

Supporting information for:

Theoretical Study of the Mechanism Behind the Site- and Enantio-Selectivity of C-H Functionalization Catalysed by Chiral Dirhodium Catalyst

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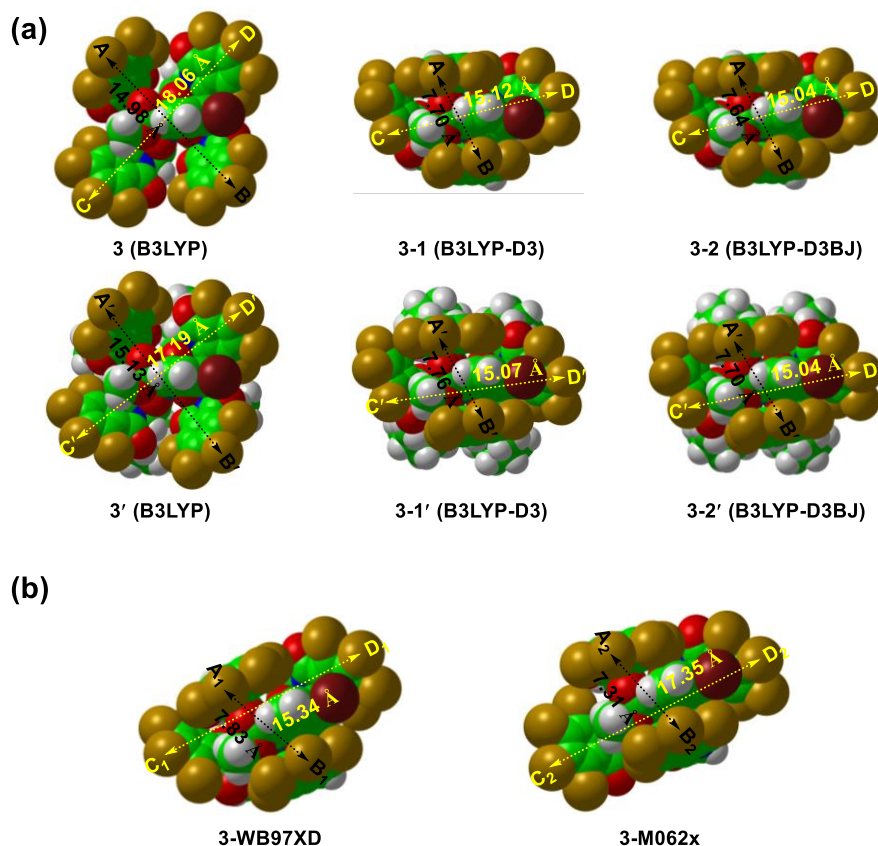


Fig. S1 (a) Space-filling models for the structures of the donor/acceptor dirhodium carbenoids $\{\text{Rh}_2(\text{S-TCPCH}_3)_4[(p\text{-Br-C}_6\text{H}_4)\text{C}(\text{COOR})]\}$ (3, 3-1 and 3-2) and $\{\text{Rh}_2(\text{S-TCPTAD})_4[(p\text{-Br-C}_6\text{H}_4)\text{C}(\text{COOR})]\}$ (3', 3-1' and 3-2'). 3 and 3' are optimized using B3LYP²¹, 3-1 and 3-1' using B3LYP-D3^{31,32}, and 3-2 and 3-2' using B3LYP-D3BJ^{31,32}. The AB, CD, A'B' and C'D' distances are defined as the ones between the two top chlorine atoms of the two opposite ligands of the dirhodium catalysts along the AB, CD, A'B' and C'D' directions, respectively. (b) Space-filling models for the structures of the donor/acceptor dirhodium carbenoids $\{\text{Rh}_2(\text{S-TCPCH}_3)_4[(p\text{-Br-C}_6\text{H}_4)\text{C}(\text{COOR})]\}$. 3-WB97XD³³ and 3-M062X³⁴ are respectively optimized using WB97XD³³ and M062X³⁴ methods. The A₁B₁, C₁D₁, A₂B₂ and C₂D₂ distances are defined as the ones between the two top chlorine atoms of the two opposite ligands of the dirhodium catalysts along the A₁B₁, C₁D₁, A₂B₂ and C₂D₂ directions, respectively. C: green, O: red, Cl: brown, H: white, Br: deep red, N: blue.

Table S1 The Natural Bond Orbital (NBO) charges in $|e|$ for selected atoms for different structures of Fig. 5

Atom	1	TS ₁₋₂	2	3
Rh1	0.557	0.490	0.486	0.486
C9	-0.158	-0.041	0.111	0.110
N1	0.121	0.079	-0.015	
N2	0.135	0.160	0.015	

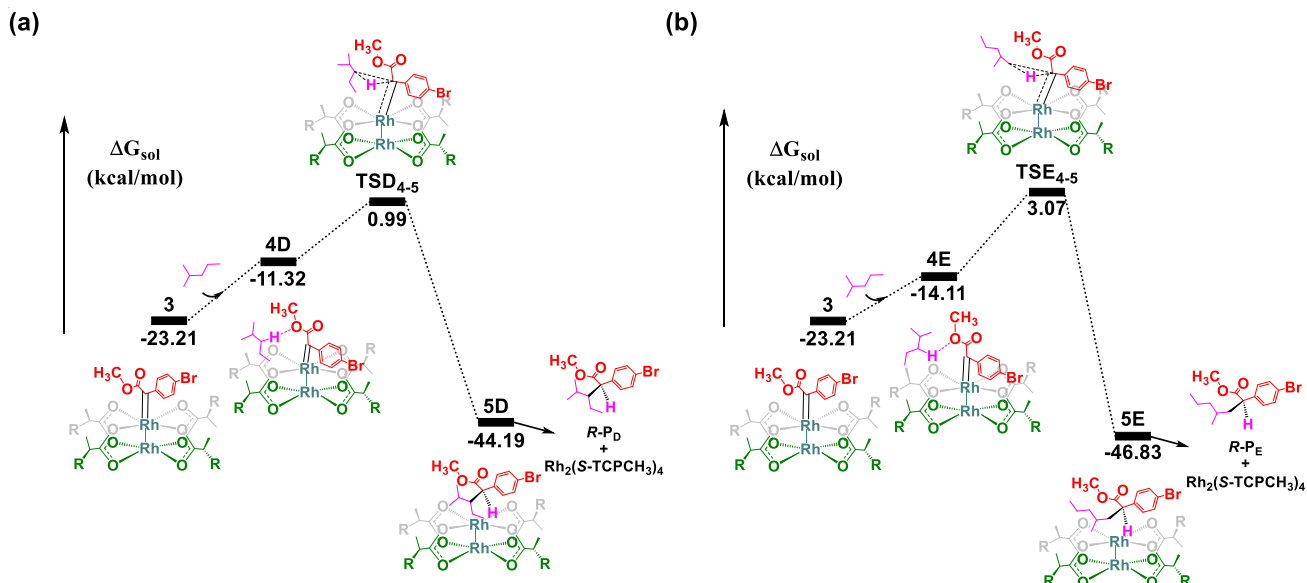


Fig. S2 Energy profiles for the two pathways for the C-H functionalization of 2-methylpentane. (a) Pathway D for the secondary C-H functionalization. In this case, the secondary carbon atom is bonded to the tertiary carbon. (b) Pathway E for the primary C-H functionalization. In this case, the primary carbon atom is bonded to the tertiary carbon. The relative free energies in dichloromethane (CH_2Cl_2) as solvent are given in kcal/mol.

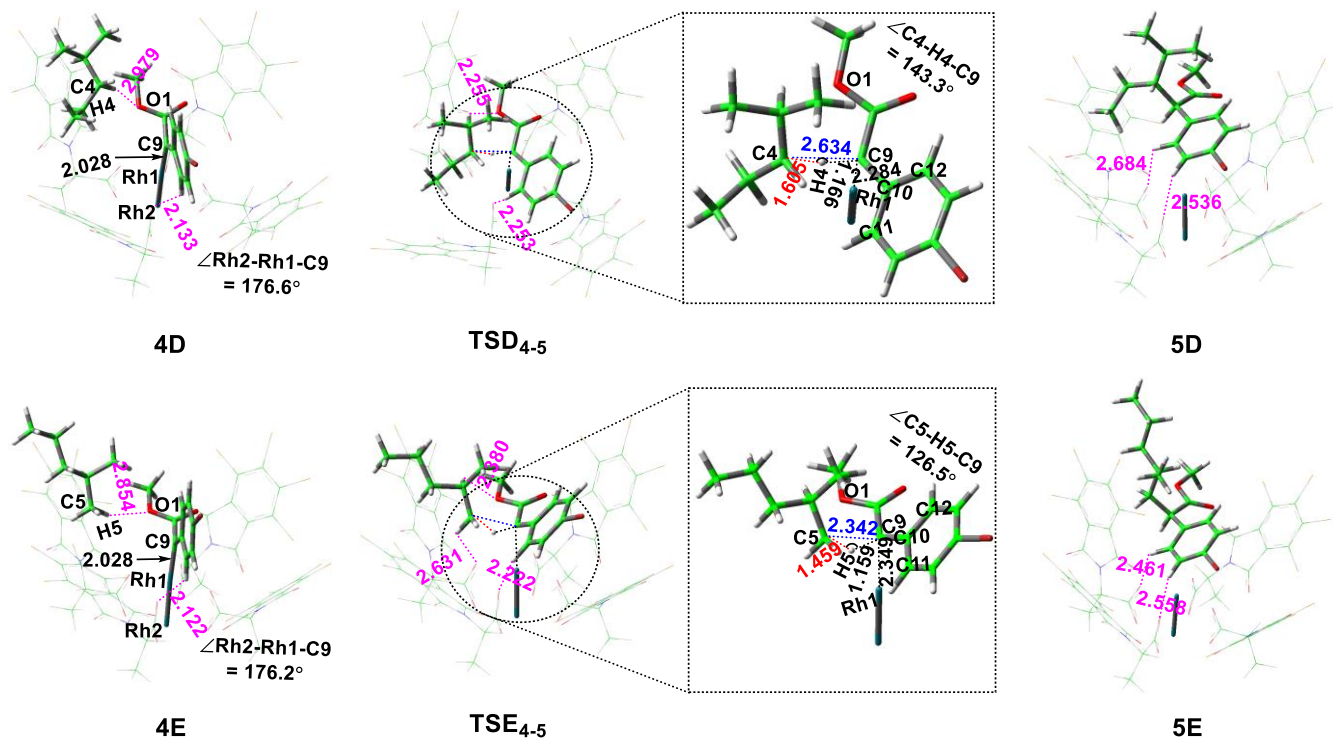


Fig. S3 Optimized structures and geometric parameters for the pathways for the C-H bond insertion reactions of Fig. S2. Blue, red, and black numbers give intramolecular distances, whereas pink numbers give intermolecular distances ($\text{\AA}$). C: green, O: red, Cl: brown, H: white, Br: deep red, N: blue. Pink numbers represent the distances between C-H and oxygen atom for the weak hydrogen bonds.

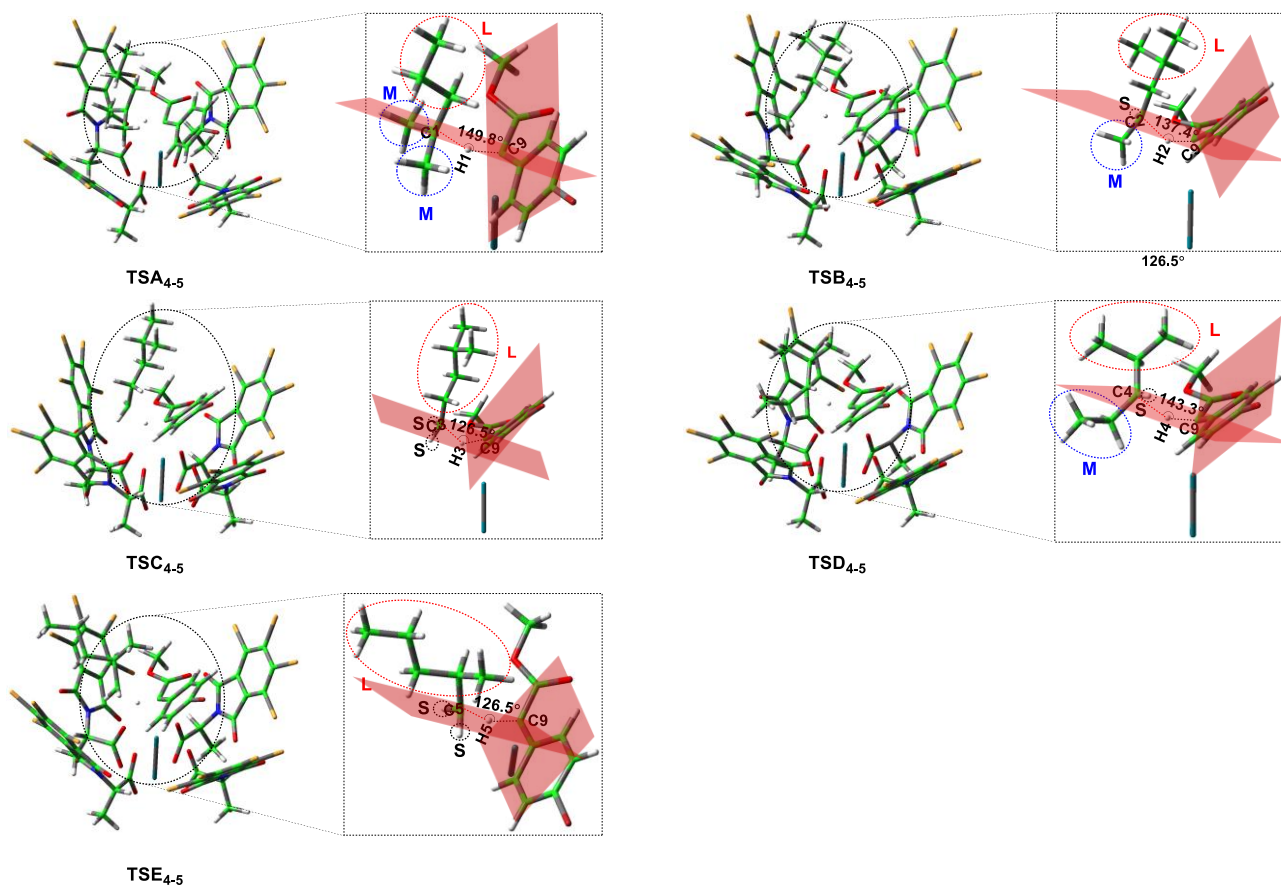


Fig. S4 The configurations for the structures of TSA₄₋₅, TSB₄₋₅, TSC₄₋₅, TSD₄₋₅ and TSE₄₋₅. L: the larger group; M: the medium-sized group; S: the smaller group. C: green, O: red, Cl: brown, H: white, Br: deep red, N: blue.

Table S2 A part of the geometric parameters for the structures shown in Figs. 7 and S3

Geometric parameter	∠Rh2-Rh1-C9	N (number of intermolecular hydrogen bonding)	
4A	175.5°	2	
4B	176.6°	2	
4C	176.8°	2	
4D	176.6°	2	
4E	176.2°	2	

Geometric parameter	∠Rh2-Rh1-C9	∠Cn-Hn-C9	N (number of intermolecular hydrogen bonding)
TSA ₄₋₅	175.3°	∠C1-H1-C9 = 149.8°	6
TSB ₄₋₅	176.7°	∠C2-H2-C9 = 137.4°	3
TSC ₄₋₅	178.1°	∠C3-H3-C9 = 126.5°	2
TSD ₄₋₅	175.8°	∠C4-H4-C9 = 143.3°	2
TSE ₄₋₅	178.1°	∠C5-H5-C9 = 126.5°	3

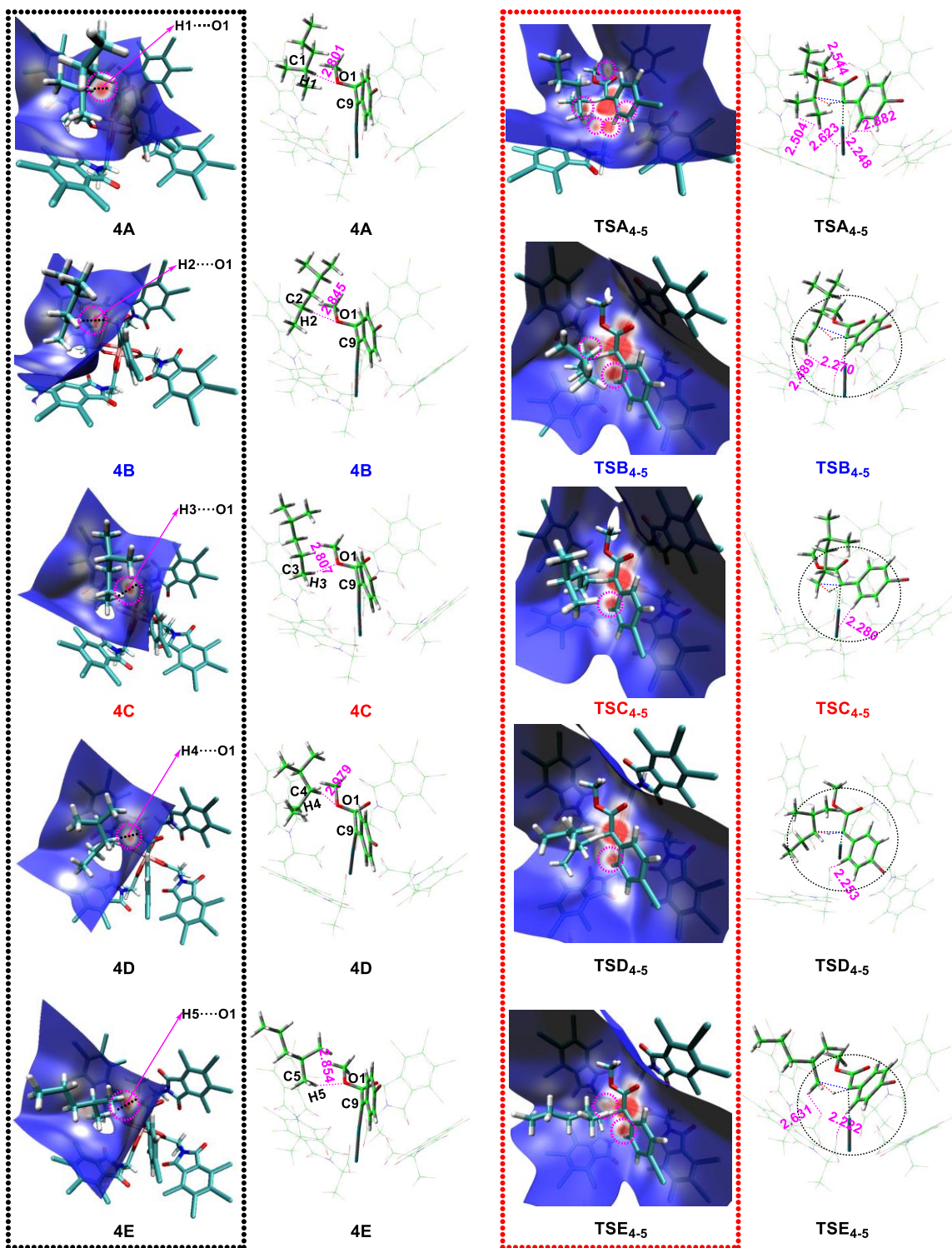


Fig. S5 The black dotted bordered rectangles represent the Hirshfeld surfaces of the second substrate $[(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3]$ for the intermediates structures. The second column: the ONIOM layers structures for the intermediates structures; The red dotted bordered rectangles represent the Hirshfeld surfaces of the complex $[(p\text{-Br-C}_6\text{H}_4)\text{C}(\text{COOR})-(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3]$. The fourth column: the ONIOM layers structures for the transition state structures. Pink numbers represent the distances between C-H and oxygen atom for the weak hydrogen bonds. For Hirshfeld surfaces, the red region implies the closer interactions with higher electron density, which mainly originate from the weak hydrogen bonding interaction; blue, no obvious interaction with very lower electron density; white, weaker interaction with less electron density. Pink circles represent the intermolecular interaction regions, and mainly due to the weak hydrogen bonding interactions.

Table S3 The Natural Bond Orbital (NBO) charges (in $|e|$) for selected atoms for the structures shown in Figs. 7 and S3

Atom	3	Atom	4A	TSA ₄₋₅	Atom	4B	TSB ₄₋₅	
Rh1	0.486	Rh1	0.487	0.542	Rh1	0.486	0.543	
C8	0.817	C8	0.819	0.859	C8	0.818	0.857	
C9	0.110	C9	0.107	-0.341	C9	0.109	-0.358	
C10	-0.165	C10	-0.165	-0.061	C10	-0.165	-0.062	
C11	-0.106	C11	-0.105	-0.185	C11	-0.105	-0.199	
C12	-0.131	C12	-0.130	-0.192	C12	-0.131	-0.195	
O1	-0.554	O1	-0.552	-0.583	O1	-0.555	-0.583	
O2	-0.611	C1	-0.250	0.181	C2	-0.460	-0.012	
		H1	0.240	0.243	H2	0.227	0.254	
Atom	4C	TSC ₄₋₅	Atom	4D	TSD ₄₋₅	Atom	4E	TSE ₄₋₅
Rh1	0.486	0.535	Rh1	0.485	0.542	Rh1	0.487	0.536
C8	0.818	0.857	C8	0.817	0.855	C8	0.818	0.856
C9	0.110	-0.306	C9	0.110	-0.350	C9	0.108	-0.311
C10	-0.164	-0.076	C10	-0.165	-0.060	C10	-0.165	-0.070
C11	-0.105	-0.194	C11	-0.105	-0.204	C11	-0.104	-0.203
C12	-0.133	-0.193	C12	-0.130	-0.195	C12	-0.129	-0.195
O1	-0.556	-0.578	O1	-0.554	-0.578	O1	-0.556	-0.575
C3	-0.689	-0.327	C4	-0.460	0.013	C5	-0.690	-0.310
H3	0.231	0.285	H4	0.227	0.246	H5	0.239	0.285

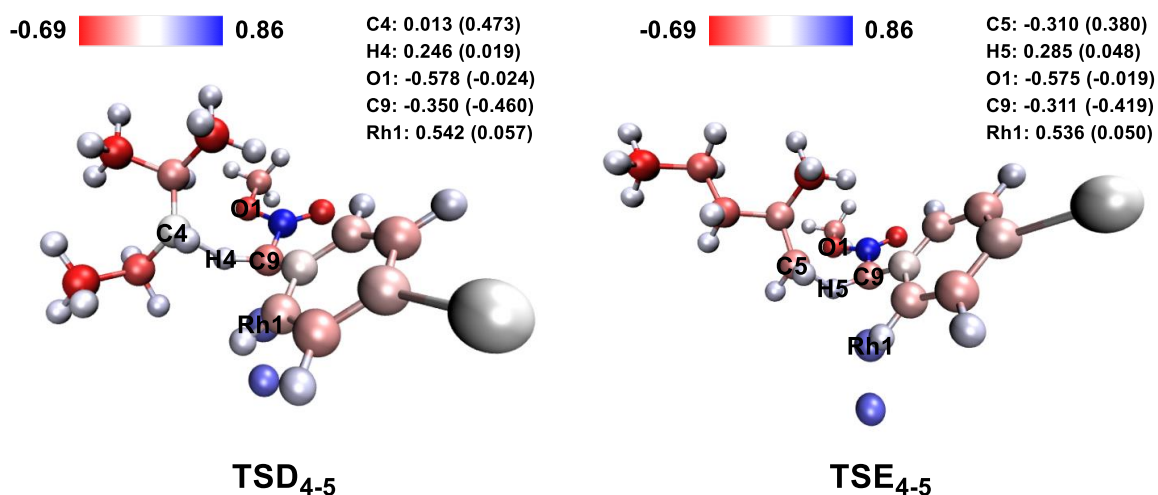


Fig. S6 The Natural Bond Orbital (NBO) charges (in $|e|$) for selected atoms for the structures shown in Fig. S3 and Table S3. In bracket, the charge differences for TSD₄₋₅ and TSE₄₋₅ compared with 4D, and 4E, respectively. Blue and red colors represent positive and negative charge, respectively.

Table S4. The Natural Bond Orbital (NBO) charges (in $|e|$) for selected atoms for the structures shown in Fig. 9

Atom	4S	TS _{4S-5S}
Rh1	0.486	0.539
C8	0.817	0.861
C9	0.110	-0.327
C10	-0.168	-0.069
C11	-0.101	-0.192
C12	-0.133	-0.197
O2	-0.611	-0.666
C1	-0.246	0.186
H1	0.232	0.242

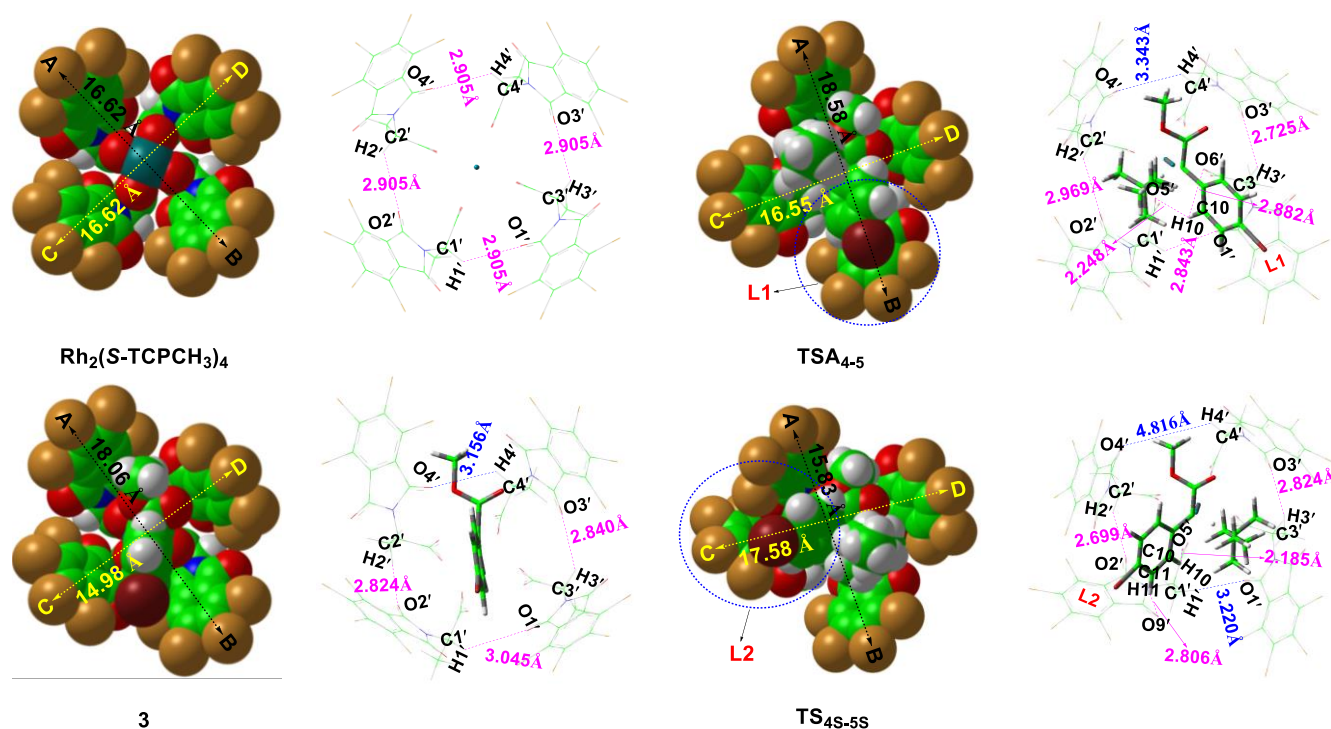


Fig. S7 Space-filling models and ONIOM layer structures. The AB and CD distances are defined as the ones between the two top chlorine atoms of the two opposite ligands of $\text{Rh}_2(\text{S-TCPCH}_3)_4$ along the AB and CD direction, respectively. C: green, O: red, Cl: brown, H: white, Br: deep red, N: blue. Also shown are the geometric parameters for the structures $\text{Rh}_2(\text{S-TCPCH}_3)_4$, 3, TSA_{4-5} and TS_{4S-5S} with blue numbers being intramolecular and pink numbers being intermolecular distances (in Å).

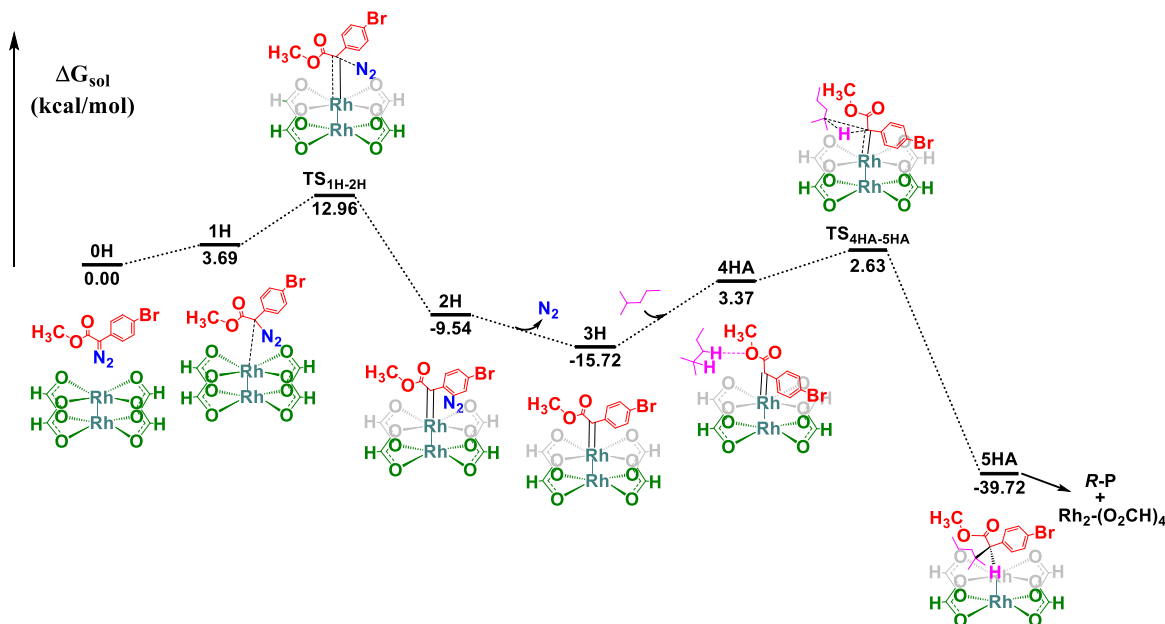


Fig. S8 Energy profiles for the pathway HA for the tertiary C-H functionalization reactions of $(p\text{-Br-C}_6\text{H}_4)\text{CN}=\text{N}(\text{COOCH}_3)$ with 2-methylpentane catalyzed by $\text{Rh}_2(\text{O}_2\text{CH})_4$. The relative free energies in dichloromethane (CH_2Cl_2) as solvent are given in kcal/mol.

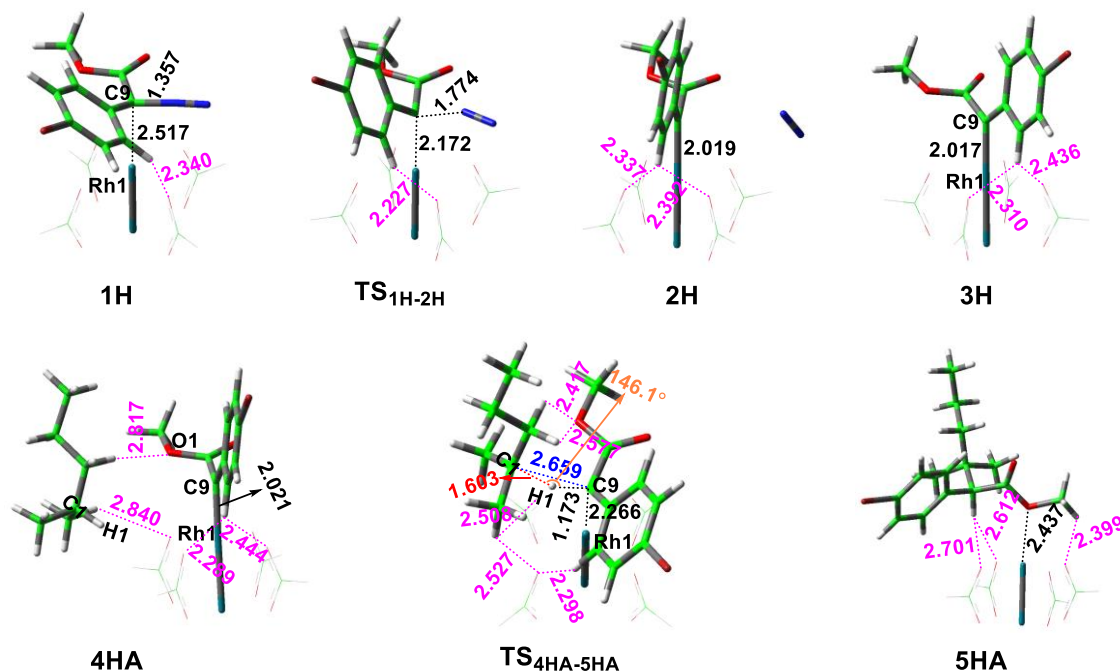


Fig. S9 Optimized structures and geometric parameters for the tertiary C-H bond functionalization reactions of $(p\text{-Br-C}_6\text{H}_4)\text{CN}=\text{N}(\text{COOCH}_3)$ with 2-methylpentane catalyzed by $\text{Rh}_2(\text{O}_2\text{CH})_4$ in Fig. S8. Blue, red, and black numbers give intramolecular bond lengths, pink numbers intermolecular bond lengths (in Å). C: green, O: red, H: white, Br: deep red, N: blue. Pink numbers represent the distances between C-H and O for the weak hydrogen bonds)

Cartesian coordinates (in Å) for optimized structures of this study

Rh ₂ (S-TCPC ₃) ₄			
-3567.243430			
Rh	-0.00025400	-0.00001300	-3.56885500
O	-0.11279500	2.04951500	-3.51044900
O	0.11230200	-2.04956000	-3.51082400
O	-0.06339300	2.05249300	-1.24462700
O	0.06312900	-2.05293100	-1.24499400
O	2.04928400	0.11252300	-3.51073800
O	-2.04978600	-0.11255600	-3.51053600
O	-2.05284800	-0.06345000	-1.24470400
O	2.05258200	0.06301100	-1.24491800
C	-2.62181400	-0.08708600	-2.37984700
C	2.62143500	0.08683500	-2.38011200
C	-0.08715300	2.62150600	-2.37974300
C	0.08679200	-2.62174400	-2.38021100
Rh	-0.00013000	-0.00022900	-1.18616400
C	4.15636900	0.13518400	-2.37689300
C	4.23338600	-2.06157800	-1.13808600
C	5.62250800	-0.34539600	-0.38653900
O	3.43118600	-2.63946100	-1.84168100
C	4.97473200	-2.55843300	0.06982900
C	6.15574400	0.74088600	-0.35127400
C	5.82178300	-1.53502200	0.50972600
C	4.92323700	-3.77862100	0.72351200
C	6.64887200	-1.71194400	1.60602300
Cl	3.81698500	-5.04726400	0.19341100
C	5.75907800	-3.97159800	1.83846900
C	6.61671100	-2.94949700	2.27349800
Cl	7.71817400	-0.41739500	2.15554200
Cl	5.72418000	-5.51517400	2.69681700
Cl	7.66205600	-3.21349300	3.67330300
C	-0.13545800	4.15644000	-2.37631500
N	0.74570300	4.66345800	-1.32478400
C	2.06123100	4.23317200	-1.13736200
O	0.34511800	5.62239600	-0.38583600
C	2.63910200	3.43099600	-1.84099400
C	2.55807100	4.97440200	0.07063000
O	-0.74111300	6.15573900	-0.35062700
C	1.53471600	5.82153700	0.51049800
C	3.77820400	4.92273800	0.72440200
C	1.71164800	6.64855400	1.60684600
Cl	5.04674800	3.81634800	0.19435200
C	3.97119300	5.75851300	1.83940600
C	2.94915200	6.61623500	2.27440200
Cl	0.41717000	7.71796300	2.15632800
Cl	3.21316500	7.66149700	3.67426700
C	-4.15674300	-0.13539900	-2.37648300
N	-4.66380000	0.74557500	-1.32481700
C	-4.23348900	2.06106400	-1.13715200
C	-5.62245800	0.34470600	-0.38570700
O	-3.43140100	2.63909500	-1.84075200
C	-4.97451200	2.55760700	0.07108600
O	-6.15567200	-0.74159100	-0.35056600
C	-5.82149300	1.53410500	0.51091100
C	-4.92281000	3.77761100	0.72509100
C	-6.64831500	1.71075900	1.60745300
Cl	-3.81662500	5.04635000	0.19506800
C	-5.75837700	3.97031800	1.84030000
C	-6.61594700	2.94813000	2.27525600
Cl	-7.71754700	0.41610800	2.15686700
Cl	-5.72320400	5.51365300	2.69906900
Cl	-7.66095700	3.21178800	3.67537500
C	0.13514400	-4.15667300	-2.37704000
N	-0.74588900	-4.66389600	-1.32550200
C	-2.06141300	-4.23367200	-1.13786500
O	-0.34515500	-5.62291200	-0.38670400
C	-2.63938000	-3.43140400	-1.84131200
C	-2.55808300	-4.97506300	0.07009600
O	0.74111400	-6.15619000	-0.35165700
C	-1.53463800	-5.82219900	0.50975100
C	-3.77815100	-4.92353900	0.72400400
C	-1.71141000	-6.64935500	1.60602100
Cl	-5.04680100	-3.81714800	0.19422800
C	-3.97097300	-5.75945100	1.83893500
C	-2.94884300	-6.61717500	2.27371700
Cl	-0.41682000	-7.71876500	2.15523600

(Energies are gas-phase electronic energies in Hartree a.u.)

Cl	-5.51439500	-5.72452700	2.69756200
Cl	-3.21264800	-7.66260900	3.67349300
H	1.14909400	-4.42448400	-2.05745400
H	-4.42454600	-1.14936300	-2.05693500
H	-1.14936300	4.42423800	-2.05657700
H	4.42418300	1.14908200	-2.05714900
Cl	5.51470300	5.72340600	2.69786300
N	4.66357600	-0.74601200	-1.32547900
C	0.16873400	4.78589700	-3.73759300
H	-0.53776500	4.41734400	-4.48461500
H	0.07105800	5.87349700	-3.66682200
H	1.18071500	4.53482700	-4.06585900
C	-4.78614700	0.16904300	-3.73772900
H	-4.41757700	-0.53733000	-4.48486200
H	-5.87375100	0.07137200	-3.66700900
H	-4.53505200	1.18108000	-4.06580400
C	-0.16916700	-4.78592700	-3.73838600
H	0.53725000	-4.41725200	-4.48542400
H	-0.07147000	-5.87353700	-3.66778700
H	-1.18118600	-4.53482300	-4.06651100
C	4.78564600	-0.16892400	-3.73827500
H	4.41698100	0.53760600	-4.48521200
H	5.87325500	-0.07123700	-3.66764600
H	4.53454600	-1.18089200	-4.06655600
Sub-1: (p-Br-C ₆ H ₄)CN=N(COOCH ₃)			
-620.239555			
C	2.06826800	0.42786200	0.00020300
C	0.60011900	0.26669700	-0.00001800
C	-0.24466500	1.39260800	-0.00207100
C	0.00875900	-1.00979900	0.00191400
C	-1.62975300	1.25651400	-0.00213900
H	0.17206200	2.39584800	-0.00372200
C	-1.37806000	-1.15037000	0.00178200
H	0.63849100	-1.88928000	0.00340300
C	-2.19245500	-0.01954400	-0.00019900
H	-2.26236000	2.13730200	-0.00374900
H	-1.81755100	-2.14190900	0.00327400
Br	-4.10495400	-0.21653600	-0.00028600
C	3.07385000	-0.64696500	-0.00018400
O	2.82827500	-1.83837600	-0.00014400
O	4.33210000	-0.14298900	-0.00051500
N	2.55609300	1.65271100	0.00607000
N	2.95274700	2.71924400	0.00109200
C	5.38427600	-1.12115300	-0.00075700
H	5.32201900	-1.75210700	-0.89116900
H	6.31106500	-0.54710100	-0.00090400
H	5.32235000	-1.75221500	0.88959800
Sub-2: (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃			
-237.084754			
C	-4.09003700	0.20687500	0.05269900
H	-3.67097900	0.83926300	-0.74589600
C	-5.61154500	0.13785500	-0.15138500
H	-6.06433000	1.13309500	-0.06785500
H	-5.87858800	-0.26321900	-1.13491300
H	-6.07786000	-0.50309600	0.60893200
C	-3.75783000	0.87076300	1.39742700
H	-4.14901400	0.27766400	2.23461300
H	-2.67479300	0.96983600	1.53792000
H	-4.19855600	1.87250200	1.46708900
C	-3.41674300	-1.17660800	-0.04886300
C	-2.35323400	-1.06687100	0.21093500
H	-3.84719900	-1.84064800	0.71710500
C	-3.51318000	-1.85651900	-1.42144300
H	-4.56427600	-2.04647200	-1.67427900
H	-3.13282300	-1.17016200	-2.19183200
C	-2.73586900	-3.17595400	-1.48636600
H	-2.82114200	-3.64385900	-2.47389800
H	-1.66929100	-3.01859300	-1.28295000
H	-3.10997300	-3.89294400	-0.74499400
1			
-4187.493735			
Rh	-0.14274300	-0.17019000	-3.85751200
O	0.16966100	1.84338300	-3.66050900

O	-0.50085000	-2.20102800	-3.92845600
O	0.14278400	1.73296800	-1.39402300
O	-0.69326500	-2.28988300	-1.67035400
O	1.88029900	-0.48443600	-3.71318400
O	-2.16925900	0.16414300	-3.89808800
O	-2.27931100	0.14899600	-1.63587000
O	1.75024500	-0.72910000	-1.46358200
C	-2.77681600	0.29313500	-2.79762700
C	2.37454100	-0.69889700	-2.57108900
C	0.26017000	2.34514900	-2.50188600
C	-0.75195500	-2.78899100	-2.83829400
Rh	-0.27269400	-0.29149600	-1.45143300
C	3.89687000	-0.89243500	-2.48616900
C	3.66947800	-3.25028200	-1.62161100
C	4.95532600	-1.76471600	-0.36893500
O	2.92475300	-3.64064500	-2.49472000
C	4.20988900	-3.99223500	-0.43184700
O	5.46065800	-0.71801000	-0.02630100
C	4.98230200	-3.10071400	0.32001600
C	4.04912400	-5.31030600	-0.03835500
C	5.61361000	-3.50542800	1.48434100
Cl	3.06339200	-6.42758400	-0.98639500
C	4.68797200	-5.73712300	1.14013200
C	5.46312800	-4.84247300	1.89497200
Cl	6.58526300	-2.37439000	2.43126500
Cl	4.51057200	-7.41261500	1.67087900
Cl	6.25704500	-5.39693900	3.37239400
C	0.47128400	3.86400100	-2.42907100
N	1.50778400	4.18296200	-1.44499900
C	2.75769500	3.56253300	-1.38791500
C	1.38591100	5.24748700	-0.54260200
O	3.11001300	2.63289200	-2.08418100
C	3.52437000	4.29931000	-0.32560200
O	0.40855300	5.95198900	-0.42011600
C	2.70211700	5.31356100	0.17759500
C	4.81737700	4.13057400	0.14085700
C	3.15254800	6.18126900	1.15792100
Cl	5.84770000	2.83739600	-0.48062400
C	5.29175000	5.01113800	1.12944200
C	4.46630900	6.02709100	1.63400500
Cl	2.10659800	7.45680100	1.79239800
C	5.07770300	7.12128600	2.87909400
C	-4.27897600	0.60907900	-2.86745000
N	-4.62757300	1.57723000	-1.82589100
C	-3.90796300	2.74443800	-1.56669300
C	-5.75524100	1.43820100	-1.00544400
O	-2.92280800	3.10941000	-2.17458200
C	-4.61990100	3.41171700	-0.42439800
O	-6.55151500	0.52853600	-1.05986800
C	-5.73997900	2.63817900	-0.10093300
C	-4.32895100	4.57712100	0.26569400
C	-6.60556600	3.01891600	0.91047800
Cl	-2.88516200	5.52175800	-0.11051200
C	-5.20106200	4.97630700	1.29472300
C	-6.33099200	4.20680500	1.61170300
Cl	-8.01912300	2.03920200	1.31368400
Cl	-4.86537900	6.45914600	2.19503300
Cl	-7.41660300	4.72810100	2.90483900
C	-1.14335100	-4.27477900	-2.90088200
N	-2.13366300	-4.54664200	-1.85881500
C	-3.32210600	-3.82358400	-1.71112400
C	-1.88512300	-5.39793700	-0.77801700
O	-3.71489400	-2.96782400	-2.47623800
C	-3.95007600	-4.33430800	-0.44710200
O	-0.88116300	-6.06200900	-0.62920500
C	-3.09041900	-5.28715200	0.10760200
C	-5.13992900	-3.99498400	

H	-0.45703000	4.27257600	-2.01541100	C	4.29884300	4.06959200	0.62443900	O	1.32327500	-3.10631700	2.22555800
H	4.28587800	0.02343900	-2.02637700	O	1.16054900	5.65651700	0.37116700	C	1.13308300	-4.51774900	2.45578200
Cl	6.94041000	4.83439800	1.73788500	C	3.44722900	5.09170900	1.05605300	H	1.03472100	-5.03463300	1.50045500
N	4.19759000	-1.95898300	-1.52899600	C	5.58156800	3.94447800	1.13185100	H	2.03223300	-4.85477700	2.97162400
C	0.76443600	4.51029100	-3.78527000	C	3.85707800	6.01350500	2.00460600	H	0.24729500	-4.68617000	3.07007100
H	-0.05072500	4.30073100	-4.48115300	Cl	6.64069400	2.63268100	0.60459500	N	-0.85655200	-0.10913300	2.15108900
H	0.85042600	5.59442200	-3.66137500	C	6.01419000	4.87697800	2.09190200	N	-1.69211100	0.61485000	2.07173700
H	1.69122400	4.11970300	-4.21379900	C	5.15912400	5.90222300	2.52487400				
C	-4.74412000	1.06628300	-4.25218800	Cl	2.77521900	7.29953800	2.54885500				
H	-4.51222300	0.29934200	-4.99431400	Cl	5.71881400	7.06284400	3.73298600				
H	-5.82637000	1.22768100	-4.23871900	C	-3.41431100	0.21016600	-1.76978200	Rh	-0.09730900	-0.22386900	-4.01971300
C	-4.24355300	1.99264900	-4.54602100	N	-3.74657300	1.22144800	-0.76184800	O	0.19748500	1.81486800	-3.95524300
H	-1.60744200	-4.73200800	-4.28502400	C	-3.03415200	2.40573100	-0.56763700	O	-0.38016200	-2.25821700	-3.92830500
H	-0.81892300	-4.54510300	-5.01737400	C	-4.90364200	1.14932500	0.02565300	O	0.28970200	1.82649600	-1.68632300
H	-1.82431400	-5.80443100	-4.26498500	O	-2.03790300	2.73220700	-1.17915400	O	-0.47683700	-2.24197200	-1.65810600
H	-2.50323300	-4.18885900	-4.59488600	C	-3.77023100	3.14823000	0.51224600	O	1.94328100	-0.53374500	-3.93556900
C	4.56854400	-1.12535200	-3.84055200	O	-5.71463900	0.25102400	-0.00166700	O	-2.13942100	0.09562300	-3.93768500
H	4.35826400	-0.28307900	-4.50322500	C	-4.90228100	2.40169900	0.85547000	O	-2.11965300	0.16291600	-1.66811900
H	5.65169500	-1.20519300	-3.70522000	C	-3.49123100	4.35453300	1.13346300	O	1.92584500	-0.62647000	-1.66663900
H	4.19467400	-2.03721900	-4.13189600	C	-5.79088200	2.84886400	1.81858900	C	-2.67663100	0.25434300	-2.81136700
C	-0.47137600	-0.43814500	1.12394200	Cl	-2.03539100	5.26825000	0.73233200	C	2.48371100	-0.69778400	-2.81208900
C	0.57268300	0.40293100	1.80029700	C	-4.38671800	4.82144300	2.11276200	C	0.34318400	2.37395900	-2.83654600
C	1.93107200	0.21547200	1.50568000	C	-5.52801300	4.07782100	2.44973300	C	-0.51475600	-2.80430300	-2.80088200
C	0.21771700	1.35346400	2.76950400	Cl	-7.21966400	1.90196600	2.24718400	Rh	-0.10336700	-0.20563500	-1.55038000
C	2.91403700	0.93843000	2.17911000	Cl	-4.06625800	6.35741300	2.92512100	C	3.99809200	-0.97157600	-2.79123800
H	2.21783500	-0.48728400	0.73628000	Cl	-6.64341200	4.68417200	3.67895300	C	3.67487000	-3.11998500	-1.50929000
C	1.19145400	2.09183900	3.44052400	C	-0.43963100	-4.67771900	-1.91061200	C	5.18461400	-1.56655000	-0.65143900
H	-0.82449700	1.51838900	3.02963400	N	-1.44645800	-4.91363500	-0.87403600	O	2.85048300	-3.59981800	-2.25793600
C	2.53610000	1.86891500	3.14794700	C	-2.58138500	-4.11832000	-0.68802500	C	4.23259100	-3.67225700	-0.22797300
H	3.95943500	0.77583200	1.93898200	O	-1.31402300	-5.90263000	0.10367900	O	5.80625900	-0.53098300	-0.55005100
H	0.90374600	2.81665700	4.19394600	O	-2.90208100	-3.18777100	-1.39667400	C	5.15566000	-2.74920600	0.27518500
Br	3.88318100	2.85060600	4.10572400	C	-3.27024800	-4.67598500	0.52451000	C	3.96715400	-4.85795800	0.43752300
C	-0.55885300	-1.93216800	1.27476800	O	-0.39166600	-6.68635800	0.18466200	C	5.84830900	-2.99639100	1.44835200
O	-1.60074500	-2.5553200	1.21470600	C	-2.51566300	-5.75704800	0.99035900	Cl	2.76546500	-5.99406100	-0.17577000
O	0.64704800	-2.46434600	1.49927500	C	-4.43307500	-4.28491900	1.16634300	C	4.66425300	-5.12105300	1.63089900
C	0.67446300	-3.89529600	1.68608500	C	-2.90786600	-6.47717000	2.10528000	C	5.59953900	-4.20121200	2.12931400
H	0.48533200	-4.40593100	0.74048800	Cl	-5.35825500	-2.89290200	0.60242100	Cl	7.01904900	-1.83009600	2.07634400
H	1.67841200	-4.11411800	2.04907200	C	-4.84587400	-5.01167600	2.29774800	Cl	4.35487900	-6.62336000	2.50780600
H	-0.07409800	-4.19771700	2.42108600	C	-4.09173900	-6.09979100	2.76216200	Cl	6.46960900	-4.55351400	3.62671100
N	-1.71262300	0.08832000	1.15632400	Cl	-1.94150900	-7.83682500	2.69550500	C	0.54193700	3.89887900	-2.85295300
N	-2.74475000	0.53793200	1.14642600	Cl	-6.32709100	-4.54550200	3.14119600	N	1.51833000	4.29871600	-1.83623600
				Cl	-4.62723700	-7.00199900	4.18496000	C	2.74615900	3.67092100	-1.63033200
TS ₁₋₂				H	0.41496900	-5.29720500	-1.61490800	C	1.34211600	5.42942100	-1.02657300
-4187.508343				H	-3.91898600	-0.70407400	-1.43927400	O	3.15304600	2.69920200	-2.23367900
Rh	0.68303800	-0.61039800	-2.89084700	O	0.33998300	3.82621200	-1.10815700	C	3.42174800	4.45398300	-0.53855500
O	1.03429900	1.40318700	-2.69273000	H	5.17426000	-0.37765600	-1.33046300	O	0.38009000	6.16301300	-1.04853200
O	0.26936300	-2.63326800	-2.93486200	Cl	7.64617000	4.75225700	2.75536000	C	2.58388700	5.51598500	-0.18365000
O	1.04774000	1.31339100	-0.42368100	N	5.13016100	-2.27595100	-0.58139500	C	4.64789400	4.27251200	0.07851300
O	0.16469000	-2.73277100	-0.66947300	C	1.57495900	4.07011000	-2.86616600	C	2.95441300	6.42563900	0.79256200
O	2.70900400	-0.96923200	-2.80674200	H	0.77508100	3.81608800	-3.56456900	Cl	5.68560900	2.90553800	-0.35012900
O	-1.33656400	-0.23669800	-2.85002200	H	1.62260500	5.15908500	-2.76633800	C	5.04020600	5.19029400	1.06880500
O	-1.38375900	-0.25251300	-0.58337600	H	2.51876800	3.70168500	-3.27733000	C	4.20101400	6.25833500	1.42228600
O	2.65901600	-1.16095200	-0.54559000	C	-3.91985400	0.61065400	-3.15808400	Cl	1.89140000	7.76367700	1.23817000
C	-1.90910000	-0.10503200	-1.73493400	H	-3.70699600	-0.18555500	-3.87439900	Cl	4.70995500	7.40125500	2.66961900
C	3.23903000	-1.15920000	-1.67990000	H	-5.00188900	0.77080400	-3.12022000	C	-4.18275800	0.56475300	-2.76584100
C	1.13083400	1.91523500	-1.54460100	H	-3.42947600	1.52424400	-3.50465200	N	-4.44570600	1.47984400	-1.65390100
C	0.03240100	-3.21314400	-1.84136300	C	-0.92938400	-5.09587600	-3.29871200	C	-3.77303500	2.69385600	-1.47768600
Rh	0.63367000	-0.72907400	-0.44201800	H	-0.13418600	-4.94372800	-4.03165800	C	-5.21717400	1.12692900	-0.54314600
C	4.76587600	-1.34472700	-1.64816000	H	-1.20371200	-6.15534100	-3.28862200	O	-2.98631500	3.17529100	-2.26549300
C	4.60781900	-3.56709600	-0.47042300	H	-1.79466900	-4.50128500	-3.60168000	C	-4.23871200	3.22397400	-0.15249700
C	5.94909000	-1.92409100	0.49661000	C	5.36488000	-1.74502600	-2.99822100	O	-5.81777400	0.08155600	-0.41098800
C	3.84076800	-4.08359300	-1.25363700	H	5.10512500	-0.99771100	-3.75079200	C	-5.12017500	2.29015700	0.40029400
C	5.19770000	-4.13052800	0.79275200	H	6.45487200	-1.80013200	-2.91552200	C	-3.92597900	4.39676800	0.51395200
O	6.48607100	-0.84959200	0.65028600	H	4.97852400	-2.71329300	-3.32547700	C	-5.72257800	2.51387600	1.62576600
C	6.00359800	-3.14530400	1.37223900	C	0.65932200	-0.95330300	1.71486000	Cl	-2.77386400	5.54840700	-0.16606900
C	5.05140100	-5.37407600	1.38376800	C	1.65940200	-0.32893800	2.62085000	C	-4.53348400	4.63758100	1.75911100
C	6.68315300	-3.38004600	2.55595700	C	2.73784700	0.40785100	2.10497800	C	-5.42889600	3.70713100	2.30761200
Cl	4.02896800	-6.61547400	0.64811600	C	1.57892400	-0.51786200	4.01715100	Cl	-6.83658700	1.32764700	2.32209100
C	5.73262900	-5.62629400	2.04768200	C	3.72560900	0.91050200	2.95313100	Cl	-4.16324200	6.12581000	2.63790200
C	6.54259000	-4.63809400	3.16834600	H	2.82736500	0.55352400	1.03791600	Cl	-6.19354700	4.03320700	3.86827500
Cl	7.70152400	-2.13274000	3.28244600	C	2.53114100	0.01652700	4.87464800	C	-0.67678300	-4.33397100	-2.79043900
Cl	5.56311300	-7.20039900	3.37457500	H	0.75163500	-1.08442600	4.43785000	N	-1.70270000	-4.72717800	-1.82233700
Cl	7.39260500	-4.97359400	4.68097200	C	3.60867700	0.72323600	4.32947600	C	-2.97623200	-4.15871500	-1.75702300
C	1.28951000	3.44434500	-1.49833300	H	4.58114500	1.43276200	2.54162800	C	-1.52271800	-5.77174600	-0.90899000
N	2.30083600	3.83594900	-0.51179600	C	2.45099900	-0.12269600	5.94693500	O	-3.37820900	-3.25108500	-2.45318400
C	3.56592600	3.25715600	-0.47040100	Br	4.94539900	1.44061900	5.50009700	C	-3.69818500	-4.91449300	-0.67407200
C	2.14755400	4.95792100	0.31432900	C	0.22347900	-2.34980400	2.10149000	O	-0.51675900	-6.43430900	-0.78787400
O	3.95397600	2.29680900	-1.04068500	O	-0.91939600	-2.73448800	2.24307300	C	-2.82546000	-5.88194400	-0.16573500

	-4.98840000	-4.78607900	-0.18695300	O	6.41446800	-0.92837300	0.70059800	H	4.79347700	-2.85620700	-3.20156200
C	-3.22009500	-6.74250500	0.84486100	C	5.68267200	-3.11309000	1.54570700	C	0.43955100	-0.37899100	1.53574600
Cl	-6.08273300	-3.55429600	-0.82325400	C	4.44553300	-5.19398200	1.70274200	C	1.44464000	-0.06787900	2.50475000
C	-5.40417700	-5.65550600	0.83788600	C	6.314400500	-3.34341900	2.75630600	C	2.75630100	0.31817900	2.11137600
C	-4.52738700	-6.62449600	1.34987900	Cl	3.25094800	-6.32201800	1.06174500	C	1.17358200	-0.16124300	3.90161800
Cl	-2.11243000	-7.96085700	1.48612800	C	5.08129700	-5.44056800	2.93334800	C	3.74387800	0.57164900	3.05284900
Cl	-7.04394800	-5.52319400	1.48366900	C	6.01022200	-4.52622000	3.45331500	H	2.98527700	0.40950500	1.05865200
Cl	-5.06694400	-7.70591300	2.63935000	Cl	7.47453700	-2.18224800	3.41243900	C	2.15355300	0.08610900	4.84633700
H	0.26272400	-4.73161400	-2.39031700	Cl	4.70213000	-6.91482700	3.83020800	H	0.18109600	-0.44089600	4.23865400
H	-4.67922600	-0.37126700	-2.48436800	Cl	6.80226400	-4.85713300	4.99810800	C	3.43719000	0.50435000	4.41362800
H	-0.41101700	4.32702800	-2.52083700	C	1.35772800	3.57284200	-1.82808500	H	4.74348000	0.84787100	2.73656000
H	4.47367800	-0.02395700	-2.51189100	N	2.31956900	3.96400200	-0.79427000	H	1.93695200	0.00389000	5.90532800
Cl	6.60143100	4.99272800	1.87241600	C	3.52564300	3.30865200	-0.54862600	Br	4.78931600	0.79127400	5.71357600
N	4.31240000	-1.88942800	-1.69533800	C	2.15681300	5.11644300	-0.01298400	C	-0.95195600	-0.50626200	2.04732200
C	0.90697300	4.45017300	-4.23356000	O	3.92060900	2.31579600	-1.12471800	O	-1.62143700	0.48921500	2.25915600
H	0.13379500	4.18163700	-4.95618000	C	4.19700800	4.09547600	0.54319200	O	-1.36651700	-1.76496300	2.25158500
H	0.98076700	5.54102300	-4.18414500	O	1.21703500	5.87627400	-0.07380300	C	-2.74079000	-1.91700000	2.648282900
H	1.85859900	4.03781300	-4.58021300	C	3.38051300	5.18656500	0.85733000	H	-2.85667200	-2.98026100	2.84915000
C	-4.74283200	1.07884200	-0.09309300	C	5.40380600	3.89460200	1.19154300	H	-2.92858900	-1.32858300	3.54396500
H	-4.55217600	0.34528200	-4.87950100	C	3.75367300	6.10628600	1.82308300	H	-3.42101000	-1.59874200	1.85060300
H	-5.82301600	1.23075800	-4.00426600								
H	-4.26813300	2.02081700	-4.37734600								
C	-0.94812400	-4.92858900	-4.17432300								
H	-0.13932400	-4.66152900	-4.85767600								
H	-1.00159900	-6.01935900	-4.10002000								
H	-1.88562700	-4.54673500	-4.58695000								
C	4.55040100	-1.45896600	-4.13234900								
H	4.32791200	-0.72472700	-4.90939200								
H	5.63553200	-1.58291600	-4.06174500								
H	4.09584200	-2.41074200	-4.41762600								
C	-0.19080000	-0.13451800	0.46907400								
C	0.84785600	0.14678400	1.41101200								
C	2.12449000	0.61120400	0.98835600								
C	0.64445400	-0.05490800	2.80760000								
C	3.14231700	0.84359300	1.90267300								
H	2.30020000	0.78631900	-0.06401300								
C	1.65792300	0.16450600	3.72393200								
H	-0.31860000	-0.40068700	3.16697300								
C	2.90389700	0.61437600	3.26345300								
H	4.11406300	1.18589300	1.56492200								
H	1.49372100	-0.00250200	4.78238300								
Br	4.29932400	0.92562900	4.52476100								
C	-1.56407000	-0.28420700	1.02049400								
O	-2.23509700	0.70355100	1.26288600								
O	-1.96392400	-1.54781700	1.18589400								
C	-3.32440500	-1.71528100	1.65044500								
H	-3.42903600	-2.78280000	1.83993200								
H	-3.48658200	-1.14524500	2.56802900								
H	-4.02914500	-1.38676700	0.88414300								
N	-2.28030300	1.31758100	4.41878700								
N	-2.76989400	2.30350400	4.32315300								
N ₂											
-109.524129											
N	0.30404500	2.55968700	1.13193900								
N	-0.79362100	2.61719700	1.01383000								
3											
-4077.985946											
Rh	0.65066100	-0.55072900	-2.94888600								
O	0.98714900	1.48202800	-2.90782900								
O	0.32133200	-2.57628400	-2.83530800								
O	1.02319500	1.52509400	-0.63774000								
O	0.17049200	-2.52675700	-0.56858700								
O	2.68117400	-0.90619700	-2.81001100								
O	-1.38654600	-0.18772500	-2.92537200								
O	-1.41925900	-0.08800600	-0.65725500								
O	2.60580100	-0.96210800	-0.54127300								
C	-1.94677400	-0.00016700	-1.81487400								
C	3.18951300	-1.06678400	-1.67131900								
C	1.11917500	2.05394500	-1.79377100								
C	0.14632900	-3.10361200	-1.70442700								
Rh	0.58394100	-0.49655600	-0.48123600								
C	4.69443400	-1.38318900	-1.60574400								
C	4.27696600	-3.49790600	-0.29534000								
C	5.77883400	-1.95491400	0.59345200								
O	3.47235400	-3.97617100	-1.06615900								
C	4.76535200	-4.03043800	1.02212500								

Cl	-0.77349700	3.65136800	1.97006400	C	1.06767000	1.85435300	-1.89852600	H	-3.10825600	1.93639800	-2.94822000
C	-2.10084600	2.05490700	3.80360900	C	0.34588800	-3.31666200	-1.81606700	C	-0.17828200	-5.49402800	-3.06672700
C	-3.00571300	1.04693800	4.17472000	Rh	0.79322400	-0.73086600	-0.62576100	H	0.82860600	-5.50931300	-3.50462600
Cl	-4.82742400	-0.96982000	3.63793200	C	4.83089500	-1.62054900	-1.82787300	H	-0.51086500	-6.52456400	-2.92218300
Cl	-1.14563900	2.88641300	5.04802500	C	4.05938700	-3.25365900	-0.12065600	H	-0.84261900	-4.98137600	-3.75899000
Cl	-3.18294800	0.60460600	5.88140600	C	5.41365200	-1.49573900	0.57949900	C	5.27632000	-2.49596100	-2.99400400
C	-0.12202200	-4.78244600	-1.71717500	O	3.44917800	-3.97605100	-0.87640600	H	5.15227400	-1.94425000	-3.92843800
N	-1.43377300	-4.76066300	-1.05348500	C	3.96918700	-3.16390700	1.37141100	H	6.33020500	-2.76180600	-2.87264100
C	-2.52521100	-4.02045200	-1.52705100	O	6.08998900	-0.49439900	0.50884000	H	4.67793400	-3.40715500	-3.04279500
C	-1.66080600	-5.29376100	0.22043500	C	4.80550400	-2.12686700	1.79408800	C	0.80439500	-0.66768100	1.36780300
O	-2.53965600	-3.36441200	-2.54611100	C	3.17936500	-3.86178100	2.26904300	C	1.62217600	0.15114600	2.19654400
C	-3.59934600	-4.17527500	-0.49389700	C	4.88626500	-1.76981400	3.12817500	C	2.79969300	0.75829400	1.68263600
O	-0.86752500	-5.94751100	0.86209100	Cl	2.15016200	-5.18421300	1.73381300	C	1.30283400	0.35453200	3.56952500
C	-3.06246700	-4.88742000	0.58299500	C	3.20607500	-3.46539200	3.61725900	C	3.63225500	1.49043100	2.51061800
C	-4.90472800	-3.71934900	-0.47791800	C	4.04745800	-2.42667100	4.04250800	H	3.06868500	0.60407100	0.64764800
C	-3.80807800	-5.10834900	1.72810800	Cl	6.01759400	-0.52733900	3.67147900	C	2.09696300	1.14223400	4.38127100
Cl	-5.61155600	-2.95673800	-1.90796700	Cl	2.17426700	-4.28838400	4.79010400	H	0.39825100	-0.08156700	3.97877700
C	-5.66118500	-3.90146300	0.69335100	Cl	4.04741100	-1.92608400	5.73673700	C	3.26486800	1.70057500	3.84411600
C	-5.10953100	-4.57685700	1.79383800	C	1.15791100	3.38352000	-1.88764600	H	4.56881400	1.87621800	2.13719900
Cl	-3.13566000	-6.03148400	3.08417300	N	2.16067600	3.79740200	-0.91054900	H	1.82909200	1.32014100	5.41530600
Cl	-7.30569700	-3.26916200	0.77900500	C	3.44054700	3.24909300	-0.83601900	Br	4.38276800	2.76620700	4.95294600
Cl	-6.05661000	-4.76653900	3.27664000	C	1.92686200	4.77932400	0.05733900	C	-0.23596000	-1.46343400	2.05208100
H	0.54541000	-5.29249000	-1.01749300	O	3.86183700	2.35156200	-1.53529900	O	-1.35209100	-1.01674300	2.24756200
H	-3.86544700	-0.79947100	-1.74672600	C	4.12112600	3.97718100	0.28791000	O	0.18247600	-2.67313700	2.41775100
H	0.18216600	3.72709100	-1.48123800	O	0.90650400	5.41859200	0.17714900	C	-0.80348400	-3.50483900	3.07352100
H	5.44910900	-0.71059200	-1.76597900	C	3.19548400	4.85744100	0.85652900	H	-0.46157500	-4.52589500	2.94025800
Cl	7.33478000	4.52072900	2.64484100	C	5.39861600	3.85200700	0.80385600	H	-0.85128300	-3.24062000	4.13253600
N	4.99252400	-2.27687400	-0.51743100	C	3.51478100	5.61045800	1.97214700	H	-1.77851700	-3.34881300	2.61507000
C	1.41168400	3.99005300	-3.25606600	Cl	6.54732800	2.71638100	0.10001600				
H	0.63148700	3.68244200	-3.95562700	C	5.74106400	4.61795700	1.93174200				
H	1.41534200	5.08177400	-3.18113800	C	4.80564800	5.48516700	2.51386200	3'			
H	2.37452100	3.64706100	-3.64413400	Cl	2.32323300	6.67932000	2.71296200	-5478.773259			
C	-3.69122000	1.00963600	-2.91527300	Cl	5.24400000	6.41691700	3.94547900	Rh	0.78141900	-0.68307800	-2.94469100
H	-3.53632600	0.47954300	-3.85749300	C	-3.26220900	0.12536200	-1.76627100	O	1.17936200	1.34005900	-2.94354100
H	-4.75144900	1.25893900	-2.81275500	N	-3.44937900	0.74512800	-0.45254500	O	0.38054500	-2.69687500	-2.79349000
H	-3.10336600	1.92964800	-2.92735500	C	-2.57550500	1.74896800	-0.00114600	O	1.17161400	1.43710700	-0.68207700
C	-0.16934500	-5.49862600	-3.06300700	C	-4.00507900	0.02272000	0.61150100	O	0.15843300	-2.58031200	-0.54180800
H	0.83063800	-5.50847200	-3.50482300	O	-1.89369800	2.447776800	-0.71901300	O	2.79707300	-1.09600500	-2.74671100
H	-0.50572700	-6.53051500	-2.92261000	C	-2.64942900	1.71259300	1.49505100	O	-1.24274600	-0.26045900	-2.99107700
H	-0.84274300	-4.98120300	-3.74873500	O	-4.67773800	-0.97782200	0.50045100	O	-1.33636300	-0.10642900	-0.73372000
C	5.28807200	-2.48706400	-2.99938600	C	-3.54560000	0.70515700	1.85974200	O	2.66100200	-1.09762500	-0.48746000
H	5.15568200	-1.93023900	-3.92992400	C	-1.90361900	2.38276800	2.44839300	C	-1.84404600	-0.05664200	-1.90442300
H	6.34394200	-2.74876200	-2.88425000	C	-3.73965800	0.35643900	3.18255900	C	3.28578900	-1.22396600	-1.59520300
H	4.69261400	-3.40037700	-3.04943400	Cl	-0.73198400	3.61434500	1.97946500	C	1.29678600	1.94601900	-1.84576200
C	0.82088200	-0.65640300	1.37810400	C	-2.08080900	2.02933600	3.79560700	C	0.15612000	-3.19651200	-1.65916700
C	1.62893100	0.17919200	2.20372300	C	-2.99344200	1.02960700	4.16124500	Rh	0.65008800	-0.56543900	-0.48847600
C	2.82386300	0.76262600	1.69969700	Cl	-4.82241000	-0.96998000	3.62038800	C	4.79999300	-1.49107700	-1.43152200
C	1.28533800	0.42085200	3.56589200	Cl	-1.12095500	2.84338600	5.04114200	C	4.25921000	-3.64507600	-0.17992200
C	3.65455800	1.49576400	2.52993300	Cl	-3.16986500	0.57797600	5.86094000	C	5.72448600	-2.13778400	0.81117100
H	3.11238300	0.59188700	0.67190400	C	-0.12869200	-4.77418100	-1.72435400	O	3.46115400	-4.09353600	-0.97439600
C	2.07468100	1.21773500	4.37506100	N	-1.43781200	-4.75505400	-1.06001400	C	4.68145400	-4.21039500	1.14718400
H	0.36428900	0.01115100	3.96661500	C	-2.52836000	-4.01067000	-1.52752700	O	6.34724000	-1.11190300	0.98295100
C	3.26545100	1.74237400	3.85158400	C	-1.65738300	-5.28606300	0.21639400	C	5.56726200	-3.30575700	1.73932000
H	4.60531800	1.85557900	2.16461600	O	-2.54822000	-3.35650800	-2.54733500	C	4.33313200	-5.39164100	1.78200100
H	1.78404800	1.42772200	5.39731900	C	-3.59608300	-4.16068600	-0.48767800	C	6.12801600	-3.55723000	2.98024800
Br	4.38295000	2.81668300	4.95856200	O	-0.85933700	-5.93727300	0.85422900	Cl	3.20168200	-6.52522800	1.04329100
C	-0.21166100	-1.46091300	2.06621000	C	-3.05657700	-4.87894000	0.58534500	C	4.89776500	-5.66195500	3.04204500
O	-1.32001200	-1.00876800	2.29505600	C	-4.89910000	-3.70031600	-0.46313200	C	5.78797900	-4.75359800	3.63545100
O	0.20705600	-2.68215800	2.39053900	C	-3.80092900	-5.10259800	1.72999300	Cl	7.24506100	-2.40688700	3.72485400
C	-0.76880800	-3.53050000	3.04425700	Cl	-5.61621800	-2.93582100	-1.88262000	Cl	4.48036700	-7.15872700	3.88233500
H	-0.41093900	-4.54609100	2.90798200	C	-5.64947500	-3.88203400	0.71020300	Cl	6.48787700	-5.11160100	5.21820500
H	-0.82453200	-3.27004100	4.10418800	C	-5.09731700	-4.56403000	1.80327100	C	1.54275100	3.47285800	-1.86312100
H	-1.74655600	-3.39230000	2.58396700	Cl	-3.14208700	-6.04186000	3.07730600	N	2.52614900	3.80261800	-0.81906000
				Cl	-7.28608900	-3.24376600	0.80676300	C	3.71345100	3.11124900	-0.57511000
				Cl	-6.03733300	-4.75434100	3.28514000	C	2.29369900	4.81679800	0.12484400
				H	0.53765100	-5.28324700	-1.02352000	O	4.11642000	2.14760400	-1.19403200
				H	-3.86817500	-0.78515900	-1.75015400	C	4.35362400	3.80242800	0.59878000
3-2				H	0.20152600	3.73612500	-1.48718200	O	1.31239000	5.52221400	0.17290900
-4078.444842				H	5.44138400	-0.71251900	-1.71501000	C	3.49990700	4.82637600	1.01759200
Rh	0.76816200	-0.75819000	-3.09505500	Cl	7.34918100	4.45649500	2.63674700	C	5.56163800	3.57536200	1.23735500
O	0.98730500	1.28891300	-3.01993800	N	4.98249100	-2.26316700	-0.51550400	C	3.82862000	5.64680100	2.08398200
O	0.51305100	-2.80535200	-2.95174900	C	1.42738700	3.98958500	-3.26242200	Cl	6.63131700	2.26572300	0.72328800
O	1.03400300	1.30677000	-0.74798700	H	0.64132600	3.69245000	-3.95957800	C	5.91347900	4.40371800	2.31796400
O	0.48717100	-2.75425300	-0.67920900	H	1.44080000	5.08077500	-3.18440000	C	5.05402600	5.43021300	2.73850000
O	2.81876900	-1.07266800	-3.04840100	H	2.38505900	3.64079900	-3.65695800	Cl	2.74144500	6.93547400	2.61047800
O	-1.26488000	-0.41891300	-2.99213600	C	-3.69702700	1.01748400	-2.92523400	Cl	5.51183200	6.45936400	4.09990500
O	-1.23963500	-0.54010000	-0.72698200	H	-3.55202200	0.48252700	-3.86600800	C	-3.36225700	0.22423700	-1.89882300
O	2.81585400	-0.95759300	-0.78489200	H	-4.75564000	1.26966400	-2.81588800	N	-3.62681700	1.23369400	-0.86202900
C	-1.79197200	-0.31617600	-1.85669700								
C	3.35954900	-1.17306600	-1.92244500								

C	-2.91692500	2.43039600	-0.70093500	C	2.31149100	6.40328900	-4.34930700				
C	-4.43576100	0.95025100	0.24506800	H	2.51129700	7.46299500	-4.14161800	3-1'			
O	-2.06091600	2.84799500	-1.45123300	C	-3.49490700	1.64191400	-4.09398500	-5479.205074			
C	-3.43526600	3.04242300	0.56942200	H	-2.43881500	1.44988200	-4.30647900	Rh	0.85156600	-0.72426700	-3.11399800
O	-5.05396500	-0.07955300	0.41560100	H	-3.54017600	2.57810500	-3.52543700	O	1.05333700	1.33090300	-3.05143800
C	-4.35146200	2.15254200	1.13482900	C	-4.08500400	0.47791800	-3.25783000	O	0.59599400	-2.76955300	-2.94322600
C	-3.13691700	4.24794300	1.18234500	C	-4.28158600	1.80230100	-5.41363700	O	0.99802200	1.36358600	-0.78362500
C	-4.99218900	2.44282800	2.32645300	H	-3.83996800	2.62649000	-5.98942900	O	0.41844800	-2.67904400	-0.68139300
Cl	-1.96029900	5.35901200	0.48102400	C	-4.20079800	0.49767300	-6.23164100	O	2.89254500	-1.03897400	-2.91861100
C	-3.78410700	4.55818200	2.39179500	H	-3.15411500	0.68905000	-6.47522400	O	-1.17893100	-0.38900200	-3.15499400
C	-4.70441800	3.66394200	2.95880600	H	-4.73365800	0.61589700	-7.18563900	O	-1.30549600	-0.48674200	-0.89454200
Cl	-6.14599000	1.30676800	3.04120700	C	-4.03542400	-0.82935200	-4.09918700	O	2.74169600	-0.86178800	-0.66799900
Cl	-3.43238600	6.08940300	3.20290800	H	-4.46139200	-1.65786800	-3.51629400	C	-1.79024000	-0.28854400	-2.06213500
Cl	-5.50918600	4.07215500	4.48008900	H	-2.99691000	-1.09310000	-4.31548400	C	3.36918600	-1.09386100	-1.76073900
C	-0.09085500	-4.71856100	-1.53742300	C	-4.81857100	-0.65686500	-5.41678800	C	1.10901800	1.90499000	-1.93423400
N	-1.28631500	-4.92732600	-0.70456500	H	-4.75433700	-1.59074600	-5.99069800	O	0.37931200	-3.27294700	-1.81126800
C	-2.50795400	-4.26995000	-0.86465200	C	-6.29355600	-0.33848400	-5.10536600	Rh	0.71475500	-0.65669400	-0.64613700
C	-1.26176300	-5.73887600	0.43981400	H	-6.86649500	-0.23075900	-6.03695000	C	4.84807900	-1.45169600	-1.51273100
O	-2.75724000	-3.42900800	-1.70236900	H	-6.74821800	-1.16624400	-4.54343800	C	3.93218700	3.13227300	0.12513000
C	-3.40533300	-4.80994500	0.21556000	C	-5.57929000	0.79531900	-2.96983000	C	5.22083500	-1.38438700	0.93937500
O	-0.30304400	-6.35491200	0.84663400	H	-5.65977000	1.71973600	-3.28291500	O	3.34841600	-3.83619500	-0.66843200
C	-2.64947700	-5.67497500	1.01205900	H	-6.02255800	-0.00698800	-2.36429700	C	3.76242500	-3.08574900	1.61130900
C	-4.74643200	-4.58252100	0.47890000	C	-5.75750000	2.12104400	-5.10206700	O	5.86317900	-0.35692300	0.93769700
C	-3.20848200	-6.31864800	2.10368700	H	-5.83005400	3.06165100	-4.53796500	C	4.55939700	-2.05230700	2.10422300
Cl	-5.71089700	-3.51613900	-0.54584900	H	-6.32170400	2.26304200	-6.03428300	C	2.92783600	-3.81345700	2.44350000
C	-5.32967300	-5.23233000	1.58199700	C	-6.36742000	0.96404000	-4.28508800	C	4.55913300	-1.72157600	3.44832400
C	-4.56604900	-6.08906900	0.29010000	H	-7.41430000	1.19182400	-4.04365300	Cl	1.94527000	-5.13411300	1.81311300
Cl	-2.24599300	-7.40535900	3.11147100	C	-1.10352400	-5.16807500	-3.91046800	C	2.86983400	-3.44685800	3.80053900
Cl	-7.03756900	-4.96784300	1.94939900	H	-0.95089900	-4.12340100	-4.19453100	C	3.67700900	-2.41007300	4.29910000
Cl	-5.31472500	-6.89280900	3.77489000	H	-2.11882700	-5.24208200	-3.50172600	Cl	5.64046800	-0.46868100	4.07400300
H	0.73210000	-5.07456200	-0.90649000	C	-0.06349900	-5.83330600	-2.83812500	Cl	1.76554400	-4.29989300	0.84024400
H	-3.80170800	-0.69163500	-1.48343400	C	-0.98580000	-6.08158100	-5.15063200	Cl	3.57587800	-1.95072600	6.00652200
H	0.60477000	3.89988000	-1.48577700	H	-1.72389000	-5.75903300	-5.89693100	C	1.32752300	3.42465800	-1.84421800
H	5.19355900	-0.55262100	-1.02021300	C	0.43276900	-5.97367800	-5.74536900	N	2.57209600	3.62793900	-1.08367400
Cl	7.45083800	4.14654900	3.15097400	H	0.63513200	-4.93857900	-6.05321500	C	3.74052000	2.88074400	-1.25685300
N	4.97537400	-2.45179900	-0.33009800	H	0.51286100	-6.59825100	-6.64617300	C	2.62859200	4.54318100	0.05025100
C	0.44980200	-0.37753200	1.51663800	C	1.36338200	-5.31563000	-3.45221000	O	3.90595600	1.99386200	-2.06753300
C	1.42835200	-0.03981400	2.50742700	H	2.10235400	-5.81960400	-2.69955800	C	4.69131200	3.36174100	-0.20118200
C	2.77695500	0.23258100	2.14514200	H	1.59999400	-4.48293900	-3.72908900	O	1.72622700	5.14371800	0.46315200
C	1.09663700	0.00365400	3.89403700	C	1.46551300	-6.42419600	-4.69263200	C	4.01247100	4.27592200	0.60842400
C	3.74251300	0.49888700	3.10538500	H	2.47826400	-6.34125600	-5.10900200	C	6.00612200	3.00969900	0.05193800
H	3.05248500	0.21654900	1.10006700	C	1.18838800	-7.88477300	-4.28825400	C	4.61909300	4.84025700	1.71735300
C	2.05170300	0.27447500	4.485768900	H	1.27616700	-8.54649100	-5.16127300	Cl	6.89404800	1.96313700	-1.06111800
H	0.07463500	-0.17804000	4.20880100	H	1.93341600	-8.22180300	-3.55416800	C	6.62873800	3.54969000	1.19397900
C	3.37396200	0.51631100	4.45597300	C	-0.33501800	-7.06637900	-2.45457400	C	5.94018000	4.45699000	2.01917800
H	4.77115600	0.67631400	2.81193300	H	-1.34076300	-7.16371900	-2.02423400	Cl	3.74842500	5.99603200	2.73023000
H	1.78709200	0.30063700	5.90860500	H	0.37455900	-7.39079100	-1.68213400	Cl	6.74303200	5.13721600	3.44053000
Br	4.69302300	0.88088000	5.78270200	C	-1.26248100	-7.54338600	-4.74666400	C	-3.28616000	0.07294500	-2.40494700
C	-0.95834200	-0.46239400	1.99598900	H	-2.28027800	-7.63760100	-4.34232600	N	-3.50724800	0.81859900	-0.78807200
O	-1.62031400	0.54685400	2.16050600	H	-1.20571500	-8.19931500	-5.62638200	C	-2.60948200	1.80333700	-0.33623500
O	-1.39378400	-1.70998500	2.19549100	C	-0.22856200	-7.98295700	-3.69086700	C	-4.15642700	0.18654700	0.28439200
C	-2.77216100	-1.82853600	2.61854600	H	-0.43017700	-9.01741000	-3.38189100	O	-1.85374400	2.43990300	-1.03819600
H	-2.91026800	-2.88627300	2.83933900	C	5.14685500	-3.01501200	-3.52739300	C	-2.75830700	1.84751400	0.15258100
H	-2.95095500	-1.22469100	3.51147100	H	4.11177400	-2.85082800	-3.84166200	O	-4.86524500	0.19195500	0.19153700
H	-3.44402600	-1.50474900	1.82121100	H	5.15256400	-3.92051200	-2.90952200	C	-3.72719900	0.91268100	1.52009100
C	1.95378400	4.14913200	-6.21400400	C	5.64864000	-1.80197400	-2.70428700	C	-2.02154800	2.53182400	2.10461400
H	1.75262900	3.08869900	-6.41945000	C	6.04890700	-3.22961900	-4.76378500	C	-0.01148800	0.65248300	2.84792100
H	2.09688600	4.64262600	-7.18554300	H	5.66794300	-4.08705800	-5.33415700	Cl	-0.73672000	3.65115300	1.63255800
C	3.22772700	4.29066900	-5.35611200	C	6.02769200	-1.96754300	-5.64906800	C	-2.29130100	2.26916600	3.45925400
H	4.07909200	3.84073800	-5.88393000	H	5.00417900	-1.76553100	-5.99353600	C	-3.28054000	1.34303300	3.82852400
C	0.75944000	4.77996200	-5.46874000	H	6.64315200	-2.12515900	-6.54569200	Cl	-5.20449500	-0.57687100	3.29296800
H	-0.15124800	4.67309000	-6.07272700	C	5.66328600	-0.53822200	-3.61017300	Cl	-1.35444300	3.10574300	4.71356200
C	0.55170000	4.05021600	-4.12577600	H	6.03053500	0.32200400	-0.33025400	Cl	-3.58052000	1.00885300	5.54327200
H	0.30773300	3.00085800	-4.30785400	H	4.64667000	-2.9796800	-3.93135600	C	-0.00278900	-4.75521200	-0.66702600
H	-0.30059000	4.49094000	-3.58960100	C	6.56179300	-0.76571400	-4.84324500	N	-1.38998500	-4.78236500	-1.16096300
C	3.03501800	3.55710700	-4.01032900	H	6.53984800	0.13707900	-5.46785300	C	-2.45018900	-4.01506000	-1.66795300
H	3.94828500	3.65157300	-3.40911900	C	8.00612100	-1.04813800	-4.38836000	C	-1.69311000	-5.32941800	0.09455700
H	2.87702200	2.48921300	-4.18398400	H	8.65881800	-1.19572800	-5.25998400	O	-2.41404800	-3.31628500	-2.65856000
C	1.82740200	4.15464700	-3.24238300	H	8.40339100	-0.18749300	-3.83241000	C	-3.58183500	-4.18810700	-0.69766500
C	2.10793600	5.66651800	-3.00919400	C	7.11449700	-2.08280600	-2.26927200	O	-0.93714500	-5.98873100	0.77449700
H	1.27935200	6.12080100	-2.45165400	H	7.15040000	-2.97526600	-1.63033300	C	-3.10611400	-4.49195700	0.39308200
H	3.01141900	5.79113200	-2.39745900	H	7.49498700	-1.24513600	-1.66907400	C	-4.88476200	-3.72189700	-0.73577800
C	3.50806100	5.78416400	-5.09857500	C	7.49450100	-3.51119200	-4.30820000	Cl	-3.90395100	-5.14386000	1.50234000
H	3.67290600	6.31057300	-6.04891900	H	7.52775600	-4.42257100	-3.69471900	Cl	-5.53611100	-2.97410400	-2.19884900
H	4.42664200	5.89944300	-4.50578200	H	8.14003900	-3.68914400	-5.17943800	C	-5.69356300	-3.90168800	0.40052500
C	1.04081800	6.27210700	-5.21085100	C	8.01856900	-2.30697900	-3.50024600	C	-5.19937500	-4.59525400	1.51801300
H	1.17218600	6.80667000	-6.16194200	H	9.04156600	-2.50827700	-3.15533500	Cl	-3.29840300	-6.08257000	2.87828400
H	0.18647300	6.73477000	-4.69768200					Cl	-7.33563100	-3.25814200	0.41669000

Cl	-6.21393400	-4.78957900	2.95410700	H	-1.60282500	-5.47174000	-3.91689800	Cl	5.67682600	-0.32235000	4.03230400
H	0.59276000	-5.10948600	-0.82087600	C	0.28507300	-5.69982100	-2.85299400	Cl	1.83220400	-4.14277600	4.93488400
H	-3.79811200	-0.87980700	-1.87436500	C	-0.15190000	-6.38822600	-5.24791300	Cl	3.62189900	-1.76027300	5.98922000
H	0.53414200	3.77593100	-1.17646200	H	-0.73228400	-6.14907400	-6.14841000	C	1.29084100	3.43303100	-1.86974800
H	5.33835300	-0.49115500	-1.31638400	C	1.35489400	-6.27290500	-5.55808500	N	2.52257900	3.65389200	-1.09949800
Cl	8.28900700	3.08724600	1.58246600	H	1.59185800	-5.25531300	-5.89750000	C	3.70463000	2.92736900	-1.26629600
N	4.87458000	-2.13400900	-0.19905200	H	1.62535900	-6.95834400	-6.37311800	C	2.55269000	4.46972500	0.04095000
C	0.61712100	-0.55725500	1.34424800	C	1.80175400	-5.61268800	-3.17587600	O	3.88833700	2.04102800	-2.07320100
C	1.39364800	0.26291300	2.21457800	H	2.38671900	-5.82209500	-2.27032500	C	4.64047800	3.42756000	-0.20701400
C	2.58775300	0.89022000	1.76124100	H	2.05710100	-4.59680000	-3.48843400	O	1.63169700	5.13633100	0.45422200
C	1.01548000	0.45175100	3.57578100	C	2.16909000	-6.60758800	-4.29219900	C	3.93666900	4.32267400	0.60446100
C	3.37642000	1.62479700	2.62922900	H	3.24257900	-6.51864100	-4.50728300	C	5.96195700	3.10803400	0.05057700
H	2.90794800	0.74336900	0.74027200	C	1.84549300	-8.04253200	-3.83279000	C	4.52660700	4.89532700	1.71709800
C	1.76967400	1.23527300	4.43011800	H	2.11961400	-8.76313600	-4.61549900	Cl	6.88420200	2.09238400	-1.05707700
H	0.09652300	0.00724400	3.94318900	H	2.43463800	-8.29435100	-2.94017600	C	6.56613300	3.65850200	1.19565300
C	2.95418300	1.81350900	3.95122400	C	-0.03037400	-7.15170500	-2.40647100	C	5.85425400	4.54387600	2.02069400
H	4.32146000	2.03221200	2.29684500	H	-1.09879300	-7.24248000	-2.16750800	Cl	3.63197600	6.02212300	2.73584300
H	1.45600700	1.39757800	5.45419000	H	0.52136600	-7.38731300	-1.48629100	Cl	6.63509000	5.23767300	3.44205200
Br	4.02077900	2.86930700	5.11970100	C	-0.47265400	-7.82521500	-4.79039500	C	-3.29295200	0.05830400	-2.04011400
C	-0.45861900	-1.35470000	1.97420700	H	-1.54801300	-7.92413400	-4.58667800	N	-3.51667500	0.79513900	-0.78542800
O	-1.57958200	-0.90361600	2.13005200	H	-0.22809300	-8.54117700	-5.58709500	C	-2.62337600	1.78055000	-0.32581100
O	-0.05854700	-2.57447700	2.33351700	C	0.33903600	-8.15133100	-3.52079100	C	-4.16110700	0.14944000	0.28133500
C	-1.06807500	-3.42400300	2.92987800	H	0.10406800	-9.16847800	-3.18085100	O	-1.87753900	2.43269600	-1.02301500
H	-0.70126000	-4.43974500	2.81643400	C	4.95590300	-3.39066800	-3.24361300	C	-2.76957300	1.80818900	1.16339200
H	-1.18300000	-3.16553300	3.98556900	H	3.95974600	-3.13191000	-3.61469100	O	-4.86416500	-0.83162200	0.17887400
H	-2.01936100	-3.28761800	2.41594600	H	4.81715200	-4.14148100	-2.46127700	C	-3.73478700	0.86501300	1.52266400
C	0.77221300	4.50473600	-6.06484900	C	5.63884900	-2.13268900	-2.65553900	C	-2.03304070	2.48051600	2.13213300
H	0.66455100	3.44651000	-6.33935800	C	5.81412100	-3.97843100	-4.38105700	C	-4.01246700	0.58740500	2.84743600
H	0.65570300	5.09298200	-6.98539900	H	5.30598200	-4.86444600	-4.78525600	Cl	-0.74770200	3.60168400	1.67028700
C	2.16706300	4.75241300	-5.45412900	H	5.99313900	-2.92936400	-5.49544600	C	-2.30231500	2.20388300	3.47348500
C	2.94184600	4.47474300	-6.18047000	H	5.01395200	-2.64722300	-5.90578300	C	-3.28512200	1.27070900	3.83334200
C	-0.31513900	4.89657800	-5.04360600	H	6.58249300	-3.35067700	-6.32140300	Cl	-5.18615700	-0.65866400	3.28561200
H	-1.30909000	4.71481400	-5.47348900	C	5.84325700	-1.08861300	-3.78916300	Cl	-1.37387100	3.03184800	4.73318300
C	-0.15479900	4.03207300	-3.77925400	H	6.33299700	-0.19383400	-3.37878800	Cl	-3.57880500	0.91582800	5.54026200
H	-0.28442300	2.97911800	-4.03689700	H	4.87292800	-0.77163700	-4.18062900	C	0.03082300	-4.75217400	-1.66128300
H	-0.93223900	4.28103600	-3.04442100	C	6.70190800	-1.68594800	-4.92035300	N	-1.35037500	-4.79154800	-1.14795200
C	2.33866800	3.88949300	-4.18640100	H	6.82581800	-0.93245500	-5.70892800	C	-2.41853400	-4.03418000	-1.65248100
C	3.33305500	4.06574000	-3.75545100	C	8.08161300	-2.08826600	-4.36390200	C	-1.63688600	-5.32609000	0.11721700
H	2.28191400	2.82710800	-4.43501500	H	8.70860000	-2.50159100	-5.16578100	O	-2.39433600	-3.34265600	-2.64636100
C	1.24644100	4.24916600	-3.15046800	H	8.60210800	-1.20387300	-3.97070100	C	-3.54058900	-4.20775800	-0.67308300
C	1.38721100	5.75437600	-2.79780200	C	7.03527500	-2.53588600	-2.11601400	O	-0.86628600	-5.96489100	0.79972500
H	0.64059400	6.03289400	-2.04283300	H	6.92034800	-3.27082300	-1.30917600	C	-3.05255600	-4.93021300	0.41981700
H	2.37358700	5.94193100	-2.35270000	H	7.53332700	-1.65803600	-1.67955200	C	-4.84689500	-3.75338000	-0.70651400
C	2.30802900	6.24351100	-5.08898900	H	7.19415800	-4.38051300	-3.82346300	C	-3.84616800	-5.15719900	1.53076400
C	2.20755600	6.86565900	-5.98891100	H	7.07660100	-5.14345700	-3.04145700	Cl	-5.51559200	-3.01923800	-2.16448500
H	3.30659000	6.43706100	-4.67262100	H	7.81076900	-4.82422300	-4.61716300	C	-5.64760400	-3.93382900	0.43337600
C	-0.17044600	6.38511300	-4.67483700	C	7.89707600	-3.13412800	-3.24678600	C	-5.14354100	-4.61736600	1.54959100
H	-0.30049300	7.01325700	-5.56680600	H	8.87600200	-3.41650400	-2.83770000	Cl	-3.24299900	-6.09435900	2.90463100
H	-0.95279700	6.67341000	-3.95929900					Cl	-7.29059500	-3.30562100	0.45510000
C	1.22313100	6.62346700	-4.06098600					Cl	-6.14796700	-4.81084100	2.98745900
H	1.32974800	7.68003200	-3.78241100	3-2'				H	0.63177500	-5.10270400	-0.81796700
C	-3.22046200	1.98725400	-3.79213600	-5479.501261				H	-3.80915600	-0.89311500	-1.87850100
H	-2.16920500	1.77533900	-4.00683300	Rh	0.84391300	-0.71984800	-3.11549900	H	0.48964500	3.78563000	-1.21300400
H	-3.23710200	2.74088400	-2.99869800	O	1.02448400	1.33494700	-3.06633000	H	5.33652800	-0.43416800	-1.35317200
C	-3.91918600	0.69536400	-3.31007600	O	0.61494800	-2.76580300	-2.76166400	Cl	8.23184600	3.23745100	1.58720500
C	-3.92586800	2.53641100	-5.04868000	O	0.98794700	1.37300000	-0.80042200	N	4.89295700	-2.05946600	-0.20965600
H	-3.41018500	3.45009000	-5.37346300	O	0.42316300	-2.66828000	-0.68365400	C	0.61241400	-0.55401900	1.33232200
C	-3.87940700	1.48520500	-6.17453600	O	2.88684200	-1.00694500	-2.92809100	C	1.39177800	0.26553700	2.19663100
H	-2.83603000	1.25583200	-6.43113800	O	-1.18942500	-0.40893700	-3.15681300	C	2.56636300	0.91439100	1.72690400
H	-4.35768700	1.88099100	-7.08124600	O	-1.30608000	-0.48041900	-0.89730100	C	1.03451600	0.43417900	3.56473900
C	-3.89089900	-0.35144100	-4.45874000	O	2.73801000	-0.84274100	-0.67828200	C	3.35361700	1.66012600	2.58531400
H	-4.38074100	-1.27585500	-4.12970100	C	-1.79773400	-0.29820300	-2.06342700	H	2.86797500	0.77380200	0.70011500
H	-2.85750300	-0.60961100	-4.69988900	C	3.36725200	-1.06118200	-1.77208200	C	1.78795700	1.22501100	4.41154800
C	-4.60036900	0.20412500	-5.70809900	C	1.08639300	1.91320600	-1.95197200	H	0.13335400	-0.03472800	3.94446200
H	-4.56093300	-0.55178300	-6.50320800	C	0.39689800	-3.26830300	-1.81012200	C	2.94872400	1.83257100	3.91419000
C	-6.06867600	0.52729400	-5.37091600	Rh	0.71214400	-0.64664500	-0.65561300	H	4.28525100	2.08719200	2.24298600
H	-6.58987200	0.90615900	-6.26087900	C	4.84927600	-1.39966800	-1.53104700	H	1.49281200	1.37129800	5.44304300
C	-6.59110600	-0.38610900	-5.05383900	C	3.96042000	-3.06050500	0.13837900	Br	4.00852000	2.90438500	5.06889100
H	-5.40217700	1.02329500	-2.99349800	C	5.23839900	-1.28370900	0.91077500	C	-0.45701000	-1.35360300	1.96767700
H	-5.45071300	1.76259300	-2.18389600	O	3.38889700	-3.79262600	-0.63663300	O	-1.59079100	-0.92667500	2.08949400
H	-5.91470500	0.12087100	-2.63323200	C	3.79175400	-2.97884700	1.62254200	O	-0.03893600	-2.55170500	2.37628300
C	-5.39515300	2.86200000	-4.71179200	O	5.87383000	-0.25268600	0.88333800	C	-1.04590900	-3.39820500	2.97669900
H	-5.43935800	3.62618900	-3.92331900	C	4.58563400	-1.93065800	2.09105900	H	-0.67426300	-4.41306900	2.87699100
H	-5.90339900	3.27726400	-5.59298700	C	2.96910200	-3.69583300	2.47445100	H	-1.16523800	-3.12704900	4.02833800
C	-6.11173600	1.57830400	-4.24432000	C	4.59136100	-1.57721600	3.42840700	H	-1.99387100	-3.26789500	2.45689400
H	-7.15495700	1.80809000	-3.99056600	Cl	1.99990100	-5.03979500	1.88282100	C	0.74260700	4.48123500	-6.09080800
C	-0.53005500	-5.39231500	-4.13140600	C	2.91548500	-3.30212300	3.82247100	H	0.63674100	3.42126500	-6.35744800
H	-0.34529600	-4.36456800	-4.45248900	C	3.71644000	-2.25134100	4.29496000	H	0.62564400	5.06249400	-7.01523500

C	2.13434400	4.73508300	-5.48204100	C	5.98212300	-2.90614400	-5.49715900	C	-2.15478400	2.15727300	3.79228100
H	2.90970500	4.45388700	-6.20576800	H	5.00289500	-2.62665700	-5.90808900	C	-3.06166200	1.16541000	4.18003200
C	-0.34374100	4.87784800	-5.07425900	H	6.57024300	-3.33334700	-6.32041500	Cl	-4.86859200	-0.84403700	3.68692300
H	-1.33699600	4.69199300	-5.50281900	C	5.83520600	-1.05699400	-3.80611000	Cl	-1.21881100	3.00990100	5.01056400
C	-0.18238000	4.02420300	-3.80599300	H	6.32546400	-0.16073500	-3.40106100	Cl	-3.27097900	0.78917000	5.88105400
H	-0.31099500	2.96911200	-4.05344400	H	4.86389400	-0.74294600	-4.19683200	C	-0.14418400	-4.73587500	-1.73149400
H	-0.95813800	4.28059100	-3.07269800	C	6.69078100	-1.66086400	-4.93254800	N	-1.44677900	-4.72686100	-1.06645400
C	2.30756400	3.88304600	-4.21022500	H	6.81394400	-0.91321800	-5.72620200	C	-2.54216600	-3.99375400	-1.52155200
H	3.30087600	4.06754100	-3.78183600	C	8.06890300	-2.05940000	-4.37597800	C	-1.67365500	-5.31410300	0.17568800
H	2.25459300	2.81908800	-4.45109900	H	8.69431800	-2.47837300	-5.17558000	O	-2.56609900	-3.31252600	-2.51648500
C	1.21549900	4.24672900	-3.17978500	H	8.59004300	-1.17290700	-3.98958900	C	-3.62110100	-4.20195600	-0.50238400
C	1.35409900	5.75075500	-2.83659300	H	7.02698400	-2.49052500	-2.12761800	O	-0.88085500	-5.97999400	0.79358800
H	0.60646000	6.03239000	-2.08443500	C	6.91153400	-3.21903800	-1.31583600	C	-3.08528100	-4.94899600	0.54131100
H	2.34022900	5.94141600	-2.39330800	H	7.52525600	-1.60989300	-1.69828100	C	-4.93089300	-3.77108300	-0.48053600
C	2.27286300	6.22639600	-5.12727900	C	7.18246500	-4.34397500	-3.81894700	C	-3.83613400	-5.24298700	1.66094200
H	2.17106100	6.84239000	-6.03076800	H	7.06504400	-5.10055300	-3.03136700	Cl	-5.63369000	-2.95040700	-1.85765000
H	3.27083200	6.42391700	-4.71247200	H	7.79750500	-4.79381100	-4.60985200	C	-5.69679500	-4.03691400	0.66187800
C	-0.20150800	6.36666700	-4.71548300	C	7.88574000	-3.09589800	-3.25314500	C	-5.14924800	-4.75706100	1.72869100
H	-0.33141700	6.98873500	-5.61120300	H	8.86476900	-3.37571200	-2.84365600	Cl	-3.16651700	-6.19589100	2.97392100
H	-0.98453600	6.65827500	-4.00267800					Cl	-7.34579800	-3.46428600	0.75032700
C	1.18922000	6.61046600	-4.10322400					Cl	-6.11393600	-5.06630300	3.15751400
H	1.29412000	7.66848300	-3.83125800	3-WB97XD				H	0.52725500	-5.25109400	-1.03896300
C	-3.21473400	1.96608600	-3.79479300	-4077.043351				H	-3.81816100	-0.84913000	-1.68152800
H	-2.16690800	1.74464000	-4.01422900	Rh	0.78188700	-0.72724900	-3.07623800	H	0.24550500	3.74808700	-1.42559200
H	-3.22147000	2.72327300	-3.00523900	O	1.01299700	1.32118700	-2.98057400	H	5.44773600	-0.76342200	-1.75944900
C	-3.92227800	0.68504100	-3.30513100	O	0.51584500	-2.77380100	-2.94065800	Cl	7.44108100	4.54844100	2.55629200
C	-3.91926600	2.51379200	-5.04938000	O	1.07925200	1.31671100	-0.71979800	N	4.96298000	-2.30968400	-0.50653800
H	-3.39715400	3.42078200	-5.38104400	O	0.47289400	-2.72513400	-0.67836400	C	1.44984900	4.01804200	-3.20646400
C	-3.88642100	1.45792300	-6.16804700	O	2.83389000	-1.06118600	-3.03192600	H	0.65233000	3.73144700	-3.89430300
H	-2.84653100	1.21799300	-6.42731600	O	-1.25317500	-0.39324700	-2.94936400	H	1.46708200	5.10796800	-3.11659500
H	-4.36465400	1.85296300	-7.07461900	O	-1.21032400	-0.49726500	-0.69247800	H	2.39973300	3.67029500	-3.62047900
C	-3.90771000	-0.36624800	-4.44508900	O	2.82272900	-0.97898800	-0.77693700	C	-3.74074800	0.93652000	-2.88408200
H	-4.40645500	-1.28239900	-4.10735600	C	-1.77314100	-0.29829000	-1.81715500	H	-3.58343500	0.39191300	-3.81691400
H	-2.87744400	-0.63579200	-4.68622600	C	3.36477800	-1.19003100	-1.91122700	H	-4.80811500	1.14074900	-2.76511900
C	-4.61559200	0.18761300	-5.69286800	C	1.10560000	1.87388100	-1.86114600	H	-3.19582800	1.88131800	-2.93281900
H	-4.58606900	-0.57243700	-6.48385200	C	0.33453800	-3.28274300	-1.81276700	C	-0.18916300	-5.44572400	-3.07593400
C	-6.07730700	0.52499500	-5.35171700	Rh	0.81120200	-0.71348600	-0.61492100	H	0.81171100	-5.46191800	-3.51364300
H	-6.59866100	0.90381000	-6.24110000	C	4.82490400	-1.66333200	-1.81302500	H	-0.52940400	-6.47588100	-2.93691200
H	-6.60617900	-0.38173400	-5.02775300	C	4.03107800	-3.28642200	-0.12155200	H	-0.85652400	-4.92799600	-3.76720600
C	-5.39715700	1.02775100	-2.98353900	C	5.39364800	-1.55520000	0.58913200	C	5.26271600	-2.53640200	-2.98004600
H	-5.43358900	1.77200100	-2.17858900	O	3.42419200	-4.00268900	-0.87676500	H	5.14575600	-1.97939300	-3.91181500
H	-5.91576300	0.13262900	-2.61548800	C	3.92760900	-3.19871700	1.37054300	H	6.31372200	-2.81081500	-2.85753200
C	-5.38179500	2.85360500	-4.70901300	O	6.07279600	-0.56176300	0.52958700	H	4.65739800	-3.44269300	-3.03617100
H	-5.41585100	3.62192600	-3.92467100	C	4.77570600	-2.18602300	1.79997900	C	0.83224100	-0.65096400	1.38151800
H	-5.88980000	3.26830600	-5.59010000	C	3.12535100	-3.88979200	2.25688700	C	1.66971100	0.14840300	2.21093100
C	-6.10636600	1.58076000	-4.23232400	C	4.86799500	-1.84491700	3.13417600	C	2.84388600	0.73928100	1.68287300
H	-7.14608200	1.82087600	-3.97556800	Cl	2.09600000	-5.19155900	1.71654600	C	1.36526200	0.35996600	3.58161300
C	-0.49262000	-5.39729400	-4.12257700	C	3.15459200	-3.50369000	3.60371900	C	3.68973000	1.46901300	2.49614300
H	-0.31426600	-4.36975800	-4.44683700	C	4.01735800	-2.49121600	4.03916200	H	3.10074100	0.58284800	0.64292200
H	-1.56478900	-5.48518500	-3.91122700	Cl	6.02737800	-0.65318500	3.68493400	C	2.17321200	1.14389800	4.37876600
C	0.32078700	-5.69525300	-2.84421900	C	2.10906700	-4.30781100	4.75919400	H	0.46092900	-0.06396200	4.00601800
C	-0.10605800	-6.39278000	-5.23325000	Cl	4.03669200	-2.02234200	5.72829600	C	3.33748900	1.68846300	3.82787700
H	-0.68602700	-6.16028200	-6.13524000	C	1.20010600	3.40019300	-1.83676200	H	4.62536600	1.84771800	2.10707700
C	1.39804500	-6.26934500	-5.54047600	N	2.20811000	3.80892700	-0.86934300	H	1.91841400	1.32755700	5.41550300
H	1.62931300	-5.25178000	-5.88250600	C	3.48602600	3.27005300	-0.81095800	Br	4.46796500	2.74470700	4.91712100
H	1.67429700	-6.95561300	-6.35230000	C	1.99524100	4.81307100	0.07167500	C	-0.23020100	-1.41632300	2.07579700
C	1.83433300	-5.59985500	-3.16341300	O	3.90075700	2.37359900	-1.50529300	O	-1.29798900	-0.90698000	2.34103700
H	2.41674800	-5.80495300	-2.25582800	C	4.18517100	4.01532400	0.29115700	O	0.12034900	-2.65965200	2.35397800
H	2.08289000	-4.58307400	-3.47705600	O	0.98883100	5.46467800	0.18480700	C	-0.88550200	-3.46049900	2.99580500
C	2.21011700	-6.59414700	-4.27377000	C	3.27496300	4.90360400	0.85275800	H	-0.55986100	-4.49067900	2.87589800
H	3.28303800	-6.49970500	-4.88663900	C	5.46981400	3.90185400	0.78238700	H	-0.95096200	-3.19225000	4.05280500
C	1.89493700	-8.02717900	-3.81050700	C	3.61171100	5.68310600	1.94042500	H	-1.85278800	-3.29359100	2.51920700
H	2.17473300	-8.74860600	-4.58986400	Cl	6.60562100	2.77809600	0.07197700				
H	2.48366900	-8.27203400	-2.91619700	C	5.83030000	4.68830200	1.88545100				
C	0.01331700	-7.14404200	-2.39378500	C	4.90691500	5.56595400	2.46353900	3-M062x			
H	-1.05485100	-7.23993300	-2.15815200	Cl	2.44837800	6.77344800	2.65991900	-4075.763280			
H	0.56422500	-7.37182500	-1.47171300	Cl	5.36630400	6.52071900	3.85718100	Rh	-0.23561600	0.01952200	-3.90290900
C	-0.41853600	-7.82787200	-4.77219900	C	-3.25361800	0.08830600	-1.71753100	O	-0.61875300	2.06289000	-3.57332600
H	-1.49331800	-7.93251700	-4.57058500	N	-3.45122000	0.71834200	-0.41688600	O	0.10818500	-2.03903100	-3.94772200
H	-0.16769800	-8.54485600	-5.56545000	C	-2.60886100	1.75006200	0.00964800	O	-0.66253700	1.78536300	-1.32886000
C	0.39097000	-8.14385200	-3.50161800	C	-3.98979500	0.01071800	0.65716500	O	-0.08573500	-2.25739600	-1.70333200
H	0.16159800	-9.16080900	-3.15865000	O	-1.94605700	2.44671200	-0.71855500	O	1.85528700	0.26062800	-3.61682100
C	4.94871700	-3.35026500	-3.24468000	C	-2.68913800	1.75240000	1.50561700	O	-2.31558000	-0.24178300	-3.95107600
H	3.95372500	-3.09243400	-3.61845600	O	-4.62057800	-1.01321900	0.57332100	O	-2.43856100	-0.53120500	-1.71271800
H	4.80818600	-4.09427200	-2.45675600	C	-3.56496900	0.74582200	1.88988900	O	1.58042700	0.07163900	-1.38483300
C	5.63339700	-2.09126500	-2.66784700	C	-1.97025200	2.46909300	2.44011200	C	-2.93269900	-0.33678900	-2.97116200
C	5.80427600	-3.94559500	-4.37681100	C	-3.78054300	0.44778300	3.21822900	C	2.27746100	0.15496400	-2.45467300
H	5.29577700	-4.83378500	-4.77430300	Cl	-0.83167200	3.70316600	1.94832800	C	-0.67456900	2.47528500	-2.39864300

C	0.06728800	-2.69669800	-2.88618200	C	0.25305600	-4.70478600	-4.44383700	C	-5.27041300	1.50726900	-0.79811700
Rh	-0.42624300	-0.24361100	-1.44824000	H	1.04128900	-4.21032700	-5.01345900	O	-3.03868700	3.48166400	-2.60307800
C	3.79015700	0.08719700	-2.17313300	H	0.42246500	-5.78464200	-4.46005400	C	-4.27094600	3.60661500	-0.48152400
C	3.21631100	-1.89571500	-0.83325900	H	-0.70600700	-4.47407000	-4.91466900	O	-5.87800300	0.47143800	-0.62864500
C	3.88383400	0.00696200	0.29131400	C	4.59711100	-0.46960200	-3.33350200	C	-5.15081100	2.69570300	0.11028100
O	2.96201200	-2.61822000	-1.76039200	H	4.43665100	0.16160500	-4.20959200	C	-3.93550000	4.79288400	0.14881700
C	2.80622500	-2.04116000	0.60233700	H	5.65956800	-0.46966800	-3.07997600	C	-5.72597100	2.95393400	1.34181800
O	4.17642500	1.16275800	0.46382900	H	4.28090900	-1.48593900	-3.57265600	Cl	-2.78758000	5.91751300	-0.58185700
C	3.28670700	-0.93688000	1.29252800	C	-0.63635500	-0.37322000	0.51059900	C	-4.51510200	5.06881500	1.39988800
C	2.04107600	-3.00459100	1.23166900	C	-0.10033200	0.50375600	1.48398600	C	-5.40535700	4.15898900	1.98981600
C	3.07292700	-0.78527600	2.64783000	C	0.90797900	1.44421800	1.12954300	Cl	-6.83536500	1.79518000	2.08913400
Cl	1.49875000	-4.42570300	0.37509400	C	-0.53503600	0.45465800	2.84030400	Cl	-4.11459700	6.57504600	2.23482000
C	1.73523300	-2.81305500	2.58581800	C	1.47460400	2.25600400	2.09087700	Cl	-6.12711600	4.52492700	3.56248600
C	2.25855100	-1.72331000	3.29248100	H	1.26252400	1.48604500	0.10595100	C	-0.80566300	-4.07002200	-2.79891700
Cl	3.83977700	0.51164000	3.54081000	C	-0.01185300	1.31038400	3.78738300	N	-1.88630600	-4.40477500	-1.86787600
Cl	0.71278000	-3.97024300	3.41384500	H	-1.31411700	-0.24405900	3.13240600	C	-3.15412100	-3.82028800	-1.89785400
Cl	1.89848400	-1.52808300	4.99671200	C	0.99147100	2.20729800	3.40142400	C	-1.76956000	-5.40559500	-0.89670200
C	-0.76465100	3.98544800	-2.15491000	H	2.30961800	2.90246100	1.84822500	O	-3.50171900	-2.93234400	-2.64683500
N	0.31696600	4.34900400	-1.24214000	H	-0.36222700	1.29008700	4.81260100	C	-3.94935500	-5.02969700	-0.83628000
C	1.62915100	3.92715500	-1.41983000	Br	1.73810200	3.37621200	4.67794700	O	-0.77093900	-6.05155700	-0.66875700
C	0.13747300	5.08570200	-0.07278500	C	-1.60539000	-1.40013200	0.99047700	C	-3.12146100	-5.48830700	-0.24261200
O	2.01640500	3.19149100	-2.29377700	O	-2.73878100	-1.10823700	1.29603300	C	-5.26723800	-4.37556000	-0.43833700
C	2.40456500	4.52166100	-0.27958600	O	-1.09021700	-2.62029100	1.03168600	C	-3.59317200	-6.32104000	0.75841200
O	-0.89981000	5.55692500	0.31151500	C	-2.01417600	-3.64152700	1.43486300	Cl	-6.30522600	-3.15535200	-1.18139000
C	1.50110100	5.16491200	0.56003800	H	-1.48504800	-4.58358200	1.29349700	C	-5.75878100	-5.21168500	0.58063500
C	3.75089900	4.46406300	0.01774700	H	-2.28236400	-3.50877700	2.48565200	C	-4.92943200	-6.17669000	1.17281000
C	1.90807900	5.72838500	1.75132700	H	-2.91503200	-3.58600000	0.81989800	Cl	-2.54944800	-7.54346100	1.49251900
Cl	4.89601600	3.79849100	-1.12057400					Cl	-7.43489900	-5.04481600	1.11444400
C	4.17891100	5.01060700	1.23751700					Cl	-5.56598300	-7.22072500	2.44877100
C	3.26407000	5.63024000	2.09816400	4A				H	0.10588500	-4.45993900	-2.33266300
Cl	0.76366500	6.52750100	2.80346700	-4315.039871				H	-4.76177500	-0.05605200	-2.69400700
Cl	3.81663900	6.31733500	3.60959500	Rh	-0.17063300	-0.01962500	-4.19783300	H	-0.42475700	4.59248800	-2.87799200
C	-4.46476200	-0.18208200	-2.90371400	O	0.13965300	2.01860700	-4.21614400	H	4.38333700	0.21758200	-2.64529500
N	-4.86628700	0.36407100	-1.61184300	O	-0.47054600	-2.04627700	-4.02121900	Cl	6.61087300	5.33190900	1.46704500
C	-4.15593200	1.42496300	-1.04393900	O	0.23963000	2.11358200	-1.94918400	N	4.22364500	-1.64954800	-1.83167400
C	-5.49659100	-0.42527000	-0.64844400	O	-0.59134200	-1.93675800	-1.75445500	C	0.89341300	4.62838100	-4.59452800
O	-3.51289800	2.23578400	-1.66188300	O	1.86630500	-0.33640900	-4.09895700	H	0.11461600	4.34643000	-5.30592900
C	-4.35022400	1.30157900	0.43732500	O	-2.20926300	0.31977300	-4.14595900	H	0.98646500	5.71884800	-4.58661100
O	-6.11763500	-1.43086000	-0.87133700	O	-2.19849300	0.48827600	-1.88217500	H	1.83711800	4.18639000	-4.92579800
C	-5.19696100	0.22520400	0.67101700	O	1.83728600	-0.36401100	-1.82902800	C	-4.79935000	1.33498300	-4.35432900
C	-3.74919200	1.98005800	1.47171000	C	-2.75007500	0.53443300	-3.03104100	H	-4.61276600	0.57057700	-5.11180100
C	-5.49571100	-0.18866600	1.95096300	C	2.40205300	-0.46611300	-2.96930900	H	-5.87819400	1.50216400	-4.27758500
Cl	-2.62472100	3.28718800	1.17303200	C	0.29756700	2.61668700	-3.11918000	H	-4.31242600	2.26049500	-4.67006300
C	-4.04533900	1.57251600	2.78342400	C	-0.62343000	-2.54423400	-2.87408900	C	-1.01559200	-4.72739100	-4.16487400
C	-4.91149000	0.50057400	3.01934200	Rh	-0.18874100	0.09582500	-1.73126300	H	-0.16851800	-4.50430400	-4.81703000
Cl	-6.52213600	-1.57826600	2.22964500	C	3.91691000	-0.73265700	-2.93086000	H	-1.08967600	-5.81260900	-4.04197700
Cl	-3.32323300	2.42354500	4.13928000	C	3.61100600	-2.89596600	-1.66845600	H	-1.92434100	-4.35318000	-4.64320800
Cl	-5.24595300	-0.00602800	4.66404800	C	5.06564500	-1.31571100	-0.76644300	C	4.48857400	-1.21624000	-4.26502200
C	0.26706900	-4.21014200	-3.00454300	O	2.79983100	-3.38088100	-2.42829200	H	4.27281100	-0.48180000	-5.04383600
N	-0.74440700	-4.88671000	-2.20227800	C	4.17080700	-3.45514900	-0.39116700	H	5.57335600	-1.33482600	-4.18067200
C	-2.07282300	-4.47902500	-2.11539400	O	5.65540000	-0.26427300	-0.63987200	H	4.04220700	-2.16947200	-4.55787400
C	-0.50324600	-6.10128900	-1.56962500	C	5.05446900	-2.51135300	0.14334900	C	-0.31319100	0.30551500	0.28409400
O	-2.54744500	-3.50897900	-2.64753900	C	3.93958800	-4.66288600	0.24638500	C	0.67662800	0.74747600	1.21710100
C	-2.74890100	-5.51311800	-1.25552000	C	5.73516300	-2.75593100	1.32397700	C	2.00747800	1.02289800	0.79619900
O	0.55250700	-6.67941200	-1.54284600	Cl	2.79381400	-5.83334100	-0.41084200	C	0.37671000	0.90529200	2.60300300
C	-1.81507000	-6.49712800	-0.94997000	C	4.62741200	-4.92563100	1.44509800	C	2.98747600	1.39999100	1.70326000
C	-4.03743500	-5.56933800	-0.76570200	C	5.51900600	-3.98192400	1.97769200	H	2.25854800	0.92107100	-0.25051900
C	-2.14789800	-7.58215800	-0.16536600	Cl	6.85104000	-1.56018100	1.99491100	C	1.34536500	1.29247200	3.51229600
Cl	-5.16143900	-4.26512200	-1.06212600	Cl	4.36036500	-6.45574200	2.28648900	H	-0.63306800	0.73147400	2.95798300
C	-4.39470600	-6.67028600	0.02634500	Cl	6.37473700	-4.33094400	3.48385800	C	2.65029700	1.53262100	3.05543800
C	-3.46117100	-7.67094800	0.31807500	C	0.52072300	4.13624700	-3.19356600	H	4.00218500	1.58244300	1.36749000
Cl	-0.96120000	-8.80835300	0.22164900	N	1.50420000	4.55870600	-2.19330300	H	1.10359800	1.41098700	4.56237900
Cl	-6.02077000	-6.78193900	0.66055800	C	2.72518100	3.92339400	-1.96813700	Br	3.98825000	2.06095400	4.30633600
Cl	-3.92849100	-9.03956300	1.30245100	C	1.34442400	5.72036800	-1.42548600	C	-1.69750100	0.15454300	0.81252900
H	1.22768300	-4.42917000	-2.52329400	O	3.11836400	2.92631500	-2.53784300	O	-2.39866100	1.13043900	1.01573200
H	-4.89580100	-1.18965400	-2.94387500	C	3.41420700	4.73870300	-0.90857700	O	-2.07378800	-1.11348900	1.00065200
H	-1.69438100	4.15658800	-1.60068400	O	0.39084100	6.46397000	-1.47103000	C	-3.43669700	-1.29975400	1.44943300
H	4.11112900	1.10694200	-1.92989200	C	2.59055700	5.82348400	-0.59106900	H	-3.52287200	-2.36576200	1.65563400
C	5.87008400	4.93195400	1.67202300	C	4.64107500	4.56679600	-0.29012200	H	-3.62384500	-0.71783500	2.35491500
N	3.92675000	-0.68124800	-0.92625500	C	2.97629800	6.76570000	0.34765100	H	-4.13679000	-0.99539200	0.66908200
C	-0.71564900	4.80159500	-3.43644100	Cl	5.66112500	3.17295300	-0.66983900	C	-0.01090100	-3.21528900	3.55814700
H	-1.54597100	4.51394400	-0.48043800	C	5.04852700	5.51726200	0.66258600	H	-0.56587700	-2.60988200	2.82618000
H	-0.79637500	5.86596100	-3.20156900	C	4.22376300	6.60811200	0.97804300	C	1.47262300	-3.14397100	3.16267700
H	0.21687700	4.61030600	-3.97275900	Cl	1.93139400	8.13297200	0.74525800	H	1.61227800	-3.49995100	2.13506500
C	-4.94006500	0.65874000	-0.07987200	Cl	4.75226900	7.79271800	2.17758200	H	1.85154800	-2.11563800	3.21727700
H	-4.62351800	0.19218900	-5.01387600	C	-4.25288400	0.86355800	-3.00582600	H	2.09707400	-3.76676300	3.81456600
H	-6.02983200	0.73230800	-4.06209500	N	-4.51001800	1.82078800	-1.92856000	C	-0.53853400	-4.65451300	3.44999100
H	-4.50724900	1.65994400	-4.02597300	C	-3.82444800	3.03309200	-1.79508300	H	0.00674000	-5.33680800	4.11307600

H	-1.60099000	-4.71179900	3.71888200	C	-1.12465800	-5.97125100	0.28875400	O	0.02834700	1.91126200	-4.02326600
H	-0.42847000	-5.03767800	2.42898200	C	-2.85068500	-3.65492500	-1.66440000	O	-0.45236700	-2.16442800	-3.87621600
C	-0.28754100	-2.58135600	4.94093700	O	-3.32816800	-5.15703600	0.21743200	O	-0.11190000	2.01355800	-1.76148700
H	0.03390200	-1.52863000	4.91039700	O	-0.11395100	-6.56078800	0.60623800	O	-0.81514200	-2.05460800	-1.64053600
H	-1.37578900	-2.56029800	5.10420100	C	-2.49233500	-6.03731100	0.91235400	O	1.81716400	-0.34057200	-3.69599400
C	0.37336700	-3.25553000	6.15306600	C	-4.66135300	-5.00986700	0.56278500	O	-2.22795900	0.10789300	-4.21336100
H	0.04377000	-4.30012700	6.22415600	C	-2.96839700	-6.78612800	1.97550000	O	-2.48103000	0.33109500	-1.97040500
H	1.46220400	-3.28607700	6.01626000	Cl	-5.71052100	-3.89479200	-0.31599800	O	1.56768000	-0.35640200	-1.44059900
C	0.05260200	-2.53715400	7.46915400	C	-5.15998600	-5.76936400	1.63714500	C	-2.90470500	0.32742800	-3.16745600
H	0.52976300	-3.03224900	8.32261300	C	-4.31993000	-6.64821100	2.33890700	C	2.25132100	-0.41992600	-2.51170600
H	0.40309000	-1.49739200	7.44944700	Cl	-1.90558500	-7.89114000	2.85741500	C	0.05228500	2.51990900	-2.91441500
H	-1.02816900	-2.51702000	7.65733700	Cl	-6.85615100	-5.61245800	2.10404800	C	-0.73443300	-2.66665300	-2.75162500
TSA ₄₋₅				Cl	-4.96246400	-7.58974500	3.68954000	Rh	-0.48065000	-0.00932400	-1.62284800
-4315.039871				H	0.75840800	-5.16481800	-1.18733000	C	3.77664700	-0.53875700	-2.35556300
Rh	0.64898000	-0.61299500	-2.81022300	H	-4.01598700	-0.52603400	-1.50666100	C	3.57226500	-2.90043600	-1.45990900
O	0.97539400	1.40818400	-2.73095200	H	0.41744700	3.92982700	-1.18381400	C	5.11743300	-1.47885800	-0.44720700
O	0.31678900	-2.64492000	-2.75069000	Cl	5.13616000	-0.42386600	-1.06662800	O	2.70012200	-3.26794800	-2.21784800
O	0.97780100	1.42047300	-0.45935400	N	7.96625000	4.54194100	2.24657500	C	4.29861000	-3.67996600	-0.39974200
O	0.10440100	-2.64617900	-0.48809900	C	5.04050700	-2.37988600	-0.46734600	O	5.73835300	-0.46310900	-0.21924200
O	2.66961800	-0.95530200	-2.62595600	C	1.54263800	4.05197800	-3.02581500	C	5.23098800	-2.82849400	0.20286500
O	-1.38108800	-0.23783900	-2.85106100	H	0.68634000	3.81821600	-3.66198000	C	4.16959400	-4.99950200	0.00096800
O	-1.45875300	-0.17577700	-0.58279800	H	1.65066000	5.13963300	-2.96751600	C	6.05963500	-3.27592900	1.21821700
O	2.58842200	-1.06965300	-0.35897800	C	2.43708900	3.62099900	-3.48393400	Cl	2.97485200	-6.06454900	-0.74489000
C	-1.95620700	-0.04543100	-1.74602900	H	-3.90357300	0.89982500	-3.13122900	C	5.00770200	-5.46925200	1.02851400
C	3.17983000	-1.12083400	-1.48741100	H	-3.73118800	0.14327800	-3.89989800	C	5.94476700	-4.61561000	1.63116400
C	1.08748500	1.96467500	-1.60305900	H	-4.97322500	1.12864400	-3.09242900	Cl	7.23385300	-2.19561300	1.97566800
C	0.10553800	-3.19456600	-1.63727700	H	-3.35140900	1.80169000	-3.40538300	Cl	4.87667200	-7.14787600	1.56217700
Rh	0.53935300	-0.60991700	-0.35149900	C	-0.32062400	-5.29551700	-3.05784900	Cl	6.98866200	-5.22412200	2.91957300
C	4.70086700	-1.35107900	-1.45603500	H	0.55194900	-5.06699200	-3.67345700	C	0.24845900	4.04267100	-2.96492000
C	4.41465500	-3.62470900	-0.37849900	H	-0.43472600	-6.38264500	-2.99638700	N	1.20377900	4.45159000	-1.93274500
C	6.10619000	-2.24036700	0.43061200	H	-1.20140200	-4.86470000	-3.53970400	C	2.45294200	3.85831500	-1.74291700
O	3.48568800	-3.99907400	-1.06268400	C	5.30256200	-1.66880800	-2.82675200	C	0.97302700	5.52671100	-1.06535600
C	5.13378800	-4.35957100	0.72033000	H	5.07750400	-0.85946800	-3.52402400	O	2.88399100	2.91463200	-2.37297500
O	6.80991400	-1.26114700	0.53762300	H	6.38922100	-1.76681800	-2.73787700	C	3.10686900	4.63974900	-0.63822500
C	6.16050000	-3.53550000	1.19333200	H	4.88678800	-2.59530500	-3.23183900	O	-0.03007100	6.20425600	-1.04083300
C	4.91984300	-5.61814400	1.25795400	C	0.31859500	-0.46531500	1.89745700	C	2.21902600	5.64216800	-0.23264600
C	7.00648500	-3.95417500	2.20668100	C	1.07974700	0.60427400	2.58687700	C	4.35886900	4.51586200	-0.05953800
Cl	3.59219600	-6.63640800	0.69001100	C	2.42913100	0.83738400	2.23885300	C	2.56042600	6.54009800	0.76446900
C	5.77422400	-6.05866100	2.28519900	C	0.54063700	1.37391300	3.64284700	Cl	5.47110200	3.23641100	-0.56031500
C	6.81026000	-5.23542900	2.75325500	C	3.21357700	1.75455700	2.93359500	C	4.72723600	5.43286300	0.94128400
Cl	8.30000800	-2.90843900	2.80098600	H	2.86223200	0.29382900	1.40739800	C	3.83270800	6.43269000	1.35377800
Cl	5.53610500	-7.66068900	2.99166500	C	1.30734500	2.31369300	4.32730400	Cl	1.43056900	7.79749600	1.28025900
Cl	7.87401300	-5.80640200	0.40308000	H	-0.49795000	1.24830000	3.92097400	Cl	4.30770500	7.57002000	2.61946000
C	1.31704000	3.48536200	-1.62188300	C	2.64673300	2.48718200	3.97816800	C	-4.41048600	0.57580200	-3.35500900
N	2.41394000	3.85455400	-0.71893400	H	4.25444400	1.89570200	2.66475300	N	-4.85562800	1.59286600	-2.40096500
C	3.62568200	3.17265800	-0.61391100	H	0.87010800	2.89587000	5.13110000	C	-4.21907700	2.82312400	-2.22110200
C	2.40535500	5.05933100	-0.00183100	Br	3.72187600	3.74895900	4.94858600	C	-5.93028400	1.40105400	-1.52583000
O	3.90852600	2.13800700	-1.18226600	C	-1.14439400	-0.52115400	2.17499200	O	-3.27120300	3.22284400	-2.86364200
C	4.47587700	3.99885500	0.31220600	O	-1.86499100	0.46066400	2.25060900	C	-4.96328400	3.50177200	-1.10517200
O	1.48782600	5.84815400	0.02896300	O	-1.63126900	-1.78273000	2.27406800	O	-6.63174000	0.41530000	-1.47997400
C	3.75048000	5.14145900	0.66378900	C	-3.06003000	-1.88633500	2.42597100	C	-6.00131800	2.65578600	-0.70016400
C	5.75885900	3.79158300	0.78993500	H	-3.24788200	-2.93025200	2.68046100	C	-4.76364300	4.73276500	-0.50170600
C	4.29566100	6.11161000	1.48753300	H	-3.41440800	-1.22865800	3.22278900	C	-6.87275300	3.02489100	0.31061900
Cl	6.65246200	2.31672700	0.39020600	H	-3.56367700	-1.62217100	1.49490000	Cl	-3.42392100	5.77623800	-0.98265800
C	6.32770300	4.76982200	1.62441700	C	1.31154000	-2.57556700	3.15202700	C	-5.64348500	5.12090900	0.52521200
C	5.60383200	5.92193500	1.96677400	H	0.80322300	-1.52895000	2.12788300	C	-6.69009300	4.27615400	0.92575400
Cl	3.37534300	7.55465200	1.92394100	C	2.77627900	-2.28011200	3.00457400	Cl	-8.18253100	1.95221700	0.81924000
Cl	6.33640100	7.14291700	3.01359800	H	3.06520500	-2.21519700	1.95242600	Cl	-5.42366800	6.68535700	1.31693100
C	-3.43979700	0.36704900	-1.77452900	H	3.07457400	-1.36484200	3.52086100	Cl	-7.78487600	4.78227100	2.21804200
N	-3.69008200	1.31340200	-0.68574400	H	3.33255600	-3.11581100	3.45639200	C	-0.96160800	-4.18704900	-2.71051100
C	-2.95190100	2.48504100	-0.49480700	C	0.80776500	-3.78469900	2.41850700	N	-2.04812300	-4.49089200	-1.77840400
C	-4.53402800	1.02879200	0.39094000	H	1.13700600	-4.67740100	2.97460400	C	-3.29898800	-3.86928600	-1.81360100
O	-2.10779400	2.90907700	-1.25587200	H	-0.28134800	-3.79507000	2.37319100	C	-1.91728700	-5.39543700	-0.71868900
C	-3.43440100	3.05997600	0.80538200	H	1.21188700	-3.85079000	1.40777500	O	-3.64806200	-3.04434700	-2.63104400
O	-5.21902600	0.03375100	0.49884600	C	0.68133500	-2.24909000	4.47747500	C	-4.06667100	-4.44588700	-0.65727600
C	-4.39468100	2.19070300	1.33060300	H	0.89431600	-1.20550500	4.74246300	O	-0.92331700	-6.03830800	-0.46359800
C	-3.06671000	4.21344400	1.47717500	H	-0.40404000	-2.36834900	4.40741300	C	-3.24278100	-5.37215100	-0.00904000
C	-5.01668600	2.45750800	2.53689600	H	1.21410800	-3.15626500	5.62132400	C	-5.35320900	-4.19329200	-2.01009100
Cl	-1.82480400	5.28958100	0.82974400	C	1.04589800	-4.20959400	5.36430300	C	-3.68855700	-6.07424700	1.09783000
C	-3.69341500	4.49767400	2.70343000	H	2.29792800	-3.02319500	5.72391400	Cl	-6.37152600	-2.99055600	-1.00394200
C	-4.66201800	3.62865100	3.22750500	C	0.52931900	-2.83542200	6.95354000	C	-5.82040900	-4.90477400	0.90993300
Cl	-6.22608500	1.34882100	3.20263200	H	0.91248500	-3.48064400	7.75154200	C	-4.99645800	-5.83851800	1.55695700
Cl	-3.25317300	5.96258700	3.59139400	H	0.70488500	-1.79475800	7.24978500	Cl	-2.63906000	-7.23623400	1.91970100
Cl	-5.44104600	4.00376000	4.77131600	H	-0.55433200	-2.98794300	6.88994200	Cl	-7.45857000	-4.61518500	1.50570300
C	-0.12568700	-4.71761600	-1.65473800	SA				Cl	-5.60152900	-6.72218600	2.96317100
N	-1.23873600	-5.06267500	-0.76578300	-4315.130481				H	-0.06365600	-4.61763300	-2.25239200
C	-2.51469400	-4.49927600	-0.86331700	Rh	-0.19589100	-0.13106100	-4.00893400	H	-4.91247200	-0.34727000	-3.04285000
								H	-0.70892500	4.47933400	-2.66015200

H	4.10124300	0.38725000	-1.86902900	H	-2.32934900	2.03037900	2.14100000	CI	-5.11483800	4.60701100	-1.93806500
CI	6.33052200	5.33025600	1.67283800	H	-3.28702300	0.53338200	2.05794300	C	-6.81187000	3.38899600	-0.13035800
N	4.11092900	-1.61069300	-1.41161500	C	0.31569800	-2.27730700	2.63161800	C	-2.37726500	2.27906900	0.51640400
C	0.64557200	4.56755800	-4.34640100	H	0.91726700	-1.04199400	0.98541500	CI	-7.68770100	-0.42635800	0.98768500
H	-0.11209700	4.28599300	-5.08098000	C	1.60434000	-3.09942100	2.41830200	CI	-7.33182800	5.02042400	0.30548400
H	0.71897800	5.65925800	-4.31705700	H	1.87345400	-3.14251600	1.35557800	CI	-8.60500600	2.51931100	1.76476400
H	1.60383100	4.14840300	-4.66390400	H	2.45221800	-2.67295800	2.96491600	C	1.13261600	-4.02747000	-2.72830900
C	-4.80177100	0.92394700	-4.79288100	H	1.46926300	-4.13044000	2.76039000	N	0.27279700	-4.62114700	-1.70301500
H	-4.49083200	0.12126800	-5.46497000	C	-0.82945900	-2.93952500	1.83528300	C	-1.12336800	-4.54504000	-1.72613600
H	-5.88787700	1.04067500	-4.86072700	H	-0.92363900	-3.99883200	2.09460700	C	0.76448400	-5.19426600	-0.52610000
H	-4.31814800	1.84962800	-5.11497300	H	-1.79580900	-2.46270300	2.03781100	O	-1.77983300	-4.02466000	-2.60293200
C	-1.19332400	-4.81201800	-4.08794600	H	-0.64706600	-2.87881300	0.75596700	C	-1.58405300	-5.21955900	-0.46507600
H	-0.34097500	-4.60106500	-4.73720300	C	-0.02831900	-2.20530600	4.14238300	O	1.93586100	-5.30392800	-0.23390500
H	-1.30015000	-5.89649700	-3.98584200	H	0.81647600	-1.74322600	4.66960200	C	-0.44991500	-5.61334800	0.25327600
H	-2.09247200	-4.40286300	-4.55539800	H	-0.88176000	-1.53123500	4.27789600	C	-2.85928800	-5.47145200	0.01313300
C	4.51735600	-0.71121700	-3.68353300	C	-0.35462700	-3.53699500	4.84060300	C	-0.56356800	-6.27049700	1.46662600
H	4.29728900	0.13269800	-4.34079600	H	-1.22044000	-4.01383200	4.36366300	CI	-4.28599000	-4.96226500	-0.89111000
H	5.59601200	-0.74170500	-3.49971300	H	0.48108600	-4.24060200	4.73707400	C	-2.98919500	-6.13907600	1.24471700
C	4.20831800	-1.63004300	-4.18855500	C	-0.65524700	-3.33878000	6.33149900	C	-1.85166300	-6.53588300	1.96452000
H	0.58714600	-0.86099200	1.99359400	H	-0.89327400	-4.29073600	6.81979100	CI	0.87299200	-6.76868300	2.36832000
C	1.65207900	0.00647500	2.66760000	H	0.20337900	-2.90068100	6.85511800	CI	-4.59915800	-6.47930500	1.88713800
C	2.88951800	0.15690000	2.02522700	H	-1.50951000	-2.66609200	6.47779300	CI	-2.03493900	-7.37481100	3.50896500
C	1.46456500	0.66421500	3.89368600					H	2.14461600	-4.07233000	-2.30871800
C	3.92926500	0.89612400	2.59144100	4B				H	-3.77985600	-1.85614200	-2.71475000
H	3.03595800	-0.29641700	1.05018400	-4315.068672				H	-1.42495100	4.28683800	-3.10732300
C	2.48966200	1.41166900	4.47416100	Rh	0.40098000	-0.03161000	-4.25549000	H	4.45611200	1.95287700	-2.63729300
H	0.51093500	0.60413800	4.40435500	O	-0.01352500	1.99652500	-4.33174700	CI	4.44187800	6.31618700	2.38214900
C	3.71952200	1.51245800	3.82381900	O	0.83481100	-2.03557100	-4.02444800	N	5.06654700	0.19351500	-1.78900200
H	4.87764500	0.98535100	2.07325500	O	-0.06560500	2.13990400	-2.06579100	C	0.02080400	4.77266900	-4.64493700
H	2.33136900	1.90934600	5.42482300	O	0.56621900	-1.92300500	-1.77205600	H	-0.53879700	4.28762500	-5.44773200
Br	5.13509100	2.52930400	4.63679500	O	2.40636400	0.41466700	-4.09483200	H	-0.22754200	5.83846100	-4.63353200
C	-0.67157500	-0.05823300	1.71467500	O	-1.60791900	-0.48720500	-4.25878300	H	1.08791900	4.65378100	-4.84639400
O	-1.05562900	0.26308500	0.59526200	C	2.31736700	0.45247900	-1.82659700	C	-4.28550300	-0.96899200	-4.62331100
O	-1.36227200	0.30552800	2.79999300	C	-2.23107700	-0.47923300	-3.16453700	H	-3.70998900	-1.69133400	-5.20610800
C	-2.54741200	1.09917500	2.57550700	C	2.91527600	0.53518800	-2.94922300	H	-5.32759400	-1.30128400	-4.57994300
H	-2.95601700	1.28861800	3.56769000	C	-0.11375500	2.62273100	-3.24545000	H	-4.23361800	-0.00130200	-5.12854100
H	-2.28462100	2.03490900	2.07710600	C	0.80271100	-2.53139900	-2.86939900	C	1.07863300	-4.79828300	-4.04837500
H	-3.26029600	0.54646100	1.95962600	Rh	0.26594000	0.13268300	-1.79745800	H	1.76750700	-4.34590700	-4.76497100
C	0.31313100	-2.28608700	2.64608600	C	4.41088900	0.88911700	-2.89891600	H	1.37537700	-5.83841300	-3.88082800
H	0.96092900	-1.08062600	0.99022800	C	4.91089900	-1.16238700	-1.50399600	H	0.07327500	-4.77357200	-4.47524500
C	1.58929400	-3.12156000	2.41717600	C	6.00134300	0.82221200	-0.95474500	C	5.13795600	0.64789000	-4.22439800
H	1.80706400	-3.20966200	1.34640700	O	4.18976000	-1.93180000	-2.10562800	H	4.65809100	1.22086400	-5.02027200
H	2.45855000	-2.67236400	2.91020900	C	5.81438600	-1.43444400	-0.33224500	H	6.17959200	0.97165100	-4.13481400
H	1.46610900	-4.13680700	2.80616500	O	6.34019900	1.98121200	-1.03214100	H	5.10969200	-0.41039300	-4.49828500
C	-0.85138600	-2.93910000	1.87050600	C	6.47240300	-0.24409900	-0.00610600	C	0.19332100	0.38003800	0.21354700
H	-0.92998200	-4.00284700	2.11614200	C	6.05482800	-2.60065600	0.37456300	C	0.80995500	-0.39338100	1.24553200
H	-1.81260300	-2.47001900	2.11728900	C	7.38663300	-0.19104400	1.03262500	C	1.66542700	-1.48739600	0.93567100
H	-0.70255200	-2.85608000	0.78853600	CI	5.20376200	-4.09778400	-0.02747800	C	0.56734800	-0.11293500	2.62290900
C	-0.00814500	-2.20461100	4.16108900	C	6.98227900	-2.56358400	1.43090900	C	2.22455800	-2.26967500	1.93605800
H	0.85933900	-1.77920500	4.68100400	C	7.64295300	-1.36911600	1.75703000	H	1.87670700	-1.71398000	-0.10010700
H	-0.83578300	-1.50136800	4.31271300	CI	8.21142500	1.31639100	1.44070000	C	1.12122300	-0.88792500	3.62635800
C	-0.37724500	-3.52678600	4.85683700	CI	7.31461900	-4.03398300	2.35267200	H	-0.06873300	0.72155200	2.89823700
H	-1.27022200	-3.96451000	4.39345900	CI	8.80459800	-1.34119600	3.08774600	C	1.94690400	-1.96639200	3.27435800
H	0.42608900	-4.26361900	4.73259800	C	-0.35613300	4.14107400	-3.30387900	H	2.85753400	-3.11220100	1.68164900
C	-0.64047400	-3.32644100	6.35445800	N	0.32405000	4.77319100	-2.17259300	H	0.92467700	-0.66728900	4.66945400
H	-0.90958200	-4.27118800	6.84007600	C	1.68304200	4.59185000	-1.89279700	Br	2.71136200	-3.03581800	4.65475500
H	0.24586600	-2.92958400	6.86456900	C	-0.36098100	5.39398300	-1.12415000	O	-0.48020400	1.63630000	0.64070500
H	-1.46266300	-2.61956100	6.52235800	O	2.46784800	4.00181700	-2.60501400	O	0.17496200	2.63805900	0.86778300
				C	1.91507200	5.26262300	-0.57010500	O	-1.81219600	1.55521700	0.71437800
R-P				O	-1.55966600	5.57394200	-1.08116900	C	-2.49488000	2.78639100	1.05082600
-747.864638				C	0.68864300	5.75480100	-0.11420600	H	-3.53802000	2.50305300	1.18400600
C	0.56746000	-0.84040100	2.00235900	C	3.07156800	5.41725600	0.17525200	H	-2.09155200	3.20718300	1.97469900
C	1.65265900	0.00399100	2.66914000	C	0.59021200	6.42185600	1.09399500	H	-2.38726400	3.51117400	0.24169900
C	2.92114300	0.06083500	2.07177700	CI	4.60891700	4.75565300	-0.38555200	H	-3.31635200	-0.20878600	2.36316000
C	1.45306500	0.74009100	3.84801600	C	2.98592500	6.09568600	1.40390900	C	-3.06643900	0.53095800	5.06429700
C	3.96358000	0.80353100	2.62706800	C	1.75648600	6.59600800	1.85836700	H	-2.48125300	1.14322000	4.35788600
H	3.10221500	-0.48442300	1.14908800	CI	-0.96617300	7.03876500	1.66832900	C	-4.39786600	1.25488000	5.31929400
C	2.48269900	1.49118700	4.41689300	CI	1.66970900	7.44815400	3.40589100	H	-4.23009500	2.23458700	5.78238800
H	0.47986700	0.74248700	4.32396400	C	-3.71635400	-0.87856600	-3.20583900	H	-4.96321700	1.41809300	4.39579600
C	3.73414600	1.51459500	3.80319800	N	-4.50041600	0.02446600	-2.36087300	H	-5.03270300	0.67109800	5.99885800
H	4.93546800	0.83177800	2.14656000	C	-4.45069400	1.41684600	-2.45383200	C	-2.26100600	0.42072600	6.36806600
H	2.30883300	2.05447300	5.32741800	C	-5.39649200	-0.42635500	-1.86688000	H	-2.80195000	-0.17835900	7.11201800
Br	5.15743300	2.54902900	4.58300400	O	-3.73818300	2.04512400	-3.20702100	H	-1.28954400	-0.06184700	6.20153900
C	-0.71186100	-0.04189100	1.74265000	C	-5.44628900	1.92273900	-1.44634300	H	-2.07535800	1.40756300	6.80862900
O	-1.10928800	0.24458400	0.63426100	O	-5.61028900	-1.58624200	-1.11094300	C	-3.26020300	-0.85938600	4.42548800
O	-1.37262600	0.23188000	2.68667900	C	-6.01128200	0.81636500	-0.80317200	H	-2.27865100	-1.35319800	4.36043300
C	-2.56668200	1.09643600	2.65663900	C	-5.83304900	3.21358200	-1.12543400	H	-3.86546200	-1.48113800	5.10329000
H	-2.96510300	1.29616900	3.65173800	C	-6.97518200	0.97445300	0.17829700	C	-3.89817900	-0.86292400	3.02894700

H	-4.90916800	-0.43852900	3.07763300	Cl	-4.24932400	-6.04285600	-1.13744800	O	2.31683300	0.12976200	-1.34854700
C	-3.97845400	-2.26508300	2.14449600	C	-3.08416700	-7.59946200	0.82482200	C	-2.21220800	-1.07034000	-2.48554000
H	-4.45325800	-2.24358100	1.42797600	C	-1.99408000	-8.11890100	1.54018300	C	2.83831800	0.36406400	-2.48198900
H	-2.97727600	-2.70026300	2.29813500	Cl	0.69710100	-8.40058100	2.10086300	C	-0.30212400	2.22189400	-2.38872200
H	-4.56132200	-2.94321300	3.05011300	Cl	-4.72916600	-8.07188700	1.26290900	C	0.98316000	-2.86349400	-2.58583400
O	-1.76185200	-0.22738300	-2.00649900	Cl	-2.27232000	-9.24203500	2.87491100	Rh	0.32210700	-0.36565300	-1.26967200
TSB _{4,5}				H	2.24295600	-4.78702300	-1.86058100	C	4.30464700	0.81765600	-2.48671500
-4315.036613				H	-3.64687700	-2.68304300	-2.64552500	C	5.03231000	-1.42981700	-1.58625400
Rh	0.57523900	-0.85613000	-4.04520600	H	-1.00732400	3.65294500	-3.20663100	C	6.06540000	0.47524600	-0.72663900
O	0.22911900	1.17289300	-4.23803800	H	4.57860300	1.05668600	-2.15517000	O	4.29531900	-2.10281100	-2.27702300
O	0.97629900	-2.84539100	-3.72513100	Cl	4.64292100	5.43142900	2.58614200	C	6.05891500	-1.86958100	-0.58169700
O	0.05266100	1.40206200	-1.98684700	N	5.12521900	-0.78167300	-1.43274200	O	6.32319400	1.64877900	-0.57765200
O	0.58029200	-2.68456300	-1.49579500	C	0.58638600	3.90277500	-4.64632700	C	6.68905100	-0.72713500	-0.07720500
O	2.56433800	-0.43252500	-3.78779800	H	0.03572100	3.44232800	-5.46944700	C	6.41824400	-3.13592500	-0.15159800
O	-1.44619300	-1.30689300	-4.14774000	H	0.45608800	4.98831400	-4.69633600	C	7.70102500	-0.82303000	0.86262400
O	2.35120800	-0.32355900	-1.52918700	H	1.64539100	3.66114300	-4.76136900	Cl	5.58784500	-4.57152100	-0.75617400
C	-2.12925100	-1.27699200	-3.09094000	C	-4.11084700	-1.91099200	-4.61054300	C	7.44739300	-3.24853700	0.80060500
C	3.01235700	-0.29132700	-2.61369700	H	-3.49041800	-2.64940700	-5.12304000	C	8.08456900	-2.10285300	1.30160900
C	0.12653100	1.84620100	-3.17616200	H	-5.14390000	-2.27288000	-4.58986000	Cl	8.49403900	0.62366300	1.49543200
C	0.89495500	-3.31394200	-2.55774500	H	-4.06580400	-0.97451900	-5.16925600	Cl	7.93992200	-4.84794100	1.36775000
Rh	0.29718200	-0.61357500	-1.62755300	C	1.42872500	-5.54482400	-3.71480800	Cl	9.37799700	-2.26597600	2.49511800
C	4.51391100	0.01875700	-2.49852600	H	2.17438300	-5.04851200	-4.33909300	C	-0.59066400	3.73181000	-2.34767300
C	4.90884700	-2.14615800	-1.23976700	H	1.75775000	-6.57074400	-3.52090900	N	0.13847800	4.33456500	-1.23421000
C	6.13151900	-0.26892700	-0.60278700	H	0.48231000	-5.56453800	-4.26150100	C	1.49847300	4.13046300	-0.98830300
O	4.13887600	-2.83547700	-1.87650300	C	5.27408100	-0.13832700	-3.81808800	C	-0.46820100	5.16366000	-0.28599100
C	5.83817900	-2.54920900	-0.12806700	H	4.83504500	0.51028800	-4.57900600	O	2.24468500	3.48696400	-1.69639700
O	6.53359600	0.87294000	-0.61435800	C	6.32061500	0.14789200	-3.67330200	C	1.79282200	4.88035100	0.27820300
C	6.58614200	-1.42638100	0.24011800	H	5.22595800	-1.16977300	-4.17793900	O	-1.62796400	5.51515600	-0.31361500
C	6.03862000	-3.77378800	0.48633000	C	0.04499200	-0.25204600	0.63611700	C	0.61524100	5.51247600	0.69165300
C	7.56060200	-1.50378600	1.22064100	C	1.19377700	-0.64243800	1.47222600	C	2.96759800	5.00472000	1.00138000
Cl	5.05292600	-5.17835500	0.05760700	C	1.66641500	-1.97376500	1.40551200	C	0.58715800	6.29565200	1.83197000
C	7.02977100	-3.86959700	1.47868300	C	1.83313800	0.22952600	2.38098800	Cl	4.44078600	4.17680900	0.49104100
C	7.78625400	-2.74506400	1.84066500	C	2.69479500	-2.42813900	2.22697100	C	2.95064300	5.79415100	2.16501000
Cl	8.50167700	-0.08097100	1.68091400	H	1.23259700	-2.65156700	0.70837000	C	1.77211800	6.43623000	2.57497600
Cl	7.31864400	-5.41954400	2.27716900	C	2.87544200	-0.20954300	3.19408600	Cl	-0.89917000	7.10537600	2.34411500
Cl	9.02696100	-2.88396900	3.09164400	H	1.51804400	1.26312800	2.43836700	Cl	1.77395100	7.42870500	4.03832900
C	0.04886400	3.37921400	-1.31258600	C	3.28968600	-1.54059200	3.12591900	C	-3.64542900	-1.62476700	-2.48465800
N	0.70814800	3.99639500	-2.16135400	H	3.03009400	-3.45771600	2.16134900	N	-4.48475900	-0.82994800	-1.58518800
C	2.02370100	3.71658400	-1.77964600	H	3.35384500	0.47765300	3.88361400	C	-4.64664500	0.55404300	-1.69548200
C	0.02428900	4.76114100	-1.21256300	Br	4.68720400	-2.15750100	4.29157300	C	-5.23512800	-1.38532900	-0.54260700
O	2.79926600	3.02614800	-2.40664500	C	-0.51077500	1.12046000	0.75670500	O	-4.07043000	1.26449700	-2.49089400
C	2.23113600	4.44391900	-0.48325000	O	0.15730900	2.12934500	0.91812700	C	-5.64458700	0.92703200	-0.63554600
O	-1.14695500	5.07017700	-1.27753200	O	-1.86043700	1.16630300	0.61224700	O	-5.25411500	-2.55650500	-0.23596100
C	1.03392200	5.08423000	-0.15077200	C	-2.44648200	2.48088700	0.63407600	C	-5.98470000	-0.23341800	0.06722600
C	3.34329500	4.53065600	0.33686700	H	-3.52227900	2.31454400	0.70186800	C	-6.21138600	2.14905300	-0.31696100
C	0.92193500	5.83595400	1.00517200	H	-2.09254500	3.04742200	1.49825100	C	-6.88768500	-0.19684500	1.11671900
Cl	4.83876800	3.68372900	-0.06597100	H	-2.20252500	3.02813100	-0.27772700	Cl	-5.79989500	3.60637000	-1.22880500
C	3.24339600	5.29356800	1.51394000	H	-0.78008400	-1.05566600	0.61306800	C	-7.13192300	2.20092700	0.74405800
C	2.04443100	5.94322100	1.84377000	C	-1.66777300	-0.38732600	3.86986800	C	-7.46506000	1.03929200	1.45763000
Cl	-0.59835400	6.63935200	1.42440600	H	-1.18341300	0.45139000	3.35344500	Cl	-7.30714100	-1.66455700	2.00651700
Cl	1.94009400	6.90060100	3.32769200	H	-3.15857000	-0.05579000	4.03612300	Cl	-7.87343800	3.74547500	1.18250000
C	-3.59951200	-1.72825100	-3.18128900	C	-3.28750900	0.85989600	4.62378100	Cl	-8.62104300	1.12558400	2.79066200
N	-4.44029400	-0.81800100	-2.39711900	H	-3.66131300	0.09702300	3.07454400	C	1.39763000	-4.34082900	-2.65253400
C	-4.59755500	0.54188000	-2.69306900	C	-3.68336800	-0.86406800	4.56185000	N	0.73090900	-5.08730100	-1.58599700
C	-5.02163300	-1.17354500	-1.17861700	H	-0.98779000	-0.55240800	5.23752500	C	-0.63615100	-5.01101300	-1.31466500
O	-4.09804900	1.12022400	-3.63192300	H	-1.41639700	-1.39794000	5.79107700	O	1.40968300	-5.96650400	-0.73116700
C	-5.47600300	1.09182500	-1.60326100	H	0.08823300	-0.72915900	5.12909200	O	-1.43831000	-4.35136100	-1.94297000
O	-4.95210400	-2.26448300	-0.65275100	C	-1.12168200	0.34598200	5.84989800	C	-0.86125000	-5.90700200	-0.12985600
C	-5.72176400	0.06380500	-0.68818000	C	-1.45171000	-1.65589200	3.02234400	O	2.59232400	-6.21786600	-0.78343800
C	-6.00361200	2.35909000	-1.41874300	H	-0.39432200	-1.96685100	3.05577500	C	0.36238000	-6.49625400	0.20725400
C	-6.49529300	0.28146300	0.43951800	H	-1.99184600	-2.50237500	3.48613000	C	-2.01416300	-6.18875200	0.58441000
Cl	-5.69036600	3.65119600	-2.57997400	C	-1.88509500	-1.62015500	1.59683800	C	0.46022500	-7.39403300	1.25697300
C	-6.79765400	2.59219800	-0.28091500	H	-2.56393600	-0.83132700	1.28716000	Cl	-3.54244900	-5.40066900	0.18714000
C	-7.03991600	1.56194000	0.64174500	C	-1.99545500	-2.91074200	0.85152100	C	-1.92921300	-7.09982000	1.65271200
Cl	-6.79235400	-1.01850400	1.60333200	H	-1.94534300	-2.77156900	-0.23028900	C	-0.70466000	-7.70029500	1.98341800
Cl	-7.49145600	4.19374200	-0.01292600	H	-1.24163700	-3.63446900	1.17625300	Cl	2.00709300	-8.13631700	1.67619200
Cl	-8.03597600	1.87334000	2.06762200	H	-2.99446800	-3.32232600	1.06858000	Cl	-3.37932700	-7.48656500	2.58501800
C	1.28378000	-4.79248900	-2.38992200	O	-1.73143800	-0.95837200	-1.92165900	Cl	-0.62031500	-8.84593100	3.32560300
N	0.34778600	-5.46932800	-1.48604000	5B				H	2.46383700	-4.36420200	-2.39773000
C	-1.03984200	-5.43670100	-1.62811800	-4315.123896				H	-3.57839700	-2.61210000	-2.01460200
O	0.76862900	-6.30782300	-0.44604600	Rh	0.30080600	-0.28567800	-3.66370600	H	-1.64968100	3.84139400	-2.08579500
O	-1.64764200	-4.78544300	-2.45214000	O	-0.24796400	1.68731800	-3.53573300	H	4.30954100	1.80856000	-2.01953300
C	-1.57792600	-6.35079700	-0.56102100	O	0.87553500	-2.25522100	-3.69077200	Cl	4.42941000	5.97721000	3.11571500
O	1.91914000	-6.51294600	-0.13033300	O	-0.17313200	1.63430200	-1.27032700	N	5.09273400	-0.03523600	-1.59615500
C	-0.49159500	-6.87114200	0.15061200	O	0.82287400	-2.36480100	-1.42841200	C	-0.31329500	4.44270800	-3.67516200
C	-2.87841000	-6.70297500	-0.23957300	O	2.25745700	0.31013800	-3.60773900	H	-0.91019700	3.99175600	-4.47074000
C	-0.67866800	-7.75203100	1.20282500	O	-1.65345200	-0.91979400	-3.61008100	H	-0.58303900	5.49951700	-3.58635300
								H	0.74251800	4.36137700	-3.94580100

C	-4.26056600	-1.74801900	-3.87999300	H	-4.02078200	3.37513500	5.92336300	Cl	-8.07469300	3.13577700	2.45349000
H	-3.63620400	-2.39328900	-4.50209500	H	-4.39908500	2.43089600	4.47779300	C	0.80615900	-3.94225100	-2.87554200
H	-5.25752700	-2.19329600	-3.80315600	H	-4.61134100	1.71419200	6.08432900	N	-0.03327300	-4.49402200	-1.81093800
H	-4.33534100	-0.77149400	-4.36403100	C	-1.92338300	1.90647700	6.88466600	C	-1.41236300	-4.27882500	-1.72303100
C	1.17844800	-4.97927600	-4.02655200	H	-2.47699900	1.24747100	7.56668700	C	0.48168800	-5.16846000	-0.69968100
H	1.72647200	-4.41967900	-4.78742100	H	-0.87523000	1.58420900	6.88956000	O	-2.07523600	-3.65912300	-2.52746300
H	1.54622000	-6.00980500	-4.01315800	H	-1.96402300	2.92150500	7.29724000	C	-1.84578600	-4.96031700	-0.45571100
H	0.11809700	-4.97817800	-4.29268900	C	-2.40665300	0.42183000	4.91152200	O	1.65390200	-5.40659300	-0.50288900
C	4.91957200	0.89598900	-3.88625200	H	-1.36913400	0.07834900	5.01781800	C	-0.70910600	-5.50212800	0.15379800
H	4.34113600	1.58115400	-4.51002400	H	-2.99859000	-0.23048300	5.57006600	C	-3.10109600	-5.10186600	0.11280900
H	5.94558700	1.26965900	-3.81270700	C	-2.87413200	0.14310700	3.46633800	C	-0.80024700	-6.20313700	1.34430600
H	4.92512800	-0.08570600	-4.36730300	H	-3.86352800	0.59141200	3.31980400	Cl	-4.52767300	-4.39493300	-0.64608500
C	-1.96188900	0.75764500	2.25755000	C	-3.02919500	-1.37389400	3.26143500	C	-3.20815100	-5.81479400	1.32112100
C	-0.51874100	0.28586100	2.27220600	H	-3.39228200	-1.60895200	2.25359600	C	-2.06847500	-6.36187600	1.93049600
C	-0.15061800	-0.86136300	1.54268600	H	-2.07921700	-1.89986000	3.40782000	Cl	0.63945800	-6.88611800	2.10947100
C	0.45783000	0.89251100	3.07231300	H	-3.75060100	-1.78165600	3.97836100	Cl	-4.79268500	-6.02193400	2.07422100
C	1.14142900	-1.40098000	1.62322000					Cl	-2.22379900	-7.25640800	3.44660800
H	-0.90241200	-1.38616600	0.95998000	4C				H	1.83616900	-4.10650600	-2.53738200
C	1.74938200	0.36776500	3.16447900	-4315.068882				H	-3.86244500	-1.35609900	-2.50516200
H	0.22100100	1.79156100	3.62708400	Rh	0.37118300	0.16694000	-4.20316400	H	-1.00459500	4.57008900	-2.76528500
C	2.07944900	-0.77813900	2.44569300	O	0.12626000	2.22406200	-4.17291600	H	4.67506900	1.71695100	-2.75922800
H	1.39729500	-2.28711600	1.05605900	O	0.63744900	-1.87530500	-4.07082100	Cl	5.39409100	5.89779400	2.33240100
H	2.48701900	0.84692500	3.79928800	O	0.22100200	2.27475900	-1.90464300	N	5.16505000	-0.12105100	-2.00447700
Br	3.83884800	-1.53205800	2.62801800	O	0.30697400	-1.83736900	-1.80371800	C	0.36589100	4.99765200	-4.38717100
C	-2.09888900	2.27997200	2.12287000	O	2.41509900	0.43225900	-4.14440900	H	-0.29129200	4.59862400	-5.16295600
O	-1.19432400	3.09123200	2.12533300	O	-1.66574800	-0.11363900	-4.10154100	H	0.21605700	6.07954200	-4.31780200
O	-3.39552600	2.63166300	1.99799900	O	-1.67321200	0.06632400	-1.83606400	H	1.40057900	4.79483100	-4.67308900
C	-3.65611500	4.05212100	1.94048800	O	2.45380500	0.38163800	-1.87428400	C	-4.39519800	-0.31589100	-4.32727700
H	-4.74161900	4.14617600	1.95006500	C	-2.22569100	-0.09421900	-2.97334300	H	-3.91600900	-1.04377500	-4.98535400
H	-3.21938300	4.54998300	2.80922700	C	2.99425700	0.45766600	-3.02652000	H	-5.45723400	-0.56583500	-4.23877600
H	-3.23593900	4.48361300	1.03148900	C	0.14460000	2.80945000	-3.05998300	H	-4.29217900	0.67449600	-4.77810700
H	-2.39464400	0.38797600	1.28628700	C	0.62074800	-2.41603100	-2.93569500	C	0.57673300	-4.64371600	-4.21553200
C	-2.53493800	1.85606300	5.36202800	Rh	0.38896400	0.23711000	-1.73505800	H	1.25245300	-4.22945600	-4.96677300
H	-2.00615500	2.55098700	4.69513700	C	4.51669300	0.67220000	-3.05129900	H	0.77777200	-5.71448800	-4.11052000
C	-3.99803200	2.31567500	5.46531600	C	4.90249800	-1.46769700	-1.75655500	H	-0.45012400	-4.50107200	-4.56024300
H	-4.06007500	3.32746900	5.88343600	C	6.19754300	0.38928800	-1.20523700	C	5.14429900	0.41568500	-4.42408200
H	-4.49538400	2.32932200	4.49050300	O	4.08240900	-2.14644700	-2.34030000	H	4.67808700	1.06092400	-5.17123500
H	-4.56839000	1.64941800	6.12614300	C	5.84030100	-1.86398800	-0.64896900	H	6.21523200	0.63775400	-4.38416600
C	-1.85223200	1.93856200	6.73734400	O	6.63641300	1.51531200	-1.26390700	H	5.00090100	-0.62406600	-4.73083100
H	-2.33109900	1.25726600	7.45288400	C	6.62014600	-0.75019500	-0.32125200	C	0.44108900	0.39937800	0.28297400
H	-0.79202700	1.66495500	6.67724200	C	6.01137600	-3.07324500	0.00369100	C	1.00181200	-0.49245200	1.24948400
H	-1.91491100	2.95203400	7.15082100	C	7.58990400	-0.81842000	0.66491100	C	1.76322800	-1.62686400	0.85340500
C	-2.40773500	0.42026700	4.80621200	Cl	5.00745200	-4.47224800	-0.39978100	C	0.79173400	-0.28978600	2.64531400
H	-1.36607700	0.08804800	4.90894800	C	6.99354000	-3.15910700	1.00636600	C	2.26642300	-2.51774400	1.79095500
H	-2.99088600	-0.23817700	5.46699200	C	7.77643900	-2.04136200	1.33410300	H	1.94983700	-1.79446200	-0.19817600
C	-2.87303900	0.14190700	3.35991000	Cl	8.56951900	0.59271100	1.07494000	C	1.28532100	-1.17621100	3.58602900
H	-3.85982900	0.59270400	3.21176700	Cl	7.23987200	-4.68742000	1.85819000	H	0.21956200	0.56752000	2.98365300
C	-3.03372800	-1.37492400	3.15641100	Cl	9.00555100	-2.16722300	2.59692800	C	2.02076500	-2.28861600	3.15020600
H	-3.37445100	-1.62138500	2.14371200	C	0.03082300	4.34382800	-3.04581600	H	2.83055300	-3.38688500	1.47205100
H	-2.09416700	-1.91003500	3.33450400	N	0.84144600	4.86825800	-1.94566400	H	1.11141300	-1.01656300	4.64408200
H	-3.77712000	-1.77070800	3.85712100	C	2.19600400	4.56260300	-1.77356600	Br	2.70392400	-3.51032300	4.44446700
O	-1.69037600	-0.85887400	-1.34461800	C	0.28891600	5.50306300	-0.82963500	C	-0.06669700	1.79925900	0.79923000
				O	2.87382600	3.93583300	-2.56036600	O	0.70451100	2.61806000	1.00970200
				C	2.57939000	5.16098900	-0.45104900	O	-1.39076900	1.74869600	0.97537200
R-P ₀				O	-0.88341500	5.78229500	-0.69230200	C	-1.91848800	3.02286000	1.41629700
-747.868272				C	1.43523700	5.73492500	0.11084200	H	-2.96437800	2.82888000	1.65089900
C	-1.97436900	0.74125700	2.31416700	C	3.79569600	5.19263000	0.20970700	H	-1.38434500	3.37096100	2.30323000
C	-0.53230900	0.26210100	2.31463600	C	1.48119100	6.36175500	1.34339300	H	-1.82790100	3.76531300	0.62121800
C	-0.16424900	-0.78164000	1.45384100	Cl	5.22687900	4.42821500	-0.48464700	H	-2.62134900	-0.62400600	1.83167700
C	0.45570300	0.79716000	3.15604200	C	3.85722300	5.83097100	1.46115100	C	-4.34698900	0.41891900	5.61526700
C	1.13395100	-1.29335600	1.43097400	C	2.71046100	6.41250700	2.02245400	H	-4.92840100	-0.43384600	5.99905700
H	-0.90478600	-1.20759200	0.78104600	Cl	0.02763500	7.07964600	2.05345000	C	-3.06573900	0.53102500	6.45589900
C	1.75978100	0.30048400	3.14619800	Cl	2.80763700	7.21121600	3.59739300	H	-3.30314600	0.73870900	7.50600800
H	0.21881800	1.62987500	3.80652800	C	-3.74084000	-0.35948800	-2.94477200	H	-2.47212400	-0.38924800	6.42857500
C	2.08858700	-0.74523200	2.28475600	N	-4.39328900	0.55456700	-2.00507800	H	-2.43174400	1.35183600	6.09291000
H	1.39603000	-2.10088800	0.75611600	C	-4.21034600	1.93888100	-2.00881200	C	-5.20641500	1.68235100	5.77623300
H	2.51196400	0.72847800	3.79994400	C	-5.29551500	0.12530800	-1.02621400	H	-4.66862900	2.57052200	5.41785000
Br	3.88596000	-1.43517500	2.26777100	O	-3.47627200	2.54857300	-2.75672500	H	-6.14056700	1.60795900	5.20699000
C	-2.10924900	2.26075600	2.21187300	O	-5.10548600	2.46544800	-0.92050400	H	-5.46604800	1.85664300	6.82723600
O	-1.25960400	3.09393400	2.44448800	O	-5.61510600	-1.02408600	-0.81857300	C	-4.05776000	0.14831300	4.12503800
O	-3.35640700	2.58518100	1.79379600	C	-5.75997600	1.37721400	-0.33405600	H	-5.01114900	0.16532600	3.57783300
C	-3.61458500	3.99250900	1.65543500	C	-5.34138200	3.76058400	-0.48933600	H	-3.45965500	0.98165200	3.72155500
H	-4.64175700	4.06664900	1.29719100	C	-6.66816200	1.55810600	0.69516800	C	-3.34633100	-1.17696800	3.81656700
H	-3.50549000	4.49962300	2.61776600	Cl	-4.50200400	5.13027700	-1.22251300	H	-2.35452600	-1.18927000	4.28855000
H	-2.92235600	4.43975400	0.93750100	C	-6.26160000	3.95904700	0.55610300	H	-3.91073700	-2.00381100	4.27101500
H	-2.44175300	0.36940500	1.39375800	C	-6.91970900	2.86705700	1.14283800	C	-3.19036900	-1.42938500	2.31211300
C	-2.51993700	1.85857400	5.46840900	Cl	-7.49776600	0.17943400	1.42894300	H	-2.66000600	-2.36978500	2.12024800
H	-1.92755000	2.53590300	4.84099900	Cl	-6.58961200	5.59708100	1.13198300	H	-4.16389500	-1.49140500	1.81156300
C	-3.96906900	2.37201400	5.48334100								

TSC ₄₋₅	-4315.029506	Rh	0.59629400	-0.45958400	-3.97581300	Cl	-6.19398500	-6.76740100	0.29096100	C	0.80352400	-2.76605600	-3.16815500
		O	0.44923500	1.59974500	-4.12677200	Cl	-4.33846700	-7.33785200	2.78895000	Rh	0.29329400	-0.31071900	-1.70812200
		O	0.80570100	-2.49047700	-3.68019300	H	1.58599700	-4.58456400	-1.64146000	C	4.50297700	0.42457300	-2.39710900
		O	0.24582900	1.80367300	-1.87563500	H	-3.55721600	-2.28819000	-3.07382700	C	4.85613800	-1.98236000	-1.70578400
		O	0.22919200	-2.31350100	-1.49280300	H	-0.47993500	4.19971600	-3.10532700	C	5.98842100	-0.32887800	-0.51475700
		O	2.60137600	-0.22630300	-3.62806500	H	4.68143900	0.95013800	-1.81243600	O	4.12821100	-2.47730800	-2.54124600
		O	-1.45021300	-0.73844500	-4.16842900	Cl	4.97762400	5.14636100	3.05104000	C	5.70785400	-2.65642100	-0.66753500
		O	-1.81000700	-0.39488000	-1.95308900	N	4.98485300	-0.97843900	-1.19018500	O	6.35749000	0.77895800	-0.19439500
		O	2.28831900	-0.18683100	-1.37964000	C	1.21374300	4.26044000	-4.44808400	C	6.39366800	-1.66438500	0.04121400
		C	-2.17046200	-0.71155900	-3.13359300	H	0.65803900	3.88735500	-5.31102800	C	5.87870900	-3.99806400	-0.36960300
		C	3.00416500	-0.18379400	-2.42960200	H	1.22749700	5.35424600	-4.48114800	C	7.27053800	-1.98951100	1.06200300
		C	0.40821900	2.25968400	-3.05123000	C	2.23806300	3.88579300	-4.50846500	Cl	4.98665000	-5.24604800	-1.24345900
		C	0.57122300	-2.96296700	-2.53659000	H	-4.19888500	-1.02095500	-4.69302500	C	6.76931100	-4.34323200	0.66313900
		Rh	0.22637500	-0.23852100	-1.57934600	H	-3.55752400	-1.53043800	-5.41460100	C	7.46010200	-3.34809700	1.37159400
		C	4.52191400	-0.05054700	-2.22709600	H	-5.20009500	-1.46069500	-4.74047900	Cl	8.13201800	-0.73194200	1.95572200
		C	4.62636200	-2.32449600	-1.11176300	H	-4.25819200	0.03548800	-4.95943800	Cl	7.01795200	-6.04525100	1.06821700
		C	5.97917700	-0.62645900	-0.26727200	C	1.02108200	-5.25461100	-3.61837600	Cl	8.57702800	-3.80152400	2.66415100
		O	3.82223800	-2.88203800	-1.83021200	H	1.92975300	-4.86555600	-4.08324000	C	-0.06600900	3.93485200	-2.53433400
		C	5.45349400	-2.89861300	0.00567600	H	1.17205600	-6.31321200	-3.38398200	N	0.68610700	4.40564300	-1.37096200
		O	6.48635400	0.46837300	-0.16873500	H	0.19851700	-5.15426500	-4.32911800	C	1.99303200	0.01657900	-1.06704900
		C	6.27117200	-1.88035900	0.50675700	C	5.32810400	-0.21164300	-3.51834400	C	0.17916100	5.35226700	-0.47610700
		C	5.51828200	-4.18242800	0.52021400	H	5.00388400	0.52829600	-4.25320200	O	2.67016900	3.26527300	-1.73713100
		C	7.17360400	-2.12162000	1.52866700	H	6.39057900	-0.05471700	-3.30716100	C	2.34341200	4.74365200	0.19874000
		Cl	4.47221200	-5.46761800	-0.09874400	H	5.18615900	-1.20689200	-3.94828800	O	-0.91191000	5.87381100	-0.56516500
		C	6.43386800	-4.44470300	1.55441300	C	-0.09231700	0.03947900	0.70756700	C	1.26539300	5.56824100	0.53730500
		C	7.25540200	-3.42309100	2.05354000	C	0.95599400	-0.54402700	1.56322000	C	3.49108800	4.70559000	0.97350800
		Cl	8.20136400	-0.82945300	2.15682700	C	1.23304400	-1.92549300	1.46410600	C	1.31983400	6.39361300	1.64653200
		Cl	6.54681700	-6.07378300	2.22984800	C	1.69655700	0.20603000	2.50088700	Cl	4.83045800	3.62997100	0.56501700
		Cl	8.39982300	-3.77031300	3.35447900	C	2.17014100	-2.54524900	2.28470100	C	3.55367000	5.53200700	2.10939600
		C	0.53648800	3.79215000	-3.15774000	C	0.71285700	-2.52446100	0.72567600	C	2.48007000	6.37299800	2.43958400
		N	1.20028900	4.30412200	-1.95908200	H	2.65666900	-0.39953500	3.30965500	Cl	-0.02904000	7.46267000	2.05536500
		C	2.44486500	3.85379200	-1.50754900	H	1.53218300	1.27254300	2.57983000	Cl	2.58404700	7.41442200	3.86481800
		C	0.55966400	5.13207200	-1.03267000	C	2.87534500	-1.77387400	3.21099600	C	-3.65020200	-0.85477000	-3.43812900
		O	3.16599800	3.08414400	-2.10665500	H	2.34145500	-3.61259400	2.19610000	N	-4.42673300	-0.04540600	-2.49648200
		C	2.65884500	4.52337700	-0.18115300	H	3.22057300	0.19505100	4.02031400	C	-4.28205000	1.33678600	-2.35881300
		O	-0.55762000	5.58698600	-1.15979200	Br	4.15467300	-2.61434200	4.37302100	C	-5.39607100	-0.58107200	-1.63926700
		C	1.53141800	5.30189400	0.09687000	C	-0.51087100	1.45779600	0.86284500	O	-3.49148100	2.02316800	-2.97111200
		C	3.71998800	4.45617500	0.70599300	O	0.26178200	2.36168600	1.13749600	C	-5.28321200	1.74447000	-1.31504100
		C	1.43956700	6.03850500	1.26454200	O	-1.81720500	1.67509000	0.59149500	O	-5.70439500	-1.74945600	-1.57039600
		Cl	5.12206000	3.43766800	0.37137500	C	-2.23522100	3.05409300	0.59700500	C	-5.94332200	0.59238600	-0.87406900
		C	3.64103400	5.20305000	1.89501900	H	-3.31735100	3.02759500	0.46920600	C	-5.59945300	2.99208600	-0.80451700
		C	2.51201200	5.98890400	2.17128500	H	-1.97053300	3.53219100	1.54296300	C	-6.92669200	0.65871400	0.09864500
		Cl	0.00610900	7.01469600	1.61350700	H	-1.77283100	3.59806600	-0.22693000	Cl	-4.78217800	4.44566700	-1.38826000
		Cl	2.43223000	6.92097700	3.67211300	H	-0.96812100	-0.69293600	0.45977900	C	-6.59820200	3.07469600	0.18148800
		C	-3.61612200	-1.21449000	-3.29090500	C	-2.03394900	-0.39642500	5.21438900	C	-7.25317300	1.91849300	0.63269900
		N	-4.46886000	-0.66624800	-2.23419300	H	-2.88728300	-1.07405700	5.37564300	Cl	-7.75342900	-0.79934800	0.65612000
		C	-4.86324800	0.67668300	-2.15785100	C	-0.76702500	-1.09607100	5.73164600	Cl	-7.03709800	4.65115400	0.85134500
		C	-4.76380700	-1.37485600	-1.06843300	H	-0.83381900	-1.26992300	6.81179500	Cl	-8.50126400	2.04250700	1.87701500
		O	-4.61306700	1.53635200	-2.97149000	C	-0.60278300	-2.06851500	5.25466500	C	1.02340700	-4.27845200	-3.32048100
		O	-5.62550800	0.79871100	-0.86568700	H	0.12314600	-0.48167800	5.54612100	N	0.11744800	-4.99619400	-2.42338900
		C	-4.41837600	-2.51200900	-0.82212900	C	-2.30302100	0.89238200	6.00555400	C	-1.25140700	-4.74104800	-2.32570400
		C	-5.56007200	-0.43334000	-0.20890300	H	-1.47984200	1.60794400	5.88161200	C	0.54654800	-6.01574000	-1.56268900
		C	-6.29987800	1.87226400	-0.30816400	H	-3.22540300	1.38302300	5.67228000	O	-1.86148400	-3.92706200	-2.98801200
		C	-6.16163600	-0.61924700	1.02449400	C	-2.40201200	0.68363000	7.07688600	C	-1.76006800	-5.67696400	-1.26587200
		Cl	-6.37683600	3.42870000	-1.14056900	H	-1.96246900	-0.08710500	3.70527000	O	1.68171700	-6.42564600	-1.47593600
		C	-6.92272900	1.69526900	0.94075000	H	-2.86232900	0.47361700	3.41610500	C	-0.68502300	-6.45451900	-0.82125800
		C	-6.85268700	0.45943400	1.60304100	H	-1.10997100	0.57861800	3.51798900	C	-3.03069100	-5.84209600	-0.73949400
		Cl	-6.06334000	-2.17781200	1.85911500	C	-1.84785800	-1.32852100	2.81049500	C	-0.85688500	-7.42581700	0.15062900
		Cl	-7.79542600	3.04046500	1.68066700	H	-0.90930700	-1.86940200	2.98457700	Cl	-4.37292300	-4.82517200	-1.26958900
		Cl	-7.63476300	0.25651700	3.17413900	H	-2.64359200	-2.04799500	3.07852400	C	-3.21957300	-6.82581400	0.24799000
		C	0.74311800	-4.47723400	-2.33246000	C	-2.03178300	-1.08737300	1.34797000	C	-2.14369600	-7.61294500	0.68662300
		N	-0.41585100	-4.99964500	-1.59934200	H	-2.08759400	-1.98079300	0.72172300	Cl	0.50344100	-8.40605300	0.70603300
		C	-1.72717300	-4.95438100	-2.08195900	H	-2.72437400	-0.30719200	1.05070700	Cl	-4.82690900	-7.06808700	0.94048000
		O	-0.34626500	-5.44810100	-0.27478300	5C				Cl	-2.40234200	-8.84608100	1.92534900
		O	-2.06575200	-4.48494900	-3.14813400	-4315.126779				H	2.02989300	-4.47682900	-2.93366400
		C	-2.57766900	-5.56104300	-1.00276300	Rh	0.55539700	-0.05128800	-4.07502200	H	-3.79842600	-1.89179500	-3.11685800
		O	0.65895100	-5.49327100	0.40048700	O	0.20959400	1.95427500	-3.83782400	H	-1.11814900	4.12312700	-2.29106800
		C	-1.75232200	-5.83309900	0.09333200	O	0.90390400	-2.06819600	-4.21886900	H	4.58360900	1.35360100	-1.82283600
		C	-3.93186300	-5.84742200	-0.97024600	O	0.02829600	1.73562800	-1.58892900	Cl	4.99998200	5.51083700	3.12528100
		C	-2.26744300	-6.37487300	1.25919800	O	0.57652900	-2.33870900	-1.99351500	N	5.07501200	-0.61365600	-1.53774900
		Cl	-4.95761800	-5.56003500	-2.37839300	O	2.54626000	0.28887700	-3.76157000	C	0.31205900	4.69706100	-3.80709100
		Cl	-4.46870600	-6.39656600	0.20744600	O	-1.45602600	-0.41896800	-4.28897900	H	-0.30392500	4.35716200	-4.64245200
		C	-3.64452900	-6.65343100	1.31430300	O	-1.73716300	-0.54522600	-2.04301800	H	0.14090600	5.76717400	-3.65487300
		Cl	-1.22210500	-6.70983300	2.64535700	O	-2.32960700	-0.06650000	-1.53210900	H	1.36186900	4.53143300	-4.06313700
						C	-2.15328200	-0.56701300	-3.24462400	C	-4.13283900	-0.67653100	-4.87885000
						C	2.99903600	0.17					

C	0.91414900	-4.77270900	-4.76507300	H	-3.71449900	3.94109100	6.83521900	C	-1.70188600	-5.20636500	-0.61640700
H	1.63551200	-4.24557300	-5.39300900	H	-2.70550000	3.48728900	8.22013800	O	1.81795600	-5.43557700	-0.53206500
H	1.13105000	-5.84469600	-4.80240400	C	-2.67441800	2.15954700	4.98970100	C	-0.55760500	-5.68051700	0.03391800
H	-0.08768300	-4.59310300	-5.16388000	H	-3.61103500	2.67631700	4.73133700	C	-2.96667800	-5.43052800	-0.09783100
C	5.27170300	0.55521800	-3.71421000	H	-1.86094600	2.78243400	4.59551900	C	-0.64992000	-6.39481600	1.21641700
H	4.85489700	1.37106000	-4.30901600	C	-2.67222700	0.78206100	4.30639000	Cl	-4.40468000	-4.80830000	-0.90723800
H	6.32254500	0.77621600	-3.50261300	H	-1.69634600	0.29618500	4.42351000	C	-3.07440200	-6.15815300	1.10131500
H	5.20538200	-0.36576400	-4.29929400	H	-3.39300800	0.13700100	4.82954300	C	-1.92725300	-6.63705200	1.75223300
C	-2.00838500	1.38742800	1.68564800	C	-3.06765500	0.77862100	2.81953000	Cl	0.79937700	-6.99292100	2.03268700
C	-0.71648600	0.58804800	1.71821500	H	-3.27258200	-0.25650400	2.51959600	Cl	-4.67146700	-6.47042600	1.79082600
C	-0.67120900	-0.61397100	0.98392300	H	-4.00296200	1.33546000	2.68434500	Cl	-2.08452100	-7.54956100	3.25715000
C	0.38650800	0.91183600	2.51381000					H	1.99432500	-4.10248200	-2.55162900
C	0.42988900	-1.47714300	1.05747500	4D				H	-3.87054900	-1.73443300	-2.76954200
H	-1.53296900	-0.91296600	0.39316000	-4315.063866				H	-1.35844600	4.37864800	-3.00318300
C	1.49615300	0.06211200	2.59560500	Rh	0.31550200	0.04363000	-4.32218700	H	4.45897800	1.86814900	-2.73740400
C	0.39531100	1.83784200	3.07421800	O	-0.04552600	2.08259400	-4.32898600	Cl	4.71567400	6.11465600	2.35984100
H	1.50659400	-1.12705600	1.87636300	O	0.69789900	-1.97693100	-4.15810900	N	5.03300500	0.06934800	-1.94771000
H	0.43595800	-2.40797900	0.50330400	O	-0.04868000	2.16054700	-2.05960200	C	0.05925300	4.86164300	-4.56780000
H	2.33653200	0.32713400	3.22827300	O	0.48946400	-1.92463500	-1.89727500	H	-0.53711000	4.41688900	-5.36745400
Br	2.99495400	-2.33001100	2.04636500	O	2.33521100	0.43123200	-4.19157600	H	-0.15443900	5.93395400	-4.52066600
C	-1.84381600	2.90167200	1.82628100	O	-1.70461600	-0.35631100	-4.29311400	H	1.11610000	4.71498500	-4.80252300
O	-0.79820300	3.51414000	1.92744500	C	2.29375500	0.40827800	-1.92148000	C	-4.40550700	-0.73460200	-4.61322400
O	-3.04694200	3.50439600	1.79520600	C	-2.30370300	-0.36907100	-3.18527600	H	-3.85804700	-1.43184000	-5.25091600
C	-3.03860100	4.94035200	1.95410800	C	2.87056100	0.50507300	-3.05402800	H	-5.45176500	-1.05202100	-4.56026300
H	-4.08794900	5.23348700	1.94872500	C	-0.10478800	2.67916000	-3.22332600	H	-4.35058500	0.25923900	-5.06476500
H	-2.56781200	5.20791400	2.90328300	O	0.68035400	-2.50604300	-3.01762200	C	0.84699500	-4.74135500	-4.27333800
H	-2.49765300	5.41205900	1.13327300	Rh	0.23710400	0.13822900	-1.85621700	H	1.52167000	-4.28525600	-5.00091900
H	-2.44344500	1.25997500	0.68442000	C	4.37678500	0.81347800	-3.02551100	H	1.12013100	-5.79394500	-4.14895900
C	-2.52152000	2.07744400	6.39953300	C	4.84192400	-1.28835700	-1.69429200	H	-0.17227500	-4.67606200	-4.66140100
H	-3.35467700	1.46294800	6.77542900	C	6.00303400	0.64753700	-1.11713700	C	5.06973400	0.58611700	-4.37154500
C	-1.20833200	1.42150300	6.85444700	O	4.08730500	-2.02054700	-2.30126900	H	4.59126100	1.19361500	-5.14224000
H	-1.13992500	1.40169600	7.94858900	C	5.75804400	-1.61725300	-0.54715400	H	6.12210800	0.87685500	-4.29528700
H	-1.11639400	0.38911000	6.50048400	O	6.37712000	1.79689800	-1.17309700	H	5.00449300	-0.46332400	-4.67184200
H	-0.34201000	1.98279300	6.47917100	C	6.45811900	-0.45604500	-0.20418300	C	0.21072500	0.33100400	0.16223100
C	-2.66172900	3.48084900	7.00828500	C	5.97466600	-2.80750900	0.12656600	C	0.81044600	-0.49649700	1.16168000
H	-1.85394000	4.14006000	6.66398300	C	7.39141200	-0.45659500	0.81884300	C	1.62809700	-1.60557600	0.80682500
H	-3.61423900	3.94576200	6.72666800	Cl	5.07099500	-4.26761400	-0.29657700	C	0.58713800	-0.25585700	2.54965000
H	-2.61588800	3.44532500	8.10316600	C	6.92070400	-2.82475900	1.16683700	C	2.16991700	-2.43875000	1.77503600
C	-2.64940300	2.14288100	4.86328300	C	7.62332000	-1.65936700	1.51005500	H	1.82411500	-1.80210800	-0.23810400
H	-3.56358100	2.69963800	4.61287700	C	8.26950100	1.01435600	1.24832600	C	1.12097700	-1.08395800	3.52101900
H	-1.81161400	2.73774600	4.47175500	Cl	7.22316500	-4.32695800	2.04665900	H	-0.02004300	0.58824700	0.58868200
C	-2.70238800	0.77293400	4.16778800	Cl	8.80719500	-1.69932900	2.82077000	C	1.90986300	-2.17443800	3.12525200
H	-1.74978900	0.24475600	4.29498300	C	-0.30070500	4.20521900	-3.23400700	H	2.77654100	-3.28982300	1.48672900
H	-3.45863400	0.15647100	4.67440800	N	0.42989800	4.78546600	-2.10637200	H	0.93699300	-0.89556800	4.57262100
C	-3.07008500	0.80109300	2.67399900	C	1.78856000	4.53203000	-1.86620800	Br	2.64806700	-3.31599100	4.46180900
H	-3.26050600	-0.22893900	2.34788500	C	-0.20532500	5.41473800	-1.03206100	C	-0.40349000	1.60197300	0.63281300
H	-4.00411800	1.35528400	2.53226700	C	2.53369900	3.94973500	-2.60919800	O	0.29702500	2.57109200	0.86570700
R-Pc				O	2.07799700	5.19322900	-0.53932800	O	-1.73588300	1.57252600	0.73438000
-747.869693				O	-1.39494600	5.63902700	-0.95685600	C	-2.36150800	2.82823300	1.09081500
C	-2.03561900	1.32622400	1.77549000	C	0.88163400	5.72003800	-0.04370000	H	-3.40876000	2.58372500	1.26243600
C	-0.74760800	0.52078200	1.73791300	C	3.25807900	5.29657600	0.17745000	H	-1.90995200	3.23793500	1.99710300
C	-0.65388500	-0.54068600	0.82668100	C	0.83752100	6.37000900	1.17701400	H	-2.25871200	3.54584300	0.27480700
C	0.33467300	0.74420300	2.60211400	Cl	4.75658900	4.59229900	-0.43357100	H	-3.04892100	-1.88211000	2.46552300
C	0.47135300	-1.36336800	0.77073900	C	3.22785200	5.95819000	1.41787000	C	-4.59227200	0.58325500	4.35043300
H	-1.47678200	-0.73226400	0.14114700	C	2.02863800	6.49228300	1.91266200	H	-5.19404700	0.79598000	3.45269300
C	1.47016400	-0.06688800	2.55885000	Cl	-0.68132200	7.02887000	1.80260300	C	-5.52070900	-0.08512900	5.37541100
H	0.30867200	1.57521000	3.29569800	Cl	2.01133600	7.32176400	3.47463200	H	-6.32108900	0.60102200	5.67772100
C	1.52883000	-1.11718600	1.64446500	C	-3.79853100	-0.73277400	-3.20853500	H	-5.99647500	-0.98453000	4.97164300
H	0.52469000	-2.17718700	0.05581400	N	-4.54094900	0.13826600	-2.29573900	H	-4.96923500	-0.37086300	6.28091200
H	2.30121600	0.12228400	3.22963000	C	-4.45729000	1.53153500	-2.30880100	C	-4.07301100	1.92278300	4.89593300
Br	3.09287200	-2.23874500	1.58264500	C	-5.43218600	-0.34758400	-1.33274400	H	-3.47657500	1.77015200	5.80521400
C	-1.84042100	2.83553700	1.90403500	O	-3.74870700	2.18624300	-3.04315300	H	-3.43612300	2.43667100	4.16519300
O	-0.84749800	3.42397200	2.27677300	C	-5.41449100	2.00151100	-1.24757100	H	-4.89920500	2.59650100	5.15201500
O	-2.97318800	3.47482700	1.53072300	O	-5.67888300	-1.51459900	-1.12713900	C	-3.41217100	-0.30750600	3.90568000
C	-2.93531300	4.90790000	1.62929000	C	-5.99593600	0.87365300	-0.65902400	H	-2.81823900	0.27517300	3.18732400
H	-3.91344100	5.24968500	1.28957800	C	-5.75510200	3.28003400	-0.83716500	H	-2.75312900	-0.48454700	4.77040600
H	-2.75710000	5.21747200	2.66264800	C	-6.92764800	0.99700500	0.35779900	C	-3.77950200	-1.66154600	3.25527300
H	-2.14336800	5.31510100	0.99536900	Cl	-5.01296500	4.70122600	-1.57792600	H	-4.74716200	-1.57213300	2.74259700
H	-2.53377600	1.19522000	0.80675500	C	-6.70306100	3.42035300	0.19269300	C	-3.81013100	-2.85371100	4.22163100
C	-2.55439300	2.11071900	6.52717200	C	-7.28293000	2.28840300	0.78630200	H	-4.08289200	-3.77811800	3.69964200
H	-3.36687000	1.46962800	6.90426500	Cl	-7.65529500	-0.43211800	1.10302900	H	-2.82514200	-3.00836200	4.68027400
C	-1.22092100	1.50479700	6.99275800	Cl	-7.16424600	5.03535600	0.74159700	H	-4.52924700	-2.70954600	5.03422700
H	-1.15768400	1.49299500	8.08746500	C	-8.46797500	2.48435800	2.08296900	O	-1.80292300	-0.16818600	-2.03050900
H	-1.09123800	0.47461000	6.64405500	C	0.96999300	-4.01464500	-2.93282200				
C	-0.37341000	2.09449000	6.61825600	N	0.12816700	-4.61649500	-1.89759300	TSD ₄₋₅			
C	-2.74723000	3.51260700	7.12467400	C	-1.26432300	-4.49203700	-1.86385600	-4315.027328			
H	-1.96189000	4.19718200	6.77827300	C	0.64167200	-5.26732400	-0.77171900	Rh	0.37740800	-0.93916300	-3.88774900
				O	-1.93396300	-3.91383700	-2.69314400	O	0.08577400	1.09343100	-4.09234700

O	0.76606300	-2.93242200	-3.54941500	N	5.06855600	-0.95872700	-1.51738400	O	6.31315300	1.16213100	-0.49985500
O	0.06629100	1.36751000	-1.83896800	C	0.46911900	3.80077900	-4.58181100	C	6.61333200	-1.25922900	-0.22161100
O	0.35828100	-2.75277100	-1.32505400	H	-0.12870000	3.32478100	-5.36182900	C	6.28863500	-3.64215500	-0.53044400
O	2.38323400	-0.56261000	-3.71394200	H	0.34590400	4.88599700	-4.65297600	C	7.61700400	-1.46980100	0.70837600
O	-1.67225100	-1.26210000	-3.91299300	H	1.51865600	3.54578200	-4.74631500	Cl	5.44529800	-4.99509700	-1.29152100
O	2.27372300	-0.51034900	-1.44671300	C	-4.39652300	-1.31440900	-4.35924700	C	7.30800100	-3.87156200	0.41124100
C	-2.32323000	-1.06609500	-2.85321200	H	-3.94181700	-2.17411900	-4.85642700	C	7.96713900	-2.79483300	1.02419600
C	2.88470100	-0.44556300	-2.55917400	H	-5.48202800	-1.45399500	-4.33487300	Cl	8.44031000	-0.11034700	1.48079900
C	0.06665000	1.78789500	-3.03957800	H	-4.15843100	-0.41943000	-4.93758100	Cl	7.76093600	-5.52956500	0.82203400
C	0.73696800	-3.37827500	-2.37150200	C	1.55752600	-5.56145300	-3.45614200	Cl	9.24795300	-3.10251800	2.20256600
Rh	0.19540000	-0.65817100	-1.45928600	H	2.23835000	-4.99165200	-4.09122200	C	-0.44416200	3.72740700	-2.66011400
C	4.38564600	-0.11488800	-2.50276500	H	2.01829600	-6.52791400	-3.22704900	N	0.29307400	4.32819300	-1.54925900
C	4.94775800	-2.34572500	-1.44791800	H	0.62637100	-5.72440600	-4.00271000	C	1.63603100	4.06710500	-1.26715600
C	6.05395300	-0.45587400	-0.65610800	C	5.07794700	-0.18017800	-3.86632600	C	-0.27938400	5.24921000	-0.66721100
O	4.18394800	-3.01799900	-2.11111700	H	4.58695200	0.50202000	-4.56344200	O	2.35959900	3.34777900	-1.92384600
O	5.95053600	-2.78978800	-0.41870100	H	6.12522000	0.12019500	-3.75953800	C	1.95174700	4.87340700	-0.04119900
C	6.38114200	0.70602800	-0.56862600	H	5.03007400	-1.18973000	-4.28323500	O	-1.41893500	5.65765900	-0.73594800
C	6.60570300	-1.65246700	0.06507000	C	0.11906300	-0.25739900	0.78834000	C	0.80941300	5.60324700	0.30415200
C	6.28923600	-4.05415100	0.03349700	C	1.30736500	-0.73093400	1.53135600	C	3.11946600	4.97272100	0.69709400
C	7.60102800	-1.74962100	1.02228400	C	1.65346000	-2.09968300	1.46437600	C	0.81506900	6.46837400	1.38404400
Cl	5.48547200	-5.49516500	-0.59962300	C	2.11155400	0.10236500	2.33804700	Cl	4.54562500	4.01861700	0.27757800
C	7.29961200	-4.16894000	1.00476900	C	2.71287100	-2.62877400	2.19452800	C	3.13450100	5.84079800	1.80313200
C	7.94696900	-3.02647500	1.49774100	H	1.09756700	-2.75422700	0.80305700	C	1.99407100	6.58589300	2.14032000
Cl	8.42048200	-0.30764600	1.63114500	C	3.18503200	-0.41126300	3.06286200	Cl	-0.61973600	7.41388200	1.80220800
Cl	7.75769400	-5.76722600	1.60460100	H	1.89943600	1.16224600	2.38798800	Cl	2.03696200	7.67988400	3.52872100
C	9.20869600	-3.19014100	2.72448600	C	3.46839000	-1.77599300	3.00215400	C	-3.77699800	-1.29948400	-3.01149600
C	-0.00076600	3.31724600	-3.20770300	H	2.94337500	-3.68643600	2.12377200	N	-4.60428300	-0.36993100	-2.23534600
N	0.72732300	3.95936600	-2.11282800	H	3.78831300	0.24637700	3.67946700	C	-4.46991600	1.02056700	-2.26373500
C	2.05491700	3.66744200	-1.78462500	Br	4.91377500	-2.49083800	4.04967100	C	-5.71594500	-0.79418400	-1.49619700
C	0.11623600	4.80249000	-1.18251300	C	-0.30407700	1.16164300	0.92212500	O	-3.60755100	1.63119600	-2.85871900
O	2.78061000	2.92599400	-2.41292200	O	0.44405100	2.11924600	1.53518700	C	-5.59634100	1.55091500	-1.42166600
C	2.34731700	4.46051800	-0.54380200	O	-1.65179100	1.30589400	0.83965400	O	-6.06479300	-1.94491700	-1.35475700
O	-1.04671900	5.14790500	-1.21004400	C	-2.14351000	2.65471700	0.92089600	C	-6.34394800	0.46230400	-0.96055600
C	1.18557800	5.15294300	-0.19042700	H	-3.21318900	2.56264700	1.11515700	C	-5.94440900	2.84998100	-1.09210300
C	3.50285300	4.56584900	0.21160400	H	-1.65422500	3.19755800	1.73263700	C	-7.45616100	0.64636900	-0.15644100
C	1.15224100	5.97344500	0.92303200	H	-1.97367300	3.18391500	-0.01801600	Cl	-5.00190100	4.22291900	-1.68349200
Cl	4.95263700	3.65539900	-0.21363100	H	-1.72702000	-2.72122400	0.10500400	C	-7.07009500	3.05150500	-0.27404000
C	3.48337300	5.39989200	1.34396000	C	-2.43250300	-0.79138000	2.88615800	C	-7.82001900	1.95989900	-0.18999800
C	2.31930900	6.09935500	1.69562800	H	-2.83928900	-0.00949000	2.23357900	Cl	-8.39497300	-0.73299700	0.42544200
Cl	-0.32427600	6.84177600	1.37003000	C	-3.65578500	-1.49092000	3.54440900	Cl	-7.54191300	4.69601800	0.17319700
Cl	2.31548000	7.14403800	3.12304700	H	-4.18000800	-0.75464700	2.16277200	Cl	-9.23177500	2.23387000	1.21590800
C	-3.85670500	-1.20606900	-2.93257500	H	-4.36354100	-1.86801400	2.80187100	C	0.98454600	-4.46662800	-2.82840000
N	-4.48752500	-0.11523000	-2.18328300	H	-3.34635900	-2.31549400	4.19591700	N	0.12771200	-5.10450000	-1.82773400
C	-4.30890900	1.24104800	-2.48137700	C	-1.54520200	-0.14716500	3.96053400	C	-1.24257700	-4.86732700	-1.71350900
C	-5.21667100	-0.31631900	-1.01036300	H	-1.16040900	-0.90309400	4.65603800	C	0.62148200	-5.94925200	-0.82399300
O	-3.62676700	1.67848900	-3.38157600	H	-0.68669500	0.37384300	3.52893200	O	-1.89700300	-4.16848500	-2.46006100
C	-5.11278100	1.98745800	-1.45319300	H	-2.12125000	0.57869700	4.54417300	C	-1.68831500	-5.64649300	-0.50900000
O	-5.43189800	-1.39098100	-0.48852100	C	-1.68240200	-1.74545400	2.00338100	O	1.77655400	-6.28721500	-0.70091800
C	-5.64696700	1.05180200	-0.56162800	H	-0.80521900	-0.95749800	0.91470100	C	-0.57278300	-6.30907200	0.01526600
C	-5.35434300	3.34287400	-1.30210600	H	-0.78319300	-2.18941000	2.43602100	C	-2.93669400	-5.76835000	0.07902200
C	-6.42527400	1.45082500	0.51176100	C	-2.37543300	-2.59435800	0.97923000	C	-0.68060900	-7.11976200	1.13268700
Cl	-4.68205400	4.51726000	-2.43372600	H	-3.29697700	-2.11854500	0.63410000	Cl	-4.33540200	-4.89843800	-0.56105700
C	-6.15233200	3.76164600	-0.22128900	C	-2.67868400	-4.00576400	1.54320400	C	-3.06070100	-6.58937000	1.21435900
Cl	-6.68009900	2.82355600	0.68024600	C	-3.14828100	-4.60344500	0.75555900	C	-1.94374700	-7.26121200	1.73483100
Cl	-7.08570400	0.26491800	1.64701700	H	-1.76038000	-4.51159000	1.86073400	Cl	0.73071200	-7.95463300	1.73844200
Cl	-6.49024900	5.48010000	-0.00006000	H	-3.36266500	-3.97536900	2.39456600	Cl	-4.63726500	-6.77236200	1.99074400
Cl	-7.67346700	3.36754700	2.03637000	O	-1.86236500	-0.79847500	-1.69640500	Cl	-2.12019300	-8.28936200	3.16063000
C	1.31593300	-4.78783800	-2.15813100					H	2.00864800	-4.62159000	-2.46899500
N	0.51711100	-5.55781700	-1.20003700	SD				H	-3.87065200	-2.26564900	-2.50512400
C	-0.79407800	-5.98189300	-1.43509000	-4315.114472				H	-1.50255900	3.86499400	-2.41039400
C	1.01307500	-5.99246900	0.03353500	Rh	0.33565800	-0.33000700	-3.91434700	H	4.34229500	1.51583800	-1.96552800
O	-1.47049100	-5.68299800	-2.39460500	O	-0.09852400	1.66874100	-3.81763300	Cl	4.60495100	5.99382400	-2.77208400
C	-1.15578300	-6.84561900	-0.25659600	O	0.76863100	-2.34037000	-3.90671600	N	5.04625400	-0.38591200	-1.67712700
O	2.09804800	-5.71389400	0.49562000	O	-0.15725000	1.62574700	-1.55130200	C	-0.13470800	4.41326100	-3.99335100
C	-0.07300300	-6.84597700	0.62816200	O	0.56738400	-2.43157500	-1.65159600	H	-0.73819900	3.97037500	-4.78851100
C	-2.31065800	-7.55514500	0.02538700	O	2.31430800	0.14656200	-3.74748300	H	-0.37393900	5.47863700	-3.91987700
C	-0.11967600	-7.55492200	1.81741700	O	-1.65556600	-0.80745300	-3.98428000	H	0.92027500	4.29716300	-4.25504300
Cl	-3.68110200	-7.53947200	-1.09117500	O	2.23848500	-0.03469600	-1.48893800	C	-4.27136200	-1.41862200	-4.45458500
C	-2.37091700	-8.28595700	1.22533500	C	-2.29516100	-0.90820600	-2.89792400	H	-3.67411500	-2.15956800	-4.99078200
C	-1.28482800	-8.28486500	2.11453800	C	2.83243500	0.17562400	-2.59138100	H	-5.31655700	-1.74336100	-4.45614500
Cl	1.24885500	-7.54833200	2.93530600	C	-0.20053000	2.21039100	-2.67758500	H	-4.18574100	-0.46350500	-4.97935500
Cl	-3.82632600	-9.20876300	1.61442300	C	0.74408800	-2.94900000	-2.79893600	O	0.81939700	-5.08989200	-4.21599600
Cl	-1.37869300	-9.20623600	3.1915400	Rh	0.20964900	-0.40364300	-1.51986800	H	1.50271800	-4.60994000	-4.91987900
H	2.27428100	-4.61874100	-1.65377800	C	4.31477100	0.56820200	-2.51320000	H	1.05383800	-6.15777000	-4.16876000
H	-4.11424700	-2.10794100	-2.36638800	C	4.94379100	-1.77352200	-1.79199200	H	-0.20202000	-4.96059400	-4.58264900
H	-1.04854400	3.60091200	-3.05435300	C	6.02484900	0.01506300	-0.75865700	C	4.97694600	0.73749600	-3.88278200
H	4.44839300	0.90299300	-2.10400800	O	4.18428100	-2.36082200	-2.53385800	H	4.44477400	1.49514800	-4.46255400
Cl	4.94083500	5.56422000	2.33129000	C	5.95887400	-2.33245700	-0.83556500	H	6.01326700	1.06301800	-3.74843500

H	4.96071300	-0.19976700	-4.44504700	H	-4.90909600	-0.07459000	3.64052200	Cl	-4.57030800	-4.55942000	-0.69961100
C	-1.90867500	1.20657100	1.98101100	C	-4.64557000	-0.32071500	1.53567300	C	-3.19882900	-5.92670300	1.26952400
C	-0.50175500	0.62101200	1.91298300	H	-5.72763700	-0.45475200	1.42401400	C	-2.03994500	-6.43472500	1.87647200
C	-0.36071900	-0.64165000	1.29912700	H	-4.29896300	0.22530400	0.65252600	Cl	0.68381200	-6.87272200	2.04663200
C	0.63757200	1.19168900	2.48924600	H	-4.18955700	-1.31917000	1.52075400	Cl	-4.77290700	-6.17980400	2.03023200
C	0.85485400	-1.33760000	1.31474000					Cl	-2.16109100	-7.32817700	3.39638200
H	-1.23198800	-1.12836000	0.86971800	4E				H	1.77448100	-4.05283400	-2.60420400
C	1.86014100	0.51134300	2.50967300	-4315.068960				H	-4.01274500	-1.51683100	-2.55330300
H	0.58523200	2.17696500	2.93035400	Rh	0.15831400	0.18324200	-4.22665000	H	-1.37836800	4.51610300	-2.75159000
C	1.95580000	-0.75413200	1.94259800	O	-0.15940400	2.22830900	-4.17851600	H	4.40252500	1.87552300	-2.76788500
H	0.93101900	-2.31598600	0.85594900	O	0.49522800	-1.85075600	-4.11543000	Cl	4.95575500	6.04768700	2.36944000
H	2.72499500	0.96682200	2.98023700	O	-0.06457500	2.26195700	-1.91024900	N	4.96173300	0.04755500	-2.03738700
Br	3.60538600	-1.73102700	2.06321600	O	0.36895500	-1.83713400	-1.84813800	C	-0.02233900	5.01120900	-4.36677300
C	-1.97987800	2.73078900	1.91305200	O	2.19141700	0.52053400	-4.16886500	H	-0.66050200	4.59287700	-5.14823700
O	-1.04307100	3.50607500	1.91116900	O	-1.86675900	-0.16849800	-4.12381900	H	-0.21586900	6.08553100	-4.28849000
O	-3.26136200	3.14064900	1.82729700	O	-1.87874900	-0.01541400	-1.85629400	H	1.02060200	4.85281000	-4.65081600
C	-3.46524000	4.57172400	1.81381300	O	2.23453300	0.44868100	-1.89946900	C	-4.58513800	-0.46299100	-4.35500500
H	-4.54537100	4.70561900	1.75820300	C	-2.42600500	-0.18320800	-2.99501900	H	-4.07746800	-1.15808200	-5.02694900
H	-3.06930900	5.01399700	2.73151900	C	2.77044900	0.55686600	-3.05126400	H	-5.63642700	-0.75653100	-4.27221500
H	-2.97211200	5.02255800	0.95218100	C	-0.16207100	2.80401800	-3.06029700	H	-4.52159900	0.53952800	-4.78593900
H	-4.60981300	1.00600500	2.08578400	C	0.50030100	-2.40183300	-2.98556300	C	0.52913500	-4.61962000	-4.28288600
C	-2.89136400	1.39282100	4.47317500	Rh	0.17693300	0.23015900	-1.75681300	H	1.18763300	-4.17592400	-5.03262400
C	-3.54274200	2.25453500	4.27145300	C	4.28368000	0.82943700	-3.07381100	H	0.76787500	-5.68349500	-4.18728000
H	-3.54013500	0.56390200	5.60052300	C	4.75424200	-1.31273700	-1.81209100	H	-0.50315600	-4.51021400	-4.62340400
H	-3.57884300	1.15297600	6.52384800	C	5.96763400	0.58775900	-1.22414100	C	4.91958400	0.61471600	-4.44985600
H	-4.56318300	0.24924500	3.57686300	O	3.96596700	-2.01539400	-2.41100100	H	4.42762300	1.25015100	-5.18886500
H	-2.94964500	-0.33773100	5.81055000	C	5.70225900	-1.68720800	-0.70560500	H	5.98097200	0.87836500	-4.40772700
C	-1.54442900	1.92364000	4.99675500	O	6.35899300	1.73205800	-1.26196200	H	4.81695400	-0.42607800	-4.76899400
H	-0.83342000	1.10467400	5.16115400	C	6.43295500	-0.54710800	-0.35571900	C	0.25207000	0.38988800	0.26391800
H	-1.08002700	2.64542500	4.32237700	C	5.92019000	-2.89836900	-0.07070700	C	0.90579800	-0.45261500	1.21582800
H	-1.69169000	2.42973100	5.95797300	C	7.39860400	-0.59014300	0.63588400	C	1.66338300	-1.58292900	0.79986700
C	-2.77641200	0.56353700	3.15701900	Cl	4.98000400	-4.33235300	-0.50360300	C	0.79794700	-0.20827800	2.61693500
H	-2.40581200	0.88934300	1.05691100	C	6.89799200	-2.95847300	0.93811200	C	2.25394900	-2.43351100	1.72335300
H	-2.24562100	-0.36076200	3.42533600	C	7.63125800	-1.81422500	1.28831200	H	1.77234800	-1.78302400	-0.25683200
C	-4.16573600	0.14984900	2.60820100	Cl	8.31614400	0.85403500	1.07375400	C	1.38450300	-1.05078200	3.54435800
H	-4.83418100	-0.07405400	3.44426600	Cl	7.20138300	-4.48774900	1.76955500	H	0.24263000	0.65313900	2.97168000
C	-4.14301500	-1.08095200	1.69164100	Cl	8.85532000	-1.90790400	2.55879900	C	2.10800800	-2.16332200	3.08940000
H	-5.15746700	-1.36916200	1.39622300	C	-0.33444800	4.33265600	-3.03210200	H	2.81017800	-3.30192300	1.38885600
H	-3.57031700	-0.91790800	0.77067800	N	0.45358100	4.87811300	-1.92590800	H	1.29006100	-0.85760400	4.60686400
H	-3.69932400	-1.94279500	2.20553700	C	1.81810900	4.62169700	-1.75257100	Br	2.91518300	-3.32697200	4.36565000
O	-1.82675000	-0.77077900	-1.72333600	C	-0.12411200	5.48764700	-0.80840800	C	-0.32236100	1.65910900	0.78779200
				O	2.52027500	4.02501100	-2.54147900	O	0.39530600	2.62050700	0.99900200
R-Pb				C	2.17637400	5.22654500	-0.42594700	O	-1.64710100	1.63500800	0.96496900
-747.861097				O	-1.30598000	5.72404300	-0.67285500	C	-2.24247800	2.88083500	1.40060500
C	-1.95926800	1.07097500	2.13315800	C	1.01099300	5.75621600	0.13583100	H	-3.28423900	2.63851300	1.60609900
C	-0.49174500	0.63080800	2.12341500	C	3.38914000	5.29818900	0.23821300	H	-1.74828100	3.24528400	2.30399300
C	-0.22466900	-0.73024700	1.90613700	C	1.03150400	6.37823700	1.37153200	H	-2.16528100	3.63277200	0.61324900
O	0.60120800	1.49973600	2.23716500	Cl	4.84831000	4.58877700	-0.45625500	H	-2.93803600	-0.82314400	1.62495900
C	1.07770500	-1.22064100	1.82782500	C	3.42460900	5.93155000	1.49316500	C	-4.08837200	-0.89478700	3.48396600
H	-1.04957700	-1.42845400	1.78529300	C	2.25650800	6.46917900	2.05413700	H	-4.78541200	-0.10644000	3.15866300
C	1.91367900	1.02764300	2.15619100	Cl	-0.44824900	7.04063600	2.08131200	C	-2.97650400	-0.22689300	4.30877300
H	0.43496200	2.55754200	2.40304500	C	2.32135500	7.26303400	3.63327200	H	-2.41814800	0.49066500	3.69475200
C	2.14370900	-0.33099400	1.95640800	C	-3.92994900	-0.50762600	-2.97273800	H	-3.36965700	0.31308000	5.17690600
H	1.25868900	-2.27687600	1.66024500	N	-4.61894200	0.36159700	-2.01692100	H	-2.26227000	-0.97627400	4.67660300
H	2.74606900	1.71683400	2.55012400	C	-4.48767400	1.75148800	-1.99143000	C	-3.50270900	-1.54860000	2.22700000
Br	3.94963700	-0.98919500	1.84735500	C	-5.51602400	-0.12043100	-1.05820900	H	-2.81633700	-2.36331200	2.49250600
C	-2.16356700	2.57693300	2.05082500	O	-3.77439900	2.40358200	-2.72347600	H	-4.29018600	-1.96858400	1.58711200
O	-1.65899700	3.41980600	2.76588700	C	-5.40642500	2.22174400	-0.89705000	C	-4.89833000	-1.91922400	4.30293400
O	-3.03993000	2.88789500	1.06747300	O	-5.80216500	-1.28417900	-0.88424700	H	-5.58852600	-2.43889600	3.62284900
C	-3.34351000	4.28689900	0.92886200	C	-6.02542600	1.09841100	-0.33881500	H	-4.21268100	-2.69154600	4.68612600
H	-4.06350600	4.34941200	0.11262700	C	-5.68840100	3.49787200	-0.43776400	C	-5.71009800	-1.33704100	5.46874900
H	-3.77273700	4.68060700	1.85389400	C	-6.94250200	1.22429600	0.69102600	H	-5.04012600	-0.85176200	6.19072600
H	-2.43904000	4.85194500	0.68901400	Cl	-4.89338900	4.91180500	-1.13581300	H	-6.37311000	-0.54751900	5.08662700
H	-4.72449900	1.44252500	2.78625200	C	-6.61782100	3.64051800	0.60861000	C	-6.54687300	-2.39566600	6.19602400
C	-2.68553900	1.09069500	4.69435200	C	-7.23926600	2.51341600	1.16832900	H	-5.91020100	-3.18532400	6.61426700
H	-3.03853200	2.12950800	4.63192900	Cl	-7.72678500	-0.19778400	1.39027500	H	-7.11841800	-1.95653100	7.02184400
C	-3.54522600	0.36738500	5.75177100	Cl	-7.00319600	5.25261400	1.22091000	H	-7.26012600	-2.87429400	5.51370700
H	-3.33097600	0.77420600	6.74644200	Cl	-8.40258000	2.71213100	2.48380300				
H	-4.62050600	0.47751600	5.58471900	C	0.73836700	-3.92124300	-2.93804900	TSE _{4,5}			
H	-3.31550900	-0.70641800	5.78102300	N	-0.07868500	-4.50846100	-1.87496000	-4315.027208			
C	-1.23008900	1.12929800	5.19075400	C	-1.46399600	-4.33992600	-1.78325500	Rh	0.44913700	-0.54163700	-3.82762900
H	-0.77752200	0.12960500	5.18541500	C	0.46180400	-5.16341600	-0.76400600	O	0.17781300	1.50776500	-3.84680300
H	-0.60892200	1.78992700	4.58626100	O	-2.14926600	-3.74227000	-2.58566800	O	0.75998500	-2.56925600	-3.67234000
H	-1.20002700	1.50069100	6.22200400	C	-1.87083200	-5.03485000	-0.51479400	O	0.16779600	1.58730800	-1.57851300
C	-2.84928000	0.44739500	3.28313500	O	1.64206600	-5.35952600	-0.56905000	O	0.55975700	-2.52775600	-1.41327400
H	-2.37655500	0.67210400	1.20577700	C	-0.71494600	-5.53717400	0.09238900	O	2.46680300	-0.21439600	-3.69876900
H	-2.51498000	-0.59747500	3.36667600	C	-3.11887700	-5.21611000	0.05800000	O	-1.59021000	-0.90198100	-3.79707700
C	-4.33778400	0.41570800	2.84741100	C	-0.77957000	-6.23758300	1.28501200	O	-1.68650900	-0.70675600	-1.53717700

O	2.42877000	-0.23999600	-1.42807000	C	-4.28994400	-1.39252600	-4.09677500	C	7.00279400	-3.83380500	0.57015700
C	-2.19017700	-0.91450300	-2.69000100	H	-3.75198300	-2.16137500	-4.65604100	C	7.64714700	-2.77271100	1.22473700
C	3.00755500	-0.16016900	-2.55626100	H	-5.34248800	-1.68400500	-4.02168900	Cl	8.16279600	-0.10008500	1.70398900
C	0.16730800	2.10996200	-2.73837100	H	-4.21161200	-0.45146300	-4.64512100	Cl	7.37411500	-5.50159000	1.02194300
C	0.72987800	-3.10880200	-2.53331500	C	0.77681700	-5.32269400	-3.83398400	Cl	8.82856200	-3.10939600	2.49547200
Rh	0.36557700	-0.45181300	-1.39267200	H	1.42650300	-4.86989800	-4.58551400	C	-0.50206800	3.83954700	-2.56790100
C	4.52252400	0.09826700	-2.53767200	H	1.02915400	-6.38367100	-3.74129200	N	0.26016800	4.38786400	-1.44572800
C	4.93979800	-2.15447600	-1.45476100	H	-0.25873200	-5.22568400	-4.17056500	C	1.60638500	4.11078700	-1.19676200
C	6.25342500	-0.35239600	-0.77897300	C	5.17680300	0.00367500	-3.91838500	C	-0.28112900	5.30899200	-0.54389700
O	4.10682900	-2.77862400	-2.07910000	H	4.70444100	0.71110900	-4.60317100	O	2.30991900	3.39671300	-1.80485500
C	5.93110900	-2.65312100	-0.43946200	H	6.23997600	0.25041000	-3.83596300	C	1.95698700	4.89760500	0.03248100
O	6.68349300	0.77868000	-0.74154100	H	5.06826500	-1.00154500	-4.33476200	O	-1.41526900	5.73550100	-0.58623400
C	6.73073900	-1.57464200	-0.04743100	C	0.25851000	-0.29183200	0.94808800	C	0.83263700	5.64026900	0.40709400
C	6.13957000	-3.92134000	0.07561000	C	1.43724400	-0.81458200	1.66753700	C	3.14104500	4.97475100	0.74715200
C	7.76395200	-1.74055000	0.85923900	C	1.89368300	-2.12510400	1.40944900	C	0.87407300	6.49694100	1.49271800
Cl	5.09251400	-5.27074700	-0.38210000	C	2.13231200	-0.05999500	2.63525300	Cl	4.54347100	4.00277000	0.29350300
C	7.19000200	-4.10670600	0.99135900	C	2.95336800	-2.68159500	2.11942100	C	3.19166100	5.83380900	1.85918400
C	7.99662900	-3.02612300	1.37819400	H	1.42207900	-2.70889900	0.62692500	C	2.06971400	6.59272800	2.22523300
Cl	8.76996900	-0.37359000	1.35068000	C	3.20912300	-0.59919300	3.33562500	Cl	-0.53752300	7.46299700	1.94715400
Cl	7.49110100	-5.71430400	1.66059500	H	1.83375600	0.96133900	2.83178400	Cl	2.15703500	7.67668800	3.61966700
Cl	9.31065900	-3.27765500	2.53298600	C	3.60151500	-1.91431700	3.08952400	C	-3.74711600	-1.17306300	-3.32312100
C	0.11671200	3.64892600	-2.76517300	H	3.27283100	-3.69725900	1.91164900	N	-4.53934600	-0.43219300	-2.33935800
N	0.87500300	4.16859100	-1.62685700	H	3.72787400	-0.00205500	4.07771100	C	-4.46640000	0.95152600	-2.16875100
C	2.20546000	3.82664600	-1.36733000	Br	5.04868900	-2.67685300	4.09819200	C	-5.45254300	-1.04245400	-1.47014200
C	0.27892200	4.86121300	-0.56928200	C	-0.25869200	1.07166800	1.22011000	O	-3.73894700	1.69672600	-2.79091500
O	2.91169000	3.16665600	-2.09655300	O	0.45135700	2.03292900	1.46816900	C	-5.44819700	1.27536400	-1.07844300
C	2.52399400	4.44178200	-0.03198200	O	-1.60101100	1.16748800	1.09408900	O	-5.69618600	-2.22721300	-1.42678900
O	-0.88646300	5.19484200	-0.52258800	C	-2.14888200	2.49007300	1.25178000	C	-6.03555700	0.07843500	-0.65424300
C	1.36870600	5.07246400	0.43960400	H	-3.22436800	2.34477100	1.35920100	C	-5.80261900	2.48840400	-0.51250200
C	3.69507400	4.44376800	0.70699200	H	-1.73701400	2.97552800	2.13908500	C	-6.98657700	0.06508400	0.35217400
C	1.35745100	5.72625900	1.65886800	H	-1.93220400	3.10172800	0.37469700	Cl	-5.07104200	3.99775100	-1.06806500
Cl	5.13929200	3.61301700	0.12502700	H	-0.59104000	-1.03607900	0.68693500	C	-6.76616500	2.48965400	0.51144100
C	3.69786900	5.10818300	1.94644000	C	-2.14089100	-1.28383700	2.84260400	C	-7.35229100	1.28910800	0.94137700
C	2.54012700	5.74547100	2.41762900	H	-2.66806200	-0.36383000	2.57024200	Cl	-7.72368800	-1.44872300	0.88555800
Cl	-0.11018700	6.51549200	2.25449000	C	-1.23285100	-1.02150700	4.04959900	Cl	-7.24493600	4.01859500	1.25897000
Cl	2.56423800	6.57545300	3.97924400	H	-0.47961700	-0.26127400	3.82678800	Cl	-8.56140700	1.31130800	2.22888100
C	-3.68879700	-1.26576200	-2.69651200	H	-1.81451500	-0.66862100	4.90580200	C	1.14983300	-4.28319100	-3.32851700
N	-4.41977000	-0.30078400	-1.86912600	H	-0.70409500	-1.93351800	4.35714400	N	0.33990000	-5.04811100	-2.38032000
C	-4.40731200	1.07936700	-2.09975800	C	-1.40741300	-1.78741200	1.63465000	C	-1.03737200	-4.88577800	-2.22073900
C	-5.12134400	-0.64969100	-0.71296700	H	-0.67241500	-2.57164400	1.81064600	C	0.87987100	-6.01487700	-1.52119300
O	-3.79986800	1.63653600	-2.98698000	H	-2.02954100	-1.95640500	0.75198300	O	-1.73381600	-4.13282400	-2.86968900
C	-5.27532200	1.67466800	-1.02692300	C	-3.23176600	-2.36810200	3.13107500	C	-1.42761100	-5.82733000	-1.11679300
O	-5.21027500	-1.76722600	-0.25031300	H	-3.82528100	-2.52211400	2.22089300	O	2.04397200	-6.34293300	-1.48185700
C	-5.70842000	0.63605900	-0.19636500	H	-2.74077100	-3.32569800	3.35746300	C	-0.28098500	-6.51878400	-0.71040600
C	-5.65696300	2.98608300	-0.79733400	C	-4.18827400	-2.00796800	4.28018100	C	-2.65614800	-6.06328400	-0.52208200
C	-6.53862100	0.88635800	0.88320000	H	-3.63223500	-1.91931000	5.22107700	C	-0.33745000	-7.47391600	0.29062100
Cl	-5.10435700	4.29055800	-1.85043500	H	-4.63464900	-1.02383400	4.08391000	Cl	-4.08904400	-5.15222800	-1.00619300
Cl	-6.49821500	3.25441500	0.29788100	C	-5.29944800	-3.05094000	4.44487900	C	-2.72785300	-7.03092200	0.49626000
C	-6.93552800	2.21264900	1.13101700	H	-4.88468300	-4.04497500	4.65167300	C	-1.58008400	-7.73223400	0.89674700
Cl	-7.10224100	-0.42941600	1.92284800	H	-5.96486600	-2.78766000	5.27472300	Cl	1.11259700	-8.34611500	0.79686500
Cl	-7.00822000	4.91343600	0.62170800	H	-5.90746500	-3.12783700	3.53621000	Cl	-4.27814800	-7.36140700	1.27664400
Cl	-7.99433500	2.56703500	2.50049200					Cl	-1.69136900	-8.94523200	2.17649000
C	0.98188200	-4.62480900	-2.48727400	5E				H	2.18483400	-4.40587500	-2.98810400
N	0.17577000	-5.23526800	-1.42743400	-4315.124083				H	-3.81322100	-2.22248100	-3.01447200
C	-1.19895100	-5.04328300	-1.28082100	Rh	0.37515400	-0.10320000	-4.10325200	H	-1.55408100	3.93869500	-2.27655300
C	0.71503100	-6.08359900	-0.45244500	O	-0.08915900	1.87903800	-3.86607700	H	4.35800900	1.61927800	-2.01200900
O	-1.89410200	-4.35529100	-1.99892100	O	0.84162700	-2.09733900	-4.24249400	Cl	4.68382500	5.95878500	2.79833400
C	-1.59252200	-5.85290800	-0.07553100	O	-0.20780800	1.66357000	-1.61247800	N	5.00029900	-0.29836200	-1.69019400
O	1.87954300	-6.40251800	-0.36555700	O	0.62361400	-2.36273600	-2.00294300	C	-0.25026800	4.61679100	-3.86245400
C	-0.44452800	-6.48265300	0.41720700	O	2.34868200	0.36507900	-3.85725000	H	-0.87024600	4.21425100	-4.66651700
C	-2.82321900	-6.02905800	0.53539700	O	-1.61804100	-0.59368000	-4.24922200	H	-0.50874300	5.66936000	-3.71106700
C	-0.49850200	-7.30539400	1.52998000	O	-1.80950900	-0.73957300	-4.9499500	H	0.79765900	4.54140700	-1.64646600
Cl	-4.26765600	-5.21875600	-0.07810400	O	2.22513400	0.03964800	-1.61612800	C	-4.29638200	-1.00712200	-4.74138300
C	-2.89309400	-6.86064700	1.66774000	C	-2.26631600	-0.78738500	-3.18107200	H	-3.70932400	-1.60917700	-5.43849000
C	-1.74185500	-7.49472500	2.15988700	C	2.84336700	0.31213100	-2.69121100	H	-5.33647400	-1.34626200	-4.77355100
Cl	0.95483700	-8.09625800	2.14711000	C	-0.22976600	2.33208200	-2.69207700	H	-4.24559300	0.03660800	-5.06156800
Cl	-4.44548700	-7.10502600	2.47633400	C	0.83223100	-2.78747900	-3.18191400	C	1.00780900	-4.80490900	-4.76050700
Cl	-1.85024200	-8.53615600	3.58249600	Rh	0.20857200	-0.35617500	-1.72710300	H	1.65861200	-4.23674100	-5.42849500
H	2.02182900	-4.74394400	-2.16084800	C	4.32988600	0.67067300	-2.55872800	H	1.29944200	-5.85906600	-4.79623800
H	-3.77425200	-2.21856500	-2.16281600	C	4.87169700	-1.68340800	-1.81182300	H	-0.02219600	-4.70351400	-5.11233300
H	-0.92233900	3.93195800	-2.56018500	C	5.92382100	0.07957300	-0.70743800	C	5.04906400	0.81987200	-3.90160800
H	4.64678200	1.10988700	-2.13625300	O	4.15786000	-2.25174900	-0.61200300	H	4.55702400	1.58663300	-4.50418500
Cl	5.17496600	5.13695800	2.91755000	C	5.79507300	-2.26523700	-0.77957100	H	6.08652100	1.12199500	-3.72770300
N	5.18248900	-0.78534200	-1.57251600	O	6.22717100	1.21938800	-0.43366800	H	5.03402500	-0.11934600	-4.46075400
C	0.56556500	4.25498200	-4.09642100	C	6.43384600	-1.20745800	-0.12398900	C	-1.99795500	1.14968500	1.56776700
H	-0.05743200	3.86586600	-4.90468600	C	6.06200700	-3.58224000	-0.44483800	C	-0.66139200	0.42934900	1.66827500
H	0.45998800	5.34369700	-4.06017900	C	7.35979100	-1.44042700	0.87847900	C	-0.52202900	-0.78698100	0.96901600
H	1.60640700	4.00091900	-4.30921600	Cl	5.22703100	-4.91332400	-1.24931300	C	0.39976300	0.84583900	2.47689900

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C	4.13936400	-0.52557200	-1.97399200	H	0.71996700	-6.57277000	-3.99212800	N	0.92022600	4.68457600	-1.74405400
C	4.49426600	-3.03534400	-1.81904800	H	-0.74071200	-5.57801200	-4.21085000	C	2.27690600	4.37983200	-1.60780800
C	5.06555200	-1.74095100	0.03015900	C	5.00686400	-0.22708000	-3.19652300	C	0.41651000	5.41609300	-0.66109300
O	4.01409900	-3.31611000	-2.89601500	H	4.69844100	0.72718600	-3.63066700	O	2.92360000	3.70788000	-2.38409000
C	5.10936700	-3.94053000	-0.79082600	H	6.05675800	-0.15272500	-2.89453500	C	2.71345500	5.04226500	-0.33164400
O	5.15237400	-0.76409800	0.74439300	H	4.90016900	-1.00380000	-3.95594000	O	-0.74026800	5.73952200	-0.50989900
C	5.44479300	-3.16460900	0.32285900	C	-0.81146000	-0.92627700	0.64254900	C	1.59962400	5.67668500	0.02891800
C	5.36658500	-5.30013200	-0.82110300	C	0.05519500	-1.63496200	1.61577600	C	3.95279200	5.09082800	0.28565700
C	6.03917900	-3.73262600	1.43717600	C	1.44046200	-1.35811900	1.66906400	C	1.70046100	6.38444800	1.41470800
Cl	4.98284600	-6.26827400	-2.24797100	C	-0.45946900	-2.52750500	2.58506200	Cl	5.34600300	4.25537200	-0.40350300
C	5.95943100	-5.89190600	0.30735900	C	2.26333900	-1.90997200	2.64869900	C	4.06970700	5.80914000	1.48964500
C	6.29217700	-5.11509100	1.42783700	H	1.88194200	-0.72009300	0.91468900	C	2.95411900	6.45231100	2.04785100
Cl	6.48529400	-2.74314400	2.83402300	C	0.35474000	-3.10288200	3.55661800	Cl	0.29011200	7.18611000	2.11691900
Cl	6.29620000	-7.62686900	0.30909200	H	-1.51359900	-2.77861600	2.58149400	Cl	3.12110400	7.35162900	3.55965000
Cl	7.04421400	-5.87567400	2.83518700	C	1.71170100	-2.77635300	3.59409100	C	-3.70710400	-0.45386500	-3.04105100
C	-0.07292400	3.47064500	-2.71850500	H	3.32028200	-1.66673600	2.66902400	N	-4.42143000	0.67662300	-2.43812700
N	0.83139000	3.99559200	-1.68793700	H	-0.06463800	-3.78178100	4.29134500	C	-4.09100800	2.02239000	-2.60648000
C	2.19113700	3.68024000	-1.60813100	Br	2.82243100	-3.52035500	4.96964500	C	-5.61112300	0.49710000	-1.72355700
O	0.42193800	4.88622100	-0.68946700	C	-2.25836000	-1.32210900	0.61230800	O	-3.10490900	2.43844300	-3.17800200
O	2.77622400	2.90567900	-2.33433400	O	-3.20999600	-0.57128700	0.76765100	C	-5.20178100	2.79538500	-1.95530900
C	2.72444800	4.47936500	-0.45115600	O	-2.40486400	-2.63332300	0.33911400	O	-6.10286500	-0.57651600	-1.44886000
O	-0.70846000	5.29090400	-0.52712300	C	-3.75779700	-3.08982000	0.14179500	C	-6.11790100	1.88006500	-1.43077500
C	1.66110600	5.19931300	0.10330000	H	-3.66727400	-4.11188500	-0.22097400	C	-5.40164700	4.15922000	-1.83045200
C	4.00301700	4.57306300	0.07275600	H	-4.31190100	-3.05794300	1.08473400	C	-7.25419800	2.30747500	-0.76867800
C	1.84966600	6.02317000	1.20020800	H	-4.26988000	-2.47145600	-0.59485800	Cl	-4.24063800	5.31634000	-2.49444200
Cl	5.34424800	3.66604800	-0.63332000	C	-1.00072400	1.43395400	1.82171100	C	-6.55388400	4.60863900	-1.16194000
C	4.21146900	5.41271200	1.18211600	H	-0.80451500	0.24165900	0.88944500	C	-7.47335000	3.68917600	-0.63529200
C	3.14295900	6.13045200	1.74219500	C	-1.96782800	2.21487600	0.97922800	Cl	-8.40870200	1.14343200	-0.09821400
Cl	0.49779200	6.91698600	1.90762200	H	-1.64877600	2.25290700	-0.06337700	Cl	-6.84542100	6.34386500	-0.98790100
C	3.42047000	7.17609200	3.13862300	H	-2.97179100	1.79816000	1.04231700	Cl	-8.91920400	4.26979500	0.20166700
Cl	-4.02606200	-0.56312500	-3.59873500	H	-1.97798800	3.25135200	1.35267000	C	0.70831500	-4.12784000	-2.97559500
N	-4.68042100	0.28157200	-2.59921300	C	0.43658800	1.87116900	1.76896400	N	-0.19506100	-4.66947800	-1.95976100
C	-4.29953600	1.59130800	-2.30652800	H	0.51595400	2.83144500	2.30098100	C	-1.53001000	-4.28721600	-1.82783700
C	-5.70340800	-0.18444600	-1.76644600	H	1.10227200	1.16389800	2.27116400	C	0.21914700	-5.56448000	-0.96421400
O	-3.40224100	2.20207100	-2.84929100	H	0.76542400	2.02248500	0.73830500	O	-2.11836700	-3.52695400	-2.56868900
C	-5.22715900	2.04481400	-1.21294500	C	-1.50632100	0.88787200	3.12634900	C	-2.03931300	-5.01232500	-0.61426800
O	-6.17268200	-1.30130500	-1.79492700	H	-2.47198900	0.40027500	2.95922300	O	1.32752000	-6.03854700	-0.86574800
C	-6.06681800	0.97561500	-0.88622800	H	-0.80737400	0.14096700	3.52097300	C	-0.99327300	-5.78758700	-0.10239400
C	-5.33760800	3.26375700	-0.56528100	C	-1.68434000	2.00363900	4.19368700	C	-3.28566800	-5.00280700	-0.01061200
C	-7.03426600	1.09673500	0.09642900	H	-0.72279000	2.49955800	4.37509100	C	-1.17111200	-6.57961900	1.01951800
C	-4.27040500	4.61283200	-0.97483500	H	-2.37016200	2.76997000	3.81247200	Cl	-4.60130500	-4.00721800	-0.64822800
C	-6.31563300	3.40236100	0.43550500	C	-2.22493900	1.43452800	5.50920800	C	-3.47953400	-5.79866300	1.13218500
C	-7.15647400	2.32813100	0.76410200	H	-1.54306900	0.68498300	5.92733600	C	-2.43267600	-6.58262900	1.64125300
Cl	-8.09139300	-0.25871400	0.50419900	H	-2.34850600	2.22873500	6.25363000	Cl	0.15143300	-7.56081100	1.65767000
Cl	-6.48337900	4.94375900	1.28550100	H	-3.20033900	0.95636800	5.36269600	Cl	-5.05566200	-5.80795700	1.93333000
Cl	-8.37952200	2.52087600	2.02577500					Cl	-2.69679800	-7.57971200	3.07631100
C	0.68339600	-4.80073100	-2.75170100	5S				H	1.71650300	-4.38019200	-2.62711600
N	0.17297700	-5.46924400	-1.55576300	-4315.121019				H	-3.91500100	-1.30916900	-2.39193100
C	-1.17252600	-5.76407600	-1.31922200	Rh	0.45117900	0.04230900	-4.09217600	H	-0.95158200	4.37269900	-2.50955200
C	0.98235400	-5.73179900	-0.44550100	O	0.21611900	2.08062400	-3.99816200	H	4.75699600	1.39796400	-2.37691900
O	-2.09592500	-5.53283300	-2.06887200	O	0.68055500	-1.99953800	-4.07162400	Cl	5.63489500	5.89948100	2.30295700
C	-1.20891000	-6.41231000	0.03967400	O	0.26034300	2.05223000	-1.73199900	N	5.13727100	-0.54940200	-1.88212300
O	2.16527800	-5.48224000	-0.36147000	O	0.52178400	-2.05325800	-1.81046600	C	0.36393200	4.84285300	-4.16304800
C	0.08383300	-6.37879800	0.56946000	O	2.48565900	0.29176800	-3.99648900	H	-0.31906800	4.45609400	-4.92243700
C	-2.25303800	-6.98978800	0.74216900	O	-1.57353200	-0.22337200	-4.08861500	H	0.21164600	5.92243100	-0.76799400
C	0.36176300	-6.90886000	1.81836700	O	-1.66596700	-0.14474400	-1.82477900	H	1.38907500	4.65034000	-4.48862100
Cl	-3.88093000	-7.07486500	0.05208500	O	2.45741400	0.14056800	-1.73624400	C	-4.21838000	-0.74314900	-4.45453600
C	-1.98959200	-7.52500500	2.01504700	C	-2.18698700	-0.23580500	-2.98027600	H	-3.71665100	-1.62696200	-4.85610500
C	-0.69330300	-7.48133100	2.55048500	C	3.03992700	0.25483600	-2.86025900	H	-5.29472400	-0.93793800	-4.41899900
Cl	2.00008700	-6.87722700	2.47831100	C	0.20546800	2.63382300	-2.86174800	H	-4.02190100	0.09876800	-5.12338600
Cl	-3.30177400	-8.26080000	2.94407700	C	0.61956800	-2.59374900	-2.95542200	C	0.46264900	-4.74131800	-4.35561200
Cl	-0.38058900	-8.15524300	4.15489600	Rh	0.38921400	-0.00597500	-1.69697600	H	1.18444400	-4.34242900	-5.07169700
H	1.77271000	-4.79528200	-2.62566000	C	4.56715700	0.41519800	-2.82353800	H	0.58354500	-5.82757200	-4.30050600
H	-4.45088300	-1.56022500	-3.43496900	C	4.85289000	-1.91730900	-1.89683000	H	-0.54352300	-4.50753100	-4.71269500
H	-1.07869100	3.73556600	-2.37585700	C	6.05597400	-0.19270000	-0.88667800	C	5.22817600	0.33143200	-4.20090300
H	4.25632200	0.26795000	-1.22997700	O	4.08952200	-2.46316700	-2.65585800	H	4.80945600	1.09515200	-4.86007400
Cl	5.82917400	5.56187900	1.87340100	C	5.68176100	-2.51129500	-0.79345300	H	6.30429700	0.50424400	-4.10136400
N	4.56387200	-1.74612300	-1.27586100	O	6.46259500	0.92862600	-0.67956200	H	5.05915500	-0.64741600	-4.65674700
C	0.19659200	4.10619100	-4.08339000	C	6.40341200	-1.47688100	-0.18792900	C	-2.04932800	1.45267800	1.94280500
H	-0.52990800	3.73535100	-4.80962300	C	5.80626700	-3.82079500	-0.35984200	C	-0.98684000	0.35771500	1.88580700
H	0.09729700	5.19398300	-4.00977000	C	7.26476600	-1.72615100	0.86715900	C	0.22209400	0.62653200	1.21431500
H	1.19749800	3.85526900	-4.44226700	Cl	4.88211200	-5.12191100	-1.11522100	C	-1.13355900	-0.90169500	2.48026100
C	-4.32920500	-0.10334000	-5.02748100	C	6.68075600	-4.08909400	0.70877900	C	1.25444200	-0.31892900	1.14935600
H	-3.86581600	-0.78875700	-5.73989900	C	7.40328800	-3.05106900	1.31717200	H	0.37599200	1.60130100	0.76159500
H	-5.41125800	-0.09789700	-5.19231100	C	8.16966500	-0.41436800	1.63041800	C	-0.11763900	-1.86071100	2.41752100
H	-3.93187200	0.89863700	-5.20680300	Cl	6.86869600	-5.74802400	1.28731500	H	-2.05193600	-1.14957300	2.99759400
C	0.33773600	-5.54840500	-4.04413500	Cl	8.49682600	-3.40777000	2.65858800	C	1.06879300	-1.56515900	1.75558000
H	0.81166500	-5.03780900	-4.88431500	C	0.07788900	4.16395200	-2.82259500	H	2.18722300	-0.07928900	0.65293100

H	-0.25336400	-2.82669300	2.89240700	O	0.06612600	-2.05756400	-1.24205700	C	0.39820000	-0.90051200	1.78056200
Br	2.46017600	-2.88514100	1.68269300	O	2.05716800	0.06467800	-3.51748400	C	1.77562900	-1.02405800	1.51158600
C	-3.44067600	0.95008400	1.55951100	O	-2.05765100	-0.06473100	-3.51727800	C	-0.10327100	-1.46319300	2.97336800
O	-4.04971100	1.36304900	0.59215500	O	-2.05747500	-0.06646300	-1.24176600	C	2.62103500	-1.68957200	2.39417000
O	-3.94931600	0.02499800	2.39679300	O	2.05722300	0.06602400	-1.24197200	H	2.18239600	-0.58489500	0.60974600
C	-5.25866200	-0.48358400	2.06166700	C	-2.61443900	-0.08274500	-2.37949400	C	0.72888000	-2.14579600	3.85342900
H	-5.49272100	-1.20705700	2.84262800	C	2.61407100	0.08249700	-2.37975300	H	-1.15789200	-1.38290700	3.21129900
H	-5.99122400	0.32649100	2.05638400	C	-0.08281000	2.61413500	-2.37938700	C	2.09001400	-2.25149900	3.55659300
H	-5.24606600	-0.96251600	1.08085600	C	0.08243300	-2.61437500	-2.37986100	H	3.67999000	-1.77693700	2.17818400
C	-2.04865000	2.34661300	3.26106000	Rh	-0.00011900	-0.00022700	-1.18484000	H	0.32972300	-2.58229500	4.76205300
H	-1.82287400	2.14898700	1.13013900	H	-0.11668100	3.71172100	-2.37928300	Br	3.24661700	-3.17921400	4.77050600
C	-3.23242700	3.33250100	3.16042900	H	-3.71202500	-0.11661400	-2.37942900	C	-1.97624900	-0.24175400	1.03132800
H	-3.23109500	3.85503400	2.19708100	H	0.11629600	-3.71196200	-2.37994100	O	-2.71897300	0.71294000	1.11875600
H	-4.19736200	2.82278600	3.26673000	H	3.71165800	0.11636000	-2.37979400	O	-2.37260000	-1.52533800	1.01732300
H	-3.17242200	4.09119900	3.94689600					C	-3.79462900	-1.72812400	0.91236900
C	-0.73647700	3.15821700	3.26280300	1H				H	-3.93091700	-2.80927800	0.91470100
H	0.14310100	2.50971000	3.34063000	-1596.067328				H	-4.31053800	-1.26851600	1.75895900
H	-0.64495400	3.75707900	2.34839800	Rh	0.02038800	0.40959300	-3.21688200	H	-4.15937800	-1.29367400	-0.02041000
H	-0.71299400	3.85482000	4.10651700	O	-0.86956300	2.26176900	-3.42081800	N	-0.25215400	1.52431700	1.25747800
C	-2.15083400	1.48335300	4.54547200	O	0.88006200	-1.43569100	-2.88784900	N	0.20877600	2.53239400	1.22908500
H	-3.03490000	0.83944000	4.46909400	O	-1.30413400	2.38106200	-1.18850200				
H	-1.28342500	0.81129300	4.58357300	O	0.41582100	-1.33350500	-0.65894300	2H			
C	-2.22615800	2.24131600	5.88214100	O	1.82943600	1.32645000	-2.82579900	-1596.083356			
H	-1.35793700	2.90221300	5.99840300	O	-1.80829800	-0.49120200	-3.50083300	Rh	0.04236600	0.73069200	-3.27187300
H	-3.11196200	2.88856400	5.90108900	O	-2.28185200	-0.37955900	-1.27601400	O	-0.97123300	2.51425700	-3.01960800
C	-2.28374200	1.28202500	7.07747500	O	1.37379300	1.45009900	-0.59928200	O	1.02399900	-1.09191100	-3.38267900
H	-1.39213400	0.64422900	7.11761200	C	-2.53405700	-0.67406100	-2.48354900	O	-1.44443400	2.02633400	-0.84190000
H	-2.34486000	1.82974900	8.02473600	C	2.09117400	1.63636800	-1.63186600	O	0.58395300	-1.56398800	-1.19540600
H	-3.15874300	0.62296400	7.01639500	C	-1.31905000	2.81923700	-2.37941900	O	1.78656900	1.63707600	-2.61408000
				C	0.87997700	-1.88144700	-1.70365700	O	-1.73382500	-0.20415200	-3.77058100
S-P				Rh	-0.46729400	0.52592000	-0.84815400	O	-2.20739200	-0.66723300	-1.58720500
-747.864661				H	-1.78095000	3.80666400	-2.51689100	O	1.32752400	1.15910400	-0.43139800
C	-2.03748900	1.45397200	1.96300900	H	-3.50815200	-1.14993100	-2.66504600	C	-2.43767600	-0.67197600	-2.83855400
C	-0.96786300	0.36404600	1.89959600	H	1.34133200	-2.86842800	-1.55899100	C	2.02345500	1.64959400	-1.37984700
C	0.20397300	0.61236300	1.16881800	H	3.05782900	2.12925800	-1.45716800	C	-1.47353800	2.74846000	-1.88865500
C	-1.09292300	-0.88557300	2.52731100	C	-0.94032900	0.68570000	1.61894500	C	1.07100200	-1.80403400	-2.34855600
C	1.22612300	-0.33260400	1.07378100	C	0.01364700	-0.20231900	2.36413600	Rh	-0.45932200	0.21303000	-0.90508800
H	0.32382100	1.56398100	0.67558800	C	1.39602200	0.03424700	2.27566600	H	-2.01145900	3.70052300	-1.77573900
C	-0.08292800	-1.84484700	2.44077900	C	-0.43702100	-1.24379200	3.18980900	H	-3.38175600	-1.15407300	-3.13242300
H	-1.99363400	-1.12299900	3.08069000	C	2.30424500	-0.73880300	2.99413700	H	1.60059100	-2.76434000	-2.43547400
C	1.07317600	-1.55968000	1.71597900	H	1.77173300	0.80861400	1.61535200	H	2.95268100	2.14523200	-1.06201600
H	2.12274900	-0.11732400	0.50279900	C	0.46795500	-2.03254600	3.89916700	C	-0.88986500	-0.22208500	1.01868400
H	-0.19883100	-2.80532200	2.93129300	H	-1.49468000	-1.45252200	3.27596000	C	0.00917500	-0.61356400	2.05743800
Br	2.46807700	-2.87994300	1.59173000	C	1.83354700	-1.77284100	3.80290800	C	1.36140300	-0.94261500	1.76566100
C	-3.41607400	0.93543500	1.54730000	H	3.36803100	-0.54399800	2.91370700	C	-0.42004200	-0.70164400	3.41371400
O	-3.97740100	1.26914200	0.52653600	H	0.10542100	-2.83647200	4.53031900	C	2.22861400	-1.35406400	2.76675800
C	-3.96495800	0.06270000	2.42715400	Br	3.07938900	-2.85125500	4.79125000	H	1.70365400	-0.89109100	0.74225700
O	-5.25199000	-0.45991600	2.05152300	C	-2.43487200	0.55499400	1.55349800	C	0.44652400	-1.08976400	4.41998100
H	-5.54011800	-1.13298900	2.85946600	O	-3.18316800	1.50417600	1.44753900	H	-1.43872800	-0.43063500	3.67024900
H	-5.97780400	0.35029400	1.94614200	O	-2.82389900	-0.72709200	1.60074700	C	1.76791400	-1.42060000	4.08637800
H	-5.18294500	-1.00057400	1.10422300	C	-4.23407100	-0.94138500	1.40011300	H	3.25401300	-1.61767000	2.53370200
C	-2.04780100	2.34218100	3.28055400	H	-4.37113600	-2.02023600	1.47136600	H	0.11354100	-1.14182300	5.45024300
H	-1.80918800	2.15652000	1.15571200	H	-4.81339500	-0.42352500	2.16827500	Br	2.96237000	-1.97513100	5.46720500
C	-3.22837000	3.33052500	3.16811200	H	-4.52290700	-0.57755200	0.41268900	C	-2.31969300	-0.05090800	1.38534300
H	-3.21862500	3.85039900	2.20289200	N	-0.62271800	2.00333300	1.69467400	O	-2.75972300	1.00726800	1.79088400
H	-4.19436000	2.82110200	3.26445400	N	-0.33266900	3.08971800	1.69360700	O	-3.03353500	-1.16776700	1.19550100
H	-3.17636100	4.09127500	3.95347600					C	-4.45892700	-1.03399700	1.36262700
C	-0.73033100	3.14588900	3.29535100	TS _{1H-2H}				H	-4.86687200	-2.02172300	1.15055900
H	0.14320500	2.49019300	3.37656600	-1596.051532				H	-4.70069800	-0.72709500	2.38343800
H	-0.62218000	3.74285700	2.38124600	Rh	0.38033200	-0.00711700	-3.71157000	H	-4.84997800	-0.29557100	0.65872000
C	-0.70757900	3.84118400	4.14041700	O	-0.55316900	1.83895000	-3.74570600	N	-0.21669800	3.09437300	2.37791900
H	-2.16379200	1.48331400	4.56726400	O	1.27868200	-1.86033000	-3.52730300	N	-0.37555400	3.87090900	1.60833500
H	-3.04862900	0.84185600	4.48492600	O	-0.94549100	1.78705200	-1.50124400				
H	-1.29782700	0.81047000	4.61491000	O	0.85994300	-1.93148600	-1.28614600	3H			
C	-2.24904200	2.24625200	5.90063400	O	2.18355900	0.91640400	-3.27054400	-1486.559446			
H	-1.38125400	2.90686000	6.02224600	O	-1.44474600	-0.91968400	-4.01410200	Rh	0.05102600	0.75552500	-3.26098900
H	-3.13447300	2.89446000	5.91072900	O	-1.87875800	-0.97166400	-1.77647300	O	-0.95813900	2.53647500	-2.97633600
C	-2.31682400	1.29135900	7.09901100	O	1.76994100	0.86450900	-1.03041000	O	1.02766300	-1.06765300	-3.40735800
H	-1.42591800	0.65325000	7.14822100	C	-2.14556800	-1.18204400	-3.00064600	O	-1.44070600	2.00356900	-0.81099100
H	-2.38528800	1.84218300	8.04411200	C	2.46061800	1.14127600	-2.06552400	O	0.57203100	-1.58853900	-1.23423600
H	-3.19149600	0.63230400	7.03298000	C	-0.99326300	2.30564300	-2.66122300	O	1.79327300	1.64368500	-2.57292000
				C	1.30791200	-2.38986700	-2.38346100	O	-1.72532900	-0.16409700	-3.78829700
Rh ₂ -(O ₂ CH) ₄				Rh	-0.06655600	-0.07389800	-1.29627800	O	-2.21329300	-0.67229600	-1.61788500
-975.819482				H	-1.48235600	3.28897200	-2.71387900	O	1.32203800	1.11302400	-0.40496700
Rh	-0.00024900	-0.00001200	-3.57440500	H	-3.11854800	-1.65762000	-3.19299300	C	-2.43618600	-0.64921400	-2.87031200
O	-0.06496200	2.05738400	-3.51719300	H	1.78433000	-3.37906800	-2.31717500	C	2.02359900	-1.62514000	-1.33723200
O	0.06444700	-2.05743400	-3.51756900	H	3.42026200	1.64049200	-1.86672500	C	-1.46417000	2.74711300	-1.84230600
O	-0.06636000	2.05713400	-1.24168100	C	-0.48384200	-0.18219700	0.83225800	C	1.06607200	-1.80332000	-2.38958700

Rh	-0.46516400	0.18628300	-0.90926200	H	-2.48443400	5.41422700	-1.32373800	C	3.43634600	-0.86028200	2.48857700
H	-2.00114700	3.69770700	-1.71162700	H	-3.52554100	4.95438500	-2.66054800	C	2.40576800	-0.06599300	-2.58449200
H	-3.38019600	-1.12151700	-3.18003000	C	-4.37888700	4.57769200	-0.71552900	C	1.04840200	-2.27914200	0.07611000
H	1.59351300	-2.76297000	-2.49510500	H	-4.89029100	5.54534300	-0.65165100	C	4.81458400	1.35087700	-0.15580100
H	2.95212300	2.11087000	-1.00251700	H	-5.11324300	3.83413900	-1.04982700	Rh	2.12038300	0.39166700	0.25128700
C	-0.90130000	-0.25676100	1.00970500	H	-4.06644400	4.29770900	0.29862500	H	0.25634900	-3.03748200	0.13876900
C	0.00509800	-0.62084500	2.05316300					H	3.64665100	-1.03069600	3.55323400
C	1.34132400	-1.00307100	1.75389700	TS _{AHA} -SHA				H	5.60744500	2.10992700	-0.20411400
C	-0.40068300	-0.62773800	3.41927800	-1723.615647				H	2.19261600	0.10053000	-3.64953500
C	2.21561800	-1.38965800	2.75903900	Rh	3.48327200	-1.17189600	-0.30658200	C	-1.41154500	1.51926200	-0.15743900
H	1.66196300	-1.02005000	0.72209800	O	2.57227500	-2.97944400	0.09872800	C	-2.41098500	0.43969300	0.25642200
C	0.47604600	-0.98488100	4.42853300	O	4.27792300	0.70669400	-0.68513900	C	-2.45163900	-0.75475900	-0.47871200
H	-1.40608300	-0.31323100	3.67859800	O	0.57168200	-1.96324200	0.50623100	C	-3.30350400	0.57975100	1.32962600
C	1.78049500	-1.37180700	4.08870200	O	2.25782100	1.72454500	-0.38865300	C	-3.35512500	-1.77271800	-0.17422900
H	3.22753700	-1.69716300	2.52094000	O	2.94714600	-1.35647100	-2.30766400	H	-1.75915700	-0.89792600	-1.30275500
H	0.16276500	-0.97197300	5.46622700	O	3.87777200	-0.92386900	1.70354000	C	-4.20830100	-0.43308900	1.65510200
Br	2.98692800	-1.88671600	5.47482500	O	1.89374100	0.14981700	2.04212700	H	-3.28356200	1.48039500	1.93146900
C	-2.33033700	-0.08741600	1.38063100	O	0.92336000	-0.36059900	-1.96825700	C	-4.23060600	-1.60175700	0.89718600
O	-2.76608700	0.96165900	1.81381800	C	3.01360400	-0.32651700	2.40247000	H	-3.37300400	-2.68639000	-0.75863500
O	-3.04746000	-1.19659400	1.16323700	C	1.82244300	-0.92831300	-2.67081400	H	-4.88678500	-0.30882700	2.49212100
C	-4.47069500	-1.06669000	1.34978300	C	1.35217300	-2.95978200	0.42116500	Br	-5.47735200	-3.00111900	1.33766400
H	-4.88159400	-2.04854100	1.11724700	C	3.50208500	1.69828700	-0.64369400	C	-0.75868300	2.17965600	1.04581300
H	-4.70049300	-0.78588900	2.38084800	Rh	1.31008900	-0.07369100	0.07168100	O	-1.32536000	2.73534500	1.95949200
H	-4.86939800	-0.31030000	0.66964700	H	0.89786300	-3.93294800	0.65908700	O	0.61775000	2.16408900	0.98658300
				H	3.25603000	-0.19652400	3.46741300	C	1.27530200	2.94612200	2.02301900
				H	3.95795700	2.67739500	-0.85801300	H	2.32182400	2.98310900	1.73053400
4HA				H	1.57447100	-1.05566200	-3.73582800	H	0.83511200	3.94359900	2.05312400
-1723.640895				C	-0.70844700	0.86695000	0.49285000	H	1.15390000	2.45462300	2.98912400
Rh	3.29786400	-0.75057500	-0.57629000	C	-1.88142000	-0.03241400	0.42434300	C	-1.99372000	2.63396800	-1.14636500
O	2.85348800	-2.74042400	-0.20275300	C	-1.99956200	-0.94759600	-0.64725900	H	-0.61673700	1.02796700	-0.72273500
O	3.60927500	1.27083700	-0.87496300	C	-2.92590400	-0.01215900	1.37701400	C	-2.39000600	1.92710600	-2.45811300
O	0.83572500	-2.20903800	0.72002100	C	-3.10334300	-1.78551400	-0.77508800	H	-1.53755500	1.38497000	-2.88547300
O	1.61543800	1.81080400	0.09546700	H	-1.19984500	-1.01087300	-1.37543200	H	-3.20730000	1.21478100	-2.30737700
O	2.32094400	-0.86997500	-2.40048300	C	-4.02839700	-0.85559900	1.26687500	H	-2.71703900	2.65952600	-3.20325900
O	4.14760800	-0.59073600	1.30016600	H	-2.85674100	0.65058400	2.22954100	C	-0.86102200	3.63637700	-1.45665300
O	2.13687100	-0.06967500	2.24424700	C	-4.11401700	-1.73391000	0.18626800	H	-1.16049300	4.31669800	-2.26042800
O	0.31278000	-0.32839600	-1.46442700	H	-3.16969600	-2.48304600	-1.60309700	H	-0.60969800	4.25320200	-0.58526500
C	3.38879400	-0.29473500	2.26088600	H	-4.81353900	-0.82825600	2.01470800	H	0.04820100	3.11726200	-1.78017000
C	1.08710700	-0.63505600	-2.43056000	Br	-5.63749400	-2.89301700	0.02364100	C	-3.21719300	3.35105200	-0.52085000
C	1.75471600	-3.00910500	0.34642300	C	-0.52671400	1.66608400	1.73544500	H	-4.00049200	2.60432500	-0.33726000
C	2.72349500	2.07044800	-0.47504500	O	-0.79429000	1.28043000	2.85850100	H	-2.93216000	3.74175200	0.46316000
Rh	1.12473000	-0.17232800	0.44817300	O	0.06375000	2.87073400	1.50974500	C	-3.83518500	4.50236700	-1.33306600
H	1.54511700	-4.07249000	0.53376300	C	0.48903700	3.56562500	2.69234500	H	-3.09108800	5.29177700	-1.49945100
H	3.85687400	-0.21668100	3.25267000	H	0.94985000	4.48887600	2.33828600	H	-4.14098700	4.15085100	-2.32686900
H	2.91976900	3.14017500	-0.63667700	H	-0.36071500	3.78514400	3.34464100	C	-5.05182500	5.10707200	-0.62147200
H	0.59690100	-0.69964200	-3.41313300	H	1.21426500	2.96035300	3.24090000	H	-5.48344600	5.93124600	-1.20088100
C	-0.63757200	0.28945300	1.32284300	C	-1.35200600	2.67285200	-1.34900400	H	-5.83748400	4.35634800	-0.47181100
C	-1.87954600	-0.40937200	1.21504300	H	-0.62929200	1.55854900	-0.45075100	H	-4.77830000	5.49945500	0.36568200
C	-2.06098600	-1.42120800	0.23235300	C	-1.72382000	1.75781300	-2.47659500				
C	-2.97859700	-0.10918800	2.07183500	H	-0.85994700	1.19961300	-2.84537800				
C	-3.27363700	-2.08147000	0.10091400	H	-2.51964900	1.06118600	-2.19915500				
H	-1.24440000	-1.65328900	-0.43600900	H	-2.10540800	2.38033100	-3.30163300				
C	-4.18341000	-0.78011800	0.96004200	C	-0.12567900	3.51431900	-1.54924400				
H	-2.86152100	0.63837900	2.84918300	H	-0.38114300	4.29487800	-2.28571600				
C	-4.32443300	-1.76116400	0.96763300	H	0.18780200	3.99831400	-0.62420200				
H	-3.40784000	-2.84116600	-0.66079000	H	0.70753100	2.93293900	-1.94744200				
H	-5.00904300	-0.55242300	2.62456700	C	-2.47365400	3.25083100	-0.53278800				
Br	-5.98925500	-2.67764000	0.79885500	H	-3.13937400	2.44639800	-0.19503500				
C	-0.58371700	1.43080200	2.27269500	H	-2.06382000	3.74895000	0.35140700				
O	-0.37464500	1.27054300	3.45952300	C	-3.31992900	4.27653700	-1.33753000				
O	-0.76586100	2.61382200	1.67145900	H	-2.66859000	5.07322200	-1.71855300				
C	-0.58916600	3.77385200	2.50944200	H	-3.76389500	3.78414100	-2.21117500				
H	-0.76919300	4.62807800	1.85794700	C	-4.42825800	4.88725300	-0.47410700				
H	-1.30139300	3.76222400	3.33842900	H	-5.01732400	5.60806100	-1.05171900				
H	0.42855200	3.79744500	2.90591900	H	-5.11239000	4.11578000	-0.10233300				
C	-1.21688200	3.24010300	-2.70727600	H	-4.01193000	5.41236600	0.39339100				
H	-0.84156700	2.20773600	-2.65394400								
C	-1.57536400	3.52628900	-4.17419100	SHA							
H	-0.70853400	3.36690800	-4.82707600	-1723.703810							
H	-2.38234100	2.87036400	-4.52448600	Rh	3.71754700	-1.30340400	-0.33986600				
H	-1.90382300	4.56319300	-4.31676000	O	2.20029700	-2.69459900	-0.24061000				
C	-0.07849500	4.15304700	-2.22465900	O	5.16433700	0.16223800	-0.40572300				
H	-0.36070900	5.21243500	-2.26607400	O	0.69223100	-1.08806500	0.32862600				
H	0.20281800	3.91048700	-1.19346500	O	3.65727000	1.77622900	0.14474600				
H	0.81162100	4.02999100	-2.85453300	O	3.27586200	-0.94483200	-2.32183100				
C	-2.44751800	3.28875900	-1.77289300	O	4.07815200	-1.58007200	1.67065900				
H	-3.16840000	2.52764200	-2.10858200	O	2.57787000	0.03757300	2.23073200				
H	-2.12691600	2.98386200	-0.76651800	O	1.74623900	0.64960000	-1.76935600				
C	-3.17890600	4.63645300	-1.66841200								