

Electronic Supplementary Information for

Rationalization of the Selectivity between 1,3- and 1,2-Migration: DFT study on Gold(I)-Catalyzed Propargylic Ester Rearrangement

Jingxing Jiang,^a Yan Liu,^b Cheng Hou,^a Yinwu Li,^a Zihong Luan,^a Cunyuan Zhao,^a and Zhuofeng Ke^{*,a}

^a MOE Key Laboratory of Bioinorganic and Synthetic Chemistry/KLGHEI of Environment and Energy Chemistry, School of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou 510275, P. R. China.

^b School of Chemical Engineering and Light Industry, Guangdong University of Technology, Higher Education Mega Center, Panyu District, Guangzhou 510006, P. R. China

E-mail: kezhf3@mail.sysu.edu.cn

Table of Contents

1.1 Overall pathways of 1,3-migration and 1,2-migration for propargylic acetates	S2
1.2 Selected optimized structures for 6- <i>endo-dig</i> or 5- <i>exo-dig</i>	S2
1.3 The rest energetic profiles in 1,3-migration and 1,2-migration	S3
1.4 Absolute energies of all species*	S4
1.5 Cartesian Coordinates of All Optimized Structures	S7

1. RESULTS AND DISCUSSION

1.1 Overall pathways of 1,3-migration and 1,2-migration for propargylic acetates

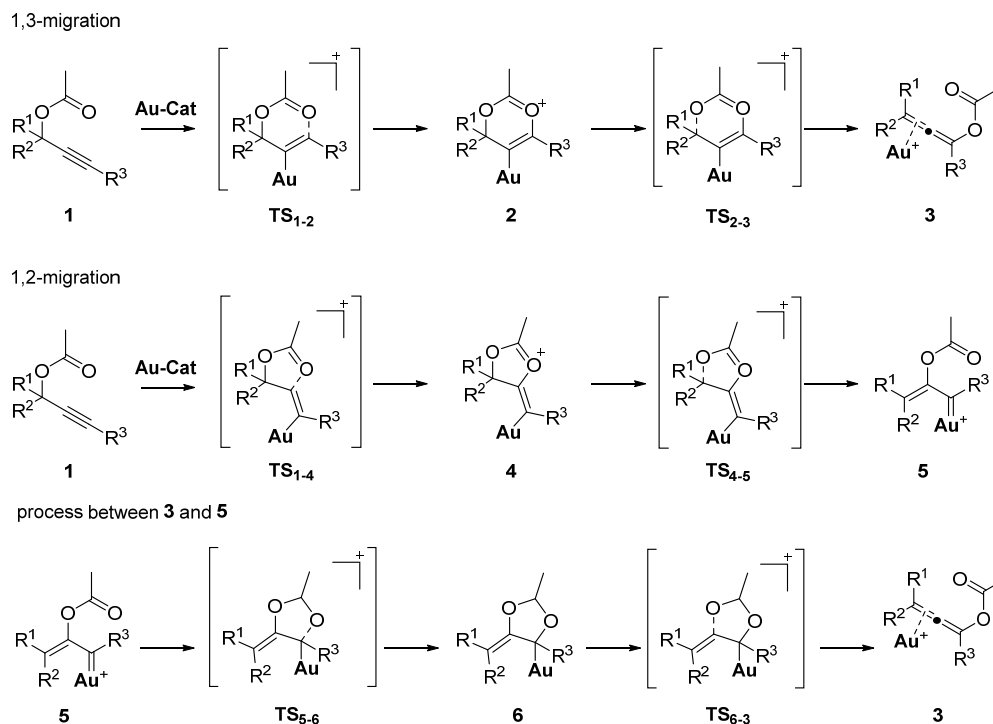


Fig. S1 Overall Pathways of 1,3-Migration and 1,2-Migration for Propargylic Acetates

1.2 Selected optimized structures for 6-endo-dig or 5-exo-dig

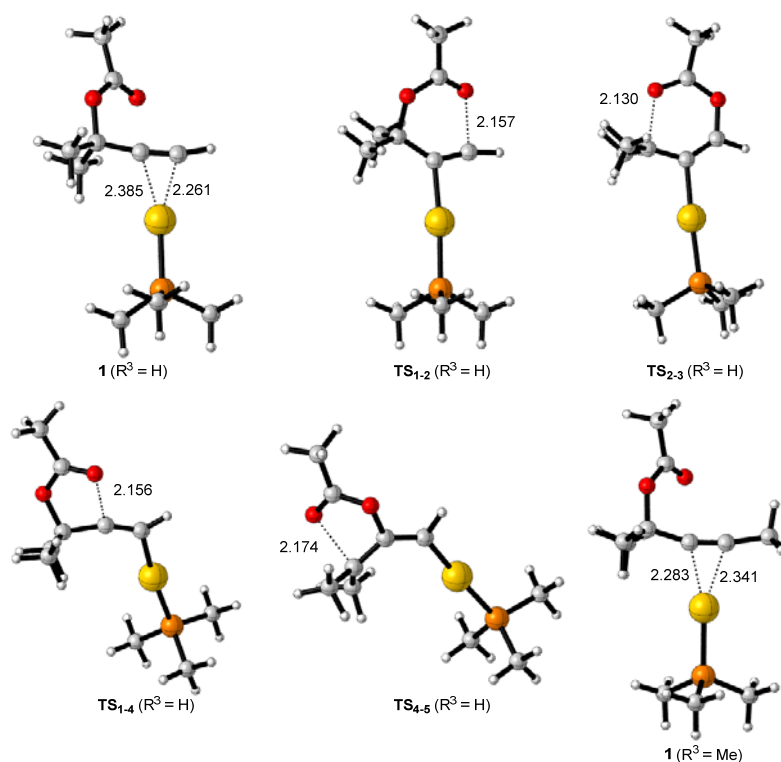


Fig. S2 Selected Optimized Structures for 6-endo-dig or 5-exo-dig, Relative bond distances in Å.

1.3 The rest energetic profiles in the 1,3-migration and 1,2-migration

Table S1 Free energetic profiles in the ring-opening steps at B3LYP-D3/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM, Relative free energies in kcal/mol.

R ³	2	TS ₂₋₃	3	4	TS ₄₋₅	5
H	-1.8	-1.5	-5.8	-1.5	7.9	1.7
Cl	-7.6	-7.9	-12.2	-10.3	-2.2	-11.6
CO ₂ Me	-4.7	-4.5	-8.7	-7.2	3.3	-3.0
<i>p</i> -C ₆ H ₄ -CF ₃	0.3	0.7	-6.0	0.7	9.6	0.5
Ph	2.8	3.7	-2.0	4.3	14.8	5.0
<i>p</i> -C ₆ H ₄ -OMe	4.2	5.0	-0.3	6.8	16.3	4.5
CMe=CH ₂	1.6	3.4	-2.9	4.4	13.8	3.8
Me	1.4	2.3	-2.1	5.4	14.3	4.7
<i>t</i> -Bu	5.5	7.4	1.4	9.6	20.0	13.2

Table S2 Free energetic profiles in the process between 3 and 5 at B3LYP-D3/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM, Relative free energies in kcal/mol.

R ³	TS ₅₋₆	6	TS ₆₋₃
H	7.4	1.1	12.5
Cl	-2.0	-9.3	4.3
CO ₂ Me	7.7	-2.9	7.9
<i>p</i> -C ₆ H ₄ -CF ₃	9.2	5.0	16.0
Ph	10.0	7.7	19.1
<i>p</i> -C ₆ H ₄ -OMe	8.7	8.7	21.6
CMe=CH ₂	8.6	6.3	18.3
Me	12.2	6.8	19.1
<i>t</i> -Bu	14.5	9.2	19.7

Table S3a Calculated $\Delta\Delta G$ value ($\Delta\Delta G = \Delta G_{TS1-2} - \Delta G_{TS1-4}$, in kcal/mol) in different functionals. Free energies calculated at X/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM level (X = B3LYP-D3, M06 and M06-L).

R ³	B3LYP-D3(hybrid GGA)	M06 (hybrid meta-GGA)	M06-L(meta-GGA)
H	3.9	3.9	5.6
Me	-2.1	-2.6	-1.7
Ph	-1.1	-0.9	-0.2

As can be seen, differences of calculated $\Delta\Delta G$ values very close to each other, leading to the same discussion and conclusions. Therefore, B3LYP-D3 is a reliable method for the studied systems.

Table S3b Absolute energies in different functionals. Free energies calculated at X/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM level (X = B3LYP-D3, M06 and M06-L).

R ³	G _{TS1-2}		G _{TS1-4}	
	M06	M06-L	M06	M06-L
H	-1019.454411	-1019.842302	-1019.460633	-1019.851175
Me	-1058.734608	-1059.151293	-1058.730470	-1059.148584
Ph	-1250.860643	-1250.316757	-1250.859225	-1250.316519

1.4 Absolute energies of all species*

Table S4 Absolute energies of species of 1,3- and 1,2- migration ($R^1 = R^2 = \text{Me}$, calculated at B3LYP-D3/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM, absolute energies in hartree)

R^3	1	TS ₁₋₂	2	TS ₂₋₃	3	TS ₁₋₄	4	TS ₄₋₅	5	TS ₅₋₆	6	TS ₆₋₃
H	-1019.990144	-1019.974481	-1019.992993	-1019.992524	-1019.999376	-1019.980713	-1019.992539	-1019.977580	-1019.987518	-1019.978293	-1019.988337	-1019.970266
Cl	-1479.612495	-1479.601058	-1479.624532	-1479.625015	-1479.631895	-1479.605677	-1479.628938	-1479.616043	-1479.631051	-1479.615636	-1479.627341	-1479.605671
CO ₂ Me	-1247.906682	-1247.890652	-1247.914198	-1247.913904	-1247.920604	-1247.901136	-1247.918098	-1247.901430	-1247.911376	-1247.894403	-1247.911308	-1247.894119
<i>p</i> -C ₆ H ₄ -CF ₃	-1588.220617	-1588.208489	-1588.220027	-1588.218663	-1588.227143	-1588.207599	-1588.218719	-1588.202350	-1588.214131	-1588.205925	-1588.212680	-1588.195154
Ph	-1251.065960	-1251.051136	-1251.061548	-1251.060126	-1251.069171	-1251.049420	-1251.059151	-1251.042387	-1251.057975	-1251.050042	-1251.053705	-1251.035499
<i>p</i> -C ₆ H ₄ -OMe	-1365.605173	-1365.590265	-1365.598483	-1365.597286	-1365.605721	-1365.585168	-1365.594399	-1365.579252	-1365.598019	-1365.591242	-1365.591366	-1365.570701
CMe=CH ₂	-1136.705998	-1136.691932	-1136.703475	-1136.700636	-1136.710620	-1136.688829	-1136.699069	-1136.683945	-1136.699970	-1136.692264	-1136.696021	-1136.676921
Me	-1059.307982	-1059.293994	-1059.305799	-1059.304382	-1059.311315	-1059.290644	-1059.299416	-1059.285201	-1059.300476	-1059.288506	-1059.297190	-1059.277499
<i>t</i> -Bu	-1177.223100	-1177.204139	-1177.214344	-1177.211352	-1177.220805	-1177.200831	-1177.207861	-1177.191304	-1177.202115	-1177.199985	-1177.208452	-1177.191746

Table S5 Absolute energies of TS species of 1,3- and 1,2- migration ($R^3 = \text{H}$, calculated at B3LYP-D3/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM, absolute energies in hartree)

R^1	R^2	1	TS ₁₋₂	TS ₁₋₄	TS ₂₋₃	TS ₄₋₅
Me	Me	-1019.990144	-1019.974481	-1019.980713	-1019.992524	-1019.977580
Me	H	-980.682684	-980.663693	-980.671399	-980.675777	-980.661477
H	H	-941.377096	-941.354414	-941.359434	-941.359549	-941.342641
Ph	H	-1172.433546	-1172.416878	-1172.425469	-1172.434917	-1172.427313
<i>p</i> -C ₆ H ₄ -OMe	H	-1286.970812	-1286.954038	-1286.961712	-1286.973694	-1286.969112
<i>p</i> -C ₆ H ₄ -CF ₃	H	-1509.590945	-1509.572892	-1509.583589	-1509.590939	-1509.580942
C ₂ H ₃	H	-1018.767670	-1018.749807	-1018.756817	-1018.765392	-1018.757093
Ph	Me	-1211.741613	-1211.722370	-1211.733145	-1211.745323	-1211.738266

Table S6 Absolute energies of species of 1,3- and 1,2- migration ($R^1 = R^2 = \text{Me}$, PPh₃ instead of PMe₃, calculated at B3LYP-D3/BS2/IEF-PCM//B3LYP/BS1/IEF-PCM, absolute energies in hartree, $\Delta\Delta G = \Delta G_{\text{TS1-2}} - \Delta G_{\text{TS1-4}}$ in kcal/mol)

R ³	H		Me		Ph	
	G	ΔG	G	ΔG	G	ΔG
1	-1595.105621	0.0	-1634.418818	0.0	-1826.155803	0.0
TS₁₋₂	-1595.090905	9.2	-1634.404730	8.8	-1826.140996	9.3
2	-1595.110756	-3.2	-1634.417785	0.7	-1826.150242	3.5
TS₂₋₃	-1595.111078	-3.4	-1634.415782	1.9	-1826.146552	5.8
3	-1595.116242	-6.7	-1634.423193	-2.8	-1826.156084	-0.2
TS₁₋₄	-1595.100437	3.3	-1634.402715	10.1	-1826.136787	11.9
4	-1595.112062	-4.0	-1634.413685	3.2	-1826.148677	4.5
TS₄₋₅	-1595.095786	6.2	-1634.397634	13.3	-1826.132200	14.8
5	-1595.108290	-1.7	-1634.412959	3.7	-1826.147927	4.9
TS₅₋₆	-1595.097575	5.1	-1634.400297	11.6	-1826.139123	10.5
6	-1595.111064	-3.4	-1634.411809	4.4	-1826.144652	7.0
TS₆₋₃	-1595.091770	8.7	-1634.390250	17.9	-1826.124156	19.9
$\Delta\Delta G$	5.9		-1.3		-2.6	

* Number of imaginary frequencies of species **1**, **2**, **3**, **4**, **5**, **6** in Table S3, **1** in Table S4 is 0, whereas that of else is 1.

1.5 Cartesian Coordinates of All Atoms (in Å)

Species with R ¹ = R ² = Me, R ³ = H:			H	-3.42312301.0792080 2.1274440	C	0.4531300 -2.33400601.1805000
1			H	-3.7309280-0.42283401.2152430	H	1.4745240 -2.69519201.0341760
C	0.2524140	-1.08379100.2041680	H	-2.8693450-0.50716502.7551520	H	0.3256900 -2.07563702.2347010
C	0.7899990	0.1494700 0.8456320	O	-1.0751370-0.88811700.9768200	H	-0.2429370-3.13491600.9154500
C	1.0498060	1.1917360 1.4441070	O	-1.31329801.3603530 0.7116500	H	-0.4056600-2.2422920-1.4486220
C	-1.9453050	-0.0500080-0.2131410	C	-0.2062420-1.1535720-1.2847140	H	0.0831540 -0.5634900-1.8077350
C	-3.4151260	-0.3146790-0.0242110	H	0.6951960 -1.3210140-1.8803500	Au	3.1227270 0.0253250 0.4972030
H	-3.98820000.5342020 -0.3959830		C	0.7476050 -2.37155400.7343200	H	0.8699280 2.0978460 1.4802840
H	-3.6992010-1.2196930-0.5703500		H	1.6609640 -2.61695600.1863980	P	5.4660250 -0.00669800.3038330
H	-3.6362710-0.48445901.0332610		H	0.9875920 -2.28392101.7968120	C	6.1648000 -1.6571350-0.1029340
O	-1.2052120-1.05514000.3300020		H	0.0243750 -3.17950800.5973720	H	5.7549040 -2.0041400-1.0549550
O	-1.46181500.9178330 -0.7663390		H	-0.8891120-1.9940070-1.4361230	H	7.2551090 -1.5995700-0.1782410
C	0.6724360 -1.2078880-1.2677360		H	-0.6825640-0.2322630-1.6271320	H	5.8939630 -2.37334000.6770300
H	1.7556930 -1.3378950-1.3314500		Au	3.2312000 0.1486800 0.3733770	C	6.3439160 0.5034010 1.8357780
C	0.6599200 -2.32290001.0150140		H	0.9131570 2.3831120 0.8204740	H	7.4270680 0.4636410 1.6850450
H	1.7462920 -2.43742401.0095940		P	5.5636220 0.0195840 0.2752650	H	6.0529190 1.5228820 2.1021240
H	0.3157240 -2.23723902.0481480		C	6.3688310 1.6306900 -0.0767890	H	6.0683490 -0.16450602.6558810
H	0.2079580 -3.20719700.5590480		H	7.4553160 1.5043790 -0.1134830	C	6.1270340 1.1068420 -1.0004310
H	0.1912240 -2.0925260-1.6934870		H	6.0155000 2.0161130 -1.0362460	H	5.8248660 2.1362110 -0.7914500
H	0.3871300 -0.3267410-1.8414290		H	6.1136670 2.3477550 0.7072960	H	7.2195710 1.0493230 -1.0321250
Au	3.1435320 0.3909480 1.1442020		C	6.3337760 -0.57457001.8303670	H	5.7211870 0.8136940 -1.9720700
H	1.0325610 2.1452350 1.9350880		H	5.9632580 -1.57520202.0655870	TS₂₋₃	
P	5.4598120 0.1432250 1.1596010		H	7.4219360 -0.60706001.7198230	C	0.5308590 -1.32449300.3322730
C	6.0934650 -0.65948802.6798190		H	6.0726950 0.0995360 2.6497370	C	1.0895610 -0.04721200.6106380
H	5.6639610 -1.65980102.7731830		C	6.1661870 -1.1183860-1.0316700	C	0.4714830 1.0832960 0.9493810
H	7.1840390 -0.73456602.6303730		H	5.8068780 -0.7791130-2.0063800	C	-1.81466200.2941290 0.9717340
H	5.8090950 -0.06855503.5537050		H	7.2603020 -1.1402620-1.0357320	C	-3.21735900.7570830 1.2176300
C	6.3242700 1.7555860 1.0490430		H	5.7846010 -2.1253850-0.8459900	H	-3.46884101.5513710 0.5080040
H	7.4068520 1.5973340 1.0624380		2		H	-3.9074120-0.07786701.1027710
H	6.0419900 2.2615370 0.1227850		C	0.2283220 -1.11963500.2871660	H	-3.29569301.1752780 2.2255610
H	6.0393680 2.3832580 1.8967830		C	1.0451530 0.0751240 0.6820060	O	-1.5219670-0.86248700.6628590
C	6.0945300 -0.8631310-0.2340700		C	0.4436490 1.1623230 1.1527000	O	-0.91582501.2726740 1.1212220
H	7.1843660 -0.9365090-0.1674140		C	-1.74741900.2749700 0.9742370	C	0.3395750 -1.7553270-1.0917820
H	5.6612670 -1.8652970-0.1927080		C	-3.21127600.4213150 1.1824540	H	1.2548880 -2.2643180-1.4191810
H	5.8186370 -0.3952680-1.1818780		H	-3.48255901.4754710 1.2355700	C	0.5908080 -2.40408701.3717310
TS₁₋₂			H	-3.7520540-0.08549900.3816160	H	1.5205120 -2.96733901.2223090
C	0.1684070 -1.06425300.1998510		H	-3.4734470-0.06252702.1308420	H	0.5916590 -1.99600702.3831750
C	1.0852390 0.1156470 0.4275550		O	-1.3021690-0.81873500.4960230	H	-0.2402780-3.10090201.2404240
C	0.8418240 1.3309620 0.6307000		O	-0.99241501.2648650 1.3092020	H	-0.4796830-2.4747000-1.1612990
C	-1.72152700.2728830 1.1246530		C	0.3007190 -1.4452730-1.1999060	H	0.1608150 -0.9065820-1.7531170
C	-3.01960100.1028620 1.8607110		H	1.3116990 -1.7876220-1.4364200	Au	3.1989840 -0.10299800.4258040

H	0.9585840	2.0274610	1.1459740	H	5.7840200	-2.1491610	2.2142080	C	1.1579260	0.9286990	1.1376030
P	5.5360330	-0.0648190	0.2549080	C	6.1302290	-0.0796820	-1.0513850	C	-2.0039480	-0.5106460	0.9555310
C	6.2766580	-1.6964200	-0.1473050	H	5.9402560	0.8979600	-0.6017360	C	-3.4535270	-0.4620110	1.2323490
H	5.8844730	-2.0505180	-1.1039690	H	7.2095360	-0.2541860	-1.0971020	H	-3.9977140	-1.0055080	0.4587000
H	7.3656380	-1.6090790	-0.2119780	H	5.7179860	-0.0895730	-2.0632900	H	-3.6349120	-0.9566880	2.1942750
H	6.0170140	-2.4200340	0.6294610					H	-3.7886230	0.5729930	1.2996210
C	6.3752940	0.4713330	1.7973650	TS₁₋₄				O	-1.4503310	-1.5301720	0.3989290
H	7.4605780	0.4652960	1.6573010	C	0.2499420	-1.3160340	1.0272320	O	-1.2139520	0.4505200	1.2769510
H	6.0494710	1.4811200	2.0596680	C	0.6644330	0.1082840	0.9634300	C	0.3814310	-1.3458290	-1.1984440
H	6.1118090	-0.2060320	2.6134210	C	1.4077940	1.1216460	0.8753360	H	1.4488200	-1.1394200	-1.3163860
C	6.1621530	1.0710030	-1.0447710	C	-1.8830560	-0.3606710	0.7001390	C	0.7196970	-2.3976490	1.0984240
H	5.8222110	2.0886660	-0.8373420	C	-3.3091770	-0.5358710	0.2845100	H	1.7990220	-2.2220700	1.0831470
H	7.2562600	1.0514430	-1.0680320	H	-3.3632940	-1.0441930	-0.6806650	H	0.3832130	-2.3850860	2.1378480
H	5.7735220	0.7628190	-2.0186240	H	-3.8152620	-1.1645660	1.0250530	H	0.5138000	-3.3771220	0.6586940
				H	-3.8024250	0.4343180	0.2387500	H	0.1649360	-2.3370730	-1.6056030
3				O	-1.1055710	-1.4235920	0.4689160	H	-0.1797560	-0.5907560	-1.7539360
C	0.6124840	-1.7473310	-0.1232290	O	-1.4074530	0.6466850	1.2221220	Au	3.1590530	0.6589560	0.7102380
C	0.8950400	-0.5449750	0.4489590	C	1.1329210	-2.1843100	1.207010	P	5.4646480	0.4461920	0.2616490
C	0.6616340	0.6243750	1.0208820	H	2.1606150	-2.1824120	0.4891620	H	0.8603080	1.8655780	1.6109990
C	-1.7785240	0.6233690	1.0875690	C	0.2116240	-1.8298320	2.4734630	C	5.9248340	-1.0269870	-0.7379550
C	-2.8859380	1.5170950	1.5720300	H	1.2190720	-1.8074430	2.8965160	H	7.0070710	-1.0556720	-0.8991810
H	-2.8192080	2.4943770	1.0848680	H	-0.4410720	-1.2123770	3.0942420	H	5.6140500	-1.9359470	-0.2164230
H	-3.8475570	1.0552340	1.3507530	H	-0.1525680	-2.8603510	2.4788110	H	5.4171020	-0.9875440	-1.7050650
H	-2.7895930	1.6786160	2.6500390	H	0.7509240	-3.2081190	1.1420690	C	6.5103840	0.3191220	1.7685820
O	-1.9099280	-0.4549680	0.5502490	H	1.1176020	-1.8136320	-0.9060370	H	7.5665290	0.2351710	1.4939460
O	-0.5621350	1.2018690	1.3405730	Au	3.4502170	0.6688280	0.4613430	H	6.3676630	1.2078070	2.3886250
C	0.3194250	-1.8655870	-1.5980030	P	5.7375000	0.3953230	0.0756270	H	6.2159600	-0.5606260	2.3468570
H	0.8180610	-2.7350880	-2.0358300	H	1.2095720	2.1788850	0.9942260	C	6.1698830	1.8681930	-0.6665530
C	0.3885770	-2.9823350	0.7135410	C	6.7315580	0.4780050	1.6159050	H	6.0148620	2.7891820	-0.0984880
H	0.8910870	-3.8534890	0.2835080	H	7.7935280	0.3512200	1.3852640	H	7.2415180	1.7223350	-0.8336180
H	0.7015780	-2.8455070	1.7488670	H	6.5780340	1.4468190	2.0976150	H	5.6632240	1.9632970	-1.6304810
H	-0.6913530	-3.1814860	0.6966120	H	6.4124520	-0.3110150	2.3012950				
H	-0.7633810	-2.0234430	-1.6909310	C	6.4464750	1.6792270	-1.0262970	TS₄₋₅			
H	0.5890930	-0.9646470	-2.1495330	H	7.5204560	1.5115170	-1.1525150	C	0.2075110	-1.5314910	0.5492020
Au	3.0030070	-1.1369030	0.1111120	H	5.9560170	1.6359450	-2.0017320	C	0.1838880	-0.1212750	0.8618880
H	1.4501080	1.3010110	1.3234210	H	6.2825810	2.6683430	-0.5919240	C	1.1996600	0.7656960	0.8708670
P	5.3276070	-1.3867570	-0.0467550	C	6.1854690	-1.2038200	-0.7043790	C	-2.0516080	-0.2142650	0.3868560
C	5.8181540	-2.9755920	-0.8199030	H	7.2686040	-1.2544050	-0.8541700	C	-3.4038950	0.4096790	0.4702700
H	5.4083300	-3.0332130	-1.8311390	H	5.8703670	-2.0290270	-0.0611500	H	-3.3513410	1.4281810	0.0717120
H	6.9092880	-3.0446930	-0.8648820	H	5.6814430	-1.2944560	-1.6697980	H	-4.1216060	-0.1757860	-0.1023090
H	5.4257130	-3.8075360	-0.2303670					H	-3.7123450	0.4782420	1.5170670
C	6.1705860	-1.3472620	1.5806790	4				O	-1.7329410	-1.1477250	-0.3539280
H	7.2484620	-1.4791670	1.4454290	C	0.0478550	-1.2970800	0.2870110	O	-1.1310820	0.3205670	1.2092840
H	5.9813380	-0.3882620	0.0689080	C	0.1627260	0.0884380	0.9046520	C	1.1037330	-2.0669060	-0.5091850

H	1.9214250	-2.6253500	-0.0358340	H	1.0770710	1.6600480	1.1418320	C	3.5293760	1.4593210	1.0949220
C	-0.3718590	-2.5235340	1.5041180	C	6.7437450	-0.24789700	0.8684840	H	4.6065030	1.4115900	1.2819590
H	0.4741130	-2.88253702	1.087310	H	7.7711870	-0.21448800	0.4934450	H	3.3085770	2.3307080	0.4733530
H	-1.1109560	-2.09781702	1.1816270	H	6.6823880	0.3094930	1.8065640	H	3.0011560	1.5629340	2.0461260
H	-0.7838030	-3.38912800	0.9804910	H	6.4612260	-1.28647401	0.0577250				
H	0.5429700	-2.7956420	-1.1046880	C	6.2764280	2.1600440	-0.7012210	6			
H	1.5112570	-1.2905190	-1.1535660	H	7.3226580	2.0873110	-1.0138520	C	-2.72406501	0.8216410	0.1015400
Au	3.2069200	0.5549150	0.4892170	H	5.6941490	2.6389600	-1.4924080	C	-2.47818600	0.5247580	-0.0950950
P	5.5360770	0.4240560	0.1162620	H	6.2105560	2.7716440	0.2021270	C	-1.4450270	-0.2555190	-0.8606330
H	0.8844710	1.7472050	1.2351600	C	5.8902270	-0.4626920	-1.9075410	C	-2.9651500	-1.63861000	0.1390210
C	6.0280780	-0.7075640	-1.2461530	H	6.9503980	-0.4298090	-2.1763520	C	-3.6554710	-2.85739800	0.6066130
H	7.1154080	-0.7051630	-1.3702680	H	5.5864500	-1.5022410	-1.7612180	H	-4.7352720	-2.72929800	0.4992220
H	5.6928740	-1.7227080	-1.0186930	H	5.2976630	-0.0342600	-2.7198420	H	-3.3097860	-3.72224500	0.0421780
H	5.5581620	-0.3839570	-2.1784170					H	-3.4372570	-2.99993701	0.6708630
C	6.4795470	-0.16775801	0.5785490	TS₅₋₆				O	-1.9584840	-1.6681190	-0.6454500
H	7.5502570	-0.20161901	0.3552460	C	-2.56696301	0.8260530	0.0906480	O	-3.3402470	-0.46014800	0.5212160
H	6.3074410	0.5071430	2.4208480	C	-2.46100800	0.5228850	-0.2838720	C	-1.82857702	0.8541160	-0.5346950
H	6.1360460	-1.16791201	0.8556830	C	-1.3344840	-0.2528510	-0.7108180	H	-2.36105603	0.3855660	-1.3337730
C	6.3104460	2.0327800	-0.3189480	C	-3.3938300	-1.50155000	0.1817380	C	-3.87544302	0.3311920	0.9284280
H	6.1351880	2.7538890	0.4834430	C	-4.5924500	-2.32511400	0.5119900	H	-4.49713601	0.5305030	1.3320730
H	7.3878280	1.9084600	-0.4656590	H	-5.3266550	-2.2444880	-0.2938410	H	-3.50075302	0.9334270	1.7655690
H	5.8620990	2.4168570	-1.2388230	H	-4.3024400	-3.36368600	0.6637750	H	-4.51125702	0.9900820	0.3242590
				H	-5.0536980	-1.93241201	0.4242830	H	-1.53145703	0.6051610	0.2071470
5				O	-2.2195660	-1.87263300	0.2837050	H	-0.92120402	0.4192640	-0.9630340
C	0.3326600	-1.63829200	0.9207160	O	-3.6578650	-0.2609160	-0.2518380	Au	0.5820800	-0.1222580	-0.2740520
C	0.3183690	-0.24211401	0.0450970	C	-1.39589902	0.7625010	0.1049560	P	2.8541780	0.0327530	0.3315310
C	1.3812490	0.6384150	0.9033920	H	-1.45551403	0.4430630	-0.7539440	H	-1.5370940	-0.1187420	-1.9407890
C	-1.55903501	0.1829980	0.6206420	C	-3.89386302	0.4431670	0.4267640	C	3.4694550	-1.41046301	0.2884750
C	-2.86491301	0.6309800	1.2097810	H	-4.72656701	0.7454210	0.3564560	H	2.8963840	-1.50780802	0.2141150
H	-2.67995902	0.1477190	2.1569400	H	-3.85025402	0.8449110	1.4470520	H	3.3409580	-2.32202400	0.6992410
H	-3.36816002	0.3025800	0.5152750	H	-4.08505303	0.2972700	-0.2338500	H	4.5290250	-1.28269001	0.5307270
H	-3.49878900	0.7661270	1.4247350	H	-1.43719803	0.3841940	1.0056410	C	3.9927170	0.1579580	-1.1051170
O	-1.07346701	0.5527840	-0.4276510	H	-0.43402802	0.2483090	0.0594490	H	3.7465310	1.0472300	-1.6909250
O	-0.93998300	0.2719620	1.4397690	Au	0.6521990	-0.1249000	-0.2354550	H	5.0302150	0.2252580	-0.7638350
C	1.5473930	-2.44024900	0.6442630	P	2.9682180	-0.06680000	0.2416560	H	3.8772370	-0.7233540	-1.7411980
H	1.6972860	-3.13643201	0.4814850	H	-1.5601490	-0.8748060	-1.5782430	C	3.2602590	1.4899420	1.3751240
C	-0.9346260	-2.39877901	0.1122100	C	3.5307460	-1.44105201	0.3225530	H	4.3290580	1.5028380	1.6103610
H	-1.3436830	-2.19927302	0.1105130	H	3.0042400	-1.39519302	0.2791080	H	2.9964770	2.4073290	0.8426080
H	-1.6968940	-2.04623200	0.4064860	H	3.3090120	-2.39856700	0.8448100	H	2.6861680	1.4469710	2.3042390
H	-0.7870990	-3.47112200	0.9849890	H	4.6081970	-1.36353801	0.4975890				
H	1.3550460	-3.0721670	-0.2326960	C	4.0233880	-0.1830960	-1.2573160	TS₆₋₃			
H	2.4509900	-1.85374800	0.4909140	H	3.8058430	0.6549520	-1.9243580	C	-2.48788401	0.9600580	0.0616500
Au	3.3316340	0.5018680	0.3291150	H	5.0813650	-0.1587710	-0.9785590	C	-2.24591000	0.7086190	-0.2547840
P	5.5974000	0.4878360	-0.3636580	H	3.8090650	-1.1159650	-1.7849960	C	-1.4917720	-0.4070290	-0.6625260

C	-3.3296800-1.49556400.1882830	C	0.9504780 2.9418440 0.9113360	C	0.8015690 -2.29670100.4144280
C	-4.0284390-2.73916700.6247520	H	1.2745380 3.2528640 1.9078250	H	1.7343940 -2.4099980-0.1436990
H	-4.2885270-3.3178310-0.2688240	H	1.5680470 3.4456550 0.1630370	H	1.0148970 -2.41092901.4802310
H	-3.3661850-3.34711001.2434210	H	-0.08952603.2564780 0.7699960	H	0.1051220 -3.07980900.1032410
H	-4.9434200-2.48801001.1608450	C	0.9060410 -1.8182070-0.8420170	H	-0.7776690-1.5504860-1.6983920
O	-2.0138860-1.60289900.0080640	H	1.9465530 -2.0573590-0.6062180	H	-0.62648300.2204380 -1.5367380
O	-3.8893750-0.4099450-0.0236970	C	0.3582370 -1.91152201.6296880	Au	3.2137410 0.1519520 0.5033120
C	-1.33768902.9068160 0.3544830	H	1.4041480 -2.09103301.8903140	P	5.5371770 0.0022590 0.3158570
H	-1.31937303.6969590 -0.4042560	H	-0.1313100-1.39484902.4585120	C	6.2306820 1.0325160 -1.0358550
C	-3.87272802.5567670 0.1445250	H	-0.1355760-2.87285001.4657610	H	5.9860670 2.0829630 -0.8601440
H	-4.65454201.8334810 -0.0772130	H	0.3632070 -2.7538530-1.0027860	H	7.3178490 0.9151130 -1.0773170
H	-4.02975602.9644240 1.1493500	H	0.8764120 -1.2205330-1.7524600	H	5.7967590 0.7247460 -1.9903600
H	-3.94526103.3922250 -0.5605260	Au	3.1093860 0.4703770 0.9853560	C	6.1291380 -1.7000840-0.0295680
H	-1.50453803.3808630 1.3279360	P	5.3939490 0.1569060 1.3230510	H	7.2203060 -1.7089420-0.1118080
H	-0.37073902.4015200 0.3588700	C	6.3767860 1.6390030 0.8766470	H	5.8211590 -2.36642300.7798850
Au	0.6005650 -0.1540420-0.2205050	H	7.4408640 1.4429580 1.0400680	H	5.6923650 -2.0571540-0.9655400
P	2.8986500 -0.03525400.2075720	H	6.2106570 1.8863670 -0.1745510	C	6.4398880 0.5264380 1.8258560
H	-1.5470150-0.6025290-1.7386410	H	6.0653700 2.4854050 1.4934480	H	7.5192540 0.4379890 1.6680060
C	3.5485120 -1.51911701.0701600	C	6.0795890 -1.21521800.3195500	H	6.1921320 1.5650830 2.0582840
H	3.0372840 -1.63936102.0285250	H	7.1525250 -1.31342200.5101290	H	6.1442010 -0.10360202.6683530
H	3.3667050 -2.40737900.4601420	H	5.5788370 -2.14988700.5824060		
H	4.6236510 -1.41132501.2430930	H	5.9161250 -1.0113210-0.7412130	2	
C	3.9239890 0.1241820 -1.3064350	C	5.8348580 -0.22713503.0597700	C	0.2518650 -1.04807000.2400140
H	4.9847210 0.1598050 -1.0391500	H	5.3344190 -1.14702103.3713330	C	1.0277530 0.1473460 0.7132550
H	3.7442520 -0.7307440-1.9629270	H	6.9179840 -0.35434403.1494640	C	0.4059210 1.2054550 1.2300500
H	3.6530800 1.0395310 -1.8385200	H	5.5104370 0.5895760 3.7088940	C	-1.76788900.2108850 1.0074920
C	3.3893680 1.3825140 1.2654530			C	-3.23442100.2825330 1.2403940
H	4.4716570 1.3731460 1.4271980	TS₁₋₂		H	-3.56930701.3199410 1.2167630
H	3.1046830 2.3190220 0.7796150	C	0.2002450 -0.92267100.1260950	H	-3.7610080-0.31999000.4997200
H	2.8784670 1.3157500 2.2290800	C	1.0795140 0.2124780 0.6123640	H	-3.4426030-0.12937402.2351730
Species with R ¹ = R ² = Me, R ³ = Me:		C	0.7340830 1.3576490 1.0418870	O	-1.2809890-0.84799600.4945000
1		C	-1.76798500.1273740 1.2051810	O	-1.05683001.2230770 1.3618920
C	0.2735190 -1.07654200.3438620	C	-3.1153700-0.18520901.7870220	C	0.9060480 2.5064440 1.7615050
C	0.8733680 0.2748280 0.5654530	H	-3.49500700.6805050 2.3293300	H	0.6216850 2.6377050 2.8120280
C	1.0122360 1.4862930 0.7575260	H	-3.8029900-0.42595200.9687660	H	1.9936510 2.5363180 1.6850680
C	-1.6666240-0.1811870-0.8921880	H	-3.0557960-1.05738702.4418560	H	0.4889770 3.3477520 1.1957890
C	-3.1722290-0.2356520-0.8997260	O	-1.0866330-0.95922500.8646640	C	0.3130430 -1.2520110-1.2707330
H	-3.55663100.4259210 -1.6756450	O	-1.35068501.2819160 1.0565270	H	1.3363060 -1.5168620-1.5494130
H	-3.5015900-1.2612220-1.0947940	C	0.8328920 2.7151610 1.5630590	C	0.5506870 -2.32156801.0247830
H	-3.56859400.0576710 0.0762920	H	0.4012430 2.7886110 2.5650940	H	1.5830890 -2.62279500.8283290
O	-1.1687370-0.90782200.1419690	H	1.8938580 2.9799310 1.6194560	H	0.4380490 -2.15589802.0990890
O	-0.97758900.4227460 -1.6915490	H	0.3310640 3.4257520 0.9006060	H	-0.1163010-3.12917800.7097000
		C	-0.1300780-0.7366420-1.3600470	H	-0.3537220-2.0645770-1.5734750
		H	0.7950260 -0.7582050-1.9422770	H	0.0371480 -0.3376000-1.8018590

Au	3.1102390	0.0857110	0.5220060	C	6.3765040	0.4570570	1.8089820	H	7.2521470	-0.3121620	-1.0385040
P	5.4517100	0.0087080	0.3118780	H	6.0965840	-0.2115100	2.6268430	H	5.7722430	-0.0937050	-2.0120360
C	6.2000950	1.5476590	-0.3587710	H	7.4617700	0.4273980	1.6718010				
H	7.2873270	1.4430500	-0.4289490	H	6.0719030	1.4745860	2.0669300	TS₁₋₄			
H	5.7915120	1.7506430	-1.3519770	C	6.2362020	-1.7150930	-0.1278180	C	0.3857970	-1.2624050	0.8924810
H	5.9600190	2.3884100	0.2971540	H	5.8368220	-2.0657230	-1.0827680	C	0.6407580	0.2098950	0.9003700
C	6.0621510	-1.3218560	-0.7996570	H	7.3267920	-1.6509180	-0.1926240	C	1.3511570	1.2640110	0.8667450
H	7.1555200	-1.3078390	-0.8452580	H	5.9611470	-2.4290500	0.6525030	C	-1.8085530	-0.4284020	0.7733340
H	5.7290990	-2.2933530	-0.4255100					C	-3.2676120	-0.6484490	0.5408160
H	5.6568060	-1.1750720	-1.8040780	3				H	-3.4226870	-1.2321690	-0.3688450
C	6.3340830	-0.2774790	1.8985290	C	0.6339590	-1.5504310	-0.2392030	H	-3.6711670	-1.2208750	1.3832410
H	7.4156270	-0.3012990	1.7334890	C	0.9037450	-0.4532180	0.5247160	H	-3.7821280	0.3098760	0.4799950
H	6.0926870	0.5239900	2.6013140	C	0.6021900	0.6087890	1.2601390	O	-1.0237060	-1.4598130	0.4934940
H	6.0129660	-1.2291820	2.3295660	C	-1.8619210	0.4681610	1.1060890	O	-1.3103750	0.6170640	1.2070000
				C	-3.0431310	1.2515460	1.6109950	C	1.0518030	2.7211950	1.0677390
TS₂₋₃				H	-2.9924580	2.2814310	1.2448940	H	1.3613050	3.3003100	0.1933090
C	0.5767680	-1.2618620	0.3209160	H	-3.9639010	0.7803580	1.2685580	H	-0.0164620	2.8727750	1.2428480
C	1.0730300	0.0371170	0.6022030	H	-3.0272590	1.2893660	2.7043710	H	1.6126780	3.1057500	1.9247730
C	0.4266060	1.1614290	0.9199450	O	-1.9123320	-0.5311520	0.4214350	C	1.2108730	-1.9917100	-0.1716900
C	-1.8398160	0.2390610	0.9357570	O	-0.7010950	1.0503630	1.5343030	H	2.2731720	-1.9245010	0.0730420
C	-3.2590210	0.6440730	1.1966940	C	1.5605760	1.5432890	1.9377440	C	0.5493330	-1.8769110	2.2889710
H	-3.5124390	1.5239320	0.5991030	H	1.3774000	1.5511950	3.0178360	H	1.5913240	-1.7843820	2.6057420
H	-3.9282150	-0.1822460	0.9595820	H	2.5943190	1.2452900	1.7574550	H	-0.0822220	-1.3662900	3.0200200
H	-3.3677020	0.9154270	2.2519260	H	1.4160590	2.5644530	1.5682730	H	0.2806260	-2.9360950	2.2571270
O	-1.5043110	-0.9087030	0.6430830	C	0.4109610	-1.4433270	-1.7278320	H	0.9165470	-3.0444940	-0.1872150
O	-0.9858670	1.2586320	1.0653870	H	0.9220970	-2.2447610	-2.2691860	H	1.0443510	-1.5544980	-1.1582360
C	0.4010890	-1.7026590	-1.1045880	C	0.3614960	-2.8977490	0.3840390	Au	3.3914010	0.7320180	0.4843290
H	1.3306700	-2.1815920	-1.4359310	H	0.8797970	-3.6990620	-0.1507340	P	5.6797620	0.4035370	0.1240170
C	0.6790070	-2.3445570	1.3570830	H	0.6231140	-2.9266450	1.4421380	C	6.4137200	1.6238780	-1.0338500
H	1.6213600	-2.8835830	1.2009610	H	-0.7174930	-3.0750420	0.2839760	H	6.2628060	2.6337750	-0.6446860
H	0.6740590	-1.9392100	2.3697000	H	-0.6677140	-1.5684440	-1.8908920	H	7.4856760	1.4361310	-1.1492450
H	-0.1345840	-3.0627700	1.2301540	H	0.7133030	-0.4739230	-2.1249530	H	5.9252180	1.5446370	-2.0081350
H	-0.3942590	-2.4488420	-1.1709860	Au	3.0068760	-1.0548260	0.1513180	C	6.6758840	0.5440220	1.6593660
H	0.1904280	-0.8612800	-1.7660930	P	5.3249410	-1.3841270	-0.0023880	H	7.7361710	0.3900010	1.4374810
Au	3.1911600	-0.0519270	0.4295790	C	6.1624570	-1.3802510	1.6287670	H	6.5373070	1.5368900	2.0944560
P	5.5297020	-0.0665030	0.2661350	H	7.2352920	-1.5510690	1.4973440	H	6.3437150	-0.2059930	2.3813130
C	0.9990140	2.5171050	1.1925010	H	6.0065080	-0.4169520	1.204100	C	6.1101540	-1.2377040	-0.5774500
H	2.0851500	2.4919180	1.0936160	H	5.7444930	-2.1699190	2.2576670	H	7.1917790	-1.3094640	-0.7283590
H	0.5949080	3.2547290	0.4895990	C	5.7654890	-2.9877810	-0.7763510	H	5.7887220	-2.0266780	1.070380
H	0.7418380	2.8502230	2.2045870	H	5.3611750	-3.0295720	-1.7905500	H	5.6013450	-1.3717810	-1.5351840
C	6.1857460	1.0502830	-1.0355240	H	6.8536600	-3.0966740	-0.8139300				
H	7.2792530	1.0069670	-1.0534820	H	5.3392910	-3.8062880	-0.1913840	4			
H	5.7952140	0.7460270	-2.0098660	C	6.1789100	-0.1023180	-0.9978110	C	0.2145550	-1.2866050	0.3978200
H	5.8673090	2.0761830	-0.8344870	H	6.0192500	0.8793190	-0.5450920	C	0.1739660	0.1640430	0.8627090

C	1.0803910	1.1218370	1.0211690	O	-1.5764630	-1.1548060	-0.4125140	C	1.5912820	-2.20314500	3.297440
C	-1.9260230	-0.64644800	0.9363970	O	-1.14955400	0.1851080	1.3086700	H	1.9395200	-2.86686001	1.1332540
C	-3.3819570	-0.72065501	1.1749480	C	1.2371120	-1.7994330	-0.6797730	C	-0.8141810	-2.27388101	0.0594180
H	-3.8497680	-1.34786300	0.4141120	H	2.1327970	-2.2841080	-0.2723470	H	-1.3609670	-1.95019701	0.9478410
H	-3.5474790	-1.18791902	0.1530290	C	-0.1513070	-2.58993401	0.2906100	H	-1.4938490	-2.14392500	0.2038790
H	-3.81327400	0.2799550	1.1808080	H	0.7371370	-2.95329401	0.8265770	H	-0.5692790	-3.33488501	0.1270860
O	-1.2554440	-1.65932000	0.5099140	H	-0.8949570	-2.29997502	0.0326170	H	1.2683500	-2.8615710	-0.4860030
O	-1.25006600	0.4194740	1.1612140	H	-0.5244880	-3.41537200	0.6805490	H	2.4209770	-1.5809300	-0.0016950
C	0.6871790	2.5000380	1.5092270	H	0.7439780	-2.5417750	-1.3157590	Au	3.3620600	0.6146070	0.3802070
H	1.2346890	2.7433790	2.4266180	H	1.5300370	-0.9335450	-1.2707150	P	5.6187490	0.5117560	-0.3193190
H	0.9766790	3.2551920	0.7698270	Au	3.1739980	0.6154280	0.6116200	C	6.7649370	-0.09212200	0.9831760
H	-0.38375602	0.6078790	1.7090820	P	5.4892890	0.4497580	0.1720950	H	6.4703050	-1.09688901	0.2965990
C	0.5851080	-1.4647510	-1.0695070	C	0.7957870	2.1837750	1.7023820	H	7.7898930	-0.11813300	0.6007440
H	1.6288390	-1.1646740	-1.1986350	H	-0.26861502	0.2959510	1.9245150	H	6.7184470	0.5733910	1.8488050
C	0.9632770	-2.22938501	0.3320930	H	1.3633890	2.3142320	2.6317490	C	6.3040240	2.1366440	-0.8320790
H	2.0233480	-1.96105501	0.3132160	H	1.1120900	3.0013580	1.0441600	H	7.3470300	2.0269790	-1.1446540
H	0.6025510	-2.13597102	0.3592770	C	6.5234510	0.2863300	1.6827830	H	5.7175470	2.5365030	-1.6631050
H	0.8538270	-3.26519900	0.9991900	H	6.2391110	-0.61860602	0.2259500	H	6.2492530	2.8371310	0.0050330
H	0.4772090	-2.5110990	-1.3680310	H	7.5826950	0.2294010	1.4133360	C	5.9087450	-0.5966200	-1.7547560
H	-0.0362560	-0.8350790	-1.7108960	H	6.3617050	1.1498700	2.3329120	H	6.9694990	-0.5972870	-2.0234220
Au	3.0988840	0.7906620	0.6174310	C	6.1813700	1.9095990	-0.7045130	H	5.5993020	-1.6139890	-1.5025100
P	5.4079080	0.5148180	0.2080790	H	7.2544880	1.7785580	-0.8741430	H	5.3198720	-0.2524840	-2.6087440
C	6.1342610	1.7941900	-0.8945660	H	5.6758410	2.0334240	-1.6656830	TS₅₋₆			
H	5.9859680	2.7839550	-0.4553330	H	6.0173200	2.8082900	-0.1044150	C	2.3954630	1.9061200	-0.1261840
H	7.2053210	1.6160610	-1.0319080	C	5.9722860	-0.9855070	-0.8702670	C	2.3622220	0.5851320	0.1706150
H	5.6358420	1.7648120	-1.8668990	H	7.0553700	-0.9941560	-1.0274970	C	1.3092030	-0.22322600	0.7704120
C	6.4414370	0.5795750	1.7273430	H	5.6726760	-1.9139240	-0.3772720	C	3.2273450	-1.4077830	-0.5331910
H	7.4985510	0.4504040	1.4757930	H	5.4675870	-0.9237210	-1.8377170	C	4.3689640	-2.1894430	-1.0919770
H	6.3029100	1.5438700	2.2231500	5				H	5.2265910	-2.1230420	-0.4173630
H	6.1335540	-0.21354302	0.4136750	C	0.4092080	-1.44847600	0.8221820	H	4.0747990	-3.2280880	-1.2352900
C	5.8658430	-1.0794250	-0.5858330	C	0.3602450	-0.07653501	0.0627770	H	4.6649290	-1.7528840	-2.0515920
H	5.3610490	-1.1667220	-1.5515310	C	1.4088540	0.8592160	1.0069640	O	2.0635750	-1.8045620	-0.4322750
H	6.9485080	-1.1318940	-0.7386870	C	-1.78615500	0.8884730	0.6276230	O	3.5373700	-0.1728920	-0.1159280
H	5.5514680	-1.91057300	0.0506730	C	-3.05486101	0.3248820	1.3025900	C	1.2435890	2.8313770	0.1443340
TS₄₋₅				H	-2.83480802	0.1014260	2.0414810	H	1.4616020	3.4499800	1.0242550
C	0.3215420	-1.44834600	0.4427470	H	-3.75191101	0.7079570	0.5582450	C	3.6357600	2.5650300	-0.6650120
C	0.2119450	-0.09492200	0.9385830	H	-3.50273200	0.4812270	1.8360820	H	4.4712950	1.8777980	-0.7893120
C	1.1605030	0.8642880	1.0674260	O	-1.53756200	0.9562080	-0.5577330	H	3.4050770	3.0209250	-1.6362960
C	-1.9971680	-0.33337200	0.4114140	O	-0.89682700	0.3812260	1.5396130	H	3.9432760	3.3827670	-0.0023510
C	-3.40278000	0.1560090	0.5018600	C	1.0821620	2.2555920	1.4292320	H	1.1138460	3.5151310	-0.7015530
H	-3.44150601	0.1856240	0.1300060	H	1.9649230	2.8028340	1.7626000	H	0.3048650	2.3045930	0.3293510
H	-4.0588820	-0.4741950	-0.0967900	H	0.7192270	2.7760550	0.5260770	Au	-0.6867970	-0.09749000	0.2393550
H	-3.72416600	0.1666570	1.5463440	H	0.2849130	2.3186360	2.1759440	P	-2.9726790	-0.0594320	-0.3599010

C	-3.4322690-1.3775980-1.5536340	H	-5.09031500.1827170 0.6884450	C	1.6642390 -0.73869302.1165810
H	-2.8536850-1.2591050-2.4732000	H	-3.9349270-0.74093301.6864510	H	1.0796290 -1.62231202.3824440
H	-3.2082650-2.3561940-1.1216300	C	-3.30561801.4785130 -1.4238570	H	2.7198910 -0.93336702.3427920
H	-4.4998370-1.3204020-1.7869240	H	-4.37023101.4766970 -1.6775210	H	1.3245010 0.0973090 2.7327160
C	-4.1120890-0.29645701.0612820	H	-3.06380802.3993240 -0.8868010	Species with R ¹ = R ² = Me, R ³ = Cl:	
H	-3.95793400.5018200 1.7914860	H	-2.71532601.4438650 -2.3431650		
H	-5.1521550-0.28084900.7212770	C	1.6860640 -0.11254402.2994190	1	
H	-3.9028800-1.25596101.5409380	H	1.0847780 -0.82866202.8652130	C	0.0140660 -1.87420100.9511100
C	-3.52216401.5055490 -1.1487630	H	2.7465120 -0.25708602.5456320	C	0.8696640 -1.26000002.0138930
H	-4.58264401.4457630 -1.4123380	H	1.3957980 0.8920400 2.6183630	C	1.3016910 -0.94334703.1307210
H	-3.36814002.3380690 -0.4574430	TS₆₋₃		C	0.1298790 -0.0163890-0.6691070
H	-2.93453801.6856960 -2.0524660			C	-0.76523400.8596890 -1.5020110
C	1.6472960 -0.94276702.0416900	C	2.3236550 2.0192050 -0.1225570	H	-0.16019301.5686760 -2.0662020
H	1.0673580 -1.86144502.1524980	C	2.1478240 0.7457420 0.1565660	H	-1.34805200.2405960 -2.1915400
H	2.7129380 -1.14193502.1927690	C	1.4655300 -0.39718000.6342620	H	-1.47618801.3912970 -0.8629120
H	1.3131280 -0.26545902.8428270	C	3.2140700 -1.3925660-0.5081920	O	-0.5984580-0.84309300.1189270
6		C	3.8903050 -2.5875000-1.0922060	O	1.3492760 0.0042150 -0.6862770
		H	4.3293960 -3.1683840-0.2733180	C	0.7732690 -2.89863700.0977770
C	2.5925730 1.8218040 -0.3106380	H	3.1649060 -3.2178220-1.6089190	H	1.1304750 -3.71293500.7341480
C	2.3794220 0.5241230 -0.0709400	H	4.6877200 -2.2751040-1.7665580	C	-1.1868750-2.52193001.6645200
C	1.4217010 -0.25106700.8020900	O	1.9407900 -1.5518860-0.1618950	H	-0.8464610-3.31681302.3324340
C	2.8273640 -1.6364150-0.3964300	O	3.7647670 -0.2955770-0.3236040	H	-1.7444150-1.77950002.2396270
C	3.4579600 -2.8411500-0.9744230	C	1.1413650 2.9658210 -0.2195600	H	-1.8503890-2.95258800.9101690
H	4.5424150 -2.7123230-0.9987820	H	1.2052360 3.7070380 0.5847940	H	0.0857930 -3.3174750-0.6423190
H	3.1835570 -3.7216940-0.3950800	C	3.6791630 2.6476200 -0.3504470	H	1.6220000 -2.4499990-0.4178100
H	3.1079320 -2.9582310-2.0064290	H	4.4951100 1.9343980 -0.2575830	Au	2.9079120 -0.27834601.6519730
O	1.8791570 -1.68411500.4531230	H	3.7050660 3.0995070 -1.3484080	P	4.9001380 0.6447410 0.8501020
O	3.1974200 -0.4484450-0.7572780	H	3.8240670 3.4552870 0.3757650	C	6.4186370 -0.02625601.6294030
C	1.7340640 2.8720770 0.3478980	H	1.1916070 3.5036150 -1.1727740	H	6.4648920 -1.10831701.4827170
H	2.2907420 3.3919510 1.1376800	H	0.1825220 2.4501950 -0.1478190	H	7.3052320 0.4354110 1.1831890
C	3.6733900 2.3202810 -1.2351830	Au	-0.6406320-0.14117100.1740970	H	6.4084910 0.1797790 2.7027350
H	4.2906360 1.5189010 -1.6434680	P	-2.9364120-0.0359950-0.2702690	C	4.9904420 2.4636180 1.0702420
H	3.2269150 2.8738200 -2.0708880	C	-3.5766270-1.5191130-1.1414840	H	5.9263100 2.8461730 0.6505680
H	4.3268820 3.0229730 -0.7039320	H	-3.0587190-1.6353970-2.0967640	H	4.1478820 2.9394670 0.5621060
H	1.4425240 3.6288590 -0.3897800	H	-3.3969530-2.4088260-0.5329270	H	4.9450740 2.7143290 2.1330930
H	0.8237580 2.4578920 0.7896260	H	-4.6508450-1.4134010-1.3214540	C	5.0833400 0.3523380 -0.9510440
Au	-0.6257800-0.10902800.2448110	C	-3.97359800.1156740 1.2366600	H	5.9820000 0.8537780 -1.3240050
P	-2.89535000.0267290 -0.3742100	H	-5.03239600.1497590 0.9616110	H	5.1640430 -0.7202020-1.1459190
C	-3.4798730-1.4236780-1.3397560	H	-3.7968550-0.74130001.8913320	H	4.2039240 0.7344230 -1.4754310
H	-2.8960550-1.5111540-2.2596970	H	-3.70913901.0296510 1.7744080	Cl	1.4759900 -0.68729304.7555610
H	-3.3441420-2.3344330-0.7509090	C	-3.42490501.3828940 -1.3280800	TS₁₋₂	
H	-4.5386250-1.3107240-1.5923780	H	-4.50619801.3716070 -1.4962590		
C	-4.05681500.1359720 1.0454590	H	-3.14479502.3191540 -0.8390770	C	0.2102330 -0.98335400.2477260
H	-3.83616501.0314870 1.6318890	H	-2.90821301.3191390 -2.2888550	C	1.0832130 0.2455640 0.4435460

C	0.7341010	1.4572400	0.5822470	H	1.3546550	-1.7551930	-1.4077810	C	6.2440960	-1.7245220	-0.1513060
C	-1.76565900	0.2332210	1.1118520	C	0.4835240	-2.2985100	1.2098900	H	5.8381960	-2.0754490	-1.1033670
C	-3.06444700	0.0247030	1.8334420	H	1.5130400	-2.6418210	1.0795420	H	7.3337690	-1.6552410	-0.2252880
H	-3.49262300	0.9876490	2.1105970	H	0.3373750	-2.0349080	2.2603010	H	5.9789350	-2.4405260	0.6305330
H	-3.7573630	-0.5004250	1.1671520	H	-0.1939140	-3.1136920	0.9406070	C	6.3883290	0.4472140	1.7882840
H	-2.9129540	-0.5998380	2.7169450	H	-0.3542310	-2.2387010	-1.4281230	H	7.4728200	0.4231540	1.6443010
O	-1.0352730	-0.8773550	1.0364240	H	0.1087310	-0.5537510	-1.7950510	H	6.0795450	1.4628670	2.0484790
O	-1.4186170	1.3183930	0.6370230	Au	3.1263370	0.0502240	0.5073980	H	6.1168170	-0.2235070	2.6071770
C	-0.1731510	-1.1223530	-1.2311240	P	5.4637560	-0.0140450	0.2997320	C	6.1702300	1.0428610	-1.0559420
H	0.7314220	-1.2512610	-1.8312770	C	6.1369630	-1.6681010	-0.1324200	H	5.8467750	2.0660940	-0.8497560
C	0.8609790	-2.2513970	0.7966160	H	5.7155680	-1.9981480	-1.0853550	H	7.2637380	1.0063260	-1.0848130
H	1.7744420	-2.4676070	0.2367970	H	7.2273150	-1.6231790	-0.2153860	H	5.7717280	0.7372420	-2.0265780
H	1.1149460	-2.1319230	1.8527070	H	5.8630700	-2.3902630	0.6409340	Cl	1.1631800	2.6654580	1.2858180
H	0.1722810	-3.0933480	0.6884780	C	6.3539920	0.4651170	1.8339240				
H	-0.8089410	-2.0025630	-1.3609710	H	7.4357630	0.4166350	1.6763880	3			
H	-0.7020290	-0.2361110	-1.5883290	H	6.0746630	1.4833440	2.1166780	C	0.6131020	-1.6546400	-0.0838830
Au	3.2283290	0.1881600	0.3614450	H	6.0760620	-0.2121630	2.6454670	C	0.9760000	-0.4608080	0.4823480
P	5.5519640	-0.0049550	0.2597120	C	6.1268970	1.1086830	-0.9948230	C	0.6371910	0.6902950	1.0321870
C	6.4019740	1.5916470	-0.0483420	H	5.8393420	2.1387210	-0.7694550	C	-1.8049670	0.5380550	1.0606740
H	7.4843370	1.4356120	-0.0888910	H	7.2182640	1.0377270	-1.0361120	C	-2.9513020	1.3897930	1.5210310
H	6.0604990	2.0133830	-0.9967430	H	5.7095380	0.8336870	-1.9668710	H	-2.9058120	2.3723680	1.0430780
H	6.1662270	2.2933510	0.7553530	Cl	1.0533980	2.7018480	1.6695780	H	-3.8895440	0.8940360	1.2747670
C	6.2977950	-0.6583220	1.8031530					H	-2.8844380	1.5444340	2.6024530
H	5.8976720	-1.6535260	2.0116770	TS₂₋₃				O	-1.8712140	-0.5562270	0.5528860
H	7.3853060	-0.7190290	1.6967310	C	0.5362500	-1.2705820	0.3485660	O	-0.6132000	1.1958750	1.3091760
H	6.0519080	0.0027010	2.6378360	C	1.0898100	0.0152850	0.6282270	C	0.3134400	-1.7628970	-1.5540050
C	6.1318550	-1.1261520	-1.0713990	C	0.4287240	1.1173350	0.9585280	H	0.7878870	-2.6448180	-1.9939430
H	5.7778160	-0.7608760	-2.0384730	C	-1.8256650	0.2702720	0.9595480	C	0.3835840	-2.8838950	0.7519490
H	7.2254570	-1.1657600	-1.0769190	C	-3.2371850	0.6983150	1.2003650	H	0.8718450	-3.7598780	0.3151810
H	5.7337210	-2.1301370	-0.9053670	H	-3.4830900	1.5389160	0.5450530	H	0.7039850	-2.7516610	1.7852800
Cl	0.8516640	3.0773490	0.7843130	H	-3.9107800	-0.1369790	1.0140900	H	-0.6987320	-3.0695060	0.7378730
				H	-3.3408350	1.0405820	2.2347460	H	-0.7733960	-1.8976200	-1.6375550
2				O	-1.4932480	-0.8731670	0.6550090	H	0.5996510	-0.8675500	-2.1057790
C	0.2486430	-1.0958730	0.3039180	O	-0.9514780	1.2809830	1.1164660	Au	3.0553830	-1.0554690	0.1555980
C	1.0439400	0.1166850	0.6968310	C	0.3719460	-1.7064200	-1.0783240	P	5.3651440	-1.4044070	-0.0531930
C	0.4003960	1.1838750	1.1505680	H	1.3059260	-2.1858400	-1.3964950	C	5.7882040	-3.0116610	-0.8283300
C	-1.7634730	0.2586240	0.9602610	C	0.6192110	-2.3492430	1.3886450	H	5.3631570	-3.0576710	-1.8338000
C	-3.2273040	0.3956530	1.1611460	H	1.5722120	-2.8752190	1.2534310	H	6.8754530	-3.1206660	-0.8877680
H	-3.5094800	1.4478610	1.1899070	H	0.5896320	-1.9425120	2.4003000	H	5.3743010	-3.8272320	-0.2306370
H	-3.7593870	-0.1364310	0.3711150	H	-0.1828040	-3.0765940	1.2440170	C	6.2344000	-1.3887120	1.5607960
H	-3.4848130	-0.0685780	2.1207860	H	-0.4239950	-2.4505270	-1.1559760	H	7.3053180	-1.5543620	1.4095480
O	-1.2942620	-0.8241170	0.4966310	H	0.1740810	-0.8630290	-1.7412100	H	6.0820400	-0.4235150	2.0498590
O	-1.0235250	1.2703800	1.2959880	Au	3.2013270	-0.0685360	0.4367920	H	5.8325950	-2.1771100	2.2017460
C	0.3366730	-1.4281160	-1.1805250	P	5.5352890	-0.0794210	0.2505390	C	6.1928100	-0.1257640	-1.0738350

H	6.0385510	0.8578690	-0.6236920	C	-1.9977850	-0.53834300	0.9456300	C	-0.2560480	-2.47162601	0.4874610
H	7.2657000	-0.3324080	-1.1347980	C	-3.4477160	-0.51960001	0.2147880	H	0.6226970	-2.79682802	0.0638830
H	5.7656540	-0.1250690	-2.0795980	H	-3.9739450	-1.09475000	0.4518810	H	-0.9959990	-2.09436002	0.1931490
Cl	1.8150820	1.8777190	1.5520110	H	-3.6205890	-0.99550502	0.1879560	H	-0.6416660	-3.34686000	0.9602050
TS₁₋₄				H	-3.80839900	0.5082820	1.2571730	H	0.6858510	-2.7522440	-1.0624520
C	0.3477740	-1.23067701	0.0382950	O	-1.4079950	-1.54015900	0.4018490	H	1.4042260	-1.1238410	-1.2622700
C	0.7246880	0.2030880	0.9860720	O	-1.23435600	0.4511800	1.2676590	Au	3.1841130	0.6118810	0.5074320
C	1.3595810	1.2889930	0.9181970	C	0.4255240	-1.3036090	-1.1870680	P	5.4965370	0.3896670	0.1327950
C	-1.8450910	-0.36993200	0.6943700	H	1.4877290	-1.0715240	-1.3036030	C	5.9313350	-0.7697770	-1.2240510
C	-3.2405880	-0.64072500	0.2220030	C	0.7843890	-2.33840101	0.1158780	H	7.0175370	-0.8184450	-1.3476400
H	-3.2243820	-1.0562230	-0.7883310	H	1.8595790	-2.13874001	0.0998180	H	5.5495520	-1.7670640	-0.9915540
H	-3.7002070	-1.38367800	0.8823080	H	0.4467120	-2.32804702	0.1547300	H	5.4769120	-0.4285180	-2.1576070
H	-3.82314900	0.2792860	0.2495770	H	0.6018470	-3.32413500	0.6801890	C	6.4200890	-0.22599001	0.5962680
O	-0.9880520	-1.37087400	0.4404140	H	0.2355390	-2.3020150	-1.5896710	H	7.4877130	-0.30022201	0.3682200
O	-1.46913100	0.6475050	1.2669310	H	-0.1532290	-0.5660740	-1.7477970	H	6.2758850	0.4610070	0.24338320
C	1.2592730	-2.09837600	0.1584800	Au	3.1412490	0.6834190	0.7092090	H	6.0415130	-1.21088701	0.8815240
H	2.2714370	-2.11568400	0.5675620	P	5.4349610	0.4299570	0.2569800	C	6.3202900	1.9685580	-0.3166920
C	0.2853810	-1.73986702	0.4864590	C	5.8597290	-1.0486560	-0.7479160	H	6.1754460	2.6989050	0.4833700
H	1.2813390	-1.69405202	0.9341570	H	6.9411260	-1.1010680	-0.9084520	H	7.3915860	1.8065210	-0.4702630
H	-0.3967830	-1.13663803	0.0886810	H	5.5281970	-1.9520370	-0.2296750	H	5.8781920	2.3627260	-1.2351830
H	-0.0548100	-2.77857202	0.4842690	H	5.3538000	-0.9932470	-1.7150430	Cl	0.7211310	2.4915780	1.4264920
H	0.8621940	-3.11663100	0.1556350	C	6.4727350	0.2793830	1.7656750	5			
H	1.2873330	-1.7194180	-0.8648760	H	7.5279440	0.1823070	1.4921280	C	0.3700580	-1.44032500	0.8382660
Au	3.3817350	0.6912590	0.4862090	H	6.3410050	1.1664530	2.3902190	C	0.3334530	-0.06141101	0.0571410
P	5.6589250	0.3611130	0.0800230	H	6.1646960	-0.59983502	0.3374480	C	1.4258660	0.8175560	0.9311750
C	6.6672930	0.3798940	1.6116950	C	6.1557380	1.8460180	-0.6659240	C	-1.79944300	0.9220610	0.6419650
H	7.7213700	0.2193240	1.3658750	H	6.0143380	2.7660210	-0.0928750	C	-3.00532301	0.4664520	1.3477040
H	6.5541270	1.3435670	2.1144100	H	7.2248520	1.6858290	-0.8355050	H	-2.71024702	0.3122800	1.9764070
H	6.3276170	-0.41157802	0.2842230	H	5.6482530	1.9519090	-1.6282020	H	-3.74251101	0.7895330	0.6137430
C	6.3853610	1.6472810	-1.0058270	Cl	0.7148040	2.5259310	1.9005310	H	-3.43445800	0.7026830	2.0025540
H	7.4520300	1.4520500	-1.1527250	TS₄₋₅				O	-1.60589400	0.8836780	-0.5522670
H	5.8781930	1.6387800	-1.9736620	C	0.2467910	-1.43453300	0.5332410	O	-0.87914400	0.4412880	1.5507810
H	6.2567430	2.6307570	-0.5477150	C	0.1567910	-0.03557600	0.8906610	C	1.5374830	-2.21383800	0.3445740
C	6.0352350	-1.2380130	-0.7349870	C	1.1663980	0.8740240	0.8856140	H	1.8711240	-2.88452401	0.1486320
H	7.1143070	-1.3279370	-0.8940280	C	-2.0487930	-0.24921400	0.3976290	C	-0.8625750	-2.23966901	0.1020040
H	5.6928950	-2.0622300	-0.1048730	C	-3.43446800	0.2912590	0.4709890	H	-1.3900180	-1.89691201	0.9950730
H	5.5211930	-1.2896960	-1.6977480	H	-3.44195701	0.3034920	0.0532500	H	-1.5517220	-2.10410800	0.2546430
Cl	1.0513450	2.9489700	1.1064460	H	-4.1145530	-0.3467040	-0.0911030	H	-0.6354290	-3.30405301	0.1754880
4				H	-3.74555800	0.3613530	1.5166890	H	1.2003500	-2.8674110	-0.4696080
C	0.0872070	-1.26010000	0.2971110	O	-1.6629610	-1.1579330	-0.3425770	H	2.3789250	-1.61063300	0.0097270
C	0.1273280	0.1313960	0.9170330	O	-1.16524900	0.3335450	1.2322940	Au	3.3953360	0.5829670	0.3561140
C	1.1360170	0.9747600	1.1405830	C	1.1533910	-1.9065180	-0.5490900	P	5.6498490	0.4499020	-0.3125910
				H	2.0750560	-2.2899050	-0.0923460	C	6.7517890	-0.30672000	0.9452230

H	7.7812860	-0.32991100	5.748710	H	-3.42115702	3.757560	-0.5250650	C	3.8098290	-2.4877360	-1.4156550
H	6.7117010	0.2767250	1.8683540	H	-3.05794701	1.6567780	-2.1096330	H	4.0662690	-3.2019350	-0.6251500
H	6.4203050	-1.32606201	1.577340	Cl	1.6902500	-1.14734901	1.9906670	H	3.0947630	-2.9701030	-2.0852730
C	6.3943630	2.0856630	-0.6817130					H	4.7144910	-2.2004710	-1.9497610
H	7.4404780	1.9638070	-0.9782710	6				O	1.8854940	-1.4480780	-0.4395370
H	5.8406930	2.5649490	-1.4928590	C	2.4403670	1.9366540	-0.3057510	O	3.7474710	-0.2237670	-0.5467910
H	6.3408860	2.7220040	0.2049950	C	2.3347990	0.6067140	-0.1933720	C	1.0553660	3.0728150	-0.1246300
C	5.9038660	-0.5470420	-1.8324830	C	1.3536190	-0.31693100	4.523030	H	1.1916570	3.7938770	0.6883980
H	6.9651900	-0.5638010	-2.0980430	C	2.9737550	-1.4594450	-0.6838280	C	3.5925190	2.7563100	-0.3251350
H	5.5571670	-1.5694390	-1.6627710	C	3.7466500	-2.5690080	-1.2699510	H	4.3981960	2.0270350	-0.3558440
H	5.3316030	-0.1125880	-2.6559630	H	4.8031310	-2.3024940	-1.3151500	H	3.5858810	3.3375330	-1.2533040
Cl	1.0586170	2.4559060	1.3552200	H	3.5915410	-3.4780580	-0.6881610	H	3.7684640	3.4567350	0.4987030
				H	3.3854900	-2.7404770	-2.2915260	H	1.0458210	3.6293820	-1.0679260
TS₅₋₆				O	1.8610900	-1.6371490	-0.0607420	H	0.1007540	2.5627900	0.0056250
C	2.3523560	1.9936900	-0.0640790	O	3.3477450	-0.2296710	-0.7895470	Au	-0.7130350	-0.12094400	0.0689750
C	2.3300740	0.6473550	0.0796340	C	1.4108610	2.8449360	0.3078070	P	-3.0239510	-0.0326100	-0.2467220
C	1.2514950	-0.19339400	5.812730	H	1.8435040	3.3653900	1.1711830	C	-3.6855540	-1.5218040	-1.0882120
C	3.1427360	-1.2595140	-0.8599080	C	3.5900170	2.6014170	-1.0119260	H	-3.2176870	-1.6263250	-2.0701500
C	4.2619670	-2.0033750	-1.5041510	H	4.3110850	1.8944710	-1.4226100	H	-3.4607590	-2.4103240	-0.4932280
H	5.0585160	-2.1587360	-0.7700710	H	3.2074940	3.2280310	-1.8262300	H	-4.7692210	-1.4303890	-1.2097230
H	3.9044260	-2.9608470	-1.8791910	H	4.1120770	3.2698740	-0.3170130	C	-3.97313300	1.039600	1.3170090
H	4.6743160	-1.4051170	-2.3220990	H	1.1152840	3.6122540	-0.4162540	H	-5.04579000	1.276360	1.1013070
O	1.9699860	-1.6380360	-0.7860720	H	0.5182810	2.3126710	0.6442400	H	-3.7509960	-0.75335801	1.9570270
O	3.4798190	-0.0841700	-0.3095700	Au	-0.7196590	-0.14363600	0.0919580	H	-3.68807301	0.0189160	1.8418850
C	1.2159450	2.8811380	0.3536410	P	-3.02376700	0.0253040	-0.3088220	C	-3.57095901	1.3862420	-1.2728540
H	1.4901210	3.4158890	1.2719380	C	-3.6900940	-1.3338780	-1.3482170	H	-4.65847901	1.3631980	-1.3914610
C	3.5729180	2.7040230	-0.5783720	H	-3.1858760	-1.3347150	-2.3178740	H	-3.27905002	3.226030	-0.7912320
H	4.3955880	2.0324080	-0.8184850	H	-3.5083040	-2.2930910	-0.8570250	H	-3.09791201	3.324030	-2.2563150
H	3.3021440	3.2713630	-1.4775400	H	-4.7658780	-1.2024110	-1.4996280	Cl	1.6957140	-0.85675502	1.282760
H	3.9144050	3.4367810	0.1621310	C	-4.0372550	-0.00698901	2.219290				
H	1.0403060	3.6396380	-0.4165550	H	-3.75223400	0.8273810	1.8676340	Species with R ¹ = R ² = Me, R ³ =			
H	0.2875710	2.3401260	0.5438160	H	-5.09999000	0.0733620	0.9741840	CO ₂ Me:			
Au	-0.7599990	-0.07860600	1.516010	H	-3.8597510	-0.94241301	1.7584840	1			
P	-3.0607570	-0.0229290	-0.3526290	C	-3.52101201	1.5674840	-1.1732980	C	0.4901350	-0.7107860	-0.3086180
C	-3.5756060	-1.3763870	-1.4807750	H	-4.60496901	1.5833100	-1.3230370	C	0.9335590	0.1867200	0.7979660
H	-3.0235710	-1.2995740	-2.4207840	H	-3.22581102	4.345240	-0.5769720	C	1.0249610	0.9109170	1.7948570
H	-3.3539980	-2.3421250	-1.0199620	H	-3.02106601	1.6218930	-2.1436440	C	-1.47926500	0.6796120	-0.7760600
H	-4.6487120	-1.3079910	-1.6831310	Cl	1.7096840	-0.42664802	2.808950	C	-2.96799400	5.799870	-0.9675040
C	-4.1393760	-0.18963401	1.227850					H	-3.37780601	1.5726000	-1.1516530
H	-3.94211000	0.6321900	1.8155620	TS₆₋₃				H	-3.1879850	-0.0748740	-1.8163350
H	-5.1916600	-0.16767100	0.8235070	C	2.2362630	2.1211860	-0.1325380	H	-3.43306200	1.393000	-0.0811640
H	-3.9255510	-1.13492301	0.6277970	C	2.0603720	0.8289340	0.0268050	O	-0.9517650	-0.5373530	-0.4620040
C	-3.61265601	1.5205810	-1.1779250	C	1.4199160	-0.36671700	3.654370	O	-0.81212301	1.6900890	-0.8749310
H	-4.68318801	1.4655420	-1.3982480	C	3.1886870	-1.2925060	-0.7805370	C	1.2202300	-0.4452260	-1.6331780

H	2.2705770	-0.7327730	-1.5400700	H	1.0299530	-1.8719230	-1.0421110	H	0.1170580	-1.7374200	-0.9566880			
C	0.6436340	-2.17578600	1.319580	H	0.2807280	-1.0738260	-2.4449880	Au	3.1637480	0.0963520	0.5183920			
H	1.6988790	-2.41363900	2.846200	H	-0.29834901	3.798720	-2.3504610	P	5.4955440	-0.07461400	3.137010			
H	0.0942680	-2.36246101	0.0571830	H	-0.08865302	3.074070	-0.8404560	C	0.8864250	2.6605720	0.1597180			
H	0.2458740	-2.8186000	-0.6572010	Au	3.4584830	0.1958230	0.4830600	O	2.0662690	2.8994060	-0.0363790			
H	0.7603230	-1.0662430	-2.4064830	P	5.7625510	-0.07349800	2.366010	C	6.4183820	1.1603220	1.3132640			
H	1.1597020	0.6023570	-1.9256870	C	1.2987610	1.1922210	3.0740330	H	6.1850450	1.0224650	2.3721310			
Au	3.1793710	0.3202180	1.3714490	O	2.4501230	1.2458970	3.4739640	H	7.4959270	1.0439150	1.1618050			
P	5.5006520	0.0887830	1.4713090	C	6.3609640	-1.72479500	7.646990	H	6.1177150	2.1682470	1.0164480			
C	0.7674440	1.8403810	2.9007700	H	7.4442120	-1.79235400	6.257170	C	6.1799810	-1.69902300	8.321280			
O	1.6371210	2.3849300	3.5528600	H	6.1193670	-1.88224301	8.185260	H	5.7393560	-2.49303000	2.237630			
C	6.1746820	-0.91180700	0.915700	H	5.8709080	-2.49958500	1.700040	H	7.2673480	-1.71091400	7.094310			
H	7.2610670	-0.99442500	1.948890	C	6.7328820	1.1407820	1.2100960	H	5.9326630	-1.88257001	1.8807000			
H	5.7327270	-1.91084200	1.096630	H	6.5097840	1.0199430	2.2727970	C	6.1131650	0.1608150	-1.4007660			
H	5.9361490	-0.4338530	-0.8613530	H	7.8033860	0.9870310	1.0425390	H	7.2037460	0.0713290	-1.4263960			
C	6.0687350	-0.73141903	0.073590	H	6.4600730	2.1538800	0.9051020	H	5.6728670	-0.5952570	-2.0557450			
H	7.1601440	-0.80829103	0.011450	C	6.3343990	0.1222620	-1.4948280	H	5.8220200	1.1502350	-1.7622060			
H	5.7504770	-0.14903603	8.751620	H	7.4192490	-0.0126000	-1.5457260	O	-0.08898403	5.731310	0.0555290			
H	5.6334050	-1.73147803	0.720820	H	5.8472150	-0.6214880	-2.1299220	C	0.3242300	4.9104100	-0.3131990			
C	6.3758470	1.6963860	1.4034210	H	6.0765400	1.1206720	-1.8563880	H	-0.59451605	4.934530	-0.3430740			
H	6.0619710	2.3203280	2.2435580	O	0.2124770	1.4471200	3.7824640	H	1.0122590	5.3097290	0.4344470			
H	7.4561820	1.5309750	1.4563850	C	0.4307380	1.8341240	5.1668150	H	0.8064960	4.8975310	-1.2925380			
H	6.1311840	2.2090570	0.4701110	H	1.0245130	2.7487560	5.2061520	TS ₂₋₃						
O	-0.54655001	1.9863520	3.0659590	H	-0.56640101	9.995010	5.5688170							
C	-0.96443002	8.944470	4.1222140	H	0.9391000	1.0296380	5.7006580							
H	-0.58198103	8.961460	3.9201210	2										
H	-2.05166802	8.781420	4.0902040				C	0.3777390	-1.07222801	0.0969750	C	0.4236090	1.2251750	0.6187350
H	-0.59573802	5.355720	5.0845170				C	1.0827540	0.1964140	0.7235100	C	-1.77804200	2.429210	0.8664730
TS ₁₋₂			C	0.3736540	1.3169570	0.5407700	H	-3.52385501	0.0649340	-0.0242030				
			C	-1.71229600	2.979130	1.0501380	H	-3.8282520	-0.26125201	1.1351010				
			C	-3.17653400	4.366230	1.2538920	H	-3.37555301	3.755440	1.7090530				
C	1.0388030	0.8059850	1.6836550	H	-3.57991301	1.858120	0.5713580	O	-1.3727170	-0.91801900	9.308400			
C	-1.59819800	2.779430	0.6731430	H	-3.6664030	-0.52752701	1.1188680	O	-0.97779701	3.040780	0.7243600			
C	-2.9958630	-0.26725300	7.320950	H	-3.34700100	7.782810	2.2819590	C	0.6147760	-2.1331040	-0.3924580			
H	-3.50772800	1.277420	1.6089190	O	-1.1637610	-0.83278501	2.457110	H	1.5722750	-2.6558800	-0.4993020			
H	-3.53748100	0.0168110	-0.1753720	O	-1.06148701	3.550450	0.7012330	C	0.7996120	-1.89674702	1.1559110			
H	-2.9663090	-1.36004500	7.723980	C	0.4456580	-2.13714800	0.0059420	H	1.7653710	-2.41161002	2.177280			
O	-0.8960100	-0.2480650	-0.3384670	H	1.4795060	-2.4765700	-0.0936050	H	0.7363360	-1.17434502	9.707300			
O	-1.15047001	1.1032540	1.4672750	C	0.7635630	-1.59404302	4.775670	H	0.0154160	-2.65090602	2.2547220			
C	0.3376090	1.5263580	-1.4731810	H	1.8060300	-1.92005202	4.551600	H	-0.1595450	-2.8876590	-0.2359280			
H	1.3283480	1.8470890	-1.8053870	H	0.6601150	-0.81388503	2.354320	H	0.4192450	-1.5721120	-1.3073440			
C	0.9645250	-0.9367050	-1.6035630	H	0.1327920	-2.44644702	7.445150	Au	3.2683360	0.0425480	0.4775030			
H	1.9558830	-0.6856830	-1.9881190	H	-0.1813300	-2.99070200	2.781570	P	5.5984190	-0.06979900	2.697150			

C	1.0190330	2.5877000	0.4570390	H	3.5441680	-1.8710910	-0.1601040	O	1.4536880	3.1681750	2.2047150
O	2.2188440	2.7871410	0.3514080	H	2.1991160	-2.37001200	0.9016970	C	6.1071360	-0.9097150	-1.1714110
C	6.2555630	-1.77736100	0.1120390	H	2.0406300	-2.5292530	-0.8616540	H	7.1868500	-1.0004980	-1.3246770
H	7.3464360	-1.75769700	0.0276230	C	2.6093070	0.7351010	1.1549990	H	5.7114580	-1.8600900	-0.8052110
H	5.9713850	-2.36259100	0.9900600	H	3.6913940	0.6882680	0.9996100	H	5.6248380	-0.6679630	-2.1214710
H	5.8327610	-2.2504960	-0.7777490	H	2.2822540	1.7770240	1.1179250	C	6.7194250	-0.03341501	0.5473360
C	6.4965660	0.6570660	1.6967430	H	2.3665010	0.3236840	2.1377750	H	7.7762260	-0.15509801	0.2897990
H	7.5770960	0.5896630	1.5365690	C	2.3380500	0.4692350	-1.7372560	H	6.6171050	0.7548830	2.2971940
H	6.2118930	1.7060100	1.8109510	H	2.0047300	1.5056960	-1.8300130	H	6.3377770	-0.96868401	0.9637170
H	6.2314110	0.1194910	2.6106260	H	3.4309800	0.4341740	-1.7779740	C	6.5657320	1.9215430	-0.6141820
C	6.2418590	0.8236460	-1.1995740	H	1.9256770	-0.1099750	-2.5669770	H	6.4507260	2.7416670	0.0984120
H	5.9541370	1.8763470	-1.1423830	O	-3.64615503	0.3879230	-0.1422690	H	7.6304380	1.7319450	-0.7805170
H	7.3328070	0.7476560	-1.2405700	C	-3.06853804	0.6976730	-0.3691890	H	6.0948790	2.2051190	-1.5585060
H	5.8144340	0.3916470	-2.1079200	H	-3.91645705	0.3792720	-0.3978440				
O	0.0994220	3.5570650	0.4420120	H	-2.39194204	0.9537630	0.4481060	4			
C	0.5955680	4.9086850	0.2895350	H	-2.52923704	0.7081560	-1.3180930	C	0.1005710	-1.32293100	0.1646580
H	-0.29138705	0.5395120	0.3013280					C	0.0931530	0.1215200	0.6438650
H	1.2605090	5.1594050	1.1182250	TS₁₋₄				C	1.0285120	1.0375610	0.8416760
H	1.1287800	5.0074830	-0.6579360	C	0.3450490	-1.23701601	0.0627540	C	-2.0315710	-0.59884200	0.6238000
				C	0.7684630	0.1804140	0.9903970	C	-3.4959370	-0.60377200	0.8016910
3				C	1.4291750	1.2427350	0.9001940	H	-3.9565250	-1.25167900	0.0545560
C	-2.7199550	-1.43335100	0.4138370	C	-1.8224340	-0.32552600	0.7329990	H	-3.7181030	-1.01025201	0.7960030
C	-2.7694040	-0.07781400	0.2431310	C	-3.2285360	-0.55735400	0.2739000	H	-3.88546000	0.4123730	0.7406640
C	-3.47163501	0.0506580	0.1586920	H	-3.2340650	-1.0176760	-0.7166200	O	-1.3878380	-1.63127700	0.2112130
C	-5.75294000	0.1836500	0.4429160	H	-3.7159690	-1.24953700	0.9688900	O	-1.31355100	0.4359800	0.8928670
C	-7.14317400	0.7494440	0.5110700	H	-3.77236600	0.3864700	0.2634560	C	0.5299570	-1.4952040	-1.2866350
H	-7.36721201	0.3015380	-0.4065120	O	-0.9951050	-1.35187100	0.4773190	H	1.5910780	-1.2421120	-1.3625520
H	-7.8579500	-0.06213800	0.6425610	O	-1.40928000	0.6804500	1.2999930	C	0.7737500	-2.29936901	0.1209500
H	-7.21837701	0.4529320	1.3457280	C	1.2408520	-2.11898300	0.1790180	H	1.8454510	-2.08226901	0.1343350
O	-5.4509010	-0.98641500	0.5287690	H	2.2605310	-2.12984800	0.5689780	H	0.3867530	-2.19379402	0.1371710
O	-4.84816801	0.1981280	0.2658720	C	0.2891640	-1.73349502	0.5151470	H	0.6267490	-3.32683500	0.7779800
C	-2.8739760	-2.3755000	-0.7510890	H	1.2907130	-1.70656502	0.9516580	H	0.3903250	-2.5321770	-1.6026610
H	-2.1310090	-3.1765140	-0.7111070	H	-0.3731740	-1.11137603	0.1202240	H	-0.0317230	-0.8314070	-1.9479200
C	-2.6590870	-2.04487601	0.7887300	H	-0.0735050	-2.76441602	0.5237210	Au	3.0769440	0.7499300	0.5381990
H	-1.9267300	-2.85563801	0.8289440	H	0.8436250	-3.13684600	0.1998540	P	5.3888310	0.4929950	0.2099170
H	-2.4465550	-1.30955702	0.5648770	H	1.2496960	-1.7555830	-0.8503080	C	0.6293510	2.4067110	1.2708440
H	-3.6501520	-2.47940801	0.9748590	Au	3.4905390	0.7222140	0.4689040	O	0.3674470	3.3187890	0.5020080
H	-3.8662750	-2.8333480	-0.6475680	P	5.7611240	0.4140030	0.0489850	C	5.8560050	-0.9918000	-0.7661490
H	-2.8212270	-1.8639070	-1.7122430	C	1.1410700	2.6978620	0.9974560	H	6.9435480	-1.0469690	-0.8755560
Au	-0.5933290	-0.17174100	0.0641430	O	0.6892160	3.3452470	0.0757080	H	5.4991280	-1.8915920	-0.2586250
P	1.7458520	-0.2262100	-0.1469260	C	1.2077870	4.5831010	2.4266840	H	5.3956130	-0.9409390	-1.7560380
C	-2.79343902	0.3683950	-0.0728540	H	0.1445540	4.7982710	2.3091050	C	6.3498000	0.3448410	1.7688820
O	-1.58089402	0.4811280	-0.1859240	H	1.5294920	4.7669970	3.4497190	H	7.4164300	0.2385020	1.5480110
C	2.4554020	-1.9156260	-0.0583300	H	1.7925020	5.1759730	1.7212530	H	6.1940410	1.2369120	2.3806640

H	6.0077380	-0.52821402	3.303850	H	7.1185130	-0.9299690	-1.0095700	C	0.4781700	3.9561290	2.6060690
C	6.1597590	1.9023850	-0.6817910	H	5.7492120	-1.8796690	-0.3739630	H	0.5660530	3.9140010	3.6897090
H	5.9960530	2.8250420	-0.1190570	O	0.9263080	2.2150030	2.8340820	H	1.2160250	4.6393680	2.1823560
H	7.2348810	1.7357700	-0.7996940	C	0.6205050	3.5117100	3.4081100	H	-0.52806704	2.562410	2.3096320
H	5.6991540	2.0075300	-1.6673660	H	0.8272730	3.4075610	4.4716840				
C	0.3317300	3.8552040	3.1305450	H	1.2587020	4.2775740	2.9632140	TS₅₋₆			
H	-0.67449604	1.553000	2.8313050	H	-0.42963803	7.581210	3.2413640	C	-2.05684302	0.0338030	-0.9173310
H	0.3970840	3.7565120	4.2129390					C	-2.12223700	0.8532260	-0.2370840
H	1.0586240	4.5838030	2.7656010	5				C	-1.1601330	-0.1999630	-0.1279350
O	0.6389710	2.5395290	2.6094690	C	-0.0387510	-1.23132200	0.0112960	C	-3.01986300	0.0640860	1.7028500
				C	-0.06350100	1.465000	0.2873290	C	-4.15879300	0.0402660	2.6653680
TS₄₋₅				C	1.0340780	0.9776490	0.4628940	H	-5.0501470	-0.35204502	1.686130
C	0.3263950	-1.56892100	4.954260	C	-2.16421200	0.9840030	-0.4856880	H	-3.9025460	-0.56923503	5.305270
C	0.2061870	-0.19720900	0.9325020	C	-3.39971801	1.6943810	-0.0188810	H	-4.37744101	0.0648190	2.9841200
C	1.1682180	0.7480330	1.0000620	H	-4.10253701	1.7850060	-0.8462240	O	-1.8815290	-0.34865601	9.196500
C	-2.0258710	-0.38234000	4.664780	H	-3.85854301	1.1528760	0.8128380	O	-3.31231300	0.5968500	0.4973330
C	-3.40614600	1.579470	0.6244240	H	-3.12838602	0.6909220	0.3440170	C	-0.87660102	4.360150	-1.7460390
H	-3.41305001	2.068430	0.3095040	O	-1.88849400	0.6674520	-1.6210640	H	-1.10990502	2.2887850	-2.8084810
H	-4.1032150	-0.41590500	0.0157810	O	-1.32473300	0.7131410	0.5759580	C	-3.22672902	0.9718180	-0.9619740
H	-3.69650200	1.250130	1.6779640	C	-1.2861510	-2.03125000	0.1307190	H	-4.11004502	0.5903960	-0.4532770
O	-1.6640710	-1.2215130	-0.3579500	H	-1.7956600	-2.0016950	-0.8452240	H	-2.93091303	0.9210370	-0.4957380
O	-1.12068400	1.275480	1.3300900	C	1.1724550	-1.9803880	-0.4021710	H	-3.47844103	0.2040610	-2.0030380
C	1.2304080	-1.9446940	-0.6218590	H	0.8974310	-2.6840960	-1.1964660	H	-0.68085003	5.044710	-1.6089760
H	2.1004550	-2.4770210	-0.2164720	H	1.9997220	-1.3517360	-0.7267630	H	0.0258670	1.8654980	-1.5192670
C	-0.1785730	-2.67426001	1.3617740	H	1.5037890	-2.59808000	0.4451290	Au	0.8974740	-0.0254160	-0.0143810
H	0.6995880	-3.04906601	1.9086970	H	-1.0598390	-3.07861400	0.3412600	P	3.2400600	0.0880660	0.2399800
H	-0.9183360	-2.35311402	0.0941500	H	-1.9775740	-1.62643300	0.8716070	C	3.8137770	-0.59035801	1.8463340
H	-0.5628610	-3.50507900	0.7657850	Au	3.0743430	0.7033410	0.2896460	H	3.3605750	-0.02604502	0.6650930
H	0.7084390	-2.6621060	-1.2647630	P	5.4228470	0.5148280	0.1494200	H	3.5110870	-1.63684301	0.9309620
H	1.5609750	-1.0888610	-1.2071260	C	0.6974450	2.3826820	0.8436730	H	4.9034780	-0.51978101	0.9170590
Au	3.1991240	0.5817640	0.5802220	O	0.4579480	3.2168010	-0.0138480	C	4.1649420	-0.8508860	-1.0377620
P	5.5147710	0.4783390	0.1742580	O	0.7445510	2.5994840	2.1543000	H	3.9291750	-0.4526660	-2.0277550
C	0.7621290	2.0904480	1.5119800	C	6.2314190	0.3080800	1.7846920	H	5.2414150	-0.7657770	-0.8603820
O	0.3722450	2.9805370	0.7734970	H	7.3152050	0.2217860	1.6606710	H	3.8732700	-1.9034190	-1.0027370
C	6.5247240	0.3374030	1.7018520	H	6.0062100	1.1706410	2.4167250	C	3.9233590	1.7899680	0.1695030
H	7.5889060	0.3038000	1.4484260	H	5.8505170	-0.59356802	0.2706920	H	5.0086430	1.7646350	0.3071170
H	6.3335760	1.1978040	2.3480270	C	6.2197770	1.9881470	-0.6007120	H	3.6922210	2.2389990	-0.7996040
H	6.2515570	-0.57339002	2.406260	H	5.9879460	2.8735440	-0.0036800	H	3.4724080	2.3991200	0.9567940
C	6.1751760	1.9572790	-0.6908360	H	7.3045520	1.8508120	-0.6412220	C	-1.6171360	-1.6162790	-0.4019440
H	5.9787560	2.8502900	-0.0922310	H	5.8354910	2.1364620	-1.6129170	O	-2.1648940	-1.6517810	-1.6261320
H	7.2536330	1.8531900	-0.8443830	C	6.0046260	-0.9071920	-0.8544140	O	-1.4325120	-2.58584000	0.3054430
H	5.6801470	2.0675190	-1.6589020	H	7.0984330	-0.9269630	-0.8791320	C	-2.4773580	-2.9659630	-2.1583240
C	6.0341820	-0.9450890	-0.8636760	H	5.6355930	-1.8394530	-0.4196610	H	-3.2292260	-3.4501360	-1.5329770
H	5.5381120	-0.8919520	-1.8359790	H	5.6218110	-0.8181690	-1.8741340	H	-2.8649320	-2.7814180	-3.1583450

H	-1.5733730-3.5765980-2.1976500	C	2.0982090 2.1545570 0.5827810	C	-1.17935700.6981440 0.6798230	
6		C	1.9552650 0.9348300 0.1199100	C	-4.2664670-0.0398420-0.7492990	
		C	1.3530640 -0.3162420-0.1150840	C	-5.7126160-0.0787090-0.3277970	
	C	-2.26628300.1535860 2.0466360	C	2.9850540 -0.4042670-1.7209330	H	-6.21553000.8264240 -0.6672760
	C	-2.1731430-0.29994900.7932990	C	3.5864730 -1.0259270-2.9337080	H	-6.2025540-0.9589780-0.7547200
	C	-1.3142480-0.0146240-0.4094830	H	3.9652220 -2.0167220-2.6590410	H	-5.7830850-0.15821600.7610980
C	-2.6888030-1.7932180-0.7811130	H	2.8237470 -1.1580140-3.7037260	O	-3.6171020-1.1550120-0.3275740	
C	-3.3603470-2.9236780-1.4508430	H	4.4109320 -0.4151240-3.2996500	O	-3.73756400.8595220 -1.3743170	
H	-4.3286660-2.5743980-1.8277440	O	1.7340190 -0.7843660-1.4352380	C	-1.9973880-1.5027370-2.1592980	
H	-2.7549620-3.2748810-2.2854580	O	3.5515440 0.4102120 -0.9811010	H	-0.9739120-1.8277020-2.3639680	
H	-3.5448540-3.7256060-0.7328250	C	0.8959560 2.9235250 1.0990840	C	-1.9043550-2.72759400.0554620	
O	-1.7090060-1.1589680-1.3092180	H	1.0216330 3.1027450 2.1725420	H	-0.8596730-3.0053600-0.1041940	
O	-3.0611080-1.37035000.3804900	C	3.4237470 2.8739670 0.6608380	H	-2.0929940-2.65349401.1290940	
C	-1.33125201.2127480 2.5661810	H	4.2505670 2.2726980 0.2898090	H	-2.5465690-3.5047210-0.3670530	
H	-1.85103102.1749260 2.6474230	H	3.3625610 3.8039250 0.0849850	H	-2.6854550-2.2552260-2.5546740	
C	-3.3106400-0.34548603.0124710	H	3.6168460 3.1479490 1.7037030	H	-2.1750870-0.5516570-2.6600490	
H	-3.9887330-1.07841502.5743980	H	0.8553270 3.8966960 0.5982440	Au	0.8517490 -0.2867410-0.1865100	
H	-2.8231970-0.79877803.8842220	H	-0.04481002.3953600 0.9380880	P	3.1140570 -0.6315040-0.6162130	
H	-3.90484400.4975380 3.3848610	Au	-0.8257380-0.0525660-0.1246200	C	-1.03125301.8779920 1.4715580	
H	-0.98965400.9400670 3.5712540	P	-3.15223600.0759370 -0.2151570	C	-0.82580501.7758420 2.8641720	
H	-0.46082301.3590860 1.9224940	C	-3.9185810-1.4069090-0.9756210	C	-1.11951003.1487590 0.8635230	
Au	0.8137050 -0.1026260-0.1254570	H	-3.5525220-1.5240510-1.9984670	C	-0.71592502.9321470 3.6331890	
P	3.1375990 -0.22137900.1551080	H	-3.6485180-2.2958480-0.4003700	H	-0.75779100.7960760 3.3254740	
C	3.9642900 -1.3663970-1.0184020	H	-5.0076160-1.3000660-0.9893580	C	-1.00829604.2970370 1.6443240	
H	3.5742420 -2.3779770-0.8805430	C	-3.93702700.2379830 1.4350160	H	-1.27865503.2202590 -0.2071600	
H	3.7620040 -1.0488550-2.0444030	H	-5.02510800.2909540 1.3302570	C	-0.80626604.1907170 3.0258790	
H	5.0449430 -1.3679520-0.8455100	H	-3.6738890-0.62512002.0513640	H	-0.56094802.8539490 4.7045980	
C	3.9825700 1.3913400 -0.0810870	H	-3.57604401.1448600 1.9261230	H	-1.08007505.2743420 1.1776670	
H	5.0619410 1.2759290 0.0564050	C	-3.77179301.4972650 -1.1951550	H	-0.71995905.0889720 3.6297330	
H	3.7838780 1.7642870 -1.0889100	H	-4.86600301.4947430 -1.2073490	C	4.2124100 0.3146600 0.5063580	
H	3.6003390 2.1150200 0.6432160	H	-3.41602302.4317570 -0.7545660	H	5.2583800 0.1094730 0.2581260	
C	3.6597280 -0.79157201.8207940	H	-3.39834101.4255150 -2.2196110	H	4.0161490 1.3837500 0.3966510	
H	4.7517570 -0.82192101.8851300	C	1.6680430 -1.41626000.8940630	H	4.0203080 0.0232690 1.5416790	
H	3.2717920 -0.10835702.5804900	O	1.5146370 -0.98153002.1486570	C	3.6163070 -2.3849190-0.4351030	
H	3.2587290 -1.79071302.0088970	O	1.9927480 -2.54523200.5809770	H	3.0520620 -3.0037870-1.1369400	
C	-1.65487901.2343540 -1.1999440	C	1.7641440 -1.94577103.2014920	H	4.6861930 -2.4863960-0.6406290	
O	-1.69556302.3066920 -0.3995770	H	1.5842580 -1.40617404.1295090	H	3.4083360 -2.72371700.5825610	
O	-1.82469301.2645990 -2.4060110	H	1.0788000 -2.78995903.1052220	C	3.6083880 -0.1486090-2.3137610	
C	-1.92939303.5839470 -1.0409360	H	2.7969030 -2.29566103.1521850	H	4.6764620 -0.3369590-2.4588470	
H	-1.92075304.3139580 -0.2334520			H	3.0357370 -0.7281490-3.0417550	
H	-1.13475403.7935620 -1.7596720	Species with R ¹ = R ² = Me, R ³ = Ph:			H	3.4027650 0.9135030 -2.4666080
H	-2.89667703.5795370 -1.5467020	1				
TS ₆₋₃		C	-2.2041610-1.3926720-0.6419840	TS ₁₋₂		
		C	-1.3853490-0.3019190-0.0244270	C	0.2747980 -0.7312840-0.0687550	

C	1.1970750	0.2407460	0.6375460	C	-2.1291020	-1.3713040	-0.8569730	TS₂₋₃	
C	0.8470820	1.3241900	1.2351580	C	-1.3342380	-0.2929830	-0.1778580	C	1.2808270 -2.1235260 -0.0650110
C	-1.67523800	0.3400350	1.0169580	C	-1.94661600	0.7345300	0.4167690	C	1.1041610 -0.7152930 -0.0596370
C	-3.08376800	1.186250	1.4785120	C	-4.1356930	-0.0372530	-0.2020310	C	2.0127400 0.2671450 -0.0319130
H	-3.62732301	0.0638730	1.4651700	C	-5.61023300	0.1448910	-0.1568730	C	4.0109810 -1.1467260 -0.0068030
H	-3.5830040	-0.62705200	0.8580590	H	-5.85773701	0.2070980	-0.1704830	C	5.5046020 -1.04584700
H	-3.0544020	-0.25173202	0.5096890	H	-6.0784490	-0.3809150	-0.9890620	H	5.7970350 -0.49944600
O	-1.0921870	-0.73695700	0.5342450	H	-5.9789330	-0.28392400	0.7826110	H	5.9414510 -2.04374700
O	-1.11424101	0.4451650	1.1223580	O	-3.6627160	-1.0755810	-0.7665070	H	5.8719560 -0.4828560 -0.8015890
C	0.1031100	-0.3325310	-1.5392580	O	-3.40846500	0.8614340	0.3625660	O	3.4055630 -2.2141310 -0.1042680
H	1.0746360	-0.3702690	-2.0395780	C	-1.9001220	-1.4450020	-2.3637800	O	3.4177910 0.0491620 0.0383790
C	0.7155400	-2.18565100	0.0874170	H	-0.8715930	-1.7639970	-2.5500360	C	1.1587030 -2.90098801
H	1.6789220	-2.3310960	-0.4073840	C	-2.0128220	-2.7282490	-0.1680100	H	0.1187250 -3.23183001
H	0.8216760	-2.44844401	0.1430760	H	-0.9880920	-3.0928010	-0.2761020	C	1.1044220 -2.8917620 -1.3446010
H	-0.0218750	-2.8482080	-0.3736600	H	-2.2403980	-2.64833800	0.8981610	H	0.0613150 -3.2238190 -1.4083440
H	-0.5764170	-1.0307250	-2.0359670	H	-2.6924070	-3.4488090	-0.6320290	H	1.3307130 -2.2809840 -2.2194990
H	-0.29069100	0.6829810	-1.6282980	H	-2.5813160	-2.1712190	-2.8163580	H	1.7327900 -3.7855000 -1.3321780
Au	3.3063790	0.0105190	0.6004110	H	-2.0482730	-0.4681790	-2.8307880	H	1.7847030 -3.79545001
P	5.6255130	-0.29180300	0.5042990	Au	0.7499750	-0.4746320	-0.2679740	H	1.4225390 -2.29650302
C	1.1076440	2.5096860	2.0025100	P	3.0873040	-0.6748540	-0.4262690	Au	-0.9994980 -0.3960250 -0.0037780
C	1.3715490	2.4098820	3.3839010	C	-1.42409001	0.8828770	1.1831100	P	-3.3104950 -0.01576500
C	1.0992810	3.7746870	1.3800290	C	-0.37306001	0.7094600	2.1008120	C	1.7709130 1.7291700 -0.0565650
C	1.6436530	3.5594560	4.1239090	C	-1.97384103	0.1675810	1.0159200	C	0.8041870 2.2843430 -0.9120060
H	1.3695490	1.4342700	3.8591230	C	0.1347080	2.7989430	2.8116730	C	2.5200360 2.5872930 0.7691590
C	1.3649180	4.9187740	2.1292210	H	0.0335920	0.7170050	2.2649720	C	0.5689090 3.6614960 -0.9186200
H	0.8867960	3.8472090	0.3183090	C	-1.46537704	0.2539110	1.7303170	H	0.2543100 1.6376910 -1.5883830
C	1.6384440	4.8119930	3.4988370	H	-2.79208503	0.3189090	0.3191740	C	2.2824080 3.9628890 0.7610240
H	1.8555390	3.4807900	5.1855940	C	-0.40726404	0.0750010	2.6278540	H	3.2801620 2.1750390 1.4246880
H	1.3612500	5.8921020	1.6487710	H	0.9435310	2.6467800	3.5204190	C	1.3039750 4.5047770 -0.0799020
H	1.8469260	5.7059220	4.0790770	H	-1.89482305	0.2405540	1.5834280	H	-0.17629504
C	6.5591480	0.7008280	1.7352570	H	-0.01512204	0.9205920	3.1851600	H	2.8611590 4.6112780 1.4123100
H	7.6330270	0.5149560	1.6344560	C	4.0077340	0.1974200	0.9037400	H	1.1242000 5.5757780 -0.0889220
H	6.3592410	1.7634070	1.5766320	H	5.0857630	0.0668610	0.7678650	C	-3.82384201
H	6.2377850	0.4296370	2.7440060	H	3.7663530	1.2630920	0.8780790	H	-4.90665401
C	6.1512450	-2.02652600	0.7975000	H	3.7151890	-0.20470901	0.8770240	H	-3.31718502
H	5.7058170	-2.67738800	0.0409270	C	3.7031140	-2.4051110	-0.3527770	H	-3.54697301
H	7.2414430	-2.10555300	0.7467600	H	3.2724450	-2.9834280	-1.1741420	C	-4.3076140 -1.2473210 -0.8167330
H	5.8106360	-2.35060201	0.7840550	H	4.7946490	-2.4238460	-0.4306590	H	-4.1192480 -2.2460730 -0.4151150
C	6.3535450	0.1577160	-1.1205350	H	3.4010550	-2.86190300	0.5931510	H	-5.3732960 -1.0156900 -0.7258980
H	7.4355300	-0.0058340	-1.1112910	C	3.7876370	-0.0015740	-1.9865300	H	-4.0221980 -1.2324060 -1.8715330
H	5.9020980	-0.4543880	-1.9053940	H	4.8759120	-0.1171220	-1.9975220	C	-3.9825190 -0.05392001
H	6.1481770	1.2097360	-1.3340240	H	3.3590660	-0.5333650	-2.8397980	H	-5.05955800
				H	3.5358830	1.0584710	-2.0728920	H	-3.7969090 -1.03399202
								H	-3.48642000

2

3

C 0.7254270 -1.6197490-0.3598460
 C 1.1008110 -0.49278600.3198400
 C 0.7666150 0.6700880 0.8666180
 C -1.38208700.9674520 1.8647330
 C -2.74341001.5460050 1.5995170
 H -3.14925601.1597100 0.6610200
 H -3.40934701.3070660 2.4281870
 H -2.66012502.6336010 1.5017260
 O -0.99407100.4844280 2.9063520
 O -0.59046901.0510370 0.7458780
 C 0.5059620 -1.6076200-1.8525370
 H 0.9823580 -2.4674700-2.3326490
 C 0.3635490 -2.89173800.3670690
 H 0.8471980 -3.7618620-0.0870530
 H 0.6024860 -2.84538901.4295990
 H -0.7202370-3.03041300.2538770
 H -0.5758260-1.7034110-2.0188920
 H 0.8518410 -0.6836820-2.3161380
 Au 3.1487930 -1.22826600.0312100
 P 5.4316280 -1.7299460-0.1908510
 C 6.1748980 -2.44986801.3229920
 H 7.2372670 -2.65373201.1572510
 H 6.0667280 -1.74917402.1542980
 H 5.6622370 -3.38078901.5766270
 C 6.4541340 -0.2617550-0.5902890
 H 7.5020270 -0.5590190-0.6959320
 H 6.1072870 0.1847130 -1.5252160
 H 6.3655590 0.4779330 0.2090310
 C 5.7643130 -2.9396080-1.5288380
 H 6.8401250 -3.1246920-1.6038710
 H 5.2487510 -3.8782220-1.3118030
 H 5.3972450 -2.5450610-2.4792600
 C 1.6453660 1.6656010 1.5152920
 C 1.4149130 3.0384530 1.3162000
 C 2.7112640 1.2642330 2.3387320
 C 2.2523200 3.9866250 1.9067740
 H 0.5889040 3.3601010 0.6900360
 C 3.5471750 2.2155340 2.9269850
 H 2.8603340 0.2092270 2.5459250
 C 3.3229370 3.5790440 2.7101130
 H 2.0690890 5.0436410 1.7382320
 H 4.3604230 1.8921400 3.5700260

H 3.9697260 4.3183550 3.1730650

TS₁₋₄

C 0.1567190 -1.15261800.0915480
 C 0.4297690 0.1091490 0.8461940
 C 1.1587700 1.0599510 1.2800640
 C -1.9033760-0.83473601.1779100
 C -3.2438010-1.34735301.5920720
 H -3.8887600-1.38605100.7073350
 H -3.1565820-2.35940301.9920920
 H -3.6864720-0.67534102.3265480
 O -1.0947150-1.72772400.6255250
 O -1.52266600.3349680 1.3044560
 C -0.0724100-0.8797600-1.4013500
 H 0.8457440 -0.4822780-1.8412620
 C 1.2204330 -2.22705900.3374590
 H 2.1787650 -1.9022100-0.0728830
 H 1.3366140 -2.41999501.4058460
 H 0.9130610 -3.1474030-0.1661110
 H -0.3354730-1.8125310-1.9071170
 H -0.8730960-0.1511980-1.5501610
 Au 3.1966240 0.6220730 0.7127510
 P 5.4522980 0.3792030 0.1593710
 C 6.0211650 -1.36534000.1098980
 H 7.0842190 -1.4055280-0.1467260
 H 5.8661080 -1.83001501.0866620
 H 5.4476280 -1.9171120-0.6390440
 C 6.5782190 1.2192720 1.3400790
 H 7.6176220 1.0911770 1.0228170
 H 6.3404500 2.2851770 1.3786070
 H 6.4491480 0.7931560 2.3380010
 C 5.8845390 1.0697750 -1.4849970
 H 5.6480510 2.1363850 -1.5080310
 H 6.9523270 0.9302660 -1.6804640
 H 5.3048170 0.5634180 -2.2606450
 C 0.9192470 2.3455770 1.9539920
 C 1.7835310 2.7957860 2.9690920
 C -0.17693303.1483820 1.5845990
 C 1.5405490 4.0069870 3.6196530
 H 2.6375900 2.1882280 3.2522630
 C -0.40514904.3661390 2.2273410
 H -0.84343202.8154590 0.7970690
 C 0.4478870 4.7976610 3.2491800
 H 2.2090590 4.3352670 4.4100420

H -1.25269204.9771900 1.9306930
 H 0.2648370 5.7441810 3.7491170

4

C 0.0978990 -1.16966700.1080440
 C 0.1094760 0.1275790 0.9072320
 C 1.0557950 0.9951880 1.2547610
 C -1.9930280-0.66713200.9156520
 C -3.4305020-0.78849501.2299870
 H -3.9613780-1.21113800.3751280
 H -3.5402950-1.47785402.0757590
 H -3.83826300.1832610 1.5068640
 O -1.3681010-1.55583200.2261870
 O -1.28401800.3189850 1.3325180
 C 0.3706200 -0.9860090-1.3802930
 H 1.4075700 -0.6596670-1.5007840
 C 0.8889550 -2.31047700.7363200
 H 1.9508080 -2.05027900.7095870
 H 0.5987920 -2.46579401.7781400
 H 0.7367110 -3.23430600.1719820
 H 0.2306890 -1.9301350-1.9138080
 H -0.2825400-0.2226520-1.8104490
 Au 3.0573920 0.7099050 0.7201840
 P 5.3369270 0.4689630 0.1744340
 C 5.9295110 -1.27115300.1627090
 H 6.9940910 -1.3094240-0.0882500
 H 5.7746210 -1.71702701.1485190
 H 5.3642540 -1.8465470-0.5749580
 C 6.4710240 1.3308830 1.3361450
 H 7.5115470 1.1869200 1.0289200
 H 6.2417020 2.3994740 1.3471400
 H 6.3336950 0.9334360 2.3450280
 C 5.7981440 1.1198500 -1.4814920
 H 5.5617270 2.1855680 -1.5349300
 H 6.8684940 0.9769630 -1.6598680
 H 5.2298450 0.5959360 -2.2542790
 C 0.7275740 2.2237840 2.0279210
 C 1.3840940 2.4938850 3.2438460
 C -0.20767603.1626450 1.5525050
 C 1.0920530 3.6474870 3.9749850
 H 2.1236810 1.7901400 3.6153940
 C -0.48428004.3266220 2.2748690
 H -0.70978602.9855340 0.6058900
 C 0.1588430 4.5720050 3.4922930

H 1.6017640 3.8292360 4.9171000
H -1.20381005.0413340 1.8848960
H -0.05847405.4755650 4.0543660

TS₄₋₅

C 0.2789010 -1.46166900.4922430
C 0.1409400 -0.07599400.8809320
C 1.0883470 0.8965060 0.9447500
C -2.0822150-0.40732300.4517820
C -3.49655300.0441940 0.5911740
H -3.58018901.0733760 0.2265930
H -4.1553320-0.60639300.0180610
H -3.77917600.0432000 1.6474030
O -1.6766940-1.2692540-0.3349410
O -1.20853100.2008910 1.2685550
C 1.1771920 -1.8683180-0.6229890
H 2.1335500 -2.1990430-0.1964720
C -0.1524240-2.54569701.4297080
H 0.7593600 -2.86730201.9538640
H -0.8694210-2.21195102.1792120
H -0.5390790-3.41357100.8907540
H 0.7472760 -2.7336940-1.1361920
H 1.3628420 -1.0619660-1.3299480
Au 3.1142280 0.6035640 0.5394270
P 5.4284390 0.3806980 0.1383390
C 5.8548230 -0.7810840-1.2206960
H 6.9400350 -0.8290770-1.3534680
H 5.4761140 -1.7785700-0.9839220
H 5.3924910 -0.4424150-2.1514160
C 6.3726880 -0.23469601.5900710
H 7.4373210 -0.31088301.3486700
H 6.2405340 0.4530870 2.4290820
H 5.9967460 -1.21879701.8819240
C 6.2579170 1.9539550 -0.3244570
H 6.1294630 2.6869570 0.4760330
H 7.3259750 1.7849450 -0.4931400
H 5.8057580 2.3503690 -1.2371540
C 0.7166770 2.2521180 1.4218940
C 1.4321980 2.8578140 2.4738570
C -0.31024502.9909790 0.7997190
C 1.1069710 4.1417440 2.9142030
H 2.2401000 2.3102080 2.9502810
C -0.60768804.2899150 1.2165180
H -0.85657102.5583130 -0.0319220

C 0.0898170 4.8666420 2.2830170
H 1.6586140 4.5820750 3.7398030
H -1.38955704.8490860 0.7105090
H -0.15028005.8730600 2.6129580

5

C 0.0841770 -1.01460000.0463470
C 0.0184060 0.1772550 0.7664480
C 1.0920830 1.0378430 1.0956150
C -2.31365600.7721610 0.6824120
C -3.51305200.9596170 1.5659710
H -4.38266101.2007530 0.9557660
H -3.69962200.0501630 2.1445180
H -3.32178801.7684800 2.2780270
O -2.27526700.9114260 -0.5223920
O -1.21415400.4257330 1.4215720
C 1.2178750 -1.4156310-0.8328300
H 1.7272120 -2.2846540-0.3951290
C -1.0514170-1.98516300.0752990
H -1.6129430-1.94973101.0103800
H -1.7458970-1.7485700-0.7430530
H -0.6844270-2.9990270-0.1034660
H 0.8023980 -1.7594190-1.7887610
H 1.9419070 -0.6266430-1.0233280
Au 3.1158040 0.6863970 0.7577690
P 5.4393720 0.3834500 0.4569040
C 5.9993930 -1.35339700.6641100
H 7.0821750 -1.42055900.5211600
H 5.7452600 -1.70349401.6677790
H 5.4981510 -1.9914430-0.0680790
C 6.4658520 1.3497940 1.6339700
H 7.5291470 1.1669530 1.4504980
H 6.2556120 2.4154290 1.5133270
H 6.2211980 1.0577200 2.6583320
C 6.0381050 0.8767020 -1.2083770
H 5.8186940 1.9337590 -1.3780000
H 7.1172870 0.7133960 -1.2862580
H 5.5272970 0.2848590 -1.9720840
C 0.8073920 2.2783720 1.8166090
C 1.6355380 2.6785150 2.8939990
C -0.23253003.1524760 1.4136210
C 1.3934050 3.8664830 3.5777580
H 2.4490250 2.0309930 3.2051200
C -0.42493004.3722970 2.0567110

H -0.84434502.9041670 0.5540200
C 0.3705290 4.7240300 3.1538630
H 2.0160370 4.1372440 4.4247620
H -1.20171905.0459570 1.7082290
H 0.2021610 5.6656820 3.6676000

TS₅₋₆

C 1.5424910 -2.2223870-1.3500140
C 1.7217510 -1.3680830-0.3255460
C 1.0880580 -0.0542960-0.0533010
C 2.4156540 -1.16556101.8447710
C 3.2588970 -1.62123302.9873040
H 4.3151710 -1.51556702.7234630
H 3.0305640 -1.03400803.8752770
H 3.0668090 -2.68148403.1789680
O 1.5195110 -0.31289001.9115870
O 2.6752630 -1.73319500.6720970
C 0.5988500 -1.9219230-2.4830850
H 1.1651490 -1.6479100-3.3825290
C 2.3284950 -3.5008590-1.4793200
H 3.0013920 -3.6786340-0.6408890
H 1.6351340 -4.3472770-1.5591220
H 2.9170280 -3.4895820-2.4049990
H 0.0173620 -2.8169020-2.7314650
H -0.0891190-1.1026170-2.2599290
Au -0.99726700.0537780 0.0180500
P -3.35000700.1647030 0.1201400
C -3.99846600.5263410 1.8004800
H -3.6817490-0.25786202.4927480
H -3.60027301.4826890 2.1488070
H -5.09167300.5738220 1.7813590
C -4.07818601.4666390 -0.9517580
H -3.79924401.2852080 -1.9927320
H -5.16887801.4633520 -0.8633230
H -3.69366202.4446740 -0.6514590
C -4.1950140-1.3864900-0.3839780
H -5.2803970-1.2667010-0.3134540
H -3.9249120-1.6335900-1.4138750
H -3.8782530-2.20471700.2677190
C 1.9027550 1.1512850 -0.2591790
C 1.3756170 2.4221680 0.0653110
C 3.2045700 1.0847710 -0.8083440
C 2.1266600 3.5776200 -0.1286250
H 0.3727290 2.4863170 0.4764220

C	3.9452960	2.2447640	-1.0245990	H	-0.49213002	3.638040	-1.0515780	C	2.4281660	3.4848250	0.2675600
H	3.6244490	0.1240730	-1.0883810	C	-3.93040502	3.361840	0.7373620	H	1.7730080	2.0711250	1.7521110
C	3.4123780	3.4919780	-0.6782320	H	-3.62007700	2.233890	0.9845430	C	2.4758190	2.6866830	-2.0099730
H	1.7098950	4.5448390	0.1345550	C	-3.42320603	5.343610	0.2279440	H	1.8694630	0.6463770	-2.3122270
H	4.9368590	2.1784180	-1.4616410	H	-1.78157504	4.4648380	-0.8237130	C	2.6815710	3.7179440	-1.0867910
H	3.9928090	4.3946790	-0.8443070	H	-4.88857602	3.227430	1.2487120	H	2.5817320	4.2761940	0.9956830
				H	-3.98319404	4.4578010	0.3430410	H	2.6708230	2.8526430	-3.0656040
6								H	3.0336760	4.6895980	-1.4200360
C	-1.7609070	-1.7935990	1.6877990	TS₆₋₃				Species with R ¹ = R ² = Me, R ³ =			
C	-1.7026220	-1.37603200	4.189840	C	1.6252910	-2.2364030	-1.3933370	<i>p</i> -C ₆ H ₄ -CF ₃ :			
C	-1.1709570	-0.1361700	-0.2589910	C	1.6638900	-1.3050120	-0.4649150	1			
C	-2.0010010	-1.6933730	-1.7707070	C	1.2413950	-0.15268800	2.349470	C	-2.1967650	-1.3756160	-0.6557020
C	-2.3760800	-2.3884440	-3.0202980	C	2.7053180	-1.06666701	1.7609690	C	-1.4081460	-0.2751310	-0.0193770
H	-3.3880760	-2.7896280	-2.9253500	C	3.3097790	-1.13022203	1.220480	C	-1.15824500	0.7091020	0.6876820
H	-2.3088210	-1.7033790	-3.8641430	H	3.9746660	-0.26732103	2.415850	C	-4.2739490	-0.0486370	-0.7615930
H	-1.6920470	-3.2306510	-3.1728400	H	2.5312130	-1.07001703	8.842920	C	-5.7274160	-0.1211810	-0.3730110
O	-1.4550270	-0.5444660	-1.7469760	H	3.8951100	-2.04309303	2.307820	H	-6.23260100	0.7942480	-0.6798080
O	-2.1963500	-2.2494190	-0.6159670	O	1.5790330	-0.36270401	6.522390	H	-6.1976290	-0.9838930	-0.8548180
C	-1.2328550	-0.92513202	8.000500	O	3.1808810	-1.60956000	7.525550	H	-5.8213530	-0.25617500	7.084470
H	-2.0592470	-0.52073603	3.983280	C	0.3702620	-2.4593280	-2.2162420	O	-3.6141650	-1.1631690	-0.3503120
C	-2.3511730	-3.12006602	0.0906590	H	0.5783050	-2.2179040	-3.2645840	O	-3.74518100	8.711620	-1.3555870
H	-2.7434060	-3.68827301	2.462680	C	2.7929260	-3.1338790	-1.7305610	C	-1.9746440	-1.4640640	-2.1722250
H	-1.5911310	-3.72930002	5.956020	H	3.6779310	-2.9153080	-1.1372320	H	-0.9433420	-1.7659640	-2.3727130
H	-3.1634740	-2.96698902	8.117650	H	2.5014390	-4.1787190	-1.5749250	C	-1.8782710	-2.71150700	0.0315420
H	-0.6099630	-1.52294203	4.757640	H	3.0353560	-3.0194240	-2.7927610	H	-0.8273840	-2.9690690	-0.1206550
H	-0.6389320	-0.08351302	4.349430	H	0.0940750	-3.5184010	-2.1665360	H	-2.0791830	-2.65212501	1.037730
Au	0.9519230	0.0417890	-0.0952790	H	-0.4689970	-1.8515710	-1.8739110	H	-2.5023070	-3.4950300	-0.4058720
P	3.2919940	0.1996560	0.0831940	Au	-0.9391190	-0.07295200	1.172790	H	-2.6442340	-2.2262160	-2.5803210
C	4.1846340	-0.4186450	-1.3989510	P	-3.26450800	1.514190	0.1291830	H	-2.1681670	-0.5113590	-2.6639810
H	3.9397210	-1.4713950	-1.5616050	C	-3.93470300	5.521760	1.7897460	Au	0.8545610	-0.2471220	-0.1500070
H	3.8759940	0.1527320	-2.2780490	H	-3.6739290	-0.24261102	4.928440	P	3.1055290	-0.6458130	-0.5953850
H	5.2653130	-0.3154180	-1.2612230	H	-3.49994401	4.907100	2.1424220	C	-1.01639601	8.953030	1.4814190
C	3.9117740	1.9130350	0.3188740	H	-5.02337200	6.519860	1.7412710	C	-0.72615901	8.001200	2.8568260
H	3.4960150	2.3297490	1.2397620	C	-3.88353901	4.839470	-0.9705340	C	-1.20353003	1.587140	0.8875820
H	5.0044720	1.9168090	0.3805050	H	-4.97469401	5.443570	-0.9107160	C	-0.63232202	9.548020	3.6275120
H	3.5950000	2.5359970	-0.5214820	H	-3.45052002	4.397470	-0.6654650	H	-0.58271900	8.264880	3.3122730
C	4.0031300	-0.75259301	4.846480	H	-3.58766701	2.770150	-2.0019180	C	-1.11032304	3.108030	1.6636800
H	5.0915860	-0.64134101	5.070640	C	-4.1573880	-1.3630210	-0.3985050	H	-1.42821303	2.295180	-0.1706490
H	3.5829990	-0.38905802	4.259320	H	-5.2381370	-1.1966120	-0.3568110	C	-0.82838304	2.064240	3.0304670
H	3.7507330	-1.81018701	3.732270	H	-3.8703630	-1.6204260	-1.4211980	H	-0.41570402	8.798660	4.6873620
C	-1.96278601	1.1396340	-0.0573730	H	-3.8936410	-2.19320900	2.613330	H	-1.26325205	2.822320	1.2074970
C	-1.46000602	3.540050	-0.5582470	C	1.7736970	1.1947980	-0.2229180	C	4.2285270	0.2826480	0.5167720
C	-3.21028801	1.1468630	0.5878260	C	1.9732460	2.2348270	0.6988550	H	5.2680800	0.0497790	0.2663170
C	-2.18591903	5.382830	-0.4267070	C	2.0247990	1.4361680	-1.5836000				

H	4.0580170	1.3553100	0.3989770	H	-3.9000450	-0.7464940	-2.1239110	C	-1.52086104	2.379490	1.7860460
H	4.0330940	0.0037370	1.5548830	H	-4.1727520	-0.46379602	1.651430	H	-2.86446103	2.961820	0.4076930
C	3.5646800	-2.4096860	-0.4051210	C	2.4302270	-3.60643701	3.770670	C	-0.43240904	0.0655150	2.6488600
H	2.9825790	-3.0187380	-1.1008370	H	2.9565350	-4.56255801	2.927240	H	0.9791990	2.6589420	3.4825980
H	4.6308410	-2.5380580	-0.6147760	H	2.7364890	-3.10900702	3.009870	H	-1.97930005	2.141390	1.6700690
H	3.3532790	-2.73682100	0.6156140	H	1.3541480	-3.79278001	4.240050	C	4.0175160	0.1936640	0.8965940
C	3.5998360	-0.1837190	-2.2980480	C	2.3780670	-3.5466140	-1.5363310	H	5.0944790	0.0579330	0.7577640
H	4.6616890	-0.4013850	-2.4478150	H	2.6488340	-3.0103920	-2.4495680	H	3.7807190	1.2601980	0.8659460
H	3.0077690	-0.7512630	-3.0198110	H	2.9090090	-4.5035750	-1.5113290	H	3.7268960	-0.20250301	8.728990
H	3.4218380	0.8828530	-2.4542170	H	1.3014170	-3.7349570	-1.5505160	C	3.6977550	-2.4146230	-0.3455960
C	-0.68531605	4.549710	3.8642640	C	4.6488890	-2.4242780	-0.0968130	H	3.2619240	-2.9950880	-1.1626910
F	-1.38013206	5.000240	3.3557380	H	5.0897750	-3.4257410	-0.1266190	H	4.7889250	-2.4383340	-0.4269470
F	-1.11208005	2.739910	5.1381980	H	4.9728070	-1.8649930	-0.9784030	H	3.3969750	-2.86511700	6.037110
F	0.6146370	5.8566190	3.9470200	H	5.0053870	-1.90363400	7.958110	C	3.7839700	-0.0193520	-1.9929270
TS₁₋₂				C	-5.4542260	-1.4650640	-0.0134550	H	4.8717370	-0.1387550	-2.0088530
C	1.6201340	2.7524710	0.1738370	F	-6.1323070	-1.2685460	-1.1644990	H	3.3492150	-0.5544760	-2.8409340
C	0.8213810	1.4626320	0.0777850	F	-5.2126040	-2.79734600	0.0871370	H	3.5354790	1.0410890	-2.0835680
C	-0.45317301	3.369970	0.1198670	F	-6.2698100	-1.12885901	0.0081830	C	0.1341690	5.2520630	3.3784010
C	-0.42164904	0.0795790	-0.2440210	2				F	-0.82216006	1.472300	3.7357580
C	-0.90840005	4.079240	-0.7421940	C	-2.1204250	-1.3641200	-0.8583220	F	1.0305700	5.9417190	2.6125970
H	-1.99218705	3.874360	-0.8550420	C	-1.3311080	-0.2901840	-0.1658260	F	0.7928570	4.9037640	4.5118160
H	-0.63816906	1.793490	-0.0123160	C	-1.95376200	7.300430	0.4316640	TS₂₋₃			
H	-0.42198405	6.618200	-1.6872470	C	-4.1343280	-0.0377710	-0.2082390	C	1.2692800	-2.1145020	-0.0586610
O	0.8809800	3.8990280	-0.4094350	C	-5.60845000	1.452030	-0.1721380	C	1.0989020	-0.7058640	-0.0638760
O	-1.17135203	2.416110	0.2734020	H	-5.85528201	2.075600	-0.1924030	C	2.0135430	0.2710880	-0.0423550
C	1.9001930	3.0922570	1.6437390	H	-6.0720670	-0.3844980	-1.0043000	C	4.0094220	-1.14375100	0.0034270
H	2.4926370	2.2936920	2.0987420	O	-5.9824140	-0.27796600	7.678570	C	5.5022400	-1.04048900	0.0760050
C	2.8987650	2.7119820	-0.6617820	O	-3.41082200	8.559750	0.3717500	H	5.7907420	-0.50322500	9.844240
H	3.5719850	1.9468530	-0.2660410	C	-1.8783740	-1.4284230	-2.3632760	H	5.9404990	-2.03774100	0.0746770
H	2.6754250	2.4771090	-1.7056100	H	-0.8501980	-1.7521670	-2.5429740	H	5.8712910	-0.4677080	-0.7803280
H	3.4024080	3.6810620	-0.6179700	C	-2.0098810	-2.7240400	-0.1744100	O	3.4021110	-2.2101400	-0.0782650
H	2.4667360	4.0256720	1.7055080	H	-0.9849000	-3.0892740	-0.2770700	O	3.4156660	0.0547580	0.0287530
H	0.9714840	3.1941520	2.2105340	H	-2.2452620	-2.64925700	8.904190	C	1.1355220	-2.88279801	2.253810
Au	1.7470200	-0.4501540	-0.0002730	H	-2.6869520	-3.4411360	-0.6471800	H	0.0958730	-3.21758901	3.225180
P	2.8155910	-2.5363760	-0.0655580	H	-2.5597790	-2.1478410	-2.8260120	C	1.1063080	-2.8885120	-1.3358740
C	-1.71095200	6.543470	0.0862910	H	-2.0172930	-0.4476920	-2.8246630	H	0.0641680	-3.2219870	-1.4078100
C	-2.25892800	2.451410	-1.1464710	Au	0.7537930	-0.4740880	-0.2596050	H	1.3407860	-2.2824680	-2.2118500
C	-2.41120300	4.008050	1.2829320	P	3.0900340	-0.6821180	-0.4257660	H	1.7350850	-3.7817030	-1.3117780
C	-3.4755430	-0.4292850	-1.1777630	C	-1.43506101	8.777850	1.2012810	H	1.7655050	-3.77495601	1.1915100
H	-1.72520000	4.552460	-2.0674350	C	-0.35514801	7.166620	2.0859070	H	1.3877360	-2.27199502	0.0931470
C	-3.6295130	-0.26928001	2.469920	C	-2.02087303	1.1506980	1.0732290	Au	-1.0082360	-0.3974620	-0.0099230
H	-1.99718700	7.344200	2.2283760	C	0.1500950	2.8026640	2.7985420	P	-3.3220310	-0.03043400	1.001570
C	-4.1574860	-0.68375700	0.0179870	H	0.0794050	0.7337030	2.2292270	C	1.7747630	1.7339600	-0.0682570

C	0.7888920	2.2898310	-0.8978330	H	0.8712630	-0.6710100	-2.3173000	H	2.1413240	-1.9117580	-0.1740950
C	2.5527530	2.5931100	0.7302800	Au	3.1605850	-1.22375800	0.0293480	H	1.3617900	-2.41868501	3.3430660
C	0.5573690	3.6659040	-0.9085050	P	5.4410380	-1.7361310	-0.2011500	H	0.8677200	-3.1511870	-0.2055510
H	0.2155880	1.6475660	-1.5574600	C	6.1868270	-2.45705101	3.107070	H	-0.4472070	-1.8153020	-1.8988960
C	2.3257010	3.9662470	0.7232420	H	7.2466690	-2.66905701	1.1392450	H	-0.9564980	-0.1480790	-1.5289110
H	3.3309070	2.1842140	1.3649660	H	6.0888660	-1.75350702	1.1408320	Au	3.2147640	0.6184190	0.6890940
C	1.3241860	4.5043010	-0.0955780	H	5.6689260	-3.38362601	1.5695260	P	5.4768240	0.3951450	0.1577670
H	-0.20204904	0.0806930	-1.5613260	C	6.4678720	-0.2736270	-0.6092300	C	6.0653070	-1.34268100	1.1347120
H	2.9269340	4.6145920	1.3524530	H	7.5132640	-0.5767500	-0.7223530	H	7.1307380	-1.3723100	-0.1133140
C	-3.84184501	1.5985500	-0.5675260	H	6.1166350	0.1738400	-1.5420310	H	5.9083750	-1.79618301	1.163130
H	-4.92562201	1.7156150	-0.4710330	H	6.3897220	0.4671680	0.1901470	H	5.5048060	-1.9110300	-0.6114710
H	-3.34196202	3.972660	-0.0140470	C	5.7590200	-2.9506410	-1.5379990	C	6.5789600	1.2615790	1.3410950
H	-3.56230301	1.6708410	-1.6214290	H	6.8332200	-3.1432830	-1.6166580	H	7.6229900	1.1399880	1.0366910
C	-4.3078300	-1.2678860	-0.8312530	H	5.2378950	-3.8851600	-1.3166690	H	6.3302010	2.3253590	1.3641680
H	-4.1127600	-2.2658230	-0.4308820	H	5.3910890	-2.5555110	-2.4878210	H	6.4429670	0.8454610	2.3422690
H	-5.3752520	-1.0440820	-0.7413130	C	1.6396490	1.6666210	1.5277810	C	5.9135370	1.0732210	-1.4899740
H	-4.0211620	-1.2489300	-1.8856160	C	1.3931680	3.0382110	1.3457670	H	5.6648640	2.1366090	-1.5265780
C	-3.9953820	-0.07487201	1.8071590	C	2.7103300	1.2685540	2.3447790	H	6.9846160	0.9442310	-1.6740830
H	-5.07366600	1.112360	1.7889330	C	2.2167920	3.9902630	1.9429440	H	5.3469000	0.5510650	-2.2647600
H	-3.8038590	-1.05412302	2.2524640	H	0.5623000	3.3607580	0.7278330	C	0.9318290	2.3280650	1.9386240
H	-3.50560200	0.6901810	2.4145450	C	3.5367450	2.2174540	2.9436180	C	1.7098830	2.7051960	3.0458320
C	1.0852750	5.9888340	-0.0735680	H	2.8744650	0.2148040	2.5423040	C	-0.08478803	1.910100	1.4883930
F	2.2332010	6.6970970	-0.2537710	C	3.2902850	3.5798080	2.7416960	C	1.4635350	3.9072090	3.7084190
F	0.2176370	6.3983780	-1.0296760	H	2.0204710	5.0457670	1.7889060	H	2.5006730	2.0500680	3.3956360
F	0.5727750	6.4048900	1.1205550	H	4.3519180	1.8967510	3.5829440	C	-0.32149504	3.981820	2.1397650
3				C	4.2062130	4.6072230	3.3488700	H	-0.68699402	9.124610	0.6314640
C	0.7307560	-1.6098510	-0.3635460	F	3.5651700	5.7652610	3.6453990	C	0.4485310	4.7545320	3.2544740
C	1.1152720	-0.48731200	3.201230	F	5.2258060	4.9422640	2.5037930	H	2.0617820	4.1802220	4.5702140
C	0.7671950	0.6689360	0.8723610	F	4.7907350	4.1729570	4.4933440	H	-1.10915205	0.0548260	1.7848590
C	-1.37803300	0.9673430	1.8729380	TS₁₋₄				C	0.1958490	6.0770900	3.9245660
C	-2.74606701	1.5258490	1.6031760	C	0.1302640	-1.15320800	0.0738040	F	0.7825300	6.1711530	5.1419470
H	-3.15319801	1.1137650	0.6762620	C	0.4451670	0.1067160	0.8102150	F	0.6685080	7.1230580	3.1858580
H	-3.40429601	1.2987310	2.4411950	C	1.1711850	1.0498420	1.2536810	F	-1.13044706	3.165330	4.1052590
H	-2.67478102	1.6116640	1.4797620	C	-1.9027810	-0.81688301	2.133480	4			
O	-0.97849500	1.5041320	2.9186110	C	-3.2259990	-1.33669501	1.6732700	C	0.0905020	-1.18341500	1.167600
O	-0.58875001	1.0450400	0.7493020	H	-3.8985990	-1.38365500	1.8096690	C	0.1068910	0.1150450	0.9129700
C	0.5176000	-1.5930840	-1.8560590	H	-3.1205320	-2.34563702	0.0763790	C	1.0544020	0.9848150	1.2472720
H	0.9886870	-2.4561530	-2.3354600	H	-3.6497350	-0.66243702	1.4169720	C	-1.9937670	-0.67940800	1.9405390
C	0.3600250	-2.87889800	1.3621300	O	-1.0982310	-1.71912200	1.6630100	C	-3.4281240	-0.79815001	1.2675980
H	0.8389540	-3.7514150	-0.0922640	O	-1.53345300	1.3583340	1.3006080	H	-3.9646670	-1.23610800	1.4242220
H	0.5969760	-2.83483001	1.4251170	C	-0.1562310	-0.8821700	-1.4095650	H	-3.5289480	-1.47337302	1.1259440
H	-0.7243810	-3.01016400	1.2459410	H	0.7460590	-0.4951750	-1.8896650	H	-3.83568000	1.1771120	1.5324150
H	-0.5644950	-1.6809050	-2.0250920	C	1.2007370	-2.23014500	1.2797920	O	-1.3749900	-1.56789500	1.2468030

O	-1.27942000.3070380 1.3520010	H	-3.55272201.1092070 0.2064320	C	0.0160250 0.1567110 0.7795420
C	0.3534950 -1.0012530-1.3733220	H	-4.1654300-0.56455700.0942580	C	1.0935720 1.0079520 1.0838950
H	1.3889410 -0.6728290-1.5008020	H	-3.74503900.1580190 1.6832570	C	-2.30011200.7924740 0.6830890
C	0.8864180 -2.32174100.7429980	O	-1.6944500-1.2479370-0.3164030	C	-3.49849201.0143650 1.5585190
H	1.9478530 -2.06065700.7082290	O	-1.19022700.2048140 1.2945230	H	-4.36467501.2477420 0.9405560
H	0.6034990 -2.47502401.7871020	C	1.1849500 -1.8896890-0.5916910	H	-3.69349100.1232500 2.1621220
H	0.7311850 -3.24684600.1817640	H	2.1116100 -2.2943580-0.1641710	H	-3.30008601.8413520 2.2476020
H	0.2126350 -1.9467610-1.9038990	C	-0.1677540-2.55462801.4493700	O	-2.24816500.9183990 -0.5221420
H	-0.3041250-0.2403600-1.8009200	H	0.7332080 -2.88597101.9866730	O	-1.21068200.4263590 1.4319790
Au	3.0571160 0.7173290 0.7065150	H	-0.8929550-2.21627302.1885540	C	1.1995670 -1.4615040-0.8076200
P	5.3367330 0.4912720 0.1605350	H	-0.5525270-3.41875400.9030020	H	1.7178140 -2.3131910-0.3461720
C	5.9385780 -1.24521700.1448830	H	0.7139610 -2.7112830-1.1408490	C	-1.0718570-2.00380800.1131670
H	7.0031100 -1.2763160-0.1071850	H	1.4255990 -1.0725170-1.2687250	H	-1.6359060-1.94544701.0453040
H	5.7873870 -1.69381901.1299990	Au	3.1262810 0.6036630 0.5275570	H	-1.7608310-1.7674950-0.7107390
H	5.3761120 -1.8223380-0.5935220	P	5.4383610 0.3938460 0.1120940	H	-0.7179840-3.0241370-0.0541360
C	6.4620960 1.3575110 1.3270210	C	5.8579390 -0.7644870-1.2515240	H	0.7810720 -1.8397420-1.7488080
H	7.5040760 1.2209000 1.0215100	H	6.9424620 -0.8105500-1.3902790	H	1.9164780 -0.6725850-1.0229900
H	6.2260320 2.4245920 1.3402420	H	5.4819420 -1.7629860-1.0147720	Au	3.1150720 0.6895030 0.7269600
H	6.3252140 0.9563180 2.3344530	H	5.3900230 -0.4242310-2.1788430	P	5.4429070 0.4135390 0.4320950
C	5.7933710 1.1502760 -1.4930340	C	6.3917880 -0.21989701.5580550	C	6.0180750 -1.31850500.6350340
H	5.5496830 2.2144730 -1.5435460	H	7.4551170 -0.29283701.3102050	H	7.1014910 -1.37509300.4921970
H	6.8648230 1.0152430 -1.6707900	H	6.2627050 0.4670340 2.3982080	H	5.7670900 -1.67342201.6377900
H	5.2293920 0.6243630 -2.2675930	H	6.0203410 -1.20534201.8510700	H	5.5231810 -1.9590720-0.0992140
C	0.7245910 2.2087750 2.0236160	C	6.2556740 1.9721700 -0.3534710	C	6.4488750 1.3868670 1.6204380
C	1.3123880 2.4331410 3.2827870	H	6.1293590 2.7028990 0.4493900	H	7.5155390 1.2156480 1.4459590
C	-0.14474803.1883080 1.5085810	H	7.3233050 1.8087420 -0.5301020	H	6.2286700 2.4505930 1.5009910
C	1.0218950 3.5818500 4.0154510	H	5.7950350 2.3677020 -1.2622710	H	6.1981660 1.0888460 2.6415920
H	1.9989140 1.6974160 3.6901950	C	0.7273600 2.2331590 1.4278840	C	6.0408770 0.9208050 -1.2287230
C	-0.42619704.3480390 2.2294580	C	1.3707890 2.8012180 2.5416330	H	5.8098960 1.9758930 -1.3947130
H	-0.59663303.0458690 0.5320610	C	-0.23769603.0011230 0.7453260	H	7.1221020 0.7701940 -1.3031370
C	0.1500060 4.5434980 3.4895510	C	1.0415020 4.0820060 2.9841280	H	5.5396910 0.3259210 -1.9963980
H	1.4748160 3.7286770 4.9902920	H	2.1299820 2.2321580 3.0685380	C	0.8090860 2.2501330 1.8192920
H	-1.09752605.0917050 1.8130060	C	-0.54632504.2921270 1.1641570	C	1.5619430 2.5909850 2.9636570
C	-0.11254505.8126310 4.2471480	H	-0.73283602.5937450 -0.1296830	C	-0.16007803.1665320 1.3537420
F	-1.33546506.3393410 3.9782500	C	0.0852260 4.8315210 2.2923640	C	1.3183320 3.7765120 3.6503080
F	-0.04523605.6417180 5.5931550	H	1.5369650 4.4957380 3.8551380	H	2.3241750 1.9093320 3.3259820
F	0.7932140 6.7921770 3.9468890	H	-1.28307904.8729470 0.6181010	C	-0.36106904.3800630 2.0042590
		C	-0.26576406.2278170 2.7223560	H	-0.72283402.9519930 0.4522180
		F	-1.60681506.3873670 2.9037950	C	0.3619380 4.6764770 3.1655030
		F	0.3306410 6.5908660 3.8828630	H	1.8822420 4.0058540 4.5475540
		F	0.0955650 7.1577550 1.7914740	H	-1.09048205.0831450 1.6169500
TS₄₋₅				C	0.1539540 5.9989790 3.8555530
C	0.2881770 -1.47589300.5203240	5		F	-1.12534706.4380760 3.7544190
C	0.1497130 -0.08817700.8999790	C	0.0707150 -1.04668100.0675560	F	0.4535570 5.9473730 5.1763640
C	1.1022280 0.8785260 0.9477760				
C	-2.0805010-0.38531700.4758490				
C	-3.48312600.0987200 0.6238280				

F	0.9385080	6.9779680	3.3204550	H	-4.55830500.8438210	-1.2948150	C	3.5876520	0.2799790	0.9097730	
TS ₅₋₆				C	-5.3089960-1.5705300-0.2334030		H	2.0743560	1.6783930	1.5001490	
				F	-5.8201630-1.77268901.0114200		C	3.9496480	-0.72598500.0137370		
				F	-5.2443540-2.7959250-0.8204050		H	3.3215410	-1.9212570-1.6780950		
C	0.6637060	2.8877360	-1.4467800	F	-6.2243000-0.8520920-0.9224820		H	4.2818540	0.6088920	1.6749440	
C	0.0524190	2.3075150	-0.3922480				C	5.2871650	-1.40404300.1132350		
C	-0.07192400.8884450	-0.0245170		6			F	5.8940050	-1.5238790-1.0990250		
C	-0.57970902.6714730	1.7756690		C	-0.45502802.6973480	1.7327700	F	5.1836810	-2.67319400.6056090		
C	-1.04235403.5968170	2.8497630		C	-0.21120102.3715710	0.4587540	F	6.1532150	-0.74797900.9225350		
H	-1.98383704.0653020	2.5509050		C	0.0318270	1.0849050	-0.2870730				
H	-1.16607003.0509490	3.7838060		C	-0.12620102.8995340	-1.7070300	TS ₆₋₃				
H	-0.29997204.3910750	2.9803970		C	-0.18132203.7328320	-2.9255750	C	-0.79743202.7575870	1.7717620		
O	-0.19255701.5094510	1.9482800		H	0.4824290	4.5928700	-2.8083540	C	-0.31960202.2474140	0.6574370	
O	-0.59920503.1708710	0.5395920		H	0.0993760	3.1420100	-3.7962240	C	0.0019760	1.2372050	-0.2759720
C	1.3432390	2.0883090	-2.5232610	H	-1.20292904.1095630	-3.0484360	C	0.2146570	3.1113700	-1.5965260	
H	0.7280160	2.0875220	-3.4321630	O	-0.02438501.6282440	-1.7368240	C	0.3757000	3.7647250	-2.9261660	
C	0.6298640	4.3759560	-1.6693890	O	-0.20321103.4274260	-0.5279050	H	1.4052800	3.6030330	-3.2650350	
H	0.0976040	4.9171930	-0.8882010	C	-0.52742301.6369070	2.8005320	H	-0.29854503.3096650	-3.6535710		
H	1.6580640	4.7551440	-1.7241100	H	0.3309370	1.7135100	3.4797430	H	0.1963730	4.8363040	-2.8418400
H	0.1624530	4.6004390	-2.6356780	C	-0.66111804.1191830	2.1878060	O	-0.12727401.8212400	-1.6162440		
H	2.2987350	2.5557600	-2.7850960	H	-0.57984504.8449650	1.3780390	O	0.3816650	3.6757790	-0.5059020	
H	1.5197920	1.0483250	-2.2391920	H	-1.65114204.2214770	2.6489350	C	-1.73566501.9562260	2.6549030		
Au	1.6149300	-0.33339200.0132880		H	0.0750140	4.3766170	2.9588490	H	-1.24777801.7595380	3.6160250	
P	3.5226830	-1.71946200.0935020		H	-1.42807901.7850080	3.4077650	C	-0.45862404.1428790	2.2707880		
C	3.8951150	-2.35658101.7753930		H	-0.54666300.6228200	2.3930390	H	0.2388360	4.6668030	1.6212230	
H	4.0636120	-1.51815702.4558750		Au	-1.5422680	-0.3514890	-0.1049250	H	-1.38035604.7284540	2.3609370	
H	3.0487040	-2.94210402.1431260		P	-3.2764510	-1.92628800.0771360		H	-0.02519004.0633260	3.2737080	
H	4.7887270	-2.98767601.7500810		C	-4.4270900	-1.9194110	-1.3547240	H	-2.63275502.5530920	2.8524970	
C	3.3917740	-3.2182950	-0.9605600	H	-4.8906730	-0.9340280	-1.4481980	H	-2.02745501.0053270	2.2059480	
H	3.2493310	-2.9231550	-2.0032170	H	-3.8727620	-2.1347510	-2.2716770	Au	-1.5306740	-0.3208040	-0.1177830
H	4.3015370	-3.8203570	-0.8752950	H	-5.2068220	-2.6748120	-1.2174410	P	-3.0781610	-2.0695010	-0.0942280
H	2.5324200	-3.8150110	-0.6443510	C	-2.6947320	-3.66395500.2025070		C	-3.8149640	-2.3996920	-1.7419990
C	5.0709530	-0.8944870	-0.4489880	H	-2.0665040	-3.77697001.0896090		H	-4.3435390	-1.5103420	-2.0939390
H	5.9118730	-1.5918610	-0.3867530	H	-3.5481770	-4.34531100.2737760		H	-3.0230840	-2.6433990	-2.4544050
H	4.9623650	-0.5507220	-1.4806410	H	-2.1026550	-3.9167900	-0.6807050	H	-4.5161290	-3.2375160	-1.6779090
H	5.2693100	-0.03041600.1902990		C	-4.3539010	-1.68383201.5451200		C	-2.3504530	-3.66820100.4371620	
C	-1.42149400.2928990	-0.0525430		H	-5.1406220	-2.44416201.5680230		H	-3.1135930	-4.45235700.4184890	
C	-1.6513290	-0.97528000.5260600		H	-3.7543910	-1.75656402.4561240		H	-1.5337160	-3.9408910	-0.2356760
C	-2.49258500.9394560	-0.7023580		H	-4.8112260	-0.69201001.5040030		H	-1.9542620	-3.57211801.4510790	
C	-2.9087910	-1.56157400.4803070		C	1.4123940	0.4720580	-0.1656300	C	-4.5062260	-1.79524801.0253870	
H	-0.8331920	-1.48917701.0198800		C	1.7890970	-0.5536060	-1.0550480	H	-5.1893850	-2.64863300.9747820	
C	-3.74961800.3409590	-0.7774580		C	2.3298030	0.8823230	0.8105020	H	-4.1519380	-1.67684202.0523820	
H	-2.33846001.9031340	-1.1754620		C	3.0464400	-1.1400690	-0.9768560	H	-5.0378490	-0.88801400.7280470	
C	-3.9581620	-0.9037690	-0.1793620	H	1.0895150	-0.8918420	-1.8128890	C	1.3450510	0.5460320	-0.1436370
H	-3.0716620	-2.53060200.9405670									

C	2.0350590	0.0970670	-1.2809350	C	-0.87442204	0.0915650	3.1605040	C	1.0887430	3.7406470	1.4530840
C	1.8928990	0.2941330	1.1248640	H	-0.63389202	0.7069180	4.8207360	C	1.6557340	3.4508920	4.1883560
C	3.2488290	-0.5780060	-1.1537790	H	-1.13889605	0.2044020	1.3345780	H	1.3600750	1.3485310	3.8731390
H	1.6252620	0.2693660	-2.2692450	C	4.2522980	0.2026990	0.4357990	C	1.3685570	4.8596580	2.2174770
C	3.1040050	-0.3805600	1.2551540	H	5.2945420	0.0396550	0.1445240	H	0.8682530	3.8488990	0.3959480
H	1.3719050	0.6231980	2.0178420	H	4.0398260	1.2744300	0.4387610	C	1.6555700	4.7241760	3.5917240
C	3.7850520	-0.82215000	1.143340	H	4.0899420	-0.1929460	1.4411560	H	1.8752870	3.3255620	5.2412350
H	3.7684520	-0.9178990	-2.0434060	C	3.6598570	-2.4014800	-0.7426920	H	1.3742990	5.8516690	1.7781170
H	3.5130800	-0.56380202	2.2428090	H	3.0855520	-2.9578140	-1.4873730	C	6.5416950	0.7013160	1.7196200
C	5.1140350	-1.50963600	2.455570	H	4.7258540	-2.4744070	-0.9787180	H	7.6168260	0.5231130	1.6184820
F	5.3212740	-2.4314800	-0.7306780	H	3.4760310	-2.83600000	2.2427680	H	6.3345730	1.7628720	1.5630450
F	6.1588920	-0.63302100	1.635970	C	3.5978770	-0.0003350	-2.4008080	H	6.2225700	0.4264020	2.7281160
F	5.2544030	-2.1536360	1.4320510	H	4.6652920	-0.1621650	-2.5794270	C	6.1583260	-2.02541700	7.736840
Species with R ¹ = R ² = Me, R ³ =				H	3.0186930	-0.5153700	-3.1710480	H	5.7165820	-2.67881900	0.171020
<i>p</i> -C ₆ H ₄ -OMe:				H	3.3797960	1.0691140	-2.4512900	H	7.2491170	-2.09340300	7.183370
1				O	-0.79269805	2.529930	3.8398370	H	5.8249670	-2.3560190	1.7605960
C	-2.1872030	-1.4510100	-0.5307000	C	-0.59175305	2.268910	5.2618030	C	6.3362980	0.1659490	-1.1364200
C	-1.3061410	-0.37426800	0.0348530	H	-0.55840206	2.712580	5.5690610	H	7.4198860	0.0134010	-1.1285080
C	-1.18842300	0.6318780	0.7633540	H	-1.42270004	7.205650	5.7626690	H	5.8905310	-0.4483770	-1.9228420
C	-4.13179500	0.0227490	-0.9000170	H	0.3549290	4.7374750	5.5112170	H	6.1201500	1.2163810	-1.3471340
C	-5.59797300	0.1323830	-0.5677580	TS_{1,2}				O	1.9190680	5.8754260	4.2509450
H	-6.0046910	1.0428760	-1.0072270	C	0.2748260	-0.7510990	-0.0845830	C	2.2120160	5.8271100	5.6543810
H	-6.1335360	-0.7385460	-0.9579540	C	1.1867980	0.2183570	0.6369590	H	2.3810510	6.8611700	5.9526220
H	-5.73808900	1.461000	0.5170750	C	0.8064000	1.2907330	1.2505110	H	1.3671520	5.4147490	6.2154430
O	-3.5942450	-1.0824350	-0.3277190	C	-1.68619700	0.3201700	0.9780080	H	3.1138440	5.2362370	5.8449420
O	-3.50434500	0.8109320	-1.5825610	C	-3.11245000	0.1246730	1.3922540	2			
C	-1.9156700	-1.7360090	-2.0142080	H	-3.6247880	1.0868730	1.4139650	C	-2.1360870	-1.3826480	-0.8770260
H	-0.9198700	-2.1747480	-2.1234360	H	-3.6177530	-0.57138000	0.7209140	C	-1.3304070	-0.3111110	-0.1997330
C	-2.0306860	-2.72627600	0.3111700	H	-3.1228600	-0.30017102	4.025730	C	-1.93035800	0.7167770	0.4072810
H	-1.0021450	-3.08954200	2.487930	O	-1.1115950	-0.75204600	4.859350	C	-4.1294220	-0.0326940	-0.2154890
H	-2.2755490	-2.5299030	1.3577250	O	-1.1045060	1.4122150	1.1304660	C	-5.60259800	0.1632320	-0.1727930
H	-2.7032360	-3.4973090	-0.0743990	C	0.1303320	-0.3590340	-1.5595960	H	-5.8398390	1.2278170	-0.1826280
H	-2.6528010	-2.4579610	-2.3771630	H	1.1104630	-0.4043940	-2.0422110	H	-6.0739770	-0.3544590	-1.0083010
H	-1.9719670	-0.8296480	-2.6162180	C	0.7038200	-2.20754300	0.0852730	H	-5.9778140	-0.26584900	0.7639230
Au	0.8765010	-0.3744680	-0.2488840	H	1.6748290	-2.3601920	-0.3920640	O	-3.6664520	-1.0741220	-0.7832940
P	3.1356930	-0.6442760	-0.7475060	H	0.7906000	-2.4666010	1.1436730	O	-3.39480000	0.8562230	0.3535630
C	-1.0668060	1.7908360	1.5612610	H	-0.0288650	-2.8682510	-0.3860680	C	-1.9123410	-1.4592340	-2.3846400
C	-0.8743830	1.6836160	2.9571150	H	-0.5444360	-1.0550230	-2.0659580	H	-0.8867090	-1.7858630	-2.5738080
C	-1.1599650	0.0817180	0.9784910	H	-0.25537100	0.6586710	-1.6604880	C	-2.0292800	-2.7410220	-0.1889730
C	-0.7794160	2.8174910	3.7536690	Au	3.2898460	-0.01154100	5.887120	H	-1.0070820	-3.1125390	-0.2978190
H	-0.80056400	0.7007460	3.4110230	P	5.6127040	-0.29512400	4.875660	H	-2.2553020	-2.65969300	0.8774410
C	-1.06657304	2.121450	1.7669800	C	1.0903240	2.4523280	2.0372660	H	-2.7140550	-3.4570720	-0.6524620
H	-1.3083480	3.1746800	-0.0920690	C	1.3650260	2.3314600	3.4128950	H	-2.6001090	-2.1806750	-2.8350560

H	-2.0546410-0.4815490-2.8518010	C	1.1027130 -2.9224770-1.3294370	H	-2.62678702.6432100 1.5034910
Au	0.7517210 -0.5037380-0.2959420	H	0.0607020 -3.2591110-1.3868100	O	-1.00985200.4280740 2.8704310
P	3.0880460 -0.7135080-0.4586090	H	1.3224880 -2.3159500-2.2089860	O	-0.56985301.0580980 0.7343330
C	-1.40321801.8458540 1.1923780	H	1.7348560 -3.8135200-1.3148360	C	0.4869360 -1.6130740-1.8662690
C	-0.36401201.6580600 2.1152830	H	1.8030470 -3.80880101.1840080	H	0.9535040 -2.4752460-2.3519410
C	-1.93381803.1446300 1.0462050	H	1.4395610 -2.30673202.0934440	C	0.3502330 -2.90388500.3487740
C	0.1589020 2.7233820 2.8532600	Au	-1.0116300-0.4333610-0.0047540	H	0.8256270 -3.7753970-0.1114740
H	0.0372220 0.6620660 2.2717380	P	-3.3252450-0.07067400.1128070	H	0.5956180 -2.86341401.4101060
C	-1.42592904.2111810 1.7760550	C	1.7450080 1.7108260 -0.0806220	H	-0.7350710-3.03553900.2417990
H	-2.74496303.3226350 0.3474720	C	0.7845150 2.2561040 -0.9436950	H	-0.5965730-1.6997680-2.0264280
C	-0.37144804.0102510 2.6841680	C	2.4867800 2.5950670 0.7298430	H	0.8371890 -0.6906370-2.3296490
H	0.9571970 2.5339560 3.5605400	C	0.5369660 3.6315060 -0.9873600	Au	3.1405520 -1.26303300.0084500
H	-1.83105105.2108540 1.6552180	H	0.2335740 1.6019880 -1.6120980	P	5.4182140 -1.7813250-0.2239040
C	4.0148740 0.1597160 0.8666020	C	2.2511690 3.9630080 0.6972150	C	6.1651500 -2.50553401.2862130
H	5.0921820 0.0254070 0.7286870	H	3.2471690 2.2045290 1.3981870	H	7.2245320 -2.71913701.1137460
H	3.7768020 1.2260750 0.8383100	C	1.2709440 4.4932540 -0.1605600	H	6.0686650 -1.80293702.1173500
H	3.7233960 -0.23873301.8417520	H	-0.20635804.0129020 -1.6766360	H	5.6459520 -3.43154201.5445530
C	3.6988480 -2.4454310-0.3804000	H	2.8161520 4.6402790 1.3298650	C	6.4494810 -0.3210760-0.6302480
H	3.2647070 -3.0252830-1.1988640	C	-3.85298001.5573840 -0.5521680	H	7.4946530 -0.6257770-0.7413290
H	4.7901710 -2.4679000-0.4604410	H	-4.93645701.6727270 -0.4500430	H	6.1006530 0.1270990 -1.5636300
H	3.3972800 -2.89801700.5677030	H	-3.35122702.3569680 -0.0015880	H	6.3703730 0.4200700 0.1687550
C	3.7885980 -0.0481340-2.0222500	H	-3.57879101.6300890 -1.6074800	C	5.7362100 -2.9951190-1.5617550
H	4.8764320 -0.1677240-2.0348860	C	-4.3150920-1.3085180-0.8145950	H	6.8101460 -3.1895000-1.6400170
H	3.3564920 -0.5812830-2.8728940	H	-4.1177270-2.3063820-0.4150630	H	5.2134000 -3.9290670-1.3418680
H	3.5404800 1.0125120 -2.1119070	H	-5.3823870-1.0856680-0.7206420	H	5.3693940 -2.5986490-2.5114630
O	0.0569560 5.1163240 3.3535980	H	-4.0325000-1.2897670-1.8700950	C	1.6653100 1.6357840 1.5211640
C	1.1261840 4.9793950 4.2943190	C	-3.9954290-0.11591901.8215330	C	1.4491660 3.0182960 1.3490240
H	1.2979580 5.9789990 4.6932650	H	-5.07407600.0685790 1.8063720	C	2.7235980 1.2265990 2.3450630
H	0.8496890 4.3020260 5.1099720	H	-3.8012520-1.09483502.2665280	C	2.2786350 3.9502010 1.9579040
H	2.0376540 4.6181670 3.8050580	H	-3.50497800.6496110 2.4278330	H	0.6312600 3.3619290 0.7239380
TS₂₋₃		O	1.1177360 5.8462450 -0.1243860	C	3.5654630 2.1540270 2.9640170
C	1.2818400 -2.1448330-0.0555250	C	0.1452050 6.4518030 -0.9811750	H	2.8739500 0.1691940 2.5388190
C	1.0928400 -0.7379750-0.0563290	H	0.1980830 7.5212670 -0.7778400	C	3.3459240 3.5257760 2.7698540
C	1.9919010 0.2538600 -0.0310450	H	0.3791470 6.2675520 -2.0356550	H	2.1168900 5.0143400 1.8187510
C	4.0011470 -1.14743200.0037930	H	-0.86244806.0851660 -0.7553740	H	4.3625860 1.7989260 3.6056990
C	5.4937490 -1.03753400.0851900	3		O	4.0964650 4.5135250 3.3290030
H	5.7754550 -0.49120300.9901130	C	0.7161640 -1.6303610-0.3746530	C	5.1845910 4.1518060 4.1852450
H	5.9370110 -2.03261100.0928110	C	1.1004780 -0.50776500.3067930	H	5.6292460 5.0923260 4.5099140
H	5.8645190 -0.4704070-0.7743540	C	0.7837840 0.6587430 0.8575960	H	4.8296890 3.5932290 5.0583690
O	3.4046090 -2.2190020-0.1070210	C	-1.37608900.9499020 1.8394200	H	5.9318680 3.5605020 3.6445660
O	3.3998570 0.0432830 0.0525410	C	-2.72648501.5550450 1.5756620	TS₁₋₄	
C	1.1731460 -2.91703101.2294600	H	-3.12887501.1963540 0.6247050	C	0.1814470 -1.14050800.0680730
H	0.1353880 -3.25195901.3453510	H	-3.40396001.3065200 2.3920770	C	0.4388960 0.1093870 0.8490710

C	1.1756270	1.0504570	1.3011080	H	2.0582860	6.6681750	4.5180610	H	-1.37595804	4.8816200	2.1786750
C	-1.8856680	-0.83882801	1.1385240					O	-0.14796505	6.6561200	4.2670430
C	-3.2328240	-1.34636201	5.351530	4				C	0.6110680	6.0293160	5.4192750
H	-3.8668600	-1.38338500	6.425460	C	0.1117830	-1.17389900	0.0805370	H	0.1675240	6.9581960	5.7782110
H	-3.1531290	-2.35903901	9.354850	C	0.1111450	0.1042850	0.9111860	H	0.5436990	5.2653440	6.2022340
H	-3.6821960	-0.67388302	2.650190	C	1.0547450	0.9646650	1.2916710	H	1.6623330	6.2014930	5.1612510
O	-1.0782810	-1.72504900	5.779510	C	-1.9919640	-0.69146800	0.8683220				
O	-1.49677400	3.268330	1.2879760	C	-3.4413430	-0.80498601	1.1280960	TS₄₋₅			
C	-0.0324740	-0.8485910	-1.4233040	H	-3.9746170	-0.82328000	1.1724470	C	0.2988730	-1.43385000	4.212250
H	0.8912160	-0.4474940	-1.8480130	H	-3.6396650	-1.75265001	1.6383120	C	0.1467440	-0.06024700	0.8527030
C	1.2411680	-2.21939900	3.102520	H	-3.78148000	0.0312060	1.7367350	C	1.0795940	0.9248330	0.9702630
H	2.2046300	-1.8896980	-0.0842430	O	-1.3554480	-1.56368000	1.1672840	C	-2.0571910	-0.45006900	0.3853990
H	1.3452510	-2.42775701	3.770230	O	-1.28891400	2.807000	1.3238850	C	-3.4888330	-0.04441800	0.4802450
H	0.9391200	-3.1323990	-0.2097790	C	0.4057760	-0.9574620	-1.3996030	H	-3.63434000	0.8634360	-0.1163450
H	-0.2924150	-1.7736090	-1.9448620	H	1.4461200	-0.6348750	-1.4991550	H	-4.1278360	-0.83347300	0.0849010
H	-0.8296500	-0.1158570	-1.5708180	C	0.8925420	-2.33118500	0.6922870	H	-3.74710900	1.1861560	1.5156280
Au	3.2064600	0.6066080	0.7193270	H	1.9550900	-2.07265500	0.6885050	O	-1.6059250	-1.2951500	-0.3995580
P	5.4520840	0.3257360	0.1420880	H	0.5859190	-2.51182201	1.7252820	O	-1.22148700	1.1761840	1.2202810
C	5.9837690	-1.43097300	0.0982560	H	0.7477380	-3.24075200	1.1031520	C	1.2083140	-1.8018930	-0.7015340
H	7.0401910	-1.4976380	-0.1793740	H	0.2677590	-1.8880960	-1.9568620	H	2.1716050	-2.1216910	-0.2829420
H	5.8385640	-1.88289301	0.0825360	H	-0.2370190	-0.1805050	-1.8209800	C	-0.0913190	-2.54723901	1.3472110
H	5.3825080	-1.9771930	-0.6329080	Au	3.0556740	0.6709440	0.7509160	H	0.8314340	-2.84354101	0.8659380
C	6.6108480	1.1505360	1.3019360	P	5.3307080	0.4253310	0.1849060	H	-0.8173510	-2.24619202	1.1022750
H	7.6432780	1.0008120	0.9714580	C	5.9179300	-1.31661500	1.1566210	H	-0.4533140	-3.41961800	0.7985200
H	6.3941090	2.2210780	1.3368010	H	6.9799870	-1.3568970	-0.1045450	H	0.7943010	-2.6639780	-1.2328910
H	6.4873500	0.7332380	2.3043330	H	5.7706300	-1.76856701	1.1408520	H	1.3766210	-0.9782620	-1.3932540
C	5.8816910	0.9944000	-1.5124050	H	5.3438890	-1.8853270	-0.5794580	Au	3.1092480	0.5997030	0.5776580
H	5.6692000	2.0658970	-1.5413330	C	6.4798890	1.2764930	1.3399970	P	5.4149480	0.3135290	0.1677570
H	6.9438790	0.8291270	-1.7181970	H	7.5167420	1.1310770	1.0212910	C	5.7943340	-0.8754290	-1.1821230
H	5.2823990	0.4956360	-2.2780350	H	6.2543790	2.3458010	1.3594320	H	6.8765300	-0.9689560	-1.3149700
C	0.9434360	2.3229880	1.9948580	H	6.3517680	0.8737180	2.3479980	H	5.3750080	-1.8546750	-0.9370590
C	1.8548250	2.8035250	2.9490050	C	5.7795980	1.0842700	-1.4715110	H	5.3451280	-0.5264080	-2.1155020
C	-0.19956903	1.1040440	1.7159680	H	5.5466890	2.1511700	-1.5166610	C	6.3585120	-0.31526401	1.6144540
C	1.6346770	4.0017730	3.6324200	H	6.8477430	0.9384060	-1.6606500	H	7.4172390	-0.42546801	1.3601390
H	2.7461820	2.2255690	3.1734700	H	5.2022400	0.5671900	-2.2422130	H	6.2578030	0.3838150	2.4484440
C	-0.41966004	3.049850	2.3759570	C	0.7346280	2.1800800	2.0842390	H	5.9574350	-1.28487801	0.9208720
H	-0.91406302	2.7647410	0.9751570	C	1.5083260	2.5205260	3.2062210	C	6.2869010	1.8566560	-0.3188300
C	0.4915740	4.7617990	3.3451780	C	-0.31218903	0.0584450	1.7296040	H	6.1859770	2.6013780	0.4748970
H	2.3560710	4.3282200	4.3715960	C	1.2403160	3.6579590	3.9741540	H	7.3483360	1.6556670	-0.4939990
H	-1.29641104	0.9062310	2.1565990	H	2.3367210	1.8785160	3.4920250	H	5.8390000	2.2569040	-1.2319600
O	0.1819360	5.9459640	3.9407570	C	-0.57672704	2.062280	2.4685620	C	0.7128880	2.2624550	1.4813750
C	1.0662250	6.4674030	4.9375950	H	-0.91538802	0.8504850	0.8514790	C	1.5603930	2.9273920	2.3891960
H	0.6155530	7.4018670	5.2715350	C	0.1920590	4.5117220	3.6036110	C	-0.44325702	0.9593290	1.0536060
H	1.1538130	5.7789040	5.7852730	H	1.8572090	3.8690840	4.8394790	C	1.2652200	4.1956860	2.8909600

H	2.4677320	2.4324300	2.7223240	H	5.6234350	0.0867320	-1.8420830	H	-5.2942110	-1.5174740	1.5865810
C	-0.7289020	4.2378320	1.5107500	C	0.8187550	2.3733730	1.7870240	H	-3.6907970	-1.6366720	2.3601570
H	-1.1087610	2.5093780	0.3267620	C	1.7910400	2.9552120	2.6499640	C	-4.6818160	-0.3147790	-1.1406380
C	0.1139840	4.8633550	2.4466980	C	-0.4044590	3.0970380	1.6256470	H	-5.6653720	-0.7883550	-1.0623340
H	1.9398580	4.6533010	3.6043400	C	1.5513490	4.1156540	3.3659260	H	-4.7674750	0.7423510	-0.8764220
H	-1.6051200	4.7716440	1.1561790	H	2.7434850	2.4498540	2.7740240	H	-4.3250710	-0.3903530	-2.1709540
O	-0.2616640	6.1076490	2.8476440	C	-0.6325720	4.2852380	2.2831830	C	1.7918520	-0.2397220	-0.0247540
C	0.5533300	6.8022310	3.7974080	H	-1.1436000	2.7541090	0.9135430	C	1.7087300	-1.6019860	-0.4080400
H	0.0580400	7.7580800	3.9671000	C	0.3300110	4.7974070	3.1844440	C	3.0514870	0.2422680	0.3954010
H	0.6166130	6.2490740	4.7409080	H	2.3102210	4.4960120	4.0380510	C	2.8174210	-2.4274510	-0.3856980
H	1.5593180	6.9759390	3.3999720	H	-1.5456730	4.8486840	2.1226310	H	0.7503940	-1.9988140	-0.7295090
5				O	-0.0007390	5.9411890	3.8011090	C	4.1734790	-0.5782380	0.4411860
C	0.1387010	-0.7669040	-0.2256150	C	0.9158050	6.5422190	4.7335990	H	3.1527290	1.2753230	0.7133940
C	0.0745840	0.2597760	0.6961350	H	0.4117450	7.4364320	5.0967030	C	4.0631870	-1.9232500	0.0423850
C	1.1241890	1.1673970	1.0668580	H	1.1170800	5.8640590	5.5679420	H	2.7497640	-3.4685880	-0.6836810
C	-2.3102430	0.5756990	0.9875190	H	1.8485420	6.8184970	4.2334390	H	5.1166470	-0.1722880	0.7853610
C	-3.3871560	0.4368430	2.0260380	TS₅₋₆				O	5.0851920	-2.8060080	0.0432050
H	-4.3462850	0.7285850	1.5996430	C	0.5007970	2.5166980	1.6582910	C	6.3871490	-2.3742150	0.4655750
H	-3.4354090	-0.6003540	2.3720810	C	0.7480420	2.0176840	0.4373700	H	7.0278350	-3.2505470	0.3751400
H	-3.1541700	1.0618940	2.8930000	C	0.6066290	0.6165430	-0.0749240	H	6.7617800	-1.5748860	-0.1816850
O	-2.4673020	0.9057520	-0.1699600	C	1.1247630	2.4162660	-1.7780030	H	6.3674520	-2.0372880	1.5069470
O	-1.0829420	0.2937520	1.5203940	C	1.5102680	3.3129900	-2.9038850	6			
C	1.2106740	-0.9012490	-1.2600870	H	2.5212990	3.6951840	-2.7363400	C	0.6605600	2.3539230	1.7812030
H	1.7804830	-1.8237910	-1.0903350	H	1.4634460	2.7677340	-3.8451590	C	0.6616230	2.0368680	0.4821740
C	-0.9296990	-1.8147160	-0.3094570	H	0.8294610	4.1693580	-2.9333400	C	0.6092430	0.7315060	-0.2762440
H	-1.4366050	-1.9793940	0.6429940	O	0.7193450	1.2476190	-1.9044020	C	0.6633640	2.5973690	-1.6812540
H	-1.6843540	-1.5226690	-1.0513870	O	1.2307730	2.9164970	-0.5599920	C	0.6588450	3.4782140	-2.8696460
H	-0.4943040	-2.7573740	-0.6541430	C	0.0162370	1.6349480	2.7793920	H	1.4455500	4.2303520	-2.7698800
H	0.7282110	-1.0155470	-2.2397990	H	0.8273910	1.4450780	3.4942770	H	0.8023520	2.8874510	-3.7730960
H	1.8929230	-0.0550370	-1.3120340	C	0.7371860	3.9629650	2.0103400	H	-0.3026350	4.0009010	-2.9176110
Au	3.1393810	0.6862660	0.7923920	H	1.1101090	4.5525630	1.1725520	O	0.6401440	1.3297390	-1.7488510
P	5.4341000	0.1640630	0.5824960	H	-0.1975120	4.4147570	2.3656120	O	0.6744810	3.1028300	-0.4853660
C	5.8141810	-1.6224500	0.7788720	H	1.4560560	4.0375450	2.8357430	C	0.6210170	1.2715710	2.8289410
H	6.8894040	-1.7954480	0.6717360	H	-0.7867660	2.1362430	3.3318900	H	1.5871700	1.1986270	3.3444100
H	5.4903050	-1.9598880	1.7667020	H	-0.3522910	0.6673010	2.4283400	C	0.7004110	3.7746980	2.2813300
H	5.2783430	-2.1967540	0.0188920	Au	-1.3210760	-0.2106910	-0.0553180	H	0.7649660	4.5095630	1.4778220
C	6.5041810	1.0067100	1.8155080	P	-3.4879110	-1.1378060	-0.0120400	H	-0.1976160	3.9882330	2.8746240
H	7.5495500	0.7153530	1.6740230	C	-3.5383730	-2.9108040	-0.4904860	H	1.5600060	3.9150640	2.9482420
H	6.4126670	2.0897810	1.7006120	H	-3.1548820	-3.0275080	-1.5073300	H	-0.1304870	1.5161430	3.5890260
H	6.1865600	0.7324350	2.8247210	H	-2.9092240	-3.4903890	0.1898150	H	0.3862580	0.2885360	2.4138940
C	6.1517100	0.6188970	-1.0468680	H	-4.5644340	-3.2881980	-0.4445350	Au	-1.2886580	-0.2280190	-0.0976440
H	6.0378100	1.6937100	-1.2087360	C	-4.2928890	-1.0788810	1.6384930	P	-3.3993870	-1.2471930	0.1155540
H	7.2139060	0.3576000	-1.0807740	H	-4.3700100	-0.0414680	1.9736650	C	-4.5466370	-0.8766580	-1.2712380

H	-4.71409600.2018560 -1.3301020	H	-1.49263702.8812980 2.9383250	O	-0.89276700.4137440 -1.7516670
H	-4.1062370-1.2146440-2.2127070	H	-1.33166301.2449240 2.2474670	C	0.9053560 2.9895700 0.9653750
H	-5.5041200-1.3836860-1.1170770	Au	-1.2488590-0.1205880-0.1068620	C	0.9481950 -1.8062690-0.8069650
C	-3.3372230-3.08202300.1901160	P	-3.2034480-1.4003290-0.0485900	H	1.9760410 -2.0676740-0.5414580
H	-2.7421090-3.39343401.0523790	C	-4.0972310-1.4344580-1.6510740	C	0.3423370 -1.85928901.6521530
H	-4.3472350-3.49386000.2795980	H	-4.3729680-0.4168270-1.9386410	H	1.3796060 -2.04009901.9440380
H	-2.8677050-3.4699980-0.7174590	H	-3.4486830-1.8549200-2.4234650	H	-0.1667230-1.32879902.4602090
C	-4.3212190-0.74967401.6255450	H	-5.0013640-2.0447300-1.5646530	H	-0.1520580-2.82026201.4877090
H	-5.2915860-1.25423701.6633810	C	-2.9033650-3.16079800.3754740	H	0.3892760 -2.7313100-0.9742960
H	-3.7409370-1.01464602.5131360	H	-3.8469190-3.71495200.3847930	H	0.9568940 -1.2175660-1.7234970
H	-4.47704000.3321430 1.6187040	H	-2.2294200-3.6044660-0.3615120	Au	3.1366440 0.4732470 0.9821680
C	1.8325080 -0.1430930-0.1875630	H	-2.4363800-3.22419801.3614830	P	5.4208030 0.1161890 1.2931670
C	1.7757060 -1.4906620-0.5965370	C	-4.4404150-0.81510801.1745080	C	6.4382800 1.5508390 0.7755260
C	3.0692260 0.3511590 0.2535240	H	-5.3265010-1.45686001.1496940	H	7.4971290 1.3372300 0.9498010
C	2.9007260 -2.3034720-0.5697350	H	-4.0054630-0.83739902.1767630	H	6.2780040 1.7505160 -0.2865780
H	0.8297980 -1.9011940-0.9387290	H	-4.73113300.2114380 0.9386260	H	6.1482830 2.4336100 1.3503940
C	4.2100930 -0.45466100.3003490	C	1.7657160 -0.0325290-0.2042480	C	6.0506260 -1.31349700.3340160
H	3.1536830 1.3827640 0.5821610	C	2.1407410 -0.7748350-1.3395090	H	7.1238890 -1.43460300.5096780
C	4.1296690 -1.7915400-0.1162980	C	2.4263350 -0.29136901.0018090	H	5.5292690 -2.22218900.6441770
H	2.8485920 -3.3405020-0.8859220	C	3.1470170 -1.7320780-1.2679060	H	5.8730330 -1.1482730-0.7312360
H	5.1416980 -0.03362700.6586010	H	1.6429960 -0.6024550-2.2879820	C	5.8863120 -0.21525903.0344360
O	5.1728540 -2.6646340-0.1133490	C	3.4354100 -1.25680201.0889440	H	5.3626050 -1.10485803.3924400
C	6.4529500 -2.20880600.3367970	H	2.1590460 0.2616090 1.8970800	H	6.9664520 -0.37612803.1047400
H	6.4108300 -1.88764001.3834130	C	3.8017090 -1.9842490-0.0513720	H	5.6053890 0.6364640 3.6583830
H	7.1196810 -3.06598000.2447340	H	3.4358560 -2.2983740-2.1478700	C	-0.59989603.3166060 0.7727380
H	6.8210400 -1.3885840-0.2891990	H	3.9243380 -1.42205802.0415020	H	-0.94210503.0293340 -0.2249250
		O	4.7689590 -2.9471640-0.0799850	H	-1.21476002.8043050 1.5185050
		C	5.4617860 -3.25679601.1315990	H	-0.74132404.3955640 0.8919570
TS₆₋₃		H	6.1687250 -4.04588100.8750590	C	1.7437730 3.7291060 -0.1027330
C	0.2920680 2.6304140 1.7815830	H	6.0080730 -2.38478901.5086300	H	1.5984650 4.8079490 0.0109950
C	0.5989010 2.0267840 0.6530690	H	4.7703960 -3.62041901.9004050	H	2.8101160 3.5131830 0.0127700
C	0.6300160 0.9729360 -0.2879620			H	1.4372680 3.4428470 -1.1128220
C	1.3077870 2.7423880 -1.6013210			C	1.3534410 3.4067480 2.3846460
C	1.6265300 3.3461350 -2.9266660	Species with R ¹ = R ² = Me, R ³ =		H	2.4138980 3.1911920 2.5447020
H	2.5749170 2.9217930 -3.2757190	t-Bu:		H	1.2006190 4.4836370 2.5066030
H	0.8518360 3.0940330 -3.6527020	1		H	0.7723580 2.8865650 3.1518490
H	1.7377780 4.4260570 -2.8312780	C	0.2980690 -1.04024400.3538530		
O	0.6321530 1.5954500 -1.6270440	C	0.9061860 0.3084790 0.5799120	TS₁₋₂	
O	1.6357130 3.2297010 -0.5086210	C	1.0306780 1.5207270 0.7912930	C	0.2723100 -0.87578200.1617250
C	-0.78782502.0790870 2.6936440	C	-1.6048070-0.1647320-0.9536240	C	1.0995550 0.2948540 0.6710920
H	-0.32940101.7420390 3.6302140	H	-3.47196300.4305620 -1.7991150	C	0.6747390 1.4243390 1.0956230
C	0.9774520 3.8838750 2.2742430	H	-3.4345360-1.2460260-1.1880260	C	-1.75607800.0814860 1.1811500
H	1.7766920 4.2152850 1.6152230	H	-3.53280100.0926790 -0.0418560	C	-3.1146380-0.26112801.7157600
H	0.2351450 4.6840970 2.3731620	O	-1.1376150-0.86015100.1154950	H	-3.50200900.5690930 2.3064070
H	1.3879290 3.6976690 3.2726870				

H	-3.7866020-0.43725400.8682280	C	-1.70970600.1789860 1.0024900	C	0.7225430 -1.14051300.3665440
H	-3.0737630-1.17632602.3097280	C	-3.18295900.1841720 1.2075070	C	1.1531770 0.1835190 0.6594130
O	-1.0280080-0.97805300.8716940	H	-3.56565301.2042580 1.1631010	C	0.4401320 1.2686340 0.9792370
O	-1.36795201.2477970 1.0356290	H	-3.6665030-0.45144600.4650980	C	-1.77312800.1879080 0.8747770
C	0.7525780 2.8053050 1.6270160	H	-3.3912180-0.22393802.2037180	C	-3.22633400.5142120 1.0489820
C	-0.0363130-0.6958870-1.3302180	O	-1.1673940-0.86196000.5065170	H	-3.51951001.2766460 0.3206660
H	0.9009680 -0.6760960-1.8926870	O	-1.05220301.2192660 1.3586490	H	-3.8260520-0.38433300.9082670
C	0.9159040 -2.23096900.4527030	C	0.7876950 2.6630310 1.8291760	H	-3.39459300.9269950 2.0480430
H	1.8554100 -2.3170670-0.0986700	C	0.4615760 -1.1681440-1.2344450	O	-1.3650630-0.93708000.5801810
H	1.1245620 -2.34087101.5199320	H	1.4989600 -1.3818860-1.5035930	O	-0.98732501.2421560 1.0714330
H	0.2449270 -3.03388800.1354880	C	0.7184730 -2.23825501.0590380	C	0.6363430 -1.6065020-1.0633780
H	-0.6421490-1.5341980-1.6858900	H	1.7608860 -2.50245500.8648140	H	1.5841430 -2.0838380-1.3382020
H	-0.56778700.2407640 -1.5139290	H	0.5975380 -2.08129102.1336130	C	0.8273780 -2.21435201.4171960
Au	3.2272070 0.1722320 0.5142990	H	0.0805160 -3.06750700.7397490	H	1.7901010 -2.72584501.3031400
P	5.5368300 -0.07834900.2621950	H	-0.1629540-2.0104810-1.5461980	H	0.7690600 -1.80185002.4254840
C	6.2335750 0.8787080 -1.1411600	H	0.1461750 -0.2668760-1.7665250	H	0.0403470 -2.95725501.2671810
H	6.0284280 1.9424030 -0.9968600	Au	3.1798460 0.1071140 0.5307040	H	-0.1505480-2.3585040-1.1594820
H	7.3150510 0.7227620 -1.2025980	P	5.4973870 -0.15166400.2384580	H	0.4515630 -0.7779900-1.7486550
H	5.7675290 0.5534500 -2.0745380	C	6.3453460 1.3309670 -0.4409130	Au	3.2706650 -0.01313500.4412200
C	6.0567890 -1.8123920-0.0409780	H	7.4182530 1.1418280 -0.5448130	P	5.5879460 -0.25901200.1790580
H	7.1442380 -1.8650970-0.1508760	H	5.9254530 1.5765170 -1.4196770	C	0.8544050 2.7039750 1.3054850
H	5.7476500 -2.43995900.7985350	H	6.1919730 2.1807360 0.2291060	C	6.2824490 0.7303670 -1.2034120
H	5.5823080 -2.1841660-0.9525760	C	5.9638660 -1.5108640-0.9075920	H	7.3638810 0.5765430 -1.2703580
C	6.5071510 0.4576180 1.7260020	H	7.0530220 -1.5808790-0.9901640	H	5.8152280 0.4264800 -2.1433780
H	7.5760790 0.3117920 1.5418240	H	5.5688960 -2.4584590-0.5326350	H	6.0774730 1.7905930 -1.0352500
H	6.3157640 1.5147630 1.9256350	H	5.5379130 -1.3200460-1.8959610	C	6.5595990 0.2486090 1.6525340
H	6.2074460 -0.12614202.5998620	C	6.4086120 -0.53057801.7892660	H	6.2666420 -0.35781102.5131860
C	0.1014980 2.8994130 3.0290870	H	7.4773310 -0.64494601.5834510	H	7.6291520 0.1153830 1.4626400
H	0.2404490 3.9141230 3.4149180	H	6.2632640 0.2801640 2.5077280	H	6.3611390 1.2991870 1.8785030
H	-0.96851002.6903990 2.9833100	H	6.0231170 -1.45641802.2238390	C	6.1173830 -1.9840770-0.1625310
H	0.5693680 2.1983930 3.7270790	C	0.1083310 3.7594350 0.9674240	H	5.6444350 -2.3378680-1.0820510
C	0.0874130 3.8043070 0.6489280	H	-0.98068703.6629590 0.9684880	H	7.2050950 -2.0296040-0.2737090
H	-0.97996203.6040640 0.5438330	H	0.3588080 4.7467080 1.3693330	H	5.8112580 -2.63145900.6628940
H	0.2144880 4.8189500 1.0391240	H	0.4595570 3.7142120 -0.0690610	C	2.3754430 2.9094930 1.2712560
H	0.5541200 3.7549330 -0.3395900	C	0.2837610 2.7685100 3.2923250	H	2.8889370 2.2859830 2.0103850
C	2.2604430 3.1661370 1.7584700	H	0.5400470 3.7536030 3.6959080	H	2.7952690 2.7008570 0.2817620
H	2.7743610 2.4947060 2.4515110	H	-0.80080802.6497950 3.3603830	H	2.5956750 3.9553180 1.5102930
H	2.7662630 3.1343050 0.7899620	H	0.7563830 2.0083810 3.9236520	C	0.2086890 3.6611170 0.2701370
H	2.3263110 4.1860570 2.1502560	C	2.3041390 2.9118180 1.8216070	H	-0.88221103.5980780 0.2856790
		H	2.8387830 2.1847870 2.4403140	H	0.4919330 4.6937160 0.4999740
2		H	2.7177340 2.8765780 0.8093360	H	0.5551760 3.4313370 -0.7434430
C	0.3698360 -0.97318500.2779500	H	2.4976850 3.9093670 2.2302160	C	0.3484970 3.0622560 2.7272900
C	1.0957060 0.2561170 0.7651140			H	0.6356880 4.0910390 2.9683280
C	0.4258370 1.2934590 1.2694370	TS₂₋₃		H	-0.73912902.9881570 2.8017530

H	0.7935730	2.4007420	3.4786780	C	1.0937860	1.5377410	3.7135730	H	1.3394220	4.6675890	-0.1542470
3				H	1.6008670	2.3288770	4.2758520	H	2.5511740	3.4053640	-0.4536760
C	0.7537250	-1.56851600	0.0257510	H	0.0197340	1.6237660	3.8974260	H	0.9234800	3.2548620	-1.1433590
C	1.0937240	-0.44183000	0.7315850	H	1.4349910	0.5714040	4.1000670	C	-0.47266103	0.2224700	1.2580670
C	0.6769530	0.5951350	1.4451600	TS₁₋₄				H	-1.10641202	0.9128090	0.4236500
C	-1.54637801	0.0570890	0.6024610	C	0.4714960	-1.21973500	0.8195430	H	-0.85592002	0.7559480	2.1685720
C	-2.97369801	1.1439740	1.0704810	C	0.5404610	0.2875600	0.8558390	H	-0.55632404	0.3092910	1.3676770
H	-3.06510801	0.9264970	1.8301980	C	1.2333930	1.3623830	0.8375990	4			
H	-3.62225001	0.3738990	0.2257240	C	-1.7966830	-0.63672600	0.8428270	C	0.3052200	-1.25379000	0.3899260
H	-3.27749000	0.2003030	1.5324980	C	-3.2414790	-0.99667000	0.7413650	C	0.1321210	0.1897990	0.8722720
O	-1.14799901	0.2765730	-0.5216620	H	-3.4164920	-1.5862300	-0.1615550	C	0.9797220	1.1993780	1.0480560
O	-0.72721600	0.6953530	1.6374030	H	-3.5105270	-1.61483201	0.6044280	C	-1.8899690	-0.82332900	0.8993350
C	1.4253460	1.6814390	2.2057060	H	-3.8508230	-0.09395100	0.7375440	C	-3.3362060	-1.03793901	1.1146390
C	0.4479420	-1.5273060	-1.4520980	O	-0.9362260	-1.59897400	0.5743600	H	-3.7343120	-1.68502400	0.3309490
H	0.9519100	-2.3396870	-1.9841510	O	-1.36806300	0.4814680	1.1631290	H	-3.4698400	-1.54560302	0.0773130
C	0.4884520	-2.87938900	0.7285970	C	1.0076060	2.8631940	1.0131050	H	-3.8593750	-0.08260201	1.1394200
H	0.9740950	-3.71413800	0.2144020	C	1.2448740	-1.8319990	-0.3512780	O	-1.1223720	-1.76369900	0.4724840
H	0.7944680	-2.85960901	0.7748720	H	2.3155460	-1.6588200	-0.2221310	O	-1.32231900	0.2974490	1.1451000
H	-0.5946090	-3.05782500	0.6807130	C	0.8575180	-1.83409102	0.1710680	C	0.6497000	2.6211910	1.5385940
H	-0.6324960	-1.6895980	-1.5625780	H	1.9060410	-1.61125802	0.3842020	C	0.7043370	-1.3857110	-1.0754310
H	0.7017080	-0.5678480	-1.9011610	H	0.2441910	-1.42283402	0.9768700	H	1.7192880	-0.9969340	-1.1955530
Au	3.1329880	-1.10718000	0.2258190	H	0.7242390	-2.91865402	0.1337790	C	1.1123650	-2.14715001	0.3250540
P	5.3960780	-1.5853040	-0.1995930	H	1.0616790	-2.9097300	-0.3721470	H	2.1548350	-1.81801701	0.3094680
C	6.4511250	-1.46984501	0.2958380	H	0.9259050	-1.3924700	-1.2988180	H	0.7434850	-2.07659802	0.3512200
H	7.4886790	-1.70319801	0.0382390	Au	3.2950000	0.7685380	0.5099620	H	1.0649650	-3.18716800	0.9903430
H	6.3986950	-0.45846001	0.7061830	P	5.5758520	0.3472620	0.2093250	H	0.6876620	-2.4351650	-1.3821980
H	6.0972040	-2.17653602	0.0503990	C	6.4098460	1.5898280	-0.8543180	H	0.0352830	-0.8073540	-1.7173890
C	5.6654080	-3.2763000	-0.8581180	H	6.2999570	2.5830890	-0.4120930	Au	3.0169890	0.8262820	0.6314070
H	5.1327300	-3.3920580	-1.8050160	H	7.4738750	1.3529170	-0.9517990	P	5.3125660	0.4759810	0.2119420
H	6.7343280	-3.4457470	-1.0201680	H	5.9480300	1.5931760	-1.8448700	C	6.0764670	1.7285500	-0.8960880
H	5.2858030	-4.0121500	-0.1452090	C	6.5298590	0.3460510	1.7785200	H	5.9658190	2.7229000	-0.4560830
C	6.1536750	-0.4517680	-1.4257980	H	7.5851830	0.1369530	1.5785400	H	7.1398380	1.5133480	-1.0403040
H	6.0932640	0.5762730	-1.0608030	H	6.4392910	1.3213350	2.2633220	H	5.5709520	1.7168460	-1.8651720
H	7.2028630	-0.7186240	-1.5854490	H	6.1308090	-0.41830902	0.4499780	C	6.3575230	0.5055450	1.7245830
H	5.6125030	-0.5226180	-2.3723450	C	5.9468010	-1.2726970	-0.5709590	H	7.4081120	0.3420720	1.4653570
C	2.9465380	1.5777270	2.0176670	H	7.0287520	-1.4006640	-0.6748110	H	6.2543760	1.4730040	2.2228370
H	3.3366180	0.6219500	2.3841890	H	5.5458960	-2.07924400	0.0477930	H	6.0289140	-0.27839502	0.4119210
H	3.2348340	1.6986700	0.9679270	H	5.4803510	-1.3206890	-1.5580100	C	5.7107400	-1.1345990	-0.5813160
H	3.4362060	2.3728920	2.5895360	C	1.8392840	3.3482640	2.2248630	H	5.2017500	-1.2048540	-1.5461270
C	0.9553390	3.0706620	1.7076810	H	2.9090720	3.1710520	2.0745710	H	6.7903460	-1.2276770	-0.7355200
H	-0.11590003	0.2193320	1.8693570	H	1.6861340	4.4238390	2.3655450	H	5.3671710	-1.95276800	0.0567830
H	1.4853200	3.8517420	2.2623780	H	1.5319500	2.8367920	3.1429080	C	1.1190960	3.6229800	0.4536890
H	1.1677740	3.2032550	0.6421870	C	1.4881910	3.5880020	-0.2663630	H	0.9351370	4.6500230	0.7897990

H	2.1888290	3.5159080	0.2466350	H	5.3438150	-0.9765690	-1.8296240	C	5.4795160	-0.5170020	-2.0440740
H	0.5749080	3.4698950	-0.4848940	C	1.2826630	3.4395330	0.7887510	H	6.4912760	-0.5535010	-2.4594460
C	-0.8380460	2.9205730	1.8369190	H	1.1032260	4.4176860	1.2488600	H	5.1428280	-1.5327620	-1.8221640
H	-1.4682440	2.7931590	0.9522470	H	2.3558870	3.3401590	0.5999940	H	4.8023790	-0.0762040	-2.7800640
H	-1.2335410	2.2875230	2.6357960	H	0.7632300	3.4178010	-0.1754600	C	2.4243080	3.0512770	2.3103800
H	-0.9284800	3.9627700	2.1626560	C	1.5498580	2.3776480	3.0653370	H	2.9046750	2.4530770	3.0912950
C	1.4503210	2.8771740	2.8401260	H	2.6249680	2.2504970	2.9048080	H	3.1423640	3.1957910	1.4973430
H	1.1457870	2.1840160	3.6321240	H	1.3869700	3.3500350	3.5437410	H	2.1897420	4.0340340	2.7329530
H	2.5262140	2.7554760	2.6779860	H	1.2119710	1.5975180	3.7559610	C	0.5562090	3.2535890	0.6489010
H	1.2695760	3.8988260	3.1940060	C	-0.7198980	2.6445590	2.0489650	H	0.4646920	4.2816940	1.0151110
TS₄₋₅				H	-1.3463950	2.6281200	1.1528550	H	1.2337020	3.2581070	-0.2102130
C	0.4470610	-1.3829780	0.4043950	H	-1.1465300	1.9572780	2.7818890	H	-0.4283480	2.9231320	0.3174760
C	0.1852340	-0.0490280	0.9042400	H	-0.7682890	3.6552070	2.4693780	C	0.1323330	2.3665460	3.0100910
C	1.0698600	0.9718420	1.0618480	5				H	-0.8676100	2.0369110	2.7350380
C	-2.0027100	-0.5147010	0.3671340	C	0.4875210	-1.3389240	1.0929510	H	0.5068000	1.7185570	3.8100280
C	-3.4490340	-0.1748520	0.5116390	C	0.3678210	0.0507000	1.0774730	H	0.0609430	3.3817850	3.4130760
H	-3.5946230	0.8812330	0.2618350	C	1.4095960	0.9904880	1.2479650	TS₅₋₆			
H	-4.0475610	-0.7979690	-0.1512570	C	-1.6388650	0.5758560	-0.1114090	C	-1.9557800	2.1059500	-0.6475820
H	-3.7575810	-0.3146460	1.5512660	C	-3.0541200	1.0404540	0.0866020	C	-2.0612660	0.8381260	-0.1620800
O	-1.5232480	-1.2602600	-0.4900260	H	-3.0848770	1.9373240	0.7104890	C	-1.1842580	-0.2958180	-0.4015610
O	-1.1973650	0.0627470	1.2722980	H	-3.5114120	1.2363910	-0.8827270	C	-2.9188810	-0.2271810	1.7084100
C	1.3585420	-1.6608660	-0.7406050	H	-3.6206350	0.2593310	0.6045990	C	-4.0193860	-0.2729870	2.7220820
H	2.2789410	-2.1319560	-0.3755170	O	-1.1244100	0.2689290	-1.1655980	H	-4.9848690	-0.3902780	2.237240
C	0.0630600	-2.5671590	1.2357400	O	-0.9724110	0.5191400	1.0872730	H	-3.8465560	-1.0912830	3.4197920
H	0.9794310	-2.8650570	1.7660700	C	1.1204350	2.3805340	1.8122960	H	-4.0395660	0.6762190	3.2680070
H	-0.6991640	-2.3464240	1.9822740	C	1.7522730	-2.1247410	1.0920190	O	-1.8592370	-0.8381890	1.7679400
H	-0.2409960	-3.4141150	0.6166740	H	1.9079780	-2.5352870	0.0992280	O	-3.1875520	0.5833270	0.6639830
H	0.8709370	-2.3992280	-1.3872350	C	-0.7499880	-2.1773510	1.1804860	C	-0.8546670	2.5503830	-1.5658810
H	1.6028170	-0.7702350	-1.3164270	H	-1.5465120	-1.6931350	1.7482070	H	-1.2282550	2.5998880	-2.5968660
Au	3.1042700	0.6709240	0.6012360	H	-1.1283850	-2.3402900	0.1601480	C	-3.0130180	3.1416990	-0.3811450
P	5.4104910	0.4003130	0.1771200	H	-0.5281310	-3.1577320	1.6057570	H	-3.8527840	2.7655080	0.2003740
C	0.7596560	2.3217670	1.7305180	H	1.6317890	-2.9860950	0.4252210	H	-2.5567640	3.9806280	0.1608360
C	6.4278360	0.1979110	1.6943880	H	2.6393960	-1.5573150	0.8125080	H	-3.3853720	3.5502710	-1.3278850
H	6.1051420	-0.6940690	2.2373700	Au	3.3282270	0.6750700	0.5007180	H	-0.5360610	3.5624190	-1.2943120
H	7.4854570	0.0986880	1.4312710	P	5.4606830	0.4904050	-0.5086310	H	0.0103970	1.8837290	-1.5580760
H	6.2966940	1.0683450	2.3421560	C	6.7264580	-0.2805870	0.5771350	Au	0.8583400	-0.0738970	-0.0869110
C	6.1744580	1.8241140	-0.6997050	H	6.4094550	-1.2894900	0.8529680	P	3.1623290	0.1301580	0.4013090
H	7.2426350	1.6462340	-0.8577690	H	7.6874220	-0.3327490	0.0562520	C	3.6952770	-0.9216200	1.8098550
H	5.6842660	1.9656380	-1.6663120	H	6.8403910	0.3131660	1.4877210	H	3.1375480	-0.6408180	2.7067590
H	6.0436090	2.7318780	-0.1050700	C	6.1840120	2.1055560	-0.9988810	H	3.4879930	-1.9703430	1.5829240
C	5.8341860	-1.0601600	-0.8563970	H	7.1707410	1.9568270	-1.4482100	H	4.7664000	-0.7954290	1.9948080
H	6.9171420	-1.1240420	-1.0021040	H	5.5277690	2.5968280	-1.7217310	C	4.2637000	-0.3465720	-0.9893440
H	5.4828860	-1.9708250	-0.3643160	H	6.2805810	2.7470060	-0.1194030	H	4.0602740	0.2918450	-1.8528080

H	5.3125050	-0.2360860	-0.6971440	H	4.8774250	-0.3267850	1.9201210	C	-3.7769010	-1.0349990	-1.6318990
H	4.0735920	-1.3859730	-1.2688580	C	4.1396500	-0.7527540	-1.0038890	H	-3.3180120	-0.7333170	-2.5765940
C	3.6890520	1.8297460	0.8561970	H	3.8823000	-0.3850140	-2.0004590	H	-3.5228100	-2.0794780	-1.4351460
H	4.7600450	1.8475480	1.0800250	H	5.2086200	-0.5989600	-0.8264220	H	-4.8639280	-0.9342590	-1.7086940
H	3.4818010	2.5117960	0.0277660	H	3.9156270	-1.8215380	-0.9567530	C	-4.0794540	-0.4991270	1.2156980
H	3.1307290	2.1635150	1.7344600	C	3.7258330	1.8822360	0.1563750	H	-5.1551540	-0.4271750	1.0275760
C	-1.7154720	-1.5584990	-1.0493260	H	4.8118390	1.9313140	0.2823050	H	-3.8245620	-1.5318870	1.4664010
C	-3.2417810	-1.7892450	-1.0257750	H	3.4557300	2.3019080	-0.8161050	H	-3.8165400	0.1430420	2.0599250
H	-3.6027130	-2.0543340	-0.0286030	H	3.2446750	2.4741500	0.9392370	C	-3.7461980	1.7108890	-0.6572330
H	-3.7974700	-0.9174070	-1.3814360	C	-1.8011710	-1.2693300	-1.3332590	H	-4.8351840	1.7058400	-0.7650130
H	-3.4811920	-2.6285320	-1.6856620	C	-1.1166340	-2.6511200	-1.2682920	H	-3.4646700	2.3927070	0.1490070
C	-0.9915200	-2.8231680	-0.5418390	H	-1.4591120	-3.2699410	-2.1046690	H	-3.2915590	2.0596600	-1.5878720
H	-1.3195200	-3.6876960	-1.1280610	H	-0.0278580	-2.5559060	-1.3372410	C	1.8080000	-1.1502010	1.4210410
H	0.0942190	-2.7316290	-0.6414080	H	-1.3548820	-3.1795400	-0.3404540	C	1.1368130	-2.5394440	1.4067000
H	-1.2263000	-3.0070210	0.5095920	C	-1.4269810	-0.5904950	-2.6666050	H	1.4557750	-3.1098410	2.2856870
C	-1.3046350	-1.3185330	-2.5495490	H	-0.3497030	-0.4080540	-2.7364600	H	0.0451570	-2.4540810	1.4351050
H	-1.8007710	-0.4405000	-2.9728410	H	-1.7143880	-1.2474360	-3.4942560	H	1.4119760	-3.1110220	0.5154370
H	-0.2240610	-1.2064110	-2.6636710	H	-1.9507280	0.3593810	-2.8025140	C	3.3421000	-1.3359300	1.4594350
H	-1.6269510	-2.1989090	-3.1152470	C	-3.3348430	-1.4650100	-1.2995420	H	3.6195020	-1.8846430	2.3653850
6				H	-3.6485140	-2.0572700	-2.1651840	H	3.7075280	-1.9200980	0.6087640
				H	-3.6634610	-2.0097230	-0.4079250	H	3.8669980	-0.3756220	1.4746570
				H	-3.8675250	-0.5090370	-1.3461220	C	1.3700270	-0.3847310	2.6848970
C	-2.0959560	2.1420810	-0.3802770					H	0.2831060	-0.2549990	2.7198180
C	-2.0819070	0.8927320	0.1023670					H	1.6724020	-0.9487240	3.5732930
C	-1.2955030	-0.3738140	-0.1493010	TS ₆₋₃				H	1.8352090	0.6044160	2.7429660
C	-2.6478370	-0.5280550	1.7267550	C	1.8994140	2.2792090	0.1996190				
C	-3.2915020	-1.0209480	2.9630060	C	1.8557330	0.9778530	-0.0013480				
H	-4.3636300	-0.8174190	2.9264710	C	1.3585640	-0.3388410	0.1555430				
H	-3.1000720	-2.0859840	3.0878530	C	2.8292840	-0.6187920	-1.6253690	Species with R ¹ = Me, R ² = H, R ³ =			
H	-2.8715630	-0.4739340	3.8151340	C	3.4023310	-1.4301680	-2.7400360	H:			
O	-1.7174170	-1.1574060	1.1263090	H	4.2482870	-2.0068490	-2.3505400	1			
O	-2.98144900	0.6087990	1.2074410	H	2.6564940	-2.1201370	-3.1352400	C	0.4608050	-0.4404670	-1.3717500
C	-1.12229502	0.6045050	-1.4326290	H	3.7748820	-0.7683840	-3.5235920	C	1.1458960	0.8383750	-1.0933730
H	-1.62615502	0.7576510	-2.3948300	O	1.7265500	-1.0949100	-1.0612860	C	1.6576630	1.9542840	-1.0186830
C	-3.07167803	0.1867130	0.1031880	O	3.3205110	0.4427500	-1.2118390	C	-0.9705980	-0.39023800	0.5919610
H	-3.79188902	0.8046820	0.8268690	C	0.6916830	3.0382950	0.7161070	C	-1.4208260	-1.23349301	0.7536200
H	-2.52665904	0.0210980	0.5622200	H	0.9096740	3.4296470	1.7163330	H	-2.1236130	-0.66698302	0.3637170
H	-3.62415103	0.6016660	-0.7484650	C	3.1316710	3.1202190	-0.0446180	H	-1.9001660	-2.14578401	0.3857760
H	-0.70335103	0.5733980	-1.1355410	H	3.9821820	2.5343100	-0.3857950	H	-0.5591120	-1.53394102	0.3567900
H	-0.29933601	0.9032470	-1.5860900	H	2.9019360	3.8907590	-0.7895750	O	-0.0582220	-1.0584930	-0.1672140
Au	0.8204210	-0.12400500	0.0165320	H	3.4018370	3.6369820	0.8831280	O	-1.34529100	0.7374180	0.3390830
P	3.1473610	0.1406880	0.2587330	H	0.4990100	3.8941750	0.0595150	C	-0.5978880	-0.2892730	-2.4717120
C	3.7933470	-0.46688501	0.8684100	H	-0.20455502	0.4179490	0.7702440	H	-0.11022600	0.0123400	-3.4024870
H	3.3183200	0.0828050	2.6850890	Au	-0.8177050	-0.1002410	-0.0084460	H	-1.0731400	-1.2612780	-2.6278470
H	3.5605200	-1.52900301	0.9793260	P	-3.13941300	0.0214620	-0.2729450	H	-1.35297000	0.4495270	-2.2042470

1

Au	3.1936080	0.7810170	0.1447450	H	5.7855170	-0.8478650	-1.9840090	H	-3.8191480	-1.12032300	9.865800
H	1.8540870	3.0079240	-1.0685650	H	7.2109640	-1.2355940	-0.9824470	H	-3.76511300	4.836830	0.2140990
P	5.0302750	0.0443620	1.3696640	H	5.6993760	-2.1644180	-0.7930980	O	-1.1020070	-1.42633900	3.954630
C	4.5834970	-0.6707690	2.9965860	H	0.6427490	-1.86546300	4.717990	O	-1.37266700	6.097510	1.2314580
H	3.9157880	-1.5233950	2.8522870					C	1.1616670	-2.23802600	1.980530
H	5.4878310	-1.0024680	3.5159610	TS₂₋₃				H	2.1524960	-2.23730900	6.571290
H	4.0718520	0.0821070	3.6008070	C	0.5947410	-1.22042600	2.256860	H	0.7586700	-3.25298500	2.332100
C	6.2134790	1.3988660	1.7241240	C	1.0786980	0.0573920	0.5326100	H	1.2442940	-1.9132370	-0.8412110
H	7.0602310	1.0116650	2.2990830	C	0.4407980	1.1637080	0.9045600	Au	3.4445100	0.6813470	0.4751580
H	6.5764380	1.8236340	0.7852260	C	-1.80615500	2.592410	1.0325440	P	5.7294970	0.4073630	0.0679480
H	5.7137930	2.1827430	2.2981390	C	-3.21867000	6.880180	1.2868350	H	1.1906350	2.1573080	1.0540420
C	5.9983350	-1.24999000	5.065890	H	-3.52840501	3.973600	0.5127400	C	6.7403090	0.4673340	1.5987390
H	6.8513230	-1.54735501	1.1242000	H	-3.8749720	-0.18131701	2.777680	H	7.7991010	0.3364980	1.3557660
H	5.3650790	-2.12048100	3.189280	H	-3.28215401	2.005020	2.2511710	H	6.5980360	1.4312480	2.0936570
H	6.3595510	-0.8614040	-0.4484580	O	-1.4748180	-0.90264500	8.000860	H	6.4235550	-0.32764702	2.783860
H	1.2141540	-1.1605630	-1.6998940	O	-0.94736301	2.914140	1.0888610	C	6.4339380	1.7009340	-1.0261710
				C	0.3577730	-1.7157250	-1.1586010	H	7.5059450	1.5306960	-1.1650220
TS₁₋₂				H	1.2237420	-2.3167690	-1.4648820	H	5.9337470	1.6711080	-1.9972380
C	0.1787400	-0.94857100	1.095100	H	-0.5055230	-2.3873720	-1.1572190	H	6.2782840	2.6857940	-0.5792270
C	1.0701010	0.2297930	0.3881740	H	0.2152080	-0.9021980	-1.8713970	C	6.1664100	-1.1841050	-0.7344240
C	0.7929170	1.4251830	0.6561660	Au	3.1892930	-0.06410200	3.666290	H	7.2480250	-1.2363370	-0.8943430
C	-1.72926800	2.433880	1.1291280	H	0.9023450	2.1171590	1.1172770	H	5.8543890	-2.0157460	-0.0979880
C	-2.97330900	0.003390	1.9332280	P	5.5330120	-0.06959500	2.498230	H	5.6536980	-1.2627880	-1.6963340
H	-3.60488700	8.881310	1.9082600	C	6.2489950	-1.7190530	-0.1208450	H	0.1368120	-1.65154002	0.0199530
H	-3.5145030	-0.86797201	5.510490	H	5.8688860	-2.0758890	-1.0812690				
H	-2.6884380	-0.20987902	9.700600	H	7.3405070	-1.6526050	-0.1645000	TS₄₋₅			
O	-1.0535730	-0.88747100	8.945740	H	5.9601400	-2.42860700	6.584450	C	2.5340780	1.3403500	0.7716450
O	-1.36723101	3.618080	0.7579470	C	6.3416150	0.4650740	1.8081720	C	2.4218950	-0.00289700	3.150170
C	-0.1577520	-1.0726880	-1.3758170	H	7.4296180	0.4393290	1.6939800	C	1.3305420	-0.7120630	-0.0589650
H	0.7640290	-1.2234860	-1.9446330	H	6.0271880	1.4824340	2.0542110	C	4.6269690	0.2274230	-0.2417820
H	-0.8109860	-1.9350530	-1.5305480	H	6.0465880	-0.20110302	6.225510	C	5.9219180	-0.4009680	-0.6300090
H	-0.6514940	-0.1695180	-1.7424450	C	6.2063200	1.0445940	-1.0442720	H	5.7641980	-1.0107290	-1.5260500
Au	3.2101750	0.2193610	0.3500010	H	5.8747580	2.0687110	-0.8560270	H	6.6658240	0.3677120	-0.8338100
H	0.8327780	2.4678920	0.9000790	H	7.3002500	1.0102890	-1.0382900	H	6.2617100	-1.06532500	1.687780
P	5.5377760	0.0119530	0.2757880	H	5.8393640	0.7308460	-2.0246790	O	4.3493820	1.4260960	-0.3548480
C	6.3959460	1.5890170	-0.1038590	H	0.6662680	-1.98325301	0.0004280	O	3.7119860	-0.62205700	2.584380
H	7.4784420	1.4297800	-0.1242870					Au	-0.6570460	-0.2121270	-0.1079320
H	6.0652210	1.9619970	-1.0762030	TS₁₋₄				P	-2.97235400	2.586900	-0.1832100
H	6.1535860	2.3318650	0.6601130	C	0.2310500	-1.31606100	9.808780	H	1.5759640	-1.7491850	-0.3027240
C	6.2712990	-0.56953001	8.531050	C	0.6426620	0.1028340	0.9652860	C	-3.37932001	9.051740	-0.8894410
H	5.8664100	-1.55211402	1.073880	C	1.4079680	1.1069830	0.9030900	H	-4.46242602	0.0602790	-0.8954940
H	7.3589340	-0.63887201	7.553090	C	-1.8694930	-0.36773800	6.672110	H	-2.90523802	6.878780	-0.2918030
H	6.0233070	0.1317710	2.6534340	C	-3.2974010	-0.49948800	2.500530	H	-3.00005101	9.672770	-1.9126610
C	6.1182910	-1.1758380	-0.9961810	H	-3.3643640	-0.9984140	-0.7189950	C	-3.78619900	2.389180	1.4639950

H -4.85371900.4578720 1.3635730
H -3.6602320-0.74594301.9208860
H -3.32330400.9873440 2.1120820
C -3.9371670-0.9344140-1.1938280
H -3.8204620-1.9401050-0.7820710
H -4.9976430-0.6640670-1.1932730
H -3.5631190-0.9307690-2.2208550
H 3.2328710 1.5265530 1.5831210
C 1.5970420 2.4376080 0.4728430
H 0.9300440 2.2237550 -0.3610380
H 1.0131130 2.6412890 1.3821820
H 2.1724410 3.3513340 0.2834050

Species with $R^1 = H$, $R^2 = H$, $R^3 = H$:

1

C 0.1080590 -0.94417301.3065550
C 0.7168840 0.3730770 1.5836590
C 1.0121660 1.5349810 1.8552360
C -1.5175700-0.4931550-0.3777670
C -2.9930200-0.3914780-0.6399600
H -3.1632520-0.2050600-1.6997180
H -3.4937530-1.3147270-0.3348710
H -3.41625800.4252860 -0.0470640
O -1.2708220-0.79175900.9323600
O -0.6264230-0.3367840-1.1880650
Au 3.0353470 0.5836130 1.4022980
H 1.0688690 2.5705810 2.1278640
P 5.3065250 0.1903290 1.0633630
C 6.0260400 -0.98766902.2682390
H 5.5243630 -1.95428302.1812860
H 7.0953090 -1.11426202.0726270
H 5.8851360 -0.60408103.2814520
C 6.3002340 1.7229760 1.2093050
H 7.3569240 1.4941140 1.0417610
H 5.9636500 2.4512120 0.4678690
H 6.1747720 2.1480060 2.2079350
C 5.6770520 -0.4924720-0.5962600
H 6.7553110 -0.6445160-0.7040030
H 5.1614230 -1.4471470-0.7245600
H 5.3302460 0.2035460 -1.3637620
H 0.1023280 -1.54685802.2166170
H 0.6606750 -1.46661500.5233660

TS₁₋₂

C 0.1771860 -0.93720500.1275940
C 1.0773410 0.2329330 0.3932220
C 0.7618450 1.4253650 0.6424240
C -1.72721200.2192500 1.1141640
C -2.95448000.0036290 1.9483440
H -3.66097400.8153570 1.7735770
H -3.4116020-0.96277901.7290420
H -2.66277600.0132900 3.0048320
O -1.0341420-0.90898100.9226880
O -1.38025601.3214190 0.6821540
Au 3.2113950 0.2118260 0.3585240
H 0.7813460 2.4702030 0.8811010
P 5.5394960 0.0064910 0.2819850
C 6.3973470 1.5874090 -0.0820210
H 7.4797070 1.4279160 -0.1066170
H 6.0648450 1.9715670 -1.0493870
H 6.1568810 2.3216860 0.6907670
C 6.2747610 -0.59011901.8529610
H 5.8718310 -1.57600202.0973030
H 7.3625720 -0.65628501.7544980
H 6.0255270 0.1024640 2.6605010
C 6.1190420 -1.1677260-1.0029620
H 5.7839150 -0.8296650-1.9866330
H 7.2117860 -1.2265300-0.9921210
H 5.7011990 -2.1586630-0.8092420
H 0.6418760 -1.88789600.3779600
H -0.1040260-0.9357470-0.9302280

TS₂₋₃

C 0.7244090 -1.13457600.4768660
C 1.0886110 0.1815800 0.6950880
C 0.3938630 1.2784570 0.9658770
C -1.80927700.2463730 0.9599780
C -3.24890100.6105050 1.1575130
H -3.53461401.3842970 0.4385520
H -3.8734730-0.27231601.0266980
H -3.38748001.0229680 2.1616940
O -1.4236590-0.89350800.7063690
O -1.00319601.3194370 1.0965240
Au 3.1866830 -0.01485900.4717990
H 0.7940740 2.2699850 1.1198800
P 5.5301960 -0.07742000.2525450
C 6.1804380 -1.7378600-0.1812570

H 5.7460460 -2.0648900-1.1290420
H 7.2700400 -1.6987350-0.2755100
H 5.9091370 -2.45487100.5974100
C 6.4117900 0.4042630 1.7884330
H 7.4937870 0.3556900 1.6331890
H 6.1314140 1.4229740 2.0679980
H 6.1316690 -0.27298202.5990290
C 6.1715180 1.0455600 -1.0491580
H 5.8800610 2.0744020 -0.8241100
H 7.2628010 0.9797780 -1.0977680
H 5.7482660 0.7636170 -2.0164740
H 0.7815490 -1.87002001.2763510
H 0.6255750 -1.5266740-0.5329100

TS₁₋₄

C 0.3225320 -1.21826600.9167610
C 0.6472960 0.2163980 1.0014380
C 1.3906150 1.2405730 1.0027300
C -1.8124350-0.39168000.6477310
C -3.2325590-0.57739100.2301760
H -3.2767380-1.0266960-0.7642370
H -3.7151740-1.26514300.9330420
H -3.75239300.3795580 0.2477870
O -0.9927360-1.40068000.3394320
O -1.35787000.5897570 1.2425100
Au 3.4139780 0.7776460 0.5514270
P 5.6777030 0.4144400 0.0957760
H 1.1621280 2.2783170 1.2090140
C 6.7369050 0.4638060 1.5934650
H 7.7833330 0.2986820 1.3186710
H 6.6390980 1.4375400 2.0796740
H 6.4193660 -0.31361502.2927770
C 6.4042990 1.6531910 -1.0462080
H 7.4641640 1.4363110 -1.2116210
H 5.8750490 1.6256210 -2.0017630
H 6.3024590 2.6520870 -0.6149850
C 6.0172870 -1.2153730-0.6767050
H 7.0914850 -1.3341880-0.8482020
H 5.6666730 -2.0121770-0.0162110
H 5.4875950 -1.2875730-1.6298970
H 0.3216940 -1.68656901.9058550
H 1.0281760 -1.73071500.2615900

TS₄₋₅

C	2.4280570	1.1159780	0.9756150	P	5.4639340	0.0801410	1.2832240	C	6.3085850	-0.58302301	1.7685940
C	2.4362520	-0.16776200	0.4089130	C	5.8759890	-0.82746402	0.8208120	H	5.9126620	-1.57209902	0.0111700
C	1.3680680	-0.8677730	-0.0646720	H	5.3250860	-1.77052802	0.8488240	H	7.3919070	-0.64969201	0.6297680
C	4.5889620	0.2983250	-0.1415180	H	6.9503330	-1.03318902	0.8542470	H	6.0904800	0.0966630	2.5959080
C	5.9164230	-0.1748890	-0.6246900	H	5.5940000	-0.22683703	0.6888980	C	6.0500440	-1.1084630	-1.0917720
H	5.7795910	-0.6956220	-1.5785270	C	6.5232930	1.5754330	1.2857840	H	5.6635680	-0.7613790	-2.0531170
H	6.5903010	0.6698310	-0.7583090	H	7.5736140	1.2825900	1.3775910	H	7.1427190	-1.1513860	-1.1339960
H	6.3306310	-0.89148100	0.0895780	H	6.3802010	2.1294640	0.3549610	H	5.6553320	-2.1078070	-0.8926980
O	4.2152440	1.4761390	-0.1177160	H	6.2515710	2.2185420	2.1260890	H	0.5993350	-1.84094800	0.5375740
O	3.7582610	-0.67839200	0.2807960	C	6.0768600	-0.9622940	-0.0936620	C	-0.1360270	-1.0508730	-1.3106980
Au	-0.5941950	-0.2931450	-0.0843330	H	7.1461820	-1.15438800	0.0365020	C	-0.2017850	-2.3395630	-1.8594990
P	-2.88084100	0.3124160	-0.1500010	H	5.5366120	-1.9118130	-0.1059690	C	-0.37933400	0.0614890	-2.1291200
H	1.6232060	-1.8779080	-0.3954280	H	5.9129130	-0.4486160	-1.0437760	C	-0.5096690	-2.5163950	-3.2109900
C	-3.19911501	0.9770240	-0.8581450	H	0.8581650	-1.58506100	0.5845040	H	-0.0127820	-3.2049450	-1.2298680
H	-4.27335202	0.1857360	-0.8635650	C	0.7032470	-0.9761330	-1.4574960	C	-0.6921520	-0.1170300	-3.4786520
H	-2.68586602	0.7350220	-0.2610040	C	0.7888190	-2.2943980	-1.9301140	H	-0.32465301	0.0640410	-1.7174730
H	-2.81765002	0.0187140	-1.8815100	C	0.8944300	0.0898370	-2.3459080	C	-0.7567870	-1.4047360	-4.0221530
C	-3.67918200	0.3442310	1.5044500	C	1.0518310	-2.5442650	-3.2787240	H	-0.5549310	-3.5182070	-3.6273410
H	-4.73215700	0.6277670	1.4130070	H	0.6492520	-3.1259180	-1.2440690	H	-0.88084100	0.7492360	-4.1056480
H	-3.6098110	-0.64549901	0.9629810	C	1.1653270	-0.1618670	-3.6935360	H	-0.9958100	-1.5400820	-5.0728360
H	-3.16520301	0.0647130	2.1457540	H	0.8234930	1.1119160	-1.9901510				
C	-3.9172690	-0.8274070	-1.1500560	C	1.2418890	-1.4769710	-4.1629490	TS ₂₋₃			
H	-3.8504250	-1.8380710	-0.7394300	H	1.1151540	-3.5678930	-3.6353810	C	0.4760860	-1.16194800	0.1962230
H	-4.9611160	-0.4994130	-1.1377970	H	1.3119230	0.6700730	-4.3758810	C	1.1378530	0.0798470	0.5202660
H	-3.5547660	-0.8430900	-2.1810550	H	1.4510970	-1.6694060	-5.2111050	C	0.5056610	1.1881580	0.9005870
H	3.0735030	1.3812600	1.8044380				C	-1.71796700	0.2874910	0.9833640	
H	1.6003660	1.7842770	0.7571530	TS ₁₋₂			C	-3.15911700	0.6289820	1.1783010	
				C	0.1563790	-0.91449700	0.1736370	H	-3.53853301	0.0774950	0.2528470
				C	1.0517620	0.2389610	0.5101970	H	-3.7282830	-0.27442401	0.3957410
Species with R ¹ = Ph, R ² = H, R ³ =				C	0.8160980	1.4147080	0.8783740	H	-3.26994501	0.3621250	1.9800130
H:				C	-1.76653900	0.2617020	1.2311980	O	-1.3383870	-0.87976900	0.7726940
1				C	-3.0830770	-0.02646201	0.8931960	O	-0.90166801	0.3255740	1.0396780
C	0.3928670	-0.77460700	0.0184770	H	-3.47862400	0.8861130	2.3384110	Au	3.2297370	-0.03024400	0.4007470
C	0.8798740	0.4981800	0.5955000	H	-3.7849900	-0.39530701	1.1374790	H	0.9574290	2.1354600	1.1560580
C	1.1565010	1.5649520	1.1392290	H	-2.9680810	-0.80616902	0.6500160	P	5.5753670	-0.09552800	0.3015110
C	-1.9325590	-0.0530020	-0.0837570	O	-1.1053140	-0.86450800	0.9302160	C	6.2629850	-1.7594680	-0.0635590
C	-3.3317500	-0.51208900	0.2217990	O	-1.36024201	0.3995210	0.9934040	H	5.8799150	-2.1110140	-1.0248770
H	-4.03114900	0.3014830	0.0312810	Au	3.1928100	0.2327620	0.3996620	H	7.3559040	-1.7165710	-0.1023250
H	-3.5795320	-1.3646630	-0.4191360	H	0.8819060	2.4353020	1.1983340	H	5.9558530	-2.46248900	0.7148660
H	-3.4087440	-0.84442401	0.2602170	P	5.5164930	0.0393500	0.2358180	C	6.3953310	0.4194210	1.8623770
O	-1.0178330	-0.97339200	0.3329080	C	6.3527470	1.6309090	-0.1307920	H	7.4829420	0.3714100	1.7515910
O	-1.62092400	0.9865720	-0.6280980	H	7.4343240	1.4774540	-0.1950500	H	6.1016930	1.4426240	2.1104780
Au	3.2014060	0.5921220	1.0873850	H	5.9851400	2.0285240	-1.0798210	H	6.0844800	-0.24142202	0.6754100
H	1.1503340	2.5559910	1.5496280	H	6.1353370	2.3511260	0.6617230	C	6.2927090	1.0000620	-0.9869090

H	5.9866530	2.0329510	-0.8028400	C	1.8167460	-3.26548700	.6541880	H	1.2468580	-0.1963270	-1.8997890
H	7.3852370	0.9376250	-0.9713700	C	1.2436710	-1.9942930	-1.3321640	C	2.5417350	-3.2346900	-2.7230270
H	5.9266640	0.6961500	-1.9708650	C	2.6194700	-4.1100860	-0.1191200	H	2.3170140	-5.0499410	-1.5718760
H	0.5942840	-1.96004200	.9257530	H	1.7233770	-3.43426101	.7233830	H	2.5851040	-1.2961260	-3.6753720
C	0.2735030	-1.6224900	-1.1792930	C	2.0380680	-2.8443110	-2.1019760	H	3.1223330	-3.7137960	-3.5057510
C	0.0162860	-2.9883040	-1.4076200	H	0.7098320	-1.1749310	-1.8043260	Species with $R^1 = p\text{-C}_6\text{H}_4\text{-OMe}$, $R^2 = \text{H}$, $R^3 = \text{H}$:			
C	0.3100040	-0.7302000	-2.2690890	C	2.7287290	-3.9016950	-1.4964970				
C	-0.1967030	-3.4554500	-2.7035420	H	3.1493540	-4.93107600	.3540480				
H	-0.0149050	-3.6765330	-0.5675850	H	2.1184820	-2.6829630	-3.1726830				
C	0.0931350	-1.1996110	-3.5615230	H	3.3466340	-4.5612130	-2.0985630				
H	0.5157200	0.3214160	-2.0957090	TS₄₋₅				1			
C	-0.1598070	-2.5612200	-3.7795140					C	1.3517760	-1.27135500	.7321760
H	-0.3909120	-4.5092530	-2.8759770					C	0.3073860	-1.7049300	-0.2226880
H	0.1232970	-0.5113480	-4.4003410					C	-0.5114650	-2.1864470	-1.0026510
H	-0.3257250	-2.9242470	-4.7894630					C	2.8802550	-3.07963200	.1373020
TS₁₋₄				C	1.2822590	0.8704670	0.8189970	C	3.7920180	-4.11245000	.7417350
				C	-1.9925780	-0.24318800	.4243020	H	4.1766050	-4.7621770	-0.0441000
				C	-3.37613400	.2999270	0.5303970	H	4.6278790	-3.60789901	.2377990
				H	-3.43986101	.2126110	-0.0722080	H	3.2633650	-4.69951201	.4968820
				H	-4.0952640	-0.43066200	.1629380	O	2.2007650	-2.40438101	.1038930
C	0.2404780	-1.32342200	.8992730	H	-3.58961700	.5678510	1.5678720	O	2.7469520	-2.8500330	-1.0481470
C	0.6612600	0.0957860	0.9184060	O	-1.6692270	-1.2345400	-0.2506800	Au	-1.7284960	-0.4610260	-0.1983650
C	1.4208920	1.1039140	0.8916910	O	-1.05308300	.4132310	1.0985970	H	-1.0129670	-2.7617200	-1.7565110
C	-1.8817410	-0.36118700	.7304480	Au	3.3041460	0.6333450	0.5187110	P	-3.39001601	.1059310	0.2556440
C	-3.3283290	-0.48833700	.3778880	P	5.6436630	0.4677320	0.2616190	C	-4.38921400	.7051030	1.7383810
H	-3.4419830	-0.9761620	-0.5923150	H	0.9576390	1.8349690	1.2176810	H	-3.74151900	.6653450	2.6173700
H	-3.8154720	-1.11654401	.1317200	C	6.1888010	-0.6554230	-1.0876470	H	-5.15759101	.4698680	1.8874830
H	-3.79577900	.4957580	0.3761250	H	7.2813550	-0.6767720	-1.1486900	H	-4.8677220	-0.26821701	.6063220
O	-1.1288820	-1.41246100	.3901290	H	5.8171150	-1.6650300	-0.8949210	C	-4.58549201	.2705610	-1.1235310
O	-1.36185400	.6008850	1.2970260	H	5.7811460	-0.3084500	-2.0405490	H	-5.33675602	.0251530	-0.8719550
Au	3.4609830	0.6902640	0.4529230	C	6.5121560	-0.15497501	.7572200	H	-4.05873301	.5715630	-2.0320790
P	5.7510180	0.4491800	0.0631620	H	7.5911330	-0.20176001	.5805400	H	-5.07864300	.3117610	-1.2999930
H	1.2088600	2.1470960	1.0902150	H	6.3124530	0.5116370	2.6000460	C	-2.72171502	.7885110	0.5405900
C	6.7462480	0.5583200	1.6010040	H	6.1429610	-1.15315402	.0060790	H	-3.54351603	.4865060	0.7275530
H	7.8096830	0.4447890	1.3701060	C	6.4658870	2.0686140	-0.1136420	H	-2.05246002	.7762890	1.4040410
H	6.5794140	1.5288130	2.0747810	H	6.2666010	2.7804800	0.6914700	H	-2.16036403	.1138690	-0.3383780
H	6.4388930	-0.22935702	.2932360	H	7.5466550	1.9273970	-0.2126060	H	0.8564740	-1.05648001	.6820970
C	6.4424900	1.7340270	-1.0490430	H	6.0674770	2.4756170	-1.0465420	C	2.1364520	-0.04479100	.3093890
H	7.5190110	1.5807210	-1.1723650	H	-0.1145120	-2.10342501	.0883290	C	2.6370020	0.7947190	1.3112410
H	5.9541950	1.6745510	-2.0247120	C	1.0404340	-1.9980910	-0.7134380	C	2.3960090	0.2791940	-1.0331660
H	6.2636370	2.7245670	-0.6239180	C	1.3276440	-3.3817320	-0.6423360	C	3.3911080	1.9293690	1.0012570
C	6.2230610	-1.1477910	-0.7063770	C	1.4985290	-1.2474420	-1.8224590	H	2.4413440	0.5666720	2.3557660
H	7.3058830	-1.1802560	-0.8632380	C	2.0870340	-3.9915040	-1.6348190	C	3.1378790	1.4081020	-1.3575020
H	5.9259780	-1.9730860	-0.0548950	H	0.9599110	-3.96134200	.1991990	H	2.0228810	-0.3581240	-1.8272320
H	5.7136830	-1.2547410	-1.6671890	C	2.2423930	-1.8679410	-2.8191480	C	3.6442710	2.2402890	-0.3431900
H	0.2091670	-1.69782401	.9278910								
C	1.1291330	-2.20749600	.0491120								

H 3.7627530 2.5549800 1.8034580
H 3.3402170 1.6620970 -2.3931020
O 4.3583920 3.3197190 -0.7622780
C 4.9141730 4.2020280 0.2182590
H 5.6198760 3.6731610 0.8681860
H 5.4421040 4.9719740 -0.3439940
H 4.1266370 4.6649430 0.8231910

TS₁₋₂

C 1.3162800 1.1314180 -0.8096870
C 0.1487360 1.3345620 0.1067950
C -0.04852702.1143280 1.0693530
C 2.2833210 3.3030850 -0.0615660
C 3.1944500 4.3984700 -0.5368040
H 3.1465550 5.2421680 0.1513460
H 4.2200010 4.0147810 -0.5681030
H 2.9236280 4.7099990 -1.5484410
O 2.0644220 2.3890050 -1.0150310
O 1.8082030 3.2610120 1.0742710
Au -1.68149000.2180200 0.0752740
H -0.45549602.6610960 1.8961790
P -3.6144210-1.0837330-0.1104290
C -4.5697530-1.18819601.4523940
H -5.4628210-1.80339701.3050420
H -3.9478270-1.63213502.2335100
H -4.8690590-0.18528301.7662650
C -4.8005260-0.4573630-1.3611620
H -4.3218540-0.4351560-2.3432790
H -5.6804190-1.1067050-1.4004760
H -5.10985200.5565520 -1.0961840
C -3.2706720-2.8206330-0.5907900
H -2.6197760-3.28511200.1540250
H -4.2063740-3.3839820-0.6571110
H -2.7677030-2.8404550-1.5606420
H 0.9606100 0.9229980 -1.8181180
C 2.2561910 0.0287160 -0.3722260
C 2.8867950 -0.7430580-1.3549700
C 2.5603000 -0.22071500.9774890
C 3.8061400 -1.7403610-1.0190180
H 2.6640300 -0.5680280-2.4043240
C 3.4736770 -1.20700801.3273180
H 2.0809190 0.3561710 1.7615760
C 4.1057270 -1.97334700.3314340
H 4.2723540 -2.3193500-1.8066580

H 3.7108640 -1.40222102.3682380
O 4.9825770 -2.91382100.7746090
C 5.6741410 -3.7198310-0.1855120
H 6.3169190 -4.38167500.3945320
H 4.9720460 -4.3169370-0.7776550
H 6.2879530 -3.1008880-0.8490490

TS₂₋₃

C 1.2141710 1.0281640 -0.8159870
C 0.1007130 1.4592750 0.0284690
C 0.1504060 2.5784800 0.7476690
C 2.2366770 3.3776360 -0.0974190
C 3.2945900 4.4239590 0.0051790
H 4.0048680 4.1198590 0.7832060
H 3.8281490 4.5058040 -0.9418710
H 2.8571530 5.3811870 0.2934550
O 2.3097290 2.4624700 -0.9514900
O 1.2584520 3.4806420 0.7704630
Au -1.58894500.2299230 0.0018160
H -0.61134502.9770660 1.4012490
P -3.5141640-1.1182830-0.0260880
C -3.3662720-2.6141350-1.0837440
H -2.5430750-3.2369890-0.7247480
H -4.2958670-3.1909640-1.0557490
H -3.1566490-2.3160120-2.1142350
C -5.0111580-0.2550980-0.6503400
H -5.8718970-0.9307720-0.6408060
H -5.22371000.6113890 -0.0189450
H -4.83445500.0907840 -1.6719810
C -4.0018200-1.76142901.6245720
H -4.2012880-0.92438802.2985340
H -4.8997900-2.38160101.5414990
H -3.1867100-2.35916402.0404090
H 0.9969750 1.0260630 -1.8817470
C 2.1169690 -0.0474710-0.3950090
C 2.8486400 -0.7536370-1.3658680
C 2.3000580 -0.38227300.9649210
C 3.7385970 -1.7640750-1.0107250
H 2.7207570 -0.5088680-2.4168530
C 3.1821100 -1.38252901.3334430
H 1.7389410 0.1452730 1.7301010
C 3.9120100 -2.08062100.3482280
H 4.2843680 -2.2911190-1.7832920
H 3.3268340 -1.64768102.3755610

O 4.7497560 -3.03693400.8086210
C 5.5389820 -3.7858840-0.1265820
H 6.1302780 -4.47401400.4763990
H 4.8998390 -4.3518400-0.8119210
H 6.2042040 -3.1253110-0.6920120

TS₁₋₄

C 2.6577470 -0.25223900.6887550
C 1.8840140 -1.45358800.3050120
C 0.8910710 -2.19448900.0568520
C 4.4383820 -1.5433800-0.1058110
C 5.8354130 -1.6320090-0.6299520
H 5.9739330 -0.9290120-1.4545550
H 6.5293210 -1.35277900.1700010
H 6.0451160 -2.6514000-0.9516420
O 3.9688560 -0.29986500.0285990
O 3.7247910 -2.50024700.2003880
Au -1.0061050-1.23885800.0154950
P -3.1783200-0.3828320-0.0494820
H 0.8562360 -3.2624300-0.1215970
C -4.1342710-0.71321101.4816300
H -5.1438540-0.30094901.3909670
H -4.1973830-1.79135901.6478070
H -3.6301780-0.25401402.3355210
C -4.1912050-1.0866000-1.4078220
H -5.1971360-0.6559510-1.3883090
H -3.7205010-0.8658760-2.3690910
H -4.2584290-2.1707420-1.2889950
C -3.25207201.4353470 -0.2835980
H -4.29347801.7715790 -0.2924770
H -2.71687401.9307150 0.5301150
H -2.77729201.7023270 -1.2308340
H 2.8584470 -0.28990001.7645840
C 1.9757430 1.0453910 0.3320920
C 1.6821990 1.9685090 1.3383410
C 1.6528570 1.3585040 -1.0002540
C 1.0738930 3.1917740 1.0392700
H 1.9309060 1.7439810 2.3719120
C 1.0576320 2.5718530 -1.3120000
H 1.8729170 0.6532130 -1.7959900
C 0.7608530 3.4977580 -0.2927290
H 0.8612470 3.8873810 1.8414630
H 0.8123540 2.8259560 -2.3381170
O 0.1730670 4.6535320 -0.6996150

C -0.14566605.6491490 0.2792480
H -0.59598206.4723640 -0.2748280
H -0.86259305.2644560 1.0127830
H 0.7570960 6.0007320 0.7902490

H 0.7193810 6.6806110 -0.4954280
H 0.3677760 5.6964410 0.9532400
H 2.0662490 5.9706940 0.4391140

C -4.8439650-2.2380820-0.1736460
F -5.8389370-2.15221300.7440830
F -5.4241670-2.1606300-1.3965680
F -4.3371320-3.5016310-0.0699550

TS₄₋₅

C 2.3725040 -0.47396200.7794060
C 1.8850190 -1.71392800.1447410
C 0.6604170 -2.0933950-0.2288420
C 4.1459060 -2.0356920-0.0119120
C 5.3333620 -2.8569470-0.3750850
H 5.3194870 -3.0291770-1.4570710
H 6.2490540 -2.3340380-0.1025850
H 5.2772180 -3.82850100.1209780
O 4.1840070 -0.81403500.2428150
O 2.9788510 -2.65017900.0186230
Au -1.1381790-1.1016780-0.0723290
P -3.2617470-0.09095900.1108750
H 0.6284780 -3.1213940-0.5975480
C -3.27796701.7316230 -0.1292170
H -4.29711902.1194470 -0.0348240
H -2.64009802.2068650 0.6202840
H -2.89036501.9730800 -1.1222830
C -4.0640750-0.34596501.7453590
H -5.04436200.1398730 1.7718720
H -4.1861290-1.41669201.9280280
H -3.43205900.0722170 2.5330490
C -4.4880640-0.7214770-1.1051640
H -4.6142420-1.7990620-0.9722290
H -5.4534590-0.2243750-0.9687450
H -4.1258450-0.5347840-2.1194560
H 2.6717650 -0.56631501.8220400
C 1.9782340 0.8435150 0.3759710
C 2.0807420 1.9016270 1.3076920
C 1.5406100 1.1407000 -0.9415080
C 1.7371480 3.2015700 0.9670890
H 2.4280660 1.6926740 2.3155560
C 1.2094720 2.4314940 -1.2962100
H 1.4778720 0.3470050 -1.6769700
C 1.2998480 3.4743680 -0.3451600
H 1.8142150 3.9887150 1.7061730
H 0.8815390 2.6727010 -2.3016840
O 0.9524110 4.6947850 -0.7886310
C 1.0373110 5.8242070 0.0973290

Species with $R^1 = p\text{-C}_6\text{H}_4\text{-CF}_3$, $R^2 =$
H, $R^3 = \text{H}$:

1

C -0.65467601.7091700 0.7075380
C 0.3839510 1.8286310 -0.3393420
C 1.2216110 2.0667800 -1.2058330
C -1.80750003.7519780 0.0719170
C -2.38746005.0168050 0.6402980
H -2.79929005.6218250 -0.1667700
H -3.17662504.7687810 1.3569600
H -1.61736005.5778630 1.1770190
O -1.19776903.0156030 1.0465490
O -1.84966703.3959080 -1.0874820
Au 2.1494160 0.2307790 -0.2543510
H 1.7744010 2.4513060 -2.0410920
P 3.5211470 -1.56396400.3083440
C 4.5408450 -1.25551701.7985500
H 3.8906100 -1.06218602.6550940
H 5.1654390 -2.12955202.0063910
H 5.1780970 -0.38348101.6341590
C 4.6991730 -1.9815640-1.0323180
H 5.3127150 -2.8362330-0.7314950
H 4.1465800 -2.2331870-1.9406950
H 5.3455580 -1.1245470-1.2360990
C 2.5881640 -3.10331200.6515740
H 3.2856480 -3.90624200.9094960
H 1.9003550 -2.93897401.4842860
H 2.0140440 -3.3898980-0.2326030
H -0.15141701.4295640 1.6360770
C -1.74277800.6804280 0.4226220
C -2.46374600.1803290 1.5161120
C -2.04661500.2322070 -0.8674130
C -3.4837980-0.74983101.3246610
H -2.23304800.5196140 2.5216690
C -3.0614150-0.7047130-1.0651340
H -1.50277100.6183640 -1.7218890
C -3.7816460-1.19085300.0304260
H -4.0392380-1.12786002.1759170
H -3.2939950-1.0438110-2.0685360

TS₁₋₂

C 0.6721750 1.5579600 -0.8465270
C -0.44687001.5061340 0.1495690
C -0.69435002.1909100 1.1714330
C 1.3202050 3.8096700 -0.0117970
C 1.9809750 5.0740530 -0.4774750
H 1.9274370 5.8273830 0.3077810
H 3.0285420 4.8648560 -0.7170540
H 1.4979450 5.4367650 -1.3887680
O 1.2072720 2.9152400 -1.0054990
O 0.9343880 3.6252290 1.1425910
Au -2.06279000.0988330 0.1233900
H -1.12843302.6144370 2.0551140
P -3.7372460-1.5161060-0.1063390
C -4.4591610-2.06331501.4890800
H -5.2291230-2.82051701.3112560
H -3.6741840-2.48603802.1207670
H -4.9041830-1.20837902.0037780
C -5.1586270-0.9475890-1.1175770
H -4.8103760-0.6668480-2.1146770
H -5.9002320-1.7474840-1.2042820
H -5.6186520-0.0756830-0.6460300
C -3.1385130-3.0458440-0.9212460
H -2.3347750-3.4865590-0.3265750
H -3.9573570-3.7654990-1.0153760
H -2.7521240-2.8051950-1.9145000
H 0.2876070 1.3467030 -1.8434710
C 1.8053370 0.5921050 -0.5338200
C 2.3802600 -0.1283880-1.5880710
C 2.3063950 0.4325360 0.7655770
C 3.4463520 -0.9981150-1.3537570
H 1.9965880 -0.0158270-2.5976810
C 3.3739550 -0.43042001.0053390
H 1.8650820 0.9752650 1.5943780
C 3.9406780 -1.1478930-0.0550950
H 3.8810720 -1.5553970-2.1759600
H 3.7548980 -0.54996502.0137820
C 5.1194650 -2.04823400.2054500
F 6.2963750 -1.35924500.1919820

F 5.0484100 -2.65402401.4180080
 F 5.2403770 -3.0304410-0.7209240

TS₂₋₃

C -0.51785801.4333630 0.8557240
 C 0.5761530 1.6781060 -0.0330950
 C 0.7527180 2.7746430 -0.7669020
 C -1.16229704.0179490 0.0027690
 C -1.95373205.2642120 -0.2309240
 H -2.55923605.1292620 -1.1344390
 H -2.61263705.4487650 0.6170220
 H -1.28510506.1120070 -0.3958650
 O -1.46484403.1899600 0.8762780
 O -0.12633303.8832920 -0.8176980
 Au 1.9508590 0.0844320 0.0040450
 H 1.5807090 2.9745950 -1.4312840
 P 3.5022280 -1.6794560-0.0051580
 C 3.1322900 -2.98719201.2302580
 H 2.1493140 -3.41800301.0237900
 H 3.8901020 -3.77556001.1860760
 H 3.1213300 -2.55178002.2325420
 C 5.2274930 -1.16282400.3528220
 H 5.8934830 -2.03092400.3302020
 H 5.5551650 -0.4357370-0.3944320
 H 5.2744680 -0.69696101.3402410
 C 3.5970620 -2.5579900-1.6148840
 H 3.8918260 -1.8550510-2.3981460
 H 4.3295830 -3.3692550-1.5624130
 H 2.6164060 -2.9707290-1.8647490
 H -0.30823801.5481560 1.9168860
 C -1.63668200.5383650 0.5435860
 C -2.45751700.0870760 1.5944090
 C -1.91617300.1410600 -0.7761730
 C -3.5375110-0.74950701.3321910
 H -2.24821000.3942790 2.6143670
 C -2.9964830-0.6949560-1.0425550
 H -1.28320700.4820950 -1.5886460
 C -3.8028880-1.13793400.0128290
 H -4.1669720-1.09584102.1449240
 H -3.2091770-1.0013810-2.0599340
 C -4.9638070-2.0678620-0.2441620
 F -6.1170920-1.59673700.2970430
 F -4.7529580-3.29255600.3102190
 F -5.1961800-2.2675200-1.5608580

TS₁₋₄

C 2.7275240 0.0753330 0.7443770
 C 2.3306030 -1.25131600.2175510
 C 1.5807810 -2.2062190-0.1266130
 C 4.7957510 -0.5461020-0.1355150
 C 6.1574340 -0.1620120-0.6141540
 H 6.0904470 0.6680480 -1.3207820
 H 6.7471910 0.1742830 0.2455330
 H 6.6444810 -1.0227050-1.0707110
 O 3.9837340 0.4857400 0.1266690
 O 4.3880090 -1.69519300.0348380
 Au -0.5014420-1.7670870-0.0547260
 P -2.8216500-1.5011300-0.0097840
 H 1.8159140 -3.2187820-0.4293950
 C -3.6199110-2.40762301.3710630
 H -4.7027110-2.25166701.3447280
 H -3.4047590-3.47509801.2801350
 H -3.2242240-2.04761202.3238750
 C -3.6533800-2.1093230-1.5272200
 H -4.7357330-1.9722580-1.4404090
 H -3.2858180-1.5557850-2.3946840
 H -3.4323090-3.1704200-1.6657700
 C -3.36843900.2398420 0.1753010
 H -4.46148100.2871490 0.1952160
 H -2.97036100.6528150 1.1052250
 H -2.99552000.8333320 -0.6628810
 H 2.9231190 -0.01155701.8183320
 C 1.6942060 1.1556160 0.4886720
 C 1.0346670 1.7386780 1.5747940
 C 1.4073830 1.5788210 -0.8159480
 C 0.0868650 2.7416270 1.3632570
 H 1.2573200 1.4162680 2.5873360
 C 0.4684630 2.5848720 -1.0307010
 H 1.9170380 1.1321630 -1.6633610
 C -0.19583903.1600310 0.0601970
 H -0.42293403.1908230 2.2082450
 H 0.2509310 2.9141260 -2.0407210
 C -1.17724504.2796390 -0.1696970
 F -0.56830305.4987110 -0.1584550
 F -2.14278104.3252990 0.7820400
 F -1.80658804.1780030 -1.3673650

TS₄₋₅

C -2.2390720-1.21502000.8114980
 C -2.8220890-0.04952400.1836870
 C -2.25983401.1061170 -0.2191640
 C -4.5859450-1.4788850-0.1402100
 C -5.9996400-1.7032220-0.5546630
 H -6.1276870-1.3374030-1.5790800
 H -6.2397230-2.7643200-0.5101170
 H -6.6672420-1.12753800.0914110
 O -3.7330740-2.3680290-0.0063200
 O -4.2440960-0.20679500.0821750
 Au -0.31659101.7638890 -0.0795720
 P 1.8731530 2.6257110 0.0992200
 H -3.00103001.8235270 -0.5803630
 C 3.0744220 1.4703440 0.8732460
 H 4.0688180 1.9253150 0.9155500
 H 2.7461150 1.2255570 1.8866800
 H 3.1230290 0.5479890 0.2886110
 C 1.9836460 4.1578430 1.1077170
 H 3.0185190 4.5101800 1.1562440
 H 1.3579520 4.9348240 0.6611130
 H 1.6223040 3.9566490 2.1194770
 C 2.6356410 3.0742840 -1.5116790
 H 2.0287800 3.8389560 -2.0032420
 H 3.6490160 3.4582380 -1.3591630
 H 2.6774690 2.1926670 -2.1561920
 H -2.6664040-1.51660301.7647790
 C -0.9364170-1.75523500.5134150
 C -0.2610790-2.47925601.5213570
 C -0.3371320-1.6058560-0.7566810
 C 1.0032490 -3.00224101.2818240
 H -0.7255290-2.61288902.4930770
 C 0.9196340 -2.1474950-1.0022310
 H -0.8697430-1.0932080-1.5484650
 C 1.5889850 -2.83228700.0196920
 H 1.5268670 -3.54078802.0637750
 H 1.3760980 -2.0401620-1.9791680
 C 2.9421660 -3.4520760-0.2439860
 F 2.8422830 -4.7920350-0.4486080
 F 3.7875780 -3.28124000.8021800
 F 3.5472440 -2.9311940-1.3354430

Species with R¹ = C₂H₃, R² = H, R³ = H:

1		Au	-0.7423950 -0.1707420 -0.0826500	C	3.8357930 -0.5922310 1.5523560
C	-2.39208200.5892480 -0.8188390	H	1.5856840 -2.0479980 -1.5404000	H	3.5372420 -1.6168260 1.7881540
C	-1.5749070 -0.6430140 -0.6900760	P	-3.0632370 -0.02696200.1579330	H	4.9258620 -0.5423750 1.4699900
C	-1.0814180 -1.7691240 -0.7002640	C	-3.9858240 -1.0285120 -1.0717870	H	3.5027460 0.0648500 2.3595580
C	-4.1939880 -0.18609200.6181070	H	-5.0628110 -0.8934060 -0.9321440	H	-1.9644490 1.2310260 -1.4162860
C	-5.6797190 -0.41582500.6473220	H	-3.7092450 -0.7138550 -2.0809170	C	-2.1233550 2.0676750 0.5718370
H	-5.9643440 -0.8304460 1.6138670	H	-3.7337630 -2.0845820 -0.9487930	C	-2.2694310 3.3317170 0.1391130
H	-6.20158000.5320660 0.4826290	C	-3.6639430 -0.5876750 1.7979770	H	-2.0734430 1.8354180 1.6321620
H	-5.9724040 -1.0979240 -0.1558830	H	-3.20586900.0196260 2.5825700	H	-2.3402870 4.1615230 0.8352130
O	-3.79552800.2595480 -0.6070390	H	-4.7522990 -0.4885090 1.8527160	H	-2.3138190 3.5680160 -0.9210050
O	-3.4223860 -0.3613770 1.5400080	H	-3.3859440 -1.6329090 1.9531930		
Au	0.7164500 -0.4729700 -0.1948620	C	-3.7048210 1.6811200 -0.0314400	TS₁₋₄	
H	-0.8534000 -2.8161620 -0.7434560	H	-3.4542330 2.0600480 -1.0252400	C	-2.70975900.8799530 -0.4138360
P	2.8544000 0.3012090 0.3118320	H	-4.7917540 1.6868860 0.0960020	C	-2.0664830 -0.4508380 -0.3431280
C	3.5352430 1.4197870 -0.9701310	H	-3.2483760 2.3301920 0.7198150	C	-1.1403580 -1.3070940 -0.2767310
H	2.8931330 2.2979650 -1.0719160	H	1.9014630 1.2266990 1.3463350	C	-4.5976600 -0.37134100.1446400
H	4.5434180 1.7369370 -0.6866000	C	2.6315460 1.9536150 -0.5373160	C	-5.9887170 -0.43691700.6853830
H	3.5752000 0.8970710 -1.9287250	C	2.4198150 3.2360240 -0.2329560	H	-6.04557400.0853900 1.6429940
C	4.0698020 -1.06011400.4785140	H	3.0346540 1.6591750 -1.5034560	H	-6.66094100.0701840 -0.0151370
H	5.0544520 -0.64531800.7146160	H	2.6480210 4.0255870 -0.9423160	H	-6.2954220 -1.47667200.7919900
H	3.7587770 -1.7362520 1.2782300	H	2.0106410 3.5377880 0.7281960	O	-4.00063600.8178250 0.2755820
H	4.1259750 -1.6199420 -0.4580280			O	-3.9914340 -1.2972960 -0.3972480
C	2.9339300 1.2359120 1.8857430	TS₂₋₃		Au	0.8051600 -0.4756370 -0.0636250
H	3.9607320 1.5686560 2.0657280	C	-2.01594600.9536830 -0.3653680	P	3.0258780 0.2181060 0.1437330
H	2.2747700 2.1054630 1.8312380	C	-1.3859440 -0.28188500.0114110	H	-1.1739440 -2.3881070 -0.3259610
H	2.6093610 0.5962950 2.7099830	C	-2.0261910 -1.40619200.3244920	C	4.0336500 -0.1431570 -1.3462550
H	-2.37273300.8807510 -1.8725420	C	-4.2635260 -0.6517000 -0.1303030	H	5.0655550 0.1861630 -1.1907810
C	-1.9196050 1.7499540 0.0246940	C	-5.7042480 -1.0430870 -0.0650480	H	4.0219530 -1.2179640 -1.5428740
C	-1.7109350 2.9594990 -0.5025260	H	-6.0166810 -1.06712200.9847700	H	3.6128840 0.3775070 -2.2099490
H	-1.7778790 1.5592840 1.0832820	H	-6.3104760 -0.3188910 -0.6078590	C	3.9122000 -0.5956180 1.5290490
H	-1.3876710 3.7907890 0.1165910	H	-5.8382320 -2.0459580 -0.4780930	H	4.9451670 -0.2372090 1.5754240
H	-1.8559580 3.1605030 -1.5614270	O	-3.89460700.4522650 -0.5679250	H	3.4072100 -0.3707620 2.4717360
		O	-3.4344910 -1.57875300.3248970	H	3.9111180 -1.6778860 1.3780150
TS₁₋₂		Au	0.7097320 -0.1444730 -0.0019490	C	3.2223780 2.0192530 0.4362530
C	2.3195480 0.8321850 0.4213550	H	-1.5769270 -2.34285500.6201230	H	4.2835910 2.2717020 0.5242020
C	1.3919750 -0.1766340 -0.2021480	P	3.0577650 -0.0712950 -0.0273570	H	2.7854140 2.5761150 -0.3962140
C	1.6481470 -1.1689950 -0.9302450	C	3.7489980 1.5969190 -0.3652630	H	2.7062570 2.2988990 1.3579450
C	4.2096390 -0.73281900.1579120	H	3.4188540 2.2945210 0.4085930	H	-2.9258590 1.1286650 -1.4584620
C	5.4773430 -1.17706300.8266860	H	4.8427410 1.5578740 -0.3752430	C	-1.8857990 1.9596520 0.2351240
H	6.0254060 -1.84725700.1652560	H	3.3906390 1.9524250 -1.3345920	C	-1.5090410 3.0573300 -0.4235770
H	6.0908030 -0.3099040 1.0847470	C	3.8105090 -1.1583350 -1.3022450	H	-1.6265900 1.7965480 1.2779030
H	5.2299160 -1.6994380 1.7567710	H	4.9019690 -1.0924820 -1.2581940	H	-0.9245030 3.8287340 0.0677400
O	3.5624230 0.1957930 0.8731070	H	3.5031740 -2.1929860 -1.1308730	H	-1.7680010 3.2208810 -1.4664360
O	3.8069440 -1.1861110 -0.9156290	H	3.4686020 -0.8508280 -2.2937260		

TS₄₋₅				H	-3.2789180-0.61519101.4084080	O	-1.31439401.4203110 1.0852760
C	2.5223060	0.9655540	0.8507490	O	-0.9667940-1.02498800.3596600	Au	3.1890150 0.1566310 0.4375680
C	2.3366820	-0.38963900.3693550		O	-1.51923300.8522250 -0.7884200	H	0.9803940 2.3188750 1.3111090
C	1.2247980	-1.04848700.0081920		Au	3.3044450 0.5831350 1.0355610	P	5.5071240 0.0320390 0.1647890
C	4.5660630	-0.1882570-0.0510430		H	1.1848010 2.4707870 1.2507600	C	6.2773080 1.6444630 -0.2516370
C	5.8750690	-0.7762530-0.4480620		P	5.5876460 0.2615050 1.3760310	H	7.3584390 1.5216450 -0.3691870
H	6.6403840	-0.0022780-0.4822050		C	5.9687770 -0.75767802.8502030	H	5.8512240 2.0235270 -1.1836910
H	6.1518880	-1.56556200.2551250		H	5.5255850 -1.74983002.7368670	H	6.0788090 2.3643060 0.5461280
H	5.7675310	-1.2319170-1.4385280		H	7.0526850 -0.85448602.9649720	C	6.3901820 -0.55881501.6601760
O	4.3085420	1.0290020 -0.0403440		H	5.5507220 -0.28267903.7409910	H	6.0337540 -1.55720501.9256850
O	3.6136470	-1.04955300.2965270		C	6.4723080 1.8473990 1.6231950	H	7.4672610 -0.59612701.4707410
Au	-0.7390490-0.44068800.0212730			H	7.5379550 1.6562880 1.7817160	H	6.1924710 0.1194040 2.4937970
P	-3.03073000.1309690 0.0187520			H	6.3435090 2.4802730 0.7420200	C	6.0085140 -1.1067000-1.1833380
H	1.4174490	-2.0884540-0.2662530		H	6.0634120 2.3644190 2.4944990	H	5.5603410 -0.7792750-2.1245500
C	-3.38054901.9289680 -0.1380050			C	6.4175930 -0.5601010-0.0365450	H	7.0981950 -1.1133390-1.2836010
H	-4.46029002.1073370 -0.1262000			H	7.4861520 -0.66977200.1716430	H	5.6592840 -2.1175060-0.9590780
H	-2.91771502.4672350 0.6930680			H	5.9770590 -1.5463730-0.1999230	C	-0.0859140-1.1367860-1.2294940
H	-2.96283102.3048320 -1.0755360			H	6.2836390 0.0412790 -0.9388020	C	-0.0757120-2.3778840-1.8818340
C	-3.9205870-0.37706101.5447070			C	0.6015490 -1.1592120-1.5442740	C	-0.35228400.0200170 -1.9807760
H	-4.9743750-0.08805801.4840700			C	-0.0643530-2.2383350-2.1453580	C	-0.3249020-2.4602990-3.2557190
H	-3.8490080-1.46084401.6663510			C	1.4185060 -0.3389940-2.3297600	H	0.1270520 -3.2905080-1.3342000
H	-3.46251400.1033540 2.4130940			C	0.0823590 -2.4870260-3.5112970	C	-0.6082110-0.0638700-3.3503810
C	-3.9796960-0.6445240-1.3507270			H	-0.7086390-2.8798460-1.5520910	H	-0.36141000.9917980 -1.4986570
H	-3.8952020-1.7321690-1.2832770			C	1.5720520 -0.5945540-3.6964940	C	-0.5935340-1.3056540-3.9940350
H	-5.0346050-0.3589530-1.2936850			H	1.9296290 0.5103960 -1.8892190	H	-0.3090190-3.4301400-3.7439890
H	-3.5683540-0.3205670-2.3102940			C	0.9044530 -1.6671870-4.2918660	H	-0.81432200.8413210 -3.9138020
H	3.0612760 1.0931230 1.7871650			H	-0.4453520-3.3212570-3.9638940	H	-0.7878470-1.3711330-5.0604580
C	1.6898910 2.0664130 0.4415890			H	2.2066040 0.0535930 -4.2936260	C	0.6508500 -2.31444900.9520340
C	1.6723600 3.2123430 1.1539980			H	1.0190800 -1.8611410-5.3541370	H	1.6058360 -2.61036300.5115470
H	1.0899780 1.9492790 -0.4550010			C	1.0783240 -2.12454700.7543000	H	0.7984490 -2.13277202.0187350
H	1.0455400 4.0483500 0.8605140			H	2.1387840 -2.21104500.5081350	H	-0.0711980-3.12467800.8354720
H	2.2803040 3.3377090 2.0460860			H	0.9635560 -1.96717601.8292670		
				H	0.5783670 -3.05319700.4724010		
Species with R ¹ = Ph, R ² = Me, R ³ = H:				TS₁₋₂			
1				C	0.1363810 -1.03605500.2863300	TS₂₋₃	
C	0.4432820	-0.9601320-0.0312810		C	1.0418960 0.1205650 0.6148150	C	0.4046020 -1.24383800.3276070
C	0.9781780	0.3426150 0.4526850		C	0.8702440 1.3025200 0.9909760	C	1.1109150 0.0111090 0.5882280
C	1.2314480	1.4500190 0.9228710		C	-1.80917900.3007540 1.2084880	C	0.5058260 1.1440690 0.9388980
C	-1.8507070-0.0972390-0.1090710			C	-3.20617400.0701320 1.7129160	C	-1.74379900.3281640 0.9339960
C	-3.2507990-0.42719200.3318870			H	-3.59040800.9852550 2.1630460	C	-3.18288400.6952820 1.0865610
H	-3.91623400.3962560 0.0740310			H	-3.8433810-0.21480900.8687470	H	-3.50592401.2277400 0.1848720
H	-3.5853680-1.3393830-0.1728810			H	-3.2219530-0.75018202.4345100	H	-3.7856460-0.20416701.2075610
				O	-1.2014730-0.85585900.9108220	H	-3.31029401.3663100 1.9390050
						O	-1.3904110-0.84219100.6780520
						O	-0.90076801.3278240 1.0744260
						Au	3.2019710 -0.07279200.4212120

H	0.9795950	2.0885770	1.1623270	C	6.7553770	0.4973690	1.6389910	H	5.7844380	-1.7377480	-0.8773880
P	5.5427230	-0.11449800	2.489850	H	7.8208410	0.3892020	1.4148020	H	5.7790740	-0.3706420	-2.0108980
C	6.2342620	-1.7692410	-0.1493870	H	6.5826280	1.4615930	2.1233650	C	6.4747490	-0.26012301	7.940580
H	5.8271070	-2.1159500	-1.1025730	H	6.4449180	-0.29960502	3.191020	H	7.5547190	-0.31880901	6.271580
H	7.3252030	-1.7166320	-0.2188710	C	6.4713770	1.7020010	-1.0012690	H	6.2755400	0.4007110	2.6415580
H	5.9553170	-2.48162800	6.311360	H	7.5482120	1.5485590	-1.1214640	H	6.0910850	-1.25601102	0.297230
C	6.4075500	0.3964630	1.7874420	H	5.9873530	1.6552500	-1.9797620	C	6.4800080	1.9786610	-0.0574910
H	7.4917210	0.3555630	1.6445140	H	6.2918750	2.6875820	-0.5650390	H	6.2850250	2.6863550	0.7523500
H	6.1155070	1.4165460	2.0501020	C	6.2505260	-1.1838480	-0.6915070	H	7.5591920	1.8213200	-0.1487570
H	6.1252270	-0.27050602	6.059330	H	7.3352940	-1.2170350	-0.8339730	H	6.0961040	2.4005520	-0.9898820
C	6.2133610	0.9950270	-1.0529410	H	5.9423120	-2.0164630	-0.0547780	C	1.0241760	-2.0052840	-0.6621930
H	5.9072800	2.0246760	-0.8514230	H	5.7542550	-1.2772870	-1.6605990	C	1.5166470	-3.3300800	-0.6221790
H	7.3062370	0.9391190	-1.0729110	C	1.1282020	-2.20872800	1.166400	C	1.2474160	-1.2304670	-1.8248920
H	5.8179020	0.6964410	-2.0271520	C	1.9795860	-3.19082100	6.355400	C	2.2282370	-3.8504330	-1.6984930
C	0.2720560	-1.6889270	-1.0896160	C	1.0532640	-2.0261300	-1.2733430	H	1.3627800	-3.94771800	2.546040
C	0.0696480	-3.0436190	-1.4108240	C	2.7403180	-3.9879400	-0.2273640	C	1.9439900	-1.7619840	-2.9049360
C	0.3314680	-0.7455590	-2.1337550	H	2.0584360	-3.35189101	7.041570	H	0.8514350	-0.2237400	-1.8812070
C	-0.0619040	-3.4438690	-2.7414470	C	1.8086650	-2.8247840	-2.1310700	C	2.4397450	-3.0700240	-2.8422300
H	0.0197850	-3.7945730	-0.6312360	H	0.3963610	-1.2673680	-1.6868030	H	2.6134890	-4.8637830	-1.6509020
C	0.1931640	-1.1457410	-3.4610230	C	2.6560100	-3.8096570	-1.6095570	H	2.0978010	-1.1624420	-3.7963130
H	0.4912760	0.3023740	-1.9026960	H	3.3927310	-4.75050100	1.871390	H	2.9847550	-3.4835040	-3.6855610
C	-0.0024440	-2.4973860	-3.7687620	H	1.7345470	-2.6800730	-3.2046640	C	-0.0687070	-2.32111501	6.377720
H	-0.2117700	-4.4935710	-2.9740260	H	3.2433760	-4.4328640	-2.2772790	H	-0.7298050	-1.80743602	3.363660
H	0.2407610	-0.4066950	-4.2548490	C	0.1971710	-1.77606402	4.978470	H	-0.5178080	-3.27057901	3.425370
H	-0.1063070	-2.8103510	-4.8034390	H	-0.4872870	-1.12844103	0.0488260	H	0.8698920	-2.52799102	1.678960
C	0.5560370	-2.29622501	4.034090	H	-0.1562530	-2.80766302	5.599640	Species with R ¹ = R ² = Me, R ³ = CMe=CH ₂ :			
H	1.5091520	-2.81424001	2.550370	H	1.1831040	-1.69949702	9.604280				
H	0.5694060	-1.83055802	3.896890	TS ₄₋₅				1			
H	-0.2504220	-3.02992801	3.623090								
TS ₁₋₄				C	0.2657970	-1.45523600	4.529880	C	0.3093540	-1.10360200	3.383090
				C	0.2497600	0.0032080	0.6838180	C	0.9416190	0.0786020	1.0032840
				C	1.2631490	0.8754280	0.7510760	C	1.0042730	1.1154000	1.6792440
				C	-2.0043180	-0.26739200	3.376580	C	-1.68248600	1.478960	-0.4041080
				C	-3.38748600	2.887920	0.3371470	C	-3.18679000	0.0974360	-0.3379010
				H	-3.41904301	1.543220	-0.3333350	H	-3.60337100	9.631110	-0.8521920
				H	-4.0941600	-0.4661000	-0.0043170	H	-3.5476370	-0.8218710	-0.8094810
				H	-3.64615700	6.342760	1.3412850	H	-3.51835400	0.0849760	0.7043660
				O	-1.6652890	-1.3348660	-0.1958460	O	-1.1398980	-0.88817800	2.863240
				O	-1.08355000	4.626570	0.9600130	O	-1.02901700	9.921110	-0.9864380
Au	3.2891390	0.5937310	0.5183710	C	0.8690190	-1.3762910	-1.0642370				
P	5.6288080	0.3878600	0.2961290	H	1.9151610	-1.6834830	-0.9831030				
H	0.9362180	1.8757410	1.0461100	C	0.4570840	-2.33614201	2.431640				
C	6.1720940	-0.7317120	-1.0570970	H	1.5150360	-2.57161901	3.818750				
H	7.2648590	-0.7677370	-1.1071980	H	0.0028690	-2.15353402	2.197900				

H	-0.0381850-3.18932500.7721490	H	-0.6611910-0.1529550-1.5567770	P	5.4923840 -0.15429400.2404140
H	0.3021210 -2.1943500-1.5173580	Au	3.2309270 0.1951510 0.3757880	C	6.0084420 -1.8859770-0.0947660
H	0.8058390 -0.4952700-1.7019690	P	5.5609390 0.0456980 0.2313800	H	5.5146270 -2.2471120-1.0005420
Au	3.1821800 0.2815840 1.1231130	C	6.3850440 1.6485730 -0.1216250	H	7.0933120 -1.9401260-0.2282230
P	5.5021620 0.1297950 0.9924250	H	7.4693450 1.5102390 -0.1754140	H	5.7157900 -2.52434500.7426800
C	6.2652340 -0.63659002.4722110	H	6.0229210 2.0460320 -1.0730040	C	6.5080620 0.3570010 1.6842580
H	5.8698320 -1.64631302.6064070	H	6.1501580 2.3639550 0.6704340	H	7.5708730 0.2008760 1.4752960
H	7.3514730 -0.68512602.3492110	C	6.3586040 -0.56598801.7676240	H	6.3340790 1.4144200 1.8989890
H	6.0265390 -0.04258703.3576460	H	5.9795650 -1.56265402.0064640	H	6.2219110 -0.23038802.5604630
C	6.3113910 1.7640160 0.8022330	H	7.4438950 -0.61287801.6357820	C	6.1753780 0.8096750 -1.1675940
H	7.3951340 1.6354020 0.7221150	H	6.1233600 0.1070680 2.5958350	H	5.9849350 1.8742560 -1.0095420
H	5.9368310 2.2549890 -0.0990550	C	6.1446710 -1.0871270-1.0904090	H	7.2536570 0.6436850 -1.2548570
H	6.0828660 2.3904270 1.6677620	H	5.7688140 -0.7454870-2.0581080	H	5.6860570 0.5001420 -2.0945820
C	6.0734420 -0.8717720-0.4320810	H	7.2386400 -1.1081460-1.1135380	C	0.8335690 2.6363770 1.7416130
H	7.1671390 -0.9053220-0.4438520	H	5.7671440 -2.0953350-0.9024350	C	-0.06211903.5643520 2.1375460
H	5.6811290 -1.8881770-0.3502180	C	0.8579510 2.8763580 0.9769460	H	0.2833950 4.5244990 2.5066540
H	5.7133320 -0.4265090-1.3624930	C	1.2423720 3.6692030 -0.0427510	H	-1.13243203.4059870 2.1085560
C	0.9607100 2.3031350 2.4869090	H	1.4254090 4.7282470 0.1155710	C	2.3112770 2.9362490 1.8156540
C	0.7635500 3.4920600 1.8829640	H	1.3979500 3.2752780 -1.0415070	H	2.8325070 2.2271050 2.4679290
H	0.6839500 4.4022190 2.4697150	C	0.6072360 3.3696150 2.3831010	H	2.7841650 2.8765990 0.8294630
H	0.6701630 3.5759570 0.8055570	H	-0.42405903.1620450 2.6848640	H	2.4656710 3.9434710 2.2100730
C	1.1000040 2.1249390 3.9827590	H	1.2677000 2.8609260 3.0940340		
H	0.3112750 1.4715550 4.3707350	H	0.7806350 4.4461780 2.4490380	TS₂₋₃	
H	2.0607230 1.6613580 4.2305040			C	0.7217840 -1.13979000.3898780
H	1.0357090 3.0907750 4.4887800	2		C	1.1469870 0.1801460 0.6883750
		C	0.3687550 -0.97814100.3136560	C	0.4339530 1.2723710 1.0136570
TS₁₋₂		C	1.0944210 0.2623760 0.7631360	C	-1.78231700.2064360 0.9210960
C	0.2423040 -0.94903900.2617910	C	0.4143200 1.3184930 1.2349000	C	-3.22973000.5507330 1.1079800
C	1.1112080 0.2705660 0.5012640	C	-1.71373900.2255200 0.9334010	H	-3.52002601.3161980 0.3817370
C	0.7033560 1.4677490 0.7185510	C	-3.19238700.2607000 1.0851370	H	-3.8408540-0.34088200.9726440
C	-1.70319100.2482820 1.2163670	H	-3.54920101.2906310 1.0732680	H	-3.38429000.9655620 2.1083440
C	-3.04490500.0478640 1.8543240	H	-3.6615530-0.32882800.2963750	O	-1.3869020-0.92007100.6235530
H	-3.39120500.9823810 2.2953650	H	-3.4480120-0.19031302.0513270	O	-0.98545801.2570970 1.1125910
H	-3.7543370-0.26695201.0809470	O	-1.1736580-0.82821400.4661380	C	0.6160710 -1.5938260-1.0423100
H	-2.9946680-0.74256702.6062420	O	-1.05144201.2594600 1.3048670	H	1.5558900 -2.0792250-1.3301810
O	-1.0322820-0.87221401.0313490	C	0.5186810 -1.2626260-1.1799580	C	0.8225560 -2.21947301.4344430
O	-1.28459001.3706710 0.8895120	H	1.5600040 -1.5163280-1.3926490	H	1.7725430 -2.75020301.3024910
C	-0.1369170-1.0509220-1.2204920	C	0.6632040 -2.19830901.1846370	H	0.7867300 -1.81158902.4455050
H	0.7710410 -1.1635050-1.8191250	H	1.7108100 -2.48220301.0582100	H	0.0185840 -2.94541501.2911260
C	0.8730070 -2.23765900.7853400	H	0.4895350 -1.97630102.2408910	H	-0.1793310-2.3374400-1.1335760
H	1.7913400 -2.44595500.2307130	H	0.0317410 -3.03851800.8816400	H	0.4319450 -0.7590140-1.7198980
H	1.1189280 -2.14624801.8463770	H	-0.1145850-2.1069060-1.4674650	Au	3.2615800 -0.02091600.4631930
H	0.1802170 -3.07252600.6496460	H	0.2481590 -0.3867410-1.7753580	P	5.5792930 -0.25800200.1918330
H	-0.7743510-1.9250360-1.3808160	Au	3.1762740 0.1085130 0.5440170	C	6.1096510 -1.9799860-0.1619100

H	5.6338570	-2.3288870	-1.0817960	H	5.2782790	-4.0770670	-0.3135920	H	7.5943500	1.3391350	-0.8230970
H	7.1969920	-2.0227480	-0.2775440	C	6.4740900	-1.6290860	1.2809190	H	6.0766780	1.5442700	-1.7385150
H	5.8077770	-2.6326470	0.6608760	H	7.5139250	-1.8380120	0.117250	H	6.3873180	2.5465200	-0.3041470
C	6.5520150	0.2442110	1.6660190	H	6.4136420	-0.6460400	1.7543060	C	6.1115090	-1.3176810	-0.4529910
H	7.6215560	0.1163250	1.4725420	H	6.1236750	-2.3848270	1.9879360	H	7.1967420	-1.4259510	-0.5441220
H	6.3501100	1.2925600	1.8991290	C	6.1948280	-0.4562700	-1.3760730	H	5.7186100	-2.1285220	0.1653110
H	6.2634940	-0.3689480	2.5233410	H	6.1420110	0.5485620	-0.9501760	H	5.6571080	-1.3779040	-1.4449680
C	6.2629740	0.7422370	-1.1877010	H	7.2425350	-0.7226130	-1.5459080	C	1.1462450	2.7189260	1.0950440
H	6.0561520	1.8007790	-1.0116880	H	5.6585210	-0.4660950	-2.3278830	C	0.7738480	3.1915110	2.2950210
H	7.3444080	0.5916130	-1.2612580	C	1.5003890	1.8214020	1.7327900	H	0.6298650	4.2572670	2.4480030
H	5.7915080	0.4429470	-2.1269650	C	0.8878930	2.8240950	2.3910380	H	0.6133570	2.5367010	3.1453410
C	0.9095020	2.6394520	1.3218690	H	1.4542500	3.6875150	2.7245790	C	1.3909880	3.5992160	-0.1082080
C	0.0437840	3.6318920	1.6112370	H	-0.1709680	2.8099930	2.6198530	H	2.4232370	3.5016840	-0.4642500
H	0.4153830	4.6265870	1.8356970	C	2.9818880	1.8661710	1.4510890	H	0.7361700	3.3114410	-0.9390980
H	-1.0287270	3.4886940	1.6320030	H	3.5095580	1.0367510	1.9374760	H	1.2013830	4.6473900	0.1363680
C	2.3927970	2.9164200	1.3126460	H	3.1865680	1.8047120	0.3761280				
H	2.9250180	2.2965090	2.0432720	H	3.4096160	2.7993280	1.8254760	4			
H	2.8367120	2.7212180	0.3295780					C	0.1493770	-1.2679290	-0.3907200
H	2.5761820	3.9642750	1.5625300	TS₁₋₄				C	0.1553940	0.1485870	-0.9536620
				C	0.3479280	-1.2343740	0.8484810	C	1.0942780	1.0675910	-1.1507020
3				C	0.6345720	0.2311410	0.8840770	C	-1.9554430	-0.6194920	-1.0411060
C	0.7751140	-1.7191530	0.2491190	C	1.3632140	1.2714290	0.8946660	C	-3.4030910	-0.6764630	-1.3276610
C	1.1471030	-0.4871290	0.7241720	C	-1.8186610	-0.3594060	0.6007050	H	-3.9141890	-1.2328260	-0.5401080
C	0.7304190	0.6516270	1.2787950	C	-3.2603650	-0.5480260	0.2579100	H	-3.5463410	-1.2125770	-2.2735270
C	-1.4786850	1.1984830	0.5356520	H	-3.3572620	-1.0958590	-0.6816950	H	-3.8070110	0.3308900	-1.4248790
C	-2.9057110	1.2611750	1.0052290	H	-3.7307480	-1.1443440	0.0473050	O	-1.3271630	-1.6087600	-0.5084960
H	-2.9986210	2.0081600	1.8000360	H	-3.7563170	0.4199260	0.1961080	O	-1.2432230	0.4088650	-1.3271590
H	-3.5521550	1.5335790	0.1715550	O	-1.0324830	-1.3989120	0.3492810	C	0.4901780	-1.3553770	1.0915450
H	-3.2112070	2.2976200	1.4220480	O	-1.3347560	0.6645060	1.0953040	H	1.5397770	-1.0761890	1.2193720
O	-1.0691540	1.5155590	-0.5603690	C	1.2287310	-1.9799220	-0.1583370	C	0.8891960	-2.2897750	-1.2463460
O	-0.6623920	0.7238590	1.5303100	H	2.2717190	-1.9445190	0.1633250	H	1.9565510	-2.0534320	-1.2197010
C	0.3664020	-1.9265890	-1.1887200	C	0.4007660	-1.8560330	2.2504070	H	0.5537360	-2.2526000	-2.2857160
H	0.8378340	-2.8191240	-1.6108580	H	1.4207350	-1.7923330	2.6379480	H	0.7399640	-3.2978120	-0.8501600
C	0.5905310	-2.8948890	1.1776100	H	-0.2669330	-1.3324130	2.9386310	H	0.3481770	-2.3762580	1.4562210
H	1.0544550	-3.7987320	0.7718590	H	0.1073430	-2.9075090	2.1930330	H	-0.1235570	-0.6685160	1.6791480
H	0.9704930	-2.6985110	2.1801750	H	0.9074290	-3.0239910	-0.2009370	Au	3.1033390	0.7260240	-0.6746930
H	-0.4893060	-3.0867730	1.2408200	H	1.1454870	-1.5348550	-1.1518970	P	5.3838430	0.4472200	-0.1449540
H	-0.7181290	-2.1027660	-1.1919760	Au	3.4154510	0.6837730	0.5812070	C	5.7453330	-0.9994050	0.9306550
H	0.5811060	-1.0587900	-1.8120260	P	5.7038560	0.2984780	0.3151420	H	6.8179250	-1.0633310	1.1389390
Au	3.1613770	-1.1802090	0.2212540	C	6.6288110	0.3245370	1.9004110	H	5.4197110	-1.9165360	0.4330300
P	5.4236740	-1.6534410	-0.2215430	H	7.6923730	0.1423900	1.7189020	H	5.2006850	-0.9000230	1.8731610
C	5.6759840	-3.3056110	-0.9771870	H	6.5044080	1.2985180	2.3800710	C	6.4707020	0.2154710	-1.6094990
H	5.1502310	-3.3548040	-1.9338140	H	6.2375990	-0.4483730	2.5665560	H	7.5142690	0.1083990	-1.2974060
H	6.7435880	-3.4820350	-1.1400440	C	6.5244770	1.5546040	-0.7416880	H	6.3793530	1.0796290	-2.2724800

H	6.1633720	-0.6794200	-2.1568100	H	6.1713530	2.6642570	0.4781620	H	4.9336900	-0.1849600	-2.7113660
C	6.1149450	1.8782980	0.7476000	H	7.3672310	1.7404720	-0.4707810	C	1.0401330	2.2392630	1.5990420
H	6.0133620	2.7798980	0.1382080	H	5.8628670	2.3187740	-1.2363410	C	0.3352860	2.4099210	2.7451820
H	7.1745550	1.6985950	0.9541720	C	0.7737370	2.2797940	1.4604840	H	0.2733580	3.3887990	3.2126280
H	5.5832780	2.0324430	1.6900950	C	0.2775770	2.4684950	2.6970890	H	-0.1238230	1.5812870	3.2728720
C	0.7649130	2.4001060	-1.7285700	H	0.1233810	3.4702930	3.0887350	C	1.6785270	3.4144460	0.8913520
C	0.0564260	3.3169860	-1.0472370	H	0.0477050	1.6377520	3.3571510	H	2.7717210	3.3653090	0.9415800
H	-0.1316810	4.3026460	-1.4647870	C	1.1145280	3.4409720	0.5493010	H	1.4008470	3.4197690	-0.1675610
H	-0.3328290	3.1164250	-0.0530950	H	2.1852340	3.4571300	0.3150350	H	1.3480660	4.3547390	1.3401420
C	1.3289990	2.6776240	-3.1045860	H	0.5808550	3.3589680	-0.4050710				
H	0.9440970	1.9559860	-3.8357810	H	0.8412430	4.3911360	1.0161290	TS ₅₋₆			
H	2.4210050	2.5766320	-3.1059070					C	-2.1783040	2.0875220	-0.2327990
H	1.0685680	3.6847700	-3.4417230	5				C	-2.2063090	0.7519750	-0.0431830
				C	0.4559530	-1.4800530	1.0876090	C	-1.2697130	-0.2958340	-0.4819370
TS ₄₋₅				C	0.3279020	-0.0987540	1.1316590	C	-2.9818510	-0.8839530	1.3549630
C	0.2834850	-1.4273920	0.5266080	C	1.3514990	0.8816570	1.1543050	C	-4.0205410	-1.4005580	2.2927650
C	0.1513000	-0.0329910	0.8830970	C	-1.5325440	1.0684580	0.1936140	H	-4.9432170	-1.5908570	1.7357470
C	1.1056670	0.9301930	0.9402150	C	-2.9581850	1.4534600	0.4641990	H	-3.6724710	-2.3179720	2.7646380
C	-2.0421530	-0.3121590	0.3043350	H	-2.9883010	2.1438300	1.3139980	H	-4.2390960	-0.6432180	3.0512790
C	-3.4453540	0.1936350	0.3166680	H	-3.3805680	1.9382850	-0.4152440	O	-1.8779280	-1.4057430	1.1533300
H	-3.4684130	1.1782300	-0.1627760	H	-3.5480510	0.5730430	0.7326480	O	-3.3091290	0.2225380	0.6918360
H	-4.0952480	-0.4917590	-0.2255760	O	-0.8786120	1.3652610	-0.7846790	C	-1.0996220	2.7631040	-1.0331730
H	-3.7861590	0.3170530	1.3476120	O	-1.0230800	0.3235730	1.2238030	H	-1.4987710	3.0774850	-2.0062310
O	-1.6080680	-1.2050790	-0.4303660	C	1.7342270	-2.2364050	1.1905130	C	-3.2758780	2.9896240	0.2655330
O	-1.2159010	0.2837850	1.1773050	H	1.6656680	-2.9110050	2.0547640	H	-4.0461470	2.4616120	0.8264150
C	1.2285600	-1.8913500	-0.5271600	C	-0.7811170	-2.3234270	1.0233040	H	-2.8410050	3.7658560	0.9074990
H	2.0888540	-2.3799330	-0.0538940	H	-1.3498940	-2.2239950	1.9571080	H	-3.7481590	3.5093720	-0.5769830
C	-0.2342500	-2.4800640	1.4576000	H	-1.4485390	-1.9889770	0.2230330	H	-0.7668980	3.6703790	-0.5168780
H	0.6251910	-2.7797330	2.0750300	H	-0.5343600	-3.3761330	0.8790240	H	-0.2357920	2.1207630	-1.2189990
H	-1.0170690	-2.1242010	2.1271760	H	1.8383220	-2.8841510	0.3106270	Au	0.7718360	-0.0999130	-0.1107480
H	-0.5703420	-3.3664240	0.9148800	H	2.6224360	-1.6161650	1.2976030	P	3.0774530	0.1078660	0.3507630
H	0.7268320	-2.6614740	-1.1230180	Au	3.2919000	0.5979180	0.4606790	C	3.6821720	-1.0925760	1.6029940
H	1.5729810	-1.0854800	-1.1726080	P	5.4790820	0.3873030	-0.4120010	H	3.1239650	-0.9651860	2.5338490
Au	3.1310000	0.6246600	0.5267060	C	6.6733350	-0.3929790	0.7453590	H	3.5277600	-2.1112530	1.2384670
P	5.4455610	0.3643370	0.1500070	H	7.6627080	-0.4543270	0.2817160	H	4.7476590	-0.9337720	1.7954430
C	5.8656460	-0.8115970	-1.1987360	H	6.7390580	0.2006310	1.6607130	C	4.1608330	-0.1514620	-1.1095350
H	6.9510240	-0.8773720	-1.3220020	H	6.3313850	-1.3986660	1.0023850	H	3.9297550	0.5933540	-1.8753330
H	5.4693100	-1.8016750	-0.9596440	C	6.2454400	1.9923360	-0.8683700	H	5.2129630	-0.0610400	-0.8223970
H	5.4163720	-0.4712640	-2.1352350	H	7.2528780	1.8314950	-1.2641380	H	3.9839250	-1.1469570	-1.5242880
C	6.3710040	-0.2543750	1.6121940	H	5.6336820	2.4878010	-1.6265020	C	3.5588020	1.7538120	1.0090840
H	7.4362080	-0.3453170	1.3783560	H	6.3017240	2.6358280	0.0131170	H	4.6334090	1.7804790	1.2138910
H	6.2415310	0.4398480	2.4462470	C	5.5691550	-0.6276430	-1.9401970	H	3.3107530	2.5283640	0.2790540
H	5.9806640	-1.2319010	1.9070330	H	6.6001560	-0.6738750	-2.3039730	H	3.0092090	1.9534000	1.9324860
C	6.2995420	1.9237510	-0.3155160	H	5.2137010	-1.6397430	-1.7309050	C	-1.7368630	-1.2760170	-1.4759940

C	-2.7110280-0.9243960-2.3451630	H	2.9732810 0.7231160 2.3184260	H	0.2220990 -2.66871101.4122950
H	-2.9685200-1.5704040-3.1795090	C	1.0850220 -2.21954102.1690530	H	1.8637760 -3.13994500.9894870
H	-3.22744600.0277230 -2.2802400	H	-0.0088170-2.15140002.1383900	H	1.4294710 -2.91803602.6937170
C	-1.0041620-2.5918910-1.5893080	H	1.3731920 -3.02881201.4890680	Species with R ¹ = R ² = Me, R ³ = H, PPh ₃ Ligand	
H	-1.4540890-3.2209530-2.3611920	H	1.3903790 -2.49869503.1804870		
H	0.0507300 -2.4304450-1.8378180				
H	-1.0341370-3.1320390-0.6380450				
6		TS ₆₋₃			
		C	2.0946240 2.1989820 0.0794500	1	
		C	1.9960210 0.8877470 0.0585700	C	0.2925470 -1.0331880-0.2008240
C	2.2947440 2.0312030 0.0054680	C	1.4174330 -0.37905300.2849450	C	0.9156730 0.2882900 0.0877640
C	2.2253250 0.7083590 -0.1790160	C	3.1010640 -0.9512780-1.1932060	C	1.2771890 1.4455420 0.3006570
C	1.3753430 -0.40362100.3785160	C	3.7688990 -1.9256210-2.1043020	C	-1.9715090-0.12313900.1158650
C	2.7729240 -1.1310480-1.3171200	H	4.2647210 -2.6859460-1.4905310	C	-3.2647280-0.41525200.8283860
C	3.4460840 -1.9757670-2.3260410	H	3.0285900 -2.4236790-2.7325940	H	-3.99650400.3539240 0.5834210
H	4.5265990 -1.8264340-2.2645730	H	4.5192640 -1.4187100-2.7107350	H	-3.6420620-1.39743600.5283260
H	3.1896630 -3.0225640-2.1694240	O	1.8639060 -1.2654330-0.8119100	H	-3.0982570-0.44195501.9093020
H	3.1180240 -1.6617330-3.3233230	O	3.6202270 0.0951590 -0.7790590	O	-1.0327590-1.05929700.4211750
O	1.8239750 -1.5505840-0.5785170	C	0.8713900 3.0703090 0.2972610	O	-1.76435800.8158110 -0.6276330
O	3.1067350 0.1096010 -1.1546320	H	0.9735730 3.6022270 1.2497000	C	0.1954440 -1.2725620-1.7167100
C	1.3680540 2.7261530 0.9687340	C	3.3989410 2.9437470 -0.0889580	H	1.2019350 -1.3483590-2.1366850
H	1.9209440 3.0846200 1.8461780	H	4.2506320 2.2792530 -0.2142330	C	1.0353810 -2.18139800.4942780
C	3.2884480 2.9066890 -0.7143310	H	3.3252290 3.6071230 -0.9580170	H	2.0373760 -2.29269000.0742540
H	3.9469930 2.3495480 -1.3815500	H	3.5629440 3.5770240 0.7898570	H	1.1088450 -2.00535401.5695520
H	2.7582370 3.6655110 -1.3030780	H	0.8216970 3.8203220 -0.4997780	H	0.4799350 -3.10637100.3210810
H	3.9083410 3.4463800 0.0118550	H	-0.05770502.4982880 0.3109610	H	-0.3258390-2.2185020-1.8872260
H	0.9268100 3.6070070 0.4875480	Au	-0.7377770-0.10913100.0208980	H	-0.3390710-0.4659260-2.2171630
H	0.5604500 2.0795140 1.3210040	P	-3.05329500.0443540 -0.2644440	Au	3.2465060 0.5034370 0.7419350
Au	-0.7230080-0.14109800.0573250	C	-3.7427960-1.2749750-1.3372390	P	5.4912590 0.1352250 1.3002960
P	-3.02618600.1591600 -0.3154050	H	-3.2799480-1.2217590-2.3256730	C	5.7230830 -1.21866702.5141600
C	-3.6709460-0.7877840-1.7517870	H	-3.5303680-2.2539730-0.9007380	C	5.0182330 -2.42168502.3356610
H	-3.1519440-0.4739320-2.6610850	H	-4.8253230-1.1487130-1.4362700	C	6.6002790 -1.08466503.6015400
H	-3.4928340-1.8549590-1.5972380	C	-4.0029590-0.06687901.3021260	C	5.1981840 -3.47920503.2284090
H	-4.7448650-0.6134950-1.8694480	H	-5.07491400.0122780 1.0967140	H	4.3302380 -2.53604301.5031320
C	-4.0844530-0.35680601.0950350	H	-3.7965250-1.02383101.7876870	C	6.7719540 -2.14557804.4962690
H	-3.82555200.2287840 1.9807920	H	-3.70192900.7413280 1.9732220	H	7.1473130 -0.16082803.7567870
H	-5.1407460-0.20157500.8543210	C	-3.59245301.6161240 -1.0431240	C	6.0744020 -3.34203004.3110540
H	-3.9148990-1.41442301.3125320	H	-4.68064601.6232530 -1.1582130	H	4.6506320 -4.40531803.0823140
C	-3.50964701.8998590 -0.6507790	H	-3.28888602.4597130 -0.4183270	H	7.4509940 -2.03285205.3359710
H	-4.58873101.9693130 -0.8190830	H	-3.12391901.7167450 -2.0253820	H	6.2088380 -4.16338605.0084580
H	-3.23559702.5272350 0.2012500	C	1.6713950 -1.07342201.6137580	C	6.2068070 1.6468910 2.0510480
H	-2.98208402.2618540 -1.5369080	C	2.1700900 -0.41860702.6726900	C	7.4652480 2.1341870 1.6671860
C	1.7198170 -0.90939601.7615170	H	2.2835740 -0.92136803.6282260	C	5.4708010 2.3255260 3.0385050
C	2.5029340 -0.21224002.6004500	H	2.4607130 0.6261170 2.6272670	C	7.9823170 3.2856160 2.2696700
H	2.6760090 -0.56401703.6132620	C	1.2757930 -2.53054101.6838330	H	8.0428350 1.6258650 0.9025160

C	5.9950500	3.4699930	3.6408120	H	7.7282320	-1.4081110	1.7893490	C	0.5110180	-2.3071830	1.2481130
H	4.4909130	1.9640850	3.3382940	C	5.9638840	-4.0012340	-0.5014870	H	1.5348350	-2.6664830	1.1147390
C	7.2511990	3.9527140	3.2559090	H	4.7111160	-2.3776950	-1.1455640	H	0.3811370	-2.0155490	2.2933600
H	8.9557500	3.6579080	1.9651640	C	7.0201280	-4.3978600	0.3268680	H	-0.1794640	-3.1209570	1.0089020
H	5.4210530	3.9865380	4.4040660	H	8.4676800	-3.7627390	1.7963960	H	-0.3434390	-2.3062220	-1.3845740
H	7.6548160	4.8472900	3.7205410	H	5.4686960	-4.7260690	-1.1405540	H	0.1326420	-0.6360770	-1.7965130
C	6.5173140	-0.2785310	-0.1586180	H	7.3469830	-5.4333790	0.3324320	Au	3.1615910	0.0410290	0.4945930
C	6.2240890	0.3266840	-1.3924030	C	6.3831420	0.8806300	1.6723530	P	5.5146720	-0.0068180	0.2921650
C	7.6016770	-1.1650940	-0.0608420	C	7.5605710	1.6291120	1.5194120	C	6.1817730	-1.7197630	0.3085890
C	7.0138840	0.0565650	-2.5114890	C	5.7904640	0.7736580	2.9426150	C	7.2885480	-2.0856110	1.0891400
H	5.3793610	1.0041520	-1.4805850	C	8.1397910	2.2564260	2.6268060	C	5.5484740	-2.6909050	-0.4874070
C	8.3850370	-1.4367740	-1.1862250	H	8.0259680	1.7285710	0.5444380	C	7.7583490	-3.4033180	1.0684750
H	7.8361240	-1.6460760	0.8831560	C	6.3771550	1.3952120	4.0462460	H	7.7855370	-1.3513930	1.7143690
C	8.0945200	-0.8262930	-2.4098090	H	4.8714060	0.2083130	3.0702400	C	6.0256360	-4.0023750	-0.5117600
H	6.7809230	0.5288720	-3.4609410	C	7.5521350	2.1388120	3.8894180	H	4.6832190	-2.4245490	-1.0885620
H	9.2201930	-2.1257040	-1.1039730	H	9.0489730	2.8362170	2.4992720	C	7.1311790	-4.3614970	0.2681270
H	8.7040520	-1.0412240	-3.2823890	H	5.9133950	1.3051450	5.0238740	H	8.6144000	-3.6763810	1.6783400
H	1.2936790	2.5156730	0.3848170	H	8.0038190	2.6283930	4.7470420	H	5.5314970	-4.7433880	-1.1330520
TS_{1,2}				C	6.3081570	0.7448730	-1.2676920	H	7.4976640	-5.3836620	0.2539490
C	0.2024160	-1.0756010	0.2204260	C	7.4376230	0.1885730	-1.8887590	C	6.3716740	0.8857920	1.6494660
C	1.1145290	0.1192030	0.3841160	C	5.7156310	1.8971920	-1.8114360	C	7.5670220	1.5911490	1.4381070
C	0.8719970	1.3429150	0.5280950	H	7.9704530	0.7843890	-3.0356650	C	5.8139440	0.8450520	2.9389220
C	-1.6864270	0.2918460	1.0977410	C	7.9010620	-0.7064420	-1.4866580	C	8.1969870	2.2402180	2.5041940
C	-2.9760510	0.1492920	1.8541600	C	6.2554810	2.4921490	-2.9534940	H	8.0066580	1.6414760	0.4472390
H	-3.3779850	1.1348650	2.0873190	H	4.8327960	2.3283170	-1.3474740	C	6.4503070	1.4884750	4.0027030
H	-3.6934970	-0.4001590	1.2356200	C	7.3829060	1.9359080	-3.5675430	H	4.8816590	0.3142220	3.1112840
H	-2.8167320	-0.4266910	2.7692470	H	8.8428950	0.3465760	-3.5112500	C	7.6424210	2.1879640	3.7865180
O	-1.0312760	-0.8706260	1.0040990	H	5.7913910	3.3826780	-3.3664540	H	9.1195480	2.7859950	2.3301070
O	-1.2913700	1.3586900	0.6236860	H	7.7977450	2.3954700	-4.4596890	H	6.0115670	1.4495880	4.9952690
C	-0.1889840	-1.2329320	-1.2542190	H	0.9356340	2.4037630	0.6651840	H	8.1333300	2.6942800	4.6123590
H	0.7060730	-1.4226560	-1.8526040	2				C	6.1171720	0.7494000	-1.2698970
C	0.7970850	-2.3541680	0.8049440	C	0.2794460	-1.1241220	0.3151600	C	7.2073690	0.2242960	-1.9813400
H	1.7073760	-2.6160630	0.2596410	C	1.0879950	0.0886510	0.6725690	C	5.4680800	1.8989650	-1.7526700
H	1.0463550	-2.2192330	1.8603040	C	0.4796280	1.1895490	1.1006990	C	7.6449750	0.8456510	-3.1551450
H	0.0789490	-3.1725760	0.7101140	C	-1.7051560	0.2844290	0.9438850	H	7.7139990	-0.6681260	-1.6283400
H	-0.8688210	-2.0828640	-1.3594660	C	-3.1708100	0.4314160	1.1373480	C	5.9130040	2.5209510	-2.9210540
H	-0.6743540	-0.3303550	-1.6319170	H	-3.4470860	1.4855490	1.1484240	H	4.6137330	2.3062210	-1.2188290
Au	3.2545820	0.1571540	0.3289280	H	-3.7038950	-0.1081080	0.3528480	C	7.0016810	1.9943170	-3.6248730
P	5.5967110	0.0178020	0.2575020	H	-3.4371150	-0.0171060	2.1017930	H	8.4877510	0.4301770	-3.6995910
C	6.1727350	-1.7235680	0.3165640	O	-1.2514600	-0.8247140	0.5114370	H	5.4053210	3.4093810	-3.2846290
C	7.2305850	-2.1258340	1.1457370	O	-0.9568000	1.2906110	1.2444310	H	7.3429110	2.4742220	-4.5373690
C	5.5372790	-2.6724030	-0.5039230	C	0.3565520	-1.4963570	-1.1608170	H	0.9010020	2.1376620	1.3968290
C	7.6494180	-3.4604480	1.1497760	H	1.3702870	-1.8379330	-1.3859980	TS_{2,3}			

C	0.5744820 -1.34858800.3574110	C	5.4330600 1.8892150 -1.7565990	C	7.1560830 -0.9856470-2.2065560
C	1.1274310 -0.06147800.5933910	C	7.7144100 1.0364870 -3.1291980	C	5.4956250 0.7482600 -1.8437830
C	0.5141780 1.0824810 0.8947830	H	7.8637900 -0.5056240-1.6367700	C	7.6781240 -0.2537590-3.2771410
C	-1.77845800.3103000 0.9416050	C	5.8555230 2.5709840 -2.8994410	H	7.5990800 -1.9410130-1.9445980
C	-3.17562000.7952740 1.1771190	H	4.5387270 2.2179820 -1.2344910	C	6.0251190 1.4780140 -2.9096380
H	-3.41912301.5753410 0.4492390	C	6.9962970 2.1445530 -3.5882120	H	4.6412490 1.1374060 -1.2968400
H	-3.8751300-0.03439601.0831280	H	8.5979920 0.6990040 -3.6626240	C	7.1160910 0.9770260 -3.6284140
H	-3.24796901.2381370 2.1749860	H	5.2902720 3.4271820 -3.2550570	H	8.5222870 -0.6480060-3.8347060
O	-1.4957270-0.85584800.6656370	H	7.3203450 2.6704060 -4.4813830	H	5.5813250 2.4305610 -3.1826860
O	-0.86978401.2861760 1.0619480	H	1.0082930 2.0291580 1.0591060	H	7.5225240 1.5415980 -4.4622020
C	0.3824120 -1.8294930-1.0496060			C	5.8760170 -3.1420760-0.2382490
H	1.2868170 -2.3731990-1.3505140	3		C	6.8870040 -3.70805700.5523460
C	0.6187590 -2.38771201.4371340	C	0.6274210 -1.7693740-0.1256370	C	5.2279770 -3.9291010-1.2064830
H	1.5421160 -2.96738501.3137730	C	0.9331410 -0.56801300.4402520	C	7.2484810 -5.04719700.3709640
H	0.6193460 -1.94155102.4322710	C	0.7092720 0.6056560 1.0084290	H	7.3921130 -3.11465601.3070670
H	-0.2193650-3.07995901.3276050	C	-1.73051100.6248090 1.0782630	C	5.5975240 -5.2622990-1.3876050
H	-0.4521880-2.5331840-1.0945610	C	-2.82936801.5276400 1.5648650	H	4.4382640 -3.5032810-1.8197290
H	0.2256660 -1.0042420-1.7452190	H	-2.75292302.5058390 1.0810260	C	6.6074590 -5.8239640-0.5973260
Au	3.2331610 -0.11960400.4094260	H	-3.79534301.0757520 1.3420540	H	8.0310430 -5.47860800.9877410
P	5.5808530 -0.06009300.2412940	H	-2.73163301.6846820 2.6434460	H	5.0946370 -5.8625630-2.1397100
C	6.3363380 -1.73376100.2172640	O	-1.8712420-0.45257600.5414530	H	6.8895310 -6.8635010-0.7348090
C	7.4582340 -2.05627200.9954170	O	-0.50871401.1933670 1.3288710	H	1.5039040 1.2767910 1.3068900
C	5.7672340 -2.7138930-0.6149900	C	0.3244870 -1.8891210-1.5977420		
C	8.0059810 -3.34218600.9368600	H	0.8027080 -2.7706980-2.0340030	TS₁₋₄	
H	7.9062700 -1.31367001.6472170	C	0.3882360 -2.99586100.7183480	C	0.3048230 -1.30741801.0708940
C	6.3220930 -3.9930480-0.6760780	H	0.8704890 -3.87846800.2888190	C	0.7275470 0.1127480 0.9950940
H	4.8928540 -2.4796580-1.2162470	H	0.7105890 -2.86020201.7508870	C	1.4630790 1.1318170 0.9130390
C	7.4418780 -4.30995900.1018010	H	-0.6955840-3.17368600.7094750	C	-1.8164420-0.36127800.6497710
H	8.8731980 -3.58292901.5444490	H	-0.7619030-2.0259490-1.6824130	C	-3.2234130-0.54815700.1770220
H	5.8775860 -4.7420230-1.3246090	H	0.6078860 -0.9963770-2.1555890	H	-3.2361290-1.0711430-0.7816950
H	7.8689000 -5.30747200.0588410	Au	3.0278840 -1.16897700.0998880	H	-3.7578710-1.16735700.9056430
C	6.3450150 0.8365470 1.6482780	P	5.3662910 -1.3914250-0.0504620	H	-3.71761800.4193240 0.0964870
C	7.4630400 1.6682370 1.4790840	C	6.1924850 -0.74405801.4506200	O	-1.0248370-1.42256000.4561760
C	5.7932520 0.6731000 2.9308170	C	7.4230300 -0.07220001.3796790	O	-1.36867700.6508740 1.1856190
C	8.0248020 2.3204470 2.5809260	C	5.5784600 -0.93738202.7001440	C	1.2217150 -2.19982100.2223760
H	7.8952400 1.8139490 0.4945190	C	8.0335130 0.3935120 2.5478160	H	2.2308670 -2.20320000.6386950
C	6.3622450 1.3203350 4.0293090	H	7.9049070 0.0937510 0.4218340	C	0.2031070 -1.78967402.5252590
H	4.9181570 0.0444040 3.0712090	C	6.1961250 -0.47615403.8641900	H	1.1911870 -1.75923702.9912920
C	7.4783810 2.1460840 3.8556120	H	4.6190900 -1.44306502.7654490	H	-0.4751460-1.15859303.1034200
H	8.8879220 2.9640970 2.4399010	C	7.4237960 0.1907730 3.7892660	H	-0.1625220-2.81962102.5361600
H	5.9295560 1.1864150 5.0161800	H	8.9837300 0.9150290 2.4844220	H	0.8271600 -3.21882600.2444470
H	7.9158710 2.6553280 4.7091690	H	5.7154970 -0.63047304.8254440	H	1.2580980 -1.8488030-0.8105830
C	6.1560420 0.7799480 -1.2853620	H	7.8998150 0.5557930 4.6944110	Au	3.5019710 0.6851830 0.4982890
C	7.2991760 0.3548520 -1.9811360	C	6.0624810 -0.4856080-1.4819000	P	5.7863860 0.3873620 0.0554300

C	6.7552710	0.0116300	1.5666520	O	-1.3936090	-1.52748600	4.042900	H	6.6618100	-4.0518440	-3.1336520
C	8.0492110	0.5221060	1.7552790	O	-1.15266300	4.605460	1.2639970	H	0.9195600	1.8804530	1.5771240
C	6.1879190	-0.81666902	5.502250	C	0.4191730	-1.3444670	-1.2140910				
C	8.7674030	0.2006950	2.9109710	H	1.4854370	-1.1410730	-1.3445320	TS₄₋₅			
H	8.4975580	1.1712030	1.0102900	C	0.7860760	-2.38821101	0.0820970	C	0.2506550	-1.53701700	4.986040
C	6.9118720	-1.14043403	6.992820	H	1.8650400	-2.21293701	0.0517170	C	0.2435430	-0.14487800	8.848700
H	5.1813800	-1.20494802	4.224590	H	0.4629570	-2.37199502	1.256760	C	1.2695550	0.7282810	0.9404450
C	8.2023520	-0.63122803	8.816590	H	0.5751240	-3.36930400	6.485150	C	-1.9917270	-0.18111700	4.040000
H	9.7665200	0.6025190	3.0500730	H	0.1963540	-2.3363670	-1.6161390	C	-3.33449800	4.579850	0.5197480
H	6.4656530	-1.78146704	4.535690	H	-0.1468990	-0.5896630	-1.7649970	H	-3.26720801	4.927690	0.1678500
H	8.7617900	-0.87721204	7.793100	Au	3.2126640	0.6700810	0.6833820	H	-4.0616800	-0.0894290	-0.0780070
C	6.5407870	1.8862870	-0.6856680	P	5.5299310	0.4363040	0.2471620	H	-3.64040400	4.834380	1.5691340
C	7.4818940	1.8043060	-1.7234960	C	6.5213360	0.2319160	1.7810830	O	-1.6850160	-1.0773120	-0.3856760
C	6.1699810	3.1462630	-0.1849780	C	7.8035180	0.7862000	1.9201280	O	-1.06450500	2.954570	1.2551160
C	8.0480520	2.9700940	-2.2488600	C	5.9735060	-0.51027902	8.417360	C	1.1406880	-2.0266470	-0.5863210
H	7.7731150	0.8398040	-2.1261620	C	8.5282500	0.5938360	3.1003000	H	1.9377860	-2.6408460	-0.1486040
C	6.7431940	4.3066090	-0.7080110	H	8.2382990	1.3709550	1.1160840	C	-0.3445970	-2.56933401	3.991720
H	5.4345290	3.2228080	0.6110310	C	6.7034890	-0.70663104	0.0160510	H	0.4960270	-2.97645801	9.802520
C	7.6819550	4.2201040	-1.7422650	H	4.9756460	-0.93064102	7.530690	H	-1.0746720	-2.16868002	1.015480
H	8.7732100	2.8978420	-3.0538560	C	7.9819850	-0.15391804	1.475240	H	-0.7726720	-3.39755700	8.298310
H	6.4516690	5.2754270	-0.3137690	H	9.5179660	1.0298260	3.1987340	H	0.5620330	-2.6958710	-1.2327520
H	8.1219130	5.1236520	-2.1536790	H	6.2707460	-1.28247404	8.286880	H	1.5740010	-1.2211800	-1.1758700
C	6.0931800	-0.9831630	-1.1249900	H	8.5464440	-0.30037905	0.0636670	Au	3.2689340	0.5162920	0.5395660
C	7.1468450	-1.8931760	-0.9496600	C	6.2458370	1.8866130	-0.6254110	P	5.6054850	0.4058680	0.1337020
C	5.2492110	-1.1071220	-2.2423160	C	7.2630800	1.7528030	-1.5837240	C	6.5869450	0.2515300	1.6791720
C	7.3549790	-2.9114050	-1.8857910	C	5.7628300	3.1678460	-0.3078340	C	7.8239990	0.8943300	1.8444710
H	7.8031770	-1.8154100	-0.0891760	C	7.7930530	2.8856630	-2.2088810	C	6.0826970	-0.54988802	7.180000
C	5.4661170	-2.1199880	-3.1777970	H	7.6414500	0.7705940	-1.8482410	C	8.5476250	0.7305140	3.0296770
H	4.4235940	-0.4145310	-2.3815600	C	6.2995630	4.2974590	-0.9294190	H	8.2244820	1.5253860	1.0576560
C	6.5187690	-3.0250280	-2.9996850	H	4.9655280	3.2837640	0.4212270	C	6.8120030	-0.71706203	8.969870
H	8.1711610	-3.6129160	-1.7414470	C	7.3148530	4.1579430	-1.8818460	H	5.1195930	-1.04052002	6.087020
H	4.8108950	-2.2061320	-4.0393610	H	8.5781020	2.7711210	-2.9504730	C	8.0458000	-0.07641904	0.0548560
H	6.6828010	-3.8170330	-3.7242800	H	5.9193480	5.2826420	-0.6762210	H	9.5021540	1.2344760	3.1487410
H	1.2583500	2.1890040	1.0213600	H	7.7268180	5.0360820	-2.3703150	H	6.4135610	-1.33947104	6.926360
				C	5.9239760	-1.0173500	-0.8077510	H	8.6096360	-0.20102904	9.745820
4				C	6.9745860	-1.8981100	-0.5101790	C	6.2326430	1.9102410	-0.7143950
C	0.1029090	-1.29169400	2.749210	C	5.1367240	-1.2455370	-1.9504930	C	7.1919150	1.8472750	-1.7365870
C	0.2203290	0.0969160	0.8853670	C	7.2364410	-2.9885770	-1.3467630	C	5.7319780	3.1614890	-0.3137620
C	1.2148830	0.9409070	1.1080840	H	7.5889160	-1.74112900	3.702100	C	7.6488560	3.0214190	-2.3438750
C	-1.9442050	-0.50460600	9.570240	C	5.4066260	-2.3296120	-2.7874790	H	7.5823000	0.8891860	-2.0637640
C	-3.3913680	-0.45547201	2.454200	H	4.3138230	-0.5767810	-2.1884560	C	6.1967420	4.3316100	-0.9169860
H	-3.9420880	-0.99158300	4.710840	C	6.4564680	-3.2048970	-2.4856540	H	4.9784930	3.2227230	0.4669070
H	-3.5666880	-0.95898302	2.038660	H	8.0509330	-3.6652750	-1.1057910	C	7.1551600	4.2631640	-1.9344590
H	-3.72417300	5.793910	1.3237890	H	4.7950030	-2.4938400	-3.6697080	H	8.3893380	2.9621370	-3.1360250

H	5.8049230	5.2931300	-0.5988610	H	9.8153940	1.7118190	2.0705630	H	0.8234860	-3.39108500	2.450840
H	7.5107160	5.1731980	-2.4085710	H	7.0889520	-0.90854804	1.1318840	H	1.9327390	-1.99543400	3.620240
C	6.0997800	-1.0148010	-0.9217830	H	9.2286510	0.3625120	4.0768980	Au	2.7370900	0.3672490	-0.4299550
C	7.2769940	-1.7427900	-0.6900040	C	6.0963050	1.9385670	-1.4183540	P	4.7300710	0.1834620	-1.7134970
C	5.2692350	-1.3718600	-1.9982250	C	6.9603130	1.8340600	-2.5197250	C	6.2441120	0.4235350	-0.7041950
C	7.6205450	-2.8082040	-1.5282280	C	5.5637960	3.1934120	-1.0745300	C	7.3915910	1.0391830	-1.2290330
H	7.9254970	-1.48693700	1.414430	C	7.2917890	2.9719170	-3.2617370	C	6.2532700	-0.03580500	6.240150
C	5.6197580	-2.4310810	-2.8378530	H	7.3733170	0.8716540	-2.8037290	C	8.5334640	1.1863620	-0.4362400
H	4.3487020	-0.8240160	-2.1799480	C	5.9030710	4.3278320	-1.8145260	H	7.3979530	1.4081740	-2.2495930
C	6.7957780	-3.1521580	-2.6029680	H	4.8844380	3.2879280	-0.2319920	C	7.3983050	0.1079290	1.4106240
H	8.5324660	-3.3667060	-1.3391750	C	6.7666320	4.2185660	-2.9099920	H	5.3673720	-0.50236901	0.0457240
H	4.9725320	-2.6963330	-3.6685320	H	7.9593940	2.8807070	-4.1132960	C	8.5396660	0.7198540	0.8817320
H	7.0646870	-3.9801900	-3.2520990	H	5.4872770	5.2926980	-1.5402300	H	9.4154160	1.6661390	-0.8499610
H	0.9685060	1.6932080	1.3564830	H	7.0242680	5.1003520	-3.4891070	H	7.3953680	-0.25036802	4.356580
				C	6.0608000	-0.9978230	-1.4035630	H	9.4275020	0.8375000	1.4959060
5				C	7.2545410	-1.7139230	-1.2271020	C	4.8091870	1.4328660	-3.0570550
C	0.3880970	-1.62978400	0.9361260	C	5.1434650	-1.4142430	-2.3845720	C	5.3024460	1.1222660	-4.3336900
C	0.3691290	-0.23076801	0.0325870	C	7.5283730	-2.8288080	-2.0261290	C	4.3690420	2.7401170	-2.7852920
C	1.4272660	0.6513720	0.8726210	H	7.9699240	-1.4103680	-0.4698710	C	5.3604210	2.1095740	-5.3224160
C	-1.51138101	1.815750	0.5825860	C	5.4249830	-2.5226430	-3.1852340	H	5.6385790	0.1163010	-4.5628120
C	-2.82115101	0.6321470	1.1606990	H	4.2102960	-0.8751080	-2.5250980	C	4.4357150	3.7241730	-3.7734150
H	-2.64208102	1.622420	2.1015650	C	6.6175770	-3.2328340	-3.0059690	H	3.9726710	2.9907910	-1.8051630
H	-3.32427502	2.2922040	0.4551330	H	8.4538100	-3.3779770	-1.8806570	C	4.9302360	3.4098780	-5.0441470
H	-3.45234300	0.7676010	1.3846300	H	4.7118360	-2.8343300	-3.9424900	H	5.7419070	1.8594210	-6.3078830
O	-1.02441201	0.5366760	-0.4699770	H	6.8327150	-4.0987640	-3.6249560	H	4.0943570	4.7312350	-3.5534670
O	-0.89001000	0.2865420	1.4181620	H	1.1215420	1.6763180	1.0930470	H	4.9748230	4.1741290	-5.8143750
C	1.6035130	-2.43349400	0.6699240					C	4.9000980	-1.4523730	-2.5290410
H	1.7674710	-3.10129401	0.5275860	TS₅₋₆				C	6.1173120	-2.1494070	-2.5608620
C	-0.8762130	-2.38933801	1.1481880	C	-0.1094630	-1.63688301	0.0152690	C	3.7665370	-2.0132250	-3.1432400
H	-1.2974290	-2.15250702	0.1328460	C	-0.0508790	-0.27975900	0.9408440	C	6.1995840	-3.3883140	-3.2050690
H	-1.6324970	-2.06877800	0.4203650	C	1.0435100	0.6086220	0.6880570	H	7.0001520	-1.7346850	-2.0857320
H	-0.7221730	-3.46483601	0.0627230	C	-1.33949601	1.4855750	0.3005300	C	3.8551270	-3.2462420	-3.7915460
H	1.4038070	-3.0952930	-0.1829130	C	-2.67518202	1.429850	0.2145030	H	2.8154340	-1.4883710	-3.1163220
H	2.5026530	-1.84890100	0.4869100	H	-3.06558602	0.3133540	1.2213300	C	5.0721330	-3.9367940	-3.8221530
Au	3.3745550	0.5090870	0.3005860	H	-2.59519503	0.0828130	-0.3295770	H	7.1455720	-3.9212250	-3.2226260
P	5.6522710	0.4809520	-0.3943650	H	-3.36922501	1.4725600	-0.3031110	H	2.9745220	-3.6692330	-4.2657020
C	6.8150130	0.4765410	1.0261770	O	-0.33001201	0.8297270	-0.3231600	H	5.1387870	-4.8989650	-4.3212240
C	8.0210110	1.1942180	1.0005340	O	-1.27562700	0.4343220	1.1304950	H	1.0553410	1.4655740	1.3624560
C	6.4837000	-0.27710102	1.655720	C	1.0955030	-2.51061600	0.8367300				
C	8.8857990	1.1512520	2.0984550	H	1.4353710	-2.87691901	0.8138870	6			
H	8.2876820	1.7893230	0.1332770	C	-1.3797920	-2.35036101	0.3770780	C	-0.3419240	-1.46827600	0.8773470
C	7.3535410	-0.32257903	0.2568200	H	-2.2142510	-1.67857001	0.5707800	C	-0.2099500	-0.14028700	0.8730270
H	5.5468210	-0.82604702	0.2028710	H	-1.6504260	-3.02773900	0.5569820	C	0.9551940	0.8108360	0.8595800
C	8.5557410	0.3925060	3.2250910	H	-1.2146220	-2.98164102	0.2581690	C	-1.03372001	0.9297800	0.9583090

C	-2.02627703.0226380 0.9858770	H	1.3363240 -0.7147420-3.4309690	C	3.0473070 4.7494540 -3.9044800
H	-2.80643102.7890440 1.7143610	C	3.0868640 -2.8417010-5.4307020	H	3.0894990 3.6309110 -2.0666610
H	-1.53763503.9649410 1.2295450	H	5.2182660 -2.7567950-5.7628890	C	3.1653140 4.6987700 -5.2979950
H	-2.49731703.0955080 -0.0007680	H	1.0000320 -2.6762850-4.8977660	H	3.5214600 3.4364020 -7.0124880
O	0.2263910 2.1348860 0.9878210	H	2.9399810 -3.7093390-6.0670810	H	2.8332920 5.6911180 -3.4079590
O	-1.39479300.6892270 0.8824970	H	1.5473660 0.7594070 1.7760580	H	3.0432430 5.6029490 -5.8869220
C	0.8882490 -2.33945900.8659220			C	3.5202400 -0.5744390-3.8586440
H	1.0046700 -2.85236201.8291570	TS₆₋₃		C	4.6341960 -1.2213290-4.4154760
C	-1.6754100-2.16822500.9049780	C	-0.0257780-1.65687400.8376490	C	2.2276090 -1.0287040-4.1729150
H	-2.5187210-1.47698600.9434130	C	0.1526780 -0.35704000.8927770	C	4.4547160 -2.3055960-5.2803930
H	-1.7869590-2.80068600.0153680	C	0.7978590 0.8796450 0.7040270	H	5.6389640 -0.8881450-4.1773170
H	-1.7343360-2.83307601.7754530	C	-1.31762101.6422230 1.1807870	C	2.0532760 -2.1061990-5.0432290
H	0.7935000 -3.11672200.0981530	C	-2.33199302.7339160 1.2481040	H	1.3586240 -0.5433250-3.7371180
H	1.8040960 -1.77541500.6691540	H	-2.10204103.3622260 2.1160300	C	3.1671390 -2.7473020-5.5971710
Au	2.2195700 0.8421510 -0.8298890	H	-2.28083903.3545490 0.3522240	H	5.3223610 -2.8021100-5.7044320
P	3.6582720 0.8769860 -2.7102330	H	-3.32883602.3118690 1.3757270	H	1.0507340 -2.4486110-5.2815710
C	5.4350860 0.9518490 -2.2530460	O	-0.21515901.9168240 0.4842120	H	3.0310330 -3.5902360-6.2681530
C	6.3662490 1.6906390 -3.0000330	O	-1.43361100.5374890 1.7307330	H	1.3912800 1.1981540 1.5675900
C	5.8688710 0.2342070 -1.1250990	C	0.8177620 -2.5077090-0.0952520		
C	7.7135460 1.7039300 -2.6263030	H	1.4542120 -3.17240800.4994350	Species with R ¹ = R ² = Me, R ³ = Me, PPh ₃ Ligand	
H	6.0463160 2.2581050 -3.8680490	C	-1.0366360-2.40261401.6766620		
C	7.2166130 0.2442160 -0.7596050	H	-1.6046680-1.74485302.3308330	1	
H	5.1547940 -0.3287890-0.5303760	H	-1.7254550-2.94132901.0164560	C	0.2979170 -1.08386500.4010120
C	8.1407980 0.9801300 -1.5092260	H	-0.5145800-3.15071002.2833490	C	0.9170220 0.2655430 0.5858310
H	8.4260920 2.2801720 -3.2089700	H	0.1549160 -3.1342220-0.7017190	C	1.0603980 1.4817200 0.7481050
H	7.5418110 -0.31442300.1129530	H	1.4511460 -1.9114530-0.7533920	C	-1.6019190-0.2003440-0.9051560
H	9.1875600 0.9934630 -1.2203280	Au	2.1674180 0.8063580 -0.9482620	C	-3.1081010-0.2209450-0.9336610
C	3.3555690 2.3332470 -3.7884020	P	3.6926960 0.8671130 -2.7363310	H	-3.46475700.3760390 -1.7725820
C	3.3078050 2.2343940 -5.1870660	C	5.4381480 0.8828070 -2.1707820	H	-3.4628430-1.2512560-1.0350400
C	3.1671470 3.5860140 -3.1782040	C	6.4264250 1.6191620 -2.8428530	H	-3.50830500.1741690 0.0045490
C	3.0813350 3.3753300 -5.9642440	C	5.7895700 0.1240030 -1.0411690	O	-1.1368570-0.89380300.1665620
H	3.4433800 1.2744080 -5.6741700	C	7.7498910 1.5893610 -2.3930590	O	-0.88690900.3561010 -1.7160300
C	2.9496120 4.7233650 -3.9577950	H	6.1703410 2.2177860 -3.7110130	C	0.9957400 2.9406380 0.8662900
H	3.1895010 3.6738230 -2.0953300	C	7.1139030 0.0917390 -0.5998580	H	1.3118010 3.2759220 1.8573760
C	2.9047600 4.6194410 -5.3528860	H	5.0300620 -0.4367740-0.5033630	H	1.6179960 3.4276150 0.1108860
H	3.0442960 3.2881240 -7.0460560	C	8.0957850 0.8252610 -1.2747860	H	-0.04394303.2491480 0.7095420
H	2.8087050 5.6867130 -3.4767860	H	8.5072820 2.1643530 -2.9173660	C	0.9353290 -1.8813160-0.7453680
H	2.7290160 5.5034660 -5.9586580	H	7.3757990 -0.49812500.2733910	H	1.9650860 -2.1376280-0.4824890
C	3.4692750 -0.6027720-3.7814890	H	9.1242380 0.8055860 -0.9266970	C	0.3406580 -1.87266101.7177850
C	4.5604910 -1.1911980-4.4401060	C	3.4730360 2.3612930 -3.7784450	H	1.3759970 -2.07679302.0003260
C	2.1859450 -1.1513890-3.9486660	C	3.5890430 2.3150890 -5.1763340	H	-0.1437990-1.31164802.5203140
C	4.3672420 -2.3072370-5.2599720	C	3.1945920 3.5859120 -3.1472050	H	-0.1812160-2.82336901.5810290
H	5.5599060 -0.7875900-4.3143400	C	3.4334750 3.4819850 -5.9311400	H	0.3729070 -2.8090170-0.8834240
C	1.9959630 -2.2613820-4.7744540	H	3.7951350 1.3762250 -5.6798330	H	0.9364030 -1.3162390-1.6767780

Au	3.1493610	0.4711420	0.9812370	H	-2.9410270	-1.0484140	2.5260620	C	6.1663590	2.3384030	-3.0076120
P	5.4481990	0.1554130	1.2995050	O	-1.0255860	-0.9645850	0.8869650	H	4.7849630	2.2357450	-1.3611130
C	5.8188730	-1.2459560	2.4203510	O	-1.3043030	1.2775820	1.0329180	C	7.2794450	1.7602670	-3.6274410
C	5.0610630	-2.4242220	2.3084250	C	0.8869870	2.7301390	1.4751140	H	8.7447330	0.1770870	-3.5441940
C	6.8576980	-1.1766150	3.3617390	H	0.4694320	2.8155450	2.4821360	H	5.6896580	3.2111630	-3.4436130
C	5.3481810	-3.5226940	3.1203310	H	1.9466480	3.0033810	1.5120550	H	7.6707360	2.1847880	-4.5471830
H	4.2481620	-2.4851100	1.5901650	H	0.3705500	3.4269160	0.8091960				
C	7.1368280	-2.2778880	4.1768020	C	-0.1441580	-0.7508550	-1.3709740	2			
H	7.4467330	-0.2712800	3.4652870	H	0.7618670	-0.7700020	-1.9825540	C	0.3046220	-1.0425130	0.2261850
C	6.3860490	-3.4504500	4.0562800	C	0.8482490	-2.3003370	0.3790050	C	1.0796990	0.1498110	0.7107250
H	4.7587610	-4.4297000	3.0267060	H	1.7600070	-2.4153070	-0.2122570	C	0.4580300	1.2040900	1.2358410
H	7.9408730	-2.2158880	4.9038620	H	1.1000040	-2.4088490	1.4369690	C	-1.7142750	0.2096860	1.0045600
H	6.6047130	-4.3034930	4.6915690	H	0.1423070	-3.0859370	0.0968720	C	-3.1806440	0.2782520	1.2381470
C	6.2222110	1.6424930	2.0421290	H	-0.7974620	-1.5699430	-1.6847700	H	-3.5150250	1.3160110	1.2323040
C	7.3988320	2.1996770	1.5196460	H	-0.6516580	0.2024650	-1.5356130	H	-3.7071390	-0.3112760	0.4869440
C	5.6128290	2.2322760	3.1640760	Au	3.2537720	0.1467440	0.4507810	H	-3.3892190	-0.1513540	0.2253480
C	7.9617210	3.3319160	2.1179620	P	5.5913030	-0.0057860	0.3169110	O	-1.2264000	-0.8449490	0.4839460
H	7.8776640	1.7603530	0.6510850	C	6.1768540	-1.7414480	0.4292560	O	-1.0036960	1.2198460	1.3663680
C	6.1830990	3.3572550	3.7607890	C	7.2463850	-2.1157440	1.2562840	C	0.9580360	2.4999140	1.7795210
H	4.6959400	1.8161840	3.5728390	C	5.5291500	-2.7173640	-0.3483820	H	0.6745460	2.6199330	2.8316240
C	7.3578880	3.9099870	3.2372830	C	7.6641280	-3.4501030	1.3006670	H	2.0454220	2.5324390	1.7022960
H	8.8712650	3.7584670	1.7060670	H	7.7541680	-1.3763190	1.8666300	H	0.5388090	3.3461780	1.2229360
H	5.7079010	3.8044430	4.6285870	C	5.9547900	-4.0457760	-0.3068970	C	0.3648100	-1.2314690	-1.2865700
H	7.7968360	4.7894140	3.6988030	H	4.6940010	-2.4415740	-0.9865750	H	1.3878360	-1.4924510	-1.5692540
C	6.3217020	-0.1817060	-0.2748520	C	7.0224370	-4.4147380	0.5197580	C	0.6050700	-2.3232250	0.9985510
C	5.8574720	0.4190220	-1.4572330	H	8.4915000	-3.7309500	1.9454300	H	1.6361100	-2.6247270	0.7960290
C	7.4547530	-1.0101900	-0.3171490	H	5.4500400	-4.7916930	-0.9134670	H	0.4963100	-2.1670430	0.0746990
C	6.5267000	0.2036190	-2.6637130	H	7.3487770	-5.4498080	0.5565030	H	-0.0642720	-3.1268430	0.6784070
H	4.9725660	1.0486650	-1.4382420	C	6.4201350	0.9148720	1.6710730	H	-0.3014260	-2.0416960	-1.5965750
C	8.1174730	-1.2267260	-1.5284110	C	7.5890350	1.6604300	1.4529980	H	0.0874550	-0.3122240	-1.8083380
H	7.8199080	-1.4899410	0.5850940	C	5.8665660	0.8579850	2.9621300	Au	3.1581990	0.0892860	0.5229450
C	7.6569370	-0.6197310	-2.7007170	C	8.1982200	2.3349350	2.5157450	P	5.5098250	0.0020250	0.3103440
H	6.1606960	0.6714830	-3.5725360	H	8.0245180	1.7206770	0.4611620	C	6.1558750	-1.7181560	0.3637530
H	8.9911690	-1.8708730	-1.5534570	C	6.4830030	1.5263210	4.0214380	C	7.2852720	-2.0720010	1.1172080
H	8.1727160	-0.7922810	-3.6405710	H	4.9550790	0.2938370	3.1402240	C	5.4857760	-2.7064470	-0.3788940
				C	7.6491450	2.2672820	3.7992110	C	7.7406370	-3.3948010	1.1221350
TS_{1,2}				H	9.1004760	2.9121930	2.3373240	H	7.8107030	-1.3242880	1.7019880
C	0.2339690	-0.9294650	0.1047840	H	6.0495930	1.4741530	5.0156470	C	5.9484070	-4.0234630	-0.3782780
C	1.1240860	0.2121030	0.5586150	H	8.1240420	2.7930930	4.6221680	H	4.6023880	-2.4489710	-0.9570660
C	0.7893930	1.3647780	0.9760720	C	6.2651900	0.6590960	-1.2549590	C	7.0765060	-4.3704160	0.3741550
C	-1.7057760	0.1241980	1.2250480	C	7.3807070	0.0813740	-1.8819620	H	8.6142230	-3.6584410	1.7109320
C	-3.0288940	-0.1863680	1.8611760	C	5.6568920	1.7879820	-1.8297510	H	5.4253060	-4.7779750	-0.9582580
H	-3.3929870	0.6856570	2.4040860	C	7.8830770	0.6318810	-3.0648200	H	7.4318280	-5.3966010	0.3798590
H	-3.7451370	-0.4419540	1.0724920	H	7.8571410	-0.7957900	-1.4562190	C	6.3839440	0.9131910	1.6446980

C	7.5761850	1.6165160	1.4110940	C	7.4122490	-2.0734140	1.0371500	H	-3.91940300	7.465220	1.2785700
C	5.8399180	0.8901710	2.9405540	C	5.7228240	-2.7116660	-0.5824460	H	-2.9660720	1.3379450	2.6711230
C	8.2165810	2.2813780	2.4613090	C	7.9349590	-3.37037600	0.9944760	O	-1.8634810	-0.57892400	0.4648490
H	8.0057890	1.6524450	0.4152140	H	7.8694940	-1.3341680	1.6863600	O	-0.6568010	1.0775370	1.4679340
C	6.4866530	1.5489520	3.9884350	C	6.2527520	-4.0019660	-0.6277480	C	1.6028360	1.6235870	1.8054920
H	4.9102360	0.3605900	3.1301780	H	4.8587710	-2.4652720	-1.1937070	H	1.4371960	1.6885240	2.8864920
C	7.6755740	2.2468020	3.7499140	C	7.3592180	-4.33412200	0.1627630	H	2.6383960	1.3328950	1.6244820
H	9.1367700	2.8253660	2.2698620	H	8.7920270	-3.6227300	1.6116840	H	1.4354770	2.6204920	1.3832030
H	6.0585360	1.5233890	4.9860730	H	5.7992810	-4.7475620	-1.2739670	C	0.4154160	-1.5555800	-1.6743970
H	8.1744860	2.7651490	4.5634020	H	7.7668850	-5.34014600	0.1320200	H	0.9222940	-2.3756840	-2.1910640
C	6.1188300	0.7143020	-1.2704070	C	6.3605840	0.8516170	1.6450450	C	0.4209520	-2.91119600	0.5043040
C	7.1961340	0.1552520	-1.9755120	C	7.4830900	1.6750460	1.4663460	H	0.9245710	-3.7365850	-0.0071220
C	5.4867180	1.8637010	-1.7756410	C	5.8133880	0.6989490	2.9309960	H	0.7122950	-2.8906780	1.5547980
C	7.6378880	0.7428300	-3.1651020	C	8.0537510	2.3300420	2.5620580	H	-0.6602820	-3.09273800	0.4431130
H	7.6897800	-0.7373650	-1.6050930	H	7.9121860	1.8118600	0.4792180	H	-0.6653250	-1.6977600	-1.8068740
C	5.9357290	2.4519970	-2.9598020	C	6.3913180	1.3486570	4.0232710	H	0.6995720	-0.6021420	-2.1205400
H	4.6421820	2.2971190	-1.2469210	H	4.9354620	0.0759920	3.0792150	Au	3.0466880	-1.05602800	0.1463450
C	7.0115830	1.8915000	-3.6571970	C	7.5118440	2.1664590	3.8400250	P	5.3782980	-1.3637670	-0.0234520
H	8.4706340	0.3010990	-3.7043080	H	8.9203840	2.9672660	2.4135850	C	6.2543580	-0.7040770	1.4458130
H	5.4411420	3.3406530	-3.3405090	H	5.9623900	1.2227370	5.0128360	C	7.4404220	0.0361230	1.3241440
H	7.3559460	2.3451950	-4.5818530	H	7.9563720	2.6776150	4.6887870	C	5.7223060	-0.9562700	2.7228290
TS₂₋₃				C	6.1827000	0.7593750	-1.2888080	C	8.0883470	0.5126780	2.4681850
C	0.6312780	-1.27298900	0.3109230	C	7.3255300	0.3036660	-1.9655650	H	7.8601300	0.2453410	0.3458600
C	1.1189480	0.0283930	0.5907600	C	5.4824080	1.8713420	-1.7872660	C	6.3772180	-0.4841460	3.8613610
C	0.4756630	1.1543290	0.9105090	H	7.7625590	0.9566860	-3.1219440	H	4.7999060	-1.5200790	2.8319510
C	-1.79429300	0.2377400	0.9424810	C	7.8731200	-0.5589190	-1.5998590	C	7.5604710	0.2525640	3.7355900
C	-3.20895500	0.6533050	1.2121130	C	5.9266430	2.5245910	-2.9386830	H	9.0044120	1.0863560	2.3648470
H	-3.4633560	1.5272960	0.6062680	H	4.5891600	2.2248180	-1.2797170	H	5.9603240	-0.6854670	4.8434850
H	-3.8844630	-0.17216000	0.9905250	C	7.0665850	2.0670770	-3.6085710	H	8.0652840	0.6251230	4.6218700
H	-3.30678000	0.9380440	2.2648270	H	8.6456230	0.5952000	-3.6402830	C	6.0843960	-0.5192550	-1.4885420
O	-1.4657610	-0.91109000	0.6508240	H	5.3788020	3.3830400	-3.3155080	C	7.1276020	-1.0916190	-2.2331890
O	-0.9338120	1.2551930	1.0636430	H	7.4072480	2.5708250	-4.5082800	C	5.5753800	0.7371560	-1.8599300
C	0.4400190	-1.7123500	-1.1124580	C	1.0534570	2.5087080	1.1789220	C	7.6578490	-0.4101030	-3.3327390
H	1.3605070	-2.2031360	-1.4517260	H	2.1390930	2.4817950	1.0759420	H	7.5254450	-2.0645340	-1.9639990
C	0.7342960	-2.3545210	1.3475230	H	0.6474900	3.2462880	0.4770830	C	6.1133500	1.4164410	-2.9545440
H	1.6685020	-2.9049820	1.1828470	H	0.8009720	2.8432420	2.1916670	H	4.7601030	1.1852890	-1.2986730
H	0.7431810	-1.9479130	2.3595190	3				C	7.1543540	0.8430230	-3.6931070
H	-0.0882420	-3.0640730	1.2292420	C	0.6709730	-1.5938740	-0.1878580	H	8.4627750	-0.8609800	-3.9052450
H	-0.3639470	-2.4500320	-1.1705780	C	0.9532170	-0.45862200	0.5172400	H	5.7148920	2.3870670	-3.2338940
H	0.2326580	-0.8694750	-1.7729840	C	0.6478630	0.6396510	1.1966820	H	7.5670350	1.3690340	-4.5487660
Au	3.2324450	-0.05705800	0.4099180	C	-1.81631400	0.4560230	1.0946300	C	5.8334620	-3.1338450	-0.1633090
P	5.5824000	-0.04657700	0.2466190	C	-3.0000490	1.2467710	1.5812690	C	6.9391910	-3.66699900	0.5167640
C	6.3038220	-1.73563200	0.2463510	H	-2.9706550	2.2581900	1.1649390	C	5.0585550	-3.9671620	-0.9883900
								C	7.2676980	-5.01790100	0.3658430

H	7.5426150	-3.03869101	1.1635320	C	6.5180980	1.8710300	-0.6593390	H	0.5176420	-2.4686670	-1.4150880
C	5.3951280	-5.3129960	-1.1410590	C	7.4581270	1.7571740	-1.6951020	H	0.0314420	-0.7795830	-1.7321210
H	4.1934580	-3.5671260	-1.5099800	C	6.1787940	3.1445390	-0.1703050	Au	3.1594870	0.7834920	0.6512100
C	6.4997970	-5.8405540	-0.4627820	C	8.0528320	2.9039060	-2.2310200	P	5.4753580	0.4829060	0.2306210
H	8.1234840	-5.42342100	0.8970130	H	7.7261410	0.7822470	-2.0885540	C	6.4580980	0.2377120	1.7630790
H	4.7920970	-5.9490580	-1.7818850	C	6.7805920	4.2857220	-0.7033290	C	7.8017200	0.6358640	1.8562890
H	6.7567840	-6.8894290	-0.5765190	H	5.4453910	3.2468830	0.6247740	C	5.8433170	-0.37493202	0.8680600
TS₁₋₄				C	7.7172820	4.1671210	-1.7363230	C	8.5193280	0.4154990	3.0351860
C	0.4455150	-1.25982000	0.9135120	H	8.7766170	2.8063680	-3.0346240	H	8.2894320	1.1212350	1.0169230
C	0.7032620	0.2112400	0.9344520	H	6.5131330	5.2649260	-0.3176920	C	6.5655730	-0.59936804	0.0427410
C	1.4027340	1.2725600	0.9138490	H	8.1793710	5.0559170	-2.1555910	H	4.7986650	-0.66786402	0.8125270
C	-1.7485230	-0.42808500	0.7665050	C	6.0163830	-0.9917940	-1.0686750	C	7.9044510	-0.20416604	0.1278510
C	-3.2015400	-0.64971400	0.4993390	C	7.0445570	-1.9255180	-0.8684810	H	9.5569040	0.7296740	3.0985490
H	-3.3346610	-1.2151980	-0.4252230	C	5.1870570	-1.1073110	-2.1979140	H	6.0804180	-1.07323004	0.8908720
H	-3.6197790	-1.24133801	0.3210350	C	7.2421870	-2.9581470	-1.7911150	H	8.4640170	-0.37191005	0.0433550
H	-3.71938000	0.3073270	0.4473970	H	7.6893780	-1.85502600	0.0012460	C	6.2444280	1.9149630	-0.6273230
O	-0.9545530	-1.45190900	0.4813380	C	5.3937130	-2.1343030	-3.1202550	C	7.2133500	1.7561600	-1.6303170
O	-1.26333300	0.6099190	1.2305530	H	4.3803900	-0.3968910	-2.3565890	C	5.8508140	3.2100900	-0.2482910
C	1.0956950	2.7259500	1.1286030	C	6.4210810	-3.0627850	-2.9170550	C	7.7837770	2.8781140	-2.2400890
H	1.6503370	3.1039450	1.9924890	H	8.0385750	-3.6778650	-1.6269890	H	7.5229290	0.7635880	-1.9412210
H	1.4059550	3.3150320	0.2612630	H	4.7498340	-2.2131340	-3.9910570	C	6.4280640	4.3278510	-0.8542480
H	0.0257620	2.8688580	1.3002110	H	6.5770820	-3.8657320	-3.6313270	H	5.0922020	3.3464910	0.5176030
C	1.2914280	-1.9867010	-0.1361030	4				C	7.3947590	4.1634690	-1.8525220
H	2.3489030	-1.92336800	0.1289090	C	0.2632850	-1.27199500	0.3701200	H	8.5311100	2.7444420	-3.0166400
C	0.5772540	-1.88163502	0.3101940	C	0.2319510	0.1711140	0.8597640	H	6.1175120	5.3238970	-0.5529850
H	1.6123280	-1.79421202	0.6500330	C	1.1439870	1.1192330	1.0453230	H	7.8381980	5.0329900	-2.3286800
H	-0.0687920	-1.37344403	0.0301030	C	-1.8758420	-0.61851800	0.8990580	C	5.8161690	-0.9750260	-0.8372550
H	0.3065320	-2.93985202	0.2662220	C	-3.3373940	-0.67626401	1.1055770	C	6.7863100	-1.9350210	-0.5139200
H	0.9949800	-3.0387030	-0.1604960	H	-3.8117190	-1.11358700	0.2233740	C	5.0578860	-1.1313590	-2.0116710
H	1.1446100	-1.5465310	-1.1244040	H	-3.5450130	-1.33253201	0.9579740	C	6.9991390	-3.0317940	-1.3564700
Au	3.4371410	0.7494930	0.5128120	H	-3.73022800	0.3198310	1.3038750	H	7.3769260	-1.83479200	0.3905130
P	5.7222410	0.3981850	0.0933270	O	-1.2109440	-1.63277200	0.4673870	C	5.2794270	-2.2218260	-2.8542430
C	6.6756490	0.0200010	1.6144480	O	-1.19045300	0.4362950	1.1477730	H	4.2955520	-0.4012720	-2.2705670
C	7.9866580	0.4875630	1.7967660	C	0.7571880	2.4912120	1.5551010	C	6.2500690	-3.1759690	-2.5268590
C	6.0775930	-0.76789102	0.6127610	H	1.2985210	2.7133770	2.4814040	H	7.7518630	-3.7697300	-1.0952460
C	8.6907490	0.1641420	2.9604910	H	1.0576050	3.2576120	0.8319400	H	4.6917150	-2.3292410	-3.7611320
H	8.4591350	1.1054770	1.0401410	H	-0.31457402	0.6021070	1.7479670	H	6.4177920	-4.0274710	-3.1796890
C	6.7872510	-1.09435903	0.7701680	C	0.6395000	-1.4293420	-1.0980460	TS₄₋₅			
H	5.0581480	-1.12256502	0.4898610	H	1.6884860	-1.1446930	-1.2161770	C	0.3833430	-1.45751400	0.4813410
C	8.0944430	-0.62762003	0.9461600	C	0.9982210	-2.23764001	0.2916410	C	0.2676040	-0.08892800	0.9312940
H	9.7032970	0.5328400	3.0943470	H	2.0619330	-1.98426401	0.2772430	C	1.2094500	0.8824500	1.0157920
H	6.3169450	-1.70406504	0.5357490	H	0.6371900	-2.15470802	0.3196040	C	-1.9470740	-0.35484400	0.4378410
H	8.6429490	-0.87536104	0.8500730	H	0.8755110	-3.26667900	0.9428170	C	-3.35387000	0.1299100	0.5361850

H	-3.40456201.1472380 0.1332700	C	6.5785370 -3.1584960-2.6033450	H	9.2950500 0.3127620 4.0776520
H	-4.0158090-0.5220210-0.0320000	H	8.1792220 -3.5804480-1.2184500	C	6.1430630 1.9491270 -1.3851290
H	-3.65848600.1713110 1.5849180	H	4.9027150 -2.4885260-3.7913240	C	6.9711330 1.8094690 -2.5097780
O	-1.5337280-1.1973350-0.3672500	H	6.8081740 -3.9982060-3.2525660	C	5.6744220 3.2252120 -1.0265410
O	-1.08954600.1952840 1.3081560	C	0.8400360 2.2221790 1.6030760	C	7.3285540 2.9329510 -3.2618240
C	1.2905090 -1.8385600-0.6373270	H	1.1353280 3.0153150 0.9062060	H	7.3356240 0.8309190 -2.8046900
H	2.2088580 -2.2695070-0.2198110	H	-0.22212202.3304190 1.8369340	C	6.0397200 4.3448400 -1.7764180
C	-0.0792750-2.57328301.3674920	H	1.4204150 2.3976070 2.5168730	H	5.0242150 3.3472760 -0.1646800
H	0.8163960 -2.92425101.8999220			C	6.8663830 4.2002140 -2.8961450
H	-0.8112210-2.26103402.1121080	S		H	7.9675470 2.8142450 -4.1317510
H	-0.4625110-3.41494200.7864070	C	0.4614350 -1.45592500.8520470	H	5.6733940 5.3263150 -1.4906460
H	0.8147250 -2.6299490-1.2251400	C	0.4088300 -0.07879501.0641990	H	7.1442420 5.0707800 -3.4828230
H	1.5461610 -0.9962290-1.2773000	C	1.4549220 0.8584700 1.0013640	C	6.0206720 -0.9838920-1.3553270
Au	3.2190500 0.6300480 0.5619010	C	-1.72488000.8940310 0.5873030	C	7.1909150 -1.7391620-1.1846630
P	5.5486720 0.4513850 0.1338090	C	-3.00492001.3349530 1.2372870	C	5.0831030 -1.3731450-2.3282280
C	6.5306710 0.2674930 1.6755890	H	-2.79664702.1100580 1.9811110	C	7.4214150 -2.8657030-1.9810390
C	7.8316820 0.7821200 1.7953010	H	-3.68536601.7212780 0.4793800	H	7.9217010 -1.4570180-0.4339080
C	5.9599130 -0.42100502.7595850	H	-3.46673300.4925750 1.7609000	C	5.3215210 -2.4932200-3.1266570
C	8.5518180 0.6016770 2.9797230	O	-1.45296100.9593490 -0.5929060	H	4.1671220 -0.8042340-2.4639530
H	8.2849040 1.3257330 0.9725540	O	-0.85433300.3852360 1.5170250	C	6.4907250 -3.2425760-2.9529490
C	6.6849500 -0.60477203.9392430	C	1.1257900 2.2600940 1.4033150	H	8.3287870 -3.4452490-1.8396080
H	4.9468930 -0.80615002.6847910	H	2.0057570 2.8080650 1.7429030	H	4.5927660 -2.7835200-3.8775510
C	7.9819390 -0.09312604.0510440	H	0.7770470 2.7724500 0.4901140	H	6.6721660 -4.1176860-3.5698320
H	9.5564470 1.0053920 3.0633550	H	0.3196430 2.3323560 2.1393680		
H	6.2340760 -1.13817804.7707320	C	1.6517980 -2.22424400.4042280	TS ₅₋₆	
H	8.5432500 -0.22975704.9706190	H	1.9724640 -2.87646301.2285560	C	0.0677000 -1.55938901.1824520
C	6.2334440 1.9240740 -0.7262200	C	-0.7687790-2.27308201.0822110	C	-0.0084380-0.22804200.9434310
C	7.2465560 1.8194010 -1.6921360	H	-1.3241180-1.93698701.9608270	C	1.0437080 0.7677300 0.7977610
C	5.7320300 3.1928740 -0.3875010	H	-1.4383170-2.14608500.2182670	C	-1.34906501.3098160 -0.0863970
C	7.7542190 2.9691220 -2.3050730	H	-0.5310490-3.33461201.1635860	C	-2.71655901.7860320 -0.4464800
H	7.6394020 0.8470150 -1.9712020	H	1.3474890 -2.8951320-0.4086100	H	-3.28285002.0009380 0.4637720
C	6.2468090 4.3391360 -0.9966660	H	2.4956800 -1.61527200.0854990	H	-2.64871202.6745410 -1.0722610
H	4.9383140 3.2864840 0.3486910	Au	3.4032560 0.6123730 0.3713190	H	-3.24199600.9911270 -0.9857170
C	7.2579800 4.2288330 -1.9574820	P	5.6661670 0.5104710 -0.3483040	O	-0.29100101.7338580 -0.5568530
H	8.5363390 2.8772990 -3.0528710	C	6.8456760 0.4810030 1.0579530	O	-1.31439500.3360960 0.8346350
H	5.8528680 5.3146250 -0.7274470	C	8.0905700 1.1269030 0.9955230	C	1.3709580 -2.28465201.3593980
H	7.6527210 5.1200820 -2.4362660	C	6.4889580 -0.21965502.2230140	H	1.5274600 -2.51115902.4218650
C	5.9833300 -0.9892360-0.9226230	C	8.9681580 1.0644830 2.0820930	C	-1.1646400-2.39697401.3881590
C	7.0552800 -1.8433460-0.6230590	H	8.3778080 1.6807910 0.1076510	H	-2.0910990-1.83000601.3107330
C	5.2059350 -1.2357100-2.0684310	C	7.3713580 -0.28505403.3033240	H	-1.1780050-3.20080700.6411080
C	7.3483840 -2.9245720-1.4610890	H	5.5222890 -0.71128502.2887820	H	-1.1264640-2.88463302.3694770
H	7.6624880 -1.67304900.2596560	C	8.6119980 0.3579220 3.2346210	H	1.3334150 -3.24394700.8320630
C	5.5070860 -2.3104310-2.9068200	H	9.9279360 1.5692530 2.0255830	H	2.2335030 -1.71397001.0088760
H	4.3655100 -0.5894590-2.3070490	H	7.0866580 -0.82982904.1984610	Au	2.7524850 0.4725740 -0.3228780

P	4.6986410	0.2266060	-1.6618680	C	-2.23331602	0.8327350	0.6308330	C	2.0686200	-1.0112280	-3.9695420
C	6.2578540	0.3647120	-0.7036540	H	-3.07337102	0.5475030	1.2674890	C	4.1899190	-2.2915840	-5.2636390
C	7.4092390	0.9586050	-1.2444150	H	-1.87048403	0.8278260	0.8851490	H	5.4651210	-0.8682040	-4.2758550
C	6.2969120	-0.15473100	0.6016510	H	-2.57773202	0.8277330	-0.4098590	C	1.8189460	-2.0935220	-4.8156240
C	8.5845060	1.0243960	-0.4901620	O	0.0885240	2.1697600	0.8217060	H	1.2414240	-0.5247800	-3.4597570
H	7.3933350	1.3734330	-2.2470990	O	-1.39021200	0.5749810	0.8187240	C	2.8799100	-2.7363540	-5.4631460
C	7.4747550	-0.09236501	0.3493400	C	1.6834500	1.0243270	2.2553070	H	5.0173480	-2.7895690	-5.7602900
H	5.4081250	-0.60431101	0.0355960	H	2.3108490	0.1412480	2.4019410	H	0.7997460	-2.4385480	-4.9620810
C	8.6201970	0.4978300	0.8044360	H	2.3348610	1.9017940	2.2595730	H	2.6861640	-3.5827270	-6.1154230
H	9.4696400	1.4875030	-0.9159470	H	0.9826100	1.0904400	3.0979560				
H	7.4948110	-0.49681402	0.3568650	C	1.1158130	-2.26565101	0.0055300	TS₆₋₃			
H	9.5341430	0.5519990	1.3884430	H	1.2835570	-2.67743802	0.0086130	C	0.1912140	-1.63371800	0.9538040
C	4.7933950	1.5096370	-2.9728680	C	-1.4478620	-2.27142400	0.9678530	C	0.2374740	-0.31952700	0.9444820
C	5.1946900	1.2093100	-4.2834160	H	-2.3409810	-1.64518900	0.9754410	C	0.8114970	0.9617100	0.7771480
C	4.4568390	2.8334050	-2.6393240	H	-1.4899530	-2.92545100	0.0878710	C	-1.42690001	0.5261640	0.9302220
C	5.2647480	2.2224150	-5.2451360	H	-1.4764220	-2.92438601	0.8486860	C	-2.54406602	0.5075350	0.8079740
H	5.4502550	0.1916550	-4.5597540	H	1.0546010	-3.11554400	0.3159090	H	-2.51360703	0.1722410	1.6786610
C	4.5350610	3.8424970	-3.6008350	H	1.9891720	-1.66704800	0.7328990	H	-2.42095903	0.1126450	-0.0913410
H	4.1323130	3.0775060	-1.6314130	Au	2.2296550	0.8875090	-0.7786110	H	-3.50124901	0.9857970	0.8011400
C	4.9379340	3.5381490	-4.9060410	P	3.6488600	0.8943930	-2.6741060	O	-0.27435301	0.8795590	0.3682990
H	5.5750510	1.9799870	-6.2571640	C	5.4325790	0.8809550	-2.2373130	O	-1.51096000	0.4382160	1.5207970
H	4.2743530	4.8620520	-3.3330600	C	6.3812700	1.6314370	-2.9492780	C	1.2244940	-2.45431500	0.2040200
H	4.9917430	4.3225510	-5.6551150	C	5.8523170	0.0845900	-1.1576360	H	1.8225110	-3.02557300	0.9227800
C	4.7610300	-1.3939240	-2.5215410	C	7.7314460	1.5796940	-2.5887690	C	-0.8542270	-2.43034401	0.7000160
C	5.9603920	-2.1009500	-2.6985140	H	6.0735460	2.2586230	-3.7796390	H	-1.5543220	-1.80068902	0.2444790
C	3.5624120	-1.9299410	-3.0235270	C	7.2024630	0.0297150	-0.8058530	H	-1.4062910	-3.05596400	0.9896490
C	5.9595050	-3.3241400	-3.3763540	H	5.1257620	-0.4901090	-0.5898680	H	-0.3527990	-3.10342102	0.4041160
H	6.8930300	-1.7061030	-2.3089490	C	8.1441590	0.7785610	-1.5203160	H	0.7090040	-3.1706500	-0.4451090
C	3.5673630	-3.1476180	-3.7066720	H	8.4574260	2.1661580	-3.1440190	H	1.8923910	-1.8380800	-0.3994720
H	2.6259520	-1.3982890	-2.8781170	H	7.5163700	-0.58985000	0.0288870	Au	2.1843840	0.8276670	-0.8941480
C	4.7664300	-3.8469840	-3.8833040	H	9.1931150	0.7415140	-1.2416320	P	3.6795490	0.8686810	-2.7095820
H	6.8918160	-3.8655160	-3.5064760	C	3.3964220	2.3809130	-3.7233640	C	5.4353070	0.8035350	-2.1831300
H	2.6365500	-3.5519170	-4.0930790	C	3.3943070	2.3166670	-5.1252380	C	6.4405210	1.4928640	-2.8799480
H	4.7691240	-4.7971700	-4.4091020	C	3.2042120	3.6209500	-3.0894090	C	5.7782140	0.0266700	-1.0634130
C	1.0188350	1.9278150	1.7462280	C	3.2089050	3.4788030	-5.8810690	C	7.7718760	1.3987010	-2.4641350
H	1.4466310	2.8269520	1.2977370	H	3.5333000	1.3668730	-5.6312030	H	6.1905950	2.1051840	-3.7404730
H	0.0393660	2.1462990	2.1829070	C	3.0274260	4.7799230	-3.8476320	C	7.1103260	-0.0697300	-0.6558010
H	1.6961690	1.6358000	2.5636620	H	3.1903900	3.6814290	-2.0045990	H	5.0060500	-0.4971580	-0.5068050
				C	3.0279660	4.7102880	-5.2453310	C	8.1087890	0.6167590	-1.3552770
6				H	3.2067630	3.4183470	-6.9653390	H	8.5426210	1.9372620	-3.0073350
C	-0.1678270	-1.47627300	0.9578460	H	2.8823530	5.7330900	-3.3479520	H	7.3657410	-0.67257900	0.2104700
C	-0.1393010	-0.14095900	0.9063880	H	2.8835470	5.6108420	-5.8348270	H	9.1436080	0.5472450	-1.0334350
C	0.9563580	0.8980780	0.9188000	C	3.3829690	-0.5529530	-3.7728680	C	3.5012630	2.4002910	-3.7055150
C	-1.14306401	0.8455300	0.7704940	C	4.4434250	-1.2027890	-4.4233910	C	3.4706850	2.3775200	-5.1079790

C	3.3969230	3.6298200	-3.0313800	H	-0.1493030	-2.6718320	1.7228020	C	1.3531560	5.0082060	-2.1894960
C	3.3432460	3.5712850	-5.8259700	H	0.5331870	-2.1680110	0.1569150	H	1.3645550	6.0892660	-0.3194480
H	3.5427130	1.4370910	-5.6442240	Au	3.1828060	0.5074900	0.9159180	H	1.3230420	3.6749880	-3.8885830
C	3.2777280	4.8188840	-3.7523600	P	5.4752630	0.1795150	1.2415910	H	1.4047220	5.9062080	-2.7976790
H	3.4077390	3.6602830	-1.9451920	C	5.8430590	-1.5554490	1.7034490				
C	3.2490810	4.7913050	-5.1514980	C	5.1619930	-2.5913310	1.0404930	TS₁₋₂			
H	3.3185270	3.5433690	-6.9112250	C	6.7946650	-1.8691250	2.6860550	C	0.3101820	-0.7277940	-0.0922110
H	3.1998220	5.7635110	-3.2225740	C	5.4407460	-3.9237040	1.3490260	C	1.2366060	0.2354940	0.6222500
H	3.1490250	5.7163120	-5.7114970	H	4.4136500	-2.3587290	0.2878550	C	0.8925310	1.3127260	1.2345150
C	3.4268860	-0.5340840	-3.8652930	C	7.0647490	-3.2057540	2.9958910	C	-1.6347890	0.3271280	1.0166720
C	4.5031190	-1.1903120	-4.4826790	H	7.3227190	-1.0807130	2.2120820	C	-3.0399210	0.0955400	1.4836280
C	2.1128690	-0.9507120	-4.1407500	C	6.3917720	-4.2325940	2.3281770	H	-3.5753680	1.0444330	1.5234220
C	4.2652610	-2.2461110	-5.3681780	H	4.9112560	-4.7176600	0.8311960	H	-3.5521600	-0.6140490	0.8318430
H	5.5238720	-0.8867840	-4.2750180	H	7.8003860	-3.4405910	3.7591610	H	-3.0028890	-0.3288070	2.4935000
C	1.8800780	-2.0000910	-5.0317610	H	6.6027170	-5.2694760	2.5721970	O	-1.0510440	-0.7442490	0.5209730
H	1.2728790	-0.4585190	-3.6582880	C	6.1420910	1.2420040	2.5773430	O	-1.0759290	1.4322510	1.1280630
C	2.9563630	-2.6504560	-5.6455820	C	7.4223120	1.8112000	2.4910720	C	0.1282720	-0.3074620	-1.5554970
H	5.1040930	-2.7503190	-5.8385670	C	5.3555970	1.4729800	3.7190750	H	1.0958990	-0.3378860	-2.0636630
H	0.8614280	-2.3138060	-5.2392930	C	7.9103490	2.5965510	3.5397610	C	0.7542170	-2.1834760	0.0403810
H	2.7748560	-3.4718300	-6.3323770	H	8.0380300	1.6498610	1.6123270	H	1.7159750	-2.3205140	-0.4596450
C	1.4988100	1.5690680	2.0066690	C	5.8506110	2.2523550	4.7660890	H	0.8644950	-2.4617210	1.0916490
H	1.9244400	2.5439170	1.7584450	H	4.3579090	1.0487470	3.7901290	H	0.0160250	-2.8401510	-0.4277270
H	0.7903640	1.6943640	2.8347330	C	7.1283510	2.8159580	4.6772740	H	-0.5548710	-0.9984780	-2.0572150
H	2.3078280	0.9129300	2.3365620	H	8.9005950	3.0354660	3.4642970	H	-0.2662160	0.7091500	-1.6268490
Species with R ¹ = R ² = Me, R ³ = Ph, PPh ₃ Ligand				H	5.2368290	2.4249640	5.6449230	Au	3.3412290	0.0061510	0.5789120
1				H	7.5096740	3.4279090	5.4892130	P	5.6707420	-0.2888250	0.4964860
C	0.1478890	-0.5467160	1.5730610	C	6.4527610	0.5463140	-0.2654310	C	6.1462800	-2.0621490	0.4583670
C	0.9542970	0.4780540	0.8343780	C	6.1200760	1.6756140	-1.0335740	C	7.2048360	-2.5669490	1.2284670
C	1.1158690	1.5162890	0.1727790	C	7.5296720	-0.2646030	-0.6559660	C	5.4241300	-2.9312580	-0.3779380
C	-1.7669420	-0.4275510	0.0220290	H	6.8651050	1.9945480	-2.1699840	C	7.5396670	-3.9231490	1.1567200
C	-3.2567700	-0.2024310	0.0181210	H	5.2812480	2.3049490	-0.7495510	H	7.7674890	-1.9113520	1.8848360
H	-3.6317870	-0.2627110	-1.0032430	C	8.2680500	0.0560410	-1.7993220	C	5.7664030	-4.2824150	-0.4520220
H	-3.7487270	-0.9571310	0.6393020	H	7.7940180	-1.1440230	-0.0780660	H	4.5952360	-2.5536200	-0.9703460
H	-3.4894950	0.7778000	0.4444930	C	7.9392590	1.1844350	-2.5552230	C	6.8245210	-4.7808500	0.3168060
O	-1.2720210	-0.3227380	1.2818660	H	6.6020540	2.8691310	-2.7571700	H	8.3591480	-4.3052090	1.7581260
O	-1.0861760	-0.6654930	-0.9573680	H	9.0980490	-0.5779610	-2.0960750	H	5.2040340	-4.9452930	-1.1027590
C	0.5488960	-1.9884680	1.2313570	H	8.5132930	1.4297660	-3.4437290	H	7.0859890	-5.8335290	0.2640670
H	1.5533750	-2.1890480	1.6133670	C	1.2182400	2.6962990	-0.6243980	C	6.5216080	0.4415650	1.9502930
C	0.2467300	-0.2894440	0.0841180	C	1.2650650	3.9651310	-0.0074740	C	7.7613720	1.0898940	1.8381130
H	1.2790010	-0.4179490	3.4183930	C	1.2426980	2.5952310	-2.0322750	C	5.9070070	0.3386010	3.2103910
H	-0.0832730	0.7236410	3.3258420	C	1.3310640	5.1133460	-0.7932160	C	8.3793310	1.6224860	2.9739010
H	-0.3876080	-1.0071010	3.6109720	H	1.2469260	4.0358830	1.0751180	H	8.2457640	1.1854580	0.8719580
				C	1.3080050	3.7516250	-2.8060330	C	6.5317380	0.8645790	4.3427880
				H	1.2053580	1.6169640	-2.4996170	H	4.9402340	-0.1478160	3.3069450

C	7.7682940	1.5089330	4.2258430	H	-0.2062550	-1.5770670	-2.0756770	C	1.9968670	4.7360280	3.2115830
H	9.3366850	2.1257440	2.8769770	H	0.2385890	0.1513930	-2.0583850	H	0.5168530	4.2954520	4.7209130
H	6.0497660	0.7786300	5.3120280	Au	3.2018060	0.1485080	0.4020200	H	3.3445980	4.9211120	1.5352190
H	8.2499170	1.9247770	5.1058630	P	5.5535870	-0.02710800	0.2683100	H	2.3795000	5.6139110	3.7237350
C	6.4338960	0.4716350	-0.9902270	C	6.1600030	-1.74186400	0.5298250				
C	7.5527450	-0.0986900	-1.6178600	C	7.3288070	-2.01816901	0.2558170	TS₂₋₃			
C	5.8887740	1.6626650	-1.4996600	C	5.4270500	-2.8044010	-0.0266070	C	0.6311240	-0.9006100	-0.2789900
C	8.1219230	0.5197310	-2.7349100	C	7.7603030	-3.33872001	0.4166700	C	1.1218580	0.2157090	0.4450660
H	7.9797710	-1.0235770	-1.2435540	H	7.9023050	-1.21101301	0.6997840	C	0.4723670	1.1553390	1.1429770
C	6.4641230	2.2800860	-2.6124370	C	5.8654020	-4.12088600	0.1292070	C	-1.79985800	0.3228590	0.7700410
H	5.0141150	2.1057880	-1.0318430	H	4.5130180	-2.6041810	-0.5788540	C	-3.21727800	0.6057120	1.1663310
C	7.5809240	1.7091470	-3.2320170	C	7.0325190	-4.39025400	0.8527730	H	-3.47356601	0.6380210	0.9109450
H	8.9858890	0.0698910	-3.2148880	H	8.6644180	-3.54193401	0.9829000	H	-3.8871200	-0.08570600	0.6565010
H	6.0354130	3.2000020	-2.9985420	H	5.2926530	-4.9342110	-0.3063570	H	-3.32198500	0.4958410	2.2502370
H	8.0233910	2.1862960	-4.1014180	H	7.3692090	-5.41485400	0.9801060	O	-1.4729630	-0.58793900	0.0109270
C	1.1516010	2.4902930	2.0125740	C	6.4188650	1.0091770	1.5149500	O	-0.93655601	0.1758630	1.3321040
C	1.3782630	2.3819570	3.4001380	C	7.5908180	1.7191570	1.2109760	C	0.5507410	-0.8437600	-1.7781770
C	1.1783230	3.7572560	1.3942280	C	5.8856670	1.0827680	2.8136810	H	1.4769730	-1.2601630	-2.1921880
C	1.6484340	3.5247530	4.1507530	C	8.2225040	2.4865480	2.1948330	C	0.6272130	-2.26523700	0.3496060
H	1.3488670	1.4050360	3.8717630	H	8.0121230	1.6807650	0.2117760	H	1.5611580	-2.77361800	0.0815420
C	1.4427260	4.8945760	2.1539610	C	6.5239070	1.8435740	3.7951610	H	0.5591310	-2.21305101	0.4369800
H	0.9946200	3.8361400	0.3275790	H	4.9711160	0.5498800	3.0588140	H	-0.1963000	-2.8581930	-0.0558490
C	1.6792600	4.7790370	3.5297050	C	7.6928890	2.5481290	3.4868100	H	-0.2743020	-1.4681970	-2.1290250
H	1.8318120	3.4397540	5.2172350	H	9.1271150	3.0345840	1.9484420	H	0.4343910	0.1782220	-2.1407310
H	1.4670390	5.8693730	1.6771870	H	6.1038260	1.8926810	4.7953030	Au	3.2394670	0.0976070	0.3236850
H	1.8872390	5.6677070	4.1181200	H	8.1844530	3.1459620	4.2486180	P	5.5901810	-0.02070900	0.2519030
				C	6.2120860	0.4953310	-1.3654000	C	6.2209310	-1.71747000	0.5564170
2				C	7.2948390	-0.1559890	-1.9762770	C	7.3888700	-1.95260201	0.2984700
C	0.3370270	-0.8269120	-0.1202180	C	5.6120830	1.5897830	-2.0120670	C	5.5159850	-2.80586400	0.0147420
C	1.1201930	0.2739890	0.5377310	C	7.7734550	0.2865230	-3.2134820	C	7.8475200	-3.25987401	0.4885100
C	0.4981160	1.2555910	1.1970400	H	7.7643490	-1.0082950	-1.4958970	H	7.9404900	-1.12491801	0.7323910
C	-1.68015000	0.3303120	0.7868900	C	6.0977340	2.0333840	-3.2438580	C	5.9819880	-4.10883800	0.1999990
C	-3.14976600	0.3855460	1.0014080	H	4.7639820	2.0928570	-1.5557980	H	4.6017710	-2.6367160	-0.5476220
H	-3.47161701	0.4177250	1.1427400	C	7.1787300	1.3812760	-3.8472680	C	7.1483550	-4.33783100	0.9384460
H	-3.6671150	-0.07876500	0.1615140	H	8.6099670	-0.2260260	-3.6791610	H	8.7503970	-3.43200802	0.0667440
H	-3.3834230	-0.18101201	0.9108190	H	5.6277350	2.8805930	-3.7343490	H	5.4311410	-4.9429890	-0.2241210
O	-1.1980040	-0.61706700	0.0863940	H	7.5516670	1.7218780	-4.8086540	H	7.5063870	-5.35200801	0.0885420
O	-0.96231501	0.2433220	1.3403400	C	1.0068590	2.4586710	1.8850190	C	6.3867880	1.0540100	1.5094520
C	0.4667210	-0.8325190	-1.6410080	C	0.4535500	2.8695650	3.1122260	C	7.5117760	1.8375200	1.2102020
H	1.4945970	-1.0909630	-1.9077910	C	2.0473460	3.2186930	1.3223920	C	5.8513910	1.0811360	2.8091860
C	0.5671890	-2.20183100	0.5014450	C	0.9487100	3.9968090	3.7702270	C	8.0953990	2.6340100	2.2007370
H	1.5954790	-2.51366200	0.3028980	H	-0.35665102	0.3011080	3.5573990	H	7.9341520	1.8327790	0.2109120
H	0.4179200	-2.17594801	0.5838730	C	2.5422130	4.3438150	1.9851090	C	6.4419130	1.8718600	3.7963160
H	-0.1128230	-2.93518800	0.0585110	H	2.4573350	2.9331060	0.3592600	H	4.9739170	0.4881250	3.0516850

C	7.5639730	2.6513430	3.4930680	H	-0.1324750	-1.5404230	-1.7900730	C	2.1620490	4.4777540	3.1459920
H	8.9642890	3.2388030	1.9588970	H	1.0401200	-0.2394330	-2.0955910	H	0.6779280	4.1107420	4.6706840
H	6.0213640	1.8851790	4.7973040	Au	3.3237240	-0.14655900	2.877630	H	3.5023570	4.5963880	1.4576690
H	8.0180160	3.2719240	4.2598960	P	5.6843310	-0.14004300	2.089680	H	2.5730070	5.3534870	3.6393890
C	6.2683660	0.4971650	-1.3733830	C	6.4015220	-1.79710600	5.263440				
C	7.3984610	-0.1178370	-1.9344470	C	7.5997320	-1.94864201	2.421960	TS₁₋₄			
C	5.6427410	1.5515750	-2.0606320	C	5.7487020	-2.93352700	0.0194380	C	0.4972940	-1.23961500	9.256310
C	7.8978890	0.3220120	-3.1641210	C	8.1392680	-3.22279901	4.414910	C	0.6984420	0.2411240	0.9230320
H	7.8892560	-0.9380230	-1.4206370	H	8.1114880	-1.08186301	6.473010	C	1.3651850	1.3230930	0.8492230
C	6.1494970	1.9925230	-3.2847740	C	6.2953230	-4.20311800	2.157640	C	-1.7359460	-0.50022100	8.847650
H	4.7594910	2.0266680	-1.6427150	H	4.8143140	-2.8306280	-0.5250200	C	-3.1898570	-0.78375400	6.895520
C	7.2772590	1.3772440	-3.8389780	C	7.4907560	-4.34947400	9.279300	H	-3.3432730	-1.3652390	-0.2218650
H	8.7710100	-0.1616700	-3.5917410	H	9.0650620	-3.33125801	9.983420	H	-3.5449470	-1.38133401	5.362510
H	5.6600110	2.8089950	-3.8071520	H	5.7844880	-5.0756890	-0.1799280	H	-3.74765200	1.1512770	0.6520260
H	7.6671050	1.7157340	-4.7943390	H	7.9114090	-5.33800201	0.0859770	O	-0.9150660	-1.49589000	5.775150
C	1.0542340	2.3194320	1.8529550	C	6.4010040	0.9861200	1.4654010	O	-1.27196100	5.636810	1.3090440
C	0.5872540	2.6774150	3.1308530	C	7.4414200	1.8746140	1.1543820	C	1.3058030	-1.9447110	-0.1684380
C	2.0681110	3.0912090	1.2603240	C	5.8939670	0.9422960	2.7759990	H	2.3740210	-1.85799800	0.0399780
C	1.1462160	3.7611160	3.8104610	C	7.9713330	2.7056560	2.1467300	C	0.7370050	-1.84112602	3.172840
H	-0.20487702	0.0995160	3.5957610	H	7.8395430	1.9244900	0.1464050	H	1.7857950	-1.70787302	5.944170
C	2.6247720	4.1759860	1.9425340	C	6.4313290	1.7688810	3.7635770	H	0.1134560	-1.35233903	0.0696880
H	2.4048200	2.8550830	0.2557220	H	5.0815220	0.2662270	3.0277250	H	0.5073160	-2.90969502	2.2971380
C	2.1687400	4.5124550	3.2204790	C	7.4699750	2.6530830	3.4498920	H	1.0327740	-3.0031780	-0.1772880
H	0.7835420	4.0176620	4.8015390	H	8.7752110	3.3916690	1.8974490	H	1.0959990	-1.5092940	-1.1474510
H	3.4041890	4.7652600	1.4684830	H	6.0342920	1.7278770	4.7732790	Au	3.4139880	0.7842720	0.4543710
H	2.5995270	5.3577370	3.7490270	H	7.8825040	3.3005320	4.2178580	P	5.7016950	0.4098720	0.1025790
				C	6.3112120	0.4064140	-1.4241750	C	6.5796560	-0.05844901	6.440140
3				C	7.4456200	-0.1778420	-2.0090820	C	7.8888940	0.3744580	1.9074830
C	1.0904890	-1.1428180	-0.1196170	C	5.6413960	1.4438530	-2.0957640	C	5.9238170	-0.88315902	5.740630
C	1.1672240	0.0560170	0.5414720	C	7.9065570	0.2773950	-3.2480320	C	8.5349780	-0.02240803	0.0821420
C	0.5349930	1.0075310	1.2199300	H	7.9686660	-0.9857870	-1.5082680	H	8.4057530	1.0211160	1.2059570
C	-1.72552701	5.610270	0.6849460	C	6.1100730	1.8991480	-3.3293750	C	6.5755820	-1.28205103	7.426300
C	-3.14156901	3.202950	1.1264000	H	4.7534600	1.8937290	-1.6603130	H	4.9042030	-1.20950102	3.895370
H	-3.28160401	7.279610	2.1329430	C	7.2428510	1.3157070	-3.9075640	C	7.8822000	-0.85197303	9.983440
H	-3.82760001	8.103610	0.4362500	H	8.7830910	-0.1818630	-3.6949070	H	9.5467950	0.3191150	3.2787020
H	-3.35060700	2.482010	1.1723020	H	5.5870430	2.7017500	-3.8403510	H	6.0609150	-1.91977504	4.4549860
O	-1.36153702	3.076150	-0.1975060	H	7.6025170	1.6656220	-4.8705260	H	8.3858770	-1.15684904	9.108030
O	-0.84995900	8.051430	1.4253790	C	1.0963780	2.2114380	1.8668430	C	6.5582090	1.8957820	-0.5480140
C	0.8999510	-1.2074900	-1.6146490	C	0.5614680	2.6585480	3.0885640	C	7.5659190	1.8003070	-1.5202790
H	1.5590110	-1.9519920	-2.0706150	C	2.1562720	2.9274710	1.2840580	C	6.2029260	3.1573730	-0.0403020
C	1.0306820	-2.45220000	6.271440	C	1.0950950	3.7812910	3.7237210	C	8.2135180	2.9538830	-1.9732760
H	1.7079280	-3.19095600	1.881890	H	-0.26223802	1.191340	3.5448480	H	7.8456770	0.8344240	-1.9277820
H	1.2446820	-2.33544601	6.895390	C	2.6885030	4.0486630	1.9233290	C	6.8571360	4.3053550	-0.4909060
H	0.0098200	-2.84193000	5.121320	H	2.5408990	2.6257750	0.3144070	H	5.4157650	3.2449510	0.7033570

C	7.8627180	4.2052320	-1.4589520	H	0.5499600	-2.7299730	-1.1129270	C	0.0678200	5.0830300	2.1759430
H	8.9904860	2.8711990	-2.7273430	H	0.0974680	-1.0736090	-1.6036450	H	0.9678010	5.6731150	0.3034460
H	6.5772100	5.2755260	-0.0916150	Au	3.1455150	0.7126760	0.6524430	H	-0.7373200	4.1794130	3.9637380
H	8.3664640	5.0995090	-1.8135650	P	5.4651000	0.4246950	0.2735010	H	-0.1896480	6.0964630	2.4696270
C	6.0117680	-0.9360020	-1.1067430	C	6.4010720	0.0491150	1.8094360				
C	7.0348300	-1.8793620	-0.9245350	C	7.6842860	0.5664350	2.0465660	TS₄₋₅			
C	5.1996150	-1.0085650	-2.2518280	C	5.8074050	-0.7878640	2.7699500	C	0.4765880	-1.5704700	0.8807920
C	7.2453080	-2.8776090	-1.8813030	C	8.3647340	0.2445170	3.2249490	C	0.2762950	-0.1541320	1.0992260
H	7.6656160	-1.8428190	-0.0424350	H	8.1538500	1.2224870	1.3208580	C	1.1687770	0.8658510	1.0185460
C	5.4190570	-2.0015910	-3.2079350	C	6.4931570	-1.1131190	3.9421720	C	-1.9033790	-0.6197250	0.5966590
H	4.3951760	-0.2925880	-2.3957670	H	4.8082720	-1.1812330	2.6049220	C	-3.3323780	-0.1954120	0.5694790
C	6.4416070	-2.9389970	-3.0229950	C	7.7728410	-0.5962020	4.1720100	H	-3.4120670	0.7311670	-0.0094020
H	8.0375480	-3.6048820	-1.7311240	H	9.3556710	0.6526970	3.4003510	H	-3.9444110	-0.9691320	0.1081120
H	4.7880200	-2.0476000	-4.0904020	H	6.0253930	-1.7610950	4.6774050	H	-3.6757110	0.0162530	1.5851430
H	6.6071760	-3.7157590	-3.7635820	H	8.3028090	-0.8428150	5.0872860	O	-1.4218150	-1.5631680	-0.0398760
C	1.0937420	2.7523440	1.0674150	C	6.2488610	1.9275770	-0.4359930	O	-1.1045480	0.1133650	1.3855500
C	1.6202690	3.7222600	0.1948220	C	7.2418670	1.8577160	-1.4253070	C	1.4176510	-2.0952110	-0.1492640
C	0.3084730	3.1667390	2.1595350	C	5.8380160	3.1844330	0.0411350	H	2.3277780	-2.4617040	0.3404750
C	1.3452340	5.0761720	0.3956580	C	7.8193350	3.0294970	-1.9247480	C	0.0474050	-2.5442020	1.9359470
H	2.2339920	3.4095440	-0.6442840	H	7.5653850	0.8964030	-1.8110900	H	0.9407790	-2.7385860	2.5465730
C	0.0511790	4.5233420	2.3643720	C	6.4227680	4.3516040	-0.4542750	H	-0.7291380	-2.1568170	2.5952940
H	-0.0939380	2.4260340	2.8414260	H	5.0606790	3.2522080	0.7972060	H	-0.2627880	-3.4963880	1.4997690
C	0.5639020	5.4814580	1.4827620	C	7.4135640	4.2759240	-1.4395190	H	0.9533140	-2.9646360	-0.6267310
H	1.7477400	5.8134690	-0.2926280	H	8.5851220	2.9649720	-2.6920680	H	1.6809830	-1.3534520	-0.9009190
H	-0.5531340	4.8313590	3.2126360	H	6.0992650	5.3172190	-0.0771900	Au	3.1975290	0.6096190	0.6119610
H	0.3590840	6.5356430	1.6442230	H	7.8628640	5.1842950	-1.8298860	P	5.5241930	0.4223140	0.2068630
				C	5.8459710	-0.9377050	-0.8996870	C	6.4802260	-0.0305620	1.7087270
4				C	6.9023790	-1.8366150	-0.6880260	C	7.7527400	0.5018960	1.9683190
C	0.2479840	-1.3743180	0.5434600	C	5.0490610	-1.0697960	-2.0504710	C	5.9175100	-0.9453580	2.6156500
C	0.2056120	0.1066800	0.9012260	C	7.1596110	-2.8501550	-1.6172190	C	8.4542480	0.1176410	3.1151820
C	1.1204100	1.0665020	1.0085500	H	7.5242950	-1.7529330	0.1971360	H	8.1978150	1.2168640	1.2841620
C	-1.9034430	-0.6688530	0.9333190	C	5.3145460	-2.0769860	-2.9800760	C	6.6245410	-1.3323060	3.7560570
C	-3.3754820	-0.6855080	1.0472350	H	4.2219590	-0.3859480	-2.2211530	H	4.9260570	-1.3512870	2.4347850
H	-3.8005770	-0.6890150	0.0367320	C	6.3696680	-2.9706900	-2.7637200	C	7.8940180	-0.8006070	4.0078680
H	-3.6949260	-1.6000720	1.5511920	H	7.9781460	-3.5421750	-1.4426180	H	9.4368400	0.5376470	3.3084810
H	-3.7213310	0.1988000	1.5810270	H	4.6950150	-2.1674240	-3.8673940	H	6.1812480	-2.0402840	4.4499490
O	-1.2307540	-1.7202660	0.6214040	H	6.5716060	-3.7582430	-3.4836800	H	8.4404020	-1.0961520	4.8986480
O	-1.2161980	0.3996590	1.1211860	C	0.7407090	2.4479220	1.4136670	C	6.2595580	1.9877390	-0.4105870
C	0.6745460	-1.6669230	-0.8901100	C	1.0649730	3.5428680	0.5902320	C	7.2827340	2.0015740	-1.3716000
H	1.7307500	-1.4057720	-0.9966790	C	0.0876820	2.7012700	2.6346790	C	5.7837060	3.2041570	0.1084260
C	0.9452330	-2.2513440	1.5762090	C	0.7191900	4.8443310	0.9605010	C	7.8264580	3.2163110	-1.8003920
H	2.0093710	-1.9999260	1.5776880	H	1.5871450	3.3669540	-0.3460650	H	7.6551660	1.0721370	-1.7901970
H	0.5474560	-2.0763790	2.5788290	C	-0.2401030	4.0060640	3.0133350	C	6.3343290	4.4147930	-0.3174260
H	0.8322220	-3.3074540	1.3169320	H	-0.1522190	1.8733200	3.2954530	H	4.9808960	3.2063850	0.8405530

C	7.3560100	4.4226190	-1.2733420	H	1.4197790	-2.4344620	-1.1370000	C	0.9157990	3.7433280	4.2097700
H	8.6162020	3.2169470	-2.5458100	H	2.3068460	-1.67280300	0.2188380	H	2.6361440	4.7056420	3.3245660
H	5.9604090	5.3489590	0.0908860	Au	3.3345690	0.5362640	0.4467620	H	-0.75426302	5.491260	4.8811730
H	7.7791490	5.3646500	-1.6093890	P	5.5718960	0.4001580	-0.3375910	H	0.8114880	4.4779180	5.0026500
C	5.9249330	-0.8511870	-1.0564310	C	6.7833860	0.9010560	0.9468640				
C	6.9841830	-1.7579530	-0.8993750	C	7.9632080	1.5909590	0.6259930	TS₅₋₆			
C	5.1338460	-0.9100180	-2.2174190	C	6.5183530	0.5725990	2.2874740	C	0.0863840	-1.53323301	0.0541100
C	7.2499960	-2.7066730	-1.8925880	C	8.8673570	1.9403000	1.6334380	C	0.0222830	-0.20553700	0.8426090
H	7.6015990	-1.7317390	-0.0074810	H	8.1785690	1.8612380	-0.4026790	C	1.0918410	0.8223640	0.8775110
C	5.4079860	-1.8522980	-3.2101720	C	7.4278130	0.9171000	3.2897790	C	-1.16902601	4.783160	-0.1438220
H	4.3030270	-0.2217060	-2.3471270	H	5.6010010	0.0527810	2.5500820	C	-2.45813602	0.0444260	-0.6347920
C	6.4658420	-2.7543680	-3.0482140	C	8.6031530	1.6024590	2.9641190	H	-3.12813202	0.2050500	0.2152720
H	8.0707880	-3.4053020	-1.7600590	H	9.7757230	2.4768210	1.3761190	H	-2.27767202	0.9846500	-1.1533080
H	4.7925820	-1.8865080	-4.1042750	H	7.2141740	0.6580430	4.3224280	H	-2.93823501	0.3276440	-1.3076380
H	6.6743130	-3.4918190	-3.8176520	H	9.3065320	1.8767030	3.7447310	O	-0.05046001	0.9784040	-0.3286970
C	0.7714790	2.2442130	1.3888660	C	5.8830940	1.4835980	-1.7867700	O	-1.25962300	0.3510070	0.5526160
C	1.1844050	3.3212560	0.5761380	C	6.7204080	1.0880330	-2.8417540	C	1.3753930	-2.22386001	0.4085400
C	0.0244710	2.5336990	2.5497600	C	5.2744820	2.7499210	-1.8255390	H	1.3837140	-2.48176402	0.4754090
C	0.8220830	4.6327610	0.8854820	C	6.9488630	1.9517410	-3.9174010	C	-1.1370820	-2.41169201	0.0291140
H	1.7806860	3.1193460	-0.3088640	H	7.1918220	0.1106990	-2.8315300	H	-2.0542800	-1.86638100	0.8083250
C	-0.30372103	0.8500760	2.8773100	C	5.5108450	3.6116900	-2.8984250	H	-1.0056410	-3.19754600	0.2746720
H	-0.28205201	0.7270570	3.2070270	H	4.6148300	3.0633110	-1.0215080	H	-1.2543430	-2.92000501	0.9938400
C	0.0821230	4.9039730	2.0416660	C	6.3472830	3.2131430	-3.9468410	H	1.4609620	-3.16313800	0.8510230
H	1.1319520	5.4437970	0.2328480	H	7.5963600	1.6361890	-4.7300530	H	2.2575630	-1.61142001	0.2063680
H	-0.86585704	0.0522570	3.7845330	H	5.0358000	4.5878860	-2.9187740	Au	2.7773070	0.5497500	-0.3196230
H	-0.18249805	0.9265750	2.2940510	H	6.5249180	3.8810670	-4.7844820	P	4.6830420	0.2424550	-1.6938410
				C	6.0468520	-1.2936920	-0.8659860	C	6.2594390	0.4213930	-0.7691250
5				C	7.2514660	-1.8910350	-0.4658810	C	7.3958360	1.0094360	-1.3464620
C	0.2078580	-1.12098500	0.0042840	C	5.1665060	-2.0053270	-1.7000480	C	6.3245300	-0.05468500	0.5520230
C	0.2621620	0.1309750	0.5917620	C	7.5723220	-3.1819680	-0.8991250	C	8.5818270	1.1126770	-0.6132710
C	1.3903010	0.8121020	1.1313880	H	7.9398620	-1.35850200	0.1817460	H	7.3603870	1.3909100	-2.3617200
C	-1.23868901	0.8848010	-0.0217890	C	5.4949380	-3.2894630	-2.1371820	C	7.5130820	0.0444440	1.2783560
C	-2.63056502	0.3989630	0.2108450	H	4.2259560	-1.5578450	-2.0094690	H	5.4476230	-0.49802601	0.0156460
H	-2.73456102	0.7053350	1.2567920	C	6.6982740	-3.8810830	-1.7353970	C	8.6433770	0.6291020	0.6969090
H	-2.81948103	0.2507790	-0.4415050	H	8.5060850	-3.6366510	-0.5819960	H	9.4548640	1.5714950	-1.0677410
H	-3.36364001	0.6095060	0.0237070	H	4.8105100	-3.8289440	-2.7850390	H	7.5528870	-0.32670802	0.2980430
O	-0.39716902	0.3809320	-0.7405230	H	6.9498620	-4.8829010	-2.0705800	H	9.5653880	0.7122690	1.2646150
O	-1.01167900	0.7458340	0.7073200	C	1.1867700	1.8298760	2.1510820	C	4.7547740	1.4568660	-3.0695570
C	1.3470750	-2.0744370	-0.1036930	C	2.0992340	2.9102720	2.2750110	C	5.2355240	1.1113950	-4.3423130
H	1.1187800	-2.95679300	0.5106570	C	0.1421140	1.7304570	3.1110280	C	4.3215840	2.7722390	-2.8288260
C	-1.1108750	-1.6345340	-0.4956010	C	1.9449790	3.8707260	3.2680750	C	5.2891960	2.0721970	-5.3566840
H	-1.8585110	-1.63351600	0.3057350	H	2.9138440	2.9948490	1.5630680	H	5.5646950	0.0978950	-4.5477240
H	-1.5041810	-0.9786230	-1.2814710	C	0.0293260	2.6605990	4.1382790	C	4.3834900	3.7304280	-3.8427260
H	-1.0166180	-2.6459520	-0.8928480	H	-0.55142900	0.8994530	3.0680810	H	3.9316730	3.0474660	-1.8528290

C	4.8665510	3.3813470	-5.1085580	H	1.1384840	-3.1369460	-0.0043760	C	3.1573520	0.9752650	4.7868810
H	5.6609260	1.7949970	-6.3386540	H	2.0610760	-1.78674500	.6889320	H	4.4965720	2.3301090	3.7680820
H	4.0468260	4.7439670	-3.6465340	Au	2.3103600	0.8269180	-0.7483800	H	1.6633810	-0.40327905	.5116100
H	4.9075890	4.1250810	-5.8988290	P	3.6528980	0.8996210	-2.6919230	H	3.6805340	1.0384710	5.7365250
C	4.7307930	-1.4161990	-2.4803660	C	5.4481290	0.9497380	-2.3082830				
C	5.9181910	-2.1545440	-2.5986840	C	6.3454950	1.7464320	-3.0362250	TS₆₋₃			
C	3.5319460	-1.9502320	-2.9841800	C	5.9295780	0.1576020	-1.2513260	C	-0.1193550	-1.57658300	.6889570
C	5.9060450	-3.4068230	-3.2215860	C	7.7064250	1.7440010	-2.7143680	C	0.1257760	-0.29655000	.8665350
H	6.8502810	-1.7614440	-2.2060700	H	5.9899410	2.3706310	-3.8494610	C	0.8763840	0.9004580	0.8410070
C	3.5258100	-3.1971600	-3.6119180	C	7.2902510	0.1522400	-0.9383490	C	-1.24528301	.7430210	1.1500330
H	2.6036610	-1.3942650	-2.8841230	H	5.2429060	-0.4523950	-0.6710220	C	-2.21088002	.8779200	1.1932620
C	4.7134860	-3.9278600	-3.7309940	C	8.1808140	0.9468140	-1.6688450	H	-2.04551803	.4319810	2.1242640
H	6.8294840	-3.9718170	-3.3069460	H	8.3924970	2.3658030	-3.2817730	H	-2.03719403	.5547800	0.3553810
H	2.5950630	-3.5998720	-4.0001590	H	7.6518040	-0.4644820	-0.1209960	H	-3.23338602	.5003920	1.1873330
H	4.7072220	-4.9006390	-4.2136680	H	9.2379460	0.9479970	-1.4202350	O	-0.06791901	.9982730	0.5790350
C	1.1244880	1.7353620	2.0284510	C	3.3096680	2.3789740	-3.7248870	O	-1.46505500	.6121860	1.6078820
C	2.0782070	2.7774850	2.0753470	C	3.3107570	2.3251960	-5.1275020	C	0.7723000	-2.4250980	-0.1985080
C	0.2369920	1.5873060	3.1197250	C	3.0478910	3.6013710	-3.0816930	H	1.2769970	-3.17965500	.4150470
C	2.1282800	3.6513930	3.1572180	C	3.0607740	3.4806040	-5.8745660	C	-1.2692640	-2.30854601	.3413230
H	2.7716880	2.8920450	1.2479510	H	3.5025840	1.3883990	-5.6404940	H	-1.8524910	-1.67343802	.0041550
C	0.3040150	2.4487850	4.2123590	C	2.8065970	4.7543410	-3.8315030	H	-1.9231350	-2.71687500	.5624800
H	-0.48889100	.7806220	3.1208680	H	3.0307240	3.6528430	-1.9964960	H	-0.8739670	-3.15691201	.9104140
C	1.2431790	3.4867970	4.2304820	C	2.8113820	4.6953340	-5.2295270	H	0.1488890	-2.9522690	-0.9289790
H	2.8615300	4.4517060	3.1731880	H	3.0620170	3.4282920	-6.9592410	H	1.5256110	-1.8380760	-0.7259230
H	-0.37390102	.3127600	5.0492870	H	2.6082580	5.6940970	-3.3248050	Au	2.2070590	0.7951200	-0.8827180
H	1.2916420	4.1593700	5.0817270	H	2.6171330	5.5908360	-5.8123540	P	3.6900780	0.8572010	-2.7006510
				C	3.4047360	-0.5518910	-3.7894780	C	5.4428660	0.9571880	-2.1688800
6				C	4.4721470	-1.1818130	-4.4477390	C	6.3809720	1.7388980	-2.8612160
C	-0.1039670	-1.57378900	.7741060	C	2.0976220	-1.0347720	-3.9758960	C	5.8514350	0.2207400	-1.0436640
C	-0.0460810	-0.24134800	.8673610	C	4.2326830	-2.2754920	-5.2859610	C	7.7123050	1.7758780	-2.4356570
C	1.0792910	0.7579940	0.9905730	H	5.4883300	-0.8275070	-4.3087120	H	6.0799270	2.3203540	-3.7265310
C	-1.00610901	.7739260	0.8644000	C	1.8620030	-2.1216190	-4.8199430	C	7.1835150	0.2553360	-0.6270190
C	-2.08193802	.7839120	0.7795180	H	1.2646920	-0.5639200	-3.4608250	H	5.1308800	-0.3749760	-0.4901700
H	-2.92325402	.4787210	1.4056670	C	2.9299450	-2.7448250	-5.4753880	C	8.1156240	1.0339720	-1.3218270
H	-1.70378603	.7590550	1.0833690	H	5.0655970	-2.7577520	-5.7888990	H	8.4307120	2.3856100	-2.9753120
H	-2.43158202	.8350020	-0.2579510	H	0.8483230	-2.4854800	-4.9588820	H	7.4898980	-0.31740800	.2431120
O	0.2266300	2.0735650	0.9663530	H	2.7470500	-3.5947680	-6.1261360	H	9.1499040	1.0661900	-0.9924710
O	-1.27604000	.5072250	0.8105210	C	1.8075320	0.7997550	2.3184450	C	3.3916100	2.3087670	-3.7822770
C	1.1594780	-2.39383000	.8013600	C	2.9522890	1.6048450	2.4574020	C	3.4813330	2.2206080	-5.1800470
H	1.2398000	-2.94611401	.7462700	C	1.3513070	0.0848320	3.4379470	C	3.0797570	3.5425790	-3.1854050
C	-1.3987450	-2.33375100	.6483400	C	3.6160830	1.7003030	3.6809410	C	3.2667890	3.3551590	-5.9689280
H	-2.2773420	-1.68747200	.6570840	H	3.3216800	2.1548130	1.5964010	H	3.7141160	1.2742050	-5.6570540
H	-1.4026960	-2.9127350	-0.2835000	C	2.0259620	0.1650830	4.6600280	C	2.8738480	4.6740770	-3.9768310
H	-1.4920960	-3.05568201	.4689450	H	0.4712500	-0.54525603	.3565600	H	2.9950360	3.6202890	-2.1050830

C	2.9656850	4.5815810	-5.3701460
H	3.3355210	3.2770720	-7.0498050
H	2.6350500	5.6232480	-3.5066030
H	2.7985060	5.4606920	-5.9853490
C	3.5510310	-0.6230890	-3.7756690
C	4.6798720	-1.2571490	-4.3169520
C	2.2697240	-1.1202760	-4.0708860
C	4.5260730	-2.3711860	-5.1483380
H	5.6762090	-0.8901310	-4.0936060
C	2.1209830	-2.2272870	-4.9081500
H	1.3897410	-0.6452820	-3.6459750
C	3.2495880	-2.8553920	-5.4470230
H	5.4051020	-2.8571430	-5.5609960
H	1.1270550	-2.6025060	-5.1327140
H	3.1335580	-3.7209390	-6.0924860
C	1.7253620	1.2355670	2.0563950
C	2.3019660	0.2143830	2.8287480
C	1.9867740	2.5729210	2.3949230
C	3.1141120	0.5248270	3.9212540
H	2.1153340	-0.8257590	2.5796890
C	2.7977260	2.8790370	3.4919390
H	1.5589890	3.3752920	1.8036470
C	3.3657020	1.8588430	4.2598700
H	3.5462130	-0.2786790	4.5108060
H	2.9850670	3.9193480	3.7421850
H	3.9965060	2.0986700	5.1105530