

Supporting Information

Theoretical Evaluation of the Carbene-Based Site-Selectivity in Gold(III)- Catalyzed Annulations of Alkynes with Anthranils

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Computational Details

All DFT calculations were carried out with the Gaussian 09 programs.¹ The geometries of all stationary points were fully optimized at the B3LYP² level in gas phase with SDD³ basis set for Au atom and 6-31g (d) basis set for all other atoms. Vibrational frequencies were conducted at the same level of theory to verify all stationary points as local minima (zero imaginary frequencies) or first-order saddle points (one imaginary frequency) and the free energies were provided at 298.15 K. IRC⁴ calculations have been also performed to ensure that all transition-state structures connected two relevant minima. The solvent effects of DCE were evaluated by single-point calculations employing a self-consistent reaction field (SCRF) method⁵ with the PCM model⁶ at the M06⁷ level, in which the 6-311+g(d,p) basis set is used for the non-metallic atoms and SDD basis set for Au. To confirm the reliability of B3LYP//M06 method for describing the present system, we have implemented benchmark calculations for crucial selective-determining transition states, including **TS3-5** and **TS3-4** in Fig. S1, **TS3'-5'** and **TS3'-4'** in Fig. S3, and **TS15-16** and **TS15-20** in Fig. S2 by using PBE0,⁸ WB97XD,⁹ and M06-2X-D3¹⁰ functionals with different basis sets, respectively. The computed energy differences for two selective-determining stationary points in three catalytic systems, **TS3-5 – TS3-4**, **TS3'-5' – TS3'-4'**, and **TS15-16 – TS15-20**, are displayed in Table S1 in the Supporting Information. All the functionals are found to give comparable energy differences and consistent trends.

These facts ensure the quality and accuracy of the B3LYP//M06 method used in the system under study.

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Table S1 Calculated free-energy differences (kcal mol⁻¹) calculated using different functions and basis sets for the energy differences of two crucial selective-determining transition states in three catalytic systems.

		TS3-5–TS3-4	TS3'-5'–TS3'-4'	TS15-16–TS15-20
Optimization	B3LYP// Single-point M06	-3.2	6.3	-6.2
Optimization	B3LYP ^a //lanl2dz	-4.8	4.5	-2.7
	PBE0 ^a //lanl2dz	-2.1	3.2	-3.8
Single-point	WB97XD ^b //SDD	-3.1	3.6	-5.9
	M06-2X-D3 ^b //SDD	-3.8	1.9	-6.3

^a 6-31G (d, p) for C, H, O, and N atoms in the gas phase.

^b 6-311+G(d, p) for C, H, O, and N atoms.

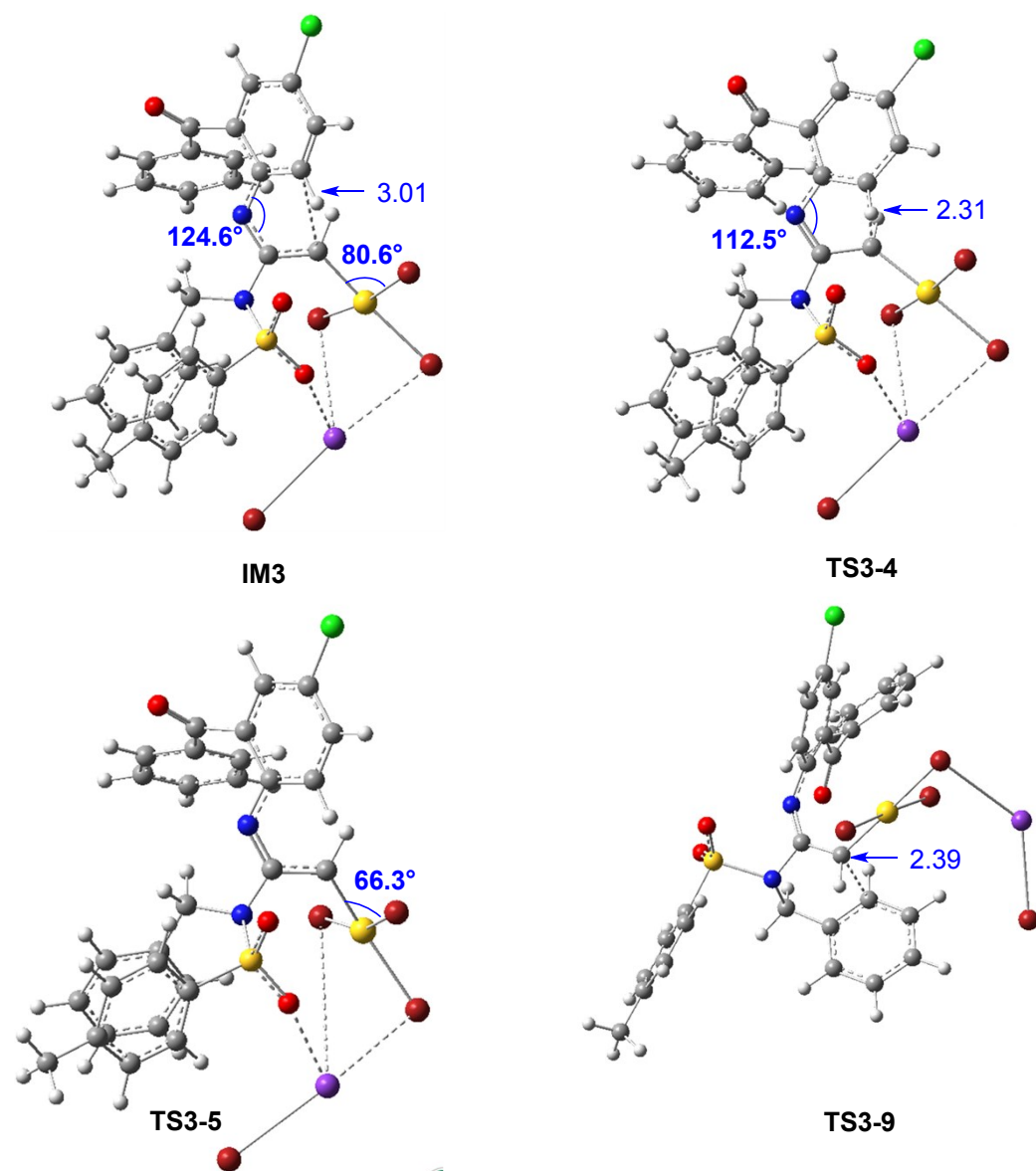


Fig. S1 Optimized structures with selected structural parameters for key stationary points shown in Fig. 1. The bond distance and bond angle are given in Å and °, respectively.

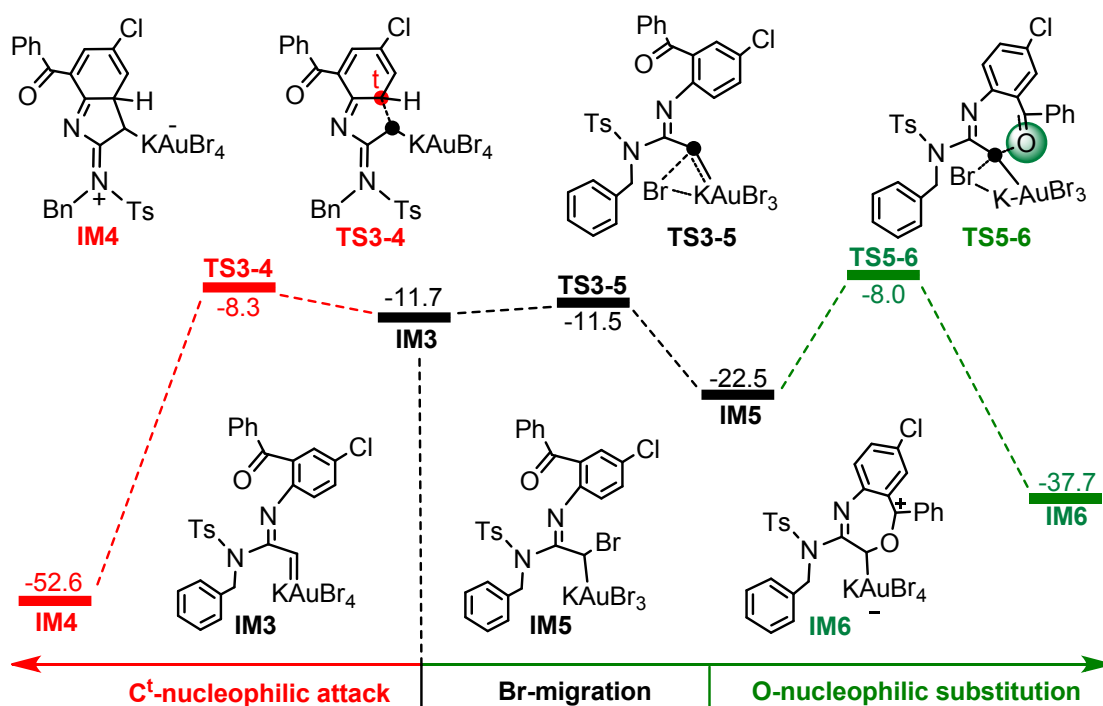


Fig. S2 Calculated free energy profile in DCE solvent for a-imino gold carbene electrophilic addition step along potential pathways in the **1a**-system. The relative free energies are given in kcal mol⁻¹.

For the **1a** system, starting from **IM3**, the reaction can possibly undergo either direct C^t-nucleophilic attack via **TS3-4** or Br-migration (**TS3-5**) followed by O-nucleophilic substitution (**TS5-6**). The two selective-determining transition states, **TS3-4** and **TS5-6** are found to be energetically comparable (-8.3 and -8.0 kcal mol⁻¹), both of which, however, are less stable in energy than **TS3-5** in Fig. 1 (-11.5 kcal mol⁻¹). Therefore, these two competitive pathways are theoretically ruled out. (Fig. S2)

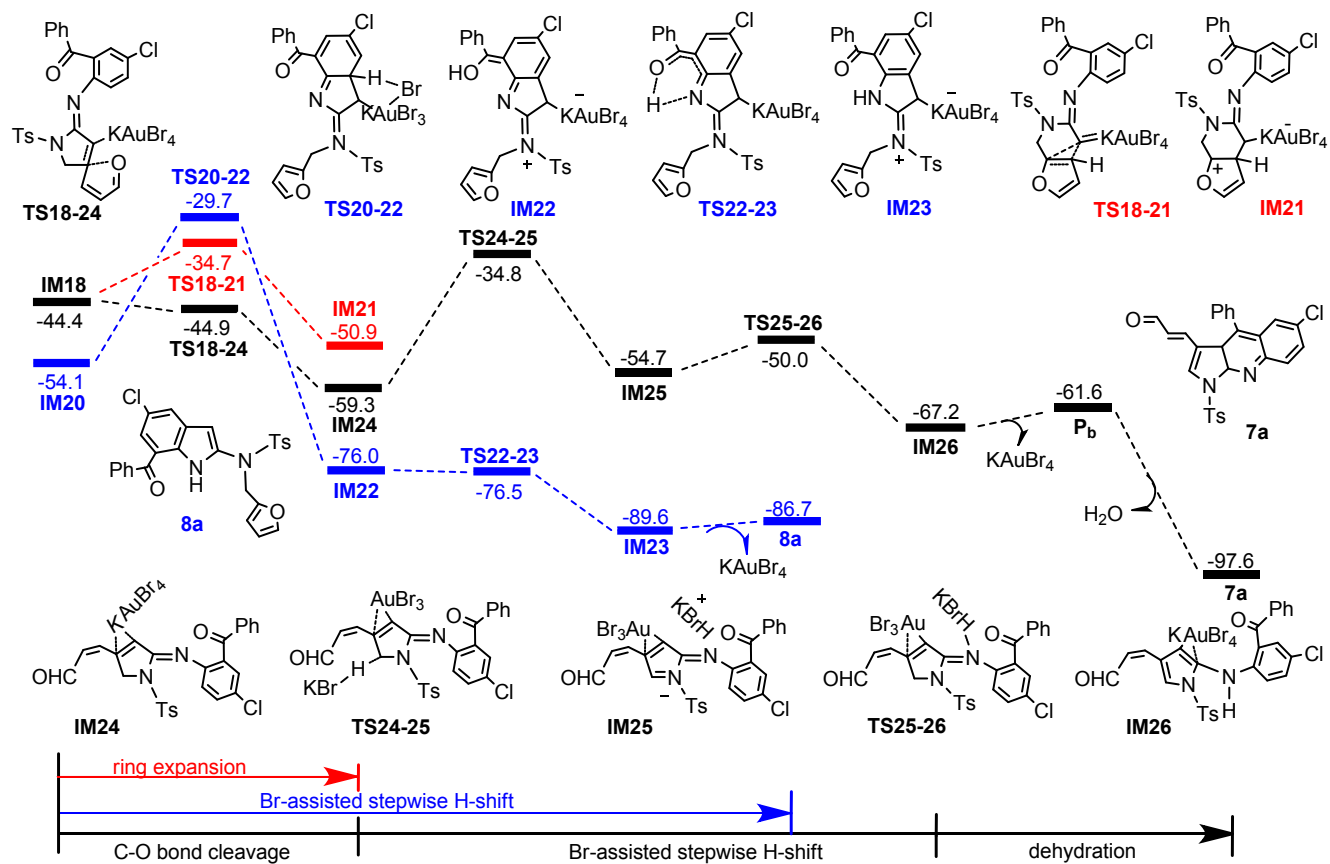


Fig. S3 Calculated free energy profiles in DCE solvent for possible pathways starting from **IM18** and **IM20**, respectively (**1b**-system). The relative free energies are given in kcal mol⁻¹.

For the **1b** annulation, from **IM18**, the alternative ring expansion through C(Au)-migration (**TS18-21**, Fig.S3) was also explored and found to be energetically disfavored over C^b-O cleavage via **TS18-24** (-34.7 vs -44.9 kcal mol⁻¹). The calculated NBO charges demonstrate that the stronger electrostatic attraction involved in **TS18-24** facilitates the C^b-O bond rupture, thereby producing a relatively lower energy requirement. (Fig. S3)

In addition, after C^t-nucleophilic attack of **IM15** to give **IM20** (blue line, Fig. S4), the stepwise Br-assisted H-shift is possibly followed, from which the 7-acylindole product **8a** is obtained, and simultaneously, KAuBr₄ is regenerated (Fig. S3). Unfortunately, the Br-assisted H-abstraction process via **TS20-22** is 15.2 kcal mol⁻¹ higher as compared to C^b-O cleavage (**TS18-24**, black line). Consequently, the alternative C^t-nucleophilic attack pathway is kinetically unfavored (Fig. S3).

For the **1b** system, we also examined the direct C^b- and C^t-nucleophilic attack of **IM15** (pink- and blue- line, respectively), as well as the nucleophilic substitution of the carbonyl O atom from **IM16** (red line), all of which are computed to be unfavorable over the pathway along Br-migration → N-donation/abstraction substitution (black line) due to higher energy demands involved (Fig. S4)

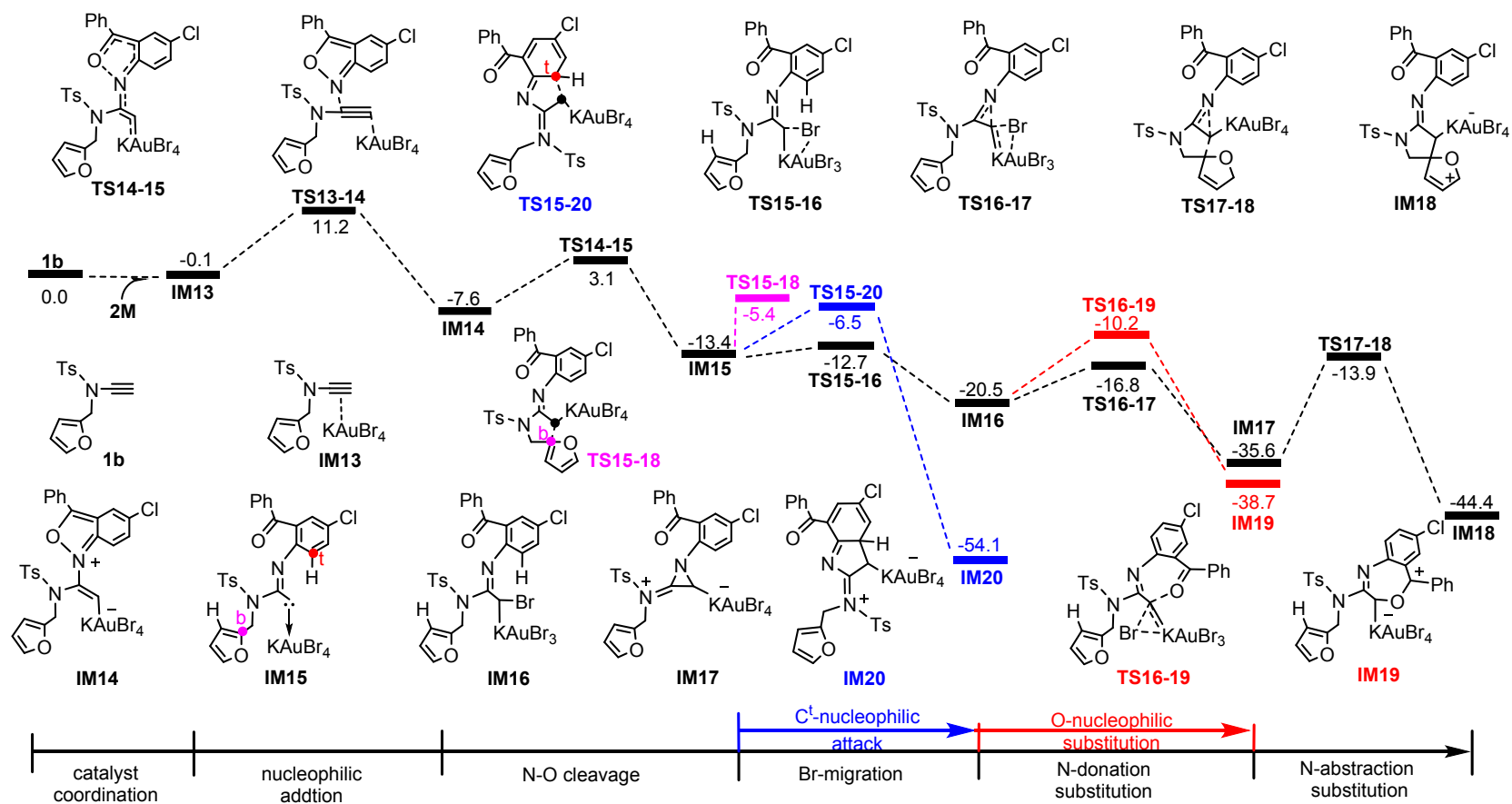


Fig. S4 Calculated free energy profiles in DCE solvent for all possible pathways from the KAuBr_3 -catalyzed annulation reaction of **1b** with **2M** (**1b**-system). The relative free energies are given in kcal mol^{-1} .

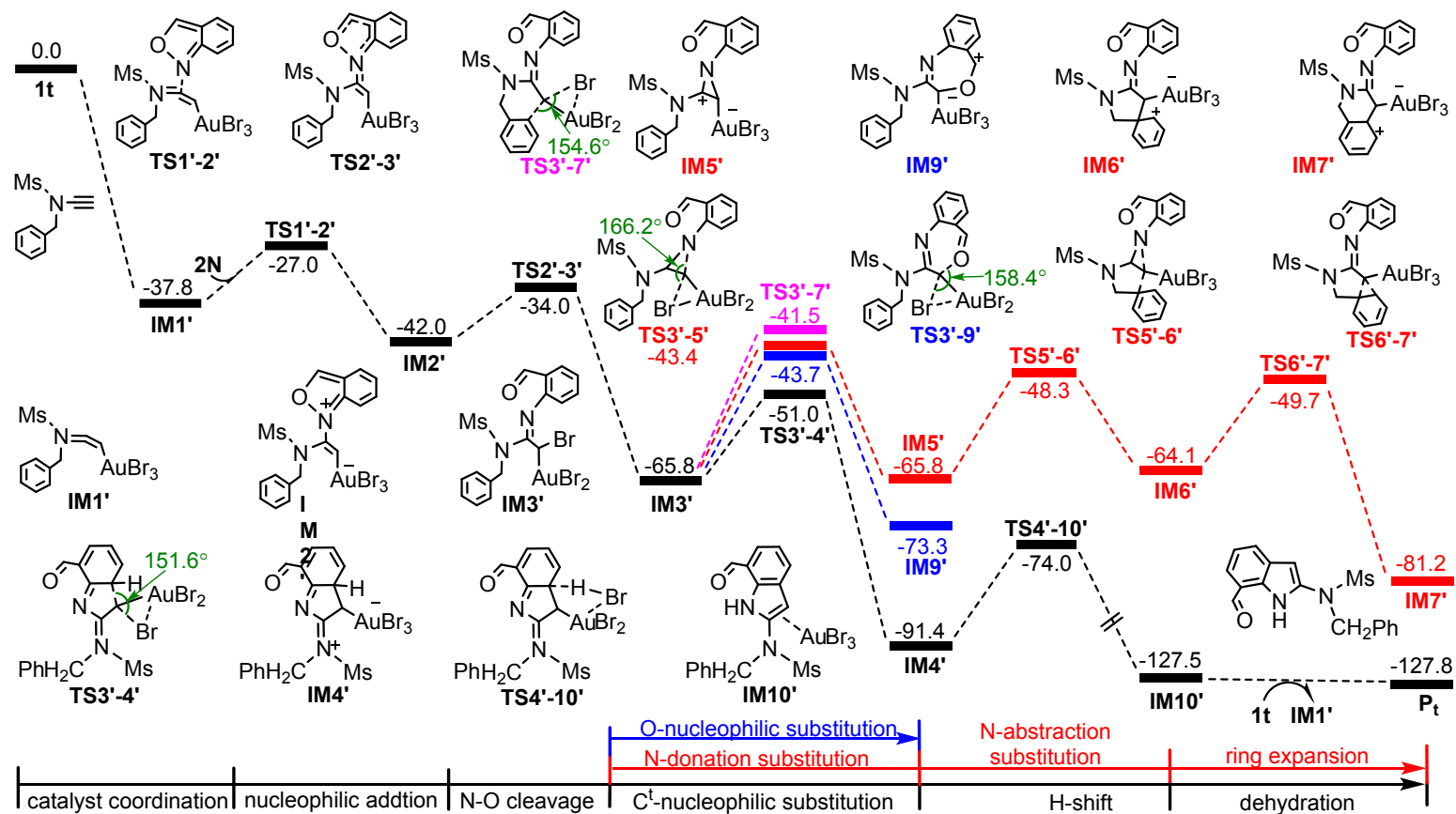


Fig. S5 Calculated free energy profiles in DCE solvent for all possible pathways from AuBr₃-catalyzed annulation of **1t** and **2b** (**1t**-system). The relative free energies are given in kcal mol⁻¹ and the bond angles are given in °.

Similar to the **1a** system, for the **1t** system, a series of the possible pathways from **IM3'**—the N-donation substitution via **TS3'-5'** (-43.4 kcal mol⁻¹), the C^a-nucleophilic substitution via **TS3'-7'** (-41.5 kcal mol⁻¹), and the O nucleophilic substitution via **TS3'-9'** (-43.7 kcal mol⁻¹)—are examined and compared with the C^t-nucleophilic substitution via **TS3'-4'** (-51.0 kcal mol⁻¹). Clearly, in all these transition states, **TS3'-4'** exhibits the highest stability, which is predicted to be related to the weakest Br *trans*-influence involved with the Br-C(Au)-C^t bond angle of 151.6°. In comparison, the Br-C(Au)-N bond angle in **TS3'-5'**, Br-C(Au)-C^a bond angle in **TS3'-7'** and Br-C(Au)-O bond angle in **TS3'-9'** are 166.2°, 154.6° and 158.4°, respectively. As a result, the smallest *trans*-influence in **TS3'-4'** renders the C^t attack the easiest (Fig. S5).

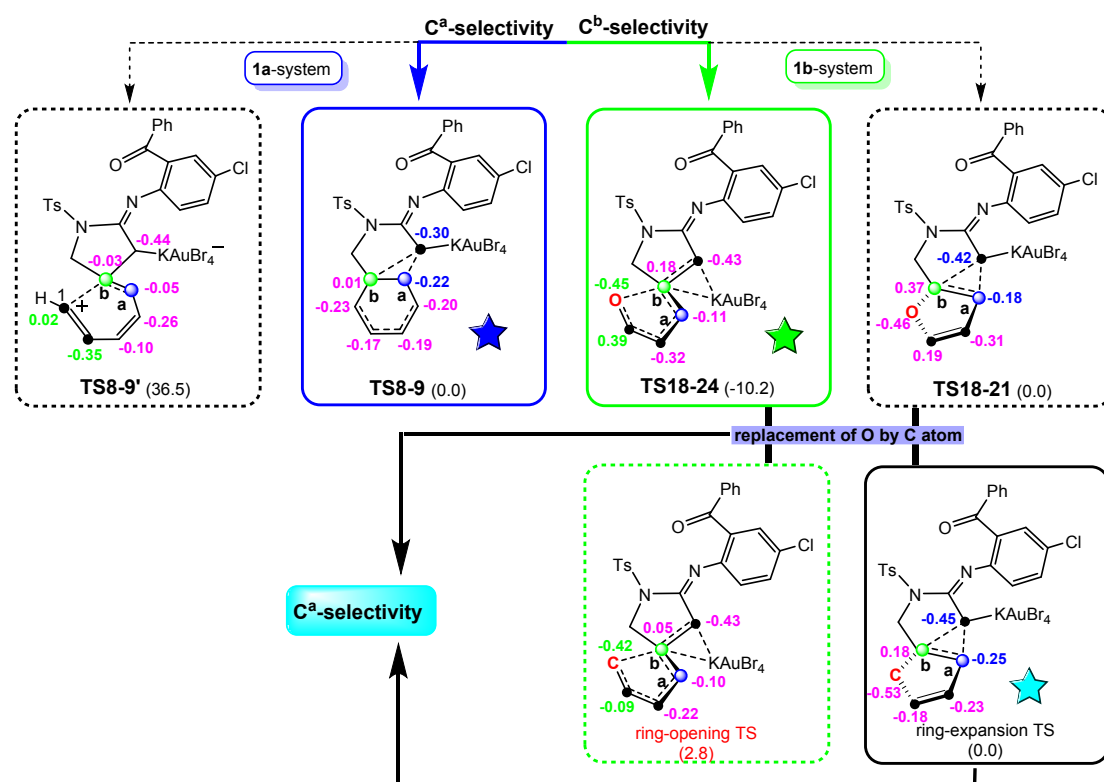


Fig. S6 Calculated NBO charges (in e) for ring-opening transition state and ring-expansion transition states in **1a**-, **1b**-systems, and the system with the replacement of O by C atom. The relative free energies are given in kcal mol⁻¹.

Table S2 Calculated Gibbs free energies in the gas-phase using B3LYP functional, single-point HF energies in DCM solvent using M06 functional, and imaginary frequencies for all structures in the present work. The relative energies and the imaginary frequencies are given in Hartree and cm^{-1} , respectively.

Structure	Gibbs Free Energy (B3LYP gas-phase optimized calculation)	Solvation Energy (M06 single-point calculation)	Imaginary Frequency
1a	-1221.594638	-1221.445757	
KAuBr₄	-217.850853	-217.6980519	
2M	-1090.155347	-1089.983608	
IM1	-1439.46876	-1439.163857	
TS1-2	-2529.604163	-2529.158119	-215.66
IM2	-2529.616048	-2529.188087	
TS2-3	-2529.603121	-2529.168868	-226.52
IM3	-2529.618688	-2529.191134	
TS3-9	-2529.60191	-2529.183739	-125.86
TS3-5	-2529.616548	-2529.192621	-57.47
IM5	-2529.632182	-2529.209229	
TS5-7	-2529.621323	-2529.201873	-80.26
IM7	-2529.639126	-2529.23108	
TS7-8	-2529.608464	-2529.194208	-209.92
IM8	-2529.628492	-2529.219556	
TS8-9	-2529.612408	-2529.19527	-180.32
IM9	-2529.634218	-2529.247041	
TS9-10	-2529.634894	-2529.234866	-243.48
IM10	-2529.690684	-2529.28571	
TS10-11	-2529.689996	-2529.281032	-51.33
IM11	-2529.70456	-2529.288047	
TS11-12	-2529.67725	-2529.27215	-110.24
IM12	-2529.700565	-2529.303911	
P_a	-2235.477624	-2235.173989	
TS3-4	-2529.608438	-2529.189294	-93.30
IM4	-2529.660672	-2529.261844	
TS5-6	-2529.616132	-2529.190423	-154.46
IM6	-2529.654386	-2529.241438	
1t	-990.617382	-990.5144337	
IM1'	-1166.662364	-1166.444464	
TS1'-2'	-1566.222783	-1565.944362	-212.32

IM2'	-1566.229893	-1565.9719	
TS2'-3'	-1566.223907	-1565.956887	-387.20
IM3'	-1566.263118	-1566.007985	
TS3'-7'	-1797.210063	-1796.907904	-38.53
TS3'-9'	-1566.238192	-1565.975048	-175.46
IM9'	-1566.271356	-1566.024312	
TS3'-5'	-1566.227624	-1565.969775	-108.31
IM5'	-1566.244549	-1566.004573	
TS5'-6'	-1566.236585	-1565.980844	-174.96
IM6'	-1566.24554	-1566.008491	
TS6'-7'	-1566.231474	-1565.98363	-119.39
IM7'	-1566.254634	-1566.035348	
TS3'-4'	-1566.242459	-1565.98537	-71.20
IM4'	-1566.280682	-1566.052193	
TS4'-10'	-1566.266021	-1566.018412	-637.26
IM10'	-1566.347183	-1566.111578	
P_t	-1390.335314	-1390.181329	
1b	-1219.39921	-1219.263008	
IM13	-1437.274439	-1436.981352	
TS13-14	-2527.412877	-2526.974482	-207.26
IM14	-2527.425646	-2527.009653	
TS14-15	-2527.414278	-2526.990151	-40.7
IM15	-2527.427894	-2527.012666	
TS15-18	-2527.412833	-2526.999216	-58.45
TS15-20	-2527.413772	-2527.003157	-96.74
IM20	-2527.466251	-2527.079443	
TS16-17	-2527.42282	-2527.0132	-53.62
IM17	-2527.443684	-2527.048994	
TS16-19	-2527.418024	-2527.015511	-152.19
IM19	-2527.45985	-2527.060168	
TS15-16	-2527.416629	-2527.010648	-71.94
IM16	-2527.457325	-2527.047606	
TS17-18	-2527.426632	-2527.013493	-161.08
IM18	-2527.454703	-2527.066251	
TS18-21	-2527.420273	-2527.027913	-291.90
IM21	-2527.443274	-2527.066253	
TS18-24	-2527.446451	-2527.06333	-202.80
IM24	-2527.471953	-2527.070842	
TS24-25	-2527.45318	-2527.041537	-756.74
IM25	-2527.501174	-2527.081245	
TS25-26	-2527.474121	-2527.061571	-163.42
IM26	-2527.513722	-2527.1009	
P_b	-2309.643293	-2309.369422	

7a	-2233.286097	-2232.972821	
TS20-22	-2527.444466	-2527.038002	-815.18
IM22	-2527.517136	-2527.117441	
TS22-23	-2527.518949	-2527.115875	-815.07
IM23	-2527.537246	-2527.140131	
8a	-2309.678006	-2309.41106	

Cartesian coordinates for the stationary points given in Fig. 1

KAuBr₄

Au	0.24761100	-0.00006200	-0.19067700
Br	1.92464000	1.77375600	0.42735100
Br	1.92413000	-1.77457100	0.42670900
Br	-1.46897200	-1.85097900	-0.75046000
Br	-1.46845200	1.85155200	-0.74979700
K	-3.39639600	0.00030500	1.08020800

2M

C	1.25384100	1.74656700	0.08915700
C	0.58283600	0.47508800	0.04424500
C	1.33431800	-0.73063500	-0.04460600
C	2.69582400	-0.61173400	-0.05382600
C	3.38028000	0.64382600	0.01418100
C	2.68005600	1.81715600	0.08043500
C	-0.76510400	0.81740600	0.06639200
H	0.86100600	-1.70176100	-0.11996500
H	4.46470800	0.64395400	0.00420300
H	3.17985800	2.77887800	0.12211000
O	-0.85187200	2.16321200	0.11206400
N	0.40215200	2.76516400	0.12790900
Cl	3.70914400	-2.09312100	-0.16904000
C	-3.20661300	0.69949900	-0.37887700
C	-4.40123300	-0.01376900	-0.41661100
C	-4.43170300	-1.36076800	-0.04518200
C	-3.25754500	-1.98981600	0.37494200
C	-2.05899400	-1.28155700	0.41946500
C	-2.01683000	0.07080500	0.03471900
H	-3.18180800	1.74296900	-0.67456800
H	-5.31152500	0.48245900	-0.74121300
H	-5.36543600	-1.91502200	-0.07828000
H	-3.27563600	-3.03264200	0.67886800
H	-1.16149800	-1.77003600	0.78405100

1a

C	-0.65300900	0.11601600	1.67325400
C	-0.49601200	-0.31736200	2.79544500
H	-0.42907000	-0.63667600	3.80923400
N	-0.82290300	0.59590700	0.43303500
C	-3.33527000	-1.79869600	-0.08197200
C	-2.83602700	-0.53550100	-0.41234200
C	-3.72920000	0.53283300	-0.57186500
C	-5.09887500	0.33581400	-0.40898600

C	-5.59247800	-0.93203800	-0.08530200
C	-4.70889600	-1.99886800	0.07791700
H	-2.64696300	-2.63023500	0.05062800
H	-3.34169900	1.51839600	-0.81628600
H	-5.78325900	1.17030400	-0.53616700
H	-6.66112100	-1.08481300	0.04008500
H	-5.08502700	-2.98608700	0.33287200
C	-1.35031100	-0.31944200	-0.60691000
H	-0.81637200	-1.27897200	-0.59261600
H	-1.16022400	0.17786800	-1.56263100
C	3.55023900	-0.98760300	-1.36707200
C	2.44831300	-0.13359000	-1.36978000
C	2.12883900	0.52634300	-0.18920300
C	2.85792200	0.36724600	0.98359700
C	3.95389400	-0.49407900	0.96127500
C	4.31264700	-1.18537300	-0.20576000
H	3.82683400	-1.50144100	-2.28412300
H	1.86630200	0.04123200	-2.26846300
H	2.58496800	0.91732800	1.87692700
H	4.54349000	-0.62590700	1.86482500
C	5.48580700	-2.13633800	-0.20713800
H	5.94326100	-2.20758600	-1.19910300
H	6.25723200	-1.82201900	0.50314700
H	5.16973900	-3.14781500	0.08064800
S	0.66057900	1.63863700	-0.16752200
O	0.86536900	2.69065100	0.92179000
O	0.29681500	1.99318900	-1.61689500

IMI

C	-1.17586500	0.97733900	0.27220100
C	-0.91201500	-0.01388800	1.06593300
H	-1.44264300	-0.18111000	1.99774700
N	-1.45048400	1.83051400	-0.58879800
C	-1.92972400	4.71243400	0.87270700
C	-0.79977900	4.00049000	0.44654700
C	0.37975400	4.05712300	1.20063700
C	0.42442000	4.81954100	2.36986900
C	-0.70509100	5.52231000	2.79287900
C	-1.88348200	5.46906400	2.04251600
H	-2.84203800	4.67940100	0.28096400
H	1.26186500	3.51469400	0.87102000
H	1.34523700	4.86546200	2.94396900
H	-0.66713000	6.11630400	3.70195500
H	-2.76087000	6.02349900	2.36404000

C	-0.85111200	3.18193300	-0.81917600
H	-1.48001900	3.64855300	-1.58245000
H	0.14576300	3.00976600	-1.23512200
C	-6.18932700	0.37394300	-0.32521300
C	-5.17304900	1.04101400	-1.00323000
C	-4.03342700	0.31108300	-1.32908100
C	-3.85002700	-1.02666800	-0.99300300
C	-4.88307500	-1.66197400	-0.30652400
C	-6.06172600	-0.97970700	0.03210400
H	-7.09721500	0.91331200	-0.06960900
H	-5.26500100	2.08382300	-1.28681800
H	-2.94052800	-1.56021100	-1.24629100
H	-4.75483700	-2.70246800	-0.02292600
C	-7.17933600	-1.69418600	0.75038900
H	-7.82506400	-0.99348300	1.28819400
H	-7.80879100	-2.24185800	0.03673900
H	-6.78987800	-2.42462100	1.46652800
S	-2.68305700	1.17567600	-2.20443600
O	-1.80620600	0.19147100	-2.97593600
O	-3.15795500	2.50848700	-2.79222900
Au	0.52128700	-1.38997600	0.54381000
Br	-1.28100200	-3.22551000	0.98246000
Br	2.33279000	-3.11183700	-0.09100400
Br	2.17438600	0.57143900	0.10415300
Br	4.72255300	2.22242500	-0.76430400
K	4.80351700	-0.98337700	-0.91810800

TS1-2

C	-1.14319800	0.52311500	-0.18574500
C	-1.20803900	-0.77481300	0.03854800
H	-2.14857600	-1.31029000	0.05490100
N	-0.36636600	1.53266400	-0.39617200
C	2.01003300	2.95220800	0.96975000
C	0.84965900	3.55354400	0.46366300
C	0.89371000	4.89422700	0.06231000
C	2.08048900	5.62338000	0.16990400
C	3.23422600	5.01221500	0.66576700
C	3.20213100	3.67181300	1.06301100
H	1.98296100	1.91058800	1.27844100
H	0.00300700	5.36253200	-0.34822200
H	2.10307000	6.66403500	-0.14292000
H	4.16143600	5.57404500	0.73944000
H	4.10477800	3.17978600	1.41727100
C	-0.45168100	2.78683900	0.38588800

H	-0.77811800	2.47319000	1.38444700
H	-1.24307900	3.40803700	-0.04921000
C	3.52858100	-0.02633400	-2.91956000
C	2.16004200	0.22415600	-2.83021400
C	1.76540700	1.53806700	-2.59753200
C	2.65533300	2.59709300	-2.44650800
C	4.01313800	2.31149500	-2.54294700
C	4.47345600	1.00147700	-2.76440000
H	3.86461900	-1.04292300	-3.10390400
H	1.43102400	-0.57177500	-2.94130800
H	2.30206000	3.60269200	-2.24839700
H	4.73198400	3.11548400	-2.41759600
C	5.94991900	0.71143700	-2.77944200
H	6.49963400	1.46779100	-3.35054600
H	6.33486300	0.73292200	-1.74951900
H	6.16429900	-0.27216300	-3.20854900
S	-0.01835500	1.86539200	-2.39045500
O	-0.37020900	3.34344600	-2.59056900
O	-0.83913500	0.75030600	-3.05428600
Au	0.43365100	-1.95412600	0.35533500
Br	-0.19345700	-3.06677600	-1.83043700
Br	2.43518600	-3.54219100	0.67504500
Br	0.87709000	-0.76483900	2.57683200
Br	6.20649700	1.11620400	1.20440200
K	4.30727400	-1.17047900	2.06763600
C	-4.01571800	0.63676200	-1.06752000
C	-5.23087800	0.52821100	-0.31983000
C	-6.43775000	0.14637200	-0.96553000
C	-6.35684300	-0.14839800	-2.30030400
C	-5.13897500	-0.07692800	-3.04232500
C	-3.96502200	0.31831200	-2.45089900
C	-4.87624900	0.90222300	0.98095400
H	-7.38364900	0.10536000	-0.44091300
H	-5.15845100	-0.33395400	-4.09573400
H	-3.03064700	0.39387400	-2.99656800
O	-3.56885400	1.21372900	0.99092400
N	-3.02053800	1.08595600	-0.28420900
Cl	-7.83500200	-0.63596300	-3.18149800
C	-5.09330400	1.86902000	3.25599500
C	-5.78395100	1.99578400	4.45662600
C	-6.97695200	1.29585600	4.65973100
C	-7.47609500	0.45972300	3.65770400
C	-6.79271900	0.32690900	2.45249200
C	-5.59606300	1.03630000	2.23716500

H	-4.17230700	2.41888800	3.09482200
H	-5.39235500	2.64356800	5.23505300
H	-7.51310600	1.39761300	5.59872200
H	-8.39380800	-0.09781100	3.81863400
H	-7.16575800	-0.35578300	1.69695200

IM2

C	1.46176100	-0.08538000	0.03384600
C	1.12115000	-1.29504000	-0.44425900
H	1.91112800	-1.99079500	-0.71716600
N	0.59581500	0.92692600	0.44713100
C	-1.40573600	3.09247500	-0.43833200
C	-0.16106400	3.31003000	0.16759700
C	0.05721500	4.50267300	0.86767500
C	-0.95368500	5.46279900	0.95949700
C	-2.19489900	5.23016100	0.36363000
C	-2.42482700	4.04014300	-0.33408900
H	-1.57488600	2.16668500	-0.98113600
H	1.01367100	4.67131400	1.35574000
H	-0.77246100	6.38523100	1.50536900
H	-2.98786600	5.96867600	0.44450200
H	-3.40135100	3.84052500	-0.76925500
C	0.95903600	2.30147700	0.02561300
H	1.22178200	2.20009100	-1.03509600
H	1.84808300	2.66040300	0.56177100
C	-3.53883900	-0.16538800	2.76847300
C	-2.15435700	-0.23699100	2.61219000
C	-1.43808600	0.95327000	2.67662900
C	-2.02944000	2.19128300	2.89772200
C	-3.41233800	2.22909400	3.05201800
C	-4.19009900	1.06174500	2.97465000
H	-4.12011200	-1.08266500	2.72623300
H	-1.65225900	-1.18627600	2.45576100
H	-1.43223600	3.09504400	2.93319500
H	-3.90009500	3.18602600	3.21252400
C	-5.69143500	1.14234100	3.06398100
H	-6.09886400	1.49062200	2.10391400
H	-6.13482100	0.16769900	3.29139500
H	-6.00785100	1.85503500	3.83350300
S	0.37016400	0.88041200	2.40857200
O	1.07647000	2.12916200	2.97084100
O	0.87433700	-0.52550600	2.80230900
Au	-0.74648600	-2.03273000	-0.71236500
Br	-0.15317000	-3.68558900	1.10992900

Br	-3.09719500	-3.05825900	-0.99381500
Br	-1.07235900	-0.42726400	-2.67984900
Br	-5.97549100	2.35717700	-0.81082100
K	-4.43352900	-0.13454800	-1.80501300
C	3.91561000	-0.13327200	0.91395500
C	5.14569600	0.24255200	0.29596300
C	6.37122800	0.08096000	0.99471400
C	6.30268800	-0.48115600	2.24266400
C	5.07262500	-0.87985500	2.84341600
C	3.86706400	-0.71111500	2.20327800
C	4.79283600	0.75719000	-0.96037700
H	7.31621800	0.40123800	0.57622200
H	5.09727900	-1.31299600	3.83746300
H	2.91255700	-0.96081200	2.65674000
O	3.45821100	0.70603400	-1.09235600
N	2.90177900	0.16893100	0.07514500
Cl	7.80111900	-0.71713200	3.18106700
C	4.89299500	2.17116900	-2.99372700
C	5.60535200	2.69816900	-4.06491900
C	6.95395100	2.37274900	-4.24065300
C	7.59154300	1.51098200	-3.34361100
C	6.88970800	0.98003500	-2.26641500
C	5.53344500	1.31133200	-2.07814600
H	3.84922500	2.43084600	-2.85259500
H	5.10905800	3.36507200	-4.76292500
H	7.50598600	2.78597600	-5.07957200
H	8.63368700	1.24439000	-3.48957300
H	7.37960300	0.27802800	-1.60096400

TS2-3

C	1.40714700	0.28942100	0.27706800
C	1.24327200	-0.91269400	-0.37555000
H	2.14042300	-1.46413300	-0.65176000
N	0.31558700	1.14022400	0.58339400
C	-1.96288600	2.98475100	-0.41347200
C	-0.75857300	3.38187300	0.18273000
C	-0.70432400	4.61282200	0.84782700
C	-1.83401500	5.43212000	0.91393400
C	-3.03189900	5.02060900	0.32636400
C	-3.09897400	3.79134700	-0.33676300
H	-2.00538000	2.02924600	-0.92887900
H	0.21942400	4.91913100	1.33104700
H	-1.77849900	6.38525700	1.43363000
H	-3.91598000	5.64950100	0.38688900

H	-4.03813800	3.45335800	-0.76810900
C	0.48692300	2.52837100	0.07625000
H	0.75983400	2.39776200	-0.97867400
H	1.32702100	3.02561500	0.57640400
C	-3.53466300	-0.54051200	2.88696100
C	-2.15500500	-0.37310600	2.76483700
C	-1.65805100	0.92484200	2.78432700
C	-2.46318800	2.04740800	2.93463600
C	-3.83581400	1.84863400	3.05695700
C	-4.39581400	0.56091000	3.01751300
H	-3.94622300	-1.54620900	2.87486300
H	-1.48984600	-1.22429600	2.66443300
H	-2.03395500	3.04274200	2.93819000
H	-4.48767400	2.71117600	3.16035600
C	-5.89096200	0.38177700	3.06850500
H	-6.32989900	0.65429400	2.09841400
H	-6.16574100	-0.65431100	3.28982400
H	-6.34451600	1.02934400	3.82715200
S	0.14041600	1.16292100	2.52992000
O	0.59205900	2.53890300	3.04598800
O	0.89016700	-0.11510600	2.96734700
Au	-0.47640000	-1.84614400	-0.83167000
Br	0.22214000	-3.41409800	1.03549500
Br	-2.61722300	-3.16928100	-1.32056200
Br	-0.83733300	-0.23135500	-2.77562000
Br	-6.37520200	1.56820500	-0.85431600
K	-4.33914300	-0.42916100	-2.05076400
C	3.73090100	-0.12335100	0.95131200
C	4.96074400	0.22625100	0.34229400
C	6.15917600	-0.38825500	0.74982100
C	6.08684600	-1.37759700	1.71107600
C	4.86386000	-1.76119300	2.28962300
C	3.67899800	-1.13963500	1.92497500
C	4.73870000	1.28608000	-0.61809600
H	7.11342100	-0.09869300	0.32988600
H	4.85131800	-2.54260100	3.04190700
H	2.73562900	-1.36947100	2.40664000
O	3.52725800	1.63978800	-0.72683300
N	2.66090800	0.68716100	0.64773700
Cl	7.58529000	-2.19629000	2.23653600
C	5.55526000	3.37359000	-1.66871200
C	6.49008300	4.07785600	-2.42026600
C	7.60874600	3.42074400	-2.94182800
C	7.79201900	2.05454000	-2.71318000

C	6.87259100	1.34461800	-1.94447600
C	5.75264100	2.00497900	-1.40799100
H	4.68004400	3.87149800	-1.26513400
H	6.34457100	5.13782800	-2.60461900
H	8.33294300	3.97180600	-3.53468700
H	8.64776800	1.53947100	-3.13877600
H	6.99905700	0.27623100	-1.80724800

IM3

C	1.31503100	0.56215900	0.17313100
C	1.55645900	-0.83010500	0.05593200
H	2.60265700	-1.12153300	0.02291600
N	0.00717200	1.06496500	0.00148500
C	-2.13394200	2.03754900	-1.78456400
C	-1.39566600	2.90300800	-0.96764900
C	-1.85647600	4.21009300	-0.76628200
C	-3.03884400	4.64530400	-1.36564700
C	-3.78017000	3.77265900	-2.16470100
C	-3.32527200	2.46824800	-2.37099300
H	-1.77345900	1.02758800	-1.95454800
H	-1.29124800	4.88853800	-0.13074000
H	-3.38641200	5.66135100	-1.19824900
H	-4.71079500	4.10142200	-2.61807400
H	-3.90551000	1.78281300	-2.98135900
C	-0.06644100	2.49198800	-0.37134000
H	0.72424100	2.61972100	-1.12016500
H	0.21378400	3.15560100	0.45977200
C	-4.23978100	3.04032700	2.07193000
C	-3.39866200	2.01152100	1.65708600
C	-2.08892000	2.03054800	2.12047400
C	-1.58056100	3.01640800	2.96038000
C	-2.44595700	4.03684500	3.35041500
C	-3.78098500	4.06414400	2.91576100
H	-5.26872100	3.03035100	1.72297300
H	-3.78659300	1.23806100	1.00150400
H	-0.55802200	2.97004000	3.31847900
H	-2.07965200	4.81695900	4.01230500
C	-4.71777300	5.15926900	3.36282200
H	-5.31224900	5.53817800	2.52451500
H	-5.42441700	4.78285700	4.11347200
H	-4.17526400	5.99877200	3.80787800
S	-0.95798100	0.65270600	1.66957000
O	0.14456100	0.55431300	2.74059000
O	-1.79560600	-0.58851400	1.29647000

Au	0.29510400	-2.36491400	-0.19842300
Br	1.30434600	-3.02482300	2.04655200
Br	-1.21830300	-4.42071600	-0.31814400
Br	-0.37068000	-1.59997300	-2.52984500
Br	-5.95864600	0.03427100	-0.28842800
K	-3.50997400	-1.96493100	-0.29016300
C	3.57468600	1.13431700	0.66909200
C	4.68691000	1.86997500	0.14634400
C	5.94835000	1.68492600	0.69287300
C	6.12631500	0.77541900	1.74160500
C	5.05633000	0.06819700	2.29568200
C	3.78802500	0.24974800	1.76831400
C	4.53065200	2.90742800	-0.94767800
H	6.78991300	2.25027600	0.30875500
H	5.21373800	-0.58724900	3.14501400
H	2.92902100	-0.20422300	2.25220300
O	4.99543100	4.01877300	-0.73852400
N	2.33200800	1.42433200	0.20444400
Cl	7.75447600	0.55244200	2.41528800
C	3.42114100	3.59982600	-3.05761000
C	2.81667500	3.31660100	-4.27830500
C	2.67048900	1.98886600	-4.69643800
C	3.13109600	0.94371700	-3.89137900
C	3.71844500	1.22473900	-2.65874500
C	3.86286600	2.55412900	-2.22879700
H	3.55928100	4.62258200	-2.72224100
H	2.46215200	4.12692400	-4.90868400
H	2.20155800	1.76919200	-5.65139700
H	3.02852500	-0.08571100	-4.22101500
H	4.08679300	0.40924600	-2.04262000

TS3-9

C	1.62823600	0.52489800	0.04316700
C	0.84902700	-0.69499600	-0.11050600
H	1.42696400	-1.60682200	-0.19719100
N	2.96720700	0.27998300	0.47546200
C	0.85213600	-1.17699700	2.22789500
C	2.27488100	-1.24093300	2.18479600
C	2.89855400	-2.48602600	2.19981000
C	2.13772500	-3.65857700	2.29337900
C	0.73819600	-3.60630900	2.35748800
C	0.09996500	-2.37276800	2.33921300
H	0.35922000	-0.22137800	2.38694400
H	3.98158200	-2.54553500	2.13276600

H	2.64207600	-4.62096300	2.31496200
H	0.13385500	-4.50591900	2.43309400
H	-0.98100600	-2.33953000	2.41811500
C	3.06408600	0.02045500	1.93896900
H	2.68295800	0.87477700	2.51094200
H	4.11888300	-0.13098100	2.18243200
C	7.13705800	-0.94377900	-1.13249700
C	5.94310500	-0.22738500	-1.13191700
C	5.71325400	0.65746900	-0.08434700
C	6.62359800	0.86257400	0.94272300
C	7.81392900	0.13270000	0.92016600
C	8.08764300	-0.77622600	-0.11073700
H	7.33726500	-1.64098700	-1.94206500
H	5.21384100	-0.34170500	-1.92703900
H	6.40886000	1.58354900	1.72467600
H	8.54156900	0.27909300	1.71393100
C	9.38693700	-1.54489700	-0.14373400
H	9.22033200	-2.60052400	-0.38537600
H	10.06074400	-1.14075900	-0.91003600
H	9.90904900	-1.49323100	0.81626100
S	4.14844000	1.63216900	-0.08094900
O	4.27162800	2.71778100	0.99728200
O	3.75875900	1.94026600	-1.53263500
Au	-0.99858000	-0.83140300	-0.96780200
Br	-2.38586700	-0.06158000	1.03459100
Br	-3.15426500	-1.15759400	-2.33364500
Br	0.42750400	-1.67255500	-2.90293600
Br	-2.79684800	-4.80760500	2.28890000
K	-4.24715700	-2.93805900	0.30006200
C	0.15353700	2.26379300	-0.74158500
C	-0.76099500	3.12621500	-0.07388200
C	-1.69460700	3.84369000	-0.83247500
C	-1.74778700	3.68039800	-2.21078100
C	-0.88492000	2.81138800	-2.87208400
C	0.06671800	2.10805700	-2.13856700
C	-0.66281300	3.22112300	1.40756500
H	-2.37759000	4.52935100	-0.34858900
H	-0.94221500	2.69080900	-3.94821200
H	0.79507900	1.48544000	-2.64508000
O	0.22980500	2.61087400	1.99642200
N	1.24031600	1.74861900	-0.06580800
Cl	-2.95963000	4.60524900	-3.15210300
C	-1.06774100	4.87519700	3.21891200
C	-1.90528400	5.63885800	4.02826200

C	-3.29127800	5.57751900	3.85741700
C	-3.83668700	4.75003400	2.87419000
C	-3.00063300	4.00173700	2.04375300
C	-1.60769400	4.06785000	2.20586400
H	0.00857700	4.89674300	3.35818800
H	-1.47849400	6.27526000	4.79832600
H	-3.94444500	6.16655000	4.49531300
H	-4.91415000	4.68253700	2.75331500
H	-3.43192800	3.33900400	1.29968400

TS3-5

C	-1.36287400	0.35912900	-0.30091900
C	-1.53561700	-1.06633200	-0.31434500
H	-2.55820700	-1.42938300	-0.35796900
N	-0.08553400	0.86026400	0.05045600
C	1.95285400	1.49914300	2.07407600
C	1.19230300	2.49402200	1.44571400
C	1.60416200	3.82891200	1.54220800
C	2.76018400	4.16563200	2.24709900
C	3.52434100	3.16793600	2.85561800
C	3.11774000	1.83494000	2.76645700
H	1.62939800	0.46453000	2.01937500
H	1.02378300	4.60809300	1.05279900
H	3.07037800	5.20534000	2.30971300
H	4.43470900	3.42441200	3.38962800
H	3.71246400	1.05411400	3.23138300
C	-0.10439200	2.17133000	0.73382400
H	-0.91830500	2.08769000	1.46460200
H	-0.39977300	2.99017300	0.06338400
C	4.00387400	3.62892300	-1.48791500
C	3.26504200	2.46233400	-1.31138100
C	1.94969600	2.46634200	-1.75713300
C	1.33685700	3.56507500	-2.35154000
C	2.09984200	4.72188700	-2.50104300
C	3.43706100	4.77125700	-2.07501300
H	5.04017700	3.62936100	-1.16103100
H	3.73817600	1.59743100	-0.85501200
H	0.31559800	3.50712200	-2.71178400
H	1.65162600	5.59404700	-2.96929100
C	4.26319500	6.02069700	-2.25783300
H	4.73067200	6.32587600	-1.31467600
H	5.07473200	5.84897900	-2.97571000
H	3.65910500	6.85513000	-2.62612100
S	0.95769000	0.92039500	-1.63636400

O	-0.11155700	0.94380900	-2.74610200
O	1.91408100	-0.28227400	-1.49858400
Au	-0.13619500	-2.41881900	0.20522000
Br	-0.80221500	-2.51765300	-2.28874500
Br	1.67284800	-4.21357000	0.37057700
Br	-0.22396800	-1.94563900	2.67067700
Br	6.10866300	0.30073000	-0.26737600
K	3.87834200	-1.87111100	-0.66233300
C	-3.63066600	0.91544900	-0.85457700
C	-4.74627900	1.61929500	-0.31051400
C	-6.00287800	1.46919300	-0.88655700
C	-6.16515900	0.62899600	-1.98951800
C	-5.08521400	-0.04063500	-2.56743600
C	-3.82598800	0.10442500	-2.00403000
C	-4.60899400	2.60910300	0.82952500
H	-6.84813200	2.01591300	-0.48411000
H	-5.22741900	-0.64309700	-3.45771200
H	-2.96269800	-0.32934600	-2.49592400
O	-5.03011500	3.74190800	0.64460300
N	-2.38739000	1.18454300	-0.34658000
Cl	-7.78510600	0.44522300	-2.70452100
C	-3.62977900	3.18717800	3.03602900
C	-3.10716200	2.84013600	4.27766100
C	-2.99209200	1.49220200	4.63713700
C	-3.40000000	0.49164200	3.75138800
C	-3.90575200	0.83713600	2.49880600
C	-4.02062800	2.18685600	2.12889600
H	-3.74411500	4.22601300	2.74398900
H	-2.79310200	3.61585400	4.97005300
H	-2.58864700	1.22252700	5.60911400
H	-3.31968000	-0.55373800	4.03295900
H	-4.23335100	0.05588600	1.81871900

IM5

C	-1.16735400	0.42913400	-0.70155000
C	-1.29763000	-1.02732000	-0.31481600
H	-2.09051500	-1.11795600	0.42835300
N	0.05374100	1.07725700	-0.44085400
C	1.63302000	2.51196100	1.57590900
C	1.11254800	3.16386700	0.45128300
C	1.57926000	4.44306200	0.12520200
C	2.55600100	5.06036300	0.90715200
C	3.08688600	4.39763900	2.01566700
C	2.62494400	3.12209000	2.34616000

H	1.26978800	1.52285500	1.83813100
H	1.18364000	4.95516100	-0.74953400
H	2.91166400	6.05266100	0.64227600
H	3.86311800	4.86596800	2.61377300
H	3.04741300	2.59571400	3.19650400
C	-0.00114300	2.55544300	-0.37476900
H	-0.96852400	2.76836000	0.09101500
H	-0.04994900	3.00934800	-1.37352500
C	4.63786600	2.88331700	-1.68866700
C	3.72261300	1.90864200	-1.30210700
C	2.58720400	1.75420100	-2.08692500
C	2.31656000	2.51499500	-3.22014100
C	3.24894200	3.48909500	-3.57328900
C	4.41547300	3.68808100	-2.81743100
H	5.53605200	2.99863500	-1.08797900
H	3.93607200	1.30941300	-0.42185500
H	1.43023600	2.33280000	-3.81795000
H	3.07123300	4.09408800	-4.45822900
C	5.42122500	4.74353900	-3.20589300
H	5.51162900	5.50405800	-2.42077900
H	6.41662400	4.30495400	-3.34134200
H	5.14123100	5.24750500	-4.13555500
S	1.38604300	0.42143400	-1.68427100
O	0.59606000	0.05266300	-2.95109200
O	2.11410900	-0.70722800	-0.90379800
Au	0.23785200	-2.32728400	0.18115800
Br	-1.74647100	-2.27475800	-1.82473200
Br	1.83671800	-4.31769900	0.23879300
Br	0.47713800	-1.43728100	2.54826800
Br	5.89794000	0.59881700	1.36451900
K	3.84750500	-1.74026300	1.05807300
C	-3.49967200	0.71458400	-1.28312200
C	-4.48471600	0.75131300	-0.26429600
C	-5.82088200	0.47644400	-0.59403400
C	-6.17264800	0.17213000	-1.90199900
C	-5.22191500	0.15949700	-2.91835900
C	-3.89605100	0.44660500	-2.60662500
C	-4.10585200	0.97796200	1.17080000
H	-6.57806800	0.48353300	0.18180700
H	-5.51169500	-0.06257100	-3.93955600
H	-3.14486700	0.47313800	-3.38932100
O	-3.11549500	0.40922200	1.62759100
N	-2.17563800	1.11423100	-1.08183500
Cl	-7.88449400	-0.19603800	-2.28877400

C	-4.79969700	1.74207700	3.42777900
C	-5.51922000	2.57317300	4.27965400
C	-6.36638900	3.55296600	3.75043800
C	-6.49202400	3.69819500	2.36730600
C	-5.78305200	2.85735900	1.50986200
C	-4.93308700	1.86850200	2.03355100
H	-4.12821500	0.98502100	3.81912200
H	-5.41980500	2.46283900	5.35566100
H	-6.92467000	4.20475900	4.41689200
H	-7.13972900	4.46691400	1.95581600
H	-5.87359400	2.98394900	0.43598200

TS5-7

C	-0.72789500	1.28396700	-0.60488100
C	-1.33701300	0.07671700	-1.05205900
H	-2.24548800	0.19796600	-1.63141100
N	0.50284100	1.74866800	-0.56873000
C	1.62050500	1.91597600	2.23944500
C	1.76925700	2.92251700	1.27816900
C	2.75712800	3.89803200	1.45269700
C	3.58851400	3.86866900	2.57318900
C	3.44855300	2.85193400	3.51992000
C	2.46368800	1.87616400	3.34775700
H	0.85492800	1.15428400	2.11823900
H	2.88224300	4.68176700	0.70776000
H	4.35352300	4.63131500	2.69965400
H	4.10569500	2.81396200	4.38323400
H	2.35912100	1.07824500	4.07696900
C	0.83902200	3.02807600	0.08835200
H	-0.12372100	3.45617000	0.38980000
H	1.26842000	3.69110000	-0.67247600
C	5.50937000	2.11644400	-0.59870500
C	4.31487200	1.39942500	-0.61901500
C	3.37481400	1.76937200	-1.57195000
C	3.54856500	2.80572900	-2.48863600
C	4.74904200	3.50788500	-2.42936100
C	5.74241900	3.17525400	-1.48963700
H	6.25875900	1.82213500	0.12971700
H	4.18423100	0.57491900	0.08184800
H	2.79315900	3.03225300	-3.23197800
H	4.92189300	4.31943900	-3.13147800
C	7.05459100	3.91867200	-1.46404100
H	7.41706800	4.05074700	-0.44013400
H	7.82529100	3.35564000	-2.00817000

H	6.97003200	4.90392300	-1.93321300
S	1.83070800	0.79413000	-1.70312000
O	1.20933300	0.94274100	-3.08786200
O	1.98587600	-0.57560300	-1.04089800
Au	-0.77612600	-1.84170400	-0.70476300
Br	-1.28542600	-2.09864800	-3.17986800
Br	0.00286600	-4.26583700	-0.52456900
Br	-0.42250800	-1.49098900	1.79629800
Br	5.34518600	-1.17616300	1.66097100
K	2.76023300	-2.66642300	0.73240900
C	-2.93941800	2.24484200	-0.30746800
C	-4.00044300	2.38224600	0.61674300
C	-5.19556600	2.96936900	0.20599500
C	-5.33446500	3.41105100	-1.10903800
C	-4.29408800	3.30027400	-2.03119400
C	-3.09761600	2.72002100	-1.62749700
C	-3.81188700	1.99029500	2.07501700
H	-6.01559300	3.08823700	0.90772200
H	-4.41907700	3.66977600	-3.04315600
H	-2.27037500	2.65280500	-2.32898000
O	-3.41181300	2.84908100	2.84739100
N	-1.74727600	1.70234400	0.15801000
Cl	-6.87692800	4.15438400	-1.61880000
C	-3.87124100	0.23328900	3.82743700
C	-4.15204300	-1.05640500	4.25964100
C	-4.70446000	-1.98759200	3.37246300
C	-4.97973000	-1.62340000	2.05272800
C	-4.69327300	-0.33194800	1.61547000
C	-4.13450400	0.60550600	2.49851800
H	-3.44360500	0.97385000	4.49742200
H	-3.94263000	-1.34344200	5.28783800
H	-4.92164200	-2.99699400	3.71299500
H	-5.41325700	-2.34652600	1.36604600
H	-4.91343800	-0.04930400	0.58831400

IM7

C	-0.27226500	0.00140300	1.19191400
C	-1.46736700	0.42823600	0.45559000
H	-2.11071700	1.16452600	0.93410100
N	0.23114700	-0.72186000	2.13980200
C	-0.58337700	-1.63050600	2.99492700
H	0.06987100	-1.89622800	3.83041500
H	-0.80295200	-2.52414900	2.40443900
C	3.99544300	-3.24480100	-0.12505300

C	3.47764100	-2.08839300	0.45561300
C	2.83865300	-2.22831500	1.68050700
C	2.68274000	-3.44281100	2.34776400
C	3.19511700	-4.57780300	1.72818300
C	3.84890600	-4.49930100	0.48455700
H	4.54202200	-3.14170000	-1.05796200
H	3.65396800	-1.12743400	-0.02059500
H	2.20993000	-3.49914100	3.32199400
H	3.09804300	-5.53893900	2.22498800
C	4.38301800	-5.74039600	-0.18476600
H	3.68436600	-6.09186400	-0.95505000
H	5.33902300	-5.54229100	-0.67972300
H	4.52481700	-6.55611900	0.53039700
S	2.16318400	-0.73405500	2.48860300
O	2.18243900	-0.87167300	4.00927500
O	2.62733000	0.55291200	1.79491700
Au	-2.44835700	-0.72528700	-0.97892100
Br	-3.73611500	-2.06021500	-2.72273600
Br	-3.89873400	1.31096700	-1.39449200
Br	5.82301500	0.16466300	-1.00494600
Br	-0.90810300	-2.71969200	-0.55009100
K	4.55293500	2.27314300	0.88064300
C	0.82606100	1.30098300	-0.77635900
C	1.39656400	2.58455100	-0.77295000
C	2.21116000	2.96365100	-1.84853200
C	2.41073300	2.08799300	-2.91050600
C	1.85949800	0.80902300	-2.90737700
C	1.06722800	0.41438000	-1.83086600
C	1.29943600	3.54241800	0.39147900
H	2.66811700	3.94749000	-1.85960500
H	2.04974600	0.12753700	-3.72834100
H	0.63581400	-0.58127800	-1.81181200
O	2.35474200	3.87841800	0.93750600
N	-0.04455300	0.92862100	0.29220800
Cl	3.39939200	2.61771000	-4.29333700
C	-0.05715900	4.81962900	2.02748300
C	-1.25607800	5.37955900	2.45174500
C	-2.41122400	5.23021400	1.67433800
C	-2.36505300	4.51918200	0.47303500
C	-1.16605900	3.94879700	0.04729100
C	-0.00292400	4.09169700	0.82362200
H	0.85057600	4.93210100	2.61089500
H	-1.29545300	5.93550400	3.38410800
H	-3.34749900	5.67085400	2.00561700

H	-3.25819100	4.40033900	-0.13189300
H	-1.13912800	3.40658800	-0.89261400
C	-1.84582200	-0.97257300	3.50232200
C	-3.09353900	-1.36401000	3.00284100
C	-1.77463900	0.02496700	4.48484900
C	-4.26071100	-0.76068700	3.47853100
H	-3.15295500	-2.13917600	2.24299500
C	-2.93977200	0.62846900	4.95546400
H	-0.80574600	0.32099400	4.88112000
C	-4.18436100	0.23696000	4.45159600
H	-5.22473600	-1.07034900	3.08577200
H	-2.87877900	1.39791700	5.72006100
H	-5.09183900	0.70662500	4.82049500

TS7-8

C	-0.21935800	-1.04914500	0.73722700
C	1.24997400	-1.06646900	0.53849800
H	1.64467700	-2.04014200	0.25976600
N	-0.69120600	-0.48465700	1.89198600
C	0.33527900	-0.14500600	2.87892000
H	-0.11277700	-0.25448700	3.87176100
H	0.62257500	0.90166800	2.74405300
C	-5.72011000	0.53937600	0.99283200
C	-4.77915400	-0.36811500	1.47805900
C	-3.56484200	0.14369300	1.91875400
C	-3.24857700	1.49707800	1.89976900
C	-4.19986600	2.37834100	1.39160400
C	-5.44793500	1.91501800	0.94223000
H	-6.67426900	0.16593700	0.63143800
H	-4.97016300	-1.43565900	1.48903500
H	-2.28145500	1.86613100	2.22259000
H	-3.94366000	3.43188800	1.32064800
C	-6.47704600	2.88771900	0.42003900
H	-7.20495800	2.39287700	-0.23022300
H	-7.03174700	3.34663600	1.24898100
H	-6.00511500	3.70016800	-0.14185600
S	-2.36151200	-1.04761300	2.62075000
O	-2.14765500	-0.80329500	4.11883700
O	-2.62717400	-2.46253100	2.09930500
Au	2.31322500	0.46625300	-0.31727200
Br	3.67743900	2.35799500	-1.43788900
Br	4.12810800	-1.26632400	-0.92535900
Br	-1.44055000	4.92515900	0.12075200
Br	0.45421300	2.19938800	0.17488300

K	1.40731700	4.89391700	-1.31191800
C	-1.96065800	-1.44086900	-0.94293100
C	-2.67852900	-2.57584700	-1.39290400
C	-3.88353400	-2.38653300	-2.08070500
C	-4.31315600	-1.10493400	-2.39468700
C	-3.59376900	0.02204900	-2.00164700
C	-2.43058800	-0.14961000	-1.26180700
C	-2.32168800	-4.00817100	-1.06207200
H	-4.46756100	-3.25428500	-2.36463300
H	-3.94083700	1.01736000	-2.25572000
H	-1.86336300	0.71621100	-0.93731100
O	-3.21579900	-4.75391800	-0.68428300
N	-0.75226400	-1.59785200	-0.28182300
Cl	-5.83874100	-0.89151300	-3.31870500
C	-0.57797100	-5.71888400	-0.61346100
C	0.68369500	-6.27467800	-0.80802200
C	1.59475000	-5.65611500	-1.67074500
C	1.24031800	-4.47986700	-2.33700100
C	-0.01714700	-3.91324400	-2.12911800
C	-0.93409500	-4.52515800	-1.26147200
H	-1.30763400	-6.19316600	0.03487600
H	0.95602400	-7.19419100	-0.29673400
H	2.57738800	-6.09258200	-1.82907900
H	1.94332100	-4.00289000	-3.01362800
H	-0.28954600	-3.00094400	-2.64980600
C	1.56357700	-1.04654300	2.74331400
C	2.86113400	-0.47944200	2.85792400
C	1.43539100	-2.45724100	2.89117100
C	3.97745100	-1.28318200	3.04397000
H	2.97119000	0.59906800	2.78411200
C	2.55589800	-3.25534900	3.07331900
H	0.44680100	-2.90845300	2.84734000
C	3.82671700	-2.67043100	3.15076400
H	4.96446200	-0.83553900	3.09734000
H	2.44392700	-4.33114200	3.16545000
H	4.70173700	-3.29810900	3.29200500

IM8

C	0.64572500	0.10093400	0.48816600
C	-0.72311900	0.47607500	1.00084500
H	-0.70749800	1.47657000	1.42850500
N	0.95493800	-1.25033600	0.81306000
C	-0.20710300	-1.86208900	1.39417600
H	0.05377300	-2.60716900	2.14716700

H	-0.82902100	-2.32046300	0.61776800
C	6.13194300	-1.65379400	0.38142500
C	5.01626400	-1.14527400	1.04341500
C	3.92662800	-1.99455800	1.19695500
C	3.89965800	-3.30609800	0.74088400
C	5.02837700	-3.78045900	0.07453400
C	6.15375300	-2.96508000	-0.11878500
H	6.99673800	-1.01143800	0.24051000
H	4.99257200	-0.12466500	1.41258800
H	3.03560300	-3.94094400	0.90490700
H	5.03283100	-4.80080600	-0.29849600
C	7.36604700	-3.47232800	-0.86117100
H	7.54268000	-2.87606300	-1.76447500
H	8.26857900	-3.39777100	-0.24298200
H	7.24720700	-4.51727700	-1.16173900
S	2.47570000	-1.37347100	2.12702300
O	1.98129000	-2.47060100	3.08633400
O	2.75070200	0.04883800	2.64565700
Au	-2.21255900	0.71840300	-0.53399300
Br	-4.17398400	1.00859700	-2.24801900
Br	-3.37164500	2.27305900	1.09502400
Br	-3.34427200	-3.83793100	0.46850200
Br	-1.08562300	-0.91778200	-2.15274000
K	-4.13554200	-2.32646000	-2.21265300
C	2.56393100	0.72426200	-0.78918800
C	3.67058300	1.58348300	-0.59923600
C	4.83580500	1.38495700	-1.35051900
C	4.87251800	0.39451100	-2.32059700
C	3.78549900	-0.44692200	-2.54348700
C	2.64455900	-0.29043100	-1.76525300
C	3.75631700	2.60321100	0.51498000
H	5.70329000	2.00747600	-1.16211700
H	3.83230300	-1.21648100	-3.30627200
H	1.78758700	-0.93459900	-1.92070300
O	4.69538700	2.50844300	1.29938500
N	1.37565400	0.96447400	-0.09988100
Cl	6.37228600	0.16780900	-3.29033600
C	2.75297900	4.48072300	1.79186100
C	1.87226600	5.55086900	1.91749700
C	1.01380700	5.87679300	0.86185800
C	1.03861400	5.12985100	-0.31900200
C	1.91078100	4.04933600	-0.44153100
C	2.77207000	3.71492800	0.61445300
H	3.43519600	4.21523000	2.59280300

H	1.85382100	6.13439600	2.83389100
H	0.32703800	6.71341500	0.95888600
H	0.37622300	5.38651300	-1.14077400
H	1.92482300	3.46732900	-1.35715300
C	-1.10092900	-0.62387000	2.04739200
C	-2.50076500	-1.06600100	2.10311600
C	-0.51585800	-0.29877700	3.36949300
C	-3.15628200	-1.30231000	3.29688700
H	-3.01760900	-1.25852200	1.17292300
C	-1.19888700	-0.49726500	4.53804400
H	0.49716100	0.09462600	3.39553800
C	-2.51654400	-1.01250700	4.50364200
H	-4.16782100	-1.69224000	3.28332800
H	-0.73395000	-0.26466900	5.49059500
H	-3.04572600	-1.17422500	5.43932500

TS8-9

C	-0.53375200	-0.32440600	-0.72844600
C	0.92418200	-0.39632600	-1.07412600
H	1.29688800	0.55827600	-1.43893000
N	-1.40129400	-1.32412600	-1.18490700
C	-0.71774700	-2.46040300	-1.79303500
H	-1.37247300	-2.87422900	-2.57144300
H	-0.58408900	-3.22258400	-1.01993400
C	-6.04950700	0.87888300	-0.59394800
C	-4.82920100	0.80238400	-1.26265800
C	-4.32686800	-0.46705400	-1.52152900
C	-4.97366500	-1.64233100	-1.16034200
C	-6.18647000	-1.52978700	-0.48358400
C	-6.73771300	-0.27407000	-0.18595000
H	-6.46392200	1.85880000	-0.37400600
H	-4.29061900	1.69902300	-1.55279600
H	-4.55442500	-2.61288100	-1.40166300
H	-6.70893400	-2.43279600	-0.18090400
C	-8.03227700	-0.15344800	0.58002600
H	-7.85350300	0.29442400	1.56530700
H	-8.74582600	0.49208200	0.05498000
H	-8.50324500	-1.12869200	0.73297800
S	-2.75422200	-0.60662300	-2.45210000
O	-2.87443900	-1.75393900	-3.46929900
O	-2.25650700	0.78039600	-2.88853900
Au	2.36835500	-1.15657700	0.20425300
Br	4.19064500	-2.05719100	1.81063800
Br	4.08882600	0.43541700	-0.91206000

Br	-0.86946300	-4.23894100	3.87534400
Br	0.61394000	-2.57468100	1.48774400
K	2.22159500	-3.53567900	4.11664200
C	-1.92278100	0.95315000	0.75790900
C	-2.50224300	2.24105800	0.74742600
C	-3.59969700	2.50831200	1.57483700
C	-4.05888400	1.53143700	2.44640200
C	-3.47795000	0.26619300	2.49894100
C	-2.42204900	-0.02443200	1.64235500
C	-2.12466600	3.31114300	-0.25308300
H	-4.08307900	3.47765700	1.52582000
H	-3.84289100	-0.48440800	3.19152400
H	-1.95986900	-1.00502700	1.67228500
O	-3.00450600	3.73164200	-0.99923600
N	-0.79244400	0.70631900	-0.02364400
Cl	-5.45911700	1.90138500	3.51546500
C	-0.39304100	4.69891800	-1.36644800
C	0.87534300	5.26805100	-1.42623600
C	1.79814700	5.02747100	-0.40231300
C	1.44848900	4.21772300	0.68163800
C	0.18165100	3.63914000	0.73855800
C	-0.74713400	3.87218300	-0.28713500
H	-1.12787300	4.87738900	-2.14465200
H	1.14783400	5.90012500	-2.26697000
H	2.78914300	5.47085100	-0.44869600
H	2.16451700	4.03316300	1.47713400
H	-0.08841400	3.00837100	1.57919600
C	0.62402800	-2.10840600	-2.41144600
C	1.66057500	-3.08095400	-2.41304900
C	0.81199100	-0.91245800	-3.15767300
C	2.82220900	-2.85969200	-3.12095100
H	1.52087900	-3.99706100	-1.84715200
C	2.02420800	-0.69619200	-3.86204900
H	-0.01994800	-0.23276000	-3.32337800
C	3.01377400	-1.65424100	-3.84041300
H	3.60771700	-3.60949200	-3.11692200
H	2.15274700	0.22431200	-4.42176100
H	3.94356700	-1.49179300	-4.37579600

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C	-0.83259400	-0.76872300	-0.29114100
C	0.41867500	-0.53235600	-1.09176500
H	0.15890300	0.05349500	-1.97192300
N	-1.19573200	-2.11549000	0.04964600

C	-0.09157400	-3.02373700	0.37860300
H	-0.47892200	-4.04627200	0.28645200
H	0.14552400	-2.85982200	1.43645800
C	-5.84556000	-1.06176700	-1.29094900
C	-4.51668400	-1.35594100	-1.59118100
C	-3.97712400	-2.51756500	-1.05666600
C	-4.69656700	-3.39969100	-0.25851700
C	-6.02551700	-3.08615600	0.01534500
C	-6.61399800	-1.91184400	-0.48263300
H	-6.26824500	-0.13987100	-1.67760100
H	-3.93015100	-0.69127100	-2.21412600
H	-4.23531000	-4.30569800	0.11864300
H	-6.61331800	-3.76228500	0.63050500
C	-8.03330900	-1.54982400	-0.11916800
H	-8.04965200	-0.93596500	0.79116600
H	-8.51516500	-0.97058300	-0.91299700
H	-8.63980100	-2.44036800	0.07436300
S	-2.22709800	-2.91966100	-1.41183100
O	-2.00795300	-4.42907300	-1.20594100
O	-1.79409900	-2.23331500	-2.72584700
Au	1.71792500	0.87116500	-0.10146700
Br	3.31032300	2.66443000	1.02343300
Br	2.04757200	1.99583300	-2.34713600
Br	5.34353900	-2.85328200	0.61436400
Br	1.48428200	-0.34506900	2.16112200
K	4.81856600	-0.02384100	2.03648500
C	-2.67462600	0.32519800	0.80853800
C	-3.63015100	1.31504300	0.48477200
C	-4.78333500	1.45664700	1.26124100
C	-4.94169800	0.67026000	2.39453600
C	-3.98612600	-0.27118300	2.77121500
C	-2.86414800	-0.45082400	1.97003500
C	-3.51973500	2.15499500	-0.77333000
H	-5.54026300	2.18212400	0.98388200
H	-4.12321700	-0.86076500	3.67107600
H	-2.12189800	-1.19081700	2.24036200
O	-4.31320100	1.93677800	-1.68500600
N	-1.54437000	0.25789300	-0.00572100
Cl	-6.42351900	0.86495800	3.39533700
C	-2.40032100	3.96232000	-2.05307900
C	-1.47810300	4.99762100	-2.16600300
C	-0.66360200	5.32968800	-1.07791500
C	-0.77805800	4.62903500	0.12553800
C	-1.70122400	3.59120400	0.24089400

C	-2.51583200	3.24636100	-0.84936100
H	-3.04162700	3.68661500	-2.88378400
H	-1.38750300	5.54468400	-3.10026300
H	0.06343300	6.13187800	-1.16898800
H	-0.14055100	4.88292300	0.96707400
H	-1.78524300	3.04547400	1.17520800
C	1.16485800	-2.86745700	-0.44469000
C	2.24608500	-3.67410700	-0.26957800
C	1.13065100	-1.83483900	-1.52032200
C	3.41549700	-3.51561500	-1.07506100
H	2.23567800	-4.46185900	0.47839900
C	2.40775700	-1.66414300	-2.26819200
H	0.41898200	-2.24057200	-2.27948300
C	3.47035400	-2.48010600	-2.07001400
H	4.10636500	-4.34421600	-1.15091000
H	2.43232600	-0.89289200	-3.03198000
H	4.37292200	-2.37655300	-2.66273300

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C	-0.07423300	-0.43792000	0.03989900
C	1.07868900	-1.09675600	-0.65701600
H	1.16138500	-0.69307100	-1.66711200
N	-1.19149000	-1.28486600	0.44943600
C	-0.77865600	-2.53732800	1.10874400
H	-1.66611500	-3.16620200	1.24560400
H	-0.43127400	-2.24685900	2.10729500
C	-5.97294800	-2.31568700	0.30019400
C	-4.80777400	-1.67443300	-0.11333700
C	-3.75490500	-2.47756800	-0.53267700
C	-3.80349400	-3.87037400	-0.56333700
C	-4.98108900	-4.47775700	-0.13288800
C	-6.07694900	-3.71547100	0.30588000
H	-6.81128000	-1.69168900	0.59838700
H	-4.79189100	-0.58499900	-0.13952300
H	-2.96912000	-4.45190700	-0.93893300
H	-5.05372400	-5.56161700	-0.15367300
C	-7.35117000	-4.38076600	0.76308200
H	-7.55219600	-4.15681100	1.81770300
H	-8.20992400	-4.01367000	0.18949000
H	-7.30424600	-5.46775700	0.65041400
S	-2.22540000	-1.65886400	-1.11199200
O	-1.42451800	-2.71722900	-1.98282500
O	-2.48896000	-0.28398000	-1.73972500
Au	2.97949700	-0.49970500	0.17295300

Br	5.23458400	0.28620500	1.10352000
Br	3.74474300	-0.03043900	-2.20942500
Br	-6.27331600	1.52097500	-0.53499000
Br	2.23597600	-1.22918800	2.50482700
K	-3.61266700	2.21142100	-2.01450200
C	-1.01243300	1.62800100	0.84792100
C	-1.17062500	2.94173500	0.34969900
C	-2.04955700	3.83066400	0.97668400
C	-2.71054900	3.43756800	2.13596800
C	-2.54013300	2.16076800	2.66782500
C	-1.70402600	1.25916800	2.01833100
C	-0.50832300	3.38996700	-0.93713200
H	-2.19402700	4.82989600	0.57907600
H	-3.06033000	1.87563900	3.57526900
H	-1.56395200	0.26769900	2.42921700
O	-1.22907600	3.50487200	-1.93540900
N	-0.07993600	0.82578500	0.19160300
Cl	-3.78462600	4.59891400	2.96318800
C	1.49950800	4.15076700	-2.17547200
C	2.85038200	4.47185400	-2.23428200
C	3.64361800	4.36940400	-1.08557600
C	3.08256700	3.95570200	0.12538800
C	1.72787600	3.64055100	0.19020200
C	0.92624600	3.72873100	-0.96133400
H	0.86961000	4.21413500	-3.05646100
H	3.29181900	4.79298600	-3.17327700
H	4.70273500	4.60520400	-1.13591500
H	3.70321000	3.86315300	1.01085000
H	1.29517300	3.31470000	1.13012500
C	0.32497600	-3.29648900	0.40332100
C	0.60260600	-4.62707300	0.67885100
C	0.98416300	-2.62505900	-0.69817300
C	1.57074500	-5.30621200	-0.06762200
H	0.07515300	-5.14096300	1.47799000
C	1.99516400	-3.36365100	-1.42309700
H	0.00500300	-2.77822100	-1.44519300
C	2.25397900	-4.68561100	-1.12908000
H	1.78811200	-6.34422600	0.16953700
H	2.53330000	-2.84745800	-2.21364200
H	2.99705400	-5.23838400	-1.69431500

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C	0.44411200	-0.41952000	-0.15026400
C	-0.59422500	-1.39206200	0.30252100

H	-0.97398600	-1.09249400	1.27591800
N	1.76068800	-0.93768700	-0.51767700
C	1.74835800	-2.30172800	-1.10017400
H	2.78454200	-2.63502300	-1.21793800
H	1.34279400	-2.13314400	-2.10644700
C	6.18836000	-0.35707200	-1.47007500
C	4.93471500	-0.18816700	-0.89144700
C	4.55698700	-1.08640300	0.10424700
C	5.36716300	-2.12337500	0.55005000
C	6.61850800	-2.26456600	-0.05190400
C	7.04777600	-1.39212300	-1.06138900
H	6.50603300	0.32973700	-2.24985400
H	4.27329600	0.61155000	-1.20933300
H	5.03731900	-2.79177600	1.33616500
H	7.27088100	-3.06813200	0.27737200
C	8.40647600	-1.54776100	-1.69838500
H	8.32158100	-1.66011700	-2.78557400
H	9.02850600	-0.66379000	-1.51298700
H	8.93646300	-2.42048300	-1.30747300
S	2.93583800	-0.78617000	0.90356000
O	2.86143400	-2.03496100	1.98821800
O	2.77857700	0.61400900	1.49398300
Au	-2.42754000	-0.99024000	-0.82175800
Br	-4.61195600	-0.47633300	-2.08840700
Br	-3.61223500	-0.53585600	1.42814000
Br	0.85214200	-1.48837300	4.18968600
Br	-1.21656300	-1.41910500	-3.02563800
K	-1.14466900	0.86485900	3.28453900
C	0.96279800	1.82510000	-0.78497800
C	0.99139300	3.13611200	-0.23603900
C	1.70320700	4.15014600	-0.89851400
C	2.34026400	3.88694100	-2.10067200
C	2.24764000	2.63312100	-2.70158000
C	1.56211900	1.61680700	-2.04636200
C	0.29315700	3.46417600	1.04103600
H	1.75836300	5.14146600	-0.46495600
H	2.69339300	2.45723300	-3.67493800
H	1.44327100	0.65460900	-2.52927400
O	0.21631900	2.64229800	1.95560900
N	0.18872700	0.83344300	-0.19471700
Cl	3.26489200	5.19064500	-2.91514200
C	-0.40959700	5.35818300	2.49968300
C	-1.04193400	6.57943600	2.71201300
C	-1.63322500	7.25569500	1.63946400

C	-1.58143900	6.71131500	0.35495700
C	-0.92621700	5.49969400	0.13419400
C	-0.33492800	4.81131500	1.20685300
H	0.04932200	4.82107500	3.32427800
H	-1.07750400	7.00550000	3.71069200
H	-2.13574200	8.20428900	1.80687700
H	-2.05341700	7.22689500	-0.47619800
H	-0.90038700	5.07480300	-0.86404700
C	0.90727000	-3.29902300	-0.34940500
C	1.24561900	-4.65230200	-0.31499800
C	-0.24090000	-2.83580200	0.31372300
C	0.44073100	-5.56139100	0.37157900
H	2.14305800	-4.99627100	-0.82503800
C	-1.03098200	-3.75619400	1.02348900
H	2.13262000	-1.82203700	2.75681200
C	-0.69702000	-5.10712300	1.04553400
H	0.70676200	-6.61419100	0.39330300
H	-1.91187700	-3.40315000	1.55198700
H	-1.31968200	-5.80549700	1.59672700

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C	0.40897600	-0.45221600	-0.19935100
C	-0.66044700	-1.40659000	0.22278700
H	-1.00231000	-1.16605600	1.22591800
N	1.69161100	-0.99704300	-0.61624000
C	1.62696600	-2.32116600	-1.27833500
H	2.65068100	-2.69092400	-1.39988400
H	1.24573200	-2.08649400	-2.28050700
C	6.11096400	-0.25529200	-1.49325800
C	4.85496400	-0.16316800	-0.90181700
C	4.49020800	-1.16232500	-0.00329900
C	5.31357800	-2.22945100	0.33256900
C	6.56646600	-2.29361700	-0.27899900
C	6.98289100	-1.31679900	-1.19392200
H	6.42081300	0.51214400	-2.19734200
H	4.18214200	0.65488700	-1.13757500
H	4.98844400	-2.97753200	1.04612900
H	7.23001200	-3.11788700	-0.03373800
C	8.33546900	-1.39970100	-1.85762400
H	8.23270000	-1.61936000	-2.92767300
H	8.87589900	-0.45018000	-1.77363200
H	8.95415900	-2.18422900	-1.41334000
S	2.86603500	-0.99201300	0.82809500
O	2.76111600	-2.31544600	1.75374000

O	2.67185600	0.34650400	1.54900100
Au	-2.50929400	-0.82992200	-0.78500500
Br	-4.70781800	-0.11355200	-1.91684800
Br	-3.53698900	-0.40632200	1.55209300
Br	1.05279500	-2.00552400	4.11400600
Br	-1.41178400	-1.22895700	-3.05058000
K	-0.75287300	0.61314400	3.25451000
C	1.00026500	1.79833000	-0.73354200
C	1.09816100	3.08795700	-0.14227000
C	1.82535600	4.09812000	-0.79441300
C	2.41322300	3.85514700	-2.02537100
C	2.25261800	2.62803300	-2.66518000
C	1.54944200	1.61619300	-2.02199800
C	0.46576000	3.40736200	1.17163100
H	1.93083900	5.07112400	-0.32971500
H	2.65916700	2.46930900	-3.65841100
H	1.37919100	0.67767900	-2.53459500
O	0.42699700	2.57610600	2.08023400
N	0.20310300	0.81270400	-0.15940600
Cl	3.36039300	5.15235800	-2.82442700
C	-0.15963400	5.27698000	2.69340400
C	-0.75727500	6.50651300	2.95163100
C	-1.35966400	7.22243500	1.91142300
C	-1.35501400	6.70854400	0.61339900
C	-0.73504100	5.48781000	0.34641900
C	-0.13138700	4.76054500	1.38614600
H	0.30589400	4.70791800	3.49221400
H	-0.75793200	6.90818000	3.96099400
H	-1.83490900	8.17801600	2.11494600
H	-1.83665800	7.25491300	-0.19208500
H	-0.74598800	5.08665200	-0.66177700
C	0.73832700	-3.32834900	-0.59591900
C	1.00464300	-4.69602700	-0.67275900
C	-0.37764900	-2.86257400	0.11757200
C	0.16060300	-5.61478700	-0.04937300
H	1.87836600	-5.04395100	-1.21986300
C	-1.20839300	-3.79503600	0.76288500
H	2.03273900	-2.15614200	2.73255500
C	-0.94559700	-5.15872600	0.67422400
H	0.37167200	-6.67816100	-0.11530000
H	-2.06783700	-3.44071000	1.32551200
H	-1.59976200	-5.86633200	1.17494000

IM11

C	-1.40451800	-0.48509600	-0.38442000
C	-0.48981900	-1.58585000	-0.83701600
H	0.03555200	-1.27656300	-1.73797200
N	-2.74604100	-0.80330500	-0.04049900
C	-2.96425600	-2.17049500	0.46698300
H	-4.04261100	-2.35735100	0.48478000
H	-2.62942200	-2.14161200	1.51167000
C	-6.94861900	1.28717100	0.56673100
C	-5.73002000	1.06826600	-0.07149600
C	-5.52071900	-0.16826100	-0.66939800
C	-6.47356900	-1.17831200	-0.66872300
C	-7.68599400	-0.93503600	-0.02184100
C	-7.93905400	0.29175000	0.60753400
H	-7.13714800	2.24986200	1.03486300
H	-4.96783800	1.83858900	-0.11371700
H	-6.27539300	-2.11498900	-1.17887400
H	-8.44830700	-1.70950200	-0.01426300
C	-9.24275100	0.53737700	1.32836300
H	-9.12807000	0.37717100	2.40846700
H	-9.58913900	1.56675400	1.18850400
H	-10.02878600	-0.13831900	0.97786800
S	-3.93020000	-0.47056000	-1.54630900
O	-4.08461500	-1.76367700	-2.36222300
O	-3.42089800	0.82758200	-2.17532200
Au	1.31429500	-1.48276000	0.43238100
Br	3.55513100	-0.90556600	1.91412800
Br	2.72667500	-1.56717900	-1.74376500
Br	6.60024500	0.18821800	0.25516200
Br	-0.04117200	-1.55114200	2.58231200
K	3.49326100	1.40999600	-0.60719400
C	-1.52038900	1.87389100	0.06478000
C	-1.07094300	3.09435700	-0.49800100
C	-1.54016100	4.31825400	-0.00977100
C	-2.43436600	4.33304600	1.05329600
C	-2.84749400	3.15214600	1.66558600
C	-2.39527800	1.93288500	1.16966100
C	-0.08234300	3.08152600	-1.63299400
H	-1.20866900	5.25137000	-0.45338700
H	-3.51077600	3.18504300	2.52339700
H	-2.70664600	1.01180700	1.64471600
O	-0.32314000	2.52809900	-2.69087400
N	-0.91914600	0.70644000	-0.39880800
Cl	-3.04130900	5.90661600	1.66920900
C	2.10333300	3.88654700	-2.53836100

C	3.37241300	4.44785400	-2.40062200
C	3.81557600	4.88141100	-1.14285300
C	2.98200400	4.75136300	-0.02714200
C	1.70620000	4.19239800	-0.16536800
C	1.25540800	3.75482400	-1.42304700
H	1.73989200	3.54315800	-3.50193600
H	4.01301400	4.56103700	-3.27104800
H	4.80037600	5.32824900	-1.03686100
H	3.31810000	5.09405700	0.94768200
H	1.06449900	4.09527000	0.70437200
C	-2.23680700	-3.26410600	-0.27394300
C	-2.74616100	-4.55900000	-0.34829500
C	-1.01243900	-2.95799900	-0.89867600
C	-2.04910200	-5.55485300	-1.03404300
H	-3.69925900	-4.78979700	0.12182400
C	-0.32827100	-3.96331100	-1.61140000
H	5.39937400	-0.46967400	0.97410800
C	-0.84050500	-5.25333000	-1.67235600
H	-2.45574200	-6.56099800	-1.08533000
H	0.61204300	-3.72154900	-2.09800900
H	-0.30424300	-6.02350500	-2.21872000

TS11-12

C	0.01729400	0.44928300	-0.39539700
C	-1.26614100	0.07393800	-0.99323800
H	-1.20413900	-0.91231500	-1.44764700
N	0.27775400	1.81884600	-0.14375300
C	-0.88618300	2.73343800	-0.29792600
H	-0.51658500	3.76144100	-0.26660500
H	-1.46306800	2.57749800	0.62163400
C	2.77127400	5.43892000	1.36188900
C	2.51781400	4.17858600	0.82635800
C	2.00381400	4.11851600	-0.46436100
C	1.74454100	5.24241600	-1.23861200
C	2.01156400	6.49076100	-0.67707300
C	2.52066600	6.60871500	0.62509300
H	3.17391300	5.51430400	2.36809900
H	2.71697800	3.27487000	1.39339500
H	1.35239500	5.13823600	-2.24473900
H	1.82113400	7.38604700	-1.26249400
C	2.77266100	7.96595800	1.23444400
H	1.89382700	8.30600200	1.79770200
H	3.61616900	7.94132400	1.93140400
H	2.98175400	8.71807000	0.46770200

S	1.72345900	2.46677300	-1.20084000
O	1.29036200	2.60281800	-2.68573400
O	2.93215100	1.54408400	-0.97011900
Au	-2.74666000	-0.59514800	0.59161400
Br	-4.59423200	-1.43084400	2.17177400
Br	-3.56922000	-2.28755800	-1.12237800
Br	0.72996300	-2.66827300	-2.08164200
Br	-1.98922900	0.95227000	2.50474000
K	2.36315800	-0.03360200	-3.37791300
C	1.93006500	-0.44675000	0.84101900
C	3.13654400	-1.18500000	0.73951300
C	4.01498900	-1.21383200	1.83661900
C	3.72245200	-0.51995100	2.99984700
C	2.52784400	0.17968800	3.12907100
C	1.64210800	0.19985600	2.05858700
C	3.66412700	-1.86885400	-0.49790800
H	4.94106400	-1.77212500	1.76365000
H	2.27342700	0.67685600	4.05898900
H	0.68477800	0.69063800	2.18181600
O	3.76836000	-1.25505700	-1.55928900
N	0.92724300	-0.48522300	-0.15832700
Cl	4.88850300	-0.55327700	4.36286700
C	5.04306900	-3.75392400	-1.35522600
C	5.49081100	-5.06944300	-1.30770900
C	5.03534200	-5.92609100	-0.29923700
C	4.13613100	-5.46112500	0.66237600
C	3.69944000	-4.13772100	0.62757800
C	4.14972800	-3.27192500	-0.38299400
H	5.37749100	-3.07885900	-2.13614400
H	6.19026800	-5.43259700	-2.05543600
H	5.37890700	-6.95643100	-0.26700500
H	3.77050000	-6.12890300	1.43671900
H	2.99034400	-3.78475400	1.36877600
C	-1.71905300	2.45751300	-1.51614500
C	-2.29015900	3.46364300	-2.29326900
C	-1.92356400	1.10438500	-1.83589500
C	-3.07887600	3.13044100	-3.39629500
H	-2.12227300	4.50725500	-2.03592400
C	-2.70235000	0.77671900	-2.95788300
H	0.82209700	-1.53906900	-0.93291100
C	-3.27790800	1.78651800	-3.72755200
H	-3.53098300	3.91448400	-3.99717600
H	-2.86974400	-0.26655300	-3.20430500
H	-3.88708200	1.52306000	-4.58759300

IM12

C	0.19973600	-0.41075100	0.49506300
C	-1.14068200	-0.41449800	1.04021900
H	-1.44118400	0.58937300	1.34863000
N	0.93691800	-1.57821500	0.41593500
C	0.20848500	-2.83130100	0.75092500
H	0.94692800	-3.62389600	0.89856300
H	-0.33388900	-3.07332200	-0.17114500
C	4.67334500	-3.74918200	-1.28207400
C	3.95512100	-2.71465400	-0.69031600
C	3.52303000	-2.89749200	0.61928600
C	3.77731700	-4.04645300	1.35632900
C	4.50079200	-5.06638200	0.73638400
C	4.95411100	-4.93718800	-0.58360600
H	5.02228700	-3.63214500	-2.30448600
H	3.73928300	-1.79849300	-1.23013700
H	3.42479000	-4.13477500	2.37846000
H	4.71402200	-5.97563100	1.29118000
C	5.72334600	-6.04835200	-1.25454100
H	5.16013200	-6.45606800	-2.10279300
H	6.67986600	-5.68481700	-1.64748400
H	5.93025300	-6.86952800	-0.56279000
S	2.60592200	-1.53781600	1.43594700
O	2.33128800	-1.90137400	2.90962400
O	3.28134800	-0.17571700	1.18435900
Au	-2.64155900	-0.55461300	-0.68253000
Br	-4.54162000	-0.67174200	-2.40136200
Br	-4.11070500	0.98345800	0.70298300
Br	-0.25948700	2.61522300	2.75957400
Br	-1.25664800	-1.99555200	-2.31413600
K	2.59340800	1.42346900	3.38023100
C	1.68020400	1.03234500	-0.92107500
C	2.41284300	2.23704400	-0.93564800
C	3.24095100	2.51958100	-2.03097600
C	3.35719500	1.61301300	-3.07538600
C	2.62310300	0.43139400	-3.08209800
C	1.78039900	0.15275200	-2.01071400
C	2.46303000	3.24623000	0.19720700
H	3.80130200	3.44791500	-2.05452900
H	2.67555600	-0.24708600	-3.92657500
H	1.15515900	-0.73137300	-2.04454800
O	3.02305800	2.93526300	1.24673300
N	0.74134800	0.76544700	0.11217400

Cl	4.44708100	1.98737400	-4.44770100
C	2.16144800	5.59903900	0.92861800
C	1.63903000	6.87524700	0.76340600
C	0.85247600	7.16857500	-0.35684000
C	0.59392700	6.18397300	-1.31251200
C	1.12559400	4.90554600	-1.15568600
C	1.91486700	4.60193000	-0.03257600
H	2.75927300	5.34801600	1.79773400
H	1.83180300	7.64154100	1.50848800
H	0.43595800	8.16453100	-0.47982700
H	-0.02619700	6.40864200	-2.17501800
H	0.91392700	4.14187900	-1.89684800
C	-0.73151500	-2.69759300	1.91465900
C	-0.93693200	-3.71490900	2.84517000
C	-1.43916700	-1.48772900	2.01578700
C	-1.86093400	-3.53720700	3.87659300
H	-0.37978300	-4.64544200	2.76364800
C	-2.35105000	-1.30583600	3.06785600
H	0.31696600	1.57658000	0.59913300
C	-2.56119600	-2.33143200	3.98726500
H	-2.02751700	-4.33304300	4.59706900
H	-2.88577300	-0.36610200	3.15358700
H	-3.27042300	-2.18726900	4.79712800

3a

C	0.35170700	-0.39114700	0.35928000
C	-1.02312900	-0.81187400	0.21396900
N	1.34278300	-1.32598400	0.70504500
C	-1.27109100	-2.26552300	0.03775900
C	-0.30632800	-3.16748700	0.53138200
C	-0.44348500	-4.54120400	0.32770800
C	-1.53956700	-5.04625800	-0.36877000
C	-2.48622200	-4.16157200	-0.88981400
C	-2.35059600	-2.78916200	-0.69801800
H	0.32135700	-5.21382600	0.70797600
H	-1.64300700	-6.11666500	-0.52340400
H	-3.32843800	-4.53872400	-1.46338900
H	-3.07949000	-2.12409800	-1.14153500
C	0.87785100	-2.59698900	1.26331100
H	0.63770200	-2.38934100	2.31693300
H	1.72272500	-3.29074600	1.25233000
C	4.93417500	1.82308600	-0.63896400
C	3.93310700	0.89528500	-0.92891200
C	3.94782000	-0.31098700	-0.24633200

C	4.90868300	-0.62977300	0.70460500
C	5.89510100	0.31418500	0.98108400
C	5.92170500	1.55165900	0.31801000
H	4.94843500	2.77233700	-1.16832800
H	3.16551800	1.09313900	-1.66781500
H	4.89400300	-1.59607800	1.19691700
H	6.66002200	0.08343100	1.71846900
C	6.99625500	2.56447000	0.63594000
H	6.90912000	2.92190800	1.66965800
H	7.99711700	2.12961800	0.52907100
H	6.93479900	3.43478100	-0.02412800
S	2.66058800	-1.56514200	-0.64343700
O	2.06183100	-1.23304500	-2.01801600
O	3.25215500	-2.95348600	-0.33215800
C	-0.15217000	1.82533300	0.04832500
C	-1.55848100	1.56428300	0.09566000
C	-2.45325800	2.67047300	0.06653300
C	-1.95478400	3.94202600	-0.06899300
C	-0.57339700	4.21200600	-0.17055600
C	0.30997600	3.16022600	-0.10559800
C	-1.99011200	0.19784500	0.16363900
H	-3.52089500	2.51268900	0.14659900
H	-0.22904400	5.23432600	-0.28052700
H	1.38266500	3.31929300	-0.14604900
N	0.76982900	0.84870500	0.22014500
Cl	-3.09622900	5.33359200	-0.11307300
C	-4.01041700	-0.70164600	1.34654900
C	-5.37866500	-0.96240900	1.41572800
C	-6.21364100	-0.62300100	0.34894000
C	-5.67284400	-0.01406900	-0.78534600
C	-4.30494400	0.25533500	-0.85202900
C	-3.45482600	-0.09204300	0.21103400
H	-3.36267800	-0.97034400	2.17600300
H	-5.79254900	-1.43157500	2.30415900
H	-7.27902600	-0.82949000	0.40200300
H	-6.31477100	0.25304400	-1.62039000
H	-3.88777300	0.72432800	-1.73902300

Cartesian coordinates for the stationary points given in Fig. S1
TS3-4

C	1.07587000	0.99265500	0.19689400
C	1.62453200	-0.32122900	-0.16586000
H	2.49030700	-0.25109600	-0.81926400
N	-0.28638800	1.26255200	0.09321400

C	-2.55619200	2.22521600	-1.47647800
C	-1.98104500	3.01717400	-0.47643000
C	-2.64667800	4.17502600	-0.05365300
C	-3.86877000	4.53513900	-0.62155500
C	-4.44686900	3.73073700	-1.60636900
C	-3.79110600	2.57296700	-2.02827700
H	-2.04649600	1.32510100	-1.80634700
H	-2.20908700	4.79482400	0.72650000
H	-4.37537900	5.43577000	-0.28445000
H	-5.40917100	3.99589900	-2.03476700
H	-4.25043500	1.92648900	-2.76898300
C	-0.62210200	2.70399900	0.11329800
H	0.15995900	3.18374400	-0.48605600
H	-0.51809200	3.13236000	1.12047400
C	-4.92085000	1.75557800	2.14572900
C	-3.85240000	1.05043100	1.59941900
C	-2.61093100	1.21675900	2.20067700
C	-2.37747000	2.04678200	3.29388600
C	-3.46875600	2.74173500	3.81050000
C	-4.74906000	2.60828300	3.24797400
H	-5.89859400	1.62557300	1.68976000
H	-4.03158300	0.40293100	0.74303200
H	-1.39140000	2.12206500	3.73880300
H	-3.32331500	3.38980100	4.67041300
C	-5.92877000	3.35074300	3.82454600
H	-6.61072300	2.65836900	4.33411600
H	-5.61635200	4.10754100	4.55025900
H	-6.50603100	3.84607400	3.03615100
S	-1.18107100	0.25600600	1.56762700
O	-0.08989300	0.18250600	2.65208300
O	-1.67973900	-1.03061500	0.88274100
Au	0.77909900	-2.15559700	-0.32600100
Br	1.74287900	-3.08307200	1.82369300
Br	-0.31626500	-4.40649400	-0.83802000
Br	0.08297800	-1.16399100	-2.59137100
Br	-5.70990900	-0.80508500	-0.97577900
K	-3.07606900	-2.47350700	-1.00375000
C	3.17068700	1.43383700	0.82135800
C	4.37705900	2.14043300	0.55028700
C	5.58209700	1.51023800	0.81184500
C	5.62080600	0.18467100	1.30086600
C	4.47166000	-0.50993300	1.62036600
C	3.23203100	0.13269600	1.43043700
C	4.41180400	3.57252500	0.04618100

H	6.51109000	2.03618300	0.61876000
H	4.50882600	-1.49752600	2.06500700
H	2.37751400	-0.22366400	2.00465700
O	5.08493400	4.37047700	0.68133300
N	1.94589800	1.93750800	0.50638900
Cl	7.21211000	-0.56122500	1.57451800
C	3.43821900	5.32068400	-1.41910600
C	2.78977900	5.73033200	-2.58007000
C	2.39968900	4.78523500	-3.53513800
C	2.66140600	3.42824500	-3.32824700
C	3.29409300	3.01454700	-2.15715200
C	3.68166300	3.95605500	-1.19022300
H	3.76143400	6.03883200	-0.67263500
H	2.59052700	6.78506100	-2.74611100
H	1.89664200	5.10671300	-4.44273800
H	2.37560700	2.69577800	-4.07747100
H	3.51225600	1.96040700	-2.01157800

IM4

C	-0.97858800	0.23075800	-0.73193100
C	-0.28777800	-0.55698400	0.34537700
H	0.14854300	0.07693600	1.11824500
N	-0.47918200	1.16823200	-1.50209200
C	-3.43510300	2.70544300	-2.13431800
C	-2.08284800	2.89191300	-2.45906300
C	-1.59213300	4.19713800	-2.61675200
C	-2.43455000	5.29599600	-2.43420100
C	-3.77671000	5.10258100	-2.10232700
C	-4.27514400	3.80557700	-1.95763500
H	-3.82267500	1.69745800	-2.02993200
H	-0.55173000	4.35056100	-2.88734800
H	-2.04239900	6.30105800	-2.56292100
H	-4.43364100	5.95765400	-1.96748600
H	-5.32279000	3.64823700	-1.71552100
C	-1.17936600	1.69572600	-2.70101000
H	-1.73775900	0.85057300	-3.10996100
H	-0.38702300	1.95631300	-3.40762400
C	2.22098900	3.58045300	2.37240400
C	2.31697600	2.84565500	1.19053600
C	1.19855300	2.82769600	0.36864400
C	0.01784100	3.51491900	0.63645100
C	-0.04367800	4.22612100	1.83255300
C	1.04817900	4.26615700	2.71745400
H	3.09763700	3.62036700	3.01319500

H	3.26697700	2.37165700	0.93961500
H	-0.81925500	3.51084800	-0.05287100
H	-0.95300300	4.76994200	2.07330800
C	0.96141300	5.02800800	4.01675800
H	0.75954600	4.34621300	4.85309500
H	1.90355100	5.53963400	4.23782800
H	0.16036600	5.77312200	3.99535900
S	1.37384900	1.94630800	-1.24650800
O	1.42541100	2.86786400	-2.46018400
O	2.38207100	0.79713100	-1.13311200
Au	1.33165300	-1.77586100	-0.31651100
Br	0.00687700	-2.36557800	-2.40409700
Br	3.31742100	-3.22045200	-1.09000700
Br	2.43224500	-1.34136000	1.95053200
Br	5.84150200	2.36954000	0.88500600
K	4.92964000	-0.33656700	-0.36351800
C	-2.62313800	-0.90037000	0.12097100
C	-3.95615100	-1.25059100	0.55716300
C	-4.06573500	-1.72542300	1.83781100
C	-2.92529100	-1.89719200	2.71525800
C	-1.65397500	-1.73287600	2.30214300
C	-1.43644300	-1.45297100	0.84971100
C	-5.13083700	-1.09769500	-0.37827700
H	-5.04476900	-1.96548700	2.23949600
H	-0.79900700	-1.90794800	2.94762000
H	-1.30486100	-2.45765900	0.39121300
O	-4.96726600	-1.37324300	-1.55772300
N	-2.32825700	-0.05832600	-0.83852300
Cl	-3.29204600	-2.36348000	4.40518200
C	-7.59461500	-0.98660000	-0.61563000
C	-8.85842400	-0.57979500	-0.20096400
C	-9.00204800	0.17620900	0.96755700
C	-7.87771300	0.52542500	1.71818000
C	-6.61027500	0.10642500	1.31303600
C	-6.45851900	-0.65971200	0.14529000
H	-7.46058200	-1.56160500	-1.52597800
H	-9.73293600	-0.84724200	-0.78702900
H	-9.98920900	0.49670500	1.28885500
H	-7.98622000	1.12610100	2.61660300
H	-5.73995200	0.40211800	1.89060700
TS5-6			
C	-1.13255300	0.72405000	-1.11499100
C	-1.49095800	-0.65350900	-0.67396000

H	-2.54679300	-0.86914400	-0.72267700
N	0.13975200	1.23688200	-0.85789900
C	1.48173800	2.56926500	1.36510100
C	1.26175800	3.23007400	0.15032000
C	1.92020800	4.44090900	-0.09844000
C	2.78980600	4.98137200	0.84877800
C	3.02123500	4.30865400	2.05077500
C	2.36734100	3.10162500	2.30455100
H	0.97572400	1.63014400	1.56866000
H	1.76006100	4.95841600	-1.04216600
H	3.29721800	5.91996900	0.64162400
H	3.71471100	4.71551800	2.78107100
H	2.55718300	2.56449800	3.22885500
C	0.27285100	2.71000500	-0.87345600
H	-0.72863700	3.09240700	-0.65637000
H	0.51049000	3.08375000	-1.87837200
C	5.05396100	2.37494600	-1.16661100
C	3.95222100	1.54342900	-0.98633400
C	2.99027900	1.53181100	-1.98718100
C	3.06607500	2.30077600	-3.14457300
C	4.17609900	3.13109600	-3.28917000
C	5.17965500	3.18229100	-2.30808200
H	5.81878000	2.36962100	-0.39450200
H	3.90139400	0.93558600	-0.08786000
H	2.30476500	2.22757700	-3.91334900
H	4.26896800	3.73702400	-4.18645400
C	6.37971100	4.08214300	-2.47139700
H	6.41076900	4.83812900	-1.67738000
H	7.31130600	3.50872500	-2.40227400
H	6.36890400	4.60157900	-3.43417400
S	1.56729900	0.37043100	-1.86235400
O	0.99127000	0.15824000	-3.26748100
O	1.97104800	-0.83993200	-0.98826600
Au	-0.34847900	-2.17098700	0.04508100
Br	-1.14847700	-2.31670400	-2.42108900
Br	0.92417100	-4.36077400	0.36239600
Br	0.07890100	-1.44121200	2.41789100
Br	5.54628300	-0.04171700	1.88365900
K	3.35818200	-2.11729800	1.09292500
C	-3.41485300	1.27323300	-1.56015100
C	-4.15206000	1.11665600	-0.35216500
C	-5.55345900	1.00055700	-0.41619300
C	-6.20123700	1.01493500	-1.64085800
C	-5.49405900	1.19646800	-2.83013100

C	-4.11525800	1.35175700	-2.77899000
C	-3.48101000	1.07680100	0.98125200
H	-6.12501200	0.87112100	0.49528000
H	-6.01832300	1.22423300	-3.77911100
H	-3.54622100	1.52040800	-3.68736600
O	-2.40328500	0.48204200	1.14010700
N	-2.04287800	1.50053800	-1.60615200
Cl	-7.97990300	0.81367700	-1.69597500
C	-3.72782000	1.31359100	3.43831000
C	-4.24088300	1.94350500	4.56700300
C	-5.10558700	3.03450800	4.42800500
C	-5.45784600	3.49399500	3.15692500
C	-4.96040200	2.85661200	2.02167500
C	-4.09449000	1.75611500	2.15327600
H	-3.04666300	0.47386500	3.52931100
H	-3.96546200	1.58890500	5.55580300
H	-5.50066700	3.52893700	5.31110100
H	-6.11684900	4.35043800	3.04903900
H	-5.22353900	3.22902400	1.03728400

IM6

C	-0.88141400	1.50176900	-0.19351900
C	-1.60126900	0.16817500	-0.41049200
H	-2.28096000	0.28011900	-1.25579500
N	0.43241600	1.59043900	0.17933900
C	2.34447600	1.64653900	2.37862900
C	2.08395700	2.79599200	1.62413000
C	2.91003100	3.91710800	1.77636700
C	3.98303600	3.88932400	2.66670000
C	4.25082100	2.73327300	3.40372000
C	3.43216000	1.61288100	3.25455800
H	1.70979300	0.77285300	2.26482500
H	2.71789300	4.81320500	1.18923900
H	4.61834000	4.76479200	2.77372700
H	5.10023200	2.69912800	4.07977900
H	3.65085500	0.70341200	3.80525700
C	0.88968600	2.89463600	0.69673100
H	0.03219700	3.30536000	1.24007900
H	1.08388300	3.60445100	-0.11908100
C	5.41891100	2.23582900	-0.74916200
C	4.25128900	1.48495000	-0.64361100
C	3.14476800	1.93175800	-1.35459700
C	3.13660700	3.07579600	-2.14769400
C	4.31929500	3.80845700	-2.22195900

C	5.47081500	3.40345200	-1.52664100
H	6.29486600	1.88421900	-0.21062800
H	4.25952000	0.58374900	-0.03324300
H	2.25314300	3.36090100	-2.70845300
H	4.35053400	4.70083500	-2.84120900
C	6.75047500	4.19741500	-1.61888500
H	7.09592600	4.50131400	-0.62377700
H	7.55133400	3.59538800	-2.06478200
H	6.62542900	5.09815800	-2.22705000
S	1.60557200	0.92677400	-1.33003500
O	0.75760100	1.25228500	-2.56517400
O	1.95263300	-0.52775200	-0.97989700
Au	-0.70255500	-1.71600700	-0.64052500
Br	-1.69558600	-1.75813100	-2.97435400
Br	0.27216100	-4.07460800	-0.99317000
Br	0.01630400	-1.77519000	1.82803400
Br	5.71268400	-1.29907700	1.21627500
K	3.04064100	-2.68541000	0.34552800
C	-2.96923900	2.62013400	-0.46893800
C	-3.95114900	1.73360300	0.09285800
C	-5.33300100	1.96488600	-0.15414900
C	-5.72380700	3.01930900	-0.94399700
C	-4.78023700	3.91069000	-1.48640900
C	-3.43798200	3.71990000	-1.23039000
C	-3.56257600	0.64830000	0.95198000
H	-6.07136900	1.27724800	0.23880000
H	-5.11373100	4.74167800	-2.09860900
H	-2.69455000	4.40354100	-1.62522900
O	-2.41922000	0.03856000	0.80039700
N	-1.61275100	2.57922600	-0.27430200
Cl	-7.45709900	3.26851000	-1.29566400
C	-4.12243100	-1.18816000	2.51020900
C	-4.83266000	-1.68681600	3.59518900
C	-5.75070500	-0.87243400	4.26717900
C	-5.95701300	0.44916800	3.85756200
C	-5.25987900	0.95670900	2.76757100
C	-4.34221800	0.13823900	2.07242700
H	-3.40199300	-1.81138500	1.99218800
H	-4.66909300	-2.70971300	3.91924800
H	-6.30012300	-1.26556400	5.11777400
H	-6.65211600	1.08550300	4.39634600
H	-5.39378500	1.99259000	2.47632700

Cartesian coordinates for the stationary points given in Fig. S3

It

C	0.73718700	1.54379100	-0.58379400
C	0.81343200	2.69643200	-0.95639900
H	0.81187000	3.66484100	-1.40047600
N	0.69544200	0.27550800	-0.15287300
C	-2.59834300	0.75343900	0.96767300
C	-1.64676300	-0.14611200	0.47854700
C	-2.03725300	-1.11367700	-0.45720500
C	-3.35987400	-1.18066100	-0.89004300
C	-4.30858800	-0.28209600	-0.39149100
C	-3.92617400	0.68477100	0.53809300
H	-2.30043000	1.51127400	1.68866700
H	-1.29722700	-1.80717500	-0.84798200
H	-3.65298600	-1.93529500	-1.61490200
H	-5.34018800	-0.33664600	-0.72875400
H	-4.65707300	1.38852700	0.92725200
C	-0.21322500	-0.08618900	0.96079500
H	-0.11731300	0.62953900	1.78836900
H	0.12053100	-1.06894700	1.30696500
C	3.41678600	0.60831700	1.00524800
H	3.01280500	0.52765300	2.01357700
H	4.43863800	0.23481500	0.93925600
H	3.31356800	1.60751700	0.58357800
S	2.39883800	-0.53480800	-0.07235400
O	2.96641200	-0.47964100	-1.48645700
O	2.17798600	-1.85233700	0.67941600

IMI'

C	1.18274500	-0.53175000	-1.57264200
C	-0.06594400	-0.80652900	-1.75614500
H	-0.46335700	-1.25933600	-2.65874800
N	2.36316000	-0.28709500	-1.25385400
C	1.95462600	2.52432600	0.20370900
C	3.10796100	1.80528700	-0.14443900
C	4.22856100	1.84464100	0.69684400
C	4.19453000	2.59455100	1.87522400
C	3.04200500	3.30342300	2.22034700
C	1.92286600	3.26816400	1.38351700
H	1.08039700	2.50690400	-0.44335000
H	5.12426400	1.29093100	0.42757300
H	5.06912400	2.62721400	2.51889800
H	3.01606100	3.88570400	3.13704400

H	1.02541700	3.82113300	1.64447200
C	3.13511400	0.97968800	-1.41025700
H	2.68135300	1.50186800	-2.25767800
H	4.15308700	0.68640500	-1.67778300
C	2.85364100	-1.71717100	1.42210900
H	3.39945500	-2.49796900	1.95477300
H	3.12350800	-0.71224800	1.74578700
H	1.77656400	-1.89939600	1.39331700
S	3.43670500	-1.84055300	-0.35211900
O	4.88346300	-1.36838800	-0.49515700
O	2.89452800	-3.09447800	-1.02183200
Au	-1.42716400	-0.24611600	-0.28972700
Br	-0.94548100	-2.42416300	0.93785600
Br	-3.10964100	0.46188500	1.44845800
Br	-1.78287500	1.87843900	-1.63941900

TS1'-2'

C	1.22748400	0.35263200	-0.26418700
C	0.73910600	-0.86790200	-0.30195100
H	1.34661400	-1.72790000	-0.55517100
N	0.95682700	1.59564800	-0.01971400
C	-1.60773300	2.94302900	-1.30595900
C	-0.37751900	3.49633800	-0.91862600
C	-0.33815200	4.80782500	-0.42771800
C	-1.51389500	5.55626000	-0.32250600
C	-2.73518200	4.99839000	-0.70413300
C	-2.78025400	3.69052700	-1.19616700
H	-1.65005600	1.92844300	-1.69450200
H	0.61077200	5.23680200	-0.11858300
H	-1.47270700	6.57359900	0.05712400
H	-3.64927300	5.57998800	-0.62133100
H	-3.72630200	3.25087400	-1.49862500
C	0.89198200	2.67950600	-1.03346200
H	0.95093700	2.17174700	-2.00048200
H	1.77930500	3.30974700	-0.91854400
C	-0.13925900	2.38940100	2.63334600
H	0.09618300	2.77112400	3.62796600
H	-0.72619400	3.08927000	2.03976100
H	-0.55328400	1.37982000	2.65764300
S	1.50021000	2.23989100	1.76399300
O	2.11381300	3.62393800	1.52214000
O	2.31397600	1.10080000	2.38381800
Au	-1.26358100	-1.23235000	-0.00360600
Br	-0.80689700	-1.47384300	2.48599600

Br	-3.74172200	-1.67645400	0.30119900
Br	-1.49314400	-1.03362300	-2.53261500
C	4.14458200	-0.52131700	-0.38322200
C	4.94099700	-1.02507800	-1.46979400
C	6.11919700	-1.78355900	-1.21315200
C	6.44656200	-2.01630900	0.09631000
C	5.64288100	-1.51135000	1.17287600
C	4.50575200	-0.76969500	0.96901000
C	4.26931900	-0.59301100	-2.59295900
H	6.72687600	-2.15968900	-2.02965400
H	5.95472200	-1.72538300	2.19100900
H	3.90451600	-0.36930100	1.77675600
O	3.18373300	0.09851400	-2.24643000
N	3.10134100	0.17402400	-0.85831900
H	7.33429500	-2.59283600	0.33696300
H	4.44027300	-0.68952800	-3.65587900

IM2'

C	1.34063700	0.44878200	-0.00669800
C	0.49108500	-0.22475300	-0.80633500
H	0.86539900	-0.55175600	-1.77499800
N	1.05405600	0.99623700	1.25251000
C	0.53224600	4.25349300	-0.07048000
C	0.24077600	3.33006700	0.93824700
C	-1.05427000	3.29334400	1.47140600
C	-2.03600800	4.16487500	1.00628400
C	-1.73466600	5.08895300	0.00171300
C	-0.44897900	5.13142500	-0.53735100
H	1.53595000	4.29379300	-0.48793600
H	-1.29562400	2.57348600	2.24928300
H	-3.03757100	4.12152100	1.42422800
H	-2.50071500	5.76956600	-0.35928200
H	-0.20741900	5.84657600	-1.31914300
C	1.33012800	2.43663900	1.49260500
H	2.30580100	2.73557500	1.09170800
H	1.40103600	2.55221600	2.57771900
C	0.36277600	-0.83725400	3.46061500
H	0.75487700	-1.38214200	4.32044000
H	-0.29344400	-0.01955800	3.75515700
H	-0.08139900	-1.49560900	2.71430600
S	1.84719400	-0.04637800	2.67211200
O	2.45681000	0.93943400	3.68483800
O	2.72764500	-1.12485500	2.01029200
Au	-1.42375000	-0.78456600	-0.43753000

Br	-0.46591100	-2.98562700	0.46187100
Br	-3.81702300	-1.46011900	0.07661000
Br	-2.12270100	1.27814800	-1.72874700
C	3.60711700	-0.39506100	-0.86751700
C	4.70056300	0.25798200	-1.52602100
C	5.80886600	-0.49692300	-2.00703300
C	5.76830000	-1.85367900	-1.82651800
C	4.66008700	-2.48978300	-1.17553800
C	3.57680700	-1.79719000	-0.68766600
C	4.35646900	1.59280700	-1.52981100
H	6.64148700	-0.00614200	-2.49929300
H	4.68162500	-3.56918300	-1.05977600
H	2.74956600	-2.27456500	-0.17751300
O	3.17112600	1.78654800	-0.95806300
N	2.70416400	0.53876200	-0.50945500
H	6.58748400	-2.47122200	-2.18033800
H	4.84759700	2.48977800	-1.88152100

TS2'-3'

C	1.41735100	0.38681600	0.19245900
C	0.59859000	-0.27996800	-0.68316000
H	1.03999800	-0.58232600	-1.63188400
N	0.97496900	0.91082000	1.43189300
C	0.33868000	4.18489000	0.13723100
C	0.07211600	3.20354800	1.09696100
C	-1.23830100	3.05519700	1.57098800
C	-2.26065100	3.87236500	1.09399700
C	-1.98472700	4.85516200	0.13901600
C	-0.68340500	5.01051800	-0.33816700
H	1.35205800	4.30640600	-0.23804100
H	-1.45989700	2.28968800	2.31022200
H	-3.27347200	3.74040800	1.46370900
H	-2.78240900	5.49260700	-0.23222500
H	-0.46148000	5.77153800	-1.08164100
C	1.20005000	2.36309200	1.65906000
H	2.16232700	2.68596500	1.24534000
H	1.27302700	2.49766400	2.74249200
C	0.33228800	-0.83677300	3.69779800
H	-0.14339000	-1.48827100	2.96518800
H	0.73221600	-1.38436300	4.55212500
H	-0.29997900	-0.00422100	4.00319700
S	1.81086600	-0.08169400	2.86588700
O	2.45001300	0.91901900	3.84462300
O	2.66116400	-1.19092300	2.21430300

Au	-1.33839100	-0.78912300	-0.46370200
Br	-0.58874900	-2.94628100	0.67598200
Br	-3.80074500	-1.31582100	-0.20807600
Br	-1.70991800	1.22606200	-1.96615300
C	3.57770500	-0.31809400	-0.80627100
C	4.44785400	0.33434500	-1.72426300
C	5.44890700	-0.37824900	-2.42357400
C	5.54421900	-1.73528800	-2.20836500
C	4.66393100	-2.38220900	-1.30118600
C	3.68359300	-1.70738300	-0.59359300
C	4.09576900	1.69357800	-1.72832500
H	6.10462300	0.13585900	-3.11933400
H	4.76205100	-3.45365300	-1.15232600
H	3.03915800	-2.19560800	0.12670500
O	3.09884100	2.00125300	-0.99612300
N	2.75260000	0.53926300	-0.13713800
H	6.28941200	-2.32116000	-2.73600800
H	4.60725800	2.50396900	-2.24991900

IM3'

C	-0.09011600	1.01590400	0.51749200
C	0.38416600	0.28883600	-0.70698000
H	1.30236400	0.70589200	-1.10572700
N	-1.21028200	0.48791400	1.24265700
C	-3.61414800	2.53069900	-0.38050400
C	-3.35671600	1.41335400	0.42144600
C	-4.10808500	0.24570000	0.22732900
C	-5.09788600	0.19378900	-0.75201000
C	-5.35235100	1.31421400	-1.54953500
C	-4.61011400	2.48047200	-1.36070200
H	-3.02394300	3.43237000	-0.25142800
H	-3.90785700	-0.63189500	0.83664700
H	-5.67156300	-0.71831800	-0.89260900
H	-6.12621100	1.27588800	-2.31163500
H	-4.80205800	3.35514600	-1.97651100
C	-2.30051500	1.47820600	1.50584800
H	-1.88632400	2.48521500	1.60023600
H	-2.74040600	1.22105700	2.47524700
C	-1.67258600	-1.51195400	3.30478700
H	-1.66680400	-2.19100700	2.45310000
H	-1.26688200	-1.96433800	4.21062400
H	-2.64407300	-1.05339300	3.48459000
S	-0.49529500	-0.13374300	2.89626900
O	-0.60459400	0.93260000	3.99380300

O	0.87872200	-0.72616900	2.50743400
Au	0.85503800	-1.74646800	-0.33101500
Br	3.28519600	-1.29307400	-0.77068500
Br	-1.19527100	-3.17081500	-0.05850200
Br	-0.91608200	0.28022100	-2.16797700
C	1.61263800	2.72877900	0.47041100
C	1.60697400	4.02120900	-0.11610000
C	2.82840800	4.65661700	-0.38168500
C	4.04096100	4.05113000	-0.06728400
C	4.03628800	2.78829200	0.53330000
C	2.83870500	2.12809100	0.80218900
C	0.35770400	4.71912500	-0.45615400
H	2.81174200	5.64101100	-0.84398500
H	4.97304400	2.30542800	0.79607600
H	2.83579500	1.16086000	1.29320400
O	-0.76385100	4.25209400	-0.35596100
N	0.42778300	2.12344000	0.87362500
H	4.97830400	4.55503500	-0.28066700
H	0.50241000	5.75785100	-0.82379500

TS3'-7'

C	-1.72719500	0.31238800	0.09311900
C	-0.73814400	-0.79232800	0.14971200
H	-1.07674800	-1.63607300	0.74089100
N	-3.06794200	-0.15054300	0.31620300
C	-1.40220200	-1.74071700	-1.67208000
C	-2.74061500	-1.93942800	-1.20522500
C	-3.15276500	-3.21649300	-0.83366100
C	-2.28344000	-4.30498900	-0.95532500
C	-0.97870100	-4.13407500	-1.44329600
C	-0.54922700	-2.87233100	-1.81907600
H	-1.15659700	-0.83058700	-2.21907400
H	-4.15513100	-3.36689700	-0.44291100
H	-2.62459200	-5.29527400	-0.66583100
H	-0.31783900	-4.98951700	-1.54177400
H	0.44534600	-2.71934000	-2.22194400
C	-3.61356600	-0.73692400	-0.94317200
H	-3.58469300	-0.00733500	-1.76037800
H	-4.64956400	-1.04059100	-0.77449200
S	-4.20296200	1.20487000	0.98297700
O	-5.08126700	1.74128200	-0.15416700
O	-3.38849700	2.11276600	1.90730400
Au	1.29951300	-0.49871300	0.29236900
Br	1.87475300	-0.34258100	-2.17856800

Br	3.74813100	-0.18815700	0.87193400
Br	0.67335900	-0.69208200	2.76495200
C	-0.39937000	2.27017200	-0.38188400
C	-0.05077900	2.79790800	-1.65287000
C	1.01663800	3.70012700	-1.75287700
C	1.74179000	4.08292600	-0.62868400
C	1.38965300	3.56163000	0.61921300
C	0.32644900	2.66750700	0.75195000
C	-0.75040700	2.36778800	-2.86601700
H	1.28428200	4.08371400	-2.73462300
H	1.94727200	3.84812400	1.50601500
H	0.02865400	2.29938700	1.72732400
O	-1.56791000	1.45912800	-2.93172400
N	-1.56267800	1.52737300	-0.25167600
C	-5.25481900	0.12158700	2.07592800
H	-5.75003100	-0.61168800	1.44112900
H	-4.57847400	-0.33094800	2.79874800
H	-5.97125400	0.79671700	2.54482700
H	-0.48206800	2.93536200	-3.78096800
H	2.57471800	4.77236900	-0.72037400

TS3'-4'

C	1.23073000	1.13899200	0.25514100
C	1.40966600	-0.14440100	-0.39973500
H	2.33947600	-0.27898500	-0.94626400
N	-0.02575700	1.73284600	0.23734600
C	-2.70810700	1.60749300	-1.48515200
C	-1.91077300	2.70328500	-1.12120400
C	-2.51313300	3.95512200	-0.93887100
C	-3.89155800	4.10803300	-1.11066600
C	-4.67877700	3.01097800	-1.46484800
C	-4.08416900	1.75955700	-1.65254200
H	-2.25568700	0.63270000	-1.64296700
H	-1.90332200	4.80482600	-0.64568800
H	-4.34699700	5.08387500	-0.96622200
H	-5.75054900	3.12987200	-1.59850900
H	-4.68718300	0.90195600	-1.93700000
C	-0.41591500	2.54631800	-0.95334900
H	0.00844800	2.01741100	-1.81365200
H	0.07057700	3.52697000	-0.88338600
S	-0.41173300	2.60621100	1.88908200
O	-0.42881800	4.12035200	1.65329500
O	0.50448200	1.95840700	2.93685200
Au	-0.10629900	-1.37560100	-0.92717200

Br	-0.58696300	-2.01109200	1.48782200
Br	-2.01108300	-2.80485300	-1.77534500
Br	0.53144000	-0.58711800	-3.26798000
C	3.22045300	0.80302400	1.21173900
C	4.59217100	1.19045700	1.25348500
C	5.55486500	0.19714300	1.35093700
C	5.20526100	-1.16779000	1.45555600
C	3.87396000	-1.55079900	1.51041900
C	2.86458400	-0.57121500	1.43169600
C	5.00342000	2.61973200	1.12738100
H	6.59729700	0.50146300	1.32993500
H	3.59835600	-2.58866200	1.67056400
H	1.86798600	-0.80730200	1.79947400
O	6.16934000	2.96020300	1.09752300
N	2.25278500	1.69661100	0.88666800
H	5.99022500	-1.91300300	1.54202900
H	4.17928400	3.35303000	1.08051700
C	-2.13390500	1.96433500	2.19834500
H	-2.77543100	2.38494900	1.42721600
H	-2.05415500	0.87864900	2.14614100
H	-2.38480400	2.31856600	3.19900900

IM4'

C	1.35862200	0.15614300	-0.21701300
C	0.17833100	0.54651300	0.62529400
H	0.27060000	0.12084200	1.62711800
N	1.73307400	-1.04136600	-0.62646600
C	5.05030100	-0.26858900	-0.37329500
C	4.22361200	-1.38211400	-0.58105600
C	4.58469100	-2.61882200	-0.02517400
C	5.74660300	-2.73673900	0.73961600
C	6.56345500	-1.62340800	0.94844400
C	6.21525100	-0.39353600	0.38642200
H	4.78063700	0.69070200	-0.80410900
H	3.96498600	-3.49197800	-0.21004100
H	6.02029100	-3.70108400	1.15939100
H	7.47161400	-1.71684700	1.53793700
H	6.85378900	0.47333200	0.53368400
C	2.97066900	-1.25727900	-1.42822500
H	3.03622800	-0.41410700	-2.11744000
H	2.80037100	-2.16918900	-2.00392700
C	0.74522500	-2.90880500	1.50110800
H	0.02333600	-2.20963500	1.92732700
H	0.44218600	-3.94550400	1.65740500

H	1.78150800	-2.73181000	1.78834500
S	0.69181400	-2.69681600	-0.35298900
O	1.61011600	-3.73168000	-0.99517900
O	-0.73060400	-2.48451000	-0.85105800
Au	-1.80375500	0.04088000	0.00900300
Br	-1.24426800	1.01987700	-2.27751500
Br	-4.21170400	-0.40532900	-0.66303600
Br	-2.24895100	-0.69799400	2.41904700
C	1.71816000	2.27425400	0.09601600
C	2.36734300	3.54846800	0.26739100
C	1.83446500	4.38387700	1.22592000
C	0.69491900	4.05892500	2.04514800
C	-0.01190600	2.92298700	1.81990200
C	0.34189000	2.07826800	0.64998900
C	3.62543200	3.94346100	-0.41205200
H	2.33833300	5.33168400	1.41075500
H	-0.89162300	2.66662000	2.40448000
H	-0.30320600	2.47665900	-0.17095300
O	4.28530600	3.24385800	-1.15071700
N	2.20985100	1.20807300	-0.49370200
H	0.41044800	4.74466700	2.83662800
H	3.93909200	4.98593100	-0.18113900

TS3'-5'

C	0.23880000	1.09836400	-0.30749300
C	0.46599700	-0.25586000	-0.74044800
H	0.72884000	-0.35520700	-1.78760800
N	-0.77894500	1.80146100	0.25142400
C	-0.70760400	3.25498200	0.53203100
H	0.28890800	3.46161400	0.93120700
H	-1.43131200	3.44163300	1.32897700
S	-2.46961800	0.96583600	0.63830500
O	-3.23260700	2.10001900	1.32038300
O	-2.15848000	-0.34606600	1.34645200
Au	0.22941400	-2.00935900	0.27415100
Br	-0.21419800	-4.25910500	1.32081300
Br	1.82255600	-1.38878600	2.13824200
Br	-1.27069700	-2.53073800	-1.74510300
C	2.47296400	2.00205600	0.24308300
C	3.63959100	2.45098100	-0.42370300
C	4.63995200	3.09882700	0.31006000
C	4.50849700	3.28426700	1.68338900
C	3.36441800	2.81774400	2.34298800
C	2.35011100	2.18094500	1.63389300

C	3.83286000	2.26173800	-1.88711800
H	5.51818600	3.44230200	-0.22745100
H	3.26564700	2.94122000	3.41739000
H	1.48975200	1.77472000	2.15453100
O	4.79640100	2.69274100	-2.49115000
N	1.49397900	1.36850900	-0.52484200
C	-3.21051500	0.66523200	-1.04762000
H	-2.62253700	-0.12682000	-1.51404900
H	-4.23290600	0.34421800	-0.84152100
H	-3.16829900	1.62466800	-1.56263700
C	-1.00806900	4.10516800	-0.68638300
C	-2.32869500	4.47641500	-0.98049500
C	0.02406100	4.52652900	-1.53527300
C	-2.61077200	5.24207900	-2.11331500
H	-3.13046000	4.17494100	-0.31123600
C	-0.25889500	5.29290200	-2.66719000
H	1.05434500	4.26687300	-1.30555300
C	-1.57697300	5.64814500	-2.96034700
H	-3.63612400	5.53065600	-2.32757900
H	0.55059400	5.61690100	-3.31518300
H	-1.79647400	6.24701200	-3.83972500
H	3.03918800	1.69438900	-2.40766500
H	5.29473700	3.78056400	2.24414900

IM5'

C	-1.09963000	0.68426000	0.66266900
C	0.32791100	0.64696900	0.94261300
H	0.60342700	0.98216600	1.94494400
N	-2.30139500	0.24053600	0.86586100
C	-4.00173600	-1.02932800	-1.41041700
C	-4.44449400	-0.14355100	-0.41796300
C	-5.79802500	-0.13347600	-0.05526500
C	-6.70240800	-1.00039200	-0.67371900
C	-6.25456500	-1.88436600	-1.65579900
C	-4.90499900	-1.89747800	-2.02070000
H	-2.95157000	-1.05417900	-1.68895000
H	-6.15250200	0.56861400	0.69760400
H	-7.75074500	-0.98096100	-0.38987000
H	-6.95393500	-2.56209600	-2.13694600
H	-4.55226300	-2.58695900	-2.78184100
C	-3.49708200	0.84663600	0.22329800
H	-3.10080800	1.54038500	-0.52782600
H	-4.02457100	1.44261200	0.97644500
S	-2.33184100	-1.49382100	1.88567500

O	-1.07655600	-1.36878500	2.73287700
O	-2.58599300	-2.64630800	0.93477100
Au	1.73772300	-0.57872100	0.03298400
Br	3.34726600	0.19949500	1.83133400
Br	3.50419500	-2.07426000	-1.00597500
Br	0.04827300	-1.22602800	-1.77051100
C	-0.56767200	3.09618800	0.04404400
C	0.24974800	3.80179800	-0.85697600
C	0.14075100	5.19708200	-0.91242900
C	-0.76389400	5.87759600	-0.10281500
C	-1.57256300	5.16356800	0.78669200
C	-1.47432700	3.77471200	0.86690600
C	1.21501600	3.11390700	-1.76765500
H	0.78240700	5.72140400	-1.61364900
H	-2.27457300	5.68746200	1.42900400
H	-2.08129500	3.22217300	1.57839000
O	1.91362300	3.72513400	-2.55090000
N	-0.44771200	1.68359200	0.11038000
H	1.25754500	2.01202300	-1.69732300
H	-0.83981400	6.95923000	-0.15870700
C	-3.84328300	-1.19383700	2.94046800
H	-3.65306500	-0.27504300	3.49336900
H	-4.68981100	-1.13558600	2.25741000
H	-3.89713100	-2.06430300	3.59630900

TS5'-6'

C	1.60243000	-0.36540300	0.09581200
C	0.36854000	0.20879600	0.57037000
H	0.51434800	0.93859100	1.36477700
N	1.92151100	-1.65699600	0.11028200
C	0.62069700	-1.58695100	2.88957500
C	0.13365300	-2.25218900	1.74669200
C	-1.22770400	-2.60146400	1.68478400
C	-2.08431600	-2.28844000	2.73719600
C	-1.59582600	-1.61908100	3.86448200
C	-0.24711400	-1.26928000	3.93650100
H	1.66968700	-1.31960100	2.95836400
H	-1.61105900	-3.11565000	0.80768900
H	-3.13513700	-2.55424600	2.67254300
H	-2.26789600	-1.36875200	4.67999800
H	0.13757400	-0.75211500	4.81064300
C	1.06105200	-2.72612200	0.64125400
H	1.73636000	-3.50703900	1.00435300
H	0.47318900	-3.14653500	-0.18095700

C	3.29382000	-1.93340300	-2.45343800
H	3.04135100	-0.88283900	-2.58386700
H	4.23422200	-2.21242300	-2.93055500
H	2.47385900	-2.60026700	-2.71489200
S	3.58812500	-2.16915500	-0.62689600
O	3.65152200	-3.66182300	-0.30984800
O	4.64782200	-1.19139300	-0.13418400
Au	-1.44507300	0.24891500	-0.34256600
Br	-0.66868500	-1.23191900	-2.28043500
Br	-3.76182100	0.31673300	-1.34296900
Br	-2.16450000	1.84455800	1.50175300
C	2.61099500	1.87067000	-0.43082600
C	3.24712200	2.38837300	0.73680100
C	3.75895200	3.69620600	0.70793000
C	3.62826800	4.51186900	-0.40955200
C	2.99470000	4.00288700	-1.54926300
C	2.51034600	2.70040900	-1.56609200
C	3.42486600	1.63753400	1.98681900
H	4.26098100	4.07044100	1.59749800
H	2.88654200	4.62230800	-2.43494000
H	2.03612200	2.29446500	-2.45404000
O	2.88850500	0.57873200	2.27650600
N	2.20678400	0.56334400	-0.58946900
H	4.01764100	5.52482300	-0.39991400
H	4.10447900	2.12797300	2.71438500

IM6'

C	-1.31355700	0.16550500	0.11667700
C	0.02692800	0.79083800	0.38987100
H	0.11666500	1.02674200	1.44888400
N	-1.80005700	0.59186200	-1.16606100
C	-0.80885400	1.46566600	-1.75267400
H	-1.27117600	2.22916800	-2.38021900
H	-0.10835800	0.85598100	-2.32914900
S	-3.53630600	1.43014600	-1.20688600
O	-3.37193200	2.60604900	-2.18456900
O	-4.02409800	1.67863300	0.22482800
Au	1.74076100	-0.47361700	0.07389900
Br	3.82837400	-1.93420800	-0.11359600
Br	2.96244900	1.13318600	1.63002100
Br	0.59627700	-1.90458000	-1.69081700
C	-2.99363400	-1.36465400	0.88937700
C	-4.03540300	-1.22176800	1.84370300
C	-5.12216000	-2.10554000	1.80549000

C	-5.19545200	-3.13006900	0.86523900
C	-4.15300200	-3.28302900	-0.05499900
C	-3.06380100	-2.41140000	-0.05106500
C	-4.02131800	-0.17978900	2.89409700
H	-5.91798800	-1.97997000	2.53671500
H	-4.18087800	-4.09228800	-0.77997600
H	-2.23693400	-2.54661100	-0.74143200
O	-3.18708200	0.69179300	3.03783600
N	-1.85852500	-0.57891200	0.98273800
C	0.02383800	2.10146000	-0.51597400
C	1.33725000	2.56728800	-0.97455600
C	-0.77688600	3.12802000	0.17812000
C	1.75386900	3.87124000	-0.82731600
H	1.97074400	1.85128800	-1.48973800
C	-0.32664500	4.41324200	0.36072200
H	-1.74914000	2.83890000	0.57300200
C	0.92825400	4.78848700	-0.15655900
H	2.72505700	4.18093800	-1.19799900
H	-0.93490900	5.13856000	0.89091500
H	1.26952800	5.81263000	-0.02824800
C	-4.55892500	0.12440700	-2.04054000
H	-4.09891700	-0.02651700	-3.01600800
H	-4.51796000	-0.76380400	-1.41285300
H	-5.56015800	0.55051600	-2.11381900
H	-4.87916800	-0.25835900	3.60023000
H	-6.04213600	-3.80960600	0.85635300

TS6'-7'

C	1.81569600	0.05598800	0.14441500
C	0.47537800	0.04831900	0.80409400
H	0.36660600	0.90494100	1.46288200
N	2.54661200	-1.09240800	0.29003800
C	0.93473100	-0.88645400	2.68119600
C	0.78113000	-1.91935600	1.71442200
C	-0.37910100	-2.74135500	1.76543800
C	-1.33333500	-2.53067600	2.73663100
C	-1.18346500	-1.48932000	3.68742700
C	-0.06930000	-0.67947900	3.66155500
H	1.87079100	-0.34245400	2.75707100
H	-0.49982500	-3.52857200	1.02824200
H	-2.21844800	-3.15883100	2.76768000
H	-1.95412700	-1.33465400	4.43585800
H	0.06220900	0.11589500	4.38752000
C	1.91832900	-2.30460700	0.79308800

H	2.66673900	-2.88800800	1.33878300
H	1.53275900	-2.92345700	-0.02361900
C	4.05072200	-0.92406600	-2.21697400
H	3.71632100	0.10725000	-2.30037000
H	5.04083100	-1.09650100	-2.64071200
H	3.31192800	-1.64244600	-2.57000800
S	4.25681800	-1.24563200	-0.39095900
O	4.54467000	-2.73588200	-0.17995600
O	5.13470600	-0.17073200	0.23432300
Au	-1.29861800	-0.22836500	-0.24805000
Br	-0.16638400	-1.65271500	-2.04513700
Br	-3.50897600	-0.50983700	-1.45074800
Br	-2.40035400	1.32816900	1.43837000
C	1.66244100	2.32329000	-0.63444500
C	1.69853600	3.30068700	0.39951500
C	1.25518500	4.60812800	0.12232800
C	0.74046800	4.95738200	-1.11834700
C	0.69057700	3.98742300	-2.12554500
C	1.16319300	2.69890200	-1.89305400
C	2.15527500	3.04702600	1.77389900
H	1.30727400	5.34923400	0.91707300
H	0.29257600	4.23863600	-3.10473600
H	1.14975900	1.95490800	-2.68369100
O	2.31397700	1.95772200	2.30861000
N	2.24776400	1.05807000	-0.52466400
H	0.38680200	5.96640800	-1.30464700
H	2.33330700	3.97248000	2.36171000

TS3'-9'

C	1.16528400	1.04628800	-0.58256800
C	-0.18860300	1.08423100	0.03556500
H	-0.46284100	2.07818500	0.35484700
N	1.83960700	-0.14401000	-0.81343400
C	3.93375800	-1.32031800	1.05658100
C	4.04124200	-1.19339500	-0.33698700
C	4.86889800	-2.07643600	-1.04026400
C	5.58485400	-3.06758200	-0.36291500
C	5.47309400	-3.18785800	1.02307200
C	4.64372900	-2.31278400	1.73169800
H	3.28236800	-0.64697200	1.60848400
H	4.94241900	-1.99424500	-2.12122000
H	6.22362900	-3.74714400	-0.92037200
H	6.02645700	-3.96035100	1.54996400
H	4.55157500	-2.40284500	2.81061900

C	3.29952700	-0.09043700	-1.06344400
H	3.62302600	0.89010100	-0.71034400
H	3.49843800	-0.12518600	-2.13845000
S	1.07967400	-1.58952300	-1.82800800
O	2.05591100	-1.82184200	-2.98262000
O	-0.38962900	-1.25448100	-2.10313200
Au	-1.69600100	-0.26453400	0.20879900
Br	-2.00216100	1.47465700	-1.70982600
Br	-3.82672200	-1.59645900	0.00856200
Br	-0.96431000	-1.54874900	2.24603900
C	1.55727700	3.38059500	-0.17263300
C	1.37493500	3.56249800	1.23468600
C	1.35393300	4.87056000	1.76506600
C	1.41470400	5.98483800	0.94442000
C	1.56774700	5.80265900	-0.43886400
C	1.67080100	4.52917400	-0.98192800
C	1.28323800	2.47196300	2.20210800
H	1.26167600	4.99080800	2.84231500
H	1.63439000	6.66691400	-1.09365800
H	1.84592300	4.38595100	-2.04320900
O	0.93944100	1.30519700	1.99203700
N	1.80172200	2.16156100	-0.77507600
C	1.16850000	-3.02458900	-0.64567600
H	2.22598000	-3.21443900	-0.47531000
H	0.63076000	-2.72496700	0.25387500
H	0.66890900	-3.83644200	-1.17673300
H	1.36094900	6.98314900	1.36625400
H	1.54482100	2.74704700	3.24058500

IM7'

C	-1.42848200	0.21535300	0.09762300
C	-0.15404200	0.73577100	0.69438500
H	-0.17706000	0.55979700	1.77024100
N	-2.32161400	1.14910200	-0.56828900
C	-1.66578900	2.13273500	-1.44085100
H	-2.39603000	2.92884300	-1.63928300
H	-1.46094800	1.63824000	-2.39573500
S	-3.36871100	2.12622500	0.69366300
O	-4.10543200	3.16949500	-0.15647600
O	-2.46756500	2.60357900	1.86796800
Au	1.57657100	-0.38735400	0.08792100
Br	3.63443800	-1.75566800	-0.58254200
Br	2.16251400	-0.61235200	2.54627600
Br	1.05322900	0.10666700	-2.36291900

C	-2.74886700	-1.72140400	-0.38191500
C	-3.56772300	-2.60497000	0.37122100
C	-4.44136100	-3.47990300	-0.29421400
C	-4.54278600	-3.48109500	-1.68022300
C	-3.73643600	-2.60824100	-2.41958300
C	-2.84877100	-1.74367400	-1.78532300
C	-3.54921100	-2.62562600	1.84101700
H	-5.05009200	-4.15815800	0.29978600
H	-3.78778700	-2.61027900	-3.50494000
H	-2.18339800	-1.11452400	-2.36647100
O	-3.13596300	-1.72593200	2.55777100
N	-1.72436500	-1.01424800	0.23781600
C	-0.38399600	2.71720900	-0.89400300
C	0.28206200	3.75418200	-1.52872700
C	0.06383800	2.24638700	0.42119300
C	1.42679400	4.30360700	-0.94591400
H	-0.07343100	4.13199800	-2.48305600
C	1.30082100	2.83100700	0.94835600
H	-0.74142600	2.70098300	1.09898200
C	1.93967700	3.84997700	0.29076200
H	1.94006600	5.11117100	-1.46185400
H	1.67454100	2.44399300	1.89261200
H	2.83953100	4.29736700	0.69941800
C	-4.54218900	0.84964900	1.33115700
H	-5.07732600	0.47598100	0.45945500
H	-3.94372400	0.08646800	1.83489700
H	-5.19285400	1.39217000	2.01858300
H	-5.22608000	-4.15875500	-2.18234400
H	-3.97774900	-3.54349000	2.29623700

IM9'

C	1.38563100	-0.16136400	0.75569700
C	0.31997800	-0.86086100	-0.09897000
H	0.27977600	-1.90296300	0.22111800
N	1.30577300	1.14696900	1.15441900
C	4.86546300	1.78210200	0.53879800
C	3.49422400	2.01894700	0.38785800
C	3.01680600	2.50757400	-0.83595000
C	3.90162600	2.75662700	-1.88653200
C	5.27060000	2.52797500	-1.72591200
C	5.75100900	2.04074400	-0.50923500
H	5.24223500	1.39507200	1.48265000
H	1.95235500	2.67713400	-0.97303700
H	3.51871800	3.13502500	-2.83061400

H	5.95765800	2.72761400	-2.54381800
H	6.81367000	1.85652600	-0.37523700
C	2.56741500	1.79576600	1.56962600
H	3.07074700	1.20864400	2.34438200
H	2.29288200	2.75345400	2.02199400
C	-1.07781000	2.91180000	1.78507200
H	-1.43869700	2.60631900	0.80471200
H	-1.88119400	3.05979300	2.50833000
H	-0.39330500	3.75808800	1.74468000
S	-0.08448400	1.50369500	2.49247700
O	0.68681300	2.04070400	3.69987600
O	-0.90253500	0.21469800	2.57691200
Au	-1.66896300	-0.23110700	-0.33940000
Br	-2.36389800	-2.45847400	0.67217800
Br	-4.09479300	0.51726500	-0.49983600
Br	-0.93627300	1.79792000	-1.72571200
C	2.90076700	-1.99440900	0.46280000
C	2.69623100	-2.38649200	-0.90979600
C	3.41597200	-3.49754500	-1.44808900
C	4.20440600	-4.27649900	-0.63857900
C	4.34437200	-3.93639100	0.73003800
C	3.73544900	-2.81642600	1.25933600
C	1.85229400	-1.67938400	-1.77939300
H	3.29295900	-3.73722500	-2.50097200
H	4.97111300	-4.55207300	1.36891300
H	3.89232100	-2.52241200	2.29153100
O	0.89448100	-0.87639100	-1.46159900
N	2.47581400	-0.82656400	1.01318400
H	4.72200300	-5.14140300	-1.03970900
H	1.96260100	-1.77605000	-2.85929200

TS4'-10'

C	0.57380500	1.07055300	-0.03998500
C	-0.26082000	0.22234000	-0.98650800
H	-0.67004400	0.81314100	-1.80717600
N	0.19545300	2.19177000	0.63700600
C	3.12324100	3.75746800	-0.03286100
C	1.89149400	4.01650300	0.58353900
C	1.29589600	5.27677200	0.42770800
C	1.91474200	6.26138000	-0.34345100
C	3.13994200	5.99654300	-0.96054000
C	3.74245700	4.74711500	-0.79981300
H	3.58925600	2.78369300	0.08849500
H	0.35497200	5.49003400	0.93088900

H	1.44838400	7.23711100	-0.45192700
H	3.62610100	6.76402700	-1.55700100
H	4.70040100	4.54063200	-1.26971200
C	1.20817000	2.95589500	1.42038700
H	1.92243700	2.22781900	1.80786600
H	0.67396100	3.40884600	2.25730000
C	-2.29170900	3.30127700	-0.41960200
H	-2.38024900	2.51807000	-1.17115400
H	-3.26978400	3.67431100	-0.11273800
H	-1.60534300	4.10224700	-0.69251600
S	-1.57298800	2.54639100	1.12270100
O	-1.46189000	3.66003700	2.16597600
O	-2.27853300	1.22240100	1.47189200
Au	-1.99086800	-0.83597600	-0.22939500
Br	-0.21886200	-2.23687700	1.16058100
Br	-3.95331100	-2.18842200	0.66952300
Br	-3.36013400	0.07991500	-2.14079800
C	2.01723200	-0.33439800	-0.86369100
C	3.21984900	-0.99976300	-1.19950000
C	3.14004300	-2.03937800	-2.13598500
C	1.93859800	-2.41906200	-2.75463900
C	0.75241600	-1.76677900	-2.43364100
C	0.78083700	-0.76639300	-1.43764700
C	4.55354300	-0.62200100	-0.67356100
H	4.05743400	-2.56068500	-2.40188200
H	-0.18593700	-2.04509600	-2.90579500
H	0.62318600	-1.75303100	-0.16027400
O	4.80280000	0.32763000	0.04026800
N	1.84967500	0.72042300	0.00064600
H	1.93796600	-3.21689300	-3.48993500
H	5.36584300	-1.30526900	-1.01018500

IM10'

C	1.20644600	1.06709700	-0.00246100
C	0.38152800	0.17036900	-0.84769200
H	-0.35341200	0.67142800	-1.47032200
N	0.83503000	2.12636300	0.72647200
C	4.10563500	3.53759100	0.93952400
C	2.72331000	3.75364600	0.91889000
C	2.21620500	4.87888600	0.25356000
C	3.07815400	5.76127100	-0.39475300
C	4.45790900	5.53350100	-0.37989700
C	4.97041100	4.42407700	0.29141800
H	4.51999400	2.68210400	1.46937100

H	1.14605400	5.07028400	0.26500400
H	2.67592900	6.63299200	-0.90354800
H	5.12857800	6.22305800	-0.88477700
H	6.04089700	4.24214800	0.31371800
C	1.78134100	2.80672400	1.63917000
H	2.32467100	2.04172200	2.20685100
H	1.16476500	3.36511800	2.34945800
C	-1.83641600	2.81980900	-0.49099600
H	-2.10860500	1.85149300	-0.91503000
H	-2.71637400	3.41241400	-0.23540700
H	-1.11565500	3.38901900	-1.07671400
S	-1.03311100	2.49984400	1.16627000
O	-0.87650300	3.83892200	1.88580600
O	-1.65631600	1.28937500	1.84872900
Au	-0.87746900	-1.20122200	0.30584700
Br	0.95279800	-1.58966800	2.03233600
Br	-2.36233500	-2.89364800	1.47155400
Br	-2.65518600	-0.81883000	-1.50631200
C	2.64779600	-0.33384000	-1.04126400
C	3.83223000	-0.96456800	-1.43358100
C	3.71238500	-1.97004600	-2.41030600
C	2.46917200	-2.30536800	-2.94975100
C	1.29711700	-1.66294800	-2.52383500
C	1.39132300	-0.66400300	-1.55426700
C	5.11752700	-0.57834300	-0.84462400
H	4.60743000	-2.48915000	-2.74344800
H	0.33050000	-1.94786400	-2.92827100
H	3.30943700	1.09867000	0.34908500
O	5.24393200	0.30804800	-0.00695500
N	2.49826800	0.70495800	-0.11829500
H	2.40433700	-3.08359000	-3.70342300
H	6.00209200	-1.14047500	-1.20336100
P_t			
C	0.16891700	0.38278600	-0.38277800
C	0.80604400	0.22606300	-1.59906800
H	0.38805100	0.46488300	-2.56616900
N	-1.10188100	0.83199500	-0.02657000
C	-2.33267900	-2.16917500	-1.20889800
C	-2.61042000	-1.05447100	-0.41112200
C	-3.25316800	-1.24306800	0.82032200
C	-3.61614800	-2.52114200	1.24119400
C	-3.33932200	-3.62958100	0.43507600
C	-2.69749500	-3.45138900	-0.79068100

H	-1.82918200	-2.03270500	-2.16283100
H	-3.46787600	-0.38019900	1.44584700
H	-4.11909400	-2.65403600	2.19541400
H	-3.62443600	-4.62594000	0.76207700
H	-2.47888400	-4.30824700	-1.42235200
C	-2.22330400	0.33855400	-0.86167800
H	-1.97340500	0.34154700	-1.93023200
H	-3.05185400	1.03639800	-0.70770300
C	-0.41230400	3.13658800	1.62938200
H	0.59969300	2.73429800	1.61930700
H	-0.41802700	4.22191400	1.73298100
H	-1.05434800	2.64836700	2.36042400
S	-1.15868400	2.78750700	-0.03988600
O	-2.65100500	3.16417300	0.01155000
O	-0.22542000	3.36336900	-1.11729800
C	2.23972000	-0.35123400	0.09278300
C	3.41125500	-0.81215700	0.72725800
C	4.48970300	-1.15401200	-0.09744200
C	4.40578300	-1.04384000	-1.49478300
C	3.23805000	-0.59704900	-2.11156800
C	2.12718400	-0.24857400	-1.32379600
C	3.47963100	-0.92149800	2.18286600
H	5.40865400	-1.51152900	0.36146400
H	3.18736900	-0.52055300	-3.19444000
H	0.83986800	-0.05032900	1.62205600
O	2.55602500	-0.63840600	2.93843300
N	1.05869900	0.05421700	0.63963000
H	5.26366700	-1.31401800	-2.10308500
H	4.44555500	-1.28734100	2.59010700

Cartesian coordinates for the stationary points given in Fig. S2

1b

C	1.39249900	-1.21292700	1.65109200
C	1.20079300	-1.06128500	2.83974800
H	1.06981300	-0.98758200	3.89382600
N	1.59809600	-1.39917700	0.34400000
C	2.57080700	-0.56607700	-0.40211000
H	2.42366400	-0.81332000	-1.45780200
H	3.56302900	-0.92505100	-0.10959600
C	-2.44471000	1.27479900	-0.92547600
C	-1.41714300	0.36527100	-1.17385400
C	-1.27988500	-0.71202100	-0.30909400
C	-2.11144400	-0.91419900	0.78648100
C	-3.12692500	0.01203500	1.01576600

C	-3.30699800	1.11700000	0.16942000
H	-2.58246000	2.11732700	-1.59830900
H	-0.74866500	0.47861900	-2.01922400
H	-1.97748500	-1.78195000	1.42235000
H	-3.79418400	-0.13022900	1.86203600
C	-4.39950400	2.12251200	0.44528600
H	-4.63157300	2.71711900	-0.44356100
H	-5.32073500	1.63142200	0.77690500
H	-4.09983900	2.81886800	1.23950800
S	0.05978200	-1.93639600	-0.62596700
O	-0.35237100	-3.26046000	0.01570500
O	0.49559900	-1.82462100	-2.09422300
C	1.66848100	2.91334900	-0.52666800
C	2.64135300	3.06663900	0.41266000
C	3.17860400	1.75784600	0.64109800
C	2.49653900	0.90470100	-0.17725800
O	1.56623100	1.60668200	-0.90052100
H	0.99327700	3.59591100	-1.01984500
H	2.94268400	3.99159100	0.88410300
H	3.96882500	1.48517500	1.32684500

IM13

C	-1.13483400	1.10271100	0.41921400
C	-0.93938300	0.04192000	1.13916600
H	-1.47364800	-0.15700900	2.06236400
N	-1.35308400	2.02523200	-0.38461100
C	-0.63855300	3.33772200	-0.55459900
H	-1.31786700	3.96209700	-1.14081400
H	0.25961200	3.12941900	-1.14187400
C	-6.18547400	0.95761300	-0.19358000
C	-5.11274200	1.56873700	-0.83672800
C	-4.04412000	0.75893300	-1.21004200
C	-3.98155900	-0.60737400	-0.95257900
C	-5.06840400	-1.18572100	-0.29989100
C	-6.18102400	-0.42047300	0.08326900
H	-7.04062400	1.56103100	0.09790800
H	-5.10914500	2.63083100	-1.05677500
H	-3.12301800	-1.20395500	-1.24122500
H	-5.03673000	-2.24875400	-0.07931500
C	-7.35872300	-1.07237200	0.76416900
H	-7.95777100	-0.34355700	1.31820400
H	-8.01690700	-1.54824700	0.02551900
H	-7.03446500	-1.85311500	1.45969800
S	-2.62140100	1.54929400	-2.04017400

O	-1.81721000	0.52958800	-2.84437700
O	-2.98197600	2.93780300	-2.57667700
C	-0.70458700	5.10380200	2.55606900
C	0.62294200	4.79933100	2.60680800
C	0.90608700	4.04747900	1.42242700
C	-0.27281200	3.95940300	0.73653000
O	-1.27136700	4.60237000	1.42416900
H	-1.36954400	5.64893200	3.20883500
H	1.32007900	5.07540600	3.38505700
H	1.85625600	3.62951300	1.11654800
Au	0.40258000	-1.37679600	0.49817200
Br	2.11221700	-3.14055600	-0.28531800
Br	-1.50030800	-3.12717900	0.82562600
Br	4.76094400	2.12534800	-0.59273700
Br	2.15833800	0.51264600	0.18393700
K	4.69398900	-1.07097000	-0.98651200

TS13-14

C	1.62100900	1.17263000	0.22466400
C	1.47272600	-0.02525300	-0.30300200
H	2.29651200	-0.71351200	-0.44107300
N	1.01693600	2.23665700	0.63422700
C	1.28459700	3.57722500	0.05862700
H	1.50740200	3.38560500	-0.99802200
H	2.17835500	3.99611900	0.53358700
C	-3.20758200	0.92241000	2.71071800
C	-1.81304200	0.94836600	2.69297700
C	-1.19809600	2.19540900	2.73300400
C	-1.89513700	3.39939100	2.77978200
C	-3.28460200	3.33717300	2.79204100
C	-3.96290700	2.10557800	2.75016900
H	-3.71345700	-0.03863100	2.68362000
H	-1.23160200	0.03340200	2.65121600
H	-1.37273400	4.34889800	2.79169700
H	-3.85599600	4.26010400	2.80854300
C	-5.46735300	2.07710600	2.70722800
H	-5.85403700	1.05649900	2.78314900
H	-5.89742700	2.67080900	3.52245100
H	-5.81593500	2.51758400	1.76273300
S	0.62520100	2.24695800	2.63586200
O	1.20654200	3.57505600	3.13001100
O	1.21386500	0.90094700	3.08049000
C	-1.86660000	5.30080300	-0.19577900
C	-1.21979300	6.28112200	0.49672300

C	0.09911200	5.78822200	0.75738400
C	0.16527600	4.54364500	0.19927900
O	-1.03063400	4.23761800	-0.39554000
H	-2.87890500	5.17609700	-0.56180000
H	-1.63544400	7.23389200	0.79291700
H	0.89259000	6.28260500	1.30067000
Au	-0.35547200	-0.70065300	-0.92526600
Br	-2.66317500	-1.58613700	-1.63217600
Br	-0.18123100	-2.37114600	0.96796000
Br	-5.30221900	3.87181200	-0.85284600
Br	-0.28594800	0.97770800	-2.85770300
K	-3.59100300	1.60789200	-2.12309900
C	4.42782500	0.60683400	1.17713300
C	5.63593500	0.39048200	0.44141500
C	6.72044400	-0.31082000	1.03401700
C	6.52497800	-0.79375000	2.30030700
C	5.30784100	-0.61223900	3.02443200
C	4.25567400	0.08699400	2.48778700
C	5.41740500	1.02701100	-0.78527600
H	7.66608100	-0.44570000	0.52497900
H	5.23037500	-1.03299800	4.02098500
H	3.32612500	0.24799100	3.02294100
O	4.19268100	1.57993900	-0.76339600
N	3.56976700	1.35622300	0.46404000
Cl	7.84551700	-1.68628800	3.11192200
C	5.90824600	2.27488300	-2.87331400
C	6.66153700	2.45220900	-4.02903700
C	7.71362600	1.58019800	-4.32410000
C	8.00754100	0.52190800	-3.46040000
C	7.25996400	0.33653400	-2.30111800
C	6.20531300	1.21641300	-1.99259100
H	5.09688300	2.95593400	-2.63995000
H	6.42903200	3.27321100	-4.70044200
H	8.29917300	1.72172800	-5.22776000
H	8.81370600	-0.16657500	-3.69500400
H	7.46845000	-0.51185500	-1.65864000

IM14

C	1.39261500	-0.14909900	-0.29823600
C	1.04491500	-1.33700500	-0.81596100
H	1.81836200	-2.01622200	-1.16792000
N	0.49710300	0.86153600	0.09788700
C	0.50238100	2.09910000	-0.72961500
H	0.41651200	1.73091300	-1.75974300

H	1.44884200	2.64431900	-0.63218000
C	-3.06235300	0.19835400	3.12581200
C	-1.73366300	0.12348400	2.70953100
C	-1.03194400	1.31733400	2.57355100
C	-1.58367900	2.56150100	2.85279900
C	-2.91152900	2.60337300	3.27245000
C	-3.67701200	1.43249200	3.39999300
H	-3.63123000	-0.72088900	3.23698800
H	-1.26352700	-0.83292500	2.50430700
H	-0.99733800	3.46476800	2.73305700
H	-3.36915200	3.56505300	3.48552700
C	-5.13378400	1.50974700	3.77107300
H	-5.50021700	0.55756300	4.16715600
H	-5.31563000	2.29108500	4.51681900
H	-5.72352100	1.75896400	2.87660600
S	0.69229900	1.23284100	1.96498100
O	1.40555000	2.59006800	2.10444200
O	1.36797700	-0.04762400	2.49459200
C	-2.66263600	3.82298800	-0.36939500
C	-1.86461900	4.87612100	-0.04438600
C	-0.51952900	4.38920400	-0.07943600
C	-0.58312700	3.07186700	-0.42944500
O	-1.89676200	2.71062700	-0.62042200
H	-3.73651500	3.67633700	-0.41989300
H	-2.19770100	5.87426300	0.20231300
H	0.38516800	4.93723000	0.14472500
Au	-0.85177100	-2.03585800	-0.94555800
Br	-3.26815900	-2.89657400	-0.99821500
Br	-0.25434800	-3.46319800	1.06359300
Br	-6.06949400	2.38418800	0.00115100
Br	-1.17886000	-0.62309300	-3.04925100
K	-3.91107900	0.41996000	-1.11515300
C	3.75867200	-0.58348200	0.59416500
C	5.02308400	0.00584100	0.30209800
C	6.19276000	-0.45712200	0.96220500
C	6.03680000	-1.50045700	1.83600200
C	4.77114200	-2.10159000	2.10618600
C	3.61876600	-1.65514400	1.50492400
C	4.75711900	1.03074600	-0.61645700
H	7.16039900	-0.00072300	0.80118400
H	4.72635100	-2.91825500	2.81830200
H	2.64528600	-2.07521500	1.72581400
O	3.43819200	1.05489700	-0.87771900
N	2.81051900	0.06552300	-0.11159800

Cl	7.45977900	-2.14136300	2.69930700
C	4.99677500	3.23397200	-1.72881800
C	5.78453400	4.18421900	-2.36857100
C	7.14473200	3.94097700	-2.58312800
C	7.71876100	2.73895700	-2.15966400
C	6.94120300	1.78272000	-1.51462200
C	5.57212800	2.02525100	-1.28787600
H	3.94442900	3.42800000	-1.55094000
H	5.33859100	5.11756000	-2.69778300
H	7.75567500	4.68577600	-3.08441300
H	8.77097100	2.54268800	-2.34072300
H	7.38371400	0.83535400	-1.22708700

TS14-15

C	1.33988400	0.19244600	0.24315300
C	1.23074200	-0.99144600	-0.44577600
H	2.14237500	-1.52763500	-0.70404900
N	0.20366700	1.00354300	0.51061300
C	0.25979600	2.32927800	-0.16453700
H	0.40618400	2.08349200	-1.22447500
H	1.12545700	2.91091600	0.17401900
C	-3.61383900	-0.48289600	2.88534000
C	-2.23818100	-0.32381600	2.71288000
C	-1.73233700	0.97138600	2.71931800
C	-2.52573900	2.09771400	2.90327900
C	-3.89506200	1.90753900	3.07447700
C	-4.46345200	0.62249100	3.05791700
H	-4.03155200	-1.48609100	2.88564200
H	-1.58486300	-1.18064600	2.58514600
H	-2.08710300	3.08869600	2.89846400
H	-4.53831400	2.77264300	3.20569000
C	-5.95462200	0.45017800	3.18167300
H	-6.22478800	-0.59063900	3.38443800
H	-6.36153700	1.07645600	3.98344800
H	-6.43964300	0.75779800	2.24480700
S	0.06363300	1.19885000	2.43210200
O	0.50960100	2.61345100	2.83415900
O	0.82612600	-0.03615200	2.95673900
C	-3.06954300	3.75062500	-0.26651400
C	-2.45538500	4.81919100	0.30898300
C	-1.08409100	4.44919100	0.48966300
C	-0.94820700	3.18030700	0.00869800
O	-2.16185800	2.73823900	-0.46916200
H	-4.09456900	3.52370300	-0.53774400

H	-2.92627700	5.75302300	0.58173400
H	-0.29650700	5.03795700	0.93875900
Au	-0.49836700	-1.85407800	-0.99215400
Br	-2.74160600	-2.93251000	-1.55752000
Br	-0.03384300	-3.40601000	0.95894800
Br	-6.29324500	1.89456000	-0.56051100
Br	-0.58082000	-0.27211900	-2.99602900
K	-3.69992900	0.32860200	-1.34578700
C	3.63462300	-0.15143500	1.03858600
C	4.88120400	0.24985200	0.50007000
C	6.07847100	-0.33120700	0.95876800
C	5.98979900	-1.34029700	1.89716600
C	4.75155500	-1.77490100	2.40474800
C	3.56649400	-1.18614100	1.99071200
C	4.66668000	1.31789900	-0.44938300
H	7.04262000	-0.00160700	0.59460900
H	4.72763000	-2.57059500	3.14160700
H	2.60923500	-1.45823400	2.41888100
O	3.44454400	1.62268800	-0.61121300
N	2.55896600	0.62979300	0.68182500
Cl	7.48463700	-2.11979700	2.48670300
C	5.43891600	3.45910800	-1.42267200
C	6.37899500	4.21715700	-2.11257400
C	7.55144600	3.61913300	-2.58491700
C	7.78377000	2.25832700	-2.36857900
C	6.85858000	1.49488000	-1.66087300
C	5.68345700	2.09567100	-1.17397300
H	4.52338600	3.91141600	-1.05669800
H	6.19635500	5.27300100	-2.28712200
H	8.28004200	4.21207000	-3.13001300
H	8.68276100	1.78935700	-2.75657400
H	7.02527200	0.43076500	-1.53417600

IM15

C	-1.52947700	0.23885900	-0.28858800
C	-1.45333100	-0.99975400	0.34801200
H	-2.37659800	-1.49005300	0.64621900
N	-0.32637000	0.96579000	-0.55330200
C	-0.32795700	2.32485900	0.06349100
H	-0.47794400	2.13248200	1.13372900
H	-1.17300500	2.92236600	-0.29317000
C	3.35497600	-0.74713700	-2.99263300
C	1.99189900	-0.52372900	-2.79263100
C	1.54081900	0.79138000	-2.82411300

C	2.37677700	1.87654600	-3.06159700
C	3.73194800	1.62268300	-3.26186200
C	4.24573100	0.31549500	-3.21927100
H	3.72909400	-1.76724700	-2.97506600
H	1.30669700	-1.34860200	-2.62684200
H	1.98032800	2.88503000	-3.07942300
H	4.40598500	2.45522400	-3.44155300
C	5.72455700	0.07375900	-3.37475700
H	5.94124800	-0.97752300	-3.58682600
H	6.14472100	0.68398500	-4.18165700
H	6.24644700	0.35109300	-2.44829100
S	-0.23644500	1.10686500	-2.50469800
O	-0.61856400	2.53263300	-2.92945300
O	-1.07835100	-0.09936100	-2.96457800
C	3.05484300	3.61980400	0.09831200
C	2.47979400	4.68529100	-0.52054200
C	1.09538200	4.35847400	-0.68487000
C	0.91284000	3.11618700	-0.15283700
O	2.11201300	2.64886500	0.34173700
H	4.06871300	3.37297400	0.38646100
H	2.98272800	5.59057700	-0.82992400
H	0.32808100	4.95856100	-1.15339900
Au	0.24804100	-1.89000300	0.92662900
Br	2.45538300	-3.04561800	1.49144000
Br	-0.29816400	-3.44431600	-1.00228500
Br	6.20969700	1.54504700	0.39251500
Br	0.40043300	-0.28397000	2.90529000
K	3.45362000	0.17782400	1.14428800
C	-3.84589300	0.21266400	-0.79930500
C	-5.08754500	0.88924800	-0.54340400
C	-6.28025600	0.28370800	-0.90335000
C	-6.26477200	-0.97948900	-1.50926800
C	-5.07101600	-1.64269400	-1.81663800
C	-3.87004100	-1.05088600	-1.47282200
C	-5.15190200	2.28475100	0.04864100
H	-7.22049600	0.79208000	-0.72247300
H	-5.09262800	-2.58555400	-2.35160600
H	-2.93234200	-1.47580400	-1.81472200
O	-5.80546600	3.11406400	-0.56645900
N	-2.69771300	0.85711300	-0.50745500
Cl	-7.80655900	-1.73352300	-1.94735300
C	-4.29057300	3.94841500	1.67177200
C	-3.69958600	4.29211200	2.88324400
C	-3.31358400	3.29168100	3.78314900

C	-3.52105900	1.94597700	3.46928500
C	-4.09505900	1.59880200	2.24690900
C	-4.47930100	2.59682000	1.33650900
H	-4.61170000	4.70818700	0.96676600
H	-3.54306800	5.33753400	3.13282600
H	-2.85779200	3.56151700	4.73168400
H	-3.23597400	1.17040500	4.17381700
H	-4.26687500	0.55154800	2.01516800

TS15-16

C	-1.10883800	0.05382900	0.00282300
C	-0.86482600	-0.89110700	-1.04513600
H	-1.64437500	-1.02982100	-1.78961900
N	-0.14663700	0.09221900	1.07346300
C	-0.71163100	-0.36559700	2.38513000
H	-1.16945200	-1.33509400	2.16097600
H	-1.49820000	0.31619900	2.72325000
C	4.38657700	0.61642300	1.34264800
C	3.01161100	0.61881900	1.11353200
C	2.25617800	1.63135000	1.70084000
C	2.80993700	2.60994600	2.52020800
C	4.18811500	2.58404300	2.72588000
C	4.99947000	1.61055100	2.12347400
H	4.99291500	-0.16382100	0.89120400
H	2.54507500	-0.15753000	0.51690100
H	2.18210600	3.36952200	2.97385900
H	4.64411600	3.35119400	3.34500000
C	6.49742200	1.66503900	2.25854100
H	6.80203200	2.13847700	3.19715700
H	6.94495500	0.66741400	2.20782600
H	6.90570600	2.26119400	1.43117300
S	0.49677000	1.84618300	1.22565200
O	-0.25450900	2.66042800	2.28980000
O	0.47288800	2.35220800	-0.25116800
C	2.04861600	-1.49459400	4.37801900
C	1.68747300	-0.48545900	5.21919300
C	0.56437100	0.15736600	4.60515700
C	0.32487200	-0.51074400	3.43823400
O	1.22945300	-1.52784500	3.29194300
H	2.82151400	-2.24746100	4.40143200
H	2.15817100	-0.22878900	6.15769300
H	0.01075300	1.01078100	4.97080100
Au	0.62104300	-2.25916900	-0.96114500
Br	2.73996000	-3.60983600	-1.12138400

Br	0.99459900	-0.29062100	-2.65942900
Br	5.67183700	3.88811600	-1.16687400
Br	-0.61574500	-3.85733100	0.51954900
K	2.78663500	2.81682800	-1.58039600
C	-3.12282200	0.99921100	-0.85609900
C	-4.51796900	0.94554100	-0.56987900
C	-5.42871100	1.33023200	-1.55268100
C	-4.96907000	1.80001700	-2.78409100
C	-3.60837000	1.90571600	-3.06385400
C	-2.68891100	1.49668900	-2.10433800
C	-4.96145500	0.32075900	0.72409300
H	-6.49398400	1.24604100	-1.37237100
H	-3.27421900	2.30227200	-4.01622200
H	-1.62581300	1.62203700	-2.27648100
O	-4.29473300	-0.59622700	1.19196800
N	-2.22576800	0.70706300	0.14418900
Cl	-6.15655400	2.27985600	-4.02522500
C	-6.69626900	2.10726900	1.24778200
C	-7.82596600	2.51576600	1.95640200
C	-8.47007300	1.62605100	2.81846500
C	-7.97364300	0.32902900	2.98768700
C	-6.83736800	-0.07668900	2.29564600
C	-6.19599900	0.80403400	1.40721100
H	-6.18870100	2.81149500	0.59636900
H	-8.19966800	3.52870400	1.83825400
H	-9.35482400	1.94379100	3.36320900
H	-8.47208700	-0.36098900	3.66239400
H	-6.42847500	-1.07338600	2.42519400

IM16

C	-1.32288700	0.03057100	-0.65697000
C	-1.33293300	-1.07990700	0.35329700
H	-2.13094200	-0.97815700	1.08721100
N	-0.05052300	0.64837200	-0.89899100
C	-0.09667200	2.10145200	-0.55049700
H	-0.35708200	2.11862900	0.51624600
H	-0.90527400	2.59526200	-1.10118200
C	4.05466700	-1.14488000	-2.35995000
C	2.66692600	-1.00597100	-2.37619500
C	2.13963600	0.20206500	-2.81924200
C	2.92934200	1.25520500	-3.26366900
C	4.31245300	1.08674400	-3.24312500
C	4.89883000	-0.10316900	-2.78160200
H	4.48675900	-2.08112300	-2.01713800

H	2.02001900	-1.81955500	-2.06632100
H	2.47397000	2.17709000	-3.60504600
H	4.94932400	1.89961900	-3.57999200
C	6.39723000	-0.23705000	-2.70574900
H	6.88341600	0.23248600	-3.56751800
H	6.76916300	0.26555000	-1.80153400
H	6.70635700	-1.28588400	-2.66177000
S	0.31712300	0.41385700	-2.81952500
O	-0.06952600	1.68597700	-3.58588700
O	-0.35472800	-0.93678500	-3.13206700
C	3.24742700	3.49229600	-0.43168400
C	2.72114000	4.39977000	-1.29642900
C	1.36798000	3.99597100	-1.53248800
C	1.15310800	2.87023800	-0.79360700
O	2.30129500	2.55013700	-0.10067700
H	4.23098100	3.34392400	-0.00186900
H	3.23756700	5.24896400	-1.72109200
H	0.64259800	4.46905700	-2.17946200
Au	0.49043200	-1.59806900	1.18385800
Br	2.70167100	-2.79066700	1.57493100
Br	-1.44298000	-2.91193300	-0.45060400
Br	6.42667400	1.79799400	0.76662000
Br	0.39031300	0.28119800	2.90460400
K	3.67289000	0.46809700	1.46953200
C	-3.64216000	-0.11601300	-1.28742800
C	-4.66482400	0.24853500	-0.38127100
C	-5.95704600	-0.26395900	-0.57588300
C	-6.21782600	-1.11975400	-1.63756300
C	-5.22304100	-1.46541500	-2.54885600
C	-3.94277200	-0.94573800	-2.38236200
C	-4.36512900	1.08326100	0.83060000
H	-6.74826600	-0.00707800	0.11916100
H	-5.44609100	-2.12043700	-3.38386700
H	-3.15440800	-1.16695000	-3.09487500
O	-3.35296100	0.84317500	1.48823000
N	-2.35673900	0.44146500	-1.26425100
Cl	-7.87233900	-1.77761800	-1.84499100
C	-6.19448700	2.77312000	0.33838800
C	-7.00707500	3.82557800	0.75866500
C	-6.93620700	4.27988200	2.07720300
C	-6.04079300	3.69029600	2.97643800
C	-5.21871600	2.64975400	2.55743700
C	-5.29539800	2.17309100	1.23646400
H	-6.24305900	2.43411600	-0.69119400

H	-7.69253900	4.29159400	0.05681500
H	-7.57505700	5.09560500	2.40443200
H	-5.98487600	4.04622300	4.00114500
H	-4.51100100	2.18697500	3.23734300

TS16-17

C	0.81357700	0.98141700	-0.75913900
C	1.11662100	-0.37551900	-1.13314500
H	1.80205100	-0.49837000	-1.96366100
N	-0.29684100	1.76059200	-0.71018400
C	-0.07133700	3.22631200	-0.61046300
H	0.93974400	3.41266700	-0.99062200
H	-0.10034800	3.56251300	0.43045700
C	-4.71167700	0.87038200	-2.20067400
C	-3.49286400	0.72206100	-1.54475000
C	-3.31103800	1.45285900	-0.37688700
C	-4.26116100	2.30421000	0.17268100
C	-5.46588300	2.43106700	-0.51418500
C	-5.71229900	1.71837400	-1.69620000
H	-4.88809200	0.31204400	-3.11583100
H	-2.72452000	0.06164000	-1.93312800
H	-4.08437400	2.81382100	1.11127700
H	-6.23723800	3.07407400	-0.10096300
C	-7.04522600	1.82793700	-2.39373200
H	-6.95044700	1.66473100	-3.47203100
H	-7.74108100	1.07251500	-2.00623600
H	-7.50462400	2.80784300	-2.23106200
S	-1.76367500	1.21045500	0.56433000
O	-1.59669200	2.22746700	1.69118800
O	-1.43765600	-0.27385000	0.80745600
C	-2.03527600	4.63025200	-3.26418600
C	-2.60710700	5.37154000	-2.27549800
C	-1.97810200	4.95608200	-1.05682600
C	-1.07145500	3.99502900	-1.39856000
O	-1.09444500	3.78946800	-2.75083000
H	-2.17426200	4.57806200	-4.33327200
H	-3.37909900	6.11873200	-2.39299100
H	-2.17407200	5.32217900	-0.05840000
Au	0.41041200	-2.08968200	-0.33319600
Br	-0.68676400	-4.27438100	0.42576600
Br	1.80066500	-1.93595900	1.78138100
Br	-4.77893700	0.03563700	2.84471800
Br	-0.76761600	-2.03021900	-2.60414000
K	-2.77554300	-2.25432300	2.20800200

C	2.70682700	1.86687500	0.54767400
C	4.07232000	2.18812800	0.35827000
C	4.74348400	2.91807900	1.33879800
C	4.08167300	3.26138700	2.51476300
C	2.74475600	2.92292200	2.73432600
C	2.05519300	2.23409000	1.74595900
C	4.81233700	1.89723100	-0.93738800
H	5.77501600	3.21314200	1.18352900
H	2.25438100	3.19565000	3.66190600
H	1.01697200	1.96547400	1.91138600
O	5.19517400	2.85572000	-1.59328900
N	2.06914900	1.17268300	-0.47165400
Cl	4.96579200	4.16285700	3.77448500
C	5.67722400	0.27253300	-2.59986300
C	5.97891000	-1.02098600	-3.01321800
C	5.71086100	-2.10545900	-2.16939800
C	5.14089300	-1.89294600	-0.91120100
C	4.83280700	-0.59737200	-0.49630000
C	5.09519200	0.49416000	-1.33922400
H	5.88266300	1.12901800	-3.23369900
H	6.42428200	-1.18869400	-3.98973700
H	5.94877600	-3.11538700	-2.49223300
H	4.93233200	-2.73164800	-0.25358400
H	4.38521900	-0.44377000	0.48027500

IM17

C	-0.25835000	0.01837300	1.29942600
C	-1.46073500	0.49423600	0.60828000
H	-2.06514400	1.24533400	1.11460200
N	0.25565300	-0.73289100	2.21753300
C	-0.54585000	-1.62697500	3.10801500
H	0.03113200	-1.69705100	4.03476800
H	-0.60400000	-2.60818700	2.62943300
C	3.77300600	-3.33881300	-0.34208300
C	3.35494300	-2.18154900	0.31312500
C	2.75069300	-2.34200000	1.55273400
C	2.54032400	-3.57573800	2.16778900
C	2.95255400	-4.70893000	1.47485500
C	3.56404900	-4.61036700	0.21107700
H	4.29092400	-3.22502700	-1.29001700
H	3.57940000	-1.21082900	-0.12204300
H	2.10245000	-3.64996900	3.15726300
H	2.81020800	-5.68561200	1.92863300
C	3.98558400	-5.84913200	-0.53813100

H	3.21931500	-6.13248200	-1.27135300
H	4.91653400	-5.68152200	-1.08865200
H	4.12859600	-6.69940500	0.13549700
S	2.20915500	-0.85079400	2.46213300
O	2.30961300	-1.05680500	3.97048800
O	2.69794300	0.43869300	1.79208300
C	-3.36810800	0.25637200	4.26215400
C	-4.09730900	-0.64059300	3.54100500
C	-3.15048900	-1.53697800	2.94868100
C	-1.91678200	-1.12147100	3.36262700
O	-2.03633700	-0.02012600	4.16893400
H	-3.62607800	1.10526300	4.87676900
H	-5.17256500	-0.66518300	3.43624800
H	-3.35747600	-2.37269600	2.29442300
Au	-2.52712900	-0.61940200	-0.79458800
Br	-3.92828300	-1.90655600	-2.48765400
Br	-3.91504900	1.47004300	-1.15869800
Br	5.72902800	0.06316900	-1.13544100
Br	-1.04289500	-2.66934800	-0.42750200
K	4.63806800	2.14436100	0.88611900
C	0.81557200	1.30702600	-0.69021100
C	1.42938900	2.57033900	-0.68798300
C	2.21845900	2.93896100	-1.78575700
C	2.35090400	2.07363800	-2.86653500
C	1.75638400	0.81415100	-2.86279900
C	0.98868300	0.42934800	-1.76518100
C	1.40237900	3.51103900	0.49389500
H	2.70911600	3.90637700	-1.79818400
H	1.89432000	0.14035700	-3.70037700
H	0.52304600	-0.55080900	-1.74529600
O	2.48482900	3.80229100	1.01160900
N	-0.02983300	0.94930600	0.40285300
Cl	3.30781900	2.59102900	-4.27588900
C	0.14227100	4.80625200	2.19226300
C	-1.02259400	5.40005700	2.66310500
C	-2.20622300	5.30266300	1.92106800
C	-2.22270000	4.60904800	0.70886000
C	-1.05802100	4.00532300	0.23627200
C	0.13346000	4.09647400	0.97649200
H	1.07107000	4.87811200	2.74820900
H	-1.01301700	5.94189400	3.60450100
H	-3.11553700	5.77053200	2.28831000
H	-3.13799600	4.53032200	0.13101900
H	-1.07991100	3.47805800	-0.71216100

TS17-18

C	-0.52703600	0.41710500	1.16332700
C	-0.33235600	-1.01861300	0.94027300
H	-1.03280900	-1.67071400	1.45327900
N	0.40135000	1.17076800	1.77929600
C	1.52547300	0.47925300	2.44627100
H	1.77590400	1.06550500	3.33609500
H	2.40688700	0.44867100	1.79454500
C	1.31260400	5.51050500	-0.76603900
C	0.54690200	4.80655900	0.16363200
C	1.19843300	3.87553400	0.96383600
C	2.56205800	3.61575500	0.88347800
C	3.29789000	4.32775000	-0.06130500
C	2.69179900	5.28516400	-0.89072100
H	0.82858300	6.24842000	-1.40036300
H	-0.51925700	4.97311900	0.27049900
H	3.06106300	2.87391500	1.49938900
H	4.36101400	4.12100500	-0.14707400
C	3.51765300	6.07267700	-1.87903800
H	2.89682400	6.50348300	-2.67052500
H	4.03697600	6.90026300	-1.37850300
H	4.28476100	5.44591100	-2.34573200
S	0.19041000	2.99984200	2.22931100
O	0.86435100	3.08389200	3.59704300
O	-1.28786500	3.32436200	2.02926500
C	0.24626300	-2.34682900	4.23854400
C	1.24542300	-3.03356200	3.60491400
C	1.84712700	-2.10883100	2.71106300
C	1.15724200	-0.91525600	2.83924700
O	0.18669900	-1.06390100	3.80755400
H	-0.49146600	-2.62676600	4.97585800
H	1.50763200	-4.07153300	3.74792600
H	2.69497100	-2.27171400	2.06030700
Au	0.64069500	-1.86617300	-0.64226800
Br	1.98714000	-3.05171700	-2.49766200
Br	-0.22685800	-4.10402500	0.16389100
Br	4.98818800	0.54656100	0.94070900
Br	1.31774800	0.40343900	-1.61877800
K	4.45797000	-0.89650000	-1.76680000
C	-2.48950100	1.38204200	-0.05455500
C	-3.89823600	1.22088200	0.01879600
C	-4.72031100	2.07601400	-0.72164800
C	-4.15518100	3.05017100	-1.53771700

C	-2.77462200	3.18681500	-1.66017400
C	-1.94689300	2.34909000	-0.92216700
C	-4.50615300	0.20646300	0.95426100
H	-5.79830300	1.98705900	-0.65357600
H	-2.35428400	3.93418700	-2.32409900
H	-0.87075500	2.42183100	-1.02504500
O	-4.03586400	0.04606800	2.07207500
N	-1.69306200	0.51054800	0.65083300
Cl	-5.22981600	4.14210900	-2.46819800
C	-6.50232300	-1.17250100	1.49066000
C	-7.59368500	-1.95740100	1.13294700
C	-7.87796200	-2.18666900	-0.21767000
C	-7.06759700	-1.62710300	-1.20705800
C	-5.98241700	-0.82540800	-0.85123000
C	-5.69258000	-0.58764500	0.50221500
H	-6.25462200	-0.99659700	2.53240200
H	-8.22200700	-2.39573900	1.90330800
H	-8.72692900	-2.80487200	-0.49687200
H	-7.27716400	-1.81624600	-2.25603600
H	-5.34928600	-0.40475900	-1.62587800

TS15-18

C	-1.09052400	-0.33391500	-1.40423000
C	0.15039000	-1.07045500	-1.52944000
H	0.48490800	-1.24284400	-2.54917300
N	-2.12693100	-0.76050400	-2.21359500
C	-1.86074900	-1.61858800	-3.36466900
H	-1.20443000	-1.13393400	-4.10270300
H	-2.82663800	-1.79459800	-3.85115400
C	-4.88573100	1.51506800	1.25845000
C	-4.24242000	1.51099500	0.01947100
C	-4.44542500	0.40669000	-0.79590600
C	-5.24985300	-0.67300600	-0.44748400
C	-5.87286700	-0.64026500	0.79765000
C	-5.70291600	0.45090500	1.66593200
H	-4.74460000	2.36705800	1.91813000
H	-3.59947700	2.33137300	-0.28709200
H	-5.39528900	-1.50006300	-1.13357300
H	-6.50634100	-1.47141000	1.09610200
C	-6.41194400	0.48822800	2.99812100
H	-7.42579100	0.89490400	2.88747300
H	-6.50880100	-0.51337500	3.42961800
H	-5.88246100	1.12173800	3.71631800
S	-3.66275000	0.36375400	-2.46130800

O	-4.51155400	-0.54396400	-3.36475800
O	-3.22963500	1.74533100	-2.93623600
C	-0.00423300	-4.68596200	-3.28700000
C	-0.61304600	-4.89393600	-2.08529700
C	-1.41561200	-3.74032000	-1.84149300
C	-1.23126700	-2.90155400	-2.91840300
O	-0.36861200	-3.47677800	-3.80864600
H	0.69250200	-5.25768600	-3.88084200
H	-0.49134500	-5.75111400	-1.43947000
H	-2.04796000	-3.54930100	-0.98785200
Au	1.65905200	-1.36155300	-0.21524900
Br	3.71142100	-1.62985400	1.30720000
Br	2.72466500	0.51077700	-1.60380800
Br	5.26056400	4.28196700	0.03095700
Br	0.47551500	-3.21650500	1.08525600
K	5.22386900	1.27475500	0.68340900
C	-0.58627100	1.26262600	0.37965000
C	-0.31666300	2.66446200	0.43209100
C	0.33786100	3.19403800	1.54236200
C	0.65696000	2.36776600	2.62114100
C	0.32853700	1.01075800	2.62970500
C	-0.27912300	0.46390200	1.50908000
C	-0.85673300	3.61257600	-0.62752300
H	0.58135500	4.25027400	1.58143500
H	0.54878200	0.39455300	3.49426200
H	-0.56802700	-0.58084100	1.51649000
O	-2.07567600	3.72916100	-0.69094700
N	-1.22962300	0.77021000	-0.72042000
Cl	1.47904100	3.06827500	4.03937400
C	-0.52865300	5.22385900	-2.46886700
C	0.27456400	5.99433300	-3.29949100
C	1.66772800	5.96094300	-3.15415100
C	2.25802800	5.15025900	-2.18271000
C	1.45427600	4.36422900	-1.35581700
C	0.05513200	4.39894700	-1.48675000
H	-1.60949300	5.23522300	-2.56026500
H	-0.17934600	6.62512600	-4.05891700
H	2.29380400	6.57189500	-3.79917900
H	3.33463400	5.12641600	-2.04257200
H	1.93443100	3.74227800	-0.60815100

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C	-0.40693600	-0.82179100	0.71121600
C	0.81752700	-1.69939500	0.78617600

H	0.62494700	-2.68880400	0.37546300
N	-0.39402800	0.05275700	1.83127500
C	0.73497500	-0.26066800	2.69135400
H	0.46036900	-0.17519400	3.74550400
H	1.57448000	0.40436800	2.46348100
C	-3.95965900	3.83471100	1.76064300
C	-3.67113600	2.52836400	2.15474200
C	-2.33419100	2.16720400	2.26327000
C	-1.28627700	3.04096100	1.99906100
C	-1.60102600	4.33461300	1.58945600
C	-2.93737200	4.75148100	1.47332700
H	-4.99814600	4.13724500	1.65687800
H	-4.45782700	1.80565800	2.34150500
H	-0.25192800	2.72167600	2.05006600
H	-0.78996500	5.00852600	1.32696300
C	-3.25855400	6.16359500	1.04743800
H	-2.57731400	6.50337300	0.26032100
H	-4.28497700	6.24885700	0.67763300
H	-3.15065800	6.85821000	1.89079300
S	-1.97632900	0.45914600	2.83765000
O	-1.44895900	0.47408500	4.28441800
O	-3.12290500	-0.48045500	2.46198000
C	0.83583500	-3.44397200	3.70470200
C	2.22607400	-3.25165500	3.66594900
C	2.43871600	-2.22230800	2.78109400
C	1.14722900	-1.71225800	2.28294200
O	0.17116300	-2.62241100	2.95570200
H	0.25085100	-4.16679900	4.26477000
H	2.96283300	-3.82851700	4.20648300
H	3.38888100	-1.77431900	2.52564300
Au	2.50438600	-1.03694400	-0.35431800
Br	4.51564900	-0.37070000	-1.87734100
Br	3.43478800	-3.43984800	0.00527300
Br	1.68422600	4.72079000	-0.73293600
Br	1.77715800	1.42818700	-0.32267200
K	3.88027700	2.93956900	-2.21928400
C	-2.32556800	-0.21380700	-0.60543600
C	-3.58145600	-0.83882400	-0.82827600
C	-4.65551600	-0.06072900	-1.28427100
C	-4.47372900	1.28804200	-1.55732800
C	-3.23318600	1.89940100	-1.40862700
C	-2.16527800	1.14572200	-0.93058900
C	-3.77377400	-2.29225400	-0.51122000
H	-5.63311000	-0.50929900	-1.41389400

H	-3.09963100	2.94814200	-1.64960800
H	-1.18776400	1.60293000	-0.82094700
O	-3.12829400	-2.83672000	0.37528400
N	-1.22589400	-0.97878800	-0.24329000
Cl	-5.87684900	2.26487200	-2.12591600
C	-5.36905200	-4.19615900	-0.65807300
C	-6.26710100	-5.00980400	-1.34266000
C	-6.56414300	-4.74990800	-2.68446400
C	-5.95973100	-3.67315300	-3.33536400
C	-5.07454100	-2.84423700	-2.64414100
C	-4.77542000	-3.09478300	-1.29587000
H	-5.11041200	-4.39476900	0.37704500
H	-6.73302500	-5.85010200	-0.83493300
H	-7.26058200	-5.38856100	-3.22137200
H	-6.17483200	-3.47772900	-4.38232400
H	-4.59886900	-2.01644900	-3.16042200

TS15-20

C	-1.08777100	0.96416300	-0.13020500
C	-1.58210600	-0.38724700	0.16494800
H	-2.46781800	-0.39034300	0.79502600
N	0.26043800	1.28072900	0.02582200
C	0.50302600	2.73267200	0.17180400
H	-0.18907500	3.03299500	0.97068600
H	0.20586100	3.30942000	-0.71455900
C	4.88761600	2.07359700	-2.13726400
C	3.85803900	1.31266400	-1.58929000
C	2.59189700	1.47519600	-2.13666800
C	2.29769800	2.34968000	-3.17983900
C	3.35064700	3.09802300	-3.69893800
C	4.65479200	2.97176900	-3.19003100
H	5.88341800	1.95351900	-1.71937200
H	4.08110400	0.63687300	-0.76615100
H	1.29459200	2.41981200	-3.58561700
H	3.15743800	3.78311700	-4.52007000
C	5.79265300	3.76669800	-3.78091000
H	6.36117600	3.15519600	-4.49374000
H	5.43312100	4.65032600	-4.31715900
H	6.49368100	4.09264200	-3.00578800
S	1.21504900	0.42911800	-1.51770400
O	0.11826200	0.34709500	-2.59735400
O	1.78851300	-0.85534500	-0.89059000
C	3.79619200	2.79652800	1.63390200
C	3.88546800	4.00705100	1.01640300

C	2.65750100	4.18563200	0.30062000
C	1.90600900	3.07248800	0.54314800
O	2.58509900	2.22030300	1.36696500
H	4.48339300	2.19071100	2.20495100
H	4.73073900	4.67989200	1.04704500
H	2.37478300	5.02658500	-0.31815200
Au	-0.61612400	-2.16287200	0.28226600
Br	0.66698400	-4.32022900	0.74088700
Br	-1.44639000	-3.06951300	-1.93011700
Br	5.78503600	-0.33734300	1.11959400
Br	-0.10418900	-1.21790500	2.61756200
K	3.15090800	-2.01920200	1.20690800
C	-3.17744600	1.33076900	-0.80032800
C	-4.42602700	1.95930700	-0.53233800
C	-5.58821900	1.27277600	-0.84494500
C	-5.54229800	-0.03353200	-1.38162900
C	-4.34933000	-0.65062100	-1.70038400
C	-3.15194400	0.05150100	-1.45756500
C	-4.55767500	3.36825200	0.01941600
H	-6.54886800	1.73967300	-0.65496200
H	-4.32123700	-1.62179100	-2.18065600
H	-2.26593900	-0.23383000	-2.02453800
O	-5.28149500	4.13915400	-0.59322700
N	-1.98687500	1.88216200	-0.43176900
Cl	-7.08274400	-0.85711800	-1.71634900
C	-3.71011400	5.13245300	1.54178600
C	-3.09353100	5.55038000	2.71707300
C	-2.64128900	4.60587200	3.64494300
C	-2.80977900	3.24093300	3.39674000
C	-3.41090300	2.82055200	2.21132200
C	-3.85919400	3.76194500	1.27101600
H	-4.08037100	5.84916100	0.81608700
H	-2.96779300	6.61082200	2.91556100
H	-2.16368700	4.93348900	4.56405700
H	-2.47725300	2.50738600	4.12536700
H	-3.55677300	1.75893200	2.03402800

IM20

C	1.27134800	0.20889800	0.35608700
C	0.44746500	-0.63207300	-0.57827500
H	-0.12643300	-0.02413200	-1.27838400
N	0.85388800	1.15449500	1.15313400
C	1.74984700	1.84247600	2.09248100
H	2.61210200	1.18372900	2.23729000

H	1.21984400	1.94035700	3.04371400
C	-2.31588700	3.40092700	-2.27780200
C	-2.13526500	2.53240500	-1.20077400
C	-1.33223500	2.97968500	-0.15751300
C	-0.71071600	4.22803000	-0.12659100
C	-0.91644300	5.06377200	-1.21622400
C	-1.72008400	4.66679800	-2.30316100
H	-2.96752700	3.08757500	-3.08733400
H	-2.63240300	1.57151300	-1.17752400
H	-0.10461000	4.53867600	0.71669600
H	-0.45600800	6.04773200	-1.21876300
C	-1.97202800	5.60903600	-3.45293700
H	-2.87361200	6.20573600	-3.26243600
H	-1.13945800	6.30534000	-3.59544900
H	-2.13471200	5.06555400	-4.38863000
S	-1.12881300	1.89592000	1.29605800
O	-0.95937200	2.67510100	2.59393900
O	-2.05295500	0.67848700	1.21324200
C	3.05198400	4.62162900	0.20964500
C	2.74704300	5.34486700	1.32252100
C	2.16317700	4.41965800	2.24967400
C	2.16783300	3.19981600	1.63611200
O	2.71110900	3.31076300	0.38406000
H	3.48311000	4.86918000	-0.74844900
H	2.90817500	6.40383000	1.46801600
H	1.78448200	4.63281400	3.23959700
Au	-1.01318300	-1.87341600	0.35150800
Br	-2.83517100	-3.32866700	1.45792900
Br	0.61929100	-2.38587900	2.22740400
Br	-5.44851500	2.22880800	-0.32817100
Br	-2.45568200	-1.53559300	-1.73820700
K	-4.64408600	-0.54277200	0.86846800
C	2.80481800	-0.89981000	-0.72418000
C	4.05135400	-1.31094100	-1.33077800
C	3.95700300	-1.82890300	-2.59753100
C	2.70902100	-1.94166100	-3.32003400
C	1.51442200	-1.76452100	-2.72458500
C	1.52653100	-1.49748000	-1.25256500
C	5.43309200	-1.31653900	-0.69656400
H	4.86875400	-2.14725400	-3.09292500
H	0.57066000	-1.91586700	-3.23868200
H	1.50384300	-2.50418400	-0.78417800
O	6.13676800	-2.28603700	-0.94905200
N	2.63340500	-0.04657500	0.25440600

Cl	2.82252900	-2.37925100	-5.05193000
C	7.01038900	-0.50246600	1.02077300
C	7.57191200	0.49734700	1.80742200
C	7.08123000	1.80493200	1.72812200
C	6.02599500	2.10611500	0.86465300
C	5.44659500	1.10144300	0.08995500
C	5.93263100	-0.21218500	0.16506500
H	7.38942100	-1.51845200	1.05222700
H	8.39387100	0.26262700	2.47760700
H	7.52371600	2.58838600	2.33757700
H	5.65084300	3.12289900	0.79523700
H	4.62409800	1.34618500	-0.57105400

TS16-19

C	-0.70910500	0.12729400	0.93858700
C	-0.91717000	0.07566000	-0.52943900
H	-1.78779200	0.59216500	-0.91001900
N	0.50805500	-0.48693000	1.39098200
C	0.27035100	-1.90122800	1.83842300
H	-0.27329400	-2.36301300	1.00649300
H	-0.37659700	-1.90432400	2.72372400
C	4.92933100	0.03224700	0.80565900
C	3.56064200	0.16674800	1.03980100
C	3.12065100	0.15856200	2.35991300
C	3.98206200	0.01937200	3.44104900
C	5.34657000	-0.10579700	3.17930500
C	5.84021800	-0.10139900	1.86579900
H	5.28353000	0.01502800	-0.22171600
H	2.86382900	0.22790100	0.21090100
H	3.59248800	-0.00062600	4.45342200
H	6.03719300	-0.21599900	4.01132800
C	7.31450400	-0.28035600	1.59380200
H	7.92356300	0.06008500	2.43713200
H	7.55115400	-1.33878400	1.42382100
H	7.62714100	0.26809300	0.69955700
S	1.34454200	0.49404000	2.73462500
O	1.00974400	-0.00197900	4.14908700
O	1.09966900	1.98790700	2.38941400
C	3.32395000	-3.76037300	1.55859600
C	3.20921500	-3.90213100	2.90960300
C	2.02519300	-3.18789700	3.28131100
C	1.50862500	-2.66788400	2.12823500
O	2.29731900	-3.01733300	1.06794100
H	4.03260100	-4.11441400	0.82571800

H	3.87763100	-4.44870000	3.55992800
H	1.61257000	-3.06184000	4.27238800
Au	0.47634100	-0.67496800	-1.79354900
Br	2.55058200	-0.91775800	-3.23146800
Br	0.49206300	1.95978200	-1.42695900
Br	0.39305900	5.15763300	-1.20032400
Br	-0.14694900	-3.14088000	-1.99108100
K	2.16452500	3.91767700	1.03023500
C	-2.76498600	1.16304200	1.41757500
C	-3.78548200	0.39580900	0.79270700
C	-5.03490200	0.99844100	0.55086800
C	-5.24672600	2.32505700	0.89113200
C	-4.25847300	3.07878500	1.52535700
C	-3.03725000	2.48268300	1.81251600
C	-3.58123600	-1.03145500	0.40575300
H	-5.82240900	0.43360900	0.06653100
H	-4.44620300	4.11216900	1.79459300
H	-2.25845000	3.03570700	2.32671600
O	-2.50093800	-1.43268200	-0.06076800
N	-1.52518700	0.62955500	1.78516700
Cl	-6.82760900	3.07939000	0.52383000
C	-5.68286400	-1.88214400	1.54432600
C	-6.65053100	-2.87367800	1.69507100
C	-6.62860000	-4.00317900	0.87348600
C	-5.62696900	-4.15223500	-0.09178900
C	-4.64760800	-3.17532100	-0.23591100
C	-4.67607400	-2.02248200	0.57216100
H	-5.69479900	-1.01508500	2.19624800
H	-7.41927000	-2.76551700	2.45453100
H	-7.38957100	-4.77027800	0.98765400
H	-5.60962000	-5.03183600	-0.72844000
H	-3.85676600	-3.28175700	-0.97145300

IM19

C	-1.25419600	1.36103100	0.29705800
C	-1.67240800	0.04242500	-0.33812200
H	-2.19556700	0.21839300	-1.28100100
N	0.09766000	1.60346600	0.57085900
C	0.30432400	2.47288800	1.75569000
H	-0.15455200	1.91406200	2.58353200
H	-0.23141100	3.42348700	1.66260900
C	3.72115800	0.42766700	-2.63505600
C	2.44942300	0.93511200	-2.36075400
C	2.36358000	2.01138000	-1.48435700

C	3.47152800	2.59593300	-0.87551700
C	4.72413400	2.06175500	-1.16286300
C	4.87145700	0.97174500	-2.04193300
H	3.81216300	-0.41216500	-3.31784900
H	1.56316700	0.51114200	-2.82025900
H	3.36028000	3.42920400	-0.19162700
H	5.60213800	2.47928300	-0.68024800
C	6.23810000	0.39553800	-2.30104400
H	6.92061500	1.16370600	-2.68417600
H	6.66512400	0.01872100	-1.36180800
H	6.20015200	-0.42277000	-3.02601300
S	0.69743200	2.66536700	-1.09874600
O	0.75652000	4.13542700	-0.66328700
O	-0.31321100	2.21091800	-2.16356100
C	3.80862500	2.30180800	2.65852700
C	3.68453700	3.65398000	2.74040100
C	2.33842400	3.96059400	2.35864900
C	1.72721900	2.77515700	2.07172300
O	2.61813300	1.74239900	2.25817800
H	4.63813100	1.61415200	2.77484000
H	4.46173900	4.34831400	3.02683500
H	1.87941000	4.93715300	2.29128900
Au	-0.19600900	-1.41194000	-0.62065800
Br	1.70199100	-3.10037500	-1.00941000
Br	-0.77679600	-1.40721400	-3.08349900
Br	6.34734600	-0.24710300	1.63138000
Br	0.08672500	-1.62622500	1.92505100
K	3.34656000	-1.00687900	1.14554200
C	-3.47505300	2.19149900	0.15665000
C	-4.33378800	1.04739500	0.20784800
C	-5.68965600	1.16696500	-0.19709000
C	-6.16631900	2.37499600	-0.65537100
C	-5.34545900	3.51363600	-0.68999500
C	-4.03239400	3.41881500	-0.26670000
C	-3.86082200	-0.20978400	0.73054900
H	-6.33334500	0.29629600	-0.19143900
H	-5.74508400	4.45802600	-1.04341200
H	-3.38091100	4.28576100	-0.27244500
O	-2.61941400	-0.57605200	0.59900300
N	-2.14897700	2.26320900	0.53516700
Cl	-7.85667100	2.50086500	-1.21274400
C	-5.79748200	-0.74561600	2.22287300
C	-6.52183900	-1.67267200	2.96259900
C	-6.13585500	-3.01720900	2.97145600

C	-5.01227200	-3.43697900	2.25027100
C	-4.27436100	-2.51827200	1.51534200
C	-4.66964100	-1.16073500	1.47947400
H	-6.07562400	0.30195600	2.25059600
H	-7.37951700	-1.34723700	3.54284800
H	-6.70688100	-3.73842000	3.54903300
H	-4.71218000	-4.47991900	2.26393000
H	-3.40039900	-2.83626400	0.95810100

Cartesian coordinates for the stationary points given in Fig. S4

TS18-24

C	-0.03751400	-0.91243100	0.72048600
C	0.71749500	-2.20516700	0.62224200
H	0.17688200	-3.04627500	0.19857100
N	0.51632700	-0.16804600	1.79819500
C	1.55415400	-0.96055000	2.45842300
H	1.43454200	-0.94209500	3.54600600
H	2.54706800	-0.55900700	2.21082100
C	-1.29110500	4.66538500	2.49742500
C	-1.46902100	3.31054000	2.77621000
C	-0.36742600	2.47408400	2.64944900
C	0.88809500	2.92504700	2.26176600
C	1.03620700	4.28009200	1.97323700
C	-0.04496500	5.16834900	2.09481300
H	-2.14157300	5.33691900	2.57823600
H	-2.43774100	2.91095600	3.05543500
H	1.72268800	2.24571700	2.13314500
H	2.00184200	4.63406200	1.62244200
C	0.13899100	6.63788200	1.80164600
H	0.81976700	6.79163700	0.95799000
H	-0.81372200	7.12403900	1.56979000
H	0.57277100	7.15615200	2.66697200
S	-0.60977000	0.70573000	3.08809200
O	0.10331700	0.39014800	4.41631200
O	-2.07435200	0.31334500	2.89225200
C	0.49254500	-3.98488400	3.64827000
C	1.84119500	-4.31490200	3.22048600
C	2.29214200	-3.46822100	2.27161200
C	1.42629900	-2.34813200	1.85985300
O	-0.05443800	-2.99633700	3.14459300
H	-0.04629900	-4.57808200	4.39852700
H	2.39639500	-5.16253800	3.60265600
H	3.26953300	-3.56925300	1.81115100
Au	2.38214900	-2.12558700	-0.85409300

Br	4.10296800	-2.09170600	-2.78787500
Br	2.21338100	-4.71191600	-0.95232900
Br	3.94956400	3.45526100	-0.73389100
Br	2.82581500	0.40123600	-0.53907200
K	4.90216300	1.23289500	-2.83684300
C	-1.70253700	0.50611700	-0.26141100
C	-3.11824200	0.45653500	-0.34575900
C	-3.82670500	1.63545300	-0.61778800
C	-3.14319800	2.82255200	-0.84343600
C	-1.75359700	2.87521300	-0.82829400
C	-1.04017200	1.71650900	-0.53433600
C	-3.84958300	-0.82696400	-0.07816700
H	-4.90989600	1.62334600	-0.64272300
H	-1.23225500	3.80411100	-1.03114200
H	0.04442000	1.73806900	-0.52902300
O	-3.41897700	-1.63774400	0.73043800
N	-0.97652000	-0.66864200	-0.09879600
Cl	-4.08035300	4.32627800	-1.17269100
C	-6.04376800	-1.99238700	-0.21270200
C	-7.22009600	-2.34597500	-0.86698500
C	-7.48409300	-1.85126100	-2.14843500
C	-6.56686700	-1.00206400	-2.76956600
C	-5.39538400	-0.63187900	-2.10702100
C	-5.12542300	-1.11945700	-0.81876900
H	-5.81084400	-2.38281800	0.77271400
H	-7.93054900	-3.01105600	-0.38338100
H	-8.39969600	-2.13213200	-2.66226100
H	-6.76034100	-0.62877700	-3.77149100
H	-4.68041800	0.01712600	-2.60249700

IM24

C	0.56509600	0.27767400	-0.68998100
C	-0.76067100	-0.15587900	-1.22195200
H	-0.72630000	-0.92735400	-1.98792000
N	0.58912700	1.69729600	-0.58651500
C	-0.74598300	2.21298700	-0.93604700
H	-0.67284100	3.01226800	-1.68098000
H	-1.21468700	2.65094900	-0.04698600
C	4.93284300	3.97134200	0.53755000
C	4.16962200	3.14048700	-0.28251900
C	2.92397600	3.59665000	-0.68911700
C	2.41110500	4.83443000	-0.32112000
C	3.19136800	5.64355000	0.50236200
C	4.45853200	5.22776800	0.94157400

H	5.90968800	3.63109200	0.87047700
H	4.53110400	2.16980700	-0.60241200
H	1.44199800	5.16390200	-0.68010700
H	2.81084500	6.61606600	0.80335900
C	5.30616200	6.12973500	1.80619700
H	5.98459600	5.55314300	2.44275100
H	5.92373200	6.79424500	1.18762000
H	4.68886400	6.76480400	2.44972100
S	1.92490200	2.52693400	-1.79890400
O	1.09196800	3.44498800	-2.71352700
O	2.80126200	1.40644300	-2.36264500
C	-3.59804000	3.50750900	-2.26703400
C	-3.73364300	2.01639500	-2.36159600
C	-2.78023000	1.01060800	-2.09138800
C	-1.54540500	1.04998700	-1.46354700
O	-2.65691200	4.10455700	-1.78855400
H	-4.45395200	4.04811600	-2.71212600
H	-4.52236100	1.71685700	-3.04562900
H	-3.09933800	0.01356900	-2.39000000
Au	-1.86626300	-1.28738400	0.31334700
Br	-3.24151800	-2.69322600	2.04620400
Br	-2.47843700	-2.93885700	-1.51282400
Br	-5.52674300	2.08233500	-0.58810600
Br	-1.44595300	0.50933600	2.12900600
K	-4.79393500	0.20130400	2.01625000
C	2.65152500	-0.33890800	0.28379800
C	3.80826900	-1.07798100	-0.07708200
C	4.99054800	-0.90376700	0.65503300
C	5.01101400	-0.04715800	1.74838400
C	3.86827700	0.63120200	2.16152300
C	2.69752500	0.48805900	1.42372900
C	3.78831900	-1.99256100	-1.27337900
H	5.88973000	-1.43634600	0.36752500
H	3.89377000	1.26879900	3.03855400
H	1.79675400	1.00677900	1.73250700
O	3.18068700	-1.67915600	-2.28579500
N	1.45433100	-0.58354900	-0.37746200
Cl	6.54920900	0.18503700	2.65603800
C	4.90940000	-3.88988100	-2.42487100
C	5.55940900	-5.12013600	-2.43712100
C	5.81893900	-5.78643700	-1.23480400
C	5.42589700	-5.21658500	-0.02272100
C	4.78949600	-3.97448100	-0.00725500
C	4.53012900	-3.29701400	-1.20914200

H	4.67984200	-3.36694300	-3.34763800
H	5.85968800	-5.56523200	-3.38181800
H	6.32083500	-6.75038600	-1.24454500
H	5.61071700	-5.73929300	0.91167300
H	4.47358700	-3.54484400	0.93801700

TS24-25

C	-0.64871900	-0.78609500	0.39331900
C	0.61943100	-1.58750600	0.47992500
H	0.55866600	-2.56377100	0.00461100
N	-0.71185900	-0.04006900	1.60709500
C	0.25973200	-0.52902700	2.50508200
H	0.03920100	-0.51135700	3.57577300
H	1.28586100	0.42496200	2.71464400
C	-3.13668000	4.41204500	1.08345200
C	-3.16146900	3.03576400	1.31171400
C	-2.17582200	2.49882000	2.12763200
C	-1.18213400	3.26124000	2.73013400
C	-1.17937100	4.63154900	2.48009200
C	-2.15136600	5.22646400	1.65873000
H	-3.89975300	4.85604100	0.44980900
H	-3.92250400	2.39957200	0.87646100
H	-0.43283700	2.81170300	3.37246900
H	-0.41102600	5.24867400	2.93834900
C	-2.15195400	6.71872700	1.42957700
H	-2.67735400	6.98315200	0.50688300
H	-2.65448400	7.23933500	2.25530600
H	-1.13284600	7.11473400	1.36882100
S	-2.25098900	0.69856800	2.49354400
O	-1.89862600	0.47514200	3.96609000
O	-3.50656700	0.10363200	1.86552300
C	1.93170400	-2.08387000	4.99791300
C	2.45163700	-2.60866500	3.72479600
C	2.05197000	-2.38247300	2.44193600
C	1.02986300	-1.52972300	1.88494000
O	1.07879100	-1.22229700	5.14628400
H	2.38074500	-2.56619600	5.88940400
H	3.24329600	-3.34510900	3.85069300
H	2.57194600	-2.96430700	1.68410200
Au	2.25233200	-0.74076000	-0.74688100
Br	4.44236400	0.15691800	-1.94648900
Br	3.11617800	-3.12333100	-1.01611800
Br	2.42331800	1.65640300	3.23845000
Br	1.29760700	1.66224500	-0.74500200

K	4.26024200	2.23180700	0.54784600
C	-2.59620500	-0.27248700	-0.96088100
C	-3.81730300	-0.99330100	-1.05222000
C	-4.95608100	-0.34287700	-1.54561300
C	-4.87549400	0.97250100	-1.98386500
C	-3.67348300	1.67168700	-1.95613500
C	-2.53958600	1.04862000	-1.44079500
C	-3.90055100	-2.39572700	-0.52665300
H	-5.90649500	-0.86224400	-1.57220200
H	-3.62049400	2.68901700	-2.32920400
H	-1.58667200	1.56736000	-1.42867700
O	-3.17725000	-2.76017400	0.39244700
N	-1.42888500	-0.91869400	-0.59568200
Cl	-6.35476100	1.78557800	-2.61117800
C	-5.36309500	-4.39523300	-0.31069500
C	-6.23707700	-5.34981300	-0.82234900
C	-6.62049200	-5.29879200	-2.16647600
C	-6.12653500	-4.28940000	-2.99456100
C	-5.26585800	-3.31954300	-2.47833600
C	-4.88108000	-3.36039600	-1.12894900
H	-5.03824700	-4.43073100	0.72414000
H	-6.61670900	-6.13778300	-0.17758900
H	-7.29797800	-6.04797800	-2.56755900
H	-6.40823000	-4.25692000	-4.04338800
H	-4.87367900	-2.54636800	-3.13141400

IM25

C	-1.16276900	-0.61414700	0.29080800
C	-0.17182300	-1.67512000	0.68170200
H	-0.60174300	-2.67306200	0.67305700
N	-0.91872700	0.49155000	1.20817200
C	-0.02495900	0.13755900	2.11589100
H	0.21243300	0.81104200	2.92710900
H	3.23977800	1.48485200	2.85982300
C	-0.09459800	4.68935800	-1.46134200
C	-0.95681200	3.88310300	-0.72116000
C	-0.50081900	3.42888600	0.51083200
C	0.75816000	3.71604800	1.02495200
C	1.60036000	4.51678500	0.25756400
C	1.18693700	5.01735600	-0.98793300
H	-0.42508400	5.06905100	-2.42427900
H	-1.94565000	3.62270200	-1.08137000
H	1.08051200	3.33728100	1.98800100
H	2.59423700	4.73643900	0.63759400

C	2.09482400	5.91462900	-1.79248400
H	1.93912300	5.78314100	-2.86803700
H	1.89923500	6.96977400	-1.56005700
H	3.14821700	5.72217000	-1.56731400
S	-1.62478000	2.39490000	1.51990900
O	-1.28319100	2.53552900	3.00016900
O	-3.04570200	2.45822400	0.99318900
C	2.88183500	-0.20484600	3.74656300
C	2.26457600	-1.43563000	3.71958900
C	1.31878200	-1.88521600	2.76447900
C	0.46195700	-1.17683100	1.92879500
O	2.47687600	0.83741800	3.05288200
H	3.79771300	-0.07659400	4.32514400
H	2.72478900	-2.19747700	4.34060100
H	1.33069300	-2.96139500	2.59351600
Au	1.46494100	-1.86849200	-0.74040000
Br	3.68420300	-2.15481400	-2.13352600
Br	1.47950200	-4.33736400	-0.13956500
Br	4.80692300	2.53583400	1.90484600
Br	1.35880000	0.61683800	-1.43801300
K	4.64117900	0.67190900	-0.71983600
C	-3.04255800	0.11840300	-1.01403700
C	-4.31826900	0.13768000	-0.39936200
C	-5.32483900	0.94458200	-0.94961600
C	-5.06993500	1.70428600	-2.08234100
C	-3.83192000	1.66462100	-2.71712900
C	-2.82776300	0.85694400	-2.18848800
C	-4.56535300	-0.59959400	0.88574300
H	-6.29700100	0.99424800	-0.47312600
H	-3.65865400	2.24227800	-3.61891400
H	-1.86374800	0.78293100	-2.68227900
O	-3.69288000	-0.63804500	1.74831500
N	-2.04186200	-0.76142700	-0.59685800
Cl	-6.37108800	2.74733800	-2.75403700
C	-6.25974300	-1.53776400	2.44209600
C	-7.45192600	-2.20033400	2.71557000
C	-8.27178100	-2.62695400	1.66523900
C	-7.89454800	-2.38756200	0.34259300
C	-6.70730200	-1.70897100	0.06602800
C	-5.88115900	-1.27337400	1.11477700
H	-5.60255800	-1.21254800	3.24190700
H	-7.74350200	-2.38947300	3.74494300
H	-9.20052400	-3.14924700	1.87871700
H	-8.52209800	-2.73148300	-0.47471000

H	-6.41197400	-1.53966500	-0.96434200
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TS25-26

C	-1.03849700	-0.47184000	0.50570700
C	0.24563400	-1.18799300	0.84018700
H	0.15587500	-2.27065200	0.84289400
N	-1.10934100	0.59361300	1.44551300
C	-0.05662100	0.52216200	2.31289900
H	0.02952800	1.20651300	3.14535900
H	-1.08740900	-3.50420300	-2.00347800
C	-1.25673600	4.91209600	-0.94217000
C	-1.89816000	3.83687000	-0.32951500
C	-1.47673500	3.47694300	0.94346200
C	-0.45802400	4.12869500	1.62828500
C	0.16713700	5.19665800	0.98814000
C	-0.21418600	5.59859700	-0.30160800
H	-1.57224500	5.22064400	-1.93511300
H	-2.70654700	3.30191100	-0.81541300
H	-0.16575700	3.82300000	2.62722000
H	0.96538800	5.72502800	1.50203200
C	0.50149500	6.73214200	-0.99519300
H	-0.14925600	7.23650000	-1.71643600
H	0.86270800	7.47649700	-0.27843300
H	1.37396000	6.35657000	-1.54545200
S	-2.31137500	2.06392700	1.76818400
O	-2.20086600	2.22409700	3.28084600
O	-3.62607400	1.75292500	1.07042500
C	2.56365900	0.82493100	4.41019200
C	2.71074000	-0.45432100	3.72714600
C	1.96637900	-0.98858100	2.71425700
C	0.79342900	-0.52958200	2.02228300
O	1.66356900	1.64993100	4.27605000
H	3.38957600	1.04290200	5.11986000
H	3.57412400	-1.03230600	4.04973600
H	2.33508800	-1.93928100	2.32781300
Au	1.53534500	-1.04958800	-0.95698200
Br	3.02789700	-0.94010800	-3.20829600
Br	1.45588000	-3.68570100	-1.01492200
Br	-1.79003700	-3.80001200	-3.26130800
Br	1.52683200	1.49137100	-0.83918300
K	1.61533100	-3.54873400	-4.28631800
C	-3.00306300	-0.33004100	-0.89346200
C	-4.26813800	-0.77564300	-0.43947300
C	-5.42591200	-0.28488000	-1.06114000

C	-5.32639500	0.60962900	-2.11644500
C	-4.08927100	1.02370000	-2.60000300
C	-2.93248800	0.54012400	-1.99360700
C	-4.37208000	-1.66314200	0.76511600
H	-6.40195100	-0.58631800	-0.69952900
H	-4.02884300	1.70556800	-3.44172200
H	-1.95505300	0.83016800	-2.36798900
O	-3.57562900	-1.54406600	1.68952800
N	-1.81350700	-0.87921900	-0.41275000
Cl	-6.82844400	1.23596600	-2.88641700
C	-5.84870900	-3.13924200	2.11539800
C	-6.81717300	-4.12935400	2.25001900
C	-7.39163700	-4.70589000	1.11227900
C	-6.99420300	-4.28675300	-0.15858200
C	-6.03602700	-3.28115000	-0.29585200
C	-5.45747800	-2.69510300	0.84138900
H	-5.37839600	-2.69241500	2.98527100
H	-7.12351700	-4.45672200	3.23978100
H	-8.14423000	-5.48286500	1.21757300
H	-7.42855200	-4.74203100	-1.04431000
H	-5.72460600	-2.96636600	-1.28679000

IM26

C	-0.53327200	0.23073800	0.74055800
C	0.69621200	-0.32737600	1.40585200
H	0.53871400	-1.34155100	1.77480800
N	-0.75689700	1.46061500	1.26558700
C	0.18407700	1.73572300	2.25808000
H	0.12979600	2.64702400	2.83193100
H	-0.82944600	-1.38675800	-0.41736200
C	-0.23471100	4.97345300	-2.13635900
C	-1.06202000	4.12678900	-1.40198100
C	-0.90527700	4.11537500	-0.02151800
C	0.02684500	4.89299600	0.65620900
C	0.84295000	5.72454300	-0.10813800
C	0.73292000	5.77252700	-1.50641300
H	-0.34213300	5.01118700	-3.21685200
H	-1.81022200	3.50498500	-1.88083000
H	0.11937500	4.86025900	1.73631900
H	1.57956500	6.34434000	0.39511300
C	1.65456800	6.64672600	-2.32041900
H	1.17299200	6.99003100	-3.24141900
H	1.98013400	7.52430800	-1.75339300
H	2.55497600	6.08901500	-2.60895000

S	-1.98403600	2.99835000	0.95446800
O	-2.14075200	3.52088200	2.37360100
O	-3.15967000	2.53190800	0.11572800
C	2.52148300	2.88117700	4.36082500
C	2.75523600	1.45023700	4.19102200
C	2.15479700	0.56213000	3.34722300
C	1.07036700	0.71093300	2.40691200
O	1.62865900	3.56218900	3.86323100
H	3.26958200	3.37426900	5.01609800
H	3.57708100	1.06387300	4.79001300
H	2.57690100	-0.44115600	3.35596900
Au	2.32112500	-0.66619700	0.01552200
Br	4.27657600	-1.19244200	-1.63766400
Br	3.01344500	-2.66821000	1.49069600
Br	-0.44559900	-3.36588100	-1.37249000
Br	1.70879400	1.38942900	-1.34599000
K	2.60552000	-4.05972700	-1.56991600
C	-2.41859000	-0.11960900	-0.85985900
C	-3.69661400	-0.34449200	-0.31602900
C	-4.81656800	-0.10333300	-1.12135100
C	-4.64711500	0.33754700	-2.42866200
C	-3.38543900	0.51768200	-2.98377200
C	-2.26530900	0.27080900	-2.18977100
C	-3.87539000	-0.73120900	1.12843300
H	-5.81374900	-0.24502500	-0.72168100
H	-3.27683500	0.82992700	-4.01635500
H	-1.26552400	0.37045000	-2.60052600
O	-3.18129200	-0.19440900	1.98469400
N	-1.23090100	-0.46176300	-0.13150400
Cl	-6.09894200	0.66070500	-3.43177200
C	-5.38263800	-1.74355000	2.82080500
C	-6.31854900	-2.68778200	3.22922700
C	-6.77344700	-3.65667900	2.32786700
C	-6.28995000	-3.67743300	1.01834000
C	-5.36492900	-2.72085200	0.59935200
C	-4.90745400	-1.74292500	1.49801600
H	-5.00532100	-0.99339200	3.50814900
H	-6.69234000	-2.67488100	4.24924000
H	-7.49998300	-4.39811500	2.64944400
H	-6.62836900	-4.43998900	0.32286000
H	-4.97905800	-2.75272500	-0.41444200
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C	-0.43629200	-0.29715600	0.57356100

C	0.24032700	-1.12723600	1.42931900
H	0.96040500	-0.80967400	2.17257600
N	-1.27339700	-1.11255900	-0.19446100
C	-1.12831500	-2.42259500	0.15454800
H	-1.69393800	-3.21230300	-0.31259500
H	-1.21209300	1.57303800	0.83594000
C	-4.35860100	2.72629500	-0.16267200
C	-3.45676500	1.88956400	-0.82339200
C	-3.59883000	0.51941000	-0.65227300
C	-4.59962700	-0.04934500	0.12648500
C	-5.48552000	0.80735400	0.77621900
C	-5.37737800	2.20200000	0.64603900
H	-4.27446700	3.80248000	-0.28880900
H	-2.67568200	2.28012600	-1.46746800
H	-4.69082100	-1.12769400	0.20652900
H	-6.27939800	0.38577700	1.38735900
C	-6.33940100	3.11291500	1.37069400
H	-6.28654600	4.13727900	0.99031200
H	-7.37268100	2.76407300	1.26634700
H	-6.11657600	3.14509700	2.44502300
S	-2.44151000	-0.60444600	-1.54847400
O	-3.16690300	-1.91141500	-1.86835700
O	-1.69433100	0.19522800	-2.60631900
C	-0.87184300	-5.68900200	1.08073600
C	0.09814900	-4.94748500	1.87795000
C	0.36035800	-3.60932000	1.89535600
C	-0.17350000	-2.48262000	1.17137700
O	-1.64596700	-5.24382800	0.24117600
H	-0.87712800	-6.78008500	1.29651200
H	0.68018800	-5.56674300	2.55795500
H	1.13467400	-3.31133500	2.60370500
C	0.72923500	1.88228800	0.36898300
C	1.97417500	1.45500700	-0.15691500
C	3.06102500	2.34335500	-0.14019200
C	2.92337500	3.63039500	0.35815800
C	1.70731500	4.06883000	0.86958900
C	0.63141800	3.18901200	0.88260300
C	2.15444200	0.15350600	-0.90205500
H	4.01290600	2.02511100	-0.55051300
H	1.60407200	5.07349400	1.26495600
H	-0.31497300	3.51913000	1.30590800
O	1.35484200	-0.16662100	-1.76829600
N	-0.42790600	1.09363400	0.40659600
Cl	4.33640400	4.74462400	0.34470000

C	3.67978100	-1.70265000	-1.53897600
C	4.75623800	-2.55317100	-1.30759200
C	5.50957600	-2.42593600	-0.13562900
C	5.18072900	-1.44571400	0.80268900
C	4.10825400	-0.58470200	0.56682600
C	3.35051500	-0.70262900	-0.60893700
H	3.07176900	-1.79328100	-2.43312900
H	5.00857100	-3.31869200	-2.03617600
H	6.34888900	-3.09204500	0.04621300
H	5.75901100	-1.35035000	1.71767700
H	3.85407300	0.17246700	1.30179100

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C	-0.51318700	-0.18855600	-0.61474900
C	0.79883000	-0.66657000	-0.26303300
N	-1.33185200	-1.30972100	-0.72387700
C	-0.59093400	-2.44622800	-0.50280800
H	-1.07469400	-3.41008300	-0.56791900
C	-4.95628900	1.55887600	0.69172600
C	-4.16918100	0.90421800	-0.25455800
C	-4.05210700	-0.47471100	-0.14842900
C	-4.67654400	-1.22334600	0.84104700
C	-5.45627200	-0.54214200	1.77394900
C	-5.60399900	0.85250300	1.71680500
H	-5.06940600	2.63796300	0.63068400
H	-3.65483800	1.44028600	-1.04318700
H	-4.56945400	-2.30238500	0.86488500
H	-5.96228300	-1.10462500	2.55407900
C	-6.42685000	1.58002600	2.75263600
H	-6.82125400	2.52305500	2.36167900
H	-7.27028500	0.97146100	3.09451000
H	-5.81867700	1.81950400	3.63486900
S	-3.05475700	-1.37766900	-1.40232600
O	-3.37230600	-2.87382000	-1.31222700
O	-3.06098800	-0.62761100	-2.72849700
C	2.83113800	-5.24650500	0.50932700
C	1.68472300	-4.41621000	0.11802900
C	1.76176400	-3.06436700	0.15088200
C	0.71645400	-2.12434800	-0.19352500
O	3.90936500	-4.82147300	0.89608500
H	2.65956900	-6.34258100	0.43008900
H	0.78563500	-4.93902000	-0.20303300
H	2.71292600	-2.64961000	0.47222100
C	0.06007800	1.98862000	-0.60615100

C	1.41714400	1.66003700	-0.25219300
C	2.35536100	2.72217100	-0.09999500
C	1.95194500	4.01832700	-0.28335600
C	0.62441100	4.35869100	-0.62781900
C	-0.29785200	3.35272400	-0.78528500
C	1.79118100	0.29002400	-0.07584400
H	3.38306400	2.49802600	0.15788600
H	0.35297900	5.39929300	-0.76644600
H	-1.32529400	3.57235900	-1.05708800
N	-0.90738300	1.04747100	-0.78183800
Cl	3.14385400	5.35212300	-0.08809000
C	4.08832600	-0.51320300	-0.70596800
C	5.39698400	-0.86203400	-0.36999000
C	5.82835400	-0.77544300	0.95500100
C	4.94754200	-0.33327600	1.94366100
C	3.63857600	0.01823200	1.61029400
C	3.19458700	-0.07475300	0.28276100
H	3.75254000	-0.58486000	-1.73685400
H	6.07730400	-1.20674500	-1.14358300
H	6.84482200	-1.05550900	1.21620700
H	5.27630300	-0.26595200	2.97698300
H	2.95263100	0.35849700	2.38137700

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C	-1.26768400	0.29867200	-0.37884900
C	-0.31903700	-0.45287900	0.52913800
H	0.23561500	0.18974100	1.21426100
N	-0.98004200	1.27217500	-1.29795400
C	-2.07160800	1.88330500	-2.08661500
H	-2.84486900	1.11242100	-2.12687000
H	-1.70211100	2.07007800	-3.09540300
C	2.01217100	3.78310000	2.01223900
C	1.79667700	2.90163500	0.95315500
C	0.89025000	3.28244800	-0.02772800
C	0.19874300	4.48868000	-0.00831300
C	0.43100400	5.34433700	1.06652700
C	1.33249400	5.00763000	2.08968200
H	2.73922900	3.50741500	2.77100800
H	2.34239000	1.96753100	0.89876800
H	-0.48230400	4.76068100	-0.80663400
H	-0.09157300	6.29633100	1.10172700
C	1.56213600	5.93792800	3.25544000
H	2.61347600	5.93985800	3.56049400
H	1.27131200	6.96491500	3.01447900

H	0.97279400	5.62244400	4.12633900
S	0.64657100	2.17707300	-1.48941200
O	0.39423100	3.02901400	-2.73407900
O	1.76266500	1.11623100	-1.50914500
C	-3.39854700	4.44952600	0.07046400
C	-3.41060600	5.20429400	-1.06295800
C	-2.88329700	4.36738500	-2.10135900
C	-2.60348200	3.16139400	-1.52497200
O	-2.91681100	3.19980400	-0.19365300
H	-3.67113000	4.63793900	1.09773300
H	-3.74255200	6.22926700	-1.15242200
H	-2.72386500	4.62903700	-3.13811100
Au	1.19233700	-1.60034200	-0.48937100
Br	2.99022200	-2.74160600	-1.94628700
Br	-0.86211600	-3.25615900	-1.27527100
Br	5.40727400	1.28469300	1.46115800
Br	3.00394500	-0.61943200	1.09343300
K	4.45818000	0.33097300	-1.61343500
C	-2.60356300	-1.01701700	0.73710600
C	-3.74202900	-1.68929100	1.24203800
C	-3.53421800	-2.57181700	2.30676100
C	-2.27093700	-2.76882300	2.88779100
C	-1.13448900	-2.17776600	2.37538200
C	-1.29436600	-1.38552500	1.20643800
C	-5.13779000	-1.69134800	0.65139700
H	-4.38502300	-3.13033900	2.68086400
H	-0.15309200	-2.36750700	2.79795500
H	-1.29904500	-2.43523400	0.21121700
O	-5.72409200	-2.76795100	0.64009700
N	-2.53793400	-0.06962400	-0.25091600
Cl	-2.14085500	-3.84719000	4.31191500
C	-6.94796600	-0.64949300	-0.66732700
C	-7.66946200	0.44557900	-1.12940300
C	-7.27390600	1.73952600	-0.77519600
C	-6.15237400	1.93099400	0.03378700
C	-5.41492500	0.83520200	0.48262100
C	-5.80801800	-0.46512000	0.13545500
H	-7.24881000	-1.66258600	-0.91177200
H	-8.54208400	0.29423600	-1.75861900
H	-7.84013400	2.59710700	-1.12909100
H	-5.84812500	2.93587900	0.30993600
H	-4.54022400	0.99604300	1.10168300

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C	-0.85226600	0.88827600	-0.46209000
C	-0.26406400	-0.06468600	0.53715300
H	0.51799200	0.33695300	1.17822800
N	-0.19395700	1.74006900	-1.25758200
C	-0.83749200	2.39410200	-2.41811600
H	-1.53771300	1.66701400	-2.83839300
H	-0.04322700	2.56576600	-3.14781400
C	3.23024100	3.18367800	2.44158300
C	3.03107500	2.49902900	1.24226800
C	1.91019400	2.84092500	0.49764600
C	1.00983400	3.83935600	0.85922100
C	1.23506600	4.49376600	2.06777600
C	2.33987400	4.17468600	2.87670400
H	4.11463100	2.93663700	3.02250000
H	3.77647500	1.77247900	0.91847600
H	0.16887500	4.10532000	0.22703700
H	0.54610700	5.27365900	2.38076500
C	2.56232900	4.88048900	4.19180400
H	3.62792200	5.05500400	4.37111200
H	2.04407300	5.84383300	4.22554900
H	2.18854300	4.27314700	5.02647400
S	1.71037700	2.02517100	-1.14450900
O	1.92113500	2.98574800	-2.31438500
O	2.41114200	0.65822500	-1.14769500
C	-3.20218600	4.94498600	-1.49431600
C	-2.19573300	5.80580700	-1.81045800
C	-1.09064000	4.98992700	-2.21979800
C	-1.50594700	3.69218100	-2.11979500
O	-2.80253100	3.65426200	-1.67373800
H	-4.21703300	5.07656900	-1.15108600
H	-2.23334400	6.88526600	-1.76920400
H	-0.11510800	5.31628500	-2.55315100
Au	0.77243100	-1.71104800	-0.41895000
Br	2.19923800	-3.56566300	-1.49018100
Br	-0.75978800	-1.70538600	-2.45086000
Br	6.27163000	1.00108800	0.75341000
Br	2.14616900	-1.86280400	1.73971400
K	4.55138600	-1.15300600	-0.70996200
C	-2.57745300	-0.05301700	0.48826300
C	-3.92195800	-0.37677700	0.79894400
C	-4.12667100	-1.34104600	1.83165500
C	-3.04408700	-1.85335300	2.51260300
C	-1.70548500	-1.50147200	2.21939600
C	-1.48280100	-0.60590100	1.19198600

C	-4.96324700	0.25528000	0.04254900
H	-5.12081000	-1.69536900	2.06714600
H	-0.88566500	-1.95626700	2.76558400
H	-3.62303400	1.14336500	-1.03478100
O	-4.65699300	1.03732500	-0.95152000
N	-2.19309400	0.82582500	-0.48923200
Cl	-3.32890100	-3.05453100	3.81129600
C	-7.25999100	0.07588800	-0.85002200
C	-8.63347600	-0.05612500	-0.67734400
C	-9.17395100	-0.13318700	0.61007500
C	-8.33690700	-0.07538500	1.72710400
C	-6.95816700	0.03338500	1.56319700
C	-6.40543800	0.09820600	0.26991600
H	-6.83321500	0.14271700	-1.84490800
H	-9.28432500	-0.09507100	-1.54553800
H	-10.24784700	-0.22844800	0.74234100
H	-8.75791800	-0.10742000	2.72735500
H	-6.31881200	0.11968000	2.43477300

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C	-0.90322600	0.97575900	-0.55975100
C	-0.26662600	0.03220900	0.42201000
H	0.52986100	0.45122300	1.03342200
N	-0.28816800	1.84043500	-1.37216500
C	-0.97813400	2.48603900	-2.50975900
H	-1.68675700	1.75225400	-2.90538000
H	-0.21345800	2.66250400	-3.26950600
C	3.22175100	3.36433000	2.21310900
C	2.99960700	2.66673600	1.02523300
C	1.85824200	2.99306700	0.30539700
C	0.95834900	3.98761600	0.67899600
C	1.20737100	4.65503100	1.87546500
C	2.33391200	4.35194100	2.66059800
H	4.12221200	3.13056200	2.77443500
H	3.74367600	1.94458500	0.68864100
H	0.10054400	4.24098100	0.06451200
H	0.51996700	5.43253800	2.19763100
C	2.58107900	5.07124100	3.96383400
H	3.65056300	5.23666000	4.12730000
H	2.07312900	6.04023600	3.99247300
H	2.21135000	4.47813300	4.81051600
S	1.62343500	2.16003800	-1.32289300
O	1.77319200	3.11313300	-2.50750000
O	2.34726500	0.80602300	-1.33874000

C	-3.30248900	5.01556200	-1.44277100
C	-2.34242700	5.88665300	-1.85951800
C	-1.26026200	5.08163500	-2.34489400
C	-1.64245100	3.77960100	-2.18670400
O	-2.89541500	3.72857700	-1.63154200
H	-4.28694400	5.13655000	-1.01710200
H	-2.39641500	6.96592000	-1.83536400
H	-0.32111400	5.41820800	-2.76197800
Au	0.76933000	-1.59236600	-0.57283500
Br	2.19277000	-3.42186900	-1.68967200
Br	-0.81319700	-1.59913000	-2.56584300
Br	6.24129000	1.21476000	0.44284000
Br	2.20819900	-1.72681100	1.54384000
K	4.52959300	-0.98002000	-0.96776800
C	-2.57546700	-0.01928800	0.45875600
C	-3.90094700	-0.36398700	0.78838100
C	-4.06523000	-1.32718000	1.82085900
C	-2.95084900	-1.81927000	2.47580400
C	-1.62891600	-1.44481600	2.15271500
C	-1.44899700	-0.53989500	1.11979000
C	-4.94882100	0.27194400	0.01568400
H	-5.04558700	-1.70012500	2.08469000
H	-0.78815300	-1.88534100	2.67807200
H	-3.48078500	1.15979600	-1.00909100
O	-4.61889300	1.04459000	-0.95747400
N	-2.24146500	0.87382700	-0.53335700
Cl	-3.18621100	-3.02291200	3.78322700
C	-7.24483000	0.09485300	-0.87950300
C	-8.61762100	-0.05137900	-0.71194000
C	-9.15863500	-0.16252100	0.57283000
C	-8.32317200	-0.12487900	1.69179200
C	-6.94480300	-0.00252100	1.53157000
C	-6.39213000	0.09784500	0.24118000
H	-6.81549100	0.19036300	-1.87101700
H	-9.26762700	-0.07456500	-1.58139700
H	-10.23192900	-0.26907700	0.70171800
H	-8.74504200	-0.18426000	2.69049500
H	-6.30712900	0.06679700	2.40592200

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C	-0.80681400	0.86761100	-0.55653100
C	-0.27293700	-0.06691600	0.47822700
H	0.48160700	0.35073800	1.14146300
N	-0.13654300	1.71000400	-1.33851500

C	-0.69885600	2.28855400	-2.57677400
H	-1.23205400	1.48395000	-3.09716100
H	0.15991000	2.56968400	-3.19216300
C	2.97921400	3.31942500	2.55869200
C	2.89646200	2.59660700	1.36764600
C	1.85158600	2.91651500	0.51150500
C	0.91914400	3.92241200	0.75240900
C	1.02842100	4.61350400	1.95574100
C	2.05136800	4.32079400	2.87589100
H	3.80364300	3.09588000	3.23010000
H	3.67164400	1.86618800	1.13017600
H	0.13999700	4.16454200	0.03648000
H	0.31364000	5.40096900	2.17855700
C	2.14656900	5.06651600	4.18390800
H	3.18977100	5.25487000	4.45647400
H	1.62231300	6.02609200	4.14040700
H	1.69947900	4.48067800	4.99759500
S	1.79776900	2.05138200	-1.11356000
O	2.03003500	2.98625600	-2.29776700
O	2.52147700	0.70256200	-1.04511000
C	-3.48287100	4.45082800	-1.88537000
C	-2.61376400	5.45657000	-2.17793000
C	-1.36368900	4.82848900	-2.49546700
C	-1.56293100	3.48366800	-2.37372900
O	-2.86104600	3.24154000	-1.99897800
H	-4.52385200	4.41449600	-1.60369100
H	-2.83223900	6.51505200	-2.17992800
H	-0.44093800	5.30933500	-2.79020000
Au	0.84141000	-1.69218600	-0.43831700
Br	2.34658000	-3.51483600	-1.44795300
Br	-0.59038200	-1.69812300	-2.54195100
Br	6.16072000	1.17492100	0.97643100
Br	2.13594600	-1.81582600	1.77133500
K	4.66473700	-1.11743800	-0.52216900
C	-2.60798700	-0.13644500	0.38772100
C	-3.93245800	-0.47564000	0.69508600
C	-4.10501300	-1.40194200	1.74307100
C	-3.00670400	-1.88807700	2.44655100
C	-1.69399000	-1.51315200	2.15455600
C	-1.50358800	-0.62631900	1.09779900
C	-5.04678200	0.11828600	-0.10163000
H	-5.09570700	-1.75464400	1.99814600
H	-0.85608300	-1.92005100	2.70945500
H	-2.79762900	1.21815400	-1.22360100

O	-4.78387500	0.71101900	-1.15191700
N	-2.14651600	0.75134100	-0.59313400
Cl	-3.29018600	-3.05517000	3.77713700
C	-7.45309200	-0.10405500	-0.65177300
C	-8.79989800	-0.15788400	-0.30571600
C	-9.18186600	-0.06390200	1.03627400
C	-8.21237600	0.08477100	2.02974900
C	-6.85982000	0.11538700	1.68898100
C	-6.46804800	0.01186600	0.34386800
H	-7.14286700	-0.15596200	-1.69035500
H	-9.55339000	-0.26716400	-1.08041900
H	-10.23382500	-0.09929900	1.30556900
H	-8.50756100	0.17977100	3.07071100
H	-6.11556300	0.25648000	2.46625600

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C	0.52397800	0.38885400	0.63977800
C	0.66755600	-0.61507200	1.56829300
H	-0.76101400	0.60421400	-1.03457000
N	1.30018500	1.54908500	0.51271200
C	0.55560400	2.84270400	0.62565300
H	-0.30618600	2.88152600	-0.05354900
H	1.26194200	3.62397000	0.33522500
C	3.93962500	-2.09150000	-1.46387600
C	3.02758000	-1.04172900	-1.57732100
C	3.37505100	0.18535600	-1.03028500
C	4.58486200	0.40894800	-0.38347200
C	5.47886500	-0.65403800	-0.28260400
C	5.16949000	-1.91691700	-0.81429100
H	3.69029400	-3.05949500	-1.89014600
H	2.08050400	-1.16344600	-2.09151600
H	4.82241400	1.39104900	0.01133400
H	6.43495200	-0.49980900	0.21112000
C	6.13989100	-3.06516100	-0.67224200
H	5.92727900	-3.86180400	-1.39148900
H	7.17371000	-2.73594500	-0.82278300
H	6.08242800	-3.50403100	0.33246500
S	2.19281700	1.58159100	-1.17298100
O	2.96768000	2.91066500	-1.19210200
O	1.16531900	1.24843900	-2.28176500
C	-1.35583600	2.88749600	3.66348700
C	-0.27243000	3.52385500	4.18899900
C	0.67551600	3.63744200	3.12133000
C	0.09990000	3.06397200	2.02436400

O	-1.14934300	2.59931400	2.34852700
H	-2.31104400	2.58521400	4.06513100
H	-0.16115200	3.87437900	5.20553700
H	1.65827000	4.08653400	3.16091100
C	-1.15884300	-1.05890700	0.23717100
C	-2.26435700	-1.77314300	-0.27255700
C	-2.56563800	-2.99596200	0.33611800
C	-1.82704700	-3.45363700	1.43177600
C	-0.74864500	-2.76012700	1.95475400
C	-0.39081600	-1.54968500	1.33983800
C	-3.09389300	-1.37227000	-1.45848700
H	-3.38936100	-3.58092700	-0.05518600
H	-0.19548900	-3.14882000	2.80283100
H	1.42643100	-0.64866300	2.33625500
O	-3.56253400	-2.23823500	-2.18807000
N	-0.58784900	0.12564700	-0.16020800
Cl	-2.30192900	-5.01971400	2.19052500
C	-3.67308600	0.44054400	-3.06320100
C	-3.99499500	1.75870600	-3.37361200
C	-4.04954500	2.72212600	-2.36132600
C	-3.78002600	2.36250900	-1.03890400
C	-3.43915800	1.04538800	-0.72782700
C	-3.37529900	0.07386500	-1.74024200
H	-3.64693600	-0.32571600	-3.83114300
H	-4.20773600	2.03685900	-4.40202700
H	-4.30518100	3.75028500	-2.60318600
H	-3.83625800	3.10451400	-0.24734000
H	-3.23528000	0.77350200	0.30277200

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C	-0.92486800	-0.08966600	0.91620200
C	-0.32365500	-1.44878600	1.23887300
H	-0.98863600	-2.29154200	1.05414700
N	-1.02189800	0.67254000	2.08015300
C	-1.29180700	-0.15392000	3.25699700
H	-2.35359900	-0.41130200	3.33925300
H	-0.96234400	0.35572100	4.16453000
C	0.32298200	5.11246600	-0.09041900
C	-0.66926800	4.32210600	0.49176300
C	-0.28297900	3.44516800	1.49602100
C	1.02640000	3.33459200	1.95338200
C	1.99742200	4.12297100	1.34554500
C	1.66118000	5.02164300	0.31698400
H	0.04834900	5.80777500	-0.87924500

H	-1.70511600	4.37959800	0.17912300
H	1.28799000	2.64651900	2.74911100
H	3.03524400	4.01874800	1.64567600
C	2.73534900	5.86356200	-0.32334400
H	3.09059700	6.63535700	0.37167400
H	3.59956500	5.24326300	-0.58697200
H	2.36900700	6.36716400	-1.22331300
S	-1.59265900	2.46493700	2.32254400
O	-1.45034300	2.56071200	3.84747400
O	-2.94253700	2.73191500	1.65979700
C	-0.00862800	-3.49672700	3.51219200
C	1.14405200	-2.98361500	3.02547800
C	0.85839300	-1.60243600	2.69395500
C	-0.51109900	-1.41169700	3.00750900
O	-1.01981700	-2.57578100	3.53091100
H	-0.27988900	-4.48300600	3.85956100
H	2.07857700	-3.50246700	2.87251100
H	1.57703500	-0.81067100	2.52649300
Au	1.20413300	-1.96229300	-0.24038600
Br	2.88443000	-2.58714500	-2.08693800
Br	0.01222800	-4.22404000	-0.55733000
Br	5.17978500	2.57524100	-0.09130500
Br	2.52407700	0.21844800	0.20451800
K	5.03221900	-0.00207500	-1.86816700
C	-2.07401400	1.03663300	-0.88817100
C	-3.48800300	0.93787400	-0.78291700
C	-4.28577900	1.83916700	-1.50753200
C	-3.70207100	2.79265800	-2.32677700
C	-2.32069900	2.86037700	-2.48541100
C	-1.51870700	1.97064100	-1.77834600
C	-4.14559100	-0.07263600	0.10575000
H	-5.36403800	1.80147600	-1.41063600
H	-1.87925200	3.59196700	-3.15367000
H	-0.44012800	1.99294500	-1.89571100
O	-3.62946800	-0.42926200	1.16421500
N	-1.22061300	0.10481200	-0.30173500
Cl	-4.75092900	3.94889900	-3.22095400
C	-6.31843600	-1.11931900	0.71527100
C	-7.52929600	-1.72674800	0.39750100
C	-7.88633600	-1.91676700	-0.94149500
C	-7.02906100	-1.49439800	-1.95901000
C	-5.82430100	-0.86553800	-1.64284300
C	-5.45997600	-0.66777200	-0.30112000
H	-6.01807600	-0.97996900	1.74859000

H	-8.19459600	-2.05714700	1.19043800
H	-8.82890900	-2.39724000	-1.18975000
H	-7.29589100	-1.65518900	-2.99969900
H	-5.15674200	-0.55044100	-2.43828100

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C	-0.64863000	-0.22595500	1.10028100
C	-0.13014500	-1.66297900	1.19742500
H	-0.97142500	-2.33883600	1.02821400
N	-0.80050200	0.37798100	2.36660400
C	-1.37056500	-0.43382700	3.42820900
H	-2.43135900	-0.66600700	3.24347000
H	-1.31215400	0.13016800	4.37573800
C	2.45841400	3.95050100	1.12292000
C	1.15393100	3.50025300	1.32725500
C	0.88570400	2.81246600	2.50217300
C	1.84142500	2.55878300	3.48139600
C	3.13377500	3.02436200	3.25362900
C	3.46010700	3.72228400	2.07779300
H	2.68596600	4.45709600	0.18895000
H	0.38216200	3.68687200	0.59024500
H	1.57784400	2.04256700	4.39771000
H	3.89912000	2.84919300	4.00535400
C	4.85754800	4.24638900	1.85391600
H	4.94324900	5.28232000	2.20776200
H	5.60275500	3.65247900	2.39288500
H	5.11308700	4.24632200	0.78986400
S	-0.82720900	2.23785900	2.82195600
O	-1.02224000	2.10636800	4.34573000
O	-1.83560000	3.00068600	1.97377400
C	-0.09713600	-3.80431000	3.82163800
C	0.79763800	-3.41038900	2.91613300
C	0.52820500	-1.97263100	2.59724400
C	-0.59616200	-1.68127100	3.48725500
O	-0.98378800	-2.72872400	4.14668900
H	-0.32050500	-4.71969400	4.34605000
H	1.57913800	-4.01440300	2.47653100
H	1.38413600	-1.29060700	2.70784700
Au	1.18781000	-2.12761000	-0.40031700
Br	2.70082900	-2.60017200	-2.44425800
Br	-0.44455800	-3.91515500	-1.12413900
Br	2.28056500	3.71282400	-2.57621400
Br	2.90470200	-0.49075400	0.57922200
K	3.06971900	0.71142200	-2.69189400

C	-1.67197300	1.28028200	-0.48756800
C	-3.09058700	1.24476300	-0.39828100
C	-3.82646700	2.31434100	-0.94025500
C	-3.18086000	3.36960400	-1.56401300
C	-1.79825200	3.37498900	-1.72658300
C	-1.05928900	2.31705100	-1.20782100
C	-3.82993200	0.11377700	0.24107700
H	-4.90670600	2.31990500	-0.85667500
H	-1.29173000	4.17525800	-2.25608700
H	0.01564500	2.31332900	-1.36487400
O	-3.39907700	-0.46801000	1.24021300
N	-0.88319000	0.20065700	-0.07306400
Cl	-4.15824900	4.73149900	-2.21140200
C	-6.05663500	-0.97089000	0.49438900
C	-7.25706300	-1.45846900	-0.01218500
C	-7.53628700	-1.34580200	-1.37827000
C	-6.61190000	-0.74153500	-2.23205700
C	-5.41667900	-0.23313700	-1.72279000
C	-5.12956500	-0.33890300	-0.35186700
H	-5.81758100	-1.06568000	1.54856900
H	-7.97502300	-1.93016800	0.65309500
H	-8.47087000	-1.73255800	-1.77556100
H	-6.81871400	-0.66658200	-3.29576000
H	-4.69713000	0.22446600	-2.39342600