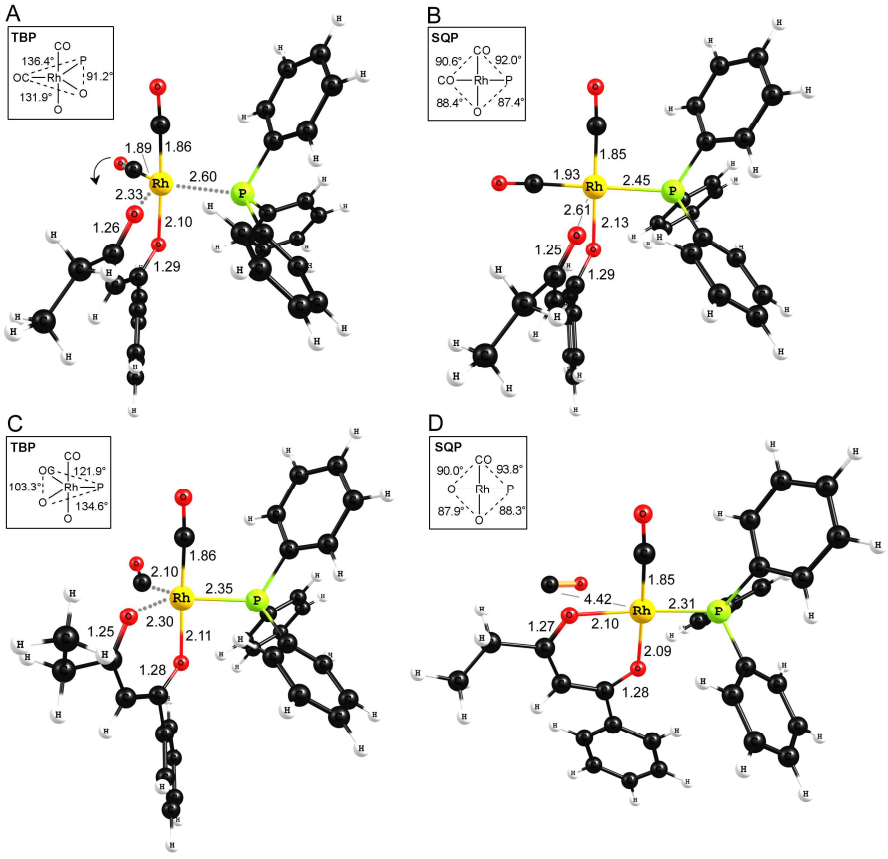

Figure S1. Optimized geometries for formation of isomer B (*SP-4*-3) of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)] (B_(*C*) pathway in Scheme 3). **A**) Transition State 1 (TS1_B), **B**) SQP intermediate (Inter_B), **C**) Transition state 2 (TS2_B), **D**) SQP product (Prod_B, isomer B in Scheme 2).

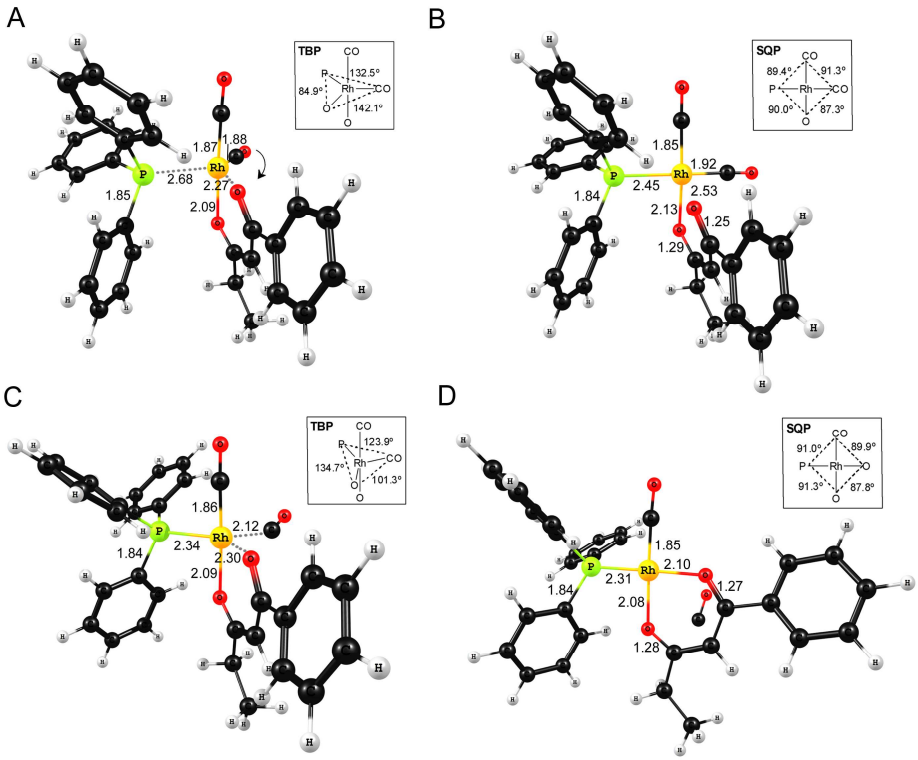

Figure S2. Optimized geometries for formation of Isomer A (*SP-4*-2) of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)] (A_(*A*) pathway in Scheme 3). A) Transition State 1 (TS1_A), **B**) Square-planar intermediate (Inter_A) **C**) Transition state 2 (TS2_A) **D**) Square-planar product (Prod_A, isomer A in Scheme 2).

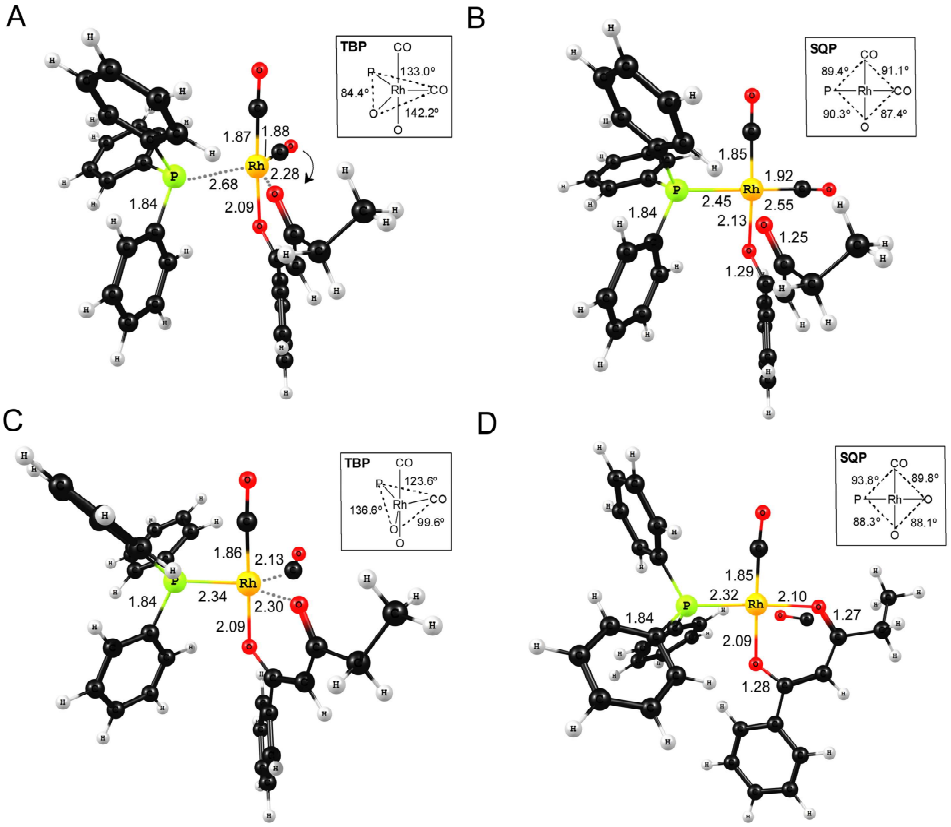

Figure S3. Optimized geometries for formation of Isomer B (*SP-4*-3) of [Rh(PhCOCHCOCH$_2$CH$_3$)(CO)(PPh$_3$)] (B_(*A*) pathway in Scheme 3). **A**) Transition State 1 (TS1_B) **B**) Square-planar intermediate (Inter_B) **C**) Transition state 2 (TS2_B) **D**) Square-planar product (Prod_B, isomer B in Scheme 2).

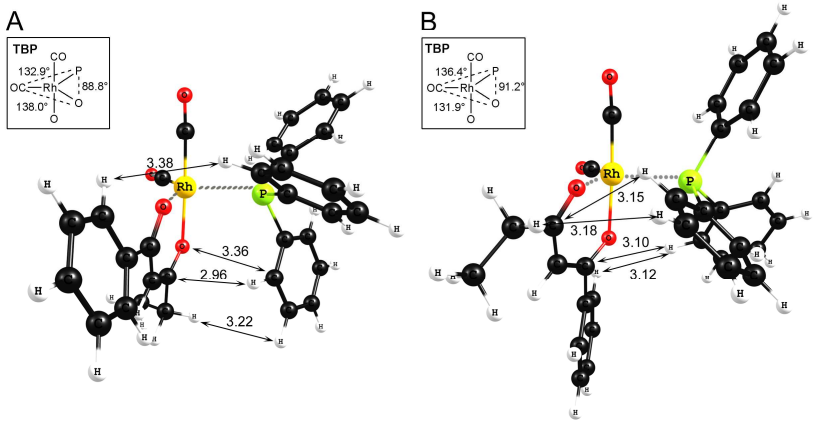

Figure S4. Selected steric interactions at the first TS for formation of **A**) isomer A (TS1_A) and **B**) isomer B (TS1_B).

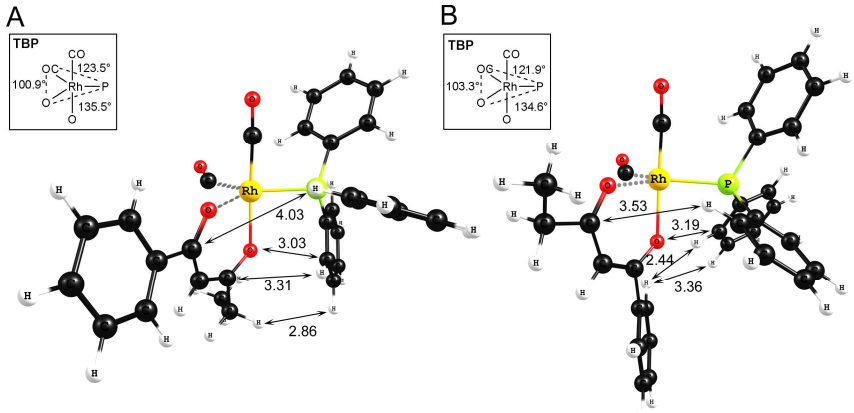

Figure S5. Selected steric interactions at the second TS for formation of **A**) isomer A (TS2_A) and **B**) isomer B (TS2_B).

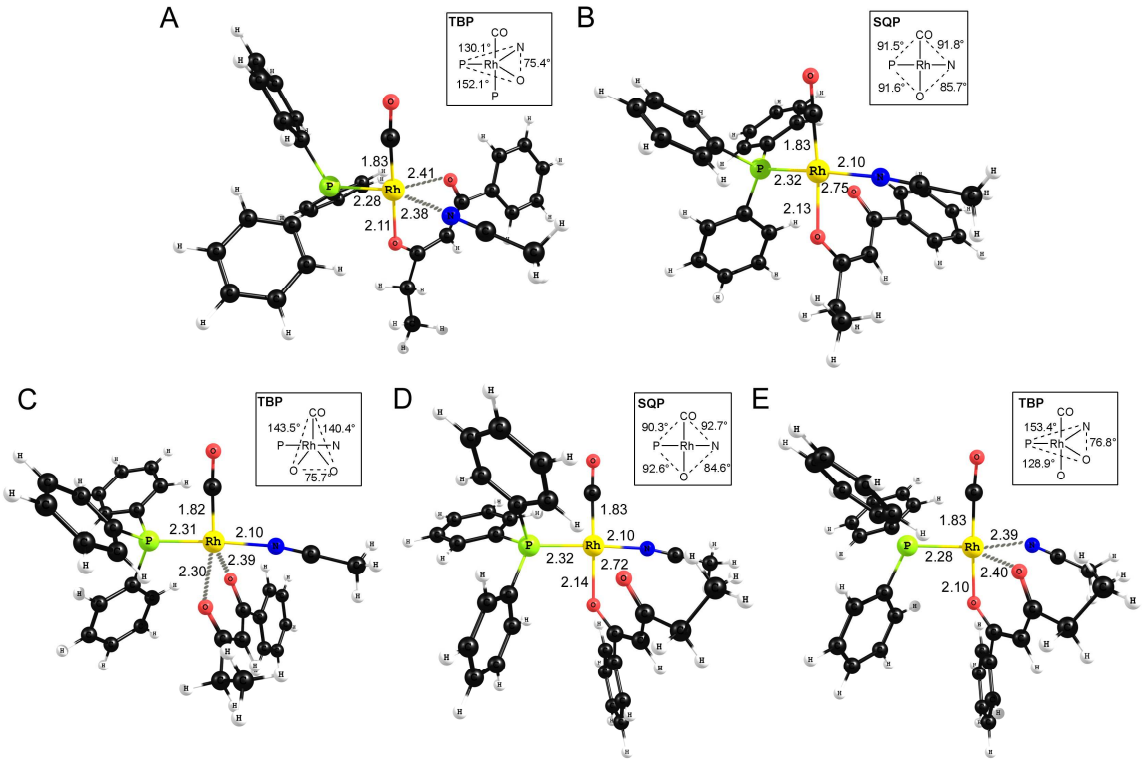

Figure S6. CH_3CN-assisted isomerisation of product isomer A to B. A) Nucleophilic attack of CH_3CN on isomer A (TS1_ CH3CN_A), B) Solvent-coordinated SQP intermediate, C) TS for isomerisation (TSi_ CH3CN), D) Isomerised solvent-coordinated SQP intermediate, E) TS for CH_3CN release (TS2_ CH3CN _B). Distances are in Angstrom. Insets show overall conformation and angles in degrees.

Optimized Cartesian coordinates (**Å**)

Structures optimized with B3LYP, using the basis set LANL2DZ for rhodium (except indicated otherwise) and 6-311G(d,p) for all other atoms

1 The reactants: $[Rh(C_6H_5COCHCOCH_2CH_3)(CO)_2]$ + (PPh_3)

C	5.562767	-2.566665	-0.531406
C	6.010936	-1.290084	-0.164736
C	7.372450	-1.108030	0.113936
C	8.262849	-2.172493	0.016131
C	7.808944	-3.432793	-0.367590
C	6.455496	-3.626362	-0.640055
C	5.012680	-0.180446	-0.063888
C	5.437118	1.155852	-0.165333
C	4.616498	2.288079	-0.078957
O	3.355213	2.299461	0.113848
Rh	2.133587	0.641698	0.300636
C	0.645847	1.771318	0.495200
O	-0.226822	2.494192	0.615984
P	-3.394646	-0.171366	-0.236056
C	-4.222801	-1.505525	-1.221677
C	-5.144158	-2.421405	-0.699995
C	-5.696144	-3.411591	-1.511867
C	-5.341505	-3.497524	-2.855778
C	-4.423703	-2.591935	-3.386014
C	-3.862167	-1.612016	-2.572878
C	-3.841825	-0.624605	1.505405
C	-3.013526	-1.554415	2.151971
C	-3.263784	-1.937927	3.466336
C	-4.334904	-1.382133	4.164607
C	-5.154431	-0.446607	3.538239
C	-4.912849	-0.071640	2.217083
C	-4.478814	1.296617	-0.562783
C	-5.759747	1.225977	-1.123838
C	-6.497120	2.386579	-1.352896
C	-5.968489	3.631946	-1.020924
C	-4.692945	3.714428	-0.465225
C	-3.950393	2.557008	-0.247614
O	3.803986	-0.562491	0.090814
C	1.060499	-0.891865	0.471936
O	0.451363	-1.849057	0.578772
C	5.238194	3.665271	-0.224056
C	4.654311	4.446844	-1.410519
H	6.484398	1.335411	-0.354909
H	5.032139	4.209692	0.704088
H	6.322784	3.577436	-0.318600
H	-5.429132	-2.366071	0.343731
H	-3.133517	-0.923278	-2.988360
H	-6.405778	-4.115827	-1.091159
H	-4.135910	-2.656420	-4.429606
H	-5.771966	-4.268554	-3.485014

H	-6.181183	0.263357	-1.387701
H	-2.949497	2.631264	0.164247
H	-7.486838	2.315920	-1.791067
H	-4.270151	4.680541	-0.212521
H	-6.543891	4.533318	-1.200586
H	-2.166375	-1.977826	1.622427
H	-5.558010	0.657381	1.741943
H	-2.615755	-2.661429	3.948668
H	-5.986255	-0.005890	4.077066
H	-4.524602	-1.671947	5.192116
H	7.737836	-0.141376	0.436980
H	9.311170	-2.018702	0.245563
H	8.504859	-4.260354	-0.447492
H	6.095462	-4.605437	-0.935309
H	4.508754	-2.708065	-0.730488
H	5.077568	5.453268	-1.452507
H	4.875545	3.946708	-2.357230
H	3.571012	4.530975	-1.314296

2 Transition State 1_A_(*C*)

C	-4.332359	1.129343	-1.385181
C	-4.001811	0.442998	-0.209113
C	-4.844923	0.569393	0.902213
C	-5.992533	1.354684	0.835788
C	-6.320823	2.017188	-0.345015
C	-5.486643	1.901117	-1.456348
C	-2.739714	-0.375867	-0.189184
C	-2.663007	-1.476701	0.704427
C	-1.600283	-2.370907	0.863802
O	-0.472474	-2.374268	0.261335
Rh	0.089343	-1.195550	-1.366093
C	0.554250	-0.190740	-2.868191
O	0.786768	0.442459	-3.789719
P	1.356721	0.500703	0.214150
C	0.640821	2.156070	0.606817
C	1.027363	2.897404	1.733006
C	0.478339	4.154220	1.970537
C	-0.464410	4.684631	1.090443
C	-0.863455	3.949403	-0.022165
C	-0.318587	2.689183	-0.261973
C	1.743651	-0.180458	1.886220
C	0.671786	-0.431437	2.755172
C	0.898457	-0.963660	4.019951
C	2.195515	-1.270104	4.431204
C	3.263139	-1.034730	3.570558
C	3.041189	-0.491667	2.305232
C	3.017691	0.885479	-0.505946
C	3.589488	2.162473	-0.482837
C	4.839201	2.386845	-1.058570
C	5.536657	1.340505	-1.655878
C	4.975056	0.065073	-1.685235
C	3.720855	-0.158360	-1.124733
O	-1.842935	-0.021211	-0.999660
C	0.619215	-2.788520	-2.227594
O	0.976645	-3.773605	-2.689007
C	-1.747497	-3.501815	1.871085

C	-1.650324	-4.885803	1.212599
H	-3.542781	-1.688464	1.294028
H	-0.935582	-3.390818	2.597946
H	-2.691439	-3.400758	2.411687
H	1.751590	2.489500	2.428263
H	-0.671193	2.101204	-1.099387
H	0.784564	4.717910	2.844906
H	-1.612760	4.345787	-0.697746
H	-0.894237	5.661976	1.279712
H	3.059380	2.987303	-0.024139
H	3.277049	-1.146584	-1.171938
H	5.265354	3.383770	-1.039842
H	5.506777	-0.754419	-2.155672
H	6.508173	1.518244	-2.103137
H	-0.342604	-0.206812	2.445052
H	3.883670	-0.306737	1.650965
H	0.060072	-1.143894	4.683683
H	4.275301	-1.268495	3.881672
H	2.370367	-1.689907	5.415414
H	-4.592486	0.076653	1.832949
H	-6.628586	1.452236	1.708546
H	-7.218507	2.623163	-0.397775
H	-5.737059	2.413248	-2.378870
H	-3.671455	1.038637	-2.237771
H	-1.706188	-5.675548	1.966149
H	-2.465244	-5.039918	0.499985
H	-0.705291	-4.986485	0.677112

3 Intermediate_A_(*C*)

C	-4.321260	1.526366	-1.039742
C	-4.130660	0.559638	-0.043964
C	-5.143046	0.370141	0.905414
C	-6.315766	1.119433	0.853787
C	-6.500349	2.063953	-0.153417
C	-5.497698	2.264454	-1.101598
C	-2.825493	-0.202325	-0.034776
C	-2.782146	-1.465048	0.625985
C	-1.672026	-2.301085	0.745169
O	-0.509180	-2.144439	0.231392
Rh	0.189651	-0.951724	-1.390391
C	1.105573	-0.179231	-2.801867
O	1.664366	0.284650	-3.688441
P	1.508123	0.390464	0.161414
C	1.099502	2.182230	0.210775
C	1.532874	2.995150	1.268610
C	1.235079	4.354169	1.278395
C	0.493840	4.914677	0.238785
C	0.042574	4.109833	-0.803019
C	0.338102	2.748200	-0.816786
C	1.359910	-0.122430	1.922405
C	0.106291	-0.000450	2.536582
C	-0.057532	-0.366071	3.867754
C	1.021541	-0.865109	4.597653
C	2.266433	-0.994876	3.989519
C	2.438171	-0.625006	2.655838
C	3.312392	0.283617	-0.210289
C	4.182351	1.376236	-0.136277

C	5.536894	1.216569	-0.424483
C	6.037020	-0.032774	-0.780957
C	5.175765	-1.125967	-0.860287
C	3.820614	-0.967931	-0.586469
O	-1.855699	0.334921	-0.616749
C	-0.582625	-2.273401	-2.554708
O	-1.023433	-3.097647	-3.203385
C	-1.797313	-3.558530	1.596827
C	-1.442716	-4.836856	0.825213
H	-3.692764	-1.823583	1.082999
H	-1.104498	-3.441157	2.438147
H	-2.804970	-3.628864	2.013736
H	2.089844	2.563535	2.092088
H	-0.055325	2.120283	-1.604629
H	1.574385	4.973056	2.101402
H	-0.554554	4.535487	-1.601146
H	0.257211	5.972709	0.250257
H	3.807525	2.355702	0.131365
H	3.146707	-1.812919	-0.676646
H	6.199268	2.073349	-0.372819
H	5.555322	-2.099854	-1.147862
H	7.090795	-0.153103	-1.005575
H	-0.738955	0.373636	1.972331
H	3.412543	-0.727255	2.195188
H	-1.031957	-0.267586	4.332467
H	3.109760	-1.381983	4.550356
H	0.890051	-1.152397	5.634869
H	-5.010559	-0.347164	1.705804
H	-7.084931	0.966859	1.603008
H	-7.416629	2.642419	-0.196705
H	-5.633978	2.998856	-1.888106
H	-3.526957	1.681466	-1.758756
H	-1.487982	-5.711097	1.480057
H	-2.137398	-5.000488	-0.003685
H	-0.434298	-4.764618	0.415282

4 Transition State 2_A_(*C*)

C	-0.474136	-1.571965	2.354645
C	-1.572214	-0.792998	1.975618
C	-2.547546	-0.476914	2.932699
C	-2.431621	-0.949164	4.236830
C	-1.340694	-1.737662	4.601831
C	-0.362462	-2.045855	3.660637
P	-1.692672	-0.206587	0.227093
Rh	0.322752	-0.257997	-0.958041
C	0.015441	-2.037529	-1.400794
O	-0.088878	-3.148153	-1.654980
C	-3.034189	-1.228970	-0.529229
C	-3.211930	-1.156997	-1.918649
C	-4.211489	-1.896335	-2.543653
C	-5.035093	-2.733696	-1.793113
C	-4.855087	-2.823767	-0.415892
C	-3.864078	-2.073700	0.215495
C	-2.440515	1.468547	0.413009
C	-1.786865	2.408443	1.222563
C	-2.311486	3.687088	1.378296
C	-3.485679	4.050827	0.720482
C	-4.135425	3.125765	-0.091223

C	-3.618035	1.840436	-0.244771
C	0.504052	0.340262	-2.957066
O	0.054278	0.445073	-4.001418
O	0.731521	1.680888	-0.288862
C	1.895978	2.184691	-0.104154
C	3.127627	1.532388	-0.063313
C	3.373961	0.133149	-0.148217
C	4.770056	-0.363584	0.123075
C	5.160494	-1.586708	-0.437904
C	6.435651	-2.094351	-0.217136
C	7.337548	-1.396493	0.585565
C	6.954042	-0.189188	1.165408
C	5.681597	0.326058	0.932719
O	2.527965	-0.745624	-0.445062
C	1.871609	3.692155	0.114795
C	1.232611	4.444588	-1.060779
H	3.985887	2.167496	0.099469
H	1.288447	3.881184	1.023461
H	2.884070	4.058140	0.299037
H	-3.391211	0.147061	2.661779
H	0.303859	-1.786878	1.630611
H	-3.190174	-0.696792	4.969405
H	0.495705	-2.645609	3.941530
H	-1.250094	-2.100775	5.619457
H	-3.734220	-2.160755	1.286384
H	-2.558432	-0.527735	-2.511980
H	-5.483952	-3.481849	0.173190
H	-4.337079	-1.827300	-3.618224
H	-5.805929	-3.319214	-2.281259
H	-0.866925	2.139749	1.723839
H	-4.141621	1.129615	-0.870946
H	-1.799075	4.402707	2.011518
H	-5.051011	3.398206	-0.604117
H	-3.890745	5.049224	0.841530
H	5.389422	1.255214	1.406099
H	7.644792	0.350837	1.803524
H	8.330908	-1.793883	0.762507
H	6.727173	-3.036012	-0.669141
H	4.445482	-2.124298	-1.047456
H	1.190163	5.517475	-0.855069
H	1.810879	4.299348	-1.977456
H	0.218109	4.084888	-1.236330

5 The products: [Rh(acac)(CO)(PPh_3)]_A_(*C*) + CO

C	-5.835399	0.696855	-0.854632
C	-4.828821	-0.163702	-0.396658
C	-5.168389	-1.485739	-0.078032
C	-6.481642	-1.927497	-0.190370
C	-7.476685	-1.060928	-0.640620
C	-7.147590	0.250079	-0.978640
C	-3.396979	0.262501	-0.257969
O	-2.553451	-0.686928	-0.275794
Rh	-0.461836	-0.510678	-0.184640
O	-0.708907	1.547820	0.084468
C	-1.816960	2.182546	0.061918
C	-1.688984	3.687307	0.233919
C	-1.115874	4.081346	1.603162

P	1.818422	-0.142605	-0.136512
C	2.484218	0.382898	1.503354
C	1.619524	0.997401	2.417120
C	2.093321	1.419752	3.657044
C	3.429979	1.228844	4.000230
C	4.295131	0.612738	3.098452
C	3.826643	0.190467	1.856352
C	2.267024	1.217894	-1.298062
C	1.564923	1.308266	-2.506824
C	1.885488	2.294481	-3.435639
C	2.899499	3.210512	-3.161467
C	3.591334	3.136220	-1.954849
C	3.279506	2.144254	-1.027110
C	2.940866	-1.530828	-0.608741
C	2.948256	-2.684912	0.187359
C	3.760676	-3.764227	-0.140702
C	4.571928	-3.711310	-1.273857
C	4.567217	-2.571904	-2.072073
C	3.758573	-1.484325	-1.741849
C	-0.289603	-2.329751	-0.451647
O	-0.252314	-3.463152	-0.625901
C	-1.861709	-1.184375	3.200656
O	-2.191335	-2.256429	3.081488
C	-3.093004	1.630852	-0.099549
H	-3.920822	2.322887	-0.061077
H	-1.017596	4.044537	-0.554270
H	-2.660176	4.163391	0.079975
H	3.819266	2.103253	-0.089122
H	0.759197	0.611121	-2.707961
H	4.373777	3.852739	-1.731003
H	1.335113	2.353195	-4.367907
H	3.143575	3.983559	-3.881566
H	3.768615	-0.602365	-2.369648
H	2.316927	-2.741993	1.067036
H	5.193923	-2.523089	-2.955514
H	3.754432	-4.649795	0.484490
H	5.200853	-4.555631	-1.532484
H	0.579360	1.139653	2.153495
H	4.505789	-0.300458	1.169568
H	1.412700	1.890395	4.357414
H	5.334950	0.454497	3.362138
H	3.794964	1.552270	4.968693
H	-5.593298	1.711817	-1.143894
H	-7.912665	0.925491	-1.345009
H	-8.500283	-1.406494	-0.733536
H	-6.729358	-2.950373	0.070669
H	-4.385459	-2.152947	0.257785
H	-1.018026	5.167273	1.680384
H	-1.767243	3.742348	2.413539
H	-0.128942	3.639517	1.748519

6 Transition State 1_A_(*A*)

C	0.131092	-0.350475	4.601924
C	-0.288370	-1.411761	3.799753
C	-0.751712	-1.174681	2.509998
C	-0.818785	0.134435	2.009723
C	-0.391918	1.193421	2.817683

C	0.082322	0.949197	4.106229
P	-1.431011	0.356900	0.284038
C	-1.455663	2.188468	0.044256
C	-2.597252	2.977827	0.226334
C	-2.542975	4.353700	0.011057
C	-1.350798	4.956426	-0.382972
C	-0.211363	4.176234	-0.571467
C	-0.261944	2.799291	-0.369869
Rh	-0.143960	-1.002932	-1.633693
O	0.492089	-2.431899	-0.247288
C	1.666258	-2.531978	0.255412
C	1.872150	-3.870692	0.956855
C	2.693119	-1.587770	0.220738
C	2.642586	-0.290721	-0.347941
O	1.672272	0.201577	-0.988377
C	-0.663612	-2.422972	-2.754175
O	-1.006199	-3.318808	-3.379887
C	-0.639409	0.239666	-2.934687
O	-0.893090	1.017638	-3.731122
C	-3.215250	-0.105698	0.425601
C	-3.939650	0.032598	1.617503
C	-5.288591	-0.310457	1.667015
C	-5.932039	-0.793383	0.528887
C	-5.219219	-0.939426	-0.658622
C	-3.868135	-0.604193	-0.707749
H	3.626019	-1.875146	0.678325
C	3.194604	-4.122031	1.680592
H	1.034819	-3.975899	1.654802
H	1.706700	-4.638819	0.192973
H	-3.448040	0.400670	2.509987
H	-3.309364	-0.745346	-1.625500
H	-5.836205	-0.202193	2.596723
H	-5.709824	-1.325755	-1.544918
H	-6.981566	-1.062412	0.570405
H	-3.531604	2.522095	0.529220
H	0.621202	2.192110	-0.538650
H	-3.435592	4.953398	0.151155
H	0.718618	4.636485	-0.886079
H	-1.311636	6.027173	-0.549490
H	-1.051021	-2.005855	1.882515
H	-0.430678	2.209676	2.445656
H	-0.249730	-2.427371	4.178037
H	0.408926	1.779682	4.722325
H	0.495796	-0.537747	5.605710
H	3.183376	-5.112651	2.142499
H	4.045683	-4.089617	0.995864
H	3.367012	-3.389532	2.473204
C	3.845856	0.599765	-0.209561
C	4.070821	1.575103	-1.190542
C	5.167419	2.425633	-1.107538
C	6.048544	2.328336	-0.031190
C	5.825411	1.373947	0.959020
C	4.735738	0.512200	0.868580
H	3.375991	1.646121	-2.017785
H	5.336671	3.164835	-1.882717
H	6.901420	2.994442	0.037330
H	6.498329	1.302575	1.806286
H	4.562057	-0.210613	1.656074

7 Intermediate_A_(*A*)

C	0.163933	-0.783889	4.436889
C	-0.287682	-1.786761	3.579314
C	-0.786750	-1.461975	2.322761
C	-0.847806	-0.122489	1.913554
C	-0.391402	0.878944	2.775047
C	0.113780	0.546139	4.031330
P	-1.537820	0.241747	0.247215
C	-1.678263	2.077406	0.168122
C	-2.884001	2.759731	0.361521
C	-2.925579	4.149622	0.266499
C	-1.767150	4.867956	-0.016740
C	-0.563856	4.192169	-0.213057
C	-0.514325	2.803101	-0.131390
Rh	-0.273519	-0.677946	-1.637482
O	0.520987	-2.186555	-0.368231
C	1.726930	-2.402888	0.018299
C	1.932564	-3.852037	0.455768
C	2.779086	-1.494672	0.081836
C	2.719329	-0.098366	-0.200997
O	1.711601	0.513784	-0.621434
C	0.393552	-1.700570	-3.118390
O	0.761932	-2.365833	-3.966199
C	-1.181999	0.462917	-2.781830
O	-1.722428	1.167561	-3.504998
C	-3.264961	-0.389576	0.370696
C	-3.997413	-0.272198	1.561064
C	-5.307058	-0.737436	1.629842
C	-5.899695	-1.329533	0.515086
C	-5.175560	-1.460452	-0.666446
C	-3.863250	-0.996654	-0.738319
H	3.735417	-1.885526	0.391486
C	3.312064	-4.279344	0.957128
H	1.178491	-4.041525	1.228073
H	1.632067	-4.472630	-0.395919
H	-3.540734	0.173239	2.436977
H	-3.290795	-1.124127	-1.649344
H	-5.862739	-0.642804	2.556028
H	-5.625645	-1.932304	-1.532425
H	-6.918711	-1.695428	0.572127
H	-3.793805	2.213740	0.576051
H	0.421599	2.279119	-0.298163
H	-3.866649	4.668216	0.411724
H	0.340778	4.745219	-0.439470
H	-1.802544	5.949169	-0.090340
H	-1.112162	-2.245769	1.650959
H	-0.427631	1.917501	2.472362
H	-0.247027	-2.825448	3.887686
H	0.465922	1.331193	4.690965
H	0.555055	-1.040268	5.415111
H	3.297915	-5.336601	1.235281
H	4.079908	-4.151592	0.189837
H	3.616972	-3.709837	1.838788
C	3.971748	0.719719	0.002680
C	4.141621	1.876349	-0.769173
C	5.272398	2.671594	-0.620650
C	6.245518	2.335237	0.320005

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C       6.079052    1.197762    1.106954
C       4.954301    0.392478    0.945341
H       3.373280    2.131584   -1.488422
H       5.396522    3.555049   -1.237503
H       7.125355    2.957474    0.441354
H       6.824811    0.937752    1.850200
H       4.828539   -0.479386    1.575491

8    Transition State 2_A_(A)
C       2.041943    3.945269    2.372132
C       2.034172    3.876079    0.979005
C       1.928717    2.645906    0.339326
C       1.850028    1.463770    1.088525
C       1.851596    1.539779    2.484809
C       1.945508    2.776737    3.121832
P       1.724345   -0.138477    0.190791
C       1.904655   -1.416341    1.518107
C       3.143085   -1.902454    1.953190
C       3.208194   -2.848290    2.974182
C       2.041340   -3.313550    3.576067
C       0.804399   -2.836173    3.147869
C       0.735029   -1.899625    2.119873
Rh     -0.241462   -0.376820   -1.053170
O      -0.704798    1.621576   -0.673280
C      -1.869974    2.116910   -0.471968
C      -1.830992    3.642466   -0.420850
C      -3.075735    1.440510   -0.295305
C      -3.287102    0.034515   -0.271199
O      -2.432983   -0.846266   -0.541799
C      -0.366797   -0.036437   -3.136512
O       0.134404   -0.051182   -4.161736
C       0.126789   -2.185085   -1.269380
O       0.280813   -3.312753   -1.392512
C       3.325863   -0.211847   -0.733836
C       4.487840    0.397639   -0.238715
C       5.687631    0.303835   -0.939374
C       5.744096   -0.398115   -2.141908
C       4.593434   -0.998918   -2.645613
C       3.391015   -0.900825   -1.949342
H      -3.946600    2.056006   -0.137573
C      -3.121717    4.399325   -0.108550
H      -1.056318    3.897053    0.309733
H      -1.432677    3.965318   -1.389629
H       4.453878    0.956690    0.688573
H       2.495209   -1.345864   -2.363154
H       6.577101    0.783802   -0.546682
H       4.625398   -1.535182   -3.587151
H       6.678195   -0.467612   -2.687861
H       4.058775   -1.556003    1.491193
H      -0.229812   -1.547675    1.770591
H       4.173230   -3.224007    3.295507
H      -0.109238   -3.200465    3.603612
H       2.095162   -4.051307    4.368755
H       1.899244    2.603311   -0.741919
H       1.784295    0.637560    3.079375
H       2.101747    4.783042    0.388656
H       1.948166    2.821959    4.205127
H       2.120646    4.905972    2.868676
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H	-2.928809	5.475424	-0.099949
H	-3.896934	4.211000	-0.855564
H	-3.521992	4.128750	0.871878
C	-4.658057	-0.475500	0.091247
C	-5.033427	-1.749478	-0.355319
C	-6.282993	-2.272308	-0.042601
C	-7.173780	-1.537389	0.739086
C	-6.804614	-0.277545	1.205309
C	-5.558204	0.251379	0.880906
H	-4.326650	-2.314721	-0.949225
H	-6.563017	-3.254800	-0.406407
H	-8.146889	-1.946266	0.987829
H	-7.486033	0.293113	1.826614
H	-5.276581	1.222521	1.268447

9 Product A_(*A*)

C	5.864997	0.053228	-0.860374
C	4.785878	-0.606740	-0.257481
C	5.013176	-1.849220	0.350095
C	6.287346	-2.404402	0.375219
C	7.355280	-1.735723	-0.221573
C	7.138189	-0.508613	-0.844720
C	3.390921	-0.053175	-0.258760
O	2.475346	-0.914645	-0.082943
Rh	0.404085	-0.576396	-0.061223
C	0.114433	-2.382962	0.191268
O	-0.005852	-3.513232	0.353028
P	-1.873061	-0.173257	-0.082038
C	-2.685482	-0.166157	1.577816
C	-3.897741	0.500900	1.804219
C	-4.496012	0.469029	3.061166
C	-3.891347	-0.225296	4.107533
C	-2.682542	-0.882739	3.893954
C	-2.080057	-0.850376	2.638246
C	-2.384235	1.449613	-0.793718
C	-1.971318	2.623572	-0.148596
C	-2.340771	3.867131	-0.649267
C	-3.112645	3.957675	-1.807228
C	-3.515257	2.796811	-2.460314
C	-3.155104	1.547278	-1.956545
C	-2.822879	-1.410667	-1.072436
C	-4.095445	-1.867085	-0.713150
C	-4.763873	-2.790632	-1.514773
C	-4.173800	-3.261809	-2.684723
C	-2.905407	-2.813663	-3.048906
C	-2.230019	-1.900334	-2.244382
O	0.810878	1.444026	-0.340978
C	1.960373	1.989850	-0.450136
C	3.195389	1.333962	-0.422942
C	1.863987	1.953223	3.160151
O	1.919557	0.922911	3.613538
C	1.890624	3.504054	-0.606582
C	3.177884	4.259823	-0.937375
H	4.077049	1.948161	-0.507568
H	1.131141	3.691780	-1.371951
H	1.464065	3.885396	0.328582
H	-4.369208	1.057166	1.002862
H	-1.127415	-1.341728	2.482516

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H      -5.431953    0.991878    3.223602
H      -2.200187   -1.414837    4.706007
H      -4.356646   -0.245822    5.086646
H      -4.564224   -1.516530    0.197498
H      -1.231612   -1.572993   -2.513080
H      -5.745538   -3.144286   -1.219981
H      -2.434325   -3.184227   -3.952255
H      -4.695188   -3.982112   -3.305081
H      -1.353213    2.563258    0.737269
H      -3.481209    0.652230   -2.470785
H      -2.019058    4.767632   -0.138170
H      -4.114836    2.857936   -3.361662
H      -3.396572    4.928687   -2.197437
H       2.964262    5.324909   -1.059139
H       3.923156    4.165383   -0.143545
H       3.626177    3.904187   -1.868793
H       4.173949   -2.365075    0.797861
H       6.447868   -3.361866    0.858277
H       8.348481   -2.170647   -0.206667
H       7.960268    0.010233   -1.325099
H       5.710187    0.996141   -1.369586

10   Transition State 1_B_(A)
 C     0.763983   -1.669718    4.147479
 C     1.269518   -2.031280    2.899160
 C     0.601048   -1.656610    1.738067
 C    -0.593396   -0.924512    1.811279
 C    -1.092621   -0.561820    3.067102
 C    -0.414697   -0.933166    4.227650
 P    -1.404939   -0.456548    0.222738
 C    -2.906514    0.484395    0.744443
 C    -4.175035   -0.094701    0.866335
 C    -5.269169    0.680033    1.247284
 C    -5.109035    2.037270    1.514860
 C    -3.849823    2.622191    1.391262
 C    -2.754889    1.856081    0.999859
Rh     0.100818    0.813161   -1.597841
 O     1.836903   -0.090593   -0.858252
 C     2.720365    0.451202   -0.103656
 C     3.972260   -0.362850    0.040241
 C     2.628571    1.680879    0.557408
 C     1.502667    2.535057    0.624438
 C     1.610361    3.791001    1.482743
 O     0.394060    2.360047    0.050034
 C     0.682682    0.353235   -3.325935
 O     1.061206    0.006864   -4.350012
 C    -1.383937    1.690146   -2.308294
 O    -2.273724    2.271745   -2.724844
 C    -2.075381   -2.066549   -0.388341
 C    -2.362505   -3.140165    0.465098
 C    -2.883555   -4.326968   -0.045309
 C    -3.127749   -4.456377   -1.411115
 C    -2.842048   -3.395710   -2.267796
 C    -2.312492   -2.211797   -1.760593
 H     3.506344    2.010757    1.092707
 H     0.894544    3.677256    2.305301
 H     2.604876    3.860300    1.929617
 H    -2.171437   -3.052871    1.527894
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H	-2.066172	-1.398809	-2.433712
H	-3.096804	-5.151569	0.625889
H	-3.019010	-3.492493	-3.333072
H	-3.530918	-5.382010	-1.806396
H	-4.314104	-1.148312	0.658480
H	-1.780355	2.318824	0.883222
H	-6.247474	0.220083	1.333203
H	-3.719979	3.680621	1.588038
H	-5.961981	2.638021	1.810341
H	1.014119	-1.918229	0.771307
H	-2.010775	0.007198	3.143367
H	2.191919	-2.596149	2.826412
H	-0.813315	-0.647175	5.194854
H	1.288721	-1.957806	5.051590
C	4.799775	-0.281823	1.168467
C	5.950150	-1.059729	1.260478
C	6.294569	-1.927746	0.226014
C	5.473440	-2.023089	-0.896426
C	4.318231	-1.254297	-0.984661
H	4.530428	0.370081	1.989924
H	6.575520	-0.991415	2.143662
H	7.193648	-2.529719	0.297002
H	5.733828	-2.697899	-1.704239
H	3.670169	-1.328538	-1.848046
C	1.283752	5.067021	0.694740
H	1.299249	5.941587	1.350043
H	2.012282	5.230440	-0.104137
H	0.295264	4.991662	0.239430

11 Intermediate_B_(*A*)

C	-0.735465	1.543241	4.110683
C	-1.173755	2.048581	2.887259
C	-0.519907	1.699107	1.710559
C	0.587594	0.840652	1.747980
C	1.020907	0.333107	2.976552
C	0.359026	0.684650	4.152128
P	1.426389	0.437134	0.161286
C	2.904488	-0.556848	0.631847
C	4.196045	-0.022449	0.682287
C	5.277749	-0.834369	1.019345
C	5.078894	-2.180667	1.312179
C	3.793619	-2.718398	1.260295
C	2.708246	-1.918232	0.913882
Rh	0.049601	-0.714537	-1.512299
O	-1.701983	0.166818	-0.691451
C	-2.693046	-0.348723	-0.055997
C	-3.914407	0.527894	-0.029829
C	-2.739110	-1.592108	0.574096
C	-1.646953	-2.480522	0.793977
C	-1.933479	-3.771445	1.562555
O	-0.467727	-2.291954	0.425160
C	-1.033116	-1.279175	-2.991401
O	-1.702438	-1.556634	-3.869784
C	1.593319	-1.234019	-2.396761
O	2.532145	-1.573430	-2.957651
C	2.076780	2.069291	-0.394179
C	2.536926	3.021121	0.527041

C	3.044520	4.239205	0.085041
C	3.094958	4.523798	-1.278957
C	2.630098	3.588481	-2.199346
C	2.119358	2.368633	-1.760049
H	-3.695133	-1.902164	0.970489
H	-1.329114	-3.739943	2.476417
H	-2.982208	-3.813797	1.867471
H	2.488734	2.814623	1.589604
H	1.731989	1.652486	-2.475014
H	3.395313	4.968401	0.806667
H	2.654154	3.809086	-3.260436
H	3.486724	5.475192	-1.620863
H	4.365362	1.021376	0.450510
H	1.710492	-2.342253	0.860112
H	6.275785	-0.411703	1.048926
H	3.633801	-3.768053	1.480035
H	5.922152	-2.810474	1.572870
H	-0.882366	2.072633	0.761826
H	1.871713	-0.334450	3.021814
H	-2.032752	2.708277	2.845198
H	0.703510	0.285452	5.099590
H	-1.248937	1.814711	5.026310
C	-4.877813	0.451301	0.985317
C	-5.988613	1.289855	0.975575
C	-6.157673	2.219142	-0.049168
C	-5.200876	2.311825	-1.058698
C	-4.086364	1.479860	-1.044162
H	-4.745580	-0.247983	1.801482
H	-6.720109	1.221959	1.773344
H	-7.025159	2.869797	-0.057427
H	-5.323703	3.033817	-1.858606
H	-3.331974	1.551727	-1.816851
C	-1.560568	-5.018587	0.749095
H	-1.695602	-5.927416	1.341419
H	-2.184711	-5.103270	-0.145156
H	-0.518511	-4.964507	0.429380

12 Transition State 2_B_(*A*)

C	-0.526972	-3.596578	-2.767250
C	-0.817081	-3.502923	-1.407054
C	-0.216135	-2.520018	-0.628253
C	0.693806	-1.620314	-1.200964
C	0.977591	-1.717469	-2.568015
C	0.368928	-2.701821	-3.344934
P	1.458570	-0.329437	-0.131878
C	2.738946	0.442582	-1.222398
C	4.064302	-0.002776	-1.273532
C	4.978235	0.605100	-2.132367
C	4.578245	1.655827	-2.953902
C	3.259739	2.105265	-2.909376
C	2.347602	1.508814	-2.043668
Rh	-0.050130	1.223581	0.756774
O	-1.625011	-0.101788	0.400743
C	-2.823033	0.205499	0.057786
C	-3.765901	-0.963405	0.053107
C	-3.328743	1.461979	-0.274811
C	-2.618319	2.690828	-0.367328

C	-3.389296	3.889270	-0.924343
O	-1.419437	2.881181	-0.060881
C	-0.589009	1.299973	2.818513
O	-0.261811	1.119133	3.896944
C	1.345381	2.424973	0.996940
O	2.159859	3.215474	1.144261
C	2.441341	-1.317577	1.084266
C	2.926859	-2.595989	0.775580
C	3.688456	-3.303327	1.702701
C	3.977220	-2.743524	2.945689
C	3.496418	-1.475072	3.261397
C	2.728080	-0.769062	2.339089
H	-4.383838	1.507054	-0.505818
H	-3.314480	3.829339	-2.018509
H	-4.451408	3.773479	-0.689413
H	2.701353	-3.043899	-0.184524
H	2.335323	0.205061	2.602359
H	4.052777	-4.293757	1.453636
H	3.707650	-1.037143	4.230282
H	4.567305	-3.296912	3.667542
H	4.390857	-0.816366	-0.638360
H	1.327725	1.875147	-1.994411
H	6.004787	0.256834	-2.155307
H	2.942506	2.928928	-3.538810
H	5.291811	2.128314	-3.619517
H	-0.465256	-2.443937	0.421053
H	1.675257	-1.032034	-3.031498
H	-1.525550	-4.185237	-0.951963
H	0.600122	-2.766961	-4.402305
H	-1.001172	-4.360525	-3.373140
C	-4.789298	-1.096375	-0.892714
C	-5.641806	-2.197039	-0.864299
C	-5.491890	-3.175245	0.116377
C	-4.474767	-3.052566	1.062405
C	-3.612332	-1.961882	1.023576
H	-4.902572	-0.348986	-1.668777
H	-6.421561	-2.292127	-1.611876
H	-6.161082	-4.028086	0.142251
H	-4.355522	-3.807021	1.832419
H	-2.817748	-1.861588	1.752193
C	-2.867276	5.243061	-0.443232
H	-3.412702	6.058945	-0.924745
H	-2.985585	5.348018	0.638422
H	-1.806257	5.350609	-0.670301

13 The products: [Rh(acac)(CO)(PPh_3)]_B_(*A*) + CO

C	2.862762	2.405221	0.484819
C	3.460849	1.399825	-0.287635
C	4.719337	1.644892	-0.853633
C	5.366227	2.859005	-0.643710
C	4.770108	3.844605	0.140661
C	3.516219	3.613066	0.704056
C	2.721512	0.112305	-0.492889
C	3.440391	-1.062395	-0.751866
C	2.891863	-2.339778	-0.983503
O	1.663365	-2.648698	-0.964595
Rh	0.059886	-1.355776	-0.544414
C	-1.109082	-2.778457	-0.653886

O	-1.773505	-3.711360	-0.724116
P	-1.608809	0.176639	-0.067884
C	-1.222582	1.114435	1.473473
C	-1.623022	2.441916	1.664864
C	-1.324319	3.100549	2.855661
C	-0.624346	2.441746	3.864954
C	-0.217922	1.122059	3.678662
C	-0.510809	0.462422	2.487559
C	-1.836303	1.489905	-1.349730
C	-0.707141	1.952728	-2.038608
C	-0.831393	2.961915	-2.989378
C	-2.079331	3.515767	-3.269043
C	-3.205733	3.059650	-2.589195
C	-3.087114	2.052911	-1.632435
C	-3.321237	-0.458249	0.201418
C	-3.991266	-0.310746	1.419608
C	-5.273220	-0.834411	1.586188
C	-5.899711	-1.503235	0.539372
C	-5.238258	-1.653679	-0.679166
C	-3.956945	-1.140342	-0.845841
O	1.449467	0.202533	-0.389252
C	2.929130	-2.572809	3.166048
O	2.017513	-1.973792	3.451273
C	3.836635	-3.489460	-1.303471
C	3.627246	-4.704515	-0.390250
H	4.518113	-0.994369	-0.761200
H	3.640667	-3.779388	-2.342591
H	4.872454	-3.145084	-1.255779
H	-2.159046	2.966648	0.883335
H	-0.176118	-0.556694	2.333218
H	-1.636059	4.130092	2.992342
H	0.337343	0.605653	4.453251
H	-0.390636	2.957390	4.789785
H	-3.516601	0.210979	2.240772
H	-3.449497	-1.271476	-1.795004
H	-5.779628	-0.716415	2.537615
H	-5.716539	-2.178742	-1.498102
H	-6.896127	-1.909675	0.670977
H	0.262844	1.524636	-1.819458
H	-3.972069	1.703794	-1.115054
H	0.049945	3.311856	-3.514981
H	-4.180488	3.484211	-2.802462
H	-2.173683	4.297262	-4.014816
H	5.184494	0.897045	-1.483878
H	6.334521	3.037662	-1.097840
H	5.277423	4.788431	0.307082
H	3.045342	4.375632	1.314423
H	1.886340	2.219632	0.913137
H	4.274198	-5.530981	-0.695109
H	3.859510	-4.458093	0.649298
H	2.590557	-5.040227	-0.437182

14 Transition State 1_B_(*C*)

C	-0.102628	2.714204	0.271212
C	-1.342335	2.098241	0.487662
C	-2.436169	2.882900	0.877542
C	-2.290508	4.257272	1.050626

C	-1.053255	4.862783	0.840411
C	0.037844	4.088528	0.453008
P	-1.475445	0.266769	0.274229
C	-1.207892	-0.404401	1.972344
C	-1.074358	-1.792994	2.115666
C	-0.896727	-2.354452	3.377329
C	-0.828131	-1.539242	4.506004
C	-0.939835	-0.158126	4.368030
C	-1.131903	0.408431	3.109287
Rh	0.020832	-0.616439	-1.661311
C	0.600999	0.020665	-3.346132
O	0.960003	0.488010	-4.327577
O	1.708232	0.304801	-0.816375
C	2.707374	-0.266839	-0.244911
C	2.830986	-1.609323	0.117132
C	1.830679	-2.612702	0.038203
C	2.138306	-4.027253	0.535450
C	3.570423	-4.372489	0.946652
C	3.857286	0.661417	0.015238
C	4.725281	0.493935	1.101929
C	5.777011	1.381285	1.311459
C	5.982014	2.445361	0.435378
C	5.120488	2.624500	-0.645924
C	4.061699	1.745954	-0.848839
C	-1.413059	-1.496303	-2.457060
O	-2.254095	-2.100393	-2.938033
O	0.661226	-2.456057	-0.391782
C	-3.289878	0.031292	-0.007154
C	-4.136591	-0.581964	0.921877
C	-5.493109	-0.745054	0.640870
C	-6.021071	-0.291732	-0.563960
C	-5.185087	0.325378	-1.494217
C	-3.830242	0.479238	-1.221623
H	3.792044	-1.908231	0.504736
H	1.455250	-4.203829	1.374645
H	1.799323	-4.699244	-0.259591
H	-3.742346	-0.932515	1.867091
H	-3.188375	0.955742	-1.954846
H	-6.135617	-1.225625	1.370298
H	-5.586861	0.680448	-2.436531
H	-7.075764	-0.419196	-0.780000
H	-3.403961	2.424794	1.040576
H	0.745643	2.119393	-0.044897
H	-3.145636	4.853824	1.348799
H	1.003020	4.552387	0.283151
H	-0.942172	5.933161	0.974081
H	-1.079559	-2.427532	1.238126
H	-1.220127	1.483413	3.015287
H	-0.801750	-3.430138	3.476533
H	-0.879101	0.483145	5.240353
H	-0.681085	-1.978271	5.486537
H	3.633300	-5.425071	1.235249
H	4.276124	-4.212775	0.127409
H	3.904077	-3.779246	1.801827
H	3.385453	1.881170	-1.683143
H	5.275021	3.449344	-1.332701
H	6.804828	3.132815	0.596966
H	6.433306	1.245013	2.163769

H	4.560593	-0.316719	1.801020

15 Intermediate 1_B_(*C*)

C	-4.097485	-0.157203	-0.980327
C	-3.339722	-0.257007	0.195698
C	-3.941633	-0.775060	1.346574
C	-5.274341	-1.185154	1.320844
C	-6.020498	-1.076756	0.151748
C	-5.428605	-0.558488	-0.999587
P	-1.564539	0.252700	0.161172
Rh	-0.104652	-1.012628	-1.344916
O	1.080853	-2.634718	0.325019
C	2.299372	-2.533775	0.568623
C	2.961416	-3.782336	1.168671
C	4.485978	-3.831775	1.290045
C	-1.624384	2.041927	-0.283998
C	-0.443150	2.659496	-0.716658
C	-0.438002	4.018236	-1.020272
C	-1.604456	4.771678	-0.903784
C	-2.780556	4.162589	-0.473358
C	-2.792830	2.804462	-0.161136
C	-1.051885	0.228358	1.927674
C	-0.502429	-0.947082	2.453572
C	-0.165005	-1.012534	3.804213
C	-0.359085	0.090082	4.632681
C	-0.890578	1.266652	4.108019
C	-1.237671	1.337954	2.761721
C	1.055646	-1.631117	-2.755357
O	1.769595	-1.931934	-3.587503
O	1.510008	0.174546	-0.621050
C	2.659100	-0.129181	-0.124626
C	3.634410	1.015017	-0.125841
C	4.590061	1.183487	0.883970
C	5.473353	2.259240	0.853570
C	5.421430	3.180384	-0.190573
C	4.471709	3.024862	-1.199267
C	3.580123	1.957750	-1.161287
C	-1.547900	-1.865267	-2.131301
O	-2.399200	-2.439783	-2.637087
C	3.087803	-1.360053	0.365474
H	4.129739	-1.417342	0.640777
H	2.502798	-3.920363	2.155440
H	2.601784	-4.621807	0.565367
H	-3.375151	-0.860012	2.264932
H	-3.649860	0.240556	-1.884220
H	-5.726335	-1.587930	2.220212
H	-6.000951	-0.473430	-1.916243
H	-7.056340	-1.396017	0.134256
H	-3.714095	2.343957	0.172515
H	0.464457	2.074317	-0.801211
H	-3.692031	4.742167	-0.378202
H	0.482586	4.486442	-1.349953
H	-1.597058	5.828455	-1.146574
H	-0.306075	-1.792870	1.805277
H	-1.642948	2.259547	2.362628
H	0.262038	-1.925505	4.203547
H	-1.032487	2.132390	4.745141
H	-0.088036	0.037231	5.681317

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H        4.801457   -4.803556    1.679691
H        4.972493   -3.690920    0.321233
H        4.868278   -3.067909    1.972156
H        2.838785    1.833494   -1.940721
H        4.428166    3.735041   -2.017854
H        6.112844    4.015312   -0.215778
H        6.198783    2.381548    1.650321
H        4.623446    0.483745    1.710215

16   Transition State 2_B_(C)
C       -3.989967   -0.320078   -0.746912
C       -3.197660   -0.104691    0.390358
C       -3.768630   -0.273796    1.655483
C       -5.105969   -0.649735    1.780280
C       -5.886716   -0.854428    0.647022
C       -5.325036   -0.686281   -0.618467
P       -1.423906    0.348148    0.157854
Rh      -0.072351   -1.224348   -0.951175
O        1.306031   -2.936486   -0.270931
C        2.513886   -2.776493    0.020725
C        3.307169   -4.040941    0.353014
C        2.499822   -5.083150    1.130307
C       -1.514179    2.026541   -0.612383
C       -0.353854    2.555182   -1.193443
C       -0.370867    3.827252   -1.757940
C       -1.542105    4.582801   -1.758660
C       -2.698932    4.062292   -1.184973
C       -2.687368    2.791766   -0.611338
C       -0.804520    0.677883    1.865934
C       -0.146658   -0.352996    2.546549
C        0.304749   -0.159694    3.849757
C        0.115754    1.068360    4.479770
C       -0.526256    2.103593    3.802823
C       -0.985478    1.911737    2.502169
C        0.209913   -1.172781   -3.033361
O       -0.222964   -1.033238   -4.080331
O        1.557181    0.068765   -0.617343
C        2.738052   -0.267470   -0.243051
C        3.694897    0.885343   -0.142417
C        4.651171    0.969269    0.876710
C        5.520364    2.054902    0.944290
C        5.456048    3.065338   -0.012719
C        4.508467    2.989836   -1.032456
C        3.628198    1.914443   -1.090053
C       -1.479610   -2.429251   -1.060941
O       -2.280007   -3.244390   -1.112658
C        3.222726   -1.544467    0.043198
H        4.272137   -1.607841    0.294248
H        3.624644   -4.466324   -0.608097
H        4.221818   -3.775120    0.889496
H       -3.173584   -0.114031    2.545628
H       -3.562568   -0.199043   -1.736394
H       -5.534214   -0.780990    2.767656
H       -5.924890   -0.848018   -1.506846
H       -6.925812   -1.147084    0.746198
H       -3.595452    2.400175   -0.170580
H        0.555171    1.967400   -1.190884
H       -3.614950    4.642628   -1.181907
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H	0.534218	4.227343	-2.201121
H	-1.553296	5.570914	-2.204991
H	0.021384	-1.300034	2.045373
H	-1.474900	2.725769	1.981667
H	0.814373	-0.965159	4.366270
H	-0.666194	3.064564	4.285149
H	0.475260	1.221869	5.491155
H	3.078422	-6.001083	1.261248
H	2.229323	-4.711191	2.122724
H	1.577303	-5.324260	0.601624
H	2.892126	1.849616	-1.881533
H	4.457160	3.769683	-1.784265
H	6.137641	3.907113	0.037109
H	6.245984	2.113095	1.747990
H	4.696891	0.194521	1.632588

17 Product B_(*C*)

C	-2.688042	2.590432	-0.422280
C	-3.392525	1.410996	-0.143736
C	-4.725685	1.507490	0.277373
C	-5.340321	2.749414	0.406416
C	-4.635389	3.914408	0.110299
C	-3.307244	3.829933	-0.304708
C	-2.683111	0.097634	-0.283117
C	-3.425616	-1.062332	-0.548526
C	-2.908240	-2.365449	-0.677032
C	-3.833890	-3.542762	-0.963855
C	-5.321963	-3.265308	-1.177077
O	-1.690702	-2.703620	-0.566970
Rh	-0.052375	-1.421724	-0.284466
C	-2.823559	-2.779646	2.877886
O	-2.144394	-2.013016	3.348537
P	1.657644	0.115986	-0.024548
C	1.491010	1.483759	-1.252599
C	0.975793	1.179713	-2.518955
C	0.856336	2.172753	-3.487849
C	1.237489	3.481575	-3.198450
C	1.738920	3.794072	-1.936503
C	1.866365	2.801342	-0.967049
C	3.393321	-0.475886	-0.233847
C	3.878054	-1.452271	0.647873
C	5.170496	-1.946459	0.512784
C	5.994867	-1.481255	-0.511517
C	5.519353	-0.517548	-1.395055
C	4.226111	-0.013542	-1.257154
C	1.696302	0.973356	1.612503
C	0.483591	1.212724	2.272280
C	0.471380	1.875576	3.496581
C	1.663932	2.301351	4.078256
C	2.873018	2.066281	3.428259
C	2.891474	1.406678	2.200757
O	-1.411934	0.162924	-0.161121
C	1.096986	-2.857583	-0.433186
O	1.752765	-3.792192	-0.547022
H	-4.487131	-0.940542	-0.693160
H	-3.412819	-4.048765	-1.839011
H	-3.695432	-4.240538	-0.130885
H	3.870094	0.738604	-1.949560

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 H     3.243196    -1.828342     1.442439
 H     6.152733    -0.152604    -2.195838
 H     5.530754    -2.701663     1.201970
 H     7.000107    -1.872275    -0.620633
 H     3.839080     1.222556     1.709759
 H    -0.443585     0.884370     1.820117
 H     3.805303     2.392399     3.875859
 H    -0.473161     2.053127     3.998217
 H     1.651476     2.810853     5.035364
 H     0.657345     0.165638    -2.733228
 H     2.248432     3.058004     0.013427
 H     0.454560     1.925273    -4.463882
 H     2.029382     4.812417    -1.703195
 H     1.137238     4.256158    -3.950589
 H    -5.848720    -4.199946    -1.385808
 H    -5.783705    -2.820620    -0.291743
 H    -5.493124    -2.594822    -2.023330
 H    -1.655182     2.516254    -0.736693
 H    -2.751713     4.732083    -0.535689
 H    -5.116500     4.881319     0.207592
 H    -6.368944     2.807297     0.744519
 H    -5.278639     0.612121     0.533111

18   Free Isomer A
C      -3.620710    1.705695   -1.520591
C      -2.861325    1.618195   -0.349687
C      -2.935010    2.659378    0.586442
C      -3.754565    3.758847    0.356936
C      -4.506641    3.839952   -0.814686
C      -4.436546    2.813169   -1.750781
P      -1.721655    0.204176   -0.016928
C      -2.126593   -1.021572   -1.335340
C      -1.379808   -0.987644   -2.519402
C      -1.665152   -1.870313   -3.557666
C      -2.689214   -2.805403   -3.418990
C      -3.427584   -2.853286   -2.238751
C      -3.150050   -1.965595   -1.201281
Rh      0.551261    0.608899    0.052913
C       0.351909    2.442862    0.130907
O       0.299414    3.588224    0.177238
O       2.639488    0.827797    0.072979
C       3.503595   -0.097905   -0.014845
C       3.224624   -1.479147   -0.094762
C       1.955205   -2.066399   -0.110771
C       1.850933   -3.579815   -0.212167
C       1.124510   -4.208783    0.985159
C       4.929955    0.368237   -0.009792
C       5.982550   -0.399005   -0.526688
C       7.287123    0.085587   -0.511894
C       7.562326    1.341418    0.024961
C       6.521695    2.116076    0.535631
C       5.216911    1.637454    0.511113
O       0.833124   -1.458436   -0.052109
C      -2.402888   -0.528640    1.535910
C      -1.545924   -1.271147    2.357856
C      -2.027481   -1.860864    3.523899
C      -3.364600   -1.711028    3.886088
C      -4.222087   -0.969695    3.076367
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C	-3.745677	-0.380940	1.906792
H	4.064789	-2.156545	-0.119268
H	1.292066	-3.801227	-1.128260
H	2.846772	-4.015022	-0.323410
H	-3.725752	-2.019333	-0.285627
H	-0.567034	-0.276555	-2.615375
H	-4.219300	-3.584844	-2.121314
H	-1.079747	-1.834012	-4.469532
H	-2.905985	-3.498418	-4.224283
H	-3.579506	0.912573	-2.256147
H	-2.351725	2.611747	1.498995
H	-5.017403	2.868373	-2.664648
H	-3.799812	4.556117	1.090036
H	-5.140679	4.700535	-0.995528
H	-0.505664	-1.382628	2.078926
H	-4.419465	0.202338	1.290767
H	-1.353801	-2.431370	4.153249
H	-5.262391	-0.844236	3.355302
H	-3.735542	-2.164974	4.798241
H	5.784432	-1.367200	-0.969107
H	8.088519	-0.516586	-0.925273
H	8.579718	1.716303	0.039423
H	6.727721	3.096393	0.950776
H	4.399280	2.234849	0.892505
H	1.035569	-5.290517	0.856154
H	1.669054	-4.024366	1.915705
H	0.120873	-3.793301	1.085839

19 Free Isomer B

C	3.875278	1.035603	-0.832671
C	3.252649	0.300506	0.186054
C	3.980090	-0.011649	1.338390
C	5.305232	0.403338	1.468997
C	5.917602	1.126605	0.450412
C	5.199130	1.440119	-0.703141
P	1.483808	-0.182059	-0.027745
C	1.532971	-1.363908	-1.448535
C	0.336769	-1.655892	-2.117272
C	0.327573	-2.564462	-3.172012
C	1.507811	-3.185447	-3.576408
C	2.700512	-2.898776	-2.917146
C	2.715368	-1.993914	-1.857158
Rh	-0.088367	1.508278	-0.210883
O	-1.578021	0.040770	-0.140218
C	-2.843430	0.230661	-0.143174
C	-3.484373	1.475861	-0.191698
C	-2.854319	2.732323	-0.285140
C	-3.723104	3.980221	-0.348713
C	-3.379870	4.993536	0.751765
C	-3.665386	-1.019867	-0.061863
C	-3.098212	-2.162148	0.519896
C	-3.827059	-3.342228	0.619380
C	-5.128213	-3.407372	0.123220
C	-5.695562	-2.283138	-0.473641
C	-4.971907	-1.097855	-0.562786
O	-1.607088	2.951639	-0.328781
C	1.178132	2.849672	-0.247598

O	1.908174	3.734671	-0.264477
C	1.123067	-1.248719	1.435177
C	1.413120	-2.617708	1.458036
C	1.138134	-3.375319	2.594590
C	0.574014	-2.774397	3.718202
C	0.279388	-1.412503	3.701173
C	0.546344	-0.653990	2.564173
H	-4.562480	1.483381	-0.130152
H	-3.550127	4.439259	-1.328961
H	-4.779177	3.703978	-0.302293
H	1.844680	-3.097324	0.587958
H	0.297245	0.400945	2.538639
H	1.362844	-4.436118	2.599723
H	-0.169121	-0.940953	4.568248
H	0.358672	-3.366331	4.600798
H	3.516322	-0.577030	2.136500
H	3.323987	1.293388	-1.730065
H	5.856104	0.157832	2.370032
H	5.666953	2.007907	-1.499287
H	6.947637	1.448583	0.553775
H	-0.580993	-1.176213	-1.801247
H	3.650740	-1.775770	-1.356839
H	-0.604669	-2.782601	-3.680731
H	3.623368	-3.376391	-3.227163
H	1.498578	-3.887355	-4.402863
H	-5.416603	-0.238890	-1.049918
H	-6.701352	-2.330260	-0.875991
H	-5.694572	-4.329220	0.195929
H	-3.378364	-4.213482	1.083533
H	-2.084916	-2.104263	0.895601
H	-3.972245	5.904630	0.635690
H	-3.585290	4.580588	1.743341
H	-2.322832	5.258531	0.706428

20 Reac (with LANL2DZ+*f*135)

C	5.546027	-2.577817	-0.522092
C	6.004042	-1.311511	-0.132552
C	7.360327	-1.153204	0.183728
C	8.236412	-2.230607	0.100200
C	7.773357	-3.480385	-0.306373
C	6.424791	-3.650488	-0.616114
C	5.021489	-0.187068	-0.049983
C	5.468392	1.143669	-0.122824
C	4.658323	2.284148	-0.049025
O	3.391390	2.304746	0.103947
Rh	2.144401	0.668302	0.232014
C	0.667199	1.805311	0.389009
O	-0.204177	2.533704	0.487214
P	-3.411000	-0.157281	-0.217131
C	-4.233439	-1.465235	-1.242098
C	-5.136635	-2.411551	-0.743800
C	-5.684400	-3.379650	-1.584680
C	-5.343446	-3.412883	-2.934427
C	-4.443290	-2.476838	-3.441579
C	-3.885867	-1.518949	-2.599874
C	-3.838257	-0.675957	1.511219
C	-2.977875	-1.596558	2.128132

C	-3.213569	-2.029854	3.429814
C	-4.302826	-1.534274	4.144828
C	-5.155098	-0.608456	3.548086
C	-4.927581	-0.183459	2.239719
C	-4.514359	1.308606	-0.481552
C	-5.793663	1.245449	-1.047110
C	-6.545869	2.405181	-1.227723
C	-6.034056	3.641953	-0.841976
C	-4.760185	3.717119	-0.281218
C	-4.002901	2.561237	-0.112118
O	3.801791	-0.549585	0.062659
C	1.050652	-0.845800	0.352950
O	0.426951	-1.796924	0.430321
C	5.297649	3.656178	-0.157760
C	4.755467	4.459995	-1.349141
H	6.523317	1.311597	-0.277211
H	5.071184	4.190263	0.771696
H	6.383530	3.558053	-0.222897
H	-5.410594	-2.397155	0.304194
H	-3.170803	-0.806086	-2.997950
H	-6.379861	-4.108129	-1.181958
H	-4.165951	-2.500389	-4.489721
H	-5.770586	-4.166860	-3.586203
H	-6.202434	0.289611	-1.352332
H	-3.003237	2.630891	0.303609
H	-7.534128	2.340332	-1.670089
H	-4.350193	4.676938	0.013133
H	-6.620977	4.542630	-0.983831
H	-2.116847	-1.973302	1.585951
H	-5.598175	0.537576	1.787914
H	-2.540206	-2.745072	3.889275
H	-6.001381	-0.214347	4.100339
H	-4.481557	-1.862841	5.162601
H	7.732053	-0.195156	0.524659
H	9.280535	-2.095218	0.358504
H	8.458280	-4.318054	-0.375131
H	6.057665	-4.621334	-0.929242
H	4.495701	-2.700805	-0.750650
H	5.190350	5.462176	-1.365294
H	4.997896	3.970370	-2.296146
H	3.670856	4.554628	-1.282008

21 TS1 A_(*C*) (with LANL2DZ+*f*135)

C	-4.318742	1.141091	-1.381617
C	-3.999036	0.447277	-0.206940
C	-4.853681	0.564840	0.896513
C	-6.001823	1.348808	0.823702
C	-6.319117	2.018805	-0.355883
C	-5.473419	1.911595	-1.459373
C	-2.736294	-0.370435	-0.180689
C	-2.663853	-1.474847	0.709344
C	-1.599854	-2.367119	0.868514
O	-0.471565	-2.365657	0.265998
Rh	0.097120	-1.199063	-1.361746
C	0.578450	-0.207434	-2.856733
O	0.824173	0.419834	-3.779600
P	1.355686	0.499560	0.211999
C	0.646673	2.163282	0.579690

C	1.024967	2.911591	1.703994
C	0.483541	4.175059	1.923060
C	-0.443326	4.705161	1.026152
C	-0.834046	3.963176	-0.084942
C	-0.296691	2.696450	-0.306383
C	1.719881	-0.167842	1.894542
C	0.637260	-0.404683	2.754019
C	0.847645	-0.924295	4.026829
C	2.138720	-1.231779	4.455737
C	3.216889	-1.010422	3.604576
C	3.011352	-0.480072	2.331093
C	3.026555	0.864778	-0.494750
C	3.608496	2.137177	-0.475393
C	4.865932	2.346774	-1.039698
C	5.560729	1.290096	-1.621731
C	4.988940	0.019111	-1.647173
C	3.727253	-0.189736	-1.097970
O	-1.833225	-0.013089	-0.982512
C	0.581838	-2.792256	-2.234270
O	0.917075	-3.779785	-2.707531
C	-1.744665	-3.499540	1.874060
C	-1.635286	-4.882759	1.215986
H	-3.545527	-1.689979	1.294881
H	-0.937075	-3.383397	2.605025
H	-2.691741	-3.404695	2.410323
H	1.736661	2.504078	2.412287
H	-0.643202	2.104199	-1.143180
H	0.783224	4.744121	2.796203
H	-1.571113	4.359611	-0.773815
H	-0.867381	5.687691	1.201011
H	3.080288	2.969945	-0.029053
H	3.275460	-1.174487	-1.142492
H	5.300115	3.340276	-1.024295
H	5.518634	-0.808307	-2.105852
H	6.538227	1.456378	-2.060277
H	-0.372747	-0.179381	2.430444
H	3.861734	-0.305727	1.684162
H	0.001168	-1.093914	4.683036
H	4.224476	-1.245232	3.929410
H	2.300773	-1.641588	5.446332
H	-4.610226	0.066040	1.826417
H	-6.646981	1.439380	1.690510
H	-7.217207	2.623715	-0.413731
H	-5.715225	2.429618	-2.380910
H	-3.648983	1.056931	-2.227937
H	-1.689488	-5.672946	1.969196
H	-2.445837	-5.042212	0.499558
H	-0.687141	-4.977219	0.684899

22 Inter A_(*C*) (with LANL2DZ+*f*135)

C	-4.319317	1.522951	-1.042517
C	-4.129446	0.558303	-0.044581
C	-5.141914	0.371569	0.905271
C	-6.314087	1.121573	0.852010
C	-6.497965	2.064028	-0.157258
C	-5.495213	2.261756	-1.105916
C	-2.825179	-0.204685	-0.033773
C	-2.781886	-1.465963	0.629739

C	-1.670733	-2.300091	0.749956
O	-0.508877	-2.141573	0.233722
Rh	0.189749	-0.959737	-1.387759
C	1.099172	-0.195427	-2.797836
O	1.656521	0.264985	-3.687747
P	1.506352	0.391971	0.160484
C	1.094227	2.183184	0.206137
C	1.526743	2.999493	1.261664
C	1.226361	4.357977	1.268399
C	0.483567	4.914636	0.227853
C	0.033429	4.106489	-0.811895
C	0.331464	2.745390	-0.822498
C	1.362587	-0.116619	1.923429
C	0.109795	0.004164	2.539550
C	-0.051157	-0.359091	3.871745
C	1.030082	-0.854538	4.600870
C	2.274200	-0.983076	3.990891
C	2.442994	-0.615578	2.656167
C	3.310510	0.288997	-0.213247
C	4.177552	1.384191	-0.143434
C	5.532172	1.227444	-0.432849
C	6.035302	-0.021523	-0.786431
C	5.176966	-1.117289	-0.861634
C	3.821732	-0.962168	-0.586557
O	-1.854397	0.330603	-0.616162
C	-0.578386	-2.280178	-2.545645
O	-1.017616	-3.105804	-3.194096
C	-1.792220	-3.555495	1.604629
C	-1.435528	-4.834954	0.835803
H	-3.691932	-1.823994	1.088244
H	-1.098756	-3.434456	2.444907
H	-2.799245	-3.627080	2.022814
H	2.085153	2.570900	2.085733
H	-0.060537	2.115176	-1.609228
H	1.564992	4.979468	2.089722
H	-0.564586	4.529179	-1.610937
H	0.245010	5.972258	0.236888
H	3.800306	2.363350	0.121963
H	3.150184	-1.809372	-0.673444
H	6.192256	2.086179	-0.384410
H	5.558834	-2.090927	-1.146982
H	7.089125	-0.139592	-1.012022
H	-0.737083	0.375632	1.976009
H	3.416803	-0.716907	2.194120
H	-1.024988	-0.261491	4.337897
H	3.119225	-1.367395	4.551094
H	0.900888	-1.139974	5.638886
H	-5.009968	-0.344100	1.707209
H	-7.083369	0.971194	1.601546
H	-7.413825	2.643060	-0.201792
H	-5.630989	2.994539	-1.894008
H	-3.524950	1.675850	-1.761916
H	-1.478532	-5.707669	1.492815
H	-2.130441	-5.002024	0.007800
H	-0.427540	-4.761698	0.424987

23 TS2 A_(*C*) (with LANL2DZ+*f*135)

C	5.689902	0.329363	0.932096
C	4.775364	-0.361573	0.126944
C	5.162847	-1.586693	-0.431751
C	6.438031	-2.095144	-0.213085
C	7.342897	-1.396054	0.585190
C	6.962390	-0.186679	1.162707
C	3.379368	0.135959	-0.141855
O	2.531401	-0.742223	-0.435521
Rh	0.327024	-0.258832	-0.944609
O	0.737567	1.676205	-0.284005
C	1.900335	2.185048	-0.100540
C	1.871573	3.692522	0.115165
C	1.230055	4.440691	-1.061787
P	-1.692750	-0.205700	0.225161
C	-2.428456	1.472773	0.429135
C	-1.769125	2.397833	1.251073
C	-2.284973	3.677978	1.422689
C	-3.455821	4.058355	0.768259
C	-4.111046	3.148290	-0.055820
C	-3.602586	1.861274	-0.224998
C	-1.593664	-0.817419	1.966609
C	-0.506354	-1.611549	2.345246
C	-0.411180	-2.104333	3.645540
C	-1.395327	-1.800005	4.581796
C	-2.475508	-0.996527	4.217540
C	-2.574923	-0.505458	2.918995
C	-3.036398	-1.205846	-0.556718
C	-3.201877	-1.111829	-1.946335
C	-4.201556	-1.834262	-2.590589
C	-5.037491	-2.676622	-1.859488
C	-4.869761	-2.788512	-0.482335
C	-3.878679	-2.055227	0.168411
C	0.016063	-2.029175	-1.385741
O	-0.093314	-3.139769	-1.640528
C	0.524940	0.326995	-2.944260
O	0.073982	0.424089	-3.988937
C	3.133182	1.535292	-0.058846
H	3.990933	2.171564	0.102090
H	1.287760	3.881627	1.023384
H	2.882956	4.061938	0.298544
H	-3.410240	0.130083	2.649092
H	0.276406	-1.824177	1.625747
H	-3.238543	-0.747135	4.946474
H	0.438787	-2.715839	3.926010
H	-1.317627	-2.177828	5.595122
H	-3.758417	-2.159277	1.238885
H	-2.538619	-0.478998	-2.524846
H	-5.508296	-3.450685	0.091563
H	-4.317539	-1.748343	-3.665023
H	-5.808400	-3.249132	-2.362732
H	-0.851574	2.116600	1.749985
H	-4.130624	1.162233	-0.860688
H	-1.768314	4.381823	2.065596
H	-5.024061	3.433643	-0.566270
H	-3.853984	5.057959	0.901607
H	5.400096	1.260154	1.403718
H	7.655517	0.354307	1.797413
H	8.336278	-1.794095	0.760537

H	6.727251	-3.038399	-0.663233
H	4.445555	-2.125146	-1.037851
H	1.183967	5.513771	-0.857952
H	1.808760	4.295775	-1.978241
H	0.216731	4.077295	-1.236523

24 Product A_(*C*) (with LANL2DZ+*f*135)

C	-5.832213	0.691584	-0.863754
C	-4.824449	-0.165023	-0.401106
C	-5.161589	-1.485945	-0.075546
C	-6.474033	-1.930573	-0.185949
C	-7.470345	-1.068064	-0.641224
C	-7.143529	0.241771	-0.986007
C	-3.394081	0.264770	-0.262857
O	-2.547430	-0.682209	-0.280360
Rh	-0.461565	-0.507862	-0.181916
O	-0.710066	1.544855	0.085016
C	-1.816176	2.183425	0.059816
C	-1.684835	3.687621	0.231447
C	-1.113512	4.081006	1.601656
P	1.814914	-0.144815	-0.136326
C	2.484558	0.376149	1.503840
C	1.623204	0.996487	2.416881
C	2.098327	1.415182	3.657492
C	3.433282	1.214892	4.002156
C	4.295154	0.593287	3.101072
C	3.825199	0.174656	1.858227
C	2.265201	1.218646	-1.294265
C	1.564792	1.312322	-2.503767
C	1.886727	2.300763	-3.429739
C	2.900535	3.215945	-3.151972
C	3.590772	3.138416	-1.944656
C	3.277574	2.144118	-1.019845
C	2.936485	-1.532224	-0.613903
C	2.943376	-2.689172	0.178052
C	3.755547	-3.767588	-0.153548
C	4.567057	-3.711006	-1.286315
C	4.562887	-2.568793	-2.080511
C	3.754566	-1.482103	-1.746610
C	-0.288366	-2.319283	-0.445701
O	-0.249310	-3.453168	-0.619822
C	-1.876360	-1.169617	3.205416
O	-2.206815	-2.241465	3.086689
C	-3.092489	1.633510	-0.104102
H	-3.920588	2.325313	-0.067037
H	-1.010976	4.042889	-0.555529
H	-2.654597	4.165885	0.075256
H	3.816348	2.100470	-0.081404
H	0.759379	0.615748	-2.708111
H	4.373149	3.854143	-1.718037
H	1.337682	2.361799	-4.362648
H	3.145723	3.990703	-3.869853
H	3.765232	-0.597949	-2.371281
H	2.311750	-2.749325	1.057283
H	5.189811	-2.517066	-2.963638
H	3.748759	-4.655360	0.468503
H	5.195759	-4.554627	-1.547775
H	0.584353	1.146090	2.152074

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 H     4.501754    -0.320471     1.171942
 H     1.420203     1.890375     4.357218
 H     5.333593     0.427875     3.365822
 H     3.799376     1.535381     4.971179
 H    -5.591521     1.705546    -1.157793
 H    -7.909725     0.913829    -1.356167
 H    -8.493306    -1.415896    -0.732666
 H    -6.720157    -2.952399     0.080604
 H    -4.377512    -2.149746     0.264386
 H    -1.013734     5.166765     1.678571
 H    -1.767013     3.743598     2.410967
 H    -0.127671     3.637414     1.749027

25   Reac (with LANL2DZ+f040)
C     5.604336    -2.544918    -0.528084
 C     6.048126    -1.253596    -0.210697
 C     7.418407    -1.043570    -0.003437
 C     8.320783    -2.095719    -0.122077
 C     7.870075    -3.371313    -0.456014
 C     6.508511    -3.592381    -0.657919
 C     5.037503    -0.158788    -0.083742
 C     5.430963     1.182586    -0.230174
 C     4.590094     2.297818    -0.124008
 O     3.339100     2.281909     0.129793
Rh     2.165700     0.611334     0.402312
 C     0.666099     1.704753     0.645161
 O    -0.220546     2.405927     0.793211
 P    -3.411201    -0.170454    -0.258222
 C    -4.253406    -1.434462    -1.322028
 C    -5.179402    -2.374058    -0.853971
 C    -5.740455    -3.309550    -1.722591
 C    -5.389872    -3.316471    -3.070237
 C    -4.466826    -2.386902    -3.547414
 C    -3.896543    -1.461742    -2.678223
 C    -3.873304    -0.715678     1.452772
 C    -3.030910    -1.654222     2.066981
 C    -3.293638    -2.111470     3.355280
 C    -4.392816    -1.622209     4.059339
 C    -5.227334    -0.678284     3.465566
 C    -4.972421    -0.229082     2.170486
 C    -4.475079     1.327805    -0.503528
 C    -5.748997     1.308410    -1.084313
 C    -6.470265     2.489998    -1.248800
 C    -5.932458     3.705389    -0.831805
 C    -4.663563     3.737081    -0.255825
 C    -3.937016     2.559419    -0.102439
 O     3.843284    -0.556057     0.135676
 C     1.125304    -0.926056     0.648556
 O     0.525328    -1.883738     0.800112
 C     5.170640     3.685661    -0.323081
 C     4.508424     4.433381    -1.490180
 H     6.464037     1.379632    -0.472960
 H     4.999880     4.241289     0.605637
 H     6.250703     3.620649    -0.472065
 H    -5.460816    -2.379748     0.192100
 H    -3.164203    -0.754031    -3.053399
 H    -6.453748    -4.033242    -1.343096
 H    -4.182023    -2.390146    -4.593822
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H	-5.827347	-4.045072	-3.743666
H	-6.177790	0.369855	-1.414704
H	-2.940888	2.595305	0.325905
H	-7.454646	2.458962	-1.703310
H	-4.233341	4.680093	0.063006
H	-6.495238	4.623197	-0.961194
H	-2.161603	-2.023576	1.533186
H	-5.628744	0.506302	1.720744
H	-2.633671	-2.840121	3.813025
H	-6.080769	-0.288785	4.010036
H	-4.592917	-1.969414	5.066905
H	7.782751	-0.064272	0.280311
H	9.376312	-1.920313	0.052103
H	8.575204	-4.189276	-0.552182
H	6.151159	-4.583268	-0.914409
H	4.544440	-2.707740	-0.671874
H	4.905540	5.448089	-1.570165
H	4.692329	3.922027	-2.438878
H	3.429818	4.495084	-1.339601

26 TS1 A_(*C*) (with LANL2DZ+*f*040)

C	-4.320694	1.145717	-1.379000
C	-4.005820	0.444225	-0.207557
C	-4.867267	0.551090	0.891714
C	-6.017255	1.332227	0.817917
C	-6.329564	2.010008	-0.358555
C	-5.477102	1.913477	-1.457811
C	-2.741305	-0.370257	-0.180045
C	-2.669948	-1.480476	0.702893
C	-1.602906	-2.368489	0.862651
O	-0.471656	-2.359081	0.264930
Rh	0.092516	-1.189015	-1.358839
C	0.577347	-0.198469	-2.855159
O	0.828690	0.423318	-3.780194
P	1.354277	0.499879	0.213659
C	0.653844	2.166560	0.585901
C	1.034362	2.910196	1.712539
C	0.498403	4.175527	1.934474
C	-0.425185	4.712257	1.038145
C	-0.818033	3.975111	-0.075434
C	-0.286090	2.706622	-0.299680
C	1.717723	-0.172130	1.894684
C	0.635157	-0.405463	2.755241
C	0.844624	-0.929147	4.026534
C	2.134734	-1.244224	4.452859
C	3.212802	-1.026349	3.600671
C	3.008182	-0.491947	2.328731
C	3.025854	0.858755	-0.494781
C	3.613901	2.128294	-0.472575
C	4.871469	2.333507	-1.038189
C	5.560259	1.275190	-1.624380
C	4.982300	0.007062	-1.652664
C	3.720450	-0.197382	-1.102175
O	-1.834609	-0.005468	-0.974404
C	0.588936	-2.775425	-2.237112
O	0.937282	-3.755361	-2.717205
C	-1.746792	-3.505669	1.862848
C	-1.624578	-4.885763	1.200429

H	-3.553468	-1.702425	1.283038
H	-0.944725	-3.387324	2.599573
H	-2.697762	-3.418728	2.393476
H	1.743651	2.497690	2.420351
H	-0.633669	2.118580	-1.139034
H	0.799874	4.740911	2.809391
H	-1.552358	4.376918	-0.764134
H	-0.844952	5.696222	1.215246
H	3.090364	2.962286	-0.023013
H	3.263672	-1.179702	-1.148936
H	5.310453	3.324862	-1.020561
H	5.507263	-0.821529	-2.114657
H	6.537857	1.438043	-2.063997
H	-0.374183	-0.174280	2.433689
H	3.858501	-0.320489	1.680927
H	-0.001768	-1.095939	4.683580
H	4.219630	-1.267086	3.923518
H	2.296101	-1.657200	5.442249
H	-4.627839	0.046133	1.819338
H	-6.667775	1.414504	1.681532
H	-7.229066	2.612728	-0.417213
H	-5.715000	2.437659	-2.376869
H	-3.645883	1.069718	-2.222062
H	-1.679003	-5.678974	1.950414
H	-2.429356	-5.047443	0.478027
H	-0.672406	-4.972720	0.675304

27 Inter A_(*C*) (with LANL2DZ+*f*040)

C	-4.300776	1.522837	-1.058096
C	-4.124854	0.557314	-0.058390
C	-5.150067	0.370329	0.877704
C	-6.321041	1.120896	0.809226
C	-6.490798	2.064277	-0.201657
C	-5.475269	2.262374	-1.136551
C	-2.822067	-0.206982	-0.031515
C	-2.785216	-1.465107	0.638266
C	-1.675603	-2.299154	0.768588
O	-0.510708	-2.143955	0.256882
Rh	0.179436	-0.977254	-1.373828
C	1.074524	-0.204872	-2.791088
O	1.622933	0.257958	-3.684947
P	1.494192	0.401863	0.160607
C	1.091625	2.196355	0.185848
C	1.512038	3.019729	1.240663
C	1.220184	4.380158	1.230008
C	0.498755	4.932004	0.172121
C	0.061326	4.117259	-0.867998
C	0.350432	2.754286	-0.860781
C	1.346673	-0.085506	1.929443
C	0.091208	0.038414	2.539547
C	-0.073780	-0.310093	3.875196
C	1.006126	-0.794160	4.613875
C	2.252812	-0.926308	4.009877
C	2.425612	-0.573588	2.671672
C	3.298871	0.288709	-0.208432
C	4.170405	1.380600	-0.141725
C	5.525360	1.216229	-0.425251
C	6.024245	-0.037073	-0.769549

C	5.161401	-1.129522	-0.841375
C	3.805823	-0.966881	-0.572296
O	-1.844925	0.324123	-0.607505
C	-0.487665	-2.357591	-2.521283
O	-0.842162	-3.224971	-3.168214
C	-1.801590	-3.549876	1.628991
C	-1.442467	-4.833571	0.868332
H	-3.698350	-1.820242	1.092745
H	-1.111761	-3.425158	2.471732
H	-2.810457	-3.618396	2.043189
H	2.054728	2.595299	2.077255
H	-0.031093	2.120038	-1.649503
H	1.549204	5.007061	2.051133
H	-0.519699	4.536544	-1.681256
H	0.267032	5.991171	0.167470
H	3.796362	2.362789	0.117087
H	3.130387	-1.811253	-0.656440
H	6.189116	2.072276	-0.379323
H	5.540119	-2.106521	-1.119369
H	7.078383	-0.161106	-0.990464
H	-0.754270	0.401038	1.968266
H	3.401245	-0.677929	2.214161
H	-1.049601	-0.209943	4.336636
H	3.096721	-1.302130	4.577492
H	0.873904	-1.068206	5.654579
H	-5.029424	-0.345977	1.680836
H	-7.100464	0.970238	1.548130
H	-7.405694	2.643786	-0.258069
H	-5.600068	2.995887	-1.925761
H	-3.496830	1.675535	-1.766763
H	-1.487645	-5.702568	1.530063
H	-2.134658	-5.005190	0.039016
H	-0.433135	-4.762728	0.460386

28 TS2 A_(*C*) (with LANL2DZ+*f*040)

C	5.686101	0.315282	0.931662
C	4.772481	-0.365699	0.117011
C	5.159098	-1.585811	-0.453154
C	6.432603	-2.099052	-0.235957
C	7.336541	-1.409915	0.571966
C	6.956866	-0.205660	1.160642
C	3.378507	0.137460	-0.150601
O	2.529450	-0.735163	-0.457568
Rh	0.321279	-0.245040	-0.950335
O	0.738692	1.683109	-0.277699
C	1.902916	2.188452	-0.091024
C	1.876674	3.694444	0.134228
C	1.239201	4.451271	-1.039461
P	-1.683140	-0.207836	0.225060
C	-2.410513	1.470012	0.466268
C	-1.747248	2.372702	1.309704
C	-2.255406	3.651850	1.509408
C	-3.422821	4.054139	0.862015
C	-4.082280	3.166616	0.017059
C	-3.581381	1.880604	-0.180262
C	-1.586455	-0.854552	1.955029
C	-0.502350	-1.660450	2.317682
C	-0.408239	-2.178878	3.608112

C	-1.390420	-1.888810	4.550885
C	-2.467555	-1.074085	4.202929
C	-2.565755	-0.557484	2.914225
C	-3.035368	-1.185032	-0.572176
C	-3.208390	-1.057654	-1.958272
C	-4.212627	-1.763178	-2.614052
C	-5.045549	-2.621971	-1.898762
C	-4.870273	-2.767050	-0.525684
C	-3.874543	-2.050796	0.136915
C	-0.002623	-2.012163	-1.405576
O	-0.122642	-3.118917	-1.671103
C	0.492925	0.350058	-2.943221
O	0.019213	0.465107	-3.976506
C	3.134360	1.536328	-0.052942
H	3.992791	2.169861	0.114885
H	1.290910	3.879016	1.042079
H	2.888382	4.060694	0.322032
H	-3.398837	0.086362	2.657436
H	0.279150	-1.862791	1.593809
H	-3.229215	-0.835841	4.937027
H	0.439381	-2.799268	3.875921
H	-1.313617	-2.286536	5.556636
H	-3.748139	-2.181077	1.203764
H	-2.547518	-0.412043	-2.525224
H	-5.506331	-3.442197	0.035722
H	-4.334417	-1.651321	-3.685461
H	-5.819949	-3.181387	-2.411301
H	-0.832951	2.075060	1.805235
H	-4.113478	1.199572	-0.831942
H	-1.735524	4.337710	2.168968
H	-4.992899	3.468693	-0.488026
H	-3.815093	5.052913	1.017221
H	5.396839	1.241901	1.411763
H	7.649282	0.327455	1.802725
H	8.328608	-1.811744	0.746091
H	6.721265	-3.038256	-0.694832
H	4.442543	-2.116603	-1.066839
H	1.195047	5.523115	-0.828956
H	1.819393	4.310743	-1.955651
H	0.225354	4.091387	-1.218452

29 Product A_(*C*) (with LANL2DZ+*f*040)

C	-5.833305	0.686626	-0.859395
C	-4.825418	-0.170204	-0.397155
C	-5.162406	-1.491855	-0.074059
C	-6.474559	-1.936843	-0.186399
C	-7.470880	-1.074006	-0.640932
C	-7.144299	0.236507	-0.983383
C	-3.395613	0.260426	-0.256644
O	-2.547880	-0.685953	-0.270603
Rh	-0.461143	-0.507251	-0.170929
O	-0.712168	1.544491	0.090254
C	-1.819407	2.181371	0.063174
C	-1.690422	3.685941	0.232783
C	-1.125424	4.082172	1.604866
P	1.808888	-0.145001	-0.136418
C	2.490814	0.388291	1.495560
C	1.634052	1.007051	2.413896

C	2.118232	1.436720	3.647296
C	3.457989	1.248798	3.979814
C	4.315496	0.628305	3.073769
C	3.836395	0.198948	1.838114
C	2.252573	1.211841	-1.305818
C	1.542533	1.298777	-2.510237
C	1.857799	2.281031	-3.445103
C	2.874701	3.196917	-3.181424
C	3.574746	3.126102	-1.979347
C	3.268190	2.137914	-1.045788
C	2.931627	-1.533050	-0.611460
C	2.955536	-2.679460	0.195342
C	3.768363	-3.758205	-0.133561
C	4.563422	-3.712698	-1.278420
C	4.542153	-2.581121	-2.087426
C	3.733191	-1.494031	-1.756311
C	-0.276166	-2.320721	-0.427770
O	-0.225470	-3.454816	-0.596476
C	-1.850548	-1.171236	3.212816
O	-2.179153	-2.244551	3.102087
C	-3.094922	1.629518	-0.100015
H	-3.923440	2.320861	-0.064816
H	-1.013704	4.040793	-0.551915
H	-2.660066	4.162815	0.071756
H	3.814746	2.099628	-0.111662
H	0.734742	0.601733	-2.703361
H	4.359783	3.842313	-1.763655
H	1.301241	2.336695	-4.373904
H	3.114850	3.966896	-3.906128
H	3.730775	-0.618077	-2.392536
H	2.337060	-2.730846	1.084418
H	5.156301	-2.537961	-2.979949
H	3.774969	-4.637671	0.500201
H	5.192704	-4.556587	-1.537629
H	0.591386	1.146653	2.159021
H	4.510137	-0.294892	1.148116
H	1.443391	1.910727	4.351015
H	5.357758	0.472269	3.329048
H	3.831243	1.577850	4.943220
H	-5.593003	1.701105	-1.151855
H	-7.910438	0.908860	-1.353099
H	-8.493611	-1.422126	-0.733728
H	-6.720396	-2.959273	0.078066
H	-4.378587	-2.156377	0.265024
H	-1.027272	5.168163	1.680299
H	-1.782021	3.745355	2.411901
H	-0.139692	3.640074	1.757405

30 TS Intermediate Isomerisation

C	3.875278	1.035603	-0.832671
C	3.252649	0.300506	0.186054
C	3.980090	-0.011649	1.338390
C	5.305232	0.403338	1.468997
C	5.917602	1.126605	0.450412
C	5.199130	1.440119	-0.703141
P	1.483808	-0.182059	-0.027745
C	1.532971	-1.363908	-1.448535

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C       0.336769   -1.655892   -2.117272
C       0.327573   -2.564462   -3.172012
C       1.507811   -3.185447   -3.576408
C       2.700512   -2.898776   -2.917146
C       2.715368   -1.993914   -1.857158
Rh     -0.088367    1.508278   -0.210883
O      -1.578021    0.040770   -0.140218
C      -2.843430    0.230661   -0.143174
C      -3.484373    1.475861   -0.191698
C      -2.854319    2.732323   -0.285140
C      -3.723104    3.980221   -0.348713
C      -3.379870    4.993536    0.751765
C      -3.665386   -1.019867   -0.061863
C      -3.098212   -2.162148    0.519896
C      -3.827059   -3.342228    0.619380
C      -5.128213   -3.407372    0.123220
C      -5.695562   -2.283138   -0.473641
C      -4.971907   -1.097855   -0.562786
O      -1.607088    2.951639   -0.328781
C       1.178132    2.849672   -0.247598
O       1.908174    3.734671   -0.264477
C       1.123067   -1.248719    1.435177
C       1.413120   -2.617708    1.458036
C       1.138134   -3.375319    2.594590
C       0.574014   -2.774397    3.718202
C       0.279388   -1.412503    3.701173
C       0.546344   -0.653990    2.564173
H      -4.562480    1.483381   -0.130152
H      -3.550127    4.439259   -1.328961
H      -4.779177    3.703978   -0.302293
H       1.844680   -3.097324    0.587958
H       0.297245    0.400945    2.538639
H       1.362844   -4.436118    2.599723
H      -0.169121   -0.940953    4.568248
H       0.358672   -3.366331    4.600798
H       3.516322   -0.577030    2.136500
H       3.323987    1.293388   -1.730065
H       5.856104    0.157832    2.370032
H       5.666953    2.007907   -1.499287
H       6.947637    1.448583    0.553775
H      -0.580993   -1.176213   -1.801247
H       3.650740   -1.775770   -1.356839
H      -0.604669   -2.782601   -3.680731
H       3.623368   -3.376391   -3.227163
H       1.498578   -3.887355   -4.402863
H      -5.416603   -0.238890   -1.049918
H      -6.701352   -2.330260   -0.875991
H      -5.694572   -4.329220    0.195929
H      -3.378364   -4.213482    1.083533
H      -2.084916   -2.104263    0.895601
H      -3.972245    5.904630    0.635690
H      -3.585290    4.580588    1.743341
H      -2.322832    5.258531    0.706428

31   TS for tetrahedral isomerisation
C      -3.503382   -1.764515   -1.328529
C      -2.551458   -1.798146   -0.298466
C      -2.368683   -2.987045    0.416968
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C	-3.120410	-4.119137	0.106294
C	-4.063513	-4.077129	-0.915522
C	-4.254504	-2.894913	-1.630037
P	-1.545154	-0.296004	0.063176
C	-2.775596	1.010467	0.468337
C	-2.370347	2.349177	0.377530
C	-3.257240	3.365770	0.722317
C	-4.548783	3.060533	1.148410
C	-4.954568	1.731027	1.238548
C	-4.071598	0.706584	0.903284
Rh	-0.004185	0.395527	-1.421836
O	2.022453	-0.268162	-0.857930
C	3.051465	0.290307	-0.353998
C	3.118453	1.624975	0.073081
C	2.047967	2.544389	0.021263
C	2.295157	3.971566	0.499540
C	2.080935	4.999011	-0.621403
C	4.271143	-0.583424	-0.244602
C	4.366640	-1.704200	-1.080637
C	5.470913	-2.547107	-1.017341
C	6.492962	-2.295533	-0.103114
C	6.401128	-1.194787	0.746555
C	5.302098	-0.343503	0.673899
O	0.886443	2.289530	-0.401756
C	-1.256054	0.245868	-2.717941
O	-1.988744	0.194212	-3.612168
C	-0.696476	-0.667440	1.654288
C	-1.238499	-0.259111	2.879370
C	-0.595857	-0.584699	4.071125
C	0.588836	-1.317075	4.051680
C	1.135027	-1.720535	2.835027
C	0.500605	-1.395822	1.638897
H	4.063983	1.994964	0.442210
H	1.585068	4.166958	1.311071
H	3.301399	4.066283	0.915946
H	-2.154626	0.316752	2.906912
H	0.951093	-1.678246	0.695622
H	-1.021138	-0.260457	5.014224
H	2.064201	-2.277993	2.811001
H	1.089367	-1.564872	4.981036
H	-1.643481	-3.034597	1.218574
H	-3.661953	-0.859578	-1.900876
H	-2.965560	-5.033011	0.668563
H	-4.985673	-2.852535	-2.429160
H	-4.646446	-4.958813	-1.156431
H	-1.365900	2.587529	0.042730
H	-4.396039	-0.324306	0.974667
H	-2.938923	4.399465	0.648853
H	-5.958769	1.488167	1.567357
H	-5.238516	3.856551	1.406062
H	5.236121	0.496170	1.354796
H	7.185150	-1.000077	1.470116
H	7.352224	-2.954911	-0.049360
H	5.534579	-3.402845	-1.680584
H	3.559606	-1.896247	-1.776077
H	2.186706	6.018900	-0.242446
H	2.810698	4.859965	-1.424096
H	1.083088	4.890158	-1.049828

32 Three-coordinated (without PPh_3)

C	-3.153275	1.235097	0.386046
C	-2.308108	0.192436	-0.017160
C	-2.875252	-1.041758	-0.365141
C	-4.253186	-1.219572	-0.333887
C	-5.086387	-0.174153	0.061258
C	-4.531648	1.050573	0.426957
C	-0.821089	0.343216	-0.067920
C	-0.252164	1.615741	-0.249884
C	1.116245	1.911083	-0.323404
C	1.566508	3.344890	-0.521422
C	2.473929	3.832880	0.618028
O	2.056681	1.053352	-0.237104
Rh	1.817346	-0.934914	-0.007449
O	-0.193205	-0.767888	0.045757
C	1.691599	-2.790533	0.194552
O	1.610991	-3.926314	0.314637
H	3.343315	3.181842	0.718853
H	2.822917	4.849197	0.420945
H	1.938618	3.837057	1.571238
H	0.696306	3.996341	-0.625194
H	-0.931125	2.445209	-0.377015
H	-2.220916	-1.850546	-0.661939
H	-6.160992	-0.314839	0.089794
H	-5.172439	1.862803	0.750737
H	-2.735922	2.184557	0.697082
H	2.118944	3.382893	-1.466979
H	-4.678038	-2.176002	-0.616766

33 Three-coordinated (without CO)

C	-5.974486	-0.348166	-0.290989
C	-4.870389	0.464021	0.000966
C	-5.084073	1.830441	0.230221
C	-6.366894	2.364384	0.193101
C	-7.459204	1.545510	-0.089972
C	-7.257301	0.189368	-0.338109
C	-3.469971	-0.060971	0.057303
C	-3.240664	-1.430697	0.311009
C	-2.002148	-2.077502	0.378908
C	-1.978790	-3.579490	0.616954
C	-1.860193	-4.373093	-0.695033
O	-0.836531	-1.563105	0.236228
Rh	-0.543842	0.411267	-0.067471
O	-2.553073	0.803512	-0.109076
P	1.717855	0.231405	-0.022188
C	2.404664	1.924486	-0.289861
C	1.942662	2.635888	-1.409040
C	2.360357	3.943666	-1.638091
C	3.238631	4.562115	-0.749466
C	3.696289	3.866626	0.367049
C	3.282303	2.555840	0.598482
C	2.479253	-0.344484	1.558804
C	1.726757	-0.207903	2.731658
C	2.251138	-0.611032	3.957456
C	3.527966	-1.164735	4.022871
C	4.278815	-1.315684	2.858346
C	3.758462	-0.909071	1.631831

C	2.550037	-0.808186	-1.300910
C	3.713591	-0.417226	-1.973182
C	4.291826	-1.256864	-2.924505
C	3.717416	-2.493198	-3.208485
C	2.557291	-2.887477	-2.542968
C	1.971126	-2.049141	-1.599245
H	-0.955559	-4.092888	-1.239086
H	-1.816269	-5.446624	-0.492982
H	-2.716806	-4.184475	-1.347022
H	-2.884319	-3.879565	1.150277
H	-4.105058	-2.051683	0.496611
H	-4.227976	2.458424	0.439837
H	-6.515847	3.421467	0.383688
H	-8.459757	1.962098	-0.123210
H	-8.099606	-0.451133	-0.574861
H	-5.832315	-1.399062	-0.509919
H	4.345764	-1.043415	0.731143
H	5.269191	-1.755215	2.903002
H	3.933799	-1.485549	4.975939
H	1.657833	-0.501966	4.858469
H	0.724211	0.202043	2.667660
H	1.259258	2.159018	-2.104821
H	1.997578	4.479755	-2.507884
H	3.561498	5.582076	-0.925264
H	4.376807	4.344382	1.063144
H	3.640669	2.026869	1.472981
H	1.058281	-2.342976	-1.093524
H	2.102505	-3.846229	-2.766499
H	4.168026	-3.144529	-3.949113
H	5.190438	-0.942008	-3.443640
H	4.165877	0.545155	-1.764043
H	-1.123164	-3.799859	1.260304

34 PPh_3-assisted isomerisation, Reac

C	-2.328676	-3.988486	-1.864916
C	-2.805626	-2.687617	-1.671995
C	-3.460710	-2.039237	-2.728030
C	-3.650618	-2.687121	-3.945369
C	-3.174080	-3.983803	-4.128627
C	-2.510167	-4.629853	-3.088863
P	-2.625776	-1.767751	-0.079321
Rh	-2.265084	0.498231	-0.375517
C	-0.996478	0.154562	-1.668371
O	-0.199070	0.003431	-2.482767
C	-4.145399	-2.209706	0.866713
C	-4.244185	-1.791689	2.200860
C	-5.366087	-2.114165	2.956341
C	-6.410592	-2.843104	2.387606
C	-6.325259	-3.249469	1.059554
C	-5.197198	-2.936749	0.301108
C	-1.299557	-2.661085	0.845434
C	-0.009830	-2.119804	0.894183
C	1.016661	-2.790314	1.556450
C	0.761082	-4.004974	2.187706
C	-0.523534	-4.545731	2.159219
C	-1.549103	-3.879266	1.494037
P	4.636248	-0.541597	0.472704
C	4.290728	0.936626	-0.589400

O	-3.703493	0.970641	1.055530
C	-4.034170	2.140742	1.442969
C	-3.513279	3.354673	0.980498
C	-2.526398	3.505592	-0.014105
C	-2.072917	4.882189	-0.400093
C	-2.880849	6.016377	-0.245714
C	-2.419795	7.272212	-0.629904
C	-1.141808	7.415601	-1.166129
C	-0.331874	6.292412	-1.328216
C	-0.796280	5.035693	-0.957382
O	-1.942951	2.558707	-0.626739
C	-5.124433	2.172394	2.501531
C	-6.472692	1.682139	1.950494
H	-6.377784	0.669558	1.556321
H	-7.232091	1.677039	2.736910
H	-6.824260	2.332622	1.144828
H	-5.224818	3.182471	2.905779
H	-3.887975	4.250334	1.453089
H	-0.179667	4.155921	-1.087668
H	0.663880	6.396345	-1.744807
H	-0.781660	8.395300	-1.460039
H	-3.061525	8.138643	-0.514656
H	-3.884531	5.917985	0.148881
H	-2.547050	-4.301472	1.492226
H	-0.730446	-5.485271	2.659640
H	1.557517	-4.525022	2.708355
H	2.009321	-2.354513	1.577937
H	0.187040	-1.161285	0.430572
H	-3.805921	-1.019759	-2.594851
H	-4.158611	-2.173226	-4.753588
H	-3.311314	-4.484491	-5.080511
H	-2.126884	-5.634359	-3.229250
H	-1.803087	-4.500437	-1.068860
H	-3.446670	-1.208338	2.642531
H	-5.428496	-1.790421	3.989278
H	-7.285888	-3.090447	2.977836
H	-7.132995	-3.815609	0.609313
H	-5.139174	-3.266410	-0.728409
H	-4.807785	1.518402	3.320606
C	5.721107	0.163669	1.800968
C	3.207707	0.844007	-1.474870
C	2.872297	1.910180	-2.305479
C	3.606783	3.093494	-2.250241
C	4.675488	3.203253	-1.362837
C	5.017294	2.132821	-0.538390
H	2.617055	-0.064972	-1.514065
H	2.029374	1.816326	-2.980054
H	3.342928	3.927500	-2.891150
H	5.245796	4.124386	-1.309746
H	5.847522	2.232513	0.150596
C	5.839439	-1.510614	-0.552142
C	6.418508	-1.046288	-1.738653
C	7.288239	-1.856883	-2.467422
C	7.596429	-3.138660	-2.019464
C	7.022815	-3.613477	-0.840612
C	6.144064	-2.810105	-0.120487
H	6.187198	-0.051135	-2.098284
H	7.725493	-1.482901	-3.386850

H	8.273310	-3.767010	-2.587543
H	7.250793	-4.613595	-0.488588
H	5.687563	-3.194474	0.786111
C	7.120633	0.139125	1.777828
C	7.856219	0.672723	2.835391
C	7.205855	1.243145	3.926788
C	5.812525	1.272457	3.961253
C	5.077694	0.728336	2.912008
H	7.638881	-0.300502	0.934203
H	8.940014	0.643254	2.803429
H	7.779942	1.657705	4.747934
H	5.297714	1.709394	4.809813
H	3.993266	0.740194	2.954683

35 PPh_3-assisted isomerisation, TS1_PPh_3_A

C	0.954954	-2.130335	2.699658
C	1.208615	-2.806290	1.497792
C	1.206222	-4.207177	1.496993
C	0.970196	-4.914802	2.674542
C	0.739707	-4.234882	3.868384
C	0.732098	-2.840863	3.877019
P	1.548990	-1.780008	-0.007229
Rh	-0.133893	0.358196	-0.387588
O	1.651246	1.771110	-0.705368
C	2.052948	2.612432	0.139147
C	3.096722	3.583070	-0.349199
C	4.026974	4.196303	0.499815
C	4.986002	5.067627	-0.010109
C	5.024259	5.347717	-1.374388
C	4.105535	4.739717	-2.229353
C	3.157324	3.858188	-1.722155
P	-2.446093	0.481661	-0.250991
C	-3.438167	-0.622051	-1.362411
C	-3.487328	-0.348012	-2.737149
C	-4.168806	-1.194800	-3.605362
C	-4.809377	-2.333165	-3.117963
C	-4.765172	-2.614875	-1.755614
C	-4.085907	-1.766142	-0.882304
C	-3.144117	2.156672	-0.627251
C	-4.475773	2.354398	-1.018155
C	-4.956098	3.639119	-1.261264
C	-4.115246	4.740886	-1.113435
C	-2.789959	4.552900	-0.728258
C	-2.304921	3.268258	-0.492658
C	-3.101606	0.085576	1.431709
C	-2.495782	-0.955859	2.144335
C	-2.979939	-1.333954	3.393631
C	-4.064994	-0.664114	3.955403
C	-4.661387	0.386471	3.261913
C	-4.184410	0.760372	2.006908
C	-0.219298	0.024031	-2.190904
O	-0.192059	-0.115668	-3.331213
O	0.005049	0.926369	1.651413
C	0.675487	1.903429	2.134072
C	0.400042	2.177736	3.607408
C	-1.036126	2.658619	3.861412
C	3.375944	-1.504589	0.111592
C	3.925831	-0.476543	-0.666655

C	5.295657	-0.225153	-0.637249
C	6.130754	-0.985287	0.178832
C	5.590342	-1.999195	0.967261
C	4.221925	-2.259276	0.934748
C	1.407795	-3.025334	-1.370960
C	2.512101	-3.590579	-2.018647
C	2.332210	-4.507276	-3.054256
C	1.050364	-4.877773	-3.450744
C	-0.056479	-4.320010	-2.811902
C	0.120841	-3.394819	-1.788317
C	1.599746	2.723473	1.479572
H	-1.757827	1.924761	3.501759
H	-1.206292	2.813342	4.930355
H	-1.227675	3.605956	3.349572
H	1.116984	2.907739	3.990359
H	2.015502	3.525392	2.071881
H	2.448266	3.367722	-2.377072
H	4.130564	4.951647	-3.292679
H	5.768046	6.030921	-1.769436
H	5.707227	5.524421	0.658648
H	4.023850	3.971187	1.559088
H	-4.069860	-1.995964	0.175493
H	-5.264559	-3.494476	-1.364534
H	-5.339847	-2.992711	-3.795519
H	-4.195954	-0.965248	-4.664631
H	-2.996524	0.531918	-3.135442
H	-1.266929	3.118773	-0.217501
H	-2.126996	5.403965	-0.620570
H	-4.490023	5.739996	-1.306123
H	-5.986489	3.778010	-1.569655
H	-5.136906	1.505220	-1.144997
H	-1.633898	-1.459461	1.725378
H	-2.497891	-2.144100	3.928880
H	-4.438403	-0.953130	4.931632
H	-5.498960	0.920522	3.696869
H	-4.654429	1.584200	1.485336
H	0.567308	1.241380	4.150943
H	3.276951	0.147046	-1.269499
H	5.704748	0.577126	-1.240870
H	7.195779	-0.782686	0.207674
H	6.233576	-2.589915	1.610569
H	3.813891	-3.048922	1.553614
H	3.515332	-3.314969	-1.718745
H	3.198907	-4.931583	-3.549311
H	0.913028	-5.589886	-4.256848
H	-1.059751	-4.592740	-3.119614
H	-0.746674	-2.950368	-1.312992
H	1.388892	-4.748297	0.576694
H	0.971780	-5.999281	2.657659
H	0.562480	-4.787271	4.784628
H	0.544106	-2.303390	4.800172
H	0.908321	-1.047959	2.702035

36 PPh_3-assisted isomerisation, Inter_PPh_3_A

C	3.251767	-2.990710	2.121981
C	2.623583	-1.819307	1.685265
C	2.638858	-0.682882	2.508409
C	3.297382	-0.720554	3.734932

C	3.925389	-1.888707	4.163137
C	3.896603	-3.023561	3.357089
P	1.727642	-1.686149	0.076001
Rh	-0.395674	-0.563706	0.266598
C	-0.723579	-1.543895	1.773128
O	-0.902285	-2.144669	2.739090
C	2.957095	-0.945650	-1.083577
C	2.676595	-0.979554	-2.456593
C	3.566836	-0.427565	-3.370776
C	4.742763	0.177553	-2.927487
C	5.022051	0.224461	-1.565204
C	4.135137	-0.334275	-0.645518
C	1.605729	-3.419292	-0.557228
C	0.370744	-4.075498	-0.537947
C	0.259113	-5.388071	-0.993601
C	1.378052	-6.056896	-1.481520
C	2.611522	-5.407598	-1.517237
C	2.725754	-4.097682	-1.060748
P	-2.666561	0.199459	0.174062
C	-2.855957	2.012717	-0.103261
O	-0.124985	0.434825	-1.610378
C	0.406071	1.512256	-2.055985
C	1.193808	2.438434	-1.375583
C	1.538833	2.439004	0.006854
C	2.476971	3.523007	0.496585
C	3.420797	4.151602	-0.325559
C	4.276840	5.123295	0.187588
C	4.197075	5.490553	1.529268
C	3.264794	4.868275	2.358860
C	2.421439	3.887231	1.848193
O	1.101894	1.641542	0.864829
C	0.092328	1.731464	-3.538044
C	0.696780	2.938937	-4.254719
H	1.789399	2.913578	-4.238934
H	0.381280	2.948793	-5.301885
H	0.372975	3.880916	-3.805255
H	-1.000834	1.768192	-3.609758
H	1.559276	3.267802	-1.959930
H	1.706074	3.382053	2.485507
H	3.198878	5.146569	3.405284
H	4.859922	6.251323	1.926858
H	5.009711	5.591583	-0.460616
H	3.507434	3.861829	-1.365461
H	3.686201	-3.597982	-1.106965
H	3.485333	-5.919409	-1.904995
H	1.289996	-7.076172	-1.840890
H	-0.705973	-5.881832	-0.974955
H	-0.504330	-3.543727	-0.184388
H	2.136248	0.223305	2.184703
H	3.308964	0.164837	4.360745
H	4.427487	-1.916661	5.123929
H	4.372697	-3.939832	3.688334
H	3.231344	-3.883746	1.510668
H	4.372697	-3.939832	3.688334
H	3.231344	-3.883746	1.510668
H	1.759150	-1.435129	-2.808877
H	3.340741	-0.466089	-4.430656
H	5.435434	0.609100	-3.641490

H	5.931992	0.695335	-1.210615
H	4.368112	-0.293439	0.410743
H	0.386191	0.808354	-4.049832
C	-3.611718	-0.578178	-1.213551
C	-1.923264	2.868424	0.493955
C	-2.055077	4.249528	0.362429
C	-3.107308	4.786265	-0.375247
C	-4.029909	3.937740	-0.985154
C	-3.908018	2.557208	-0.849930
H	-1.082504	2.451299	1.036040
H	-1.322013	4.901907	0.822909
H	-3.203285	5.860981	-0.483836
H	-4.845431	4.349597	-1.569430
H	-4.628857	1.908050	-1.331486
C	-3.738348	-0.123784	1.647247
C	-4.219514	0.909891	2.457337
C	-4.979481	0.623740	3.591142
C	-5.272154	-0.694347	3.926672
C	-4.797325	-1.731178	3.124399
C	-4.031753	-1.449306	1.998462
H	-4.004912	1.940770	2.206703
H	-5.343342	1.436938	4.209250
H	-5.863332	-0.914925	4.808321
H	-5.015177	-2.761963	3.380151
H	-3.663629	-2.266641	1.388983
C	-4.990131	-0.818010	-1.141123
C	-5.664453	-1.387176	-2.220032
C	-4.972122	-1.719310	-3.381881
C	-3.601521	-1.479912	-3.461324
C	-2.920501	-0.916152	-2.385053
H	-5.539846	-0.570278	-0.241425
H	-6.730784	-1.571419	-2.148988
H	-5.497544	-2.164429	-4.219631
H	-3.056447	-1.737502	-4.362785
H	-1.855925	-0.723608	-2.446537

37 PPh_3-assisted isomerisation, TSi_PPh_3

C	3.676488	-2.047222	2.412924
C	2.850405	-1.054389	1.878997
C	2.359854	-0.043655	2.721431
C	2.720922	-0.016362	4.064516
C	3.551402	-1.006366	4.590487
C	4.020891	-2.022939	3.764751
P	2.276886	-1.020183	0.127224
Rh	-0.095421	-0.761733	0.106690
C	-0.263640	-2.432232	0.799026
O	-0.374644	-3.486624	1.264300
C	3.259990	0.325518	-0.667239
C	3.118200	0.500465	-2.050245
C	3.873367	1.458331	-2.717407
C	4.768932	2.261874	-2.012581
C	4.902683	2.103129	-0.636610
C	4.153588	1.138015	0.035894
C	3.008595	-2.509331	-0.685847
C	2.180680	-3.505549	-1.211685
C	2.730244	-4.618818	-1.846932
C	4.110219	-4.745433	-1.968696
C	4.944566	-3.749175	-1.461499

C	4.398906	-2.636586	-0.830248
P	-2.477728	-0.575564	0.180798
C	-3.222765	0.981766	-0.472931
O	-0.245773	0.225258	-2.111515
C	-0.190357	1.426068	-2.487899
C	0.120514	2.531916	-1.667777
C	0.366424	2.477511	-0.286266
C	0.697287	3.761801	0.433861
C	1.313829	4.849652	-0.197928
C	1.609303	6.011186	0.510623
C	1.287528	6.110376	1.862902
C	0.680443	5.032274	2.505113
C	0.398356	3.867176	1.798868
O	0.305142	1.446428	0.452845
C	-0.491149	1.645040	-3.975666
C	-0.393442	3.058758	-4.551788
H	0.611365	3.474105	-4.437212
H	-0.625919	3.048400	-5.620489
H	-1.097025	3.741208	-4.068453
H	-1.499114	1.246334	-4.136765
H	0.129111	3.506316	-2.129683
H	-0.057741	3.018381	2.292969
H	0.429370	5.099328	3.558331
H	1.514203	7.017236	2.412771
H	2.097430	6.838506	0.006863
H	1.589792	4.777496	-1.242435
H	5.055827	-1.857826	-0.460653
H	6.020560	-3.834876	-1.564786
H	4.536360	-5.610456	-2.464605
H	2.074405	-5.382114	-2.250053
H	1.105960	-3.403070	-1.139980
H	1.690880	0.709026	2.317378
H	2.343687	0.774193	4.703739
H	3.823130	-0.988497	5.640103
H	4.655950	-2.803586	4.168670
H	4.044730	-2.848901	1.785707
H	2.408502	-0.106498	-2.599549
H	3.756700	1.582308	-3.788174
H	5.355728	3.010152	-2.533772
H	5.591666	2.728620	-0.080094
H	4.271846	1.021245	1.105452
H	0.176908	0.968692	-4.520894
C	-3.211743	-1.910610	-0.859284
C	-2.970661	2.172378	0.220825
C	-3.529456	3.370372	-0.209508
C	-4.341440	3.397552	-1.342515
C	-4.589838	2.220073	-2.041943
C	-4.034077	1.015595	-1.610950
H	-2.328567	2.162759	1.092782
H	-3.320434	4.284196	0.334684
H	-4.775067	4.332783	-1.678777
H	-5.220278	2.232741	-2.924245
H	-4.239892	0.105717	-2.159957
C	-3.290399	-0.702320	1.834272
C	-4.649884	-0.395779	1.997593
C	-5.248718	-0.488739	3.249811
C	-4.496922	-0.878903	4.357921
C	-3.144261	-1.169227	4.208218

C	-2.541835	-1.078867	2.953940
H	-5.238004	-0.071034	1.147271
H	-6.300269	-0.249085	3.362030
H	-4.963794	-0.946472	5.334287
H	-2.550505	-1.461458	5.066937
H	-1.484397	-1.284536	2.844862
C	-4.257868	-2.738843	-0.443530
C	-4.730281	-3.747783	-1.283008
C	-4.168242	-3.932518	-2.542582
C	-3.120640	-3.111585	-2.960313
C	-2.633502	-2.112533	-2.122970
H	-4.699879	-2.612664	0.536604
H	-5.536494	-4.390157	-0.946521
H	-4.538038	-4.717284	-3.193243
H	-2.671938	-3.256400	-3.936910
H	-1.802943	-1.487482	-2.437327

38 PPh_3-assisted isomerisation, Inter_PPh_3_B

C	4.271962	-1.229121	2.064532
C	3.093393	-0.607627	1.630893
C	2.462586	0.321288	2.468277
C	3.006380	0.622976	3.714344
C	4.175574	-0.002222	4.142934
C	4.806694	-0.928383	3.315790
P	2.348874	-0.938402	-0.027576
Rh	-0.048607	-0.765684	-0.048141
C	-0.222770	-2.578174	-0.168906
O	-0.361211	-3.718321	-0.256837
C	3.189789	0.251155	-1.156408
C	2.605212	0.493049	-2.405095
C	3.233536	1.335464	-3.319709
C	4.436233	1.956619	-2.990781
C	5.010834	1.735111	-1.740733
C	4.394006	0.884198	-0.826823
C	3.086337	-2.569936	-0.495464
C	2.830899	-3.685760	0.314483
C	3.337506	-4.936304	-0.021073
C	4.098785	-5.096544	-1.178127
C	4.353216	-3.996813	-1.991391
C	3.853173	-2.739684	-1.652955
P	-2.440913	-0.659278	0.256618
C	-3.271651	0.975708	0.047714
O	-0.640990	0.537699	-2.360195
C	-0.633479	1.778735	-2.502450
C	-0.202739	2.716992	-1.523981
C	0.199919	2.449328	-0.213481
C	0.633103	3.619197	0.634493
C	1.286871	4.733684	0.093169
C	1.684098	5.792201	0.905856
C	1.428949	5.761074	2.275206
C	0.786521	4.654322	2.827976
C	0.403936	3.590621	2.016513
O	0.216700	1.325961	0.400597
C	-1.127408	2.291727	-3.864512
C	-1.121944	3.795397	-4.146382
H	-0.114075	4.215428	-4.090108
H	-1.504469	3.993508	-5.151804
H	-1.753663	4.340677	-3.440664

H	-2.143512	1.896326	-3.974862
H	-0.230658	3.758903	-1.801881
H	-0.080662	2.722564	2.444934
H	0.585822	4.619404	3.893491
H	1.734713	6.587734	2.906938
H	2.200586	6.639933	0.468933
H	1.511228	4.758571	-0.965982
H	4.065076	-1.893213	-2.293247
H	4.944444	-4.111066	-2.893136
H	4.487820	-6.073197	-1.443191
H	3.129523	-5.787734	0.617002
H	2.235324	-3.578427	1.213627
H	1.557665	0.809513	2.128066
H	2.512724	1.349041	4.350481
H	4.593302	0.230762	5.116204
H	5.717037	-1.419482	3.641615
H	4.771189	-1.953706	1.433147
H	1.645952	0.048534	-2.643722
H	2.772214	1.517025	-4.283912
H	4.919025	2.619050	-3.700871
H	5.939945	2.226222	-1.473464
H	4.848916	0.721980	0.142419
H	-0.530618	1.763763	-4.616862
C	-3.328797	-1.775201	-0.916190
C	-2.960063	1.998301	0.953316
C	-3.560221	3.247388	0.842669
C	-4.476930	3.495725	-0.177963
C	-4.788636	2.486825	-1.084553
C	-4.190005	1.232055	-0.974925
H	-2.241051	1.818689	1.742445
H	-3.302265	4.029616	1.547314
H	-4.942865	4.470863	-0.265680
H	-5.502008	2.670697	-1.880368
H	-4.446081	0.455623	-1.684262
C	-3.014494	-1.163723	1.940161
C	-4.302789	-0.853726	2.400056
C	-4.714678	-1.254971	3.667522
C	-3.845911	-1.967034	4.493821
C	-2.561911	-2.270018	4.049792
C	-2.146224	-1.867233	2.781753
H	-4.980417	-0.288494	1.771157
H	-5.712697	-1.007409	4.011818
H	-4.167444	-2.275675	5.482368
H	-1.876755	-2.812045	4.691894
H	-1.138271	-2.077875	2.444286
C	-4.343322	-2.653726	-0.523229
C	-4.956008	-3.483263	-1.461323
C	-4.565548	-3.439459	-2.796743
C	-3.551676	-2.568217	-3.192635
C	-2.925701	-1.744913	-2.260496
H	-4.651907	-2.704141	0.513132
H	-5.736118	-4.166246	-1.143643
H	-5.042742	-4.086836	-3.524207
H	-3.235881	-2.535919	-4.229531
H	-2.126103	-1.077193	-2.567325

39 PPh_3-assisted isomerisation, TS2_PPh_3_B

C	3.476936	-2.188868	2.113973
C	2.450561	-1.368699	1.625378
C	1.598541	-0.733185	2.535424
C	1.775706	-0.905501	3.906320
C	2.801031	-1.718252	4.384520
C	3.649972	-2.360944	3.485668
P	2.180574	-1.100046	-0.187240
Rh	0.082167	-0.364879	-0.805242
C	-0.235404	-1.894317	-1.768747
O	-0.456477	-2.817142	-2.416296
C	3.462437	0.146185	-0.663780
C	3.295123	0.818903	-1.880786
C	4.244031	1.740235	-2.315079
C	5.362068	2.015208	-1.530069
C	5.526281	1.363896	-0.310117
C	4.584076	0.432358	0.121674
C	2.816017	-2.678142	-0.913134
C	2.184678	-3.880212	-0.563477
C	2.603743	-5.086934	-1.111690
C	3.655812	-5.112526	-2.026750
C	4.286105	-3.924644	-2.383288
C	3.871812	-2.713189	-1.829642
P	-2.511665	-0.448079	0.246675
C	-3.402651	1.132468	0.611761
O	-0.967888	1.047444	-2.302143
C	-0.804029	2.293404	-2.331972
C	-0.066662	3.064041	-1.398695
C	0.543361	2.616482	-0.221513
C	1.223933	3.626892	0.661502
C	1.752559	4.826969	0.166420
C	2.382947	5.731918	1.015059
C	2.492279	5.458659	2.377002
C	1.980079	4.264404	2.880336
C	1.362181	3.354268	2.029050
O	0.562748	1.419433	0.234099
C	-1.510136	2.994588	-3.496271
C	-1.203034	4.468139	-3.768754
H	-0.137102	4.631589	-3.949596
H	-1.743669	4.804954	-4.657407
H	-1.508254	5.110119	-2.938710
H	-2.583773	2.866107	-3.314643
H	-0.035542	4.126851	-1.575670
H	0.982261	2.416805	2.412128
H	2.067480	4.038709	3.937517
H	2.980156	6.166200	3.038244
H	2.795422	6.649442	0.610015
H	1.698963	5.044128	-0.892827
H	4.376562	-1.798328	-2.112757
H	5.105318	-3.934691	-3.093620
H	3.978398	-6.052857	-2.459306
H	2.103633	-6.006851	-0.830514
H	1.361479	-3.873926	0.142028
H	0.797221	-0.109611	2.160994
H	1.103024	-0.413046	4.599462
H	2.933756	-1.856841	5.451797
H	4.445614	-3.001425	3.850114
H	4.135730	-2.705123	1.425822
H	2.407703	0.627436	-2.473873

H	4.099992	2.253986	-3.258927
H	6.095397	2.741874	-1.861697
H	6.386305	1.583759	0.312667
H	4.721301	-0.058414	1.076835
H	-1.290493	2.391871	-4.383196
C	-3.675665	-1.321281	-0.897223
C	-2.703020	2.115674	1.325574
C	-3.305566	3.330609	1.637013
C	-4.612429	3.589208	1.226227
C	-5.311755	2.624617	0.505172
C	-4.712966	1.402873	0.199662
H	-1.678164	1.931555	1.625446
H	-2.747952	4.080180	2.187332
H	-5.079482	4.539175	1.461476
H	-6.327561	2.819663	0.178586
H	-5.267938	0.660815	-0.361060
C	-2.702372	-1.382406	1.834812
C	-3.688326	-1.100355	2.789619
C	-3.774251	-1.852088	3.959870
C	-2.881686	-2.897118	4.190923
C	-1.893998	-3.182151	3.250284
C	-1.800887	-2.424428	2.085622
H	-4.387240	-0.289778	2.621699
H	-4.540966	-1.620392	4.691246
H	-2.950646	-3.480420	5.102498
H	-1.186881	-3.984537	3.428716
H	-1.013929	-2.625150	1.367237
C	-4.581403	-2.305382	-0.484721
C	-5.414088	-2.931326	-1.411484
C	-5.355609	-2.579566	-2.757469
C	-4.452584	-1.603793	-3.177033
C	-3.610661	-0.983767	-2.258066
H	-4.637017	-2.588561	0.559159
H	-6.108438	-3.695052	-1.078177
H	-6.003368	-3.068508	-3.476757
H	-4.392223	-1.333072	-4.225450
H	-2.891801	-0.242635	-2.592364

40 PPh_3-assisted isomerisation, Prod_PPh_3_B

C	-2.306276	-1.781866	-1.792882
C	-3.326171	-1.917962	-0.839658
C	-4.234513	-2.976022	-0.969928
C	-4.131159	-3.870155	-2.034344
C	-3.122822	-3.717565	-2.983658
C	-2.211108	-2.670420	-2.861385
P	-3.351065	-0.682258	0.540969
C	-4.456185	-1.502265	1.785271
C	-5.797427	-1.165866	2.001093
C	-6.538538	-1.805199	2.995145
C	-5.954470	-2.793176	3.782920
C	-4.618241	-3.136050	3.578274
C	-3.874304	-2.488782	2.596711
Rh	1.527273	0.111254	-1.449336
O	1.210954	1.717074	-0.146286
C	0.501969	2.755950	-0.371876
C	0.546040	3.795764	0.709307
C	0.211893	5.138223	0.481672
C	0.276455	6.071474	1.511686

C	0.671997	5.679905	2.789125
C	1.016172	4.350080	3.025211
C	0.962669	3.419350	1.993527
P	2.981090	-0.764500	0.121802
C	4.056069	-2.183484	-0.368110
C	3.450800	-3.407806	-0.685465
C	4.221373	-4.491797	-1.090670
C	5.606669	-4.367572	-1.193634
C	6.214699	-3.154791	-0.885332
C	5.445544	-2.066946	-0.472492
C	2.138560	-1.384615	1.643776
C	2.719283	-2.349001	2.478967
C	2.060708	-2.769980	3.631984
C	0.816496	-2.236136	3.962222
C	0.229164	-1.283646	3.132261
C	0.883362	-0.860930	1.977116
C	4.169025	0.513800	0.720273
C	4.590065	1.497204	-0.183275
C	5.514953	2.462431	0.205976
C	6.019593	2.463964	1.504502
C	5.595304	1.496786	2.413054
C	4.675268	0.525476	2.024741
C	1.802509	-1.262284	-2.647674
O	1.929519	-2.080643	-3.442909
O	0.159243	0.999504	-2.771611
C	-0.443369	2.104800	-2.600048
C	-1.401704	2.446583	-3.735945
C	-2.095483	3.808962	-3.718911
C	-4.437920	0.659256	-0.136786
C	-4.361889	1.913281	0.485817
C	-5.140020	2.979191	0.041242
C	-5.992026	2.813829	-1.049518
C	-6.062035	1.577616	-1.688655
C	-5.293134	0.506890	-1.235231
C	-0.300133	2.972231	-1.503114
H	-1.374235	4.630736	-3.722765
H	-2.722500	3.917290	-4.607682
H	-2.742916	3.924343	-2.846416
H	-2.149439	1.645753	-3.749378
H	-0.898265	3.868477	-1.514461
H	1.244613	2.389456	2.165890
H	1.331700	4.038070	4.014652
H	0.718838	6.407283	3.592002
H	0.023421	7.107237	1.314217
H	-0.074207	5.466255	-0.509547
H	5.931976	-1.130339	-0.230767
H	7.291043	-3.049605	-0.963189
H	6.206113	-5.211970	-1.514634
H	3.738884	-5.431908	-1.332680
H	2.374371	-3.516618	-0.614512
H	0.416381	-0.130239	1.328892
H	-0.745427	-0.873905	3.370980
H	0.303811	-2.567398	4.858504
H	2.518618	-3.519272	4.268221
H	3.678864	-2.783172	2.224575
H	4.179412	1.508658	-1.186516
H	5.830346	3.220012	-0.502464
H	6.732901	3.221226	1.810126

H	5.976411	1.499293	3.428227
H	4.347307	-0.214655	2.744104
H	-0.827333	2.322935	-4.659909
H	-3.682751	2.056267	1.319875
H	-5.071277	3.940461	0.538547
H	-6.592127	3.644920	-1.403200
H	-6.717215	1.444001	-2.542723
H	-5.354966	-0.448523	-1.742504
H	-6.266842	-0.401327	1.393907
H	-7.576355	-1.530175	3.149742
H	-6.533208	-3.289940	4.553655
H	-4.153087	-3.901669	4.189731
H	-2.830759	-2.752239	2.455008
H	-5.020304	-3.107622	-0.235414
H	-4.840031	-4.686798	-2.120223
H	-3.043069	-4.415070	-3.810222
H	-1.415060	-2.549896	-3.587491
H	-1.575290	-0.985219	-1.698834

41 CH_3CN-assisted isomerisation, Reac_CH_3CN_A

C	-4.968407	2.024163	0.379205
C	-4.730469	0.645669	0.471243
C	-5.827301	-0.227171	0.464710
C	-7.125838	0.266795	0.380038
C	-7.350265	1.640033	0.306883
C	-6.266345	2.516933	0.306284
C	-3.310509	0.165814	0.543580
O	-2.448726	0.983974	0.084170
Rh	-0.360928	0.714495	0.039280
O	-0.660427	-1.198736	0.822864
C	-1.770182	-1.701637	1.196882
C	-1.670467	-3.087488	1.811851
C	-0.979434	-4.099471	0.886717
P	1.904472	0.244839	0.053783
C	2.402523	-0.478760	1.675074
C	1.801258	0.023753	2.835985
C	2.167063	-0.465197	4.087096
C	3.125850	-1.471411	4.191598
C	3.716875	-1.986154	3.040305
C	3.359461	-1.492744	1.786990
C	3.090522	1.637181	-0.203928
C	3.943788	2.091018	0.806684
C	4.796276	3.170866	0.577304
C	4.809002	3.804534	-0.661139
C	3.962198	3.356692	-1.674642
C	3.106828	2.284467	-1.447598
C	2.416872	-0.988145	-1.217258
C	1.457618	-1.876547	-1.717664
C	1.807082	-2.825997	-2.675278
C	3.118290	-2.898051	-3.139839
C	4.080284	-2.017673	-2.646769
C	3.733654	-1.064524	-1.692216
C	-0.129507	2.420473	-0.623434
O	-0.053506	3.493023	-1.025582
N	-1.803051	-2.908569	-3.068893
C	-2.292993	-1.865411	-3.095558
C	-2.904680	-0.544607	-3.121985
C	-3.033443	-1.099406	1.093361

H	0.035617	-3.774970	0.655360
H	-0.926201	-5.079982	1.366629
H	-1.522036	-4.208322	-0.055711
H	-2.666056	-3.440918	2.089975
H	-3.864802	-1.662622	1.489746
H	-4.119101	2.694730	0.368627
H	-6.433371	3.586722	0.247771
H	-8.362625	2.023592	0.245862
H	-7.962762	-0.422446	0.366873
H	-5.669921	-1.297923	0.500169
H	3.819688	-1.908751	0.899417
H	4.454940	-2.777004	3.114388
H	3.404480	-1.858317	5.165438
H	1.694539	-0.067708	4.978289
H	1.037704	0.789029	2.752541
H	2.451694	1.948920	-2.243641
H	3.963131	3.846568	-2.641697
H	5.472154	4.643821	-0.837552
H	5.451328	3.512471	1.370906
H	3.948885	1.604515	1.773793
H	0.436848	-1.825275	-1.362578
H	1.042339	-3.490885	-3.059079
H	3.389693	-3.633095	-3.889501
H	5.100905	-2.066368	-3.010064
H	4.485878	-0.374135	-1.329542
H	-1.090440	-2.987221	2.736762
H	-2.708322	-0.060124	-4.080672
H	-3.984471	-0.627670	-2.983440
H	-2.496040	0.074393	-2.319686

42 CH_3CN-assisted isomerisation, TS1_CH_3CN_A

C	-3.141292	-2.727618	0.444791
C	-2.929699	-1.639905	-0.408226
C	-3.533125	-1.643903	-1.674011
C	-4.336640	-2.706802	-2.070732
C	-4.542074	-3.788248	-1.214274
C	-3.941674	-3.796100	0.040702
P	-1.834663	-0.224367	0.052259
Rh	0.122341	0.040535	-1.083640
C	-0.319641	-1.236713	-2.324047
O	-0.519159	-2.029417	-3.132183
C	-2.991956	1.221119	0.007461
C	-2.454512	2.503533	-0.162407
C	-3.290952	3.616371	-0.186574
C	-4.669831	3.465083	-0.050328
C	-5.211287	2.192971	0.115908
C	-4.378263	1.075675	0.146861
C	-1.511088	-0.483461	1.855027
C	-0.337442	-1.150286	2.227054
C	-0.063431	-1.397452	3.570210
C	-0.952418	-0.973440	4.555397
C	-2.117681	-0.300377	4.193078
C	-2.397430	-0.056015	2.850479
N	1.508963	1.174875	-2.654388
C	2.340289	1.698309	-3.251828
C	3.404242	2.354854	-3.994317
O	0.581041	1.584008	0.283104
C	1.622696	1.775080	1.002442

C	2.806514	1.037683	1.027174
C	3.122524	-0.120016	0.257514
C	4.487190	-0.747931	0.438400
C	5.595416	-0.058156	0.947189
C	6.832277	-0.687342	1.066763
C	6.980410	-2.019465	0.686988
C	5.885948	-2.714646	0.173380
C	4.655016	-2.081569	0.042760
O	2.357116	-0.684581	-0.554944
C	1.515803	2.987278	1.920148
C	1.479472	4.307837	1.135918
H	0.654871	4.308071	0.420733
H	1.348800	5.158304	1.810547
H	2.409886	4.457574	0.580392
H	2.346483	2.997279	2.629713
H	3.544183	1.369299	1.743166
H	3.800102	-2.602154	-0.369928
H	5.994409	-3.750969	-0.127895
H	7.942341	-2.510596	0.785494
H	7.681416	-0.135216	1.454782
H	5.503688	0.982890	1.231080
H	-3.301338	0.477035	2.582562
H	-2.808999	0.040448	4.955970
H	-0.734498	-1.158415	5.601481
H	0.851962	-1.909489	3.844193
H	0.365878	-1.457669	1.461179
H	-3.374088	-0.813192	-2.352504
H	-4.796208	-2.694465	-3.052590
H	-5.163637	-4.619736	-1.526990
H	-4.093943	-4.633675	0.712305
H	-2.683502	-2.745573	1.425636
H	-1.382435	2.616802	-0.264471
H	-2.863456	4.604249	-0.318709
H	-5.319144	4.333218	-0.077788
H	-6.283448	2.065605	0.217971
H	-4.813934	0.091365	0.268159
H	0.590247	2.881043	2.494977
H	2.985413	3.054995	-4.719794
H	4.052337	2.901401	-3.306391
H	4.002328	1.610677	-4.523861

43 CH_3CN-assisted isomerisation, Inter_CH_3CN_A

C	4.493509	0.672265	-0.702257
C	3.461313	-0.226272	-0.416032
C	3.723040	-1.603022	-0.469309
C	4.997119	-2.068047	-0.778370
C	6.022125	-1.165392	-1.059222
C	5.765896	0.202131	-1.026193
P	1.740034	0.284077	0.014864
Rh	0.127415	-0.990225	-1.051211
C	0.955482	-0.716028	-2.662975
O	1.451507	-0.599006	-3.695065
C	1.684385	0.229497	1.854876
C	0.501965	0.645921	2.482377
C	0.416001	0.653553	3.869919
C	1.499878	0.239517	4.644982
C	2.672194	-0.182094	4.025340
C	2.767332	-0.187298	2.633465

C	1.640085	2.092145	-0.328669
C	0.821411	2.561477	-1.360420
C	0.742757	3.926906	-1.629126
C	1.470024	4.835312	-0.865708
C	2.269787	4.377643	0.180924
C	2.350579	3.015445	0.452560
N	-1.427898	-2.104997	-1.921262
C	-2.402292	-2.614878	-2.252326
C	-3.649789	-3.241706	-2.649864
O	-0.579471	-1.759473	0.809486
C	-1.702556	-1.774530	1.414944
C	-2.791065	-0.919065	1.229916
C	-2.814837	0.250591	0.408802
C	-4.134691	0.978789	0.238502
C	-5.382081	0.386008	0.473040
C	-6.560800	1.099710	0.267034
C	-6.511300	2.421364	-0.170863
C	-5.275255	3.021257	-0.411213
C	-4.100653	2.303445	-0.214903
O	-1.819145	0.737893	-0.162596
C	-1.823397	-2.878336	2.462884
C	-1.572110	-4.276882	1.884938
H	-0.605346	-4.307422	1.380375
H	-1.578158	-5.034894	2.673014
H	-2.344502	-4.545071	1.156766
H	-2.801438	-2.832813	2.948743
H	-3.670752	-1.136433	1.819387
H	-3.132098	2.746847	-0.409949
H	-5.229620	4.049682	-0.753421
H	-7.428627	2.978699	-0.326706
H	-7.518415	0.623083	0.447719
H	-5.436931	-0.645002	0.800992
H	2.955074	2.672236	1.284194
H	2.823583	5.081660	0.791977
H	1.403976	5.897459	-1.073971
H	0.100946	4.277927	-2.429214
H	0.219718	1.861122	-1.924502
H	2.918019	-2.305450	-0.282765
H	5.185448	-3.135182	-0.813774
H	7.012148	-1.527800	-1.312479
H	6.554827	0.909409	-1.256484
H	4.308470	1.738544	-0.688541
H	-0.347574	0.949235	1.881728
H	-0.503665	0.975332	4.345333
H	1.428131	0.244115	5.727063
H	3.518086	-0.506721	4.621218
H	3.685463	-0.515798	2.162639
H	-1.069596	-2.667984	3.230283
H	-3.926225	-4.008380	-1.923468
H	-4.441793	-2.490876	-2.689104
H	-3.545537	-3.703446	-3.633601

44 CH_3CN-assisted isomerisation, TSi_CH_3CN

C	4.448378	-0.373113	-0.024830
C	3.134567	-0.737504	0.279897
C	2.873313	-2.022697	0.780991
C	3.920017	-2.913012	0.994584
C	5.231300	-2.543210	0.693093

C	5.491676	-1.276831	0.179381
P	1.676046	0.353873	0.005720
Rh	0.040855	-0.793687	-1.150487
C	1.156219	-0.969396	-2.578863
O	1.827848	-1.144560	-3.502647
C	1.177187	0.901075	1.693701
C	0.033033	1.700029	1.816118
C	-0.350989	2.181406	3.063334
C	0.396484	1.870571	4.198602
C	1.531335	1.073366	4.082028
C	1.923507	0.589430	2.834458
C	2.327615	1.915847	-0.729192
C	1.991465	2.278394	-2.037110
C	2.477340	3.463579	-2.587578
C	3.297230	4.300216	-1.836766
C	3.625671	3.954436	-0.526239
C	3.140479	2.773943	0.026718
N	-1.459603	-1.935134	-2.073633
C	-2.384224	-2.514826	-2.430644
C	-3.568357	-3.236675	-2.859987
O	-0.580322	-1.759780	0.844233
C	-1.703885	-1.804855	1.421407
C	-2.807474	-0.966253	1.174299
C	-2.806269	0.139204	0.293954
C	-4.058781	0.978846	0.177294
C	-5.049362	1.033356	1.166805
C	-6.176579	1.834571	1.002595
C	-6.336706	2.591531	-0.156411
C	-5.353182	2.552964	-1.144138
C	-4.222326	1.761548	-0.973464
O	-1.836001	0.494901	-0.428023
C	-1.851553	-2.890200	2.486905
C	-1.649739	-4.300275	1.915502
H	-0.688321	-4.367964	1.403500
H	-1.675370	-5.053823	2.707448
H	-2.435263	-4.545749	1.193918
H	-2.825323	-2.813274	2.977744
H	-3.711607	-1.179735	1.726160
H	-3.438793	1.735635	-1.720323
H	-5.466469	3.145663	-2.045650
H	-7.216211	3.213061	-0.284570
H	-6.928051	1.872305	1.783892
H	-4.930568	0.468226	2.082870
H	3.384199	2.526758	1.053284
H	4.252634	4.608826	0.069035
H	3.671273	5.223557	-2.264883
H	2.205724	3.732980	-3.601916
H	1.333823	1.643509	-2.616605
H	1.849991	-2.316158	0.991355
H	3.710130	-3.902412	1.385445
H	6.043915	-3.243668	0.850692
H	6.506846	-0.987168	-0.068144
H	4.664113	0.606740	-0.431518
H	-0.568406	1.916211	0.941994
H	-1.242188	2.792774	3.147864
H	0.092027	2.244699	5.169866
H	2.115665	0.824071	4.960931
H	2.806210	-0.032483	2.756816

H	-1.087157	-2.695863	3.247547
H	-3.344627	-4.300070	-2.965921
H	-4.358801	-3.110617	-2.117303
H	-3.917890	-2.849535	-3.819164

45 CH_3CN-assisted isomerisation, Inter_CH_3CN_B

C	3.781113	-1.939235	-0.929769
C	3.757516	-1.103071	0.195169
C	4.748150	-1.273300	1.171728
C	5.742000	-2.236201	1.017931
C	5.766503	-3.046156	-0.116046
C	4.779504	-2.895120	-1.088880
C	2.654214	-0.080697	0.311550
O	1.592516	-0.389950	-0.333603
Rh	0.015245	0.737957	-1.227485
O	0.758787	2.131169	0.991897
C	1.936149	2.088189	1.387954
C	2.411508	3.202173	2.332618
C	1.976745	4.596907	1.872733
P	-1.614161	-0.352509	0.020811
C	-2.490141	-1.739034	-0.828389
C	-2.437741	-1.847466	-2.222100
C	-3.108887	-2.878836	-2.876281
C	-3.831138	-3.818204	-2.145649
C	-3.877449	-3.726976	-0.755251
C	-3.209891	-2.696666	-0.099354
C	-2.937420	0.813981	0.559592
C	-4.302022	0.526112	0.459858
C	-5.248459	1.462172	0.874845
C	-4.840144	2.686397	1.396200
C	-3.480167	2.978311	1.495143
C	-2.527954	2.055145	1.072118
C	-1.031807	-1.146618	1.578533
C	-0.043208	-2.136596	1.493348
C	0.396084	-2.786875	2.641370
C	-0.139139	-2.455587	3.885681
C	-1.115652	-1.468416	3.977003
C	-1.562498	-0.815147	2.828911
C	-1.283013	1.501866	-2.270136
O	-2.052400	2.007305	-2.961286
N	1.562434	1.688696	-2.283807
C	2.520109	2.164725	-2.702750
C	3.731722	2.773473	-3.221261
C	2.887109	1.069966	1.065448
H	0.899173	4.619637	1.704929
H	2.231691	5.355851	2.617444
H	2.466362	4.870694	0.932883
H	3.496597	3.157604	2.462502
H	3.876359	1.188737	1.485060
H	2.998255	-1.825278	-1.668909
H	4.785860	-3.526558	-1.971008
H	6.542119	-3.794779	-0.235133
H	6.493994	-2.360046	1.789747
H	4.725253	-0.669859	2.070743
H	-3.239064	-2.645028	0.982554
H	-4.428231	-4.462224	-0.179227
H	-4.348095	-4.623916	-2.654966
H	-3.057485	-2.950991	-3.956861

H	-1.852691	-1.134184	-2.789575
H	-1.470355	2.291931	1.134993
H	-3.156441	3.933636	1.893045
H	-5.577810	3.413485	1.717514
H	-6.304401	1.232128	0.785853
H	-4.633320	-0.419830	0.050515
H	0.401064	-2.374034	0.536114
H	1.166359	-3.545729	2.563702
H	0.208307	-2.962001	4.779444
H	-1.534066	-1.202004	4.941266
H	-2.321763	-0.048362	2.912687
H	1.968372	2.989390	3.313705
H	3.921997	3.718105	-2.707759
H	4.579214	2.105304	-3.055609
H	3.630707	2.963543	-4.291609

46 CH_3CN-assisted isomerisation, TS2_CH_3CN_B

C	3.327240	2.290079	0.876336
C	3.472592	1.438549	-0.227151
C	4.386502	1.791508	-1.227911
C	5.140980	2.957130	-1.122606
C	5.001673	3.786230	-0.011335
C	4.091268	3.447415	0.989066
C	2.629727	0.192436	-0.294490
O	1.487678	0.312359	0.271890
Rh	0.023334	-1.139677	0.683518
O	1.445780	-2.561219	-0.633135
C	2.542833	-2.204316	-1.105610
C	3.286429	-3.208564	-1.995146
C	3.039861	-4.668226	-1.611487
P	-1.654172	0.243821	-0.005886
C	-2.588579	1.169083	1.298842
C	-2.593411	0.681467	2.609831
C	-3.307513	1.340824	3.607964
C	-4.013804	2.503759	3.311002
C	-4.001626	3.007490	2.011446
C	-3.294138	2.345986	1.010781
C	-2.961109	-0.648465	-0.966186
C	-4.319696	-0.320548	-0.906605
C	-5.248070	-1.021805	-1.674114
C	-4.829924	-2.050721	-2.513956
C	-3.478411	-2.385133	-2.577475
C	-2.549925	-1.695648	-1.802718
C	-1.118765	1.594298	-1.142402
C	-0.243300	2.572786	-0.651886
C	0.193571	3.602607	-1.477789
C	-0.231234	3.667389	-2.804233
C	-1.095532	2.695987	-3.300396
C	-1.538377	1.662929	-2.475125
C	-1.217103	-2.381990	1.216162
O	-1.935966	-3.201030	1.583253
N	1.624836	-1.927117	2.270572
C	2.667905	-2.089664	2.727338
C	3.998791	-2.284894	3.278800
C	3.168383	-0.935291	-0.917005
H	1.970440	-4.878196	-1.578509
H	3.509901	-5.345162	-2.329966
H	3.449046	-4.889618	-0.621419

H	4.356233	-2.979028	-1.997943
H	4.163740	-0.831736	-1.326717
H	2.608428	2.023557	1.641031
H	3.975391	4.087561	1.857114
H	5.592912	4.691532	0.071554
H	5.833886	3.221682	-1.913922
H	4.487284	1.167552	-2.107554
H	-3.281255	2.754529	0.007296
H	-4.539695	3.919061	1.775791
H	-4.563064	3.021446	4.089563
H	-3.301319	0.950205	4.619397
H	-2.015739	-0.204233	2.846624
H	-1.502171	-1.975531	-1.830239
H	-3.146137	-3.193016	-3.219651
H	-5.554238	-2.596334	-3.108469
H	-6.299475	-0.764157	-1.610585
H	-4.661334	0.472191	-0.253390
H	0.109957	2.516083	0.368519
H	0.878720	4.346357	-1.087484
H	0.114478	4.469006	-3.447497
H	-1.430082	2.738083	-4.331053
H	-2.212311	0.915487	-2.873673
H	2.936693	-3.033783	-3.021388
H	4.177507	-3.345873	3.463860
H	4.743056	-1.918241	2.568980
H	4.104447	-1.738442	4.218017

47 CH_3CN-assisted isomerisation, Prod_CH_3CN_B

C	3.404597	-1.918523	-1.545354
C	2.132224	-1.360524	-1.369268
C	1.094191	-1.743339	-2.229098
C	1.328489	-2.667093	-3.243725
C	2.598203	-3.214803	-3.417013
C	3.634565	-2.839495	-2.566075
P	1.755811	-0.156862	-0.017511
C	3.420605	0.458576	0.489631
C	3.919117	0.275245	1.783111
C	5.164824	0.792565	2.137904
C	5.925918	1.491584	1.206418
C	5.436186	1.677438	-0.086082
C	4.191304	1.170139	-0.440987
Rh	0.147641	1.413536	-0.577775
N	-2.788801	0.508780	4.538992
C	-3.547450	0.769197	3.711664
C	-4.501301	1.095914	2.661726
O	-1.263613	-0.133528	-0.634760
C	-2.515579	-0.027923	-0.863584
C	-3.202558	1.168666	-1.123467
C	-2.625023	2.451236	-1.238730
C	-3.528002	3.623861	-1.598680
C	-3.346121	4.829245	-0.668113
C	-3.276089	-1.318915	-0.809546
C	-2.762260	-2.369530	-0.036271
C	-3.436483	-3.583157	0.045128
C	-4.624608	-3.774603	-0.658637
C	-5.134686	-2.743252	-1.445113
C	-4.468648	-1.523336	-1.517255
O	-1.403931	2.743505	-1.085881

C	1.336845	2.821941	-0.512068
O	2.015489	3.746266	-0.479506
C	1.206696	-1.208503	1.392903
C	0.385059	-0.638188	2.372936
C	-0.029752	-1.387574	3.472084
C	0.368414	-2.717562	3.594758
C	1.179231	-3.295678	2.619207
C	1.597439	-2.546707	1.521744
H	-2.301345	5.140562	-0.649272
H	-3.955021	5.671799	-1.005150
H	-3.644373	4.585959	0.355750
H	-4.571725	3.300256	-1.615161
H	-4.272413	1.109266	-1.261903
H	-1.834820	-2.215600	0.499909
H	-3.032262	-4.381478	0.657331
H	-5.146345	-4.723371	-0.600283
H	-6.048663	-2.890842	-2.009534
H	-4.862952	-0.739382	-2.152163
H	2.218778	-3.008762	0.764263
H	1.484523	-4.332478	2.708381
H	0.040879	-3.304169	4.445992
H	-0.676881	-0.932510	4.212573
H	0.061749	0.391134	2.266375
H	3.819504	1.328728	-1.447109
H	6.020119	2.225387	-0.816797
H	6.893682	1.893488	1.484289
H	5.536753	0.645770	3.145676
H	3.338741	-0.269196	2.517061
H	0.106332	-1.321869	-2.093053
H	0.517001	-2.954671	-3.902740
H	2.779459	-3.928699	-4.212802
H	4.625619	-3.260242	-2.695043
H	4.220616	-1.631242	-0.893976
H	-3.269131	3.916781	-2.623317
H	-5.021886	2.024910	2.903098
H	-3.984445	1.216406	1.706507
H	-5.236534	0.295080	2.560976