

Supporting Information

Key role of a π - π complex in diary cross-coupling between aryldiazonium salts and
arylbronic acids using photosensitizer-free gold/photoredox catalysis

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I. Estimation of Activation Barriers for Single Electron Transfer by Marcus-Hush Theory

According to the Marcus-Hush equation, the reorganization energy λ is decomposed into the inner-sphere nuclear reorganization energy λ_i and the outer-sphere solvent reorganization energy λ_o . The inner-sphere nuclear reorganization energy λ_i can be calculated from the equations (S1)-(S3):

$$\lambda_{i1} = \left| E^D(Q_P) - E^D(Q_R) \right| + \left| E^{D^+}(Q_P) - E^{D^+}(Q_R) \right| \quad (\text{S1})$$

$$\lambda_{i2} = \left| E^A(Q_P) - E^A(Q_R) \right| + \left| E^{A^-}(Q_P) - E^{A^-}(Q_R) \right| \quad (\text{S2})$$

$$\lambda_i = \frac{\lambda_{i1} + \lambda_{i2}}{2} \quad (\text{S3})$$

where λ_{i1} represents the reorganization energy of the electron-donating substrates (D), λ_{i2} is the reorganization energy of the electron-accepting substrates (A). Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively.

In addition, the outer-sphere solvent reorganization energy λ_o can be obtained according to the equation (S4):

$$\lambda_o = (332 \text{ kcal/mol}) \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon} \right) \quad (\text{S4})$$

where a_1 and a_2 are the radii of the electron-donating substrates (D) and the electron-accepting substrates (A), respectively, $R = a_1 + a_2$, ε_{op} and ε are the optical dielectric constant (2.05) and the static dielectric constant (32.6) of methanol solvent, respectively. The radius of a molecule can be obtained by calculating the molecular volume via a Monte-Carlo integration as implemented in the Gaussian 16 program.

Therefore, the overall activation barrier of single electron transfer (SET) process can be calculated from the equations (S5) and (S6):

$$\lambda = \lambda_i + \lambda_o \quad (\text{S5})$$

$$\Delta G_{SET}^{\#} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad (\text{S6})$$

where ΔG_r is the reaction energy.

II. Complexes of the Aryldiazonium Salt with the Gold(I) Catalyst and with MeOH

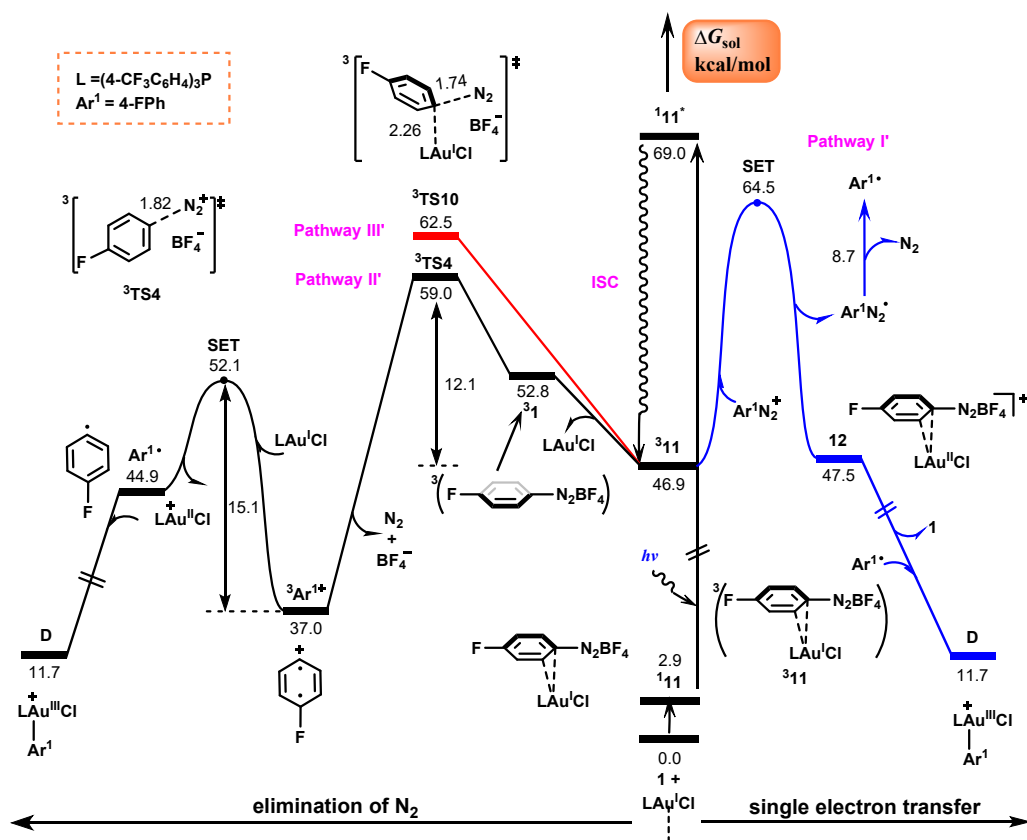


Fig. S1 Calculated Gibbs energy profiles for the generation of aryl radical **Ar¹•** (Ar¹=4-FPh) and the oxidation of gold(I) using the complex of the aryldiazonium salt with the gold(I) catalyst as a photoinitiator. Bond distances are in Å.

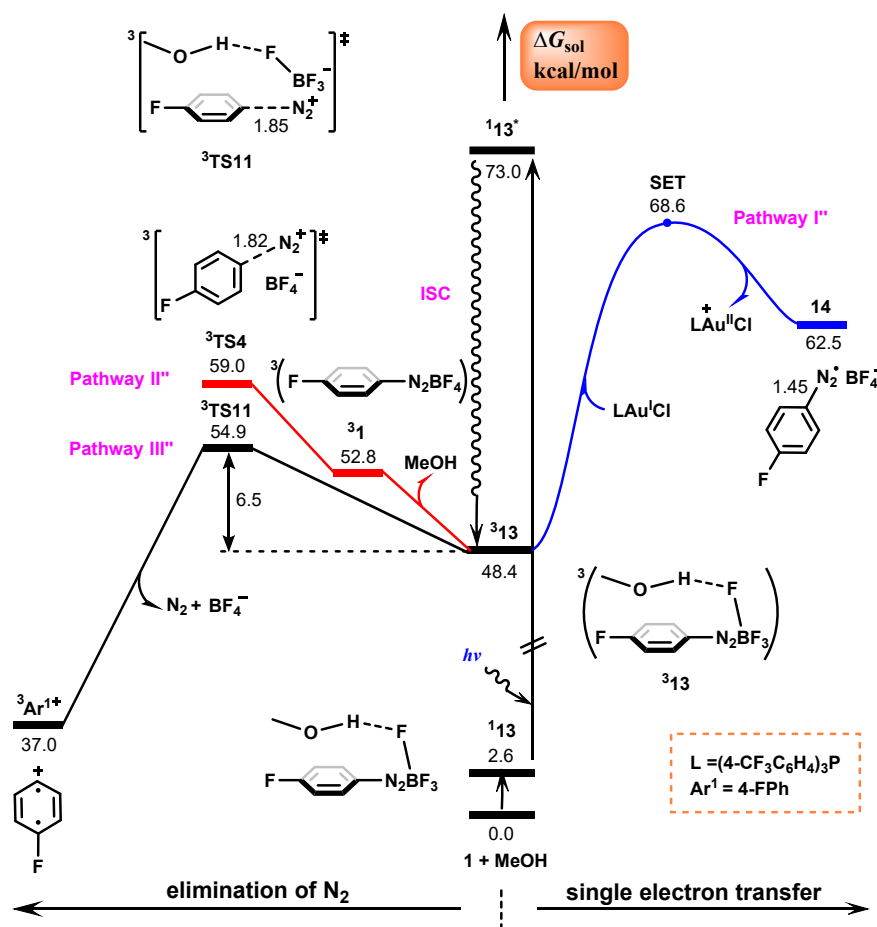


Fig. S2 Calculated Gibbs energy profiles of the generation of aryl radical $\text{Ar}^{\text{I}\bullet}$ ($\text{Ar}^{\text{I}} = 4\text{-FPh}$) and the oxidation of gold(I) using the complex of the aryldiazonium salt with MeOH as a photoinitiator. Bond distances are in Å.

III. HOMO-LUMO Orbitals Analysis

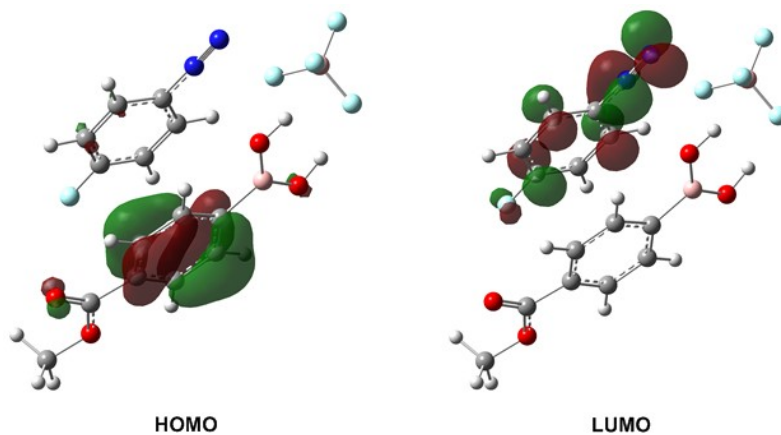
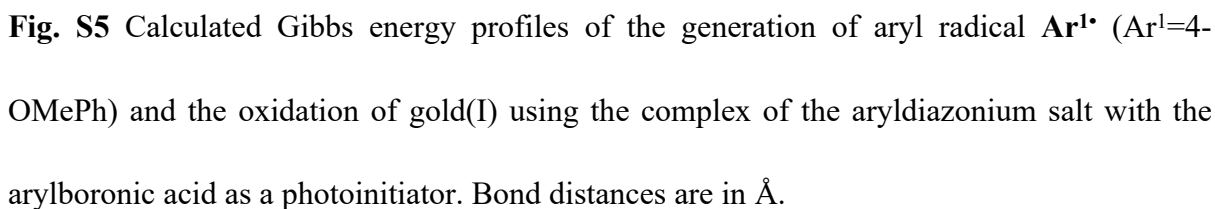


Fig. S3 Calculated HOMO and LUMO orbitals (isovalue = 0.050 a.u.) of the complex of the aryl diazonium salt with the arylboronic acid.

S7



V. Substituent Effect

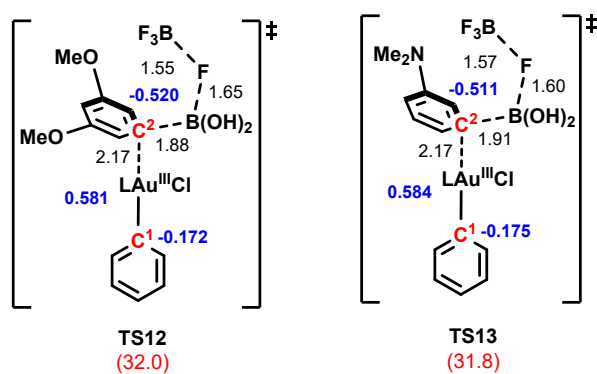


Fig. S6 Calculated transmetalation transition states involved in the reactions of boronic acids bearing -OMe and -NMe₂ groups, respectively. Gibbs free energy barriers (red) are in kcal mol⁻¹.

VI. Thermodynamic Data

Table S1. Calculated Key Structures of Zero-Point Energy (*ZPE*) Corrections, Thermal Corrections to Energies (ΔE), Thermal Correction to Gibbs Free Energies (ΔG), Energies (*E*), Enthalpies (*H*), and Gibbs Free Energies (*G*) in Methanol and the Imaginary Frequencies (IF, cm^{-1}) of the Transition States. All Energies Are Given in Hartree

Structures	<i>ZPE</i>	ΔE	ΔH	ΔG	<i>E</i>	<i>H</i>	<i>G</i>	IF
1	0.107473	0.120181	0.121125	0.066979	-864.244838	-864.243894	-864.29804	
2	0.167861	0.180214	0.181158	0.128383	-635.602844	-635.6019	-635.65468	
LAu^ICl	0.290821	0.321667	0.322611	0.219626	-2641.92079	-2641.91984	-2642.0228	
MeOH	0.051344	0.054658	0.055602	0.028616	-115.600397	-115.599453	-115.62644	
Ar^IN₂⁺	0.091041	0.097969	0.098913	0.059483	-439.780816	-439.779872	-439.8193	
Ar^IN₂[•]	0.088905	0.096049	0.096993	0.056424	-439.949028	-439.948084	-439.98865	
BF₄⁻	0.014721	0.019025	0.019969	-0.01283	-424.447044	-424.446099	-424.4789	
B(OH)₂Cl	0.035114	0.039539	0.040483	0.007694	-636.705583	-636.704639	-636.73743	
B(OH)₂F–BF₃	0.051108	0.060051	0.060995	0.015897	-600.820431	-600.819487	-600.86459	
N₂	0.005622	0.007983	0.008927	-0.01283	-109.447418	-109.446474	-109.46823	
TS1	0.396339	0.441426	0.44237	0.310364	-3506.11053	-3506.10959	-3506.2416	-426.21
E	0.397503	0.443604	0.444548	0.309863	-3506.17364	-3506.17269	-3506.3074	
TS1'	0.38116	0.419839	0.420783	0.305427	-3081.64376	-3081.64282	-3081.7582	-395.59
LAu^{II}Cl	0.371624	0.409039	0.409983	0.293309	-2972.43904	-2972.4381	-2972.5548	
¹4	0.278704	0.304599	0.305543	0.221725	-1499.87243	-1499.87149	-1499.9553	
¹11	0.399848	0.444852	0.445796	0.314067	-3506.18546	-3506.18451	-3506.3162	
¹13	0.160942	0.177973	0.178917	0.114842	-979.857189	-979.856245	-979.92032	
2-Au^I	0.462404	0.506159	0.507103	0.379622	-3277.54108	-3277.54014	-3277.6676	
2-MeOH	0.222077	0.238832	0.239777	0.175458	-751.210846	-751.209902	-751.27422	
MeOH-Au^I	0.344005	0.379512	0.380456	0.268469	-2757.5282	-2757.52726	-2757.6392	
³4	0.273896	0.30071	0.301654	0.215151	-1499.78206	-1499.78112	-1499.8676	
5	0.27533	0.301902	0.302846	0.215237	-1500.03056	-1500.02962	-1500.1172	
6	0.105433	0.118604	0.119548	0.062837	-864.401707	-864.400763	-864.45747	
7	0.290974	0.321758	0.322702	0.221142	-2641.668	-2641.66705	-2641.7686	
TS2	0.102323	0.115973	0.116917	0.058497	-864.385911	-864.384966	-864.44339	-414.36
Ar^I*	0.079327	0.084446	0.08539	0.049928	-330.499247	-330.498303	-330.53377	
8	0.54331	0.593753	0.594697	0.450483	-3607.88696	-3607.88602	-3608.0302	
³1	0.104155	0.117488	0.118432	0.061628	-864.15809	-864.157146	-864.21395	

³TS3	0.10132	0.115261	0.116206	0.056525	-864.145218	-864.144274	-864.20396	-452.24
³TS4	0.272531	0.299094	0.300038	0.21377	-1499.78245	-1499.78151	-1499.8678	-464.68
Ar¹⁺	0.079094	0.084411	0.085355	0.049098	-330.256934	-330.25599	-330.29225	
D	0.373566	0.410296	0.41124	0.298649	-2972.25697	-2972.25603	-2972.3686	
TS5	0.539956	0.590294	0.591238	0.449398	-3607.84638	-3607.84544	-3607.9873	-273.86
9	0.505999	0.550725	0.55167	0.420698	-2971.15197	-2971.15103	-2971.282	
10	0.562032	0.61733	0.618275	0.466082	-4032.36766	-4032.36671	-4032.5189	
TS6	0.558837	0.61412	0.615064	0.463955	-4032.33216	-4032.33122	-4032.4823	-287.72
F	0.507011	0.553517	0.554461	0.419799	-3431.53895	-3431.538	-3431.6727	
TS7	0.506171	0.552161	0.553105	0.420345	-3431.52678	-3431.52584	-3431.6586	-292.47
3	0.216126	0.230373	0.231317	0.173694	-789.685946	-789.685002	-789.74263	
TS8	0.570909	0.629151	0.630095	0.470926	-4270.04706	-4270.04612	-4270.2053	-289.07
TS9	0.599753	0.656573	0.657518	0.503622	-4047.54587	-4047.54493	-4047.6988	-283.34
³11	0.39776	0.442873	0.443817	0.311754	-3506.11501	-3506.11406	-3506.2461	
12	0.400585	0.445391	0.446335	0.315105	-3505.94548	-3505.94454	-3506.0758	
³TS10	0.397677	0.442395	0.443339	0.313159	-3506.09203	-3506.09109	-3506.2213	-437.9
TS	0.085754	0.093384	0.094328	0.052126	-439.933628	-439.932684	-439.97489	-424.23
³13	0.159687	0.176055	0.176999	0.114314	-979.785566	-979.784622	-979.84731	
14	0.15962	0.176728	0.177672	0.11259	-980.015029	-980.014085	-980.07917	
³TS11	0.157291	0.173922	0.174867	0.111426	-979.774483	-979.773538	-979.83698	-458.82
1_{CF3}	0.120626	0.136094	0.137039	0.075568	-1101.94873	-1101.94778	-1102.0093	
¹4'	0.293065	0.321258	0.322202	0.233774	-1737.57961	-1737.57866	-1737.6671	
³4'	0.289226	0.317732	0.318676	0.229961	-1737.49899	-1737.49804	-1737.5868	
5'	0.290424	0.319054	0.319998	0.22934	-1737.7416	-1737.74066	-1737.8313	
6'	0.11847	0.134465	0.135409	0.071119	-1102.11187	-1102.11093	-1102.1752	
TS2'	0.115536	0.131895	0.132839	0.067414	-1102.09803	-1102.09708	-1102.1625	-423.29
Ar_{CF3}[•]	0.092556	0.100354	0.101299	0.058191	-568.211794	-568.21085	-568.25396	
8'	0.55833	0.610683	0.611627	0.465886	-3845.59847	-3845.59752	-3845.7433	
³1'	0.116802	0.132904	0.133849	0.069811	-1101.85748	-1101.85654	-1101.9206	
³TS3'	0.114315	0.130627	0.131571	0.067183	-1101.84571	-1101.84476	-1101.9092	-469.08
³TS4'	0.286085	0.315124	0.316068	0.224724	-1737.49214	-1737.4912	-1737.5825	-462.17
³Ar_{CF3}⁺	0.091517	0.099602	0.100546	0.056919	-567.949459	-567.948515	-567.99214	
D'	0.388815	0.427382	0.428327	0.314032	-3209.96933	-3209.96838	-3210.0827	
Ar_{CF3}N₂⁺	0.104125	0.113824	0.114769	0.067347	-677.483861	-677.482917	-677.53034	
Ar_{CF3}N₂[•]	0.102184	0.112089	0.113033	0.064748	-677.658643	-677.657699	-677.70598	
10'	0.576995	0.634072	0.635016	0.482087	-4270.08029	-4270.07934	-4270.2323	
1_{OMe}	0.148815	0.163183	0.164127	0.106026	-879.464979	-879.464034	-879.52214	
¹4''	0.319784	0.347254	0.348199	0.260891	-1515.09692	-1515.09598	-1515.1833	
³4''	0.317466	0.345057	0.346001	0.25796	-1515.02688	-1515.02593	-1515.114	
5''	0.317221	0.344979	0.345923	0.257004	-1515.24688	-1515.24594	-1515.3349	
6''	0.145883	0.160812	0.161756	0.101028	-879.616276	-879.615331	-879.67606	
TS2''	0.142781	0.158196	0.159141	0.096662	-879.598848	-879.597903	-879.66038	-402.72
Ar_{OMe}[•]	0.119666	0.126584	0.127529	0.087884	-345.711818	-345.710874	-345.75052	
8''	0.584974	0.636592	0.637536	0.493459	-3623.10257	-3623.10163	-3623.2457	

³I''	0.146002	0.16079	0.161734	0.101578	-879.397599	-879.396655	-879.45681	
³TS3''	0.143411	0.158536	0.15948	0.098197	-879.386776	-879.385832	-879.44712	-455.97
³TS4''	0.314304	0.342472	0.343417	0.25405	-1515.01715	-1515.01621	-1515.1056	-462.33
³Ar_{OMe}⁺	0.119678	0.126785	0.127729	0.087407	-345.495017	-345.494073	-345.5344	
D''	0.415313	0.453232	0.454176	0.340992	-2987.47586	-2987.47492	-2987.5881	
Ar_{OMe}N₂⁺	0.131695	0.140373	0.141317	0.098009	-455.004168	-455.003224	-455.04653	
Ar_{OMe}N₂[•]	0.129394	0.138279	0.139224	0.094798	-455.164174	-455.16323	-455.20766	
10'	0.602197	0.659262	0.660206	0.503816	-4047.5786	-4047.57765	-4047.734	
TS12	0.588832	0.644089	0.645033	0.493659	-3934.2581	-3934.25715	-3934.4085	-265.46
TS13	0.597039	0.651204	0.652148	0.504463	-3839.20189	-3839.20095	-3839.3486	-273.59

VII. Cartesian Coordinates of All Structures Involved in this Work

1

C	-2.69559800	0.23181800	-0.37360000
C	-1.32175100	0.17064500	-0.46432700
C	-0.60316200	1.31656700	-0.08448000
C	-1.19795200	2.50196300	0.38032100
C	-2.57181900	2.53709300	0.46152000
C	-3.29291100	1.40496000	0.08243400
H	-3.31723300	-0.61318900	-0.64977500
H	-0.79746500	-0.71565000	-0.80835800
H	-0.58801000	3.35376100	0.66207300
H	-3.09801400	3.41880100	0.81053100
N	0.76461900	1.28520000	-0.15245700
N	1.87481100	1.27001000	-0.19729300
B	1.01409800	-0.94063100	-2.55010600
F	0.93641000	0.44654900	-2.73209300
F	-0.20462700	-1.52454200	-2.89470400
F	1.24168500	-1.18107400	-1.17300300
F	2.04803300	-1.47311000	-3.29798900
F	-4.60743000	1.44867800	0.16178400

2

C	-2.38797400	0.66360400	0.10010700
C	-1.16609900	0.65073000	0.77886600
C	-0.38444300	1.79770400	0.80855700
C	-0.79280300	2.97510000	0.16813100
C	-2.02121900	2.96770400	-0.50666800
C	-2.81260100	1.82921200	-0.54223600
H	-0.83718600	-0.25599100	1.27883900
H	0.56600800	1.78527800	1.33887100
H	-2.35557700	3.87264700	-1.01035700
H	-3.76552700	1.82113100	-1.06537200
B	0.09996100	4.26453000	0.20127900
O	1.27693200	4.20039200	0.88646200
H	1.79648300	5.00994600	0.88604500
O	-0.36041600	5.36491500	-0.45874200
H	0.21127500	6.13735100	-0.42023900
C	-3.26859000	-0.52730400	0.03120700
O	-2.74765100	-1.58811500	0.66169200
O	-4.34469400	-0.55387900	-0.53192000
C	-3.54434700	-2.77092600	0.63122500
H	-3.71458300	-3.09458000	-0.39968000
H	-2.98250500	-3.52889800	1.17683200

H	-4.51174800	-2.59807300	1.11177100
LAu^ICl			
P	0.03697600	0.01023200	0.41856300
Au	0.04267100	0.00003200	2.72723400
C	-1.38679200	-0.87718100	-0.29065900
C	-2.02076200	-0.43509300	-1.45563500
C	-1.81001300	-2.05272700	0.33415500
C	-3.06992200	-1.16953500	-1.99041100
H	-1.69633000	0.47880000	-1.94889600
C	-2.85625000	-2.79070600	-0.20497300
H	-1.31978200	-2.39172800	1.24594400
C	-3.48054800	-2.34464400	-1.36522100
H	-3.56746800	-0.83226700	-2.89623700
H	-3.18712000	-3.70636600	0.27595200
C	-0.04069100	1.68781300	-0.28758600
C	0.73061200	2.06570500	-1.38618600
C	-0.93816800	2.59698500	0.28507400
C	0.60766800	3.34799900	-1.91307900
H	1.43030500	1.36565000	-1.83745300
C	-1.06529200	3.87056300	-0.24427600
H	-1.53769300	2.30488500	1.14659800
C	-0.28827100	4.24229300	-1.34215100
H	1.20891800	3.64584800	-2.76653200
H	-1.76257100	4.57924800	0.19653700
C	1.51514700	-0.76853200	-0.30726000
C	1.44460500	-1.52815700	-1.47918200
C	2.74670900	-0.56136300	0.31815600
C	2.60056400	-2.07652900	-2.01598700
H	0.49042600	-1.69553300	-1.97432500
C	3.90482400	-1.10523900	-0.22359100
H	2.80193600	0.02466300	1.23467100
C	3.82499900	-1.86368900	-1.38606800
H	2.55190500	-2.67251800	-2.92443900
H	4.86355500	-0.94675400	0.26044400
C	-4.64599300	-3.08727000	-1.94609000
C	5.04609600	-2.48355900	-1.99474300
C	-0.45242900	5.63235300	-1.87677700
F	-4.53519900	-3.20779900	-3.27506700
F	-4.77285700	-4.31538500	-1.43858600
F	-5.79498700	-2.43735700	-1.71329700
F	0.34015800	5.88002700	-2.92158000
F	-0.17780700	6.54589400	-0.93611400
F	-1.71491100	5.85313200	-2.26730900

F	6.15633900	-2.21241900	-1.30538400
F	5.23376800	-2.05273500	-3.24929100
F	4.92766500	-3.81631800	-2.06210200
Cl	0.04248000	-0.00617500	5.10512700

MeOH

O	-1.21381500	-3.34740000	0.00003500
H	-1.53097800	-2.43881900	0.00163300
C	0.19348200	-3.31059700	0.00005100
H	0.54990400	-4.34573100	-0.00199100
H	0.60701000	-2.81203900	-0.88957100
H	0.60708500	-2.81554200	0.89159700

Ar¹N₂⁺

C	-2.69178700	0.22954200	-0.37434500
C	-1.31905900	0.17625100	-0.45674700
C	-0.60131500	1.32303900	-0.07274100
C	-1.19978800	2.50909100	0.38791900
C	-2.57364300	2.53833200	0.46247300
C	-3.29161500	1.40435500	0.08074000
H	-3.31008200	-0.61645700	-0.65379400
H	-0.80147800	-0.71206400	-0.80266600
H	-0.59271600	3.36231700	0.67084200
H	-3.10426200	3.41886200	0.80762600
N	0.76309700	1.28280300	-0.15317700
N	1.87416700	1.24897800	-0.22080800
F	-4.60343400	1.44560800	0.15305200

Ar¹N₂[•]

C	-2.73754700	0.21271500	-0.35039900
C	-1.35496300	0.11548900	-0.43171500
C	-0.56978400	1.21594000	-0.10628100
C	-1.13781100	2.42299200	0.30249300
C	-2.51617800	2.52720400	0.38563100
C	-3.28888300	1.41863000	0.05656000
H	-3.38749000	-0.62153500	-0.59520800
H	-0.87112100	-0.80570000	-0.74567200
H	-0.49276900	3.26285400	0.54923000
H	-3.00396000	3.44549600	0.69882600
N	0.86350500	1.04622500	-0.21343100
N	1.66136800	1.88649500	0.03181500
F	-4.61628400	1.52225500	0.13612400

BF₄⁻

B	-3.39792200	0.37216600	-0.00013100
F	-3.39841300	0.37217400	1.39761300
F	-4.05706400	-0.76913900	-0.46568000
F	-4.05706500	1.51347400	-0.46567100
F	-2.07982800	0.37216600	-0.46613000

B(OH)₂Cl

Cl	1.53828900	-0.92721300	-2.81804500
B	0.54070800	-2.01885700	-1.79671400
O	1.22720500	-2.77659900	-0.91946600
H	0.68988000	-3.35980300	-0.37322000
O	-0.78729100	-1.96393800	-2.01723300
H	-1.32022700	-2.54839400	-1.46778000

B(OH)₂F–BF₃

B	-1.33490700	-2.65967200	-2.47596900
O	-0.19058400	-2.72387000	-3.18045100
H	0.15295600	-1.85472300	-3.41032800
O	-1.94441000	-1.50867200	-2.12867600
H	-2.75246200	-1.63906900	-1.61765700
B	-4.12469000	-3.92329000	-2.12354000
F	-4.19098700	-3.01720000	-1.15984400
F	-1.88243100	-3.85073000	-2.12024900
F	-4.16579900	-3.52162700	-3.37376700
F	-4.18758500	-5.19620400	-1.82395300

N₂

N	1.32770600	2.05532500	1.26747200
N	2.14208700	1.39677100	0.91553500

TS1

C	-1.07047900	-1.42357800	0.20395900
C	-1.94878200	-1.23045500	-0.86218700
C	-1.42995600	-1.43559700	1.55533300
C	-3.25271200	-0.89690300	-0.54202600
C	-2.74305800	-1.11162500	1.84923200
C	-3.61889600	-0.83727900	0.79866700
H	-3.95968600	-0.62826500	-1.32437700
H	-3.09529300	-1.06128900	2.87473800
H	-0.70647000	-1.66340200	2.33331700
H	-1.62681800	-1.26209600	-1.89882200
N	0.12720200	-2.64932400	-0.15994400
N	0.27834200	-3.75677200	-0.26236500
Au	0.95809900	-0.54095000	-0.19418700

P	0.65125000	1.84289800	0.15850800
C	1.14567300	2.83381400	-1.28044100
C	0.48015900	4.01993700	-1.61079400
C	2.24145900	2.40709900	-2.03479200
C	0.91041600	4.76785300	-2.69620400
H	-0.37240600	4.35805700	-1.02637200
C	2.67230600	3.16241500	-3.11928100
H	2.75833800	1.48193700	-1.77852500
C	2.00180900	4.33481500	-3.44729900
H	0.39514800	5.68660400	-2.96571700
H	3.52074900	2.83226700	-3.71078200
C	1.66996300	2.38486200	1.56046500
C	1.90988500	1.49023300	2.60958400
C	2.17628800	3.68461000	1.61623600
C	2.65166000	1.89686400	3.70788800
H	1.51506000	0.47514000	2.56912800
C	2.92455900	4.08883900	2.71604600
H	1.99474900	4.38612800	0.80483400
C	3.15889000	3.19485400	3.75383100
H	2.84247100	1.20586000	4.52527300
H	3.32332700	5.09742400	2.76214100
C	-1.06956100	2.25576300	0.54022600
C	-2.01703900	2.08629800	-0.47238900
C	-1.47057300	2.62273300	1.83006000
C	-3.36773800	2.26730700	-0.19923000
H	-1.72817600	1.78000300	-1.47771800
C	-2.81935500	2.79296100	2.10215000
H	-0.73733400	2.76212300	2.62115200
C	-3.76161800	2.59828400	1.09181100
H	-4.09301000	2.10002700	-0.99226600
H	-3.14263900	3.06253700	3.10494300
Cl	3.32287100	-0.91928500	-0.68321500
C	2.43480100	5.18639100	-4.60265500
C	-5.20969300	2.71067700	1.45882800
C	3.97658700	3.58608800	4.94832900
F	2.91333300	6.36347500	-4.17676500
F	3.38635800	4.60932400	-5.33898100
F	1.40512500	5.46066400	-5.41297800
F	-5.51003100	1.87129000	2.46039700
F	-6.02241100	2.42610300	0.44037900
F	-5.51219500	3.94346400	1.88859600
F	5.08945800	2.84545600	5.03174900
F	3.29572300	3.38720400	6.08457700
F	4.34700400	4.86749000	4.91951100

F	-4.86226400	-0.49003600	1.09436000
B	-3.46840700	1.15951000	-3.57703400
F	-3.74153900	1.00827000	-4.92590200
F	-4.56278100	0.70688400	-2.81228600
F	-2.33077900	0.40140200	-3.23264400
F	-3.22745500	2.49638100	-3.26699600
E			
C	-0.98524400	-0.36451600	0.16152100
C	-1.62926700	-0.41848500	-1.06647600
C	-1.63323900	-0.63852400	1.36125600
C	-2.96199300	-0.82143700	-1.10412000
C	-2.96575400	-1.03862900	1.32134400
C	-3.59855000	-1.12426600	0.08823200
H	-3.49145400	-0.85338400	-2.05073700
H	-3.51435300	-1.27764200	2.22789300
H	-1.12396500	-0.54747900	2.31887300
H	-1.14395500	-0.11465200	-1.99168200
N	1.39776000	-2.44163400	0.16864900
N	1.58735900	-3.52818300	0.19092000
Au	1.01759900	0.02757100	0.19677400
P	0.48273300	2.31068600	0.40330900
C	0.88275500	3.12807700	-1.15261100
C	0.25555200	4.34800100	-1.44248900
C	1.83416800	2.59377000	-2.02263500
C	0.58860000	5.02382700	-2.60497300
H	-0.48018300	4.77465700	-0.76562400
C	2.15549200	3.27353100	-3.19070300
H	2.33554100	1.65645700	-1.79156800
C	1.53086000	4.48069200	-3.47669500
H	0.11138000	5.97313200	-2.83496300
H	2.88974100	2.85922000	-3.87397500
C	1.59861100	2.86164400	1.71110000
C	1.63311500	2.17729900	2.93351700
C	2.42930700	3.95879100	1.48325800
C	2.48768900	2.61142400	3.93151700
H	1.00761800	1.30225300	3.10360000
C	3.28694300	4.38814600	2.49078700
H	2.41717000	4.48225500	0.53069000
C	3.31082900	3.71529400	3.70460600
H	2.52350400	2.08934000	4.88421000
H	3.93607700	5.24181700	2.32423800
C	-1.22057700	2.68870000	0.83663500
C	-2.18940900	2.58985500	-0.16854600

C	-1.57520900	3.02171300	2.14853400
C	-3.52108800	2.81848400	0.14322100
H	-1.92872900	2.32710500	-1.19305000
C	-2.90926000	3.25327100	2.44870700
H	-0.82463900	3.10970500	2.92927600
C	-3.87397700	3.14359000	1.44919500
H	-4.26657400	2.72730200	-0.64110400
H	-3.20096700	3.51679400	3.46221600
Cl	3.44774300	0.25622500	0.21240600
C	1.84542200	5.24410400	-4.73045800
C	-5.30193900	3.40764400	1.82591800
C	4.23061900	4.14037400	4.81186600
F	2.28256800	6.47586200	-4.44159700
F	2.77808000	4.64742300	-5.47339500
F	0.75229300	5.38898400	-5.48824200
F	-5.66726400	2.65725600	2.87257300
F	-6.14918700	3.15432200	0.82857000
F	-5.47272600	4.68534200	2.18899100
F	5.09970600	3.16708900	5.10946200
F	3.54264000	4.40059800	5.92976600
F	4.93277300	5.23084300	4.50308900
F	-4.88111400	-1.49698900	0.05636000
B	-2.51342600	1.62491000	-3.73920500
F	-2.60216500	2.26289400	-4.96755300
F	-2.66230000	0.24190400	-3.90116000
F	-1.24843300	1.87856600	-3.16825800
F	-3.50545900	2.10673700	-2.87566100

TS1'

C	-1.11349700	-1.35011500	0.23033500
C	-1.80981800	-1.40756500	-0.98429400
C	-1.70951900	-1.08766400	1.47163800
C	-3.14745500	-1.05986200	-0.96629700
C	-3.04923300	-0.74898100	1.46729800
C	-3.73468400	-0.72943700	0.25340600
H	-3.74270800	-1.04758100	-1.87362100
H	-3.57474600	-0.49350500	2.38222400
H	-1.13284700	-1.12398600	2.39246500
H	-1.30806300	-1.70209200	-1.90227500
N	0.07524100	-2.57809500	0.27903700
N	0.23664000	-3.67056700	0.49029300
Au	0.93322300	-0.49982400	-0.01587900
P	0.65784400	1.90659700	0.25298800
C	1.10143400	2.88876200	-1.20422600

C	0.54720100	4.16000600	-1.40199500
C	2.04215500	2.38123900	-2.10214200
C	0.93437200	4.91304500	-2.49933200
H	-0.18148800	4.56110600	-0.70055200
C	2.42675500	3.13994900	-3.20257000
H	2.48098400	1.39667400	-1.94302900
C	1.86970500	4.39776300	-3.39631700
H	0.50946200	5.90123500	-2.65931900
H	3.15460200	2.74856500	-3.90634500
C	1.71786000	2.44346800	1.62647300
C	1.78890900	1.64333100	2.77493200
C	2.47143600	3.61444700	1.54130400
C	2.59913500	2.02429600	3.83205600
H	1.20988500	0.72253900	2.84729300
C	3.29050200	3.99010400	2.60092300
H	2.43015600	4.23752000	0.65124300
C	3.35015400	3.19572700	3.73860200
H	2.65519100	1.41081300	4.72762200
H	3.87939800	4.89977400	2.53598800
C	-1.06348500	2.29978500	0.66784100
C	-2.01856800	2.19664200	-0.34919700
C	-1.46389100	2.55480800	1.98307100
C	-3.36673000	2.34023000	-0.05347400
H	-1.71802200	1.98038900	-1.37389500
C	-2.81405400	2.68396800	2.27816800
H	-0.72767000	2.64351400	2.77851400
C	-3.75953300	2.56301200	1.26326800
H	-4.11391400	2.24697100	-0.83711100
H	-3.13485600	2.86569500	3.30096000
Cl	3.33573700	-0.75550500	-0.34353800
C	2.24394900	5.24329400	-4.57744000
C	-5.20857200	2.56787900	1.64571900
C	4.25236600	3.54341800	4.88484500
F	2.71365400	6.43403300	-4.18528700
F	3.17624400	4.67328100	-5.34236600
F	1.17785300	5.48527800	-5.35166000
F	-5.50979900	1.45237100	2.33243600
F	-6.01772800	2.61354300	0.58718100
F	-5.50782200	3.60089400	2.43934100
F	5.26842800	2.67487500	4.97141600
F	3.59760300	3.48783600	6.05134600
F	4.77626000	4.76510400	4.77196300
F	-5.00804100	-0.37503400	0.26142900

LAu^{II}Cl

Au	0.25934400	-0.34548900	1.58859400
P	1.15448200	1.75394400	2.25588300
C	0.17770300	3.17589700	1.67173800
C	0.00075300	4.32138500	2.45543500
C	-0.37688000	3.11233700	0.39145900
C	-0.72616600	5.39180900	1.95558800
H	0.42764300	4.37930600	3.45450700
C	-1.10068300	4.18733900	-0.11072800
H	-0.24731100	2.21681300	-0.21531700
C	-1.27457500	5.32030000	0.67592300
H	-0.86882600	6.28369200	2.56117900
H	-1.53326900	4.13865700	-1.10524600
C	1.21373000	1.88818700	4.06845800
C	2.41981300	1.98359400	4.76345300
C	0.00965100	1.77133400	4.77065400
C	2.42152000	1.95424200	6.15343100
H	3.36250500	2.07180700	4.22768300
C	0.01087600	1.74699500	6.15637800
H	-0.93275500	1.67789600	4.23228300
C	1.21983400	1.83465000	6.84404100
H	3.36014000	2.02559700	6.69642500
H	-0.92424600	1.65128400	6.70066700
C	2.85774100	2.03151900	1.67842700
C	3.36377500	3.32362100	1.52395700
C	3.67775100	0.92376000	1.43797200
C	4.68321800	3.50990300	1.12886100
H	2.73422200	4.19056900	1.71317100
C	4.99615400	1.11037300	1.04921800
H	3.28163100	-0.08483600	1.55310200
C	5.49182800	2.40365400	0.89409900
H	5.08049300	4.51262700	1.00524600
H	5.63826600	0.25358600	0.85930500
C	1.14130900	-1.36735500	4.46440500
C	0.03462800	-1.23846700	3.63810600
C	-1.25540100	-1.46580800	4.09381700
C	-1.45013800	-1.80659100	5.43370500
C	-0.34160700	-1.91252800	6.25991900
C	0.95251600	-1.71077100	5.80307100
H	2.15028400	-1.18669100	4.09374000
H	-2.11448900	-1.37244600	3.43105100
H	-2.44235200	-1.98544200	5.83969600
H	1.78868000	-1.81279500	6.48989200
Cl	-0.64522500	-2.14655700	0.23202900

F	-0.52762000	-2.23271700	7.54887400
C	1.24596600	1.71987900	8.33735600
C	6.91442400	2.56160300	0.44805900
C	-2.05874600	6.49925700	0.18337700
F	-2.52937400	6.32277200	-1.05259500
F	-1.30772700	7.60837600	0.17547800
F	-3.10538300	6.75160400	0.98077500
F	7.29660800	3.83942700	0.39796900
F	7.75405300	1.92045200	1.27188000
F	7.09777500	2.03733900	-0.77080900
F	1.51588100	0.46273300	8.71969700
F	2.18883400	2.49913700	8.87963100
F	0.07727700	2.05663100	8.89142900

¹⁴

C	-2.55728400	0.83855800	-0.48119800
C	-1.25278000	0.64997400	-0.88574500
C	-0.37744600	1.74278500	-0.77094200
C	-0.75303800	3.00302700	-0.27368000
C	-2.05727700	3.16186900	0.13665000
C	-2.92927100	2.07662900	0.03725800
H	-3.28880000	0.03966500	-0.53869000
H	-0.88793900	-0.29532800	-1.27864900
H	-0.03217600	3.81110200	-0.20945900
H	-2.41456900	4.10114600	0.54530900
N	0.92752300	1.57686100	-1.14915500
N	1.99277800	1.47223500	-1.45232500
B	2.17413200	-1.79543600	-1.78868200
F	0.94515500	-1.12317900	-1.87780200
F	1.97806400	-3.00408900	-1.09314700
F	3.04858900	-0.99560800	-1.01587600
F	2.70133900	-2.02615000	-3.03160400
F	-4.16996800	2.23440800	0.45564700
C	-3.09176000	0.78447800	3.22129900
C	-3.15310200	-0.54606100	2.79567200
C	-2.02258300	-1.14757900	2.25991300
C	-0.81429600	-0.44832000	2.13100900
C	-0.75992700	0.86637100	2.61301800
C	-1.88277900	1.48160000	3.14693100
H	-4.09021400	-1.09146800	2.86434100
H	-2.07976400	-2.17242500	1.89785200
H	0.17219800	1.42366100	2.53023400
H	-1.85259700	2.51323300	3.49020000
B	0.38819400	-1.07144100	1.33074200

O	0.27015900	-2.35907700	0.92041900
H	0.94222100	-2.65487200	0.28098900
O	1.42977400	-0.23901200	1.03636300
H	2.12537000	-0.63004000	0.48062900
C	-4.28273400	1.51946300	3.71046500
O	-5.37330000	0.74591600	3.77654900
O	-4.28498000	2.69714200	4.00856000
C	-6.56162600	1.40008700	4.21952700
H	-6.82599000	2.21765600	3.54248400
H	-7.34328400	0.64069800	4.21890600
H	-6.42582500	1.80493300	5.22648600
¹¹			
C	-2.35278100	0.37689000	-5.11360200
C	-1.36199800	1.31386800	-4.92278100
C	-0.25308300	0.94095400	-4.14276800
C	-0.09093000	-0.32866200	-3.56592000
C	-1.09193100	-1.25344600	-3.77825800
C	-2.20508000	-0.88190200	-4.53009500
H	-3.24193700	0.60624900	-5.69203700
H	-1.43639200	2.31033200	-5.34661000
H	0.77873800	-0.56758200	-2.95957600
H	-1.02784100	-2.25292000	-3.35787600
N	0.72018700	1.87649400	-3.93120800
N	1.50733500	2.64415400	-3.76164000
Cl	0.95232400	-2.35826800	-0.80817500
B	0.82372700	1.91038500	0.02442700
F	1.17059000	0.80694300	0.80590200
F	1.80245200	2.88548400	0.09436200
F	-0.40643600	2.41870600	0.46570700
F	0.67133600	1.49493700	-1.32063000
P	-2.94706300	0.17918800	-0.12719700
Au	-0.92900400	-0.91587300	-0.39898000
C	-3.39276300	1.29718700	-1.50388000
C	-2.52773400	2.35843200	-1.80401800
C	-4.55376600	1.10734200	-2.25622200
C	-2.84020100	3.22839600	-2.83830000
H	-1.61362900	2.49509200	-1.22850100
C	-4.85620400	1.97460600	-3.30181200
H	-5.23132600	0.28584800	-2.03642000
C	-4.00206700	3.03291200	-3.58504600
H	-2.17446700	4.05674500	-3.07241500
H	-5.75551100	1.82649100	-3.89306000
C	-3.10717600	1.16795800	1.39228400

C	-2.43792900	0.72320700	2.53677800
C	-3.89957400	2.31423000	1.44766400
C	-2.56807300	1.41698400	3.72884800
H	-1.80655400	-0.16329200	2.48853600
C	-4.02621900	3.01456400	2.64324300
H	-4.42353800	2.66726100	0.56144200
C	-3.36092900	2.56382500	3.77665100
H	-2.04687400	1.07609900	4.62045800
H	-4.64075300	3.90838400	2.68658000
C	-4.31746100	-1.02619900	-0.05200000
C	-4.20400100	-2.21600500	-0.78030800
C	-5.48246200	-0.76402300	0.67074300
C	-5.24467200	-3.13216400	-0.78363800
H	-3.29428200	-2.42715200	-1.34185000
C	-6.52377700	-1.68556100	0.67423400
H	-5.58289100	0.15953400	1.23698100
C	-6.40019000	-2.86446300	-0.05118100
H	-5.15777900	-4.05826700	-1.34708800
H	-7.42797200	-1.48596100	1.24114400
C	-7.48862700	-3.89443000	-0.04876400
C	-4.25136900	3.90320300	-4.77674000
C	-3.47637500	3.28206100	5.08636500
F	-4.22653000	4.38317600	5.00508200
F	-4.02138600	2.49198200	6.02236800
F	-2.27346200	3.64786300	5.54930000
F	-3.52034500	3.47629800	-5.82939000
F	-5.52751300	3.89238000	-5.16290300
F	-3.89912400	5.17205500	-4.55817700
F	-7.07031300	-5.03595500	0.51445500
F	-8.57301300	-3.49188000	0.61770700
F	-7.87144800	-4.20034400	-1.29559700
F	-3.17072800	-1.76240200	-4.69311000

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C	-2.74439000	0.28793900	-0.36729200
C	-1.37024800	0.23903800	-0.46253500
C	-0.65104000	1.32059100	0.07325200
C	-1.24776400	2.43007700	0.69984800
C	-2.62091000	2.45353300	0.78278700
C	-3.34192700	1.38504000	0.24678200
H	-3.36443000	-0.50349900	-0.77378700
H	-0.85466700	-0.59087700	-0.93577800
H	-0.63786100	3.23506300	1.09552900
H	-3.14742800	3.27789100	1.25094300

N	0.71578500	1.31321100	-0.01568200
N	1.82527100	1.32178700	-0.08172800
B	1.11488600	-0.86041700	-2.46831000
F	0.95105900	0.52517200	-2.63562100
F	-0.08761800	-1.47626600	-2.87288000
F	1.29709300	-1.11709200	-1.10016500
F	2.17753800	-1.32638300	-3.20620300
F	-4.65656500	1.42027900	0.32720700
C	-1.52876300	1.98947800	-3.44654900
H	-2.31923300	2.58636100	-3.91471400
H	-0.58181700	2.21502900	-3.95529300
H	-1.43113700	2.33701300	-2.40199400
O	-1.88817600	0.63732700	-3.53984300
H	-1.10436300	0.10032700	-3.35076000

2-Au^I

C	-2.91946400	0.01588500	3.57948300
C	-1.73236500	0.12795000	4.30725400
C	-1.02802100	1.32541200	4.29493800
C	-1.46699900	2.42191400	3.53860400
C	-2.64884400	2.28108300	2.79699700
C	-3.37735000	1.09966300	2.82559200
H	-1.37126500	-0.71640300	4.88921100
H	-0.11474200	1.41088300	4.88067900
H	-2.99997200	3.11588200	2.19208300
H	-4.30403900	0.99261400	2.26598100
B	-0.64376300	3.75794900	3.51827700
O	0.47124300	3.82713800	4.29787500
H	0.95661500	4.65680900	4.25396100
O	-1.08452900	4.75541300	2.69576700
H	-0.56330900	5.56419700	2.71437200
C	-3.73964700	-1.21885500	3.59412500
O	-3.13416800	-2.23037800	4.23024900
O	-4.84092500	-1.31682200	3.09129400
C	-3.88753700	-3.44020800	4.30825500
H	-4.17104100	-3.78414900	3.30898300
H	-3.23999100	-4.16954600	4.79433500
H	-4.79701500	-3.28781800	4.89671900
P	0.68584500	0.16480500	0.40298500
Au	1.52396500	0.33741100	2.55135600
C	-0.99587600	-0.53690700	0.33943600
C	-2.04067900	0.08982200	-0.34065800
C	-1.20972900	-1.77066700	0.96248700
C	-3.28416500	-0.52476200	-0.41536100

H	-1.89103900	1.05399400	-0.82105700
C	-2.44726000	-2.39410200	0.87000600
H	-0.40045000	-2.25598900	1.50814200
C	-3.48292400	-1.76554400	0.18276600
H	-4.10027600	-0.03938200	-0.94490500
H	-2.60332700	-3.36492400	1.33378000
C	0.58783700	1.73963800	-0.50576000
C	1.02088600	1.87233800	-1.82389200
C	0.00948100	2.82976100	0.15330300
C	0.87077200	3.08986500	-2.48268800
H	1.47610700	1.03393600	-2.34562200
C	-0.15468000	4.03638700	-0.50548800
H	-0.33069600	2.72173800	1.18142900
C	0.28012600	4.16148800	-1.82520400
H	1.20986800	3.19807900	-3.50835500
H	-0.61892100	4.87505600	0.00887600
C	1.69467300	-0.93836700	-0.63841500
C	1.13338900	-1.64049300	-1.71133600
C	3.06411700	-1.02888900	-0.38518000
C	1.94172300	-2.42386400	-2.52129500
H	0.06639500	-1.57363500	-1.91625800
C	3.87494300	-1.81161300	-1.19899300
H	3.50029200	-0.48956200	0.45459600
C	3.30953300	-2.50615900	-2.26139100
H	1.51030200	-2.97231900	-3.35552400
H	4.94007400	-1.88393100	-1.00233400
C	-4.81364500	-2.42892000	-0.00681600
C	4.14786600	-3.36477300	-3.15957400
C	0.08945000	5.48403600	-2.50311100
F	-4.93302000	-2.89193100	-1.26158600
F	-4.99676300	-3.46873500	0.81180400
F	-5.82449000	-1.57490400	0.18136400
F	0.52769700	5.48413700	-3.76378300
F	0.73511100	6.46037600	-1.85070600
F	-1.20454900	5.83121300	-2.52667100
F	5.43249200	-3.38242000	-2.79842600
F	4.09155500	-2.93629800	-4.42755400
F	3.71321200	-4.63157000	-3.16343900
Cl	2.55012700	0.36498900	4.70694200

2-MeOH

C	-2.19349600	0.42948600	0.22053200
C	-1.55558000	0.68565200	1.43707800
C	-0.78779200	1.83297900	1.58033800

C	-0.63376800	2.74596300	0.52761500
C	-1.28011200	2.47020300	-0.68642400
C	-2.05021200	1.32595700	-0.83999300
H	-1.66681300	-0.01479800	2.26014000
H	-0.29361200	2.03117900	2.52939200
H	-1.17103100	3.15413900	-1.52771800
H	-2.55257700	1.10786100	-1.77922400
B	0.22986200	4.03677100	0.73255600
O	0.79460900	4.23366400	1.95365000
H	1.31500400	5.03673400	2.05245100
O	0.37014700	4.90520000	-0.32121000
H	0.90040400	5.68727900	-0.13512700
C	-3.02949700	-0.77637800	0.00448200
O	-3.09791400	-1.55204600	1.09374700
O	-3.59482300	-1.04268300	-1.03708400
C	-3.89266400	-2.72955600	0.96002100
H	-3.49067500	-3.37971000	0.17762000
H	-3.85255200	-3.23234500	1.92614400
H	-4.92547100	-2.47088700	0.70934300
C	1.11809400	3.48696700	-3.14766500
H	1.15979000	3.06875000	-4.15854900
H	2.09223500	3.95304200	-2.93460900
H	0.98222500	2.65002600	-2.44280400
O	0.05548200	4.40780500	-3.09860300
H	0.05416900	4.76986200	-2.19858500

MeOH-Au^I

P	0.18093200	0.24438100	0.45098300
Au	0.26148000	0.40937600	2.75250100
C	-1.23500700	-0.75905800	-0.10855800
C	-2.18225400	-0.28561100	-1.01827600
C	-1.35185000	-2.04578200	0.42560100
C	-3.24531300	-1.10000900	-1.38784500
H	-2.09778700	0.71382600	-1.43938500
C	-2.41229700	-2.85950800	0.05000300
H	-0.60165400	-2.40390500	1.13242000
C	-3.35680400	-2.38124200	-0.85348700
H	-3.98871800	-0.73800000	-2.09448600
H	-2.50523900	-3.86001100	0.46235400
C	0.01324700	1.84738500	-0.39793300
C	0.51971400	2.05355200	-1.68193800
C	-0.68155800	2.87276900	0.25235200
C	0.33810600	3.27949500	-2.31289300
H	1.06078700	1.26223300	-2.19640200

C	-0.86930900	4.09258700	-0.37932200
H	-1.07240300	2.71375600	1.25665800
C	-0.35415900	4.29200300	-1.65936400
H	0.73707000	3.44267800	-3.30921200
H	-1.40793800	4.89285600	0.12266200
C	1.64972100	-0.55844200	-0.26980800
C	1.56548600	-1.32248700	-1.43912200
C	2.88420800	-0.37491300	0.35546500
C	2.71115700	-1.88991800	-1.97742200
H	0.60685000	-1.47623000	-1.93121000
C	4.03258800	-0.94109000	-0.18547600
H	2.94921300	0.20922300	1.27243000
C	3.93981700	-1.69694000	-1.34821000
H	2.65183800	-2.48555300	-2.88550000
H	4.99364800	-0.80014000	0.29932700
C	-4.52089900	-3.22141700	-1.28166000
C	5.15025500	-2.33503500	-1.95906000
C	-0.55902200	5.63476900	-2.29279400
F	-4.53186400	-3.39007100	-2.61157500
F	-4.51264500	-4.43400900	-0.72305200
F	-5.68464200	-2.63904100	-0.96148000
F	-0.08209000	5.69618600	-3.53764800
F	0.04218800	6.59879700	-1.58206900
F	-1.85989900	5.95170900	-2.34246000
F	6.26616100	-2.07900600	-1.27300000
F	5.34088700	-1.90847400	-3.21467100
F	5.01328400	-3.66628900	-2.02471500
Cl	0.30467100	0.56985300	5.12847100
C	0.03710800	-3.15338300	3.66978300
H	-0.42035900	-2.28655600	4.16002400
H	0.51612600	-3.77066000	4.44096900
H	-0.76157400	-3.74350800	3.19509100
O	0.96659900	-2.65165700	2.72966600
H	1.42241200	-3.39658800	2.32235700

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C	-2.61855600	0.46923300	-0.53700900
C	-1.28459100	0.54173400	-0.96148400
C	-0.52670600	1.71690700	-0.67702800
C	-1.11945400	2.78175000	0.05490500
C	-2.45027300	2.66461600	0.47788100
C	-3.19076100	1.53461300	0.14402300
H	-3.21596700	-0.40930500	-0.76569100
H	-0.81242700	-0.28344600	-1.48710200

H	-0.53903400	3.66549600	0.30013700
H	-2.92344900	3.46909400	1.03613700
N	0.73899400	1.80602200	-1.07984600
N	1.85433400	1.84443100	-1.36856300
B	2.35341800	-1.83917100	-1.77521600
F	1.15795900	-1.15514200	-1.99517700
F	2.06028500	-3.02432500	-1.05627600
F	3.18563300	-1.04751900	-0.95372700
F	2.98683000	-2.14142600	-2.95394800
F	-4.45615800	1.44436300	0.56781500
C	-2.99914500	0.93154300	3.18074600
C	-3.13428900	-0.34822800	2.69282400
C	-2.02430000	-0.96719800	2.07748900
C	-0.75285800	-0.34306900	2.00221000
C	-0.62577300	0.92188700	2.55180600
C	-1.73844800	1.57908500	3.10008100
H	-4.09376300	-0.85460200	2.72879900
H	-2.13818200	-1.95979900	1.64476400
H	0.33402400	1.43240200	2.51316000
H	-1.65334300	2.58871300	3.49722600
B	0.42551600	-1.02712700	1.19191300
O	0.14571900	-2.23396900	0.65101300
H	0.83093800	-2.59104800	0.05374300
O	1.56335800	-0.30401800	1.07962800
H	2.23233700	-0.64259300	0.45630100
C	-4.15288400	1.73154500	3.67166000
O	-5.24786400	0.99590200	3.82443900
O	-4.08815900	2.92601300	3.87300300
C	-6.41804000	1.70828300	4.24088500
H	-6.67803600	2.47129100	3.50241300
H	-7.20969900	0.96430600	4.31750100
H	-6.24699800	2.18616600	5.20906000

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C	-2.06238400	0.36961400	-1.36287200
C	-0.72613600	0.73442500	-1.30648700
C	-0.38800200	1.97204900	-0.75813900
C	-1.35685700	2.84761200	-0.27938900
C	-2.69613800	2.48620600	-0.33402300
C	-3.01903200	1.24869300	-0.87122100
H	-2.37230000	-0.59580200	-1.75334700
H	0.05491400	0.05856300	-1.65208600
H	-1.04628900	3.80168300	0.13914200
H	-3.48384400	3.13630200	0.03444300

N	0.98670800	2.40496500	-0.63639500
N	1.92783800	1.74033800	-0.91427300
B	2.56336300	-2.01069300	-1.62557500
F	1.62484600	-1.23684900	-2.30078600
F	1.88386200	-3.04199900	-0.93240600
F	3.21223800	-1.21408500	-0.65960100
F	3.48274300	-2.55367400	-2.49300000
F	-4.30350800	0.88394500	-0.91279000
C	-3.08191000	0.99113700	3.45854800
C	-3.34882100	-0.18581000	2.75177300
C	-2.33616800	-0.79417200	2.02284800
C	-1.04419400	-0.25450900	1.97172000
C	-0.79843900	0.92572400	2.68613900
C	-1.79891300	1.54357000	3.42233600
H	-4.34665600	-0.61525900	2.77841800
H	-2.54670600	-1.70539200	1.46463800
H	0.19648800	1.36732100	2.64958900
H	-1.60982100	2.46100300	3.97497400
B	0.07741700	-0.91659000	1.08389200
O	-0.26801500	-2.00736500	0.34649800
H	0.46725800	-2.39367700	-0.16228000
O	1.31011800	-0.34362600	1.11619900
H	1.96962200	-0.68398800	0.48557100
C	-4.11731700	1.69075900	4.25248700
O	-5.31233500	1.08543500	4.18861100
O	-3.92559500	2.70375000	4.89626500
C	-6.35679800	1.71369500	4.92856400
H	-6.50640100	2.74239100	4.58805900
H	-7.25404700	1.12175500	4.74774700
H	-6.12059900	1.72596500	5.99670600

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C	-1.19923800	0.30598300	0.22495200
C	0.07856700	0.46154600	0.73856300
C	0.30898700	1.45716000	1.68867500
C	-0.70847400	2.29683500	2.13121700
C	-1.98952900	2.14630500	1.61850600
C	-2.20512600	1.15164100	0.67515400
H	-1.40124000	-0.46676800	-0.51047700
H	0.89141700	-0.18123900	0.40180500
H	-0.48309600	3.05880400	2.87281300
H	-2.81400800	2.77856800	1.93376400
N	1.61836100	1.67280500	2.26691800
N	2.58697500	1.04437900	2.00125300

B	0.90552300	-1.79390400	-1.76548000
F	0.54569300	-0.59046000	-2.37138500
F	-0.18706100	-2.29178100	-1.04068900
F	1.97207000	-1.56593000	-0.87933600
F	1.28915700	-2.72132000	-2.73055100
F	-3.43631900	1.00088200	0.17766900

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Au	0.30658400	-0.20701600	1.75775900
P	1.24077100	1.84858300	2.44823700
C	0.19387600	3.18057500	1.83733400
C	-0.19080500	4.23060300	2.68041500
C	-0.19769100	3.15997600	0.49327500
C	-0.97066900	5.25662000	2.17062500
H	0.12069400	4.25472900	3.72127100
C	-0.97291900	4.19529700	-0.00965100
H	0.09492200	2.33307000	-0.15451500
C	-1.35894500	5.23327600	0.83252500
H	-1.27542300	6.07882600	2.81314700
H	-1.28388700	4.19057100	-1.04944400
C	1.28513900	1.86310700	4.24795300
C	2.48950100	2.03388200	4.94242000
C	0.07912900	1.68699900	4.94277200
C	2.47729400	2.04671600	6.32771400
H	3.42648900	2.17244900	4.40970700
C	0.07581400	1.70717600	6.32925000
H	-0.85606400	1.54086700	4.40388700
C	1.27408800	1.88589700	7.01357700
H	3.40428400	2.19023300	6.87717900
H	-0.85358100	1.58036200	6.87484600
C	2.89877900	1.99253700	1.76544900
C	3.27312300	3.13058200	1.04814800
C	3.80597200	0.94159800	1.96620400
C	4.56360900	3.22420000	0.53927500
H	2.57121300	3.94472000	0.88784700
C	5.09074700	1.04580900	1.46360500
H	3.50762700	0.04824000	2.51238300
C	5.46203300	2.18613800	0.74928000
H	4.86500200	4.10461400	-0.01917600
H	5.80395300	0.23991200	1.61641700
Cl	0.74263500	-0.36947100	-0.61494000
C	1.31590900	1.91197900	8.51448000
C	6.86477700	2.25470900	0.21800100
C	-2.22918700	6.35242700	0.33794000

F	-2.47824700	6.26700700	-0.96894500
F	-1.66045000	7.54077400	0.56858300
F	-3.40506000	6.35433200	0.97800200
F	7.08781700	3.36194300	-0.49041700
F	7.75543500	2.22310100	1.21644700
F	7.12747800	1.20639500	-0.57084800
F	2.08531200	0.92459300	8.98663500
F	1.84313600	3.06031400	8.95383600
F	0.10728500	1.78328900	9.06091100

TS2

C	-1.86337900	0.59307700	-0.92353000
C	-0.58317600	0.77525300	-0.39872100
C	-0.43452900	1.77884300	0.52755000
C	-1.42274900	2.61772700	0.98357600
C	-2.70011600	2.43077600	0.45382200
C	-2.88527800	1.42360700	-0.48513600
H	-2.04580700	-0.18776900	-1.65623900
H	0.24555500	0.14435800	-0.72362600
H	-1.22078800	3.39057000	1.72183100
H	-3.54408600	3.04614800	0.75416100
N	1.31753100	2.06355300	1.27186900
N	2.15226200	1.38854300	0.91113800
B	0.33447700	-1.51976900	-2.82117900
F	-0.01633100	-0.32178000	-3.44298300
F	-0.77321100	-2.01945100	-2.12187900
F	1.37782600	-1.27981900	-1.91029300
F	0.74762700	-2.45002200	-3.77114300
F	-4.11431400	1.24685600	-0.99180900

Ar^{1•}

C	-1.39990700	0.33335400	0.14774800
C	-0.13446600	0.52818000	0.70848200
C	-0.01310000	1.51954500	1.65397900
C	-1.03077800	2.33368300	2.09330200
C	-2.29419400	2.13472100	1.52947300
C	-2.44582600	1.14100500	0.57224700
H	-1.58166200	-0.42838500	-0.60599900
H	0.70600400	-0.08784700	0.39726100
H	-0.87981700	3.10412400	2.84587400
H	-3.15288700	2.73434500	1.82037800
F	-3.65893700	0.95252300	0.03308100

Au	0.91227900	-0.37956300	1.46812800
P	1.50803000	1.72990900	2.41318300
C	0.37642200	2.95041700	1.70738100
C	0.36602600	4.24416800	2.25081700
C	-0.47424300	2.61994500	0.65141800
C	-0.48961200	5.19825600	1.72524500
H	1.01921300	4.50591200	3.08066400
C	-1.33893000	3.57939700	0.13708800
H	-0.47636700	1.62410200	0.21212300
C	-1.34180500	4.85965200	0.67423500
H	-0.50117100	6.20425500	2.13709500
H	-2.00862800	3.32216900	-0.67790800
C	1.40972500	1.88460500	4.21304200
C	2.55286000	1.78260400	5.01177400
C	0.15119600	2.05566600	4.80012100
C	2.42990100	1.83723800	6.39281200
H	3.53847500	1.67220800	4.56906300
C	0.03340300	2.10697200	6.18074500
H	-0.74157600	2.14137000	4.18464100
C	1.17324600	1.99173700	6.97070500
H	3.31383500	1.76447200	7.02119100
H	-0.94242700	2.23413800	6.63929000
C	3.21238900	2.03343800	1.89846100
C	3.54562500	3.18916600	1.19493500
C	4.18267500	1.06129400	2.17696100
C	4.85952500	3.38386000	0.78127400
H	2.79205200	3.93515800	0.95578500
C	5.48905700	1.26398400	1.76858500
H	3.91726100	0.13847600	2.69239700
C	5.82090900	2.42432900	1.06795400
H	5.12753900	4.27835900	0.22830200
H	6.24884600	0.51517400	1.97785000
C	0.81776100	-1.42247800	4.24230300
C	0.03955600	-0.79993800	3.27213500
C	-1.31056400	-0.53882100	3.47132100
C	-1.92000700	-0.97801800	4.64643300
C	-1.14701000	-1.64008100	5.58739300
C	0.21415400	-1.85582400	5.41858400
H	1.88196700	-1.59337800	4.08505000
H	-1.90011700	-0.01536300	2.71986000
H	-2.97739400	-0.81415200	4.83312600
H	0.77925300	-2.36899800	6.19207800
Cl	2.02098200	0.21218800	-0.64102800
F	-1.72921200	-2.09298300	6.70092500

C	1.08626700	2.00677000	8.46869300
C	7.24695600	2.59942500	0.63541700
C	-2.25849200	5.92305200	0.14321900
F	-3.05369200	5.47311600	-0.82778000
F	-1.55889700	6.95309200	-0.34774900
F	-3.03835400	6.41162800	1.11472700
F	7.42933900	3.70519900	-0.08796800
F	8.06238000	2.66741900	1.69509600
F	7.65630500	1.55943800	-0.10059200
F	1.42989100	0.81614600	8.97602900
F	1.92697500	2.90698700	8.99104200
F	-0.14025000	2.29365500	8.90628400
C	-1.11554000	-3.50481000	2.10049400
C	0.12357000	-3.34647300	1.49488800
C	0.24887000	-2.51093600	0.36686200
C	-0.88526000	-1.84220600	-0.17353700
C	-2.11625000	-2.01773700	0.46503900
C	-2.23323300	-2.84999300	1.57064600
H	0.99976300	-3.84531600	1.90067800
H	1.17907100	-2.52187900	-0.20108000
H	-2.99617100	-1.50803000	0.07929800
H	-3.19264500	-2.98899700	2.06375800
B	-0.80638900	-0.98884700	-1.50580400
O	-0.16053800	-1.55651800	-2.55252200
H	-0.11659800	-1.02320400	-3.35291300
O	-1.47858100	0.19516900	-1.49800200
H	-1.46087700	0.68395700	-2.32803200
C	-1.30055300	-4.27017700	3.36172900
O	-0.15619100	-4.77997700	3.81981800
O	-2.36780200	-4.38805400	3.92587300
C	-0.25214200	-5.45679700	5.07570600
H	-0.89443800	-6.33723900	4.98897600
H	0.76374100	-5.75023700	5.33820100
H	-0.66642700	-4.78512400	5.83426500

³¹

C	-2.62791200	-0.00081000	0.10978400
C	-1.28921000	-0.19004900	0.27740500
C	-0.41852500	0.93146400	0.15389000
C	-0.89891400	2.25138900	-0.09852000
C	-2.23734500	2.44071800	-0.25801200
C	-3.08402300	1.31022100	-0.16022600
H	-3.35120900	-0.80580000	0.18099800
H	-0.85408900	-1.16250000	0.47766400

H	-0.18551900	3.06684100	-0.16986700
H	-2.67646500	3.41174200	-0.46065200
N	0.96406600	0.70860800	0.42484800
N	1.81852600	1.36978300	-0.07032400
B	0.57063400	-0.38958000	-2.59474500
F	-0.35892500	0.64317200	-2.28783000
F	0.24013600	-0.93962600	-3.82051200
F	0.48443500	-1.35526000	-1.58538600
F	1.84767300	0.15580800	-2.61841700
F	-4.35965000	1.49172700	-0.31961800

³TS3

C	-1.77447200	0.53882400	-0.96436800
C	-0.53064600	0.74320300	-0.43045400
C	-0.41114000	1.77431000	0.51725700
C	-1.44159000	2.62199700	0.96995900
C	-2.68410200	2.42432800	0.43972300
C	-2.83042000	1.38123500	-0.52149700
H	-1.95588800	-0.24348200	-1.69716000
H	0.32357200	0.13241700	-0.73494100
H	-1.23746200	3.39159000	1.70876800
H	-3.55352800	3.01483400	0.71060600
N	1.21627000	2.08482700	1.27434800
N	2.08705200	1.43251500	0.94959200
B	0.23881400	-1.48753600	-2.79508900
F	-0.13348400	-0.26210200	-3.35208500
F	-0.86698200	-2.01952900	-2.11060400
F	1.27521100	-1.26574400	-1.86724900
F	0.66054500	-2.36613200	-3.77813600
F	-4.00687800	1.19319400	-1.02480000

³TS4

C	-2.71446700	0.58225000	-0.35705100
C	-1.36561800	0.80158100	-0.55576200
C	-0.88013800	2.07251300	-0.24162500
C	-1.64434900	3.15648300	0.19501600
C	-2.98833100	2.93737700	0.38872300
C	-3.49032700	1.64177300	0.13912600
H	-3.19050000	-0.37248200	-0.56069300
H	-0.69393100	0.03818200	-0.95305700
H	-1.18179900	4.12130600	0.38499900
H	-3.66648700	3.70621100	0.74642100
N	0.92299500	2.40544500	-0.47705200
N	1.55015600	1.60700400	-0.98317400

B	2.08573700	-2.01786300	-1.84200600
F	0.85362600	-1.36613800	-1.79287600
F	1.98869300	-3.22895400	-1.11429400
F	3.05546700	-1.21876900	-1.19334600
F	2.46572000	-2.27070500	-3.13711000
F	-4.76715400	1.42778000	0.36912900
C	-2.69884200	0.93444000	3.02845200
C	-2.82037400	-0.44396300	2.71776800
C	-1.71218900	-1.16597900	2.29085800
C	-0.48273100	-0.53793400	2.10735900
C	-0.37087100	0.83695600	2.45935800
C	-1.46045300	1.55367900	2.94877200
H	-3.79491000	-0.91770400	2.80189100
H	-1.81835400	-2.21606100	2.03149500
H	0.59400900	1.32724500	2.33848200
H	-1.37363100	2.60443800	3.21258000
B	0.69704900	-1.26514400	1.34182000
O	0.49944700	-2.56436600	1.02439400
H	1.12259800	-2.91903600	0.36394400
O	1.75032900	-0.47809200	1.02172000
H	2.35095100	-0.81543700	0.33088700
C	-3.88103600	1.75881100	3.40228300
O	-4.98865400	1.02759300	3.50496900
O	-3.83877700	2.96138000	3.55317300
C	-6.18920900	1.76226600	3.76394100
H	-6.38967500	2.45287200	2.93934900
H	-6.98331600	1.02124800	3.84345800
H	-6.09721100	2.32820600	4.69434600
Ar¹⁺			
C	-1.83186300	0.56606000	-0.96047000
C	-0.60018500	0.80984100	-0.41609400
C	-0.52962800	1.85316500	0.52273000
C	-1.57878400	2.67463200	0.96810500
C	-2.81041300	2.43087800	0.42412700
C	-2.91771800	1.38068900	-0.53203800
H	-2.01569400	-0.20983900	-1.69692100
H	0.27581100	0.23115600	-0.69214900
H	-1.41901900	3.45664600	1.70379100
H	-3.70015600	2.99526200	0.68521500
F	-4.08098900	1.15377900	-1.04679200
D			
Au	0.28488700	-0.28291900	1.58283400

P	1.19051300	1.76956800	2.42167000
C	0.18338800	3.13712300	1.78631400
C	-0.33450900	4.12889500	2.62492600
C	-0.03955300	3.19325900	0.40567200
C	-1.08838200	5.15890700	2.08081400
H	-0.14808600	4.10803200	3.69509400
C	-0.79450500	4.22508300	-0.13311700
H	0.38292900	2.44152300	-0.25861100
C	-1.32178100	5.19874100	0.70857600
H	-1.49374300	5.93264900	2.72812100
H	-0.97343900	4.27096000	-1.20253500
C	1.27923400	1.87667800	4.22225300
C	2.51807800	1.91632600	4.86848200
C	0.09332900	1.85510700	4.96415100
C	2.56391900	1.94489800	6.25546400
H	3.44303600	1.92521900	4.29712300
C	0.14481600	1.88837800	6.34984400
H	-0.87463400	1.80917300	4.46798500
C	1.38091100	1.93135900	6.98849300
H	3.52300600	1.97778700	6.76612800
H	-0.77167300	1.87452400	6.93158500
C	2.85920600	1.97902000	1.74922800
C	3.34425300	3.27460600	1.54764400
C	3.67483000	0.86948700	1.49940400
C	4.64543900	3.46075700	1.09873300
H	2.71632700	4.14023000	1.74631500
C	4.97184000	1.06134100	1.04762000
H	3.30718700	-0.14336800	1.65256400
C	5.45011500	2.35499200	0.85014000
H	5.02957500	4.46392000	0.94397200
H	5.61120600	0.20564700	0.84594000
C	1.07083000	-1.44341800	4.20968600
C	-0.01702000	-1.00159500	3.48118100
C	-1.33197300	-1.04706000	3.90452000
C	-1.56765500	-1.54435000	5.18498400
C	-0.49280200	-1.97790100	5.94753700
C	0.81501200	-1.94139800	5.48672700
H	2.08874500	-1.41130200	3.83142100
H	-2.15618300	-0.71317600	3.28149000
H	-2.57601400	-1.60353200	5.58310300
H	1.62387300	-2.29858700	6.11677600
Cl	-0.63573300	-2.24566600	0.61107300
F	-0.72577800	-2.45282800	7.16957000
C	1.47894200	1.97200700	8.48546900

C	6.85594600	2.51410400	0.34780000
C	-2.16041100	6.31980600	0.16824000
F	-2.29929200	6.25877900	-1.15706100
F	-1.62408300	7.50893000	0.46675800
F	-3.38562700	6.30144000	0.70711300
F	7.22520300	3.79265700	0.26304500
F	7.72513800	1.89186400	1.15315200
F	6.99376200	1.96922500	-0.86648600
F	2.22193200	0.95854900	8.94628600
F	2.06876500	3.10149000	8.89522600
F	0.28524000	1.90145400	9.07596000

TS5

Au	0.76063700	-0.19683100	2.02559400
P	1.50950800	2.08060400	2.47701500
C	0.37591800	3.32476900	1.80156300
C	0.41602300	4.63632500	2.28626400
C	-0.51937500	2.97829100	0.78491700
C	-0.43310000	5.59774100	1.75342000
H	1.10523900	4.91107100	3.08238300
C	-1.36758900	3.94024300	0.25598400
H	-0.56131300	1.95923300	0.40552000
C	-1.32015200	5.24440600	0.74251800
H	-0.40441500	6.61685700	2.12603000
H	-2.06744800	3.67890700	-0.53371700
C	1.65513300	2.42691300	4.24908700
C	2.88943000	2.45511700	4.89603600
C	0.46699000	2.52435200	4.98590400
C	2.93894700	2.56006700	6.28377200
H	3.81530300	2.38649600	4.32947000
C	0.51948800	2.62539700	6.36395700
H	-0.49923200	2.50001800	4.48494300
C	1.75751900	2.62961900	7.00872400
H	3.89690000	2.57687700	6.79398700
H	-0.39795200	2.68463000	6.94498500
C	3.13782500	2.30293800	1.70525600
C	3.46459400	3.47839500	1.02897500
C	4.06953600	1.25894800	1.79482100
C	4.72263800	3.61886000	0.45260500
H	2.74350500	4.28747100	0.94203000
C	5.32468300	1.40591100	1.22747600
H	3.81709000	0.32751900	2.30208900
C	5.64512200	2.58586200	0.55624200
H	4.97968600	4.53080100	-0.07703900

H	6.05317100	0.60205400	1.29805800
C	1.34376900	-0.72601700	4.88907700
C	0.30366200	-0.51466600	3.99163700
C	-1.02551900	-0.50798000	4.39542700
C	-1.31941700	-0.66862600	5.74877500
C	-0.27566300	-0.84665000	6.64380200
C	1.04998200	-0.89158300	6.23985100
H	2.38153000	-0.74653000	4.56190500
H	-1.83216700	-0.37275300	3.67825900
H	-2.34394100	-0.65738100	6.10923600
H	1.83486500	-1.04229700	6.97568500
Cl	1.26458000	-0.23712500	-0.46072200
F	-0.55708700	-0.99312400	7.94176800
C	1.75969100	2.65447400	8.50664100
C	7.01675100	2.70550400	-0.03885500
C	-2.28369000	6.24329900	0.17335900
F	-2.02299000	7.48885600	0.57346400
F	-3.53953300	5.95496400	0.53878000
F	-2.25899000	6.23247700	-1.16405800
F	7.18077200	3.83973800	-0.72151600
F	7.95709600	2.66663200	0.91452200
F	7.27081500	1.68919600	-0.87244400
F	2.98414400	2.78919300	9.01848500
F	1.00835600	3.65670500	8.97964800
F	1.23923700	1.51976600	8.99644300
C	-1.86032700	-4.16726100	2.02756100
C	-0.59685900	-4.24869000	2.61951100
C	0.32170000	-3.23254700	2.40891000
C	0.01523900	-2.14381100	1.56768600
C	-1.27808900	-2.07143500	1.00271600
C	-2.20168600	-3.07769100	1.22047800
H	-0.34795900	-5.09805100	3.24827800
H	1.30592200	-3.28817600	2.86895400
H	-1.53954000	-1.23190100	0.35885800
H	-3.19316000	-3.04334400	0.77729200
B	1.42017500	-2.16481900	0.11499000
O	2.59030100	-2.36722700	0.79669300
H	3.20897100	-2.92667300	0.31446300
O	0.93216000	-2.90854800	-0.91733500
H	1.07235200	-3.85492100	-0.80100900
C	-2.89579800	-5.22160000	2.22892700
O	-2.46898500	-6.20555400	3.02036500
O	-4.00006700	-5.18367200	1.72981800
C	-3.41308200	-7.25124200	3.26459600

H	-3.69823400	-7.73415100	2.32598700
H	-2.91238700	-7.96148800	3.92144500
H	-4.30880400	-6.85067300	3.74705600

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Au	-0.83855900	-0.82469600	-0.15739300
P	0.29990500	1.39935500	-0.12476200
C	-0.59932000	2.81073000	-0.83164800
C	-0.40617300	4.10465100	-0.34087500
C	-1.46085400	2.59127700	-1.91174600
C	-1.06608900	5.17676800	-0.93028500
H	0.26180400	4.28006600	0.50027900
C	-2.11655200	3.66204400	-2.50037200
H	-1.62016200	1.58630500	-2.29810500
C	-1.91638000	4.94984300	-2.00640600
H	-0.91795100	6.18343700	-0.55170200
H	-2.78829800	3.49796900	-3.33944200
C	0.58615500	1.79542900	1.62851700
C	1.84968400	1.72088900	2.21170600
C	-0.54608700	1.99942800	2.42916700
C	1.98312000	1.81821000	3.59445100
H	2.73417800	1.56871000	1.59774600
C	-0.41159700	2.10239300	3.80223700
H	-1.53711400	2.05722000	1.98033800
C	0.85295100	1.99160600	4.38166000
H	2.96384800	1.74498000	4.05520600
H	-1.28818200	2.23789000	4.43181700
C	1.93091600	1.35279000	-0.93223400
C	2.39541500	2.40603800	-1.72008100
C	2.72570000	0.21285900	-0.74833800
C	3.65075200	2.32761500	-2.31558100
H	1.78253700	3.29036500	-1.87786100
C	3.98054200	0.14175800	-1.33116100
H	2.36909100	-0.61962400	-0.14182200
C	4.43694900	1.20053200	-2.11615200
H	4.01222100	3.14466400	-2.93254100
H	4.60371600	-0.73738900	-1.18669900
C	-0.05453500	-1.46129300	2.62559700
C	-1.16101000	-1.14025700	1.85271800
C	-2.40653200	-0.85157600	2.38803100
C	-2.53545100	-0.82832100	3.77508200
C	-1.42668900	-1.11471800	4.55718700
C	-0.19150700	-1.43284900	4.01171200
H	0.90741500	-1.69842900	2.17663700

H	-3.26324600	-0.62699800	1.75885500
H	-3.48491000	-0.59393700	4.24723000
H	0.64691400	-1.65181400	4.66652400
F	-1.55070900	-1.08539800	5.88480600
C	0.93642100	1.96927700	5.87579200
C	5.80478600	1.08512000	-2.71821300
C	-2.63988800	6.07700900	-2.68053300
F	-2.39698200	7.25782100	-2.10970500
F	-3.96454400	5.88109300	-2.66046400
F	-2.28568200	6.16969300	-3.96936900
F	6.09580500	2.10430200	-3.52867800
F	6.74582500	1.04514400	-1.76494000
F	5.92827900	-0.04456400	-3.42705800
F	2.18766600	2.08819500	6.32461800
F	0.21168300	2.95122300	6.42555100
F	0.44581100	0.81473400	6.35533100
C	-2.63134300	-5.26597700	-0.57558400
C	-1.27550400	-5.08299500	-0.29503100
C	-0.78043700	-3.80308900	-0.07195200
C	-1.64115100	-2.70983900	-0.15957200
C	-3.00171000	-2.88395900	-0.40893300
C	-3.48952000	-4.16561800	-0.63100800
H	-0.61296200	-5.94214900	-0.24353600
H	0.27396500	-3.66490700	0.16097000
H	-3.67892000	-2.03286000	-0.44607400
H	-4.54236600	-4.33261900	-0.84414000
C	-3.21798300	-6.60990300	-0.80813700
O	-2.30981600	-7.58651800	-0.71447400
O	-4.38988200	-6.80772400	-1.05519500
C	-2.80980800	-8.90845700	-0.91960400
H	-3.24544100	-9.00396900	-1.91819300
H	-1.95438700	-9.57500000	-0.81402700
H	-3.57365400	-9.14835700	-0.17462200
10			
Au	-0.18514300	-0.93410400	-1.19514500
P	0.46605100	1.19615600	-0.32946600
C	-0.37647300	2.47557900	-1.29154900
C	-0.45279400	3.77804300	-0.78575200
C	-0.87155100	2.18391200	-2.56673100
C	-1.03797300	4.78100900	-1.54775600
H	-0.05462700	4.01588800	0.19842100
C	-1.45647800	3.18855300	-3.32314100
H	-0.79405100	1.17727600	-2.97536700

C	-1.53965500	4.48011800	-2.80921000
H	-1.10074500	5.79234500	-1.15901500
H	-1.84603200	2.97042500	-4.31403000
C	0.04591700	1.41083100	1.41657200
C	0.88416800	0.90127200	2.41030500
C	-1.21235300	1.93124400	1.75396000
C	0.45490400	0.88497200	3.73258200
H	1.85505500	0.47451300	2.17864700
C	-1.62637700	1.92818900	3.07387900
H	-1.88745300	2.30976200	0.99028800
C	-0.79749000	1.38777100	4.05684500
H	1.09611700	0.46010000	4.49873000
H	-2.60471900	2.32096500	3.33959800
C	2.25414700	1.39581600	-0.58558000
C	2.69941100	2.46910900	-1.36662000
C	3.17175300	0.47907000	-0.05944700
C	4.05602800	2.63376400	-1.60120600
H	1.99908900	3.17736000	-1.79992500
C	4.52894500	0.65849400	-0.29180900
H	2.84216800	-0.39003200	0.50366900
C	4.96669400	1.72978400	-1.06196700
H	4.40248300	3.46521800	-2.21007200
H	5.24283300	-0.04925900	0.11792900
C	-1.70973400	-1.26734800	1.38532600
C	-1.78305700	-0.76559200	0.09138300
C	-2.94922800	-0.20544500	-0.41927000
C	-4.09911600	-0.20606300	0.36859800
C	-4.03278700	-0.75148300	1.64200900
C	-2.85896600	-1.26314500	2.17313700
H	-0.77684300	-1.64687700	1.79575900
H	-2.99575100	0.19816500	-1.42968000
H	-5.03883900	0.19367000	-0.00297300
H	-2.84409000	-1.63683100	3.19389100
Cl	1.57105500	-0.87062200	-2.94897000
F	-5.14677500	-0.78393600	2.38107200
C	-1.33691400	1.29157700	5.45137400
C	6.42281200	1.94154000	-1.35207900
C	-2.22025900	5.52767200	-3.64149200
F	-1.74839600	5.53322000	-4.89275800
F	-2.06538800	6.75445500	-3.14279300
F	-3.53482800	5.28650900	-3.72400200
F	6.83672400	3.13086400	-0.89608300
F	7.19738100	1.00609300	-0.80030000
F	6.65397700	1.93331900	-2.67088200

F	-2.31960400	0.38022200	5.51007100
F	-0.40654300	0.93815400	6.33885200
F	-1.86400400	2.45418300	5.85383300
C	-2.72774400	-3.57102100	-0.92328400
C	-2.10826600	-4.21565200	0.14838600
C	-0.72604100	-4.40153800	0.16671100
C	0.08514800	-3.94334000	-0.86906300
C	-0.54839800	-3.26332500	-1.94790100
C	-1.94805800	-3.10864800	-1.98022700
H	-2.71485400	-4.57902800	0.97358700
H	-0.26560300	-4.92006500	1.00411400
H	0.01585900	-3.05685600	-2.85704000
H	-2.42998200	-2.62440800	-2.82726400
B	1.63411500	-4.28740800	-0.86124200
O	2.60155800	-3.51084500	-1.40633300
H	2.31780600	-2.65505100	-1.76478000
O	1.94642300	-5.51646900	-0.36964100
H	2.89953400	-5.65726000	-0.36083100
C	-4.18816000	-3.29987600	-0.96409000
O	-4.79253800	-3.62260800	0.18209500
O	-4.76109200	-2.81695800	-1.91841400
C	-6.18850900	-3.32780100	0.25044100
H	-6.72727300	-3.81670800	-0.56518200
H	-6.52918000	-3.70459200	1.21450400
H	-6.34858000	-2.24620000	0.19195000
B	1.83934800	-2.34187000	2.11587100
F	2.93368900	-1.58741500	2.53152000
F	2.21290500	-3.62945500	1.76564900
F	1.30202000	-1.70432200	0.95470100
F	0.85699400	-2.35827100	3.09762600

TS6

Au	0.90764000	-0.32357000	2.09510600
P	1.72352200	1.93475200	2.57405400
C	0.76264300	3.11115500	1.57677700
C	0.68176900	4.46020400	1.93890000
C	0.11719200	2.66030800	0.42024000
C	-0.04894000	5.34819600	1.15890300
H	1.18087100	4.82415900	2.83486200
C	-0.61282200	3.54817400	-0.35662200
H	0.18169400	1.61455500	0.12348300
C	-0.69651600	4.88706200	0.01864100
H	-0.11514700	6.39363400	1.44289100
H	-1.12139200	3.19772700	-1.25158100

C	1.48970500	2.38670400	4.31993200
C	2.45676300	2.01287500	5.25585000
C	0.27423200	2.93058900	4.75154700
C	2.20425400	2.15692800	6.61537500
H	3.40779300	1.59426400	4.93434400
C	0.02765600	3.07972800	6.10605900
H	-0.49445400	3.21824100	4.03890900
C	0.98638100	2.67779900	7.03392200
H	2.95001200	1.85246000	7.34322000
H	-0.92119200	3.48833000	6.44657700
C	3.48487200	2.20503300	2.18794400
C	3.89645300	3.39126400	1.57310500
C	4.42546800	1.22514500	2.51969500
C	5.24214600	3.60107700	1.30794800
H	3.17529000	4.15448800	1.29358500
C	5.77298600	1.44348000	2.26054800
H	4.11613700	0.28344700	2.96662600
C	6.17553700	2.62856700	1.65525800
H	5.56645400	4.52256200	0.83062300
H	6.50636200	0.68633500	2.52067400
C	-0.09381500	-0.38150400	4.92148200
C	-0.43922000	-0.05179600	3.61523900
C	-1.68168200	0.49730900	3.31247700
C	-2.59010500	0.74711700	4.34034700
C	-2.22654000	0.43226800	5.63993900
C	-0.99981100	-0.13428200	5.95021000
H	0.87041600	-0.82287300	5.16157300
H	-1.95750600	0.73551800	2.28611900
H	-3.56650100	1.17985100	4.14167700
H	-0.75450100	-0.35240300	6.98635600
Cl	2.49735000	-0.37495800	0.17956000
F	-3.08724800	0.68757400	6.63231300
C	0.62446100	2.74730700	8.48494600
C	7.61289600	2.87894800	1.31288100
C	-1.52044500	5.80592900	-0.83406100
F	-1.08911800	5.80606200	-2.10080600
F	-1.49739500	7.06683600	-0.39947800
F	-2.79997600	5.41163300	-0.86246500
F	8.00487800	4.09275800	1.72040600
F	8.43465700	1.98260200	1.86290500
F	7.80443700	2.83904600	-0.01297500
F	-0.33379200	1.85156000	8.77170200
F	1.65958800	2.49663400	9.28810000
F	0.13530300	3.94942300	8.81355100

C	-2.34917300	-3.44573300	0.54518400
C	-2.25291600	-3.26921000	1.92733800
C	-1.13026200	-2.65959700	2.45799200
C	-0.04218500	-2.24612600	1.64074300
C	-0.20650300	-2.40389300	0.23569900
C	-1.32690100	-3.00826800	-0.30140000
H	-3.05509800	-3.61059900	2.57420300
H	-1.05232100	-2.55951400	3.53747600
H	0.59609200	-2.08115600	-0.42465200
H	-1.43275500	-3.15233200	-1.37296200
B	1.33588900	-3.42642900	2.11793800
O	2.50090000	-3.24350900	1.43418200
H	2.73718900	-2.33717700	1.18685000
O	0.79640100	-4.69366200	2.16988700
H	1.37968800	-5.30851600	1.71419900
C	-3.53428300	-4.09930300	-0.08680100
O	-4.42159000	-4.51378100	0.81592700
O	-3.66752300	-4.23483600	-1.28384700
C	-5.58845400	-5.15000600	0.28805400
H	-5.31097500	-6.03397900	-0.29248500
H	-6.19139100	-5.43393900	1.14975200
H	-6.14175900	-4.45908200	-0.35376400
B	2.76791100	-2.56655800	4.43462300
F	3.62888700	-3.59052100	4.25738200
F	1.45564800	-2.95036200	3.66527900
F	3.15525600	-1.38560300	3.84703300
F	2.33529700	-2.40180400	5.71373200

F

Au	0.53124300	-0.86189300	-0.12232800
P	0.90792100	1.58948100	0.19183300
C	-0.05813200	2.64176900	-0.93837000
C	-0.31492000	3.98353400	-0.62642800
C	-0.54761800	2.09695800	-2.12684900
C	-1.05184800	4.76721900	-1.50009700
H	0.05684000	4.41391200	0.30179300
C	-1.28882000	2.88429300	-3.00224500
H	-0.34156500	1.05706100	-2.37444200
C	-1.53993700	4.21245500	-2.68361100
H	-1.25808000	5.80806900	-1.26167100
H	-1.67288500	2.45927300	-3.92453700
C	0.43386100	2.13645100	1.86448500
C	1.37352700	2.42032300	2.85415100
C	-0.93036600	2.11419100	2.18486400

C	0.95993300	2.65353000	4.16360700
H	2.43444500	2.44862500	2.61686300
C	-1.34195000	2.35404200	3.48369800
H	-1.67243300	1.89201300	1.41946600
C	-0.39199100	2.60750600	4.47436500
H	1.69368600	2.86282500	4.93605700
H	-2.39899900	2.32980600	3.73974200
C	2.66061500	2.03503900	-0.02526400
C	3.05923900	3.14113300	-0.77404800
C	3.62470900	1.20606600	0.56388800
C	4.41260100	3.42812500	-0.92677700
H	2.31938800	3.78218300	-1.24714500
C	4.97119300	1.49929600	0.42288300
H	3.32240200	0.32585500	1.13117000
C	5.36011600	2.60909200	-0.32723100
H	4.72405500	4.28647400	-1.51427300
H	5.72350400	0.86129600	0.88022100
C	0.22093200	-0.99513000	2.84212200
C	-0.48346000	-1.05503600	1.64104800
C	-1.87001400	-1.18582600	1.64566900
C	-2.56363200	-1.22556500	2.85381800
C	-1.84415400	-1.14156000	4.03488100
C	-0.46280000	-1.03041300	4.05466700
H	1.30580400	-0.89703300	2.84714000
H	-2.42320500	-1.25288400	0.71066000
H	-3.64538200	-1.32099700	2.88721600
H	0.05514200	-0.94866000	5.00694200
Cl	1.74498100	-0.73001700	-2.27799400
F	-2.50583600	-1.17727400	5.19924800
C	-0.87668200	2.77305800	5.88074900
C	6.82547600	2.89692700	-0.44458200
C	-2.32757500	5.09977500	-3.59924800
F	-2.88212600	4.43101000	-4.61223900
F	-1.55339700	6.05838500	-4.12628100
F	-3.31207500	5.72261500	-2.93873000
F	7.08820900	3.88181900	-1.30614100
F	7.34222700	3.25096500	0.74062000
F	7.50274200	1.81384300	-0.84833300
F	-1.38872100	1.62415400	6.34992000
F	0.09224000	3.14872300	6.71878200
F	-1.85476100	3.68591600	5.95719100
C	-0.20334600	-5.61472000	-0.67861800
C	0.76862700	-5.16364400	0.21822900
C	0.96189200	-3.79953300	0.40802200

C	0.19753900	-2.88084300	-0.30948200
C	-0.77838900	-3.32610600	-1.20137500
C	-0.97539100	-4.68906500	-1.38425500
H	1.36755500	-5.88204800	0.77135400
H	1.71172100	-3.45756400	1.11969100
H	-1.38295600	-2.61462700	-1.76204600
H	-1.72872300	-5.05570600	-2.07753900
C	-0.45833100	-7.05417500	-0.91370400
O	0.33460300	-7.84256200	-0.17520700
O	-1.29010000	-7.48840300	-1.68564900
C	0.14251800	-9.24464700	-0.35508600
H	0.33998200	-9.53012500	-1.39241500
H	0.85024800	-9.73484800	0.31328500
H	-0.88188700	-9.52960900	-0.09855500

TS7

Au	0.07877100	-1.04892900	0.02660100
P	0.61935700	1.38987700	0.12714900
C	-0.20232700	2.52456800	-1.03685400
C	-0.54699900	3.82905200	-0.67491100
C	-0.44907900	2.06917400	-2.33753700
C	-1.13180900	4.67847400	-1.60732800
H	-0.35837000	4.18849100	0.33485300
C	-1.03031700	2.91935300	-3.26671000
H	-0.17621600	1.05057200	-2.61620500
C	-1.36955500	4.22027200	-2.89825500
H	-1.39932000	5.69345900	-1.32978000
H	-1.22375900	2.57232700	-4.27927400
C	0.17462300	1.96952400	1.79674900
C	1.13327500	2.28353600	2.76416900
C	-1.17591500	1.90171000	2.15380900
C	0.74512800	2.49061000	4.08141400
H	2.18632200	2.34521200	2.49951300
C	-1.56418000	2.11124100	3.46835200
H	-1.92878800	1.64902400	1.40770400
C	-0.59801200	2.38327900	4.43167800
H	1.48877600	2.71496400	4.84261200
H	-2.61004800	2.02777700	3.75047100
C	2.40643400	1.71287900	-0.03129700
C	2.90343900	2.92136300	-0.52741100
C	3.29019600	0.72500300	0.41030300
C	4.27303200	3.13585600	-0.57817400
H	2.22290500	3.69523700	-0.87603500
C	4.66212200	0.94237600	0.36843700

H	2.90362900	-0.21982200	0.79444300
C	5.14669800	2.14712200	-0.12876500
H	4.66461800	4.07377400	-0.96566600
H	5.34861800	0.17682800	0.71620200
C	0.08904400	-1.40145300	2.98931400
C	-0.77659200	-1.49746800	1.89305900
C	-2.15379700	-1.35476800	2.08228700
C	-2.66395900	-1.09105700	3.34910100
C	-1.78075000	-0.96060100	4.40960100
C	-0.41256500	-1.12623000	4.25581100
H	1.16498900	-1.50856000	2.85807600
H	-2.83986400	-1.44056100	1.24239300
H	-3.72987500	-0.96212800	3.51522700
H	0.23959400	-1.00032400	5.11618900
Cl	1.05297600	-1.27388000	-2.30881500
F	-2.25923000	-0.64279900	5.61877700
C	-0.95848900	2.45939300	5.88096700
C	6.61723400	2.42709300	-0.19673100
C	-2.00216100	5.10266200	-3.93089200
F	-3.16287300	4.58902800	-4.36106700
F	-1.21688300	5.22672800	-5.00970100
F	-2.25161100	6.33190200	-3.47340400
F	6.93796600	3.49995000	0.54003100
F	7.35691500	1.40457600	0.23868000
F	7.00141300	2.69659600	-1.45148900
F	-0.47980400	1.39258900	6.54045000
F	-0.42980900	3.54030500	6.47014900
F	-2.27711900	2.49300100	6.08423900
C	-0.55595800	-5.80019700	0.11958400
C	0.58106700	-5.24279500	0.71119800
C	0.66340500	-3.87100900	0.90840600
C	-0.38852600	-3.04380800	0.50473100
C	-1.53080600	-3.59821800	-0.08179700
C	-1.60772700	-4.96862700	-0.27469000
H	1.40130800	-5.88701200	1.01536700
H	1.55027100	-3.44522300	1.37436200
H	-2.35617100	-2.96235600	-0.39643600
H	-2.48363200	-5.41543300	-0.73852100
C	-0.69624500	-7.25438200	-0.11811500
O	0.37329400	-7.94678200	0.29476700
O	-1.66622800	-7.77425700	-0.63292700
C	0.30943700	-9.35616600	0.08121900
H	0.20220600	-9.57913600	-0.98428100
H	1.24738900	-9.76195200	0.46004400

H	-0.53726300	-9.79040100	0.62070700
3			
C	-0.30940900	-1.44213300	3.37412500
C	-1.14499800	-2.35537700	2.71760500
C	-2.49835900	-2.39758800	3.07743200
C	-3.00784300	-1.55757300	4.05869400
C	-2.14812600	-0.66636400	4.68097100
C	-0.80295100	-0.59310600	4.35581300
H	0.73977800	-1.37535500	3.09420100
H	-3.16056100	-3.11678000	2.60012900
H	-4.05339300	-1.58959700	4.35102100
H	-0.16526600	0.12607200	4.86169500
F	-2.63242900	0.14945400	5.62555900
C	0.39620600	-4.94210000	-0.32991000
C	1.17793100	-4.62359900	0.78365900
C	0.67544700	-3.78843000	1.76966400
C	-0.61423300	-3.24833000	1.66968300
C	-1.38891500	-3.57529600	0.54769000
C	-0.89119400	-4.41176400	-0.43772200
H	2.17648900	-5.04072000	0.87758700
H	1.28300900	-3.56887200	2.64515700
H	-2.38245700	-3.14600000	0.43633000
H	-1.48839300	-4.66028300	-1.31134400
C	0.87898700	-5.82644600	-1.41400700
O	2.12855000	-6.26127600	-1.20232700
O	0.22728500	-6.13267900	-2.39270900
C	2.65459600	-7.12554100	-2.20796800
H	2.67187100	-6.62236700	-3.17891700
H	3.66813400	-7.37434800	-1.89368000
H	2.05016100	-8.03348200	-2.28996100
TS8			
Au	0.90918300	-0.32634300	2.07388800
P	1.67005300	1.95521800	2.54701100
C	0.72048500	3.11342100	1.51921900
C	0.64193900	4.46709700	1.86502000
C	0.07917900	2.64936800	0.36571800
C	-0.07738600	5.34834500	1.06746700
H	1.13174700	4.83976200	2.76250100
C	-0.64074900	3.53092100	-0.42778800
H	0.14085800	1.59945400	0.08450600
C	-0.71830200	4.87545300	-0.07185700
H	-0.14082800	6.39756100	1.33774100

H	-1.14579000	3.17090700	-1.32092800
C	1.38673600	2.42538500	4.27981700
C	2.34299900	2.10633600	5.24736700
C	0.13883200	2.92338100	4.67031700
C	2.04508700	2.25585000	6.59651900
H	3.31954600	1.72404800	4.95877500
C	-0.15831600	3.06748200	6.01580100
H	-0.61965200	3.16744300	3.93016000
C	0.79032300	2.71900100	6.97509100
H	2.78281900	1.99712900	7.35001200
H	-1.13907100	3.42317400	6.32004700
C	3.43793200	2.22445500	2.20963000
C	3.87532800	3.40413200	1.60074800
C	4.35848500	1.24278800	2.58551600
C	5.23110100	3.60390500	1.38426200
H	3.16791900	4.16755500	1.28824000
C	5.71608100	1.45129400	2.37515200
H	4.02247400	0.30669900	3.02602800
C	6.14570000	2.62928300	1.77458700
H	5.57911500	4.51898100	0.91119800
H	6.43482900	0.69275100	2.66940600
C	0.03394300	-0.44380800	4.93155500
C	-0.38686800	-0.12717100	3.64606100
C	-1.66162000	0.37778400	3.40226000
C	-2.52034400	0.59720200	4.47467500
C	-2.09947800	0.30408000	5.77009600
C	-0.83054500	-0.21815300	6.00032400
H	1.02546800	-0.84898300	5.12024300
H	-1.99044500	0.60581300	2.38959400
H	-3.51553300	1.00037600	4.30104300
H	-0.50842900	-0.43082000	7.01638300
Cl	2.46268200	-0.31719000	0.13709600
C	0.38544400	2.74599300	8.41675200
C	7.59603300	2.87485200	1.48738900
C	-1.52973000	5.78846200	-0.94289200
F	-1.08470300	5.77445400	-2.20472300
F	-1.50674400	7.05352900	-0.52054400
F	-2.81020800	5.39831700	-0.98092000
F	7.98597100	4.06904100	1.95179800
F	8.39094400	1.95061200	2.03031900
F	7.82929700	2.88154400	0.16787900
F	-0.39093500	1.68692200	8.70455400
F	1.43215900	2.70588200	9.24354900
F	-0.32817600	3.83650300	8.71509400

C	-2.36275100	-3.40467300	0.55589100
C	-2.21599700	-3.27864000	1.93922500
C	-1.06659600	-2.70264500	2.44972700
C	-0.00277400	-2.27247300	1.60950400
C	-0.21453100	-2.38621200	0.20656900
C	-1.36129000	-2.95772600	-0.31059400
H	-3.00095000	-3.63085600	2.60136000
H	-0.94886800	-2.63934100	3.52863700
H	0.56915500	-2.05174400	-0.47035600
H	-1.50542800	-3.06578600	-1.38193300
B	1.40673100	-3.42085700	2.04099400
O	2.53905100	-3.23474800	1.30209600
H	2.78155100	-2.32105700	1.09457700
O	0.88293900	-4.69558300	2.11917500
H	1.47364300	-5.31142600	1.67438100
C	-3.58336200	-4.00985500	-0.05653300
O	-4.46784900	-4.39755700	0.86056100
O	-3.74548000	-4.12929100	-1.25174100
C	-5.66745100	-4.98532200	0.34963100
H	-5.43326900	-5.87432100	-0.24216500
H	-6.26523700	-5.25342100	1.21988000
H	-6.20534800	-4.26895600	-0.27710300
B	3.00054300	-2.70812100	4.25451100
F	3.63911200	-3.89360800	4.14276400
F	1.59528800	-2.91946600	3.55890300
F	3.56794900	-1.68434600	3.54774400
F	2.65511500	-2.36284300	5.52369600
C	-2.99695200	0.65356400	6.91446700
F	-3.01425300	1.98310900	7.12758100
F	-2.61898100	0.07936300	8.05869300
F	-4.26576400	0.29521900	6.68016100

TS9

Au	0.93397700	-0.39449800	2.07218000
P	1.68513800	1.87733200	2.59511600
C	0.68673600	3.05311800	1.63355600
C	0.59487600	4.39586500	2.01650300
C	0.02486800	2.61056300	0.48327600
C	-0.15821900	5.28603700	1.26070000
H	1.10536300	4.75319800	2.90881300
C	-0.72754600	3.50039200	-0.26968900
H	0.09612200	1.56966600	0.17159800
C	-0.81829500	4.83331300	0.12413000
H	-0.23133600	6.32692000	1.55944000

H	-1.24704700	3.15657800	-1.16093200
C	1.44605400	2.28464000	4.35166800
C	2.41828600	1.91030300	5.28201700
C	0.21680400	2.78768400	4.79189800
C	2.15876700	2.01869300	6.64365400
H	3.37954700	1.52000100	4.95502300
C	-0.04334800	2.88644300	6.14825500
H	-0.55345700	3.07645700	4.08177600
C	0.92461000	2.49312700	7.07027200
H	2.91091400	1.71898400	7.36691400
H	-1.00910600	3.25088700	6.49344300
C	3.43560500	2.20800200	2.20656100
C	3.81445200	3.40885300	1.59929800
C	4.40305600	1.25107500	2.52830200
C	5.15396700	3.65725700	1.33540200
H	3.07235600	4.15353400	1.32457100
C	5.74400300	1.50809100	2.27180400
H	4.11851400	0.29600700	2.96292500
C	6.11405500	2.70895800	1.67691900
H	5.45267300	4.59039000	0.86407100
H	6.49881300	0.76960100	2.52466100
C	-0.01781400	-0.54776500	4.91419000
C	-0.39469300	-0.19456700	3.62077300
C	-1.64845600	0.34041700	3.36549100
C	-2.53354300	0.57697200	4.42105700
C	-2.14921000	0.26286800	5.72551000
C	-0.89820000	-0.31998600	5.96085900
H	0.95605000	-0.98341700	5.12298000
H	-1.95757500	0.58925300	2.35094500
H	-3.50626800	1.00940300	4.20703100
H	-0.62389600	-0.55967000	6.98547200
Cl	2.50645800	-0.35195700	0.13191700
C	0.55857700	2.52552700	8.52151900
C	7.54433600	2.99875400	1.33687900
C	-1.66008600	5.75570400	-0.70687200
F	-1.24489100	5.77298900	-1.97902000
F	-1.64003500	7.01188900	-0.25858800
F	-2.93721400	5.35303700	-0.72383500
F	7.90068700	4.22584300	1.73724900
F	8.38931300	2.12972200	1.89576000
F	7.74178800	2.95503500	0.01192800
F	-0.38542000	1.61046700	8.79045400
F	1.59722800	2.27656100	9.32148600
F	0.05034500	3.71384600	8.87374200

C	-2.26658500	-3.56414200	0.50990500
C	-2.14676400	-3.41823000	1.89366100
C	-1.03019900	-2.79062400	2.41648800
C	0.02958200	-2.32918600	1.58790900
C	-0.16136400	-2.45372400	0.18270600
C	-1.27611600	-3.07510300	-0.34657900
H	-2.92521900	-3.79830700	2.54790900
H	-0.93089900	-2.71239100	3.49594500
H	0.61745800	-2.09141000	-0.48578000
H	-1.40148300	-3.19487700	-1.41908100
B	1.44287600	-3.48957400	2.00150600
O	2.58827600	-3.25350700	1.30123100
H	2.78915900	-2.33392800	1.07038300
O	0.93823200	-4.77230100	2.02352500
H	1.51868200	-5.35167300	1.52040000
C	-3.44360100	-4.23944800	-0.11388300
O	-4.30445300	-4.69337700	0.79571100
O	-3.59298100	-4.35947300	-1.31071400
C	-5.46039500	-5.35491300	0.27516500
H	-5.16669700	-6.22765800	-0.31438500
H	-6.04732600	-5.65968300	1.14080900
H	-6.03738800	-4.67400400	-0.35647400
B	2.89758900	-2.66924000	4.31420400
F	3.77928000	-3.66735900	4.09086400
F	1.58109400	-3.06399700	3.56467200
F	3.24648400	-1.46426700	3.75197500
F	2.49123500	-2.54979800	5.60722500
O	-2.90263900	0.49491800	6.82481300
C	-4.15620900	1.12084200	6.64121800
H	-4.59530600	1.23443700	7.63359100
H	-4.04413500	2.11217100	6.18091800
H	-4.82465700	0.51028200	6.01990100

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C	-2.67144000	-0.60291500	-4.41162100
C	-2.01631500	0.61307600	-4.60617500
C	-0.71649000	0.79680100	-4.13770200
C	-0.04334000	-0.20967500	-3.45925400
C	-0.69895700	-1.43227900	-3.23114200
C	-1.99903300	-1.60392700	-3.74051600
H	-3.67731100	-0.77520900	-4.78174800
H	-2.51200500	1.43479300	-5.12053800
H	0.97590000	-0.05718700	-3.11038500
H	-0.17094000	-2.28622700	-2.81245400

N	-0.10917800	2.08910000	-4.39494200
N	1.01019300	2.35836200	-4.12579200
Cl	1.25360500	-1.79745700	-0.52902600
B	0.49259500	2.20352700	0.28222800
F	0.17237800	1.07538500	1.08631500
F	1.75883400	2.64793600	0.57989400
F	-0.46386000	3.18861600	0.48680600
F	0.42723600	1.78087400	-1.06944300
P	-2.97550800	0.38697300	-0.37080200
Au	-0.82989900	-0.57120900	-0.65375500
C	-3.42424000	1.56958200	-1.66317800
C	-2.54043800	2.62379800	-1.93133200
C	-4.59990900	1.41903000	-2.40790800
C	-2.84374600	3.53233100	-2.93703700
H	-1.61842000	2.72819400	-1.36177200
C	-4.89183800	2.32645700	-3.41612600
H	-5.28041100	0.59385900	-2.21409600
C	-4.01142000	3.37414900	-3.67746500
H	-2.16509100	4.35145900	-3.15634000
H	-5.79909000	2.21498300	-4.00375000
C	-3.03932100	1.21765200	1.23482100
C	-2.77868800	0.43605300	2.37056900
C	-3.36834000	2.56649500	1.36551700
C	-2.85860000	1.00546600	3.62832700
H	-2.51825800	-0.61656300	2.26757700
C	-3.45001000	3.13413100	2.63154900
H	-3.57194600	3.17672100	0.49001800
C	-3.19387800	2.35497300	3.75306700
H	-2.65945700	0.40761600	4.51414100
H	-3.71527000	4.18089800	2.74096800
C	-4.25369900	-0.89713400	-0.30083500
C	-4.02695700	-2.14888800	-0.87920600
C	-5.48195000	-0.61301700	0.30580100
C	-5.02984900	-3.10673400	-0.87014500
H	-3.06608900	-2.38258300	-1.33038000
C	-6.48405800	-1.57397700	0.31495700
H	-5.66011800	0.35747900	0.76507700
C	-6.25415100	-2.81335800	-0.27419300
H	-4.85730900	-4.08097400	-1.32137900
H	-7.44148400	-1.36058700	0.77988700
C	-7.31276100	-3.87730400	-0.27838800
C	-4.28013600	4.25892500	-4.85758900
C	-3.29836900	2.92452100	5.13663300
F	-3.53335800	4.23757200	5.13507800

F	-4.29012100	2.33663700	5.81875400
F	-2.17503000	2.71332300	5.83244600
F	-3.91334000	3.63661700	-5.99097700
F	-5.57721100	4.55224200	-4.97666100
F	-3.60379200	5.40623700	-4.79856900
F	-6.88629700	-4.97930500	0.35009100
F	-8.43717500	-3.48024000	0.31899500
F	-7.62382900	-4.24062400	-1.52874900
F	-2.57980800	-2.78352600	-3.56466000

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C	-2.01900000	0.86888700	-5.28260200
C	-0.94683800	1.66931700	-4.95173900
C	0.01004200	1.14056200	-4.06976800
C	-0.05213100	-0.15591600	-3.53110000
C	-1.13689700	-0.93459700	-3.86776000
C	-2.10620800	-0.40335300	-4.71899700
H	-2.79973000	1.22182000	-5.94790100
H	-0.84272600	2.67566500	-5.34513400
H	0.73322600	-0.51720800	-2.87485900
H	-1.25018700	-1.93854000	-3.46680500
N	1.05212000	1.93801100	-3.68640100
N	1.89602600	2.58557300	-3.36035300
Cl	-0.94110300	-3.04647700	-1.00925600
B	0.44817400	1.95272800	0.19105700
F	0.07222100	0.88663600	1.08497400
F	1.72234500	2.35656700	0.46706100
F	-0.48068600	2.96681900	0.31965400
F	0.36490100	1.40114400	-1.11152900
P	-3.18228900	0.20988400	-0.12663700
Au	-0.99691600	-0.79180200	-0.21462700
C	-3.53743100	1.24053000	-1.56427000
C	-2.70211100	2.33472600	-1.84003500
C	-4.64560100	0.96879600	-2.37453600
C	-3.01336400	3.17443400	-2.89783200
H	-1.83106000	2.54279400	-1.22103900
C	-4.93760100	1.80685900	-3.44408800
H	-5.29192900	0.11986000	-2.17029300
C	-4.12876300	2.90973100	-3.69254200
H	-2.38906200	4.04044600	-3.10561100
H	-5.80094600	1.60823700	-4.07170700
C	-3.21451600	1.19278600	1.38117400
C	-2.84520200	0.55785500	2.57871300
C	-3.54855300	2.54945700	1.37393300

C	-2.81323100	1.28243600	3.75593300
H	-2.58002600	-0.49825400	2.59035100
C	-3.51131500	3.27183500	2.56008200
H	-3.84009600	3.04720500	0.45326000
C	-3.13798200	2.63961000	3.73948400
H	-2.52574800	0.80055400	4.68692200
H	-3.77134800	4.32552400	2.56337000
C	-4.40564100	-1.11067000	-0.02760100
C	-4.36928600	-2.13339500	-0.98587400
C	-5.39297800	-1.09724700	0.96136300
C	-5.32307900	-3.13524600	-0.95186800
H	-3.59309900	-2.15016800	-1.74972300
C	-6.34533900	-2.10984600	0.99237000
H	-5.43067400	-0.30113100	1.70031700
C	-6.30456200	-3.11996200	0.03989500
H	-5.30530500	-3.93274200	-1.68976400
H	-7.11883900	-2.10829800	1.75410100
C	-7.29000800	-4.25185500	0.07095600
C	-4.39631300	3.80522300	-4.86685900
C	-3.03940400	3.39992400	5.02972100
F	-3.44835400	4.66292800	4.91068200
F	-3.77215200	2.82169700	5.98812900
F	-1.77491900	3.42128200	5.46769200
F	-3.51408300	3.56130900	-5.85480800
F	-5.61500700	3.63036900	-5.37314000
F	-4.26298000	5.09267400	-4.54318600
F	-6.69453300	-5.38849200	0.45200100
F	-8.30085100	-4.02440800	0.91031100
F	-7.80829800	-4.47250100	-1.14250700
F	-3.16155200	-1.13864600	-4.99727100

³TS10

Au	-8.74711000	-1.61564400	-0.53762400
P	-10.59513800	0.03867800	-0.40686000
C	-10.35687500	0.97891300	1.10771200
C	-10.17206800	2.36798600	1.08270400
C	-10.25447900	0.27091600	2.31209000
C	-9.89127500	3.03875200	2.26381200
H	-10.23328300	2.92112700	0.14843200
C	-9.98733600	0.94994300	3.49057000
H	-10.32172600	-0.81571400	2.33985200
C	-9.79297800	2.32597400	3.45748800
H	-9.72573400	4.11228900	2.25149300
H	-9.85653600	0.39639800	4.41273400

C	-12.19747100	-0.79288800	-0.37764000
C	-12.62575200	-1.40368100	-1.56308000
C	-12.98998300	-0.84688400	0.77418300
C	-13.84434900	-2.06334300	-1.59762200
H	-12.00915400	-1.36873900	-2.45903300
C	-14.20593600	-1.51263300	0.73427300
H	-12.67427200	-0.35996900	1.69254500
C	-14.62543800	-2.11955200	-0.44662600
H	-14.18643400	-2.53549200	-2.51329000
H	-14.83372600	-1.55427700	1.62057700
C	-10.60775200	1.14353000	-1.83954300
C	-9.57265900	1.11616600	-2.77669500
C	-11.68669600	2.02167100	-1.99888800
C	-9.60735000	1.97758400	-3.86371600
H	-8.74731200	0.41639300	-2.66679900
C	-11.71243100	2.88861800	-3.08309400
H	-12.50366800	2.03486400	-1.27957000
C	-10.67290400	2.86201000	-4.00729800
H	-8.80804200	1.96241800	-4.60001900
H	-12.54035500	3.57941600	-3.20865100
C	-6.88765600	-0.65645500	1.55172500
C	-6.80371700	-0.67455700	0.14302500
C	-6.65685500	0.51686000	-0.60767600
C	-6.77064900	1.72832900	0.04027100
C	-6.92141500	1.72228900	1.43105300
C	-6.99416600	0.56101600	2.19828300
H	-6.87161300	-1.57744700	2.13339400
H	-6.45350800	0.46054500	-1.67604700
H	-6.70133300	2.67492100	-0.48717200
H	-7.09649100	0.62016600	3.28021000
N	-5.88652100	-2.03393700	-0.42733000
N	-5.48957300	-2.07551300	-1.50063400
Cl	-9.89458500	-3.50733600	-1.48069500
F	-6.97032000	2.88802000	2.05162600
C	-9.31015900	3.02709000	4.69183200
C	-10.67864500	3.76129300	-5.20925300
C	-15.92283900	-2.87164000	-0.42815900
F	-16.90414900	-2.13120400	0.10068600
F	-15.82064200	-3.97366400	0.32556900
F	-16.31095800	-3.25140500	-1.64659500
F	-11.66992200	4.65280600	-5.17531400
F	-9.52712400	4.43589300	-5.30930400
F	-10.81042300	3.04989600	-6.33574000
F	-9.67553100	2.39743300	5.80940500

F	-9.76331500	4.28348300	4.76289600
F	-7.97052100	3.09328200	4.68993600
B	-7.81159300	-1.54442100	4.85551600
F	-6.59454400	-1.85574700	4.23557600
F	-7.96732200	-2.29523900	6.00950400
F	-7.81617100	-0.17234800	5.17371000
F	-8.85838200	-1.81038300	3.96037300
TS			
C	-1.09683600	0.65021300	-0.68109900
C	0.17702200	0.83542100	-0.14515100
C	0.32088000	1.83589800	0.78562600
C	-0.67388600	2.66927100	1.23597500
C	-1.94688500	2.48053900	0.69697300
C	-2.12524800	1.47734900	-0.24680700
H	-1.30273800	-0.11671100	-1.42282500
H	1.01979000	0.21668100	-0.44985400
H	-0.47976800	3.44027300	1.97799500
H	-2.79396700	3.09285300	0.99398600
N	2.06502800	2.11430400	1.53408500
N	2.90087500	1.44144500	1.17267500
F	-3.34655000	1.29800600	-0.76339500
³13			
C	-1.75435000	-0.05942500	-0.51700400
C	-0.53240800	0.34555000	-0.03327800
C	-0.40216400	1.64362000	0.46992100
C	-1.49125000	2.56035300	0.50741800
C	-2.70852100	2.17414300	0.02441800
C	-2.82380200	0.87125100	-0.50968800
H	-1.89521300	-1.04312900	-0.95376900
H	0.32410700	-0.31971500	-0.06880000
H	-1.33111300	3.55223400	0.92169600
H	-3.57581000	2.82592600	0.02324800
N	0.90042000	2.01901900	0.96079400
N	1.14573100	3.10349000	1.37503500
B	-0.04145900	-1.36045300	-3.01476000
F	0.54375500	-0.09705800	-2.91482300
F	-1.42295900	-1.14964200	-3.32945400
F	0.02311900	-2.01248500	-1.78337900
F	0.54482100	-2.10995200	-4.00778300
F	-3.98547800	0.47769500	-0.94238500
C	-1.02221900	2.29945200	-2.84441200
H	-1.44787800	3.30055300	-2.74760400

H	-0.46999100	2.20019100	-3.78692300
H	-0.27721500	2.13470000	-2.04208400
O	-2.06466000	1.36616900	-2.77788800
H	-1.73217300	0.47813700	-3.06127900

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C	-1.75250200	0.19867800	-0.59752700
C	-0.51600200	0.51372700	-0.05246100
C	-0.38104300	1.66172700	0.72252900
C	-1.45992900	2.51562300	0.95763800
C	-2.69454800	2.21078700	0.40782300
C	-2.81404300	1.05655000	-0.35904400
H	-1.88032800	-0.67605200	-1.22722000
H	0.33704500	-0.13142400	-0.24418300
H	-1.31724900	3.40554900	1.56611900
H	-3.56250900	2.84572000	0.55971900
N	0.93095900	1.93175700	1.26884500
N	1.20182500	2.85872900	1.95522800
B	0.04165600	-1.48843600	-2.98924300
F	0.52860200	-0.18752900	-3.10583800
F	-1.35003100	-1.46141500	-3.26852500
F	0.22362500	-1.94613900	-1.68154600
F	0.67221400	-2.33069000	-3.89074700
F	-4.00616400	0.76628600	-0.88392100
C	-1.15786700	2.23627400	-3.34888000
H	-1.63974900	3.21629400	-3.44512800
H	-0.35974300	2.17623000	-4.10442800
H	-0.67631200	2.18938600	-2.35846900
O	-2.14365300	1.25334100	-3.51780300
H	-1.72096500	0.38565200	-3.41572300

³TS11

C	-1.74292000	-0.07103100	-0.50590200
C	-0.51511600	0.33172400	-0.02903300
C	-0.42892900	1.62825100	0.45378300
C	-1.47296000	2.56412100	0.51020400
C	-2.69636300	2.17532500	0.02843600
C	-2.80888300	0.86697700	-0.49894200
H	-1.89239900	-1.05420900	-0.94222800
H	0.34301600	-0.33244100	-0.06778300
H	-1.30359000	3.55715600	0.92156900
H	-3.56622300	2.82447500	0.02259800
N	1.23660800	2.15072400	1.06825800
N	1.34779600	3.20712400	1.46518900

B	-0.05475500	-1.36635500	-3.02010900
F	0.53746300	-0.10622100	-2.92018900
F	-1.43636000	-1.14973600	-3.32436500
F	0.01739200	-2.02394200	-1.79173000
F	0.52267000	-2.11499400	-4.02004800
F	-3.97236200	0.47413600	-0.93157500
C	-1.00440100	2.30625100	-2.83604200
H	-1.42134900	3.31125600	-2.73801800
H	-0.45076400	2.20698700	-3.77767200
H	-0.26346800	2.13556900	-2.03094500
O	-2.05628300	1.38308800	-2.77457000
H	-1.72849200	0.49409800	-3.05513800

¹CF₃

C	-2.70521000	0.24544000	-0.39091900
C	-1.32607400	0.17011300	-0.47048600
C	-0.61455900	1.31199100	-0.08715900
C	-1.19862000	2.50052900	0.36850700
C	-2.57761700	2.53621000	0.43494100
C	-3.31761900	1.41549000	0.05420900
H	-3.30663700	-0.60963900	-0.68182000
H	-0.80282700	-0.71879500	-0.80873900
H	-0.58655700	3.34998400	0.65178800
H	-3.08013500	3.43616700	0.77496800
N	0.76467200	1.27332300	-0.14493000
N	1.87267500	1.25353900	-0.18000700
B	1.01635800	-0.94235400	-2.53973400
F	0.94488000	0.44649700	-2.71656100
F	-0.20260300	-1.51992900	-2.89177600
F	1.23489200	-1.18578200	-1.16093300
F	2.05251200	-1.47587500	-3.28234300
C	-4.81786800	1.46328500	0.18704300
F	-5.41383500	0.60408700	-0.63783800
F	-5.28942800	2.68284000	-0.07434800
F	-5.17990800	1.14988600	1.43389800

^{14'}

C	-2.43900200	0.47860300	-1.20148100
C	-1.07712500	0.50734800	-1.43148400
C	-0.36681600	1.57375500	-0.86483000
C	-0.94075300	2.58689300	-0.08765100
C	-2.30520400	2.51952000	0.12668600
C	-3.04009800	1.46929000	-0.42276300
H	-3.03467200	-0.33367800	-1.60645600

H	-0.55647500	-0.26586400	-1.98596800
H	-0.33128400	3.38083300	0.33047700
H	-2.79476100	3.27627700	0.73117400
N	0.99766900	1.62834800	-1.06538300
N	2.09418600	1.68870200	-1.22698200
B	2.57095200	-1.54531800	-1.68470600
F	1.45393900	-0.83095800	-2.14493700
F	2.11305200	-2.68237100	-0.98783000
F	3.25192200	-0.72601600	-0.75549800
F	3.39371600	-1.90142900	-2.71776600
C	-3.10544700	0.89433000	3.43248200
C	-3.36943500	-0.18718600	2.58684800
C	-2.32994300	-0.78036800	1.88335200
C	-1.01204000	-0.31669200	1.99701700
C	-0.76808800	0.76097100	2.85931700
C	-1.79739200	1.36128100	3.57268400
H	-4.39075800	-0.53834300	2.46594800
H	-2.54564300	-1.60842000	1.20955900
H	0.24689400	1.14294600	2.95571000
H	-1.61066100	2.20474000	4.23290100
B	0.14134300	-0.93116000	1.12021000
O	-0.13841100	-2.03500700	0.38014400
H	0.61205300	-2.35240600	-0.15332200
O	1.33117800	-0.26185600	1.11242500
H	2.03963300	-0.63226700	0.55790900
C	-4.18198600	1.60330700	4.16473700
O	-5.39198000	1.08533400	3.92092500
O	-4.00186800	2.55400600	4.89922600
C	-6.47972800	1.73125400	4.58023300
H	-6.56323200	2.77206800	4.25408100
H	-7.37515200	1.17569100	4.30182300
H	-6.34146700	1.70969400	5.66490300
C	-4.53489500	1.42625400	-0.22828100
F	-5.14704000	2.04925900	-1.23793800
F	-4.98199000	0.16968500	-0.19743100
F	-4.90997500	2.02382700	0.90305000
34'			
C	-2.63801600	0.55080800	-0.68764900
C	-1.27822800	0.57257600	-0.99257200
C	-0.50844200	1.70312700	-0.60362900
C	-1.11786000	2.76257900	0.13550900
C	-2.48331000	2.70052000	0.40972700
C	-3.25782800	1.61934200	-0.01719200

H	-3.22982000	-0.30648700	-1.00160100
H	-0.79514700	-0.25444100	-1.50366600
H	-0.52004800	3.60537200	0.46789700
H	-2.94786200	3.51931000	0.95400000
N	0.78823600	1.76472700	-0.89413200
N	1.90490200	1.82449000	-1.14501500
B	2.44936800	-1.67075100	-1.78680500
F	1.30641700	-0.87722500	-1.91251600
F	2.06237500	-2.92571100	-1.26129400
F	3.31071200	-1.06847900	-0.84366500
F	3.08612100	-1.82794000	-2.99065000
C	-2.99044900	0.86482700	3.12965700
C	-3.14391800	-0.37580300	2.55170800
C	-2.02992700	-0.99241700	1.93126800
C	-0.74154500	-0.40749300	1.94121100
C	-0.60287100	0.82401200	2.55932600
C	-1.71461100	1.47779100	3.12484000
H	-4.11552800	-0.85876100	2.53308600
H	-2.15830200	-1.95550600	1.44001900
H	0.37071500	1.30917600	2.57966300
H	-1.61213300	2.45881000	3.58483100
B	0.45455600	-1.08548200	1.15186500
O	0.16630300	-2.24911000	0.52639900
H	0.85689300	-2.58367000	-0.07764800
O	1.61663500	-0.39389300	1.14430200
H	2.30603700	-0.71324300	0.53259500
C	-4.12922500	1.63920300	3.69473200
O	-5.26750600	0.95547800	3.64498300
O	-4.01648400	2.76637400	4.12634200
C	-6.42502800	1.64645600	4.12488700
H	-6.61275600	2.53714900	3.51860700
H	-7.25191100	0.94346900	4.03394100
H	-6.28677400	1.94234600	5.16792900
C	-4.73440200	1.60482800	0.18731100
F	-5.40013000	1.96875100	-0.91564100
F	-5.17903900	0.38328500	0.51553500
F	-5.10695600	2.44648600	1.16461900
5'			
C	-2.37586500	0.53106100	-1.33622000
C	-1.02335400	0.78170200	-1.52182800
C	-0.44375100	1.84911800	-0.84558500
C	-1.18375800	2.69145200	-0.02139900
C	-2.53683500	2.44412700	0.14646400

C	-3.12252300	1.35537300	-0.49642900
H	-2.84775900	-0.31796400	-1.82476800
H	-0.39771000	0.14460100	-2.14044800
H	-0.68988400	3.51547900	0.48789100
H	-3.13466700	3.07711300	0.79598400
N	0.98223500	2.05358200	-1.03517600
N	1.65439900	2.70578900	-0.31322400
B	2.48691400	-1.85914900	-1.72000700
F	1.51523200	-0.93059300	-2.07737100
F	1.84266400	-3.02607300	-1.24717200
F	3.24435700	-1.33154600	-0.64965200
F	3.30938700	-2.16363700	-2.77876700
C	-3.00146500	0.95916900	3.42831800
C	-3.29304100	-0.12829200	2.60080600
C	-2.27521800	-0.73552500	1.87798300
C	-0.95105700	-0.28507100	1.95584500
C	-0.67966500	0.80207600	2.79807800
C	-1.68544800	1.41799000	3.52965600
H	-4.31935800	-0.47145500	2.50238600
H	-2.51609100	-1.56376300	1.21251500
H	0.34066300	1.17854900	2.85881700
H	-1.47592200	2.26905300	4.17354700
B	0.18754100	-0.93821000	1.08181100
O	-0.13324700	-2.05381700	0.37221400
H	0.57856100	-2.41678300	-0.18372300
O	1.40629000	-0.33532400	1.10986100
H	2.07475100	-0.70340500	0.50584900
C	-4.05364500	1.68265800	4.17713500
O	-5.27788200	1.18068000	3.95931800
O	-3.85115400	2.63401600	4.90638000
C	-6.33968700	1.84095300	4.64410800
H	-6.41784400	2.88337300	4.32127800
H	-7.24947600	1.29818700	4.38733700
H	-6.17708600	1.81793000	5.72558600
C	-4.58209000	1.07160700	-0.31802200
F	-5.29623400	1.50119600	-1.36943500
F	-4.81944100	-0.24326600	-0.20729200
F	-5.08862400	1.66191900	0.77046600
6'			
C	-1.86261100	0.55303800	-0.89492100
C	-0.58688000	0.74876600	-0.38247300
C	-0.38514600	1.78549700	0.52326800
C	-1.41621200	2.62893000	0.92458800

C	-2.68712700	2.42783100	0.40900600
C	-2.90254800	1.38835600	-0.49598200
H	-2.02524200	-0.25825300	-1.59758000
H	0.23886600	0.10757800	-0.68953500
H	-1.20709600	3.42522200	1.63382300
H	-3.51270100	3.06911600	0.70773500
N	0.92224100	2.04961500	1.10416200
N	1.89014700	1.40333800	0.89030900
B	0.31683100	-1.52657100	-2.81898800
F	-0.04880300	-0.32835800	-3.43150500
F	-0.78130200	-2.03802400	-2.11087400
F	1.36457100	-1.28284500	-1.91497900
F	0.72763700	-2.44980900	-3.77582400
C	-4.28148200	1.22335000	-1.05562200
F	-4.42235800	0.09572100	-1.75648700
F	-4.59816000	2.24171700	-1.87029900
F	-5.20635400	1.21287500	-0.08456800

TS2'

C	-1.86960200	0.56764900	-0.90641400
C	-0.58550700	0.75699900	-0.39077300
C	-0.43924000	1.77592600	0.51503000
C	-1.42446600	2.62494900	0.96129600
C	-2.69763800	2.42269900	0.43594000
C	-2.90787600	1.39606700	-0.48853200
H	-2.03275400	-0.23204700	-1.62315900
H	0.24464500	0.12362100	-0.70608200
H	-1.21870900	3.40933200	1.68573600
H	-3.52924700	3.05371900	0.74332900
N	1.30282200	2.07192800	1.24619800
N	2.13641100	1.38808700	0.89758900
B	0.34474100	-1.51705800	-2.81387700
F	-0.01398400	-0.31704500	-3.42707300
F	-0.75945400	-2.02696800	-2.11508200
F	1.38739400	-1.27687100	-1.90224100
F	0.76092300	-2.43934700	-3.76953400
C	-4.28580700	1.23947600	-1.04924200
F	-4.43014100	0.11872800	-1.76207000
F	-4.60498800	2.26532100	-1.85540000
F	-5.21398100	1.22064400	-0.08008000

ArCF₃'

C	-1.81529700	0.63588500	-0.99528400
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C	-0.53466600	0.82675000	-0.47850400
C	-0.40442900	1.77744000	0.50747300
C	-1.41668300	2.54902000	1.02284100
C	-2.69432900	2.34536900	0.49339500
C	-2.88153400	1.39285400	-0.50501600
H	-1.98917500	-0.10213100	-1.77622300
H	0.30740400	0.24533400	-0.84576100
H	-1.25166600	3.28744600	1.80362500
H	-3.53848500	2.92449400	0.85808300
C	-4.22911200	1.17041900	-1.11441600
F	-4.55962600	-0.12961800	-1.11881300
F	-5.20130200	1.82617600	-0.47332200
F	-4.25835800	1.56953700	-2.39602600

8'

Au	0.87923200	-0.38748700	1.46973300
P	1.48333400	1.72905800	2.40774700
C	0.37299800	2.96022500	1.68706900
C	0.39304400	4.26187900	2.21130000
C	-0.49429200	2.63081900	0.64493900
C	-0.44705800	5.22524300	1.67784700
H	1.05824800	4.52237100	3.03200200
C	-1.34368100	3.59982600	0.12281100
H	-0.52086800	1.62897400	0.22106200
C	-1.31485700	4.88820200	0.63908400
H	-0.43407800	6.23751400	2.07396800
H	-2.02591300	3.34381900	-0.68218200
C	1.36039600	1.89329200	4.20490700
C	2.49129900	1.79564200	5.02190600
C	0.09382800	2.07852700	4.77020400
C	2.34787900	1.87148100	6.39982000
H	3.48232700	1.67337400	4.59452600
C	-0.04423500	2.15035000	6.14838300
H	-0.78897800	2.16283700	4.14019900
C	1.08314400	2.04020600	6.95635200
H	3.22150800	1.80208900	7.04273800
H	-1.02648700	2.28351300	6.59172500
C	3.19704400	2.01407800	1.91382200
C	3.55031100	3.16344200	1.20946800
C	4.15361000	1.03255300	2.20591600
C	4.87047900	3.34261800	0.80906700
H	2.80710700	3.91568500	0.95800800
C	5.46624100	1.21928900	1.80974300
H	3.87411300	0.11462000	2.72245900

C	5.81805300	2.37331800	1.10860800
H	5.15351500	4.23202100	0.25535500
H	6.21561900	0.46281800	2.02865200
C	0.82138700	-1.43381400	4.24729400
C	0.02685800	-0.83076500	3.28024000
C	-1.32042500	-0.56531200	3.49714300
C	-1.89398800	-0.95251500	4.70569300
C	-1.11148700	-1.57661900	5.67578900
C	0.24116600	-1.81841500	5.45308800
H	1.88108400	-1.61357900	4.07249000
H	-1.92390300	-0.06216400	2.74276800
H	-2.94594000	-0.75363500	4.89822900
H	0.84384300	-2.30214500	6.21707000
Cl	1.97392600	0.24023300	-0.63470700
C	0.97237900	2.06928800	8.45266900
C	7.25097200	2.53163800	0.69248600
C	-2.21547200	5.96158500	0.10052900
F	-3.01749400	5.51677800	-0.86712900
F	-1.50077500	6.97768400	-0.39758900
F	-2.98804700	6.46821500	1.06880600
F	7.45036100	3.62285800	-0.04827300
F	8.05181400	2.61429800	1.76226700
F	7.66406600	1.47591100	-0.01837600
F	1.28982700	0.87731700	8.97406600
F	1.81781400	2.96083000	8.98179200
F	-0.25674800	2.37722600	8.86778100
C	-1.11093500	-3.54457100	2.04779500
C	0.12853000	-3.34026000	1.45769200
C	0.24105500	-2.48021900	0.34532900
C	-0.90651000	-1.82447100	-0.18561400
C	-2.13346800	-2.03119400	0.45050300
C	-2.23841000	-2.89521100	1.53335200
H	1.01341800	-3.83085100	1.85444800
H	1.16994400	-2.47324900	-0.22538600
H	-3.02131900	-1.52676100	0.07627500
H	-3.19672900	-3.06549300	2.01877300
B	-0.84867100	-0.95534300	-1.50941100
O	-0.20826700	-1.50672700	-2.56765000
H	-0.18205100	-0.96791000	-3.36511800
O	-1.53421600	0.22036000	-1.48286200
H	-1.53216700	0.71728400	-2.30833000
C	-1.29002100	-4.37133100	3.27015200
O	-0.12428800	-4.76420300	3.78661400
O	-2.36963200	-4.62327300	3.76069600

C	-0.21537000	-5.47026200	5.02667500
H	-0.76677500	-6.40538500	4.89749400
H	0.81007300	-5.67114700	5.33507200
H	-0.72709800	-4.85174900	5.77105000
C	-1.76448000	-2.01125800	6.95123400
F	-0.87406900	-2.33544600	7.89293300
F	-2.53995700	-3.08884600	6.75228200
F	-2.55572100	-1.05533400	7.45148200

³1'

C	-2.14484100	0.11299100	-0.66337900
C	-0.79254900	0.25283400	-0.22844600
C	-0.35018700	1.51166700	0.29633100
C	-1.20366200	2.57941300	0.38537600
C	-2.53150000	2.42171300	-0.04423500
C	-2.98837500	1.18395700	-0.56335400
H	-2.46428000	-0.83648600	-1.07852600
H	-0.15422500	-0.62421000	-0.12587300
H	-0.84878700	3.52599000	0.78061200
H	-3.21717100	3.26409000	0.01392000
N	1.01221300	1.69747600	0.72222700
N	1.83306400	0.84599700	0.64140200
B	0.46558700	-0.85584900	-2.54734900
F	0.11797700	0.50373900	-2.10604800
F	-0.72045900	-1.56508700	-2.60770600
F	1.30201500	-1.37996100	-1.57712100
F	1.07467100	-0.74129500	-3.76653700
C	-4.42653100	1.10326000	-1.00077000
F	-4.74477500	-0.10657500	-1.44706300
F	-4.66230700	1.98622600	-1.97239900
F	-5.23544100	1.40402500	0.01651800

³TS3'

C	-2.15083600	0.10331900	-0.64959700
C	-0.80166700	0.23665900	-0.19136200
C	-0.39795400	1.49217500	0.32444200
C	-1.20334600	2.58282000	0.41618600
C	-2.52969000	2.42275900	-0.01931900
C	-2.98380300	1.18069100	-0.55026600
H	-2.47292800	-0.84134900	-1.07354000
H	-0.16032400	-0.63928900	-0.08979100
H	-0.84382600	3.53269000	0.80147200
H	-3.22100500	3.26174000	0.03486900
N	1.39251300	1.74268700	0.69918800

N	2.10844800	0.89042600	0.48732000
B	0.50219400	-0.84461400	-2.51769200
F	0.17838100	0.51094900	-2.07178600
F	-0.69508100	-1.53632500	-2.59780200
F	1.31994700	-1.39957500	-1.54580200
F	1.12800400	-0.73855600	-3.73142800
C	-4.41744800	1.11329000	-1.00283700
F	-4.74038800	-0.08929200	-1.46544700
F	-4.63905200	2.00808000	-1.96766000
F	-5.23549500	1.40882900	0.00926500

³TS4'

C	-2.25058200	0.50315100	-1.01794200
C	-0.90308000	0.85523800	-1.14456400
C	-0.51391500	1.99420100	-0.49251400
C	-1.34430100	2.82364800	0.25480900
C	-2.70188700	2.48835500	0.32268800
C	-3.13694800	1.32071200	-0.28594900
H	-2.61908400	-0.41293000	-1.47576400
H	-0.19284100	0.22520200	-1.67993100
H	-0.95258900	3.71710400	0.73717100
H	-3.39470000	3.12027800	0.87272900
N	1.29374000	2.46037500	-0.46233900
N	2.03095500	1.76174200	-0.96578200
B	2.43089500	-1.90583400	-1.82285500
F	1.38721800	-1.07585000	-2.22372500
F	1.87277900	-3.04127300	-1.18465700
F	3.21303700	-1.23074000	-0.85863400
F	3.20791300	-2.28866400	-2.88699700
C	-2.98046400	1.06450800	3.25532400
C	-3.21923000	-0.15251700	2.63660200
C	-2.17467900	-0.80488900	1.91946200
C	-0.88058800	-0.28489600	1.85650400
C	-0.65506900	0.93374500	2.49379000
C	-1.70028800	1.61852500	3.17565900
H	-4.20606600	-0.60458100	2.68732000
H	-2.39098500	-1.74673200	1.41720300
H	0.34076900	1.37386300	2.47992800
H	-1.51488500	2.58152400	3.64755500
B	0.24147500	-0.99431400	0.98953500
O	-0.16981700	-2.04686500	0.24754300
H	0.52398800	-2.46567900	-0.29722800
O	1.47438700	-0.44430700	1.05291400
H	2.14388900	-0.79344600	0.43455200

C	-4.04826800	1.84870800	3.93324700
O	-5.19590400	1.18104500	3.99076300
O	-3.87722400	2.96967600	4.36056500
C	-6.28447400	1.87529700	4.60985200
H	-6.51418300	2.78910400	4.05563000
H	-7.13060400	1.19027200	4.58285200
H	-6.03183500	2.13226300	5.64183800
C	-4.58852600	0.93577900	-0.22528100
F	-5.24199000	1.33615700	-1.31667300
F	-4.73399300	-0.39153900	-0.13772700
F	-5.19742900	1.47846300	0.83457100

³Ar_{CF₃}⁺

C	-1.79649100	0.48702100	-0.91956100
C	-0.54649700	0.70491600	-0.39785600
C	-0.42657100	1.78810800	0.49896100
C	-1.43765500	2.66655300	0.91812800
C	-2.67695200	2.43527000	0.38584200
C	-2.85254600	1.34963700	-0.53118500
H	-1.98805700	-0.32165700	-1.61736300
H	0.30699500	0.08546500	-0.65610100
H	-1.24397300	3.47270400	1.61834900
H	-3.53098700	3.05513100	0.64521900
C	-4.24199200	1.17581600	-1.11070100
F	-4.34722000	0.07295700	-1.83333700
F	-4.51254000	2.22598100	-1.88002200
F	-5.13123000	1.13568600	-0.12465700

D'

Au	0.48650700	-0.34636700	1.61058100
P	1.26202100	1.79139400	2.40093200
C	0.18744300	3.09779600	1.75313400
C	-0.28311300	4.13285600	2.56775900
C	-0.12306200	3.07558800	0.38920000
C	-1.08274900	5.12436200	2.01832800
H	-0.02478000	4.17272700	3.62251600
C	-0.92086600	4.07172300	-0.15584500
H	0.26072900	2.29132400	-0.26025400
C	-1.40389700	5.08615300	0.66370200
H	-1.45530600	5.92995700	2.64593400
H	-1.16764800	4.05649400	-1.21260700
C	1.32548500	1.87873800	4.20373700
C	2.55084700	1.78351600	4.86923400

C	0.12610200	1.87233700	4.92504400
C	2.57088900	1.65049300	6.25125700
H	3.48655800	1.79104000	4.31531800
C	0.15149200	1.74405300	6.30546000
H	-0.83411100	1.94136700	4.41646700
C	1.37345400	1.61274400	6.95943800
H	3.51792700	1.55936700	6.77650100
H	-0.77657200	1.73521400	6.86835300
C	2.92407100	2.07677800	1.73569200
C	3.31790100	3.38252200	1.42948200
C	3.82129100	1.01202700	1.58518100
C	4.61055700	3.62446600	0.98070000
H	2.62523200	4.21334900	1.54216000
C	5.10941100	1.25969800	1.13695300
H	3.52472200	-0.00909400	1.81841700
C	5.49744700	2.56421400	0.83828600
H	4.92470100	4.63644000	0.74469600
H	5.81456300	0.44108400	1.01879900
C	1.11908100	-1.35043900	4.32556700
C	0.06590300	-0.98140500	3.51485100
C	-1.26791100	-1.00174300	3.87619400
C	-1.55231600	-1.38263400	5.18531600
C	-0.52108700	-1.73197100	6.05401700
C	0.80411000	-1.71994600	5.63386900
H	2.15302800	-1.34329600	3.99270500
H	-2.06390300	-0.72833600	3.19052600
H	-2.58641700	-1.40711800	5.51976100
H	1.60385700	-1.98686800	6.31935200
Cl	-0.26454500	-2.41865100	0.72982500
C	1.42450600	1.32518600	8.43081900
C	6.89197900	2.78179500	0.32755600
C	-2.29175200	6.16797100	0.12155200
F	-2.49721000	6.05075600	-1.19092200
F	-1.76596000	7.37782300	0.34505000
F	-3.48703800	6.14833100	0.72456500
F	7.20711700	4.07471800	0.24197500
F	7.79233800	2.19466100	1.12447000
F	7.04242300	2.24533700	-0.88924500
F	1.73633100	0.03689100	8.64197500
F	2.36115300	2.05583200	9.04295200
F	0.26069400	1.55872700	9.03650500
C	-0.87489900	-2.07300100	7.47161300
F	-1.22449000	-0.97348900	8.15604200
F	0.13674900	-2.64757600	8.12310000

F	-1.91981600	-2.90577600	7.52441000
Ar_{CF₃}N₂⁺			
C	-2.70128600	0.24853400	-0.39768500
C	-1.32273800	0.18296600	-0.46852900
C	-0.61423100	1.32360800	-0.07122200
C	-1.20335000	2.50852200	0.38793900
C	-2.58297100	2.53608000	0.44588000
C	-3.31740300	1.41544500	0.05403700
H	-3.29808400	-0.60636400	-0.69750100
H	-0.80499700	-0.70497100	-0.81463200
H	-0.59558400	3.35833200	0.67871300
H	-3.09105800	3.43228000	0.78765700
N	0.76234400	1.27715800	-0.13918300
N	1.87095500	1.23731700	-0.19587200
C	-4.82017800	1.46175400	0.17715500
F	-5.28880200	2.67687900	-0.10425300
F	-5.18539800	1.16504800	1.42585300
F	-5.40730200	0.59023500	-0.63969900
Ar_{CF₃}N₂[•]			
C	-2.73027600	0.18151400	-0.29175100
C	-1.34530500	0.09168000	-0.37855000
C	-0.57680000	1.21373000	-0.10500900
C	-1.15113700	2.43304500	0.25318800
C	-2.52954100	2.51743700	0.33690800
C	-3.31209900	1.39201200	0.06573300
H	-3.35221400	-0.68383500	-0.49873400
H	-0.85149600	-0.83635800	-0.65344000
H	-0.51348100	3.28854100	0.46088700
H	-3.00831000	3.45305600	0.61611700
N	0.86458200	1.05412800	-0.21163600
N	1.64543200	1.91729300	-0.00029500
C	-4.80047200	1.54114300	0.14830600
F	-5.43987600	0.37637300	0.02489800
F	-5.25825100	2.35504500	-0.81348600
F	-5.16995400	2.08411800	1.31611500
10'			
Au	-0.19703500	-0.97520000	-1.21707500
P	0.45491100	1.16175200	-0.35591800
C	-0.39141300	2.42469900	-1.33787200

C	-0.44526600	3.74175100	-0.86637700
C	-0.93305300	2.10163700	-2.58626300
C	-1.05331100	4.72633000	-1.63403400
H	-0.01240300	4.00693500	0.09600100
C	-1.54005700	3.08848200	-3.34900400
H	-0.87748500	1.08418400	-2.97065700
C	-1.60116600	4.39377300	-2.86808000
H	-1.09885600	5.74780700	-1.27042400
H	-1.96676100	2.84309100	-4.31799500
C	-0.01211900	1.37688800	1.37851500
C	0.77523400	0.83875200	2.39930200
C	-1.26647700	1.93134400	1.67296400
C	0.30002400	0.83681000	3.70618400
H	1.74212000	0.38714700	2.19662500
C	-1.72886400	1.93568400	2.97622400
H	-1.89807600	2.33640200	0.88681600
C	-0.95117800	1.37061100	3.98718500
H	0.90165100	0.39785100	4.49589000
H	-2.70684100	2.35497000	3.20014700
C	2.24541000	1.38445000	-0.57247300
C	2.69445600	2.47583300	-1.32590500
C	3.16287000	0.47647600	-0.03167000
C	4.05453100	2.66954000	-1.51380900
H	1.99530300	3.17684800	-1.77210200
C	4.52316000	0.68505100	-0.21714300
H	2.83416200	-0.40880100	0.50526400
C	4.96487600	1.77633700	-0.95616000
H	4.40381700	3.51576900	-2.10026200
H	5.23659800	-0.01540400	0.20591000
C	-1.64166500	-1.36895000	1.38154100
C	-1.77305200	-0.84683300	0.10371600
C	-2.95226200	-0.24973700	-0.33333400
C	-4.02880700	-0.17219800	0.54794800
C	-3.90853100	-0.68713500	1.83782700
C	-2.72767000	-1.29361900	2.25079100
H	-0.70614100	-1.79703500	1.72919800
H	-3.05089100	0.14703200	-1.34304100
H	-4.95756200	0.29701500	0.22917300
H	-2.63657600	-1.69294300	3.25686800
Cl	1.55938400	-0.85240900	-2.96287200
C	-1.53093700	1.32503400	5.36926100
C	6.42553600	2.02475100	-1.18798200
C	-2.30500600	5.42034600	-3.70751700
F	-1.82689200	5.43364100	-4.95647100

F	-2.18612000	6.65282900	-3.21349300
F	-3.61179200	5.14238100	-3.79599100
F	6.79755600	3.20764000	-0.68131800
F	7.19921000	1.08836200	-0.63664800
F	6.70407900	2.06160600	-2.49710800
F	-2.67148800	0.61969400	5.38193100
F	-0.70389100	0.77005700	6.25556300
F	-1.83303900	2.55316500	5.80819100
C	-2.70122900	-3.57247000	-0.98482600
C	-2.09090200	-4.26133400	0.06225000
C	-0.71019400	-4.46865200	0.07135100
C	0.10608900	-3.98699200	-0.94830300
C	-0.52037400	-3.27204500	-2.00926400
C	-1.91844400	-3.09520800	-2.03413600
H	-2.70133200	-4.63704900	0.87903300
H	-0.25726900	-5.02111300	0.89056500
H	0.04382100	-3.05524100	-2.91591300
H	-2.39646300	-2.58616400	-2.86889100
B	1.65423700	-4.33360000	-0.95143400
O	2.61609300	-3.55200300	-1.49974800
H	2.33030000	-2.69097800	-1.84279900
O	1.96954800	-5.56519600	-0.47003200
H	2.92265600	-5.70615800	-0.46514900
C	-4.15406700	-3.26458100	-1.00994600
O	-4.75231000	-3.56691000	0.14294000
O	-4.72357400	-2.77178400	-1.96141900
C	-6.14831300	-3.26883700	0.20811100
H	-6.69847200	-3.84509900	-0.54057100
H	-6.46756900	-3.54337700	1.21328400
H	-6.31614400	-2.20164700	0.03747400
B	1.89111100	-2.42107600	2.04895000
F	2.98182500	-1.66156500	2.46176400
F	2.27226700	-3.70022000	1.67799600
F	1.33438900	-1.77158200	0.90159200
F	0.91917800	-2.46037000	3.04075500
C	-5.03198800	-0.47917600	2.80475300
F	-5.07774800	0.79659000	3.22128700
F	-4.92027300	-1.24327100	3.89330900
F	-6.22379200	-0.73818200	2.24805200
1_{OMe}			
C	-1.55045200	0.46451000	-0.24264000
C	-0.29260200	0.88087100	0.10938300
C	-0.14956100	2.14338900	0.72131400

C	-1.24614900	2.99915100	0.98148500
C	-2.48887200	2.57388600	0.60508400
C	-2.65342200	1.31511000	-0.02121600
H	-1.67031700	-0.51465100	-0.69688900
H	0.56841100	0.25324100	-0.09734700
H	-1.08983900	3.96234300	1.45616600
H	-3.36728400	3.19057400	0.76582500
B	-0.90334600	-1.60657600	-2.74972000
F	-1.57629300	-0.50384800	-3.28957100
F	-1.75180400	-2.22671900	-1.81101700
F	0.25178700	-1.17299800	-2.08502000
F	-0.57111600	-2.50574200	-3.75109300
O	-3.88638800	1.01638100	-0.38204100
C	-4.12170600	-0.20365100	-1.09895100
H	-5.17343500	-0.17746500	-1.38111600
H	-3.48004000	-0.26046600	-1.98427500
H	-3.92934100	-1.06724200	-0.45448900
N	1.08991800	2.55790700	1.06795200
N	2.11549700	2.89982800	1.35592700

14"

C	-2.44378200	0.46738200	-0.96237200
C	-1.12103900	0.41275900	-1.31012500
C	-0.34876100	1.57919300	-1.12242400
C	-0.88346700	2.78376600	-0.63165700
C	-2.21352900	2.81492900	-0.28837800
C	-2.99608300	1.64980800	-0.42243400
H	-3.08573800	-0.40300600	-1.05685700
H	-0.65083600	-0.48911300	-1.68979300
H	-0.25064700	3.65790800	-0.51777400
H	-2.63837300	3.73210900	0.10393100
N	0.98032700	1.53920900	-1.39762100
N	2.07644000	1.51389400	-1.60578600
B	2.52539100	-1.78480000	-1.61106700
F	1.32394200	-1.19250600	-2.02043200
F	2.22511600	-2.88660500	-0.78309700
F	3.22727800	-0.84367300	-0.82245400
F	3.27984000	-2.17684100	-2.68504900
C	-3.21681000	0.92826000	3.14461200
C	-3.29253300	-0.38629200	2.67202100
C	-2.17313800	-0.97513300	2.10223000
C	-0.96195800	-0.27903600	1.97846200
C	-0.90075700	1.02810400	2.47761100
C	-2.01197300	1.63025800	3.05267500

H	-4.22880900	-0.93253000	2.74442300
H	-2.23744900	-1.99143700	1.71761600
H	0.02967300	1.58706000	2.38815300
H	-1.97344000	2.65296200	3.42151100
B	0.25397700	-0.92156700	1.21187700
O	0.09180700	-2.18131700	0.73257100
H	0.84796900	-2.51840800	0.22070700
O	1.36167900	-0.14626900	1.03486900
H	2.08300300	-0.53451000	0.50999500
C	-4.38843600	1.63301300	3.71498800
O	-5.49717700	0.88241200	3.70204200
O	-4.36904000	2.77814100	4.12414400
C	-6.67537600	1.51971500	4.19504900
H	-6.92010100	2.39566400	3.58570500
H	-7.47083000	0.77798200	4.12621700
H	-6.53821400	1.83648800	5.23259400
O	-4.26229300	1.56528200	-0.04722400
C	-4.89405200	2.69698400	0.54890900
H	-4.97437500	3.52039200	-0.16855500
H	-5.89195800	2.36331000	0.83517900
H	-4.34541200	3.02680300	1.44053000
³⁴"			
C	-2.08151300	0.63291400	-1.15763100
C	-0.82429000	0.58581700	-1.68854900
C	0.05346400	1.66502400	-1.43874700
C	-0.32700500	2.78546300	-0.67444400
C	-1.59849400	2.86779600	-0.17550500
C	-2.50251600	1.78935200	-0.42389600
H	-2.80381400	-0.16699200	-1.29502900
H	-0.46169900	-0.26996800	-2.25005500
H	0.40252300	3.57070500	-0.50083700
H	-1.91375900	3.73150200	0.40022500
N	1.39996000	1.66447400	-1.93660100
N	1.71875600	1.06575300	-2.91118900
B	2.50902500	-1.86681400	-1.36551100
F	1.32634100	-1.50325300	-2.00980500
F	2.20116100	-2.87726900	-0.42533600
F	2.99429500	-0.75322100	-0.64045100
F	3.45489400	-2.30804700	-2.25497500
C	-3.59368800	0.84203900	3.18261000
C	-3.64536400	-0.41117700	2.55686200
C	-2.52542800	-0.89885100	1.89959400
C	-1.33589000	-0.16003600	1.84149500

C	-1.30811100	1.10200100	2.46804200
C	-2.42088000	1.59688200	3.13667300
H	-4.56401200	-0.98971200	2.59401300
H	-2.56352200	-1.87392000	1.41785500
H	-0.38727000	1.68155100	2.43867300
H	-2.39828200	2.56524100	3.63180200
B	-0.06092500	-0.72077800	1.10225300
O	-0.09702000	-2.01569400	0.71015500
H	0.70676500	-2.35036300	0.27151500
O	0.95936100	0.16087900	0.90490000
H	1.73374000	-0.18151000	0.42021000
C	-4.76509600	1.42171900	3.88755800
O	-5.76807100	0.54841700	4.01201700
O	-4.81231000	2.56326900	4.29956300
C	-6.93494000	1.03953300	4.67402500
H	-7.35732100	1.88875900	4.12954200
H	-7.64205700	0.21083800	4.69124100
H	-6.69309200	1.35405500	5.69306200
O	-3.74708100	1.77853000	-0.03859700
C	-4.34765400	2.93998500	0.56594300
H	-4.32013400	3.77461300	-0.13911900
H	-5.37724700	2.65529600	0.77612700
H	-3.83174400	3.19594100	1.49584700

5"

C	-1.88261500	0.69584100	-1.43235300
C	-0.53371400	0.98131800	-1.43283700
C	-0.08212800	2.12347900	-0.76217500
C	-0.97092900	2.96454400	-0.10820100
C	-2.33073700	2.67632400	-0.09891800
C	-2.78740700	1.53022300	-0.75398300
H	-2.27173700	-0.19565300	-1.91899900
H	0.18517300	0.31800700	-1.91025000
H	-0.58455400	3.84175200	0.40599700
H	-3.01483100	3.32820900	0.43504200
N	1.31408900	2.46642600	-0.69328800
N	2.19590600	1.82471300	-1.16171200
B	2.46103300	-2.11664400	-1.59636200
F	1.45509200	-1.42362700	-2.26180100
F	1.85391100	-3.12602900	-0.81067000
F	3.12110700	-1.23801300	-0.71246400
F	3.35844300	-2.67478400	-2.47665800
C	-3.22397800	0.99441900	3.32317700
C	-3.54225700	-0.04525100	2.44259200

C	-2.53554900	-0.65627300	1.70747600
C	-1.19898400	-0.25029100	1.81524900
C	-0.90260100	0.79257500	2.70223800
C	-1.89500300	1.40606500	3.45349600
H	-4.57555200	-0.36706800	2.33920200
H	-2.78787700	-1.46119400	1.01863300
H	0.12914700	1.12883400	2.79250400
H	-1.66379300	2.21519600	4.14228700
B	-0.06927800	-0.92471800	0.94494500
O	-0.40619400	-2.03090400	0.22675200
H	0.34281400	-2.43474500	-0.24597700
O	1.16801300	-0.36164400	0.99584800
H	1.83924300	-0.71775200	0.38643700
C	-4.25030800	1.69371700	4.12908300
O	-5.49638700	1.28505700	3.84369200
O	-4.01201700	2.55208200	4.95566300
C	-6.53468800	1.92427500	4.58346000
H	-6.51769600	3.00538900	4.41823600
H	-7.47092900	1.50148800	4.21875000
H	-6.42352900	1.72878000	5.65405900
O	-4.07591400	1.13368900	-0.78778200
C	-5.03452900	1.91739700	-0.10407800
H	-5.06960600	2.94210200	-0.49584800
H	-6.00036700	1.43723900	-0.26993100
H	-4.82822400	1.94619500	0.97499600

6''

C	-1.84457900	0.97837100	-0.97257500
C	-0.63649500	0.86678700	-0.30079300
C	-0.37189600	1.70261600	0.78243200
C	-1.30496200	2.65106100	1.20162300
C	-2.50774300	2.76977200	0.53173000
C	-2.78036500	1.93525300	-0.56099100
H	-2.03072900	0.31255300	-1.80908100
H	0.10327600	0.14091000	-0.63744500
H	-1.06699500	3.28659700	2.05131100
H	-3.25470300	3.50146300	0.82784200
N	0.86408400	1.63808000	1.52108400
N	1.75604500	0.88696400	1.30233300
B	0.14494600	-1.13680700	-3.09965600
F	-0.17779600	0.07586900	-3.70955300
F	-0.96548500	-1.60276500	-2.38079800
F	1.21336100	-0.94539000	-2.20921400
F	0.50390600	-2.07605800	-4.06435800

O	-3.97286000	2.12830600	-1.16113900
C	-4.27703500	1.34040400	-2.29726400
H	-4.32452700	0.27363000	-2.04451400
H	-5.25549100	1.67106200	-2.64866000
H	-3.53701800	1.48680000	-3.09442200

TS2''

C	-1.84364200	0.98316200	-0.97020300
C	-0.62443900	0.86926200	-0.29477400
C	-0.41408200	1.71626900	0.76223700
C	-1.29942500	2.66818300	1.21484700
C	-2.50651200	2.77908100	0.53429400
C	-2.77523400	1.93921500	-0.55600000
H	-2.03011600	0.31691400	-1.80700000
H	0.11632000	0.14209900	-0.63067200
H	-1.06477600	3.30652300	2.06418900
H	-3.25819900	3.50967900	0.82503700
N	1.25439000	1.58770000	1.73358100
N	1.99704500	0.80245100	1.39594800
B	0.16373300	-1.13667300	-3.09142700
F	-0.15972100	0.07579300	-3.70118200
F	-0.94600100	-1.60424600	-2.37323100
F	1.23239600	-0.94472300	-2.20107200
F	0.52412000	-2.07524900	-4.05664200
O	-3.97684500	2.13161300	-1.15524000
C	-4.27697000	1.34060900	-2.28626900
H	-4.31754600	0.27269800	-2.03352800
H	-5.25829600	1.66255400	-2.63911300
H	-3.53958100	1.48710500	-3.08691000

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C	-1.53231700	0.46533600	-0.24071400
C	-0.27391000	0.88299200	0.21286600
C	-0.18153700	2.12251400	0.79284300
C	-1.23884800	2.99064300	0.96149400
C	-2.48685500	2.57061500	0.50993600
C	-2.63368000	1.31221200	-0.08870500
H	-1.63673200	-0.51153200	-0.70436500
H	0.58752400	0.22812600	0.09848700
H	-1.12278900	3.96776100	1.42583700
H	-3.36763200	3.20151000	0.60893300
O	-3.89290300	1.00249500	-0.49049000
C	-4.09808200	-0.25235100	-1.10327000
H	-5.16113800	-0.31065500	-1.34329600

H	-3.51582900	-0.35005200	-2.02955200
H	-3.83688400	-1.07949600	-0.42936500

8"

Au	0.95749100	-0.39714400	1.45308200
P	1.52233600	1.71367200	2.40494300
C	0.36341600	2.91005700	1.69944900
C	0.31763900	4.20101700	2.24731800
C	-0.46580000	2.56677700	0.62983400
C	-0.55035100	5.13933200	1.71369200
H	0.95337100	4.47393300	3.08709000
C	-1.34187700	3.51063000	0.10618700
H	-0.44062800	1.57271800	0.18644700
C	-1.37955400	4.78819500	0.64853300
H	-0.58961700	6.14284900	2.12996200
H	-1.99181300	3.24255300	-0.72100800
C	1.43919800	1.87656400	4.20629900
C	2.59466500	1.80182600	4.98981500
C	0.18625500	2.02639400	4.81108300
C	2.49083500	1.86063200	6.37233100
H	3.57628700	1.70818500	4.53467300
C	0.08749500	2.08323200	6.19295000
H	-0.71745700	2.08515200	4.20887600
C	1.24017000	1.99390400	6.96767900
H	3.38510600	1.80816300	6.98793600
H	-0.88431800	2.19403500	6.66402000
C	3.21786100	2.05942200	1.88292800
C	3.52196000	3.23449000	1.19860000
C	4.21431200	1.11143200	2.15223900
C	4.83233000	3.47441300	0.79734800
H	2.74879100	3.96252900	0.96673100
C	5.51726500	1.35952700	1.75751300
H	3.97223600	0.17281600	2.65043000
C	5.81996100	2.54036800	1.07830700
H	5.07802100	4.38486100	0.26008100
H	6.29763100	0.63052000	1.96081000
C	0.88282300	-1.40934000	4.23671200
C	0.09315200	-0.80381300	3.26071100
C	-1.25366100	-0.55809500	3.46743800
C	-1.86148700	-1.01212900	4.64037800
C	-1.09483700	-1.67785100	5.59920300
C	0.28335500	-1.84955900	5.40496900
H	1.94922600	-1.56794900	4.08107000

H	-1.85346900	-0.03965900	2.71974200
H	-2.92589200	-0.85191700	4.78293400
H	0.85685700	-2.36364500	6.17295500
Cl	2.09245200	0.17529600	-0.65112100
C	1.17200600	2.00816700	8.46640600
C	7.24513600	2.76956400	0.66971300
C	-2.30677900	5.83705800	0.10730700
F	-3.09250800	5.37269800	-0.86470100
F	-1.61715400	6.87264500	-0.38648300
F	-3.09631100	6.32206900	1.07272900
F	7.39604900	3.87691700	-0.05846200
F	8.03713000	2.87841900	1.74395600
F	7.71058400	1.74194800	-0.05012500
F	1.51753600	0.81579500	8.96861300
F	2.02151100	2.90500000	8.98034500
F	-0.04853400	2.29815300	8.91921700
C	-1.26802800	-3.44048800	2.05453500
C	0.00841600	-3.35958500	1.51383200
C	0.23758900	-2.55498800	0.38026100
C	-0.82754500	-1.83733300	-0.23017000
C	-2.09699700	-1.92560100	0.35122300
C	-2.31700400	-2.72823600	1.46161500
H	0.83348600	-3.89336000	1.97782400
H	1.19708800	-2.62054600	-0.13379000
H	-2.92467400	-1.37414400	-0.08861100
H	-3.30464400	-2.80128600	1.91125600
B	-0.64421900	-1.03663800	-1.58414200
O	0.03893600	-1.66523600	-2.57182400
H	0.15423300	-1.15963500	-3.38309100
O	-1.28598100	0.16203500	-1.66183500
H	-1.20754400	0.61812500	-2.50637900
C	-1.56738600	-4.16740700	3.31753600
O	-0.47781900	-4.70394400	3.86712900
O	-2.67438000	-4.22930300	3.81150000
C	-0.67669200	-5.30685000	5.14921200
H	-1.39674100	-6.12649800	5.07992200
H	0.29856300	-5.68051700	5.45996300
H	-1.04509600	-4.56050400	5.86339100
O	-1.58921500	-2.19905200	6.74267100
C	-2.99567300	-2.18869300	6.91338600
H	-3.19684200	-2.71641800	7.84653000
H	-3.38368800	-1.16490600	6.98879700
H	-3.49055000	-2.70876200	6.08288000

³1''

C	-1.51523600	0.41600400	-0.22883000
C	-0.28998000	0.86550300	0.16485900
C	-0.16968200	2.15079600	0.75309300
C	-1.28088800	3.00009600	0.94555500
C	-2.51272600	2.57728100	0.54072600
C	-2.64372400	1.28218900	-0.06673500
H	-1.63289800	-0.57688900	-0.65685000
H	0.59532500	0.25062000	0.03142900
H	-1.12693000	3.97164400	1.40476500
H	-3.40689600	3.18338100	0.64505500
N	1.09884600	2.66056900	1.19097000
N	2.11242900	2.05038000	1.07347500
B	-1.01294500	-1.59341700	-2.80054400
F	-1.71047000	-0.46811600	-3.26918100
F	-1.81172800	-2.21750500	-1.81747100
F	0.18166100	-1.18410100	-2.20401600
F	-0.76569100	-2.47284900	-3.83901200
O	-3.84017200	0.97935100	-0.45640800
C	-4.11387000	-0.27324700	-1.13276300
H	-5.15573500	-0.20431000	-1.43658700
H	-3.44121700	-0.38240900	-1.98841600
H	-3.97021600	-1.09631100	-0.42828200

³TS3''

C	-1.50579000	0.41797700	-0.22222200
C	-0.27428900	0.87092000	0.17122100
C	-0.20136600	2.14398900	0.74299800
C	-1.27220700	3.01595600	0.95339600
C	-2.50588200	2.58693600	0.54746100
C	-2.63195100	1.28854800	-0.05787500
H	-1.62721300	-0.57559200	-0.64861900
H	0.61647500	0.26106200	0.03985300
H	-1.11756800	3.98878200	1.41151600
H	-3.40452900	3.18834000	0.64781300
N	1.44567300	2.76987000	1.28264700
N	2.34712400	2.10194200	1.11490000
B	-0.99783200	-1.58611200	-2.79448600
F	-1.69475000	-0.46021000	-3.26229200
F	-1.79871700	-2.21358200	-1.81535800
F	0.19511800	-1.17767700	-2.19410000
F	-0.74722200	-2.46288600	-3.83466000
O	-3.83101900	0.98466200	-0.44724500
C	-4.10264300	-0.26644100	-1.12486100

H	-5.14447100	-0.19907100	-1.42959600
H	-3.43015800	-0.37459900	-1.98079700
H	-3.95900200	-1.09135200	-0.42240400
³TS4''			
C	-2.07892900	-0.91349900	-1.30307100
C	-0.80220600	-0.42691700	-1.40085700
C	-0.63941300	0.94182900	-1.17196700
C	-1.66044500	1.85401700	-0.89308900
C	-2.94228600	1.37303500	-0.79536100
C	-3.15932000	-0.02461300	-0.98138500
H	-2.31794600	-1.96447200	-1.44086800
H	0.05486000	-1.06757700	-1.60946300
H	-1.43238300	2.90854000	-0.75809400
H	-3.77375600	2.03885800	-0.58550900
N	1.05031500	1.67798600	-1.25131700
N	1.92716200	0.97873100	-1.42159500
B	2.84197300	-2.78107800	-0.61356900
F	1.80071200	-2.17548000	-1.31591200
F	2.27909200	-3.62024300	0.37642600
F	3.58145400	-1.77949100	0.05273200
F	3.65732100	-3.50464600	-1.44765600
C	-2.87867400	1.79292400	2.46217700
C	-3.09349100	0.41823900	2.27156600
C	-2.01699100	-0.42324400	2.00520700
C	-0.71680500	0.07661100	1.88937200
C	-0.52421000	1.45461500	2.07625100
C	-1.58841400	2.30460500	2.38273300
H	-4.09837900	0.01278900	2.36391700
H	-2.18736000	-1.49009300	1.87047700
H	0.48054100	1.86242500	1.97864600
H	-1.43284400	3.37014000	2.53226600
B	0.47965300	-0.87093300	1.48099200
O	0.18722400	-2.18603600	1.32493200
H	0.92680900	-2.74205700	1.01806900
O	1.68273900	-0.27592100	1.28456800
H	2.39094600	-0.83464100	0.91596800
C	-3.99823500	2.73316200	2.71278000
O	-5.18927700	2.17205800	2.45860800
O	-3.86367400	3.88028200	3.08118400
C	-6.32626500	3.00705800	2.69181800
H	-6.28270000	3.89857000	2.06043900
H	-7.19841200	2.40504300	2.43839000
H	-6.36592000	3.31276500	3.74083100

O	-4.32815800	-0.59866300	-0.88977500
C	-5.50055400	0.16350900	-0.55638900
H	-6.30878100	-0.56200100	-0.49213500
H	-5.36364900	0.66652300	0.40787400
H	-5.70819400	0.89152600	-1.34506700
³Ar_{OMe}⁺			
C	-1.48407000	0.42740100	-0.24533600
C	-0.26329800	0.85915600	0.20513100
C	-0.20912400	2.12999400	0.78867500
C	-1.27169600	3.01663500	0.96465800
C	-2.49403800	2.59118300	0.51775800
C	-2.61340800	1.29445600	-0.09191000
H	-1.59404000	-0.54828100	-0.70767800
H	0.62262000	0.23803600	0.11357200
H	-1.14154200	3.98943300	1.42870300
H	-3.39435300	3.19345500	0.59819400
O	-3.81499500	0.99341200	-0.48013600
C	-4.11572800	-0.26671600	-1.11379400
H	-5.18386400	-0.23744100	-1.31571500
H	-3.55452200	-0.35171500	-2.04736300
H	-3.87955700	-1.08889000	-0.43411900
D''			
Au	1.12895200	-0.48160400	1.68643700
P	1.55878600	1.73728700	2.47503200
C	0.31278400	2.91827500	1.91241800
C	0.26511200	4.19009100	2.50180900
C	-0.56043600	2.58767200	0.87536700
C	-0.65146800	5.12210000	2.04329500
H	0.93969800	4.45115900	3.31454100
C	-1.48162800	3.52530200	0.42188800
H	-0.53363400	1.60154200	0.41668100
C	-1.52074700	4.78423500	1.00650900
H	-0.69415900	6.11090600	2.49303700
H	-2.16679400	3.27413000	-0.38126000
C	1.65364100	1.85830200	4.27784300
C	2.87041500	1.67857700	4.94186800
C	0.46308100	1.97657100	5.00211800
C	2.88780500	1.58905400	6.32645500
H	3.80292600	1.60175800	4.38825600
C	0.48513200	1.88526700	6.38671700
H	-0.49016600	2.10796100	4.49389600
C	1.69562600	1.67774800	7.04010400

H	3.82836000	1.44238500	6.85111800
H	-0.43956700	1.95424800	6.95344200
C	3.16501500	2.15187100	1.74563400
C	3.36472700	3.36427900	1.08332800
C	4.19937500	1.20777800	1.82607200
C	4.60227000	3.64003400	0.51229900
H	2.56372200	4.09456000	1.00289400
C	5.43162800	1.49063700	1.26030700
H	4.04464400	0.25001700	2.32216800
C	5.62567400	2.70532400	0.60320500
H	4.76346300	4.58066700	-0.00468500
H	6.23858100	0.76468400	1.31966900
C	0.87772400	-1.25082900	4.52046400
C	0.12900100	-0.83608200	3.44091200
C	-1.23801000	-0.62553700	3.45284900
C	-1.88644700	-0.82211600	4.66514200
C	-1.17131900	-1.21459300	5.80482100
C	0.20708600	-1.44304600	5.72950500
H	1.95328900	-1.39713400	4.46005200
H	-1.78787000	-0.30991000	2.57012000
H	-2.95823500	-0.66370500	4.74884100
H	0.78341400	-1.74312500	6.60000200
Cl	0.76913100	-2.67667900	0.85284900
C	1.73915800	1.45367200	8.52162800
C	6.97316200	2.96019600	-0.00664500
C	-2.50137300	5.82267900	0.54457800
F	-3.28147500	5.38347000	-0.44350000
F	-1.86825700	6.91797000	0.10818600
F	-3.29575300	6.20907900	1.54952200
F	7.03897300	4.13701000	-0.63028100
F	7.93085000	2.94059300	0.92852800
F	7.28140400	2.00923400	-0.89704200
F	1.96277700	0.15549400	8.78806100
F	2.72597400	2.14269300	9.09951200
F	0.59616300	1.78928700	9.12292700
O	-1.89775000	-1.33567800	6.93090000
C	-1.21520800	-1.64291000	8.13353000
H	-0.71656400	-2.61830100	8.07322300
H	-0.47535600	-0.86921600	8.37604100
H	-1.97268400	-1.67517200	8.91720000
AroMeN₂⁺			
C	-1.52734000	0.48783800	-0.30034300
C	-0.27704700	0.88945700	0.09897900

C	-0.14570700	2.14209000	0.72965400
C	-1.24220900	3.00178600	0.96796900
C	-2.47828400	2.58276200	0.56323600
C	-2.63777300	1.32864700	-0.07127500
H	-1.64614800	-0.47366200	-0.78693900
H	0.59485800	0.26433500	-0.06341200
H	-1.09345500	3.95949100	1.45582600
H	-3.35953900	3.19660100	0.71817400
O	-3.87409700	1.02655000	-0.41734400
C	-4.14244300	-0.21650800	-1.06928000
H	-5.21700500	-0.23290200	-1.24439300
H	-3.61162200	-0.27225500	-2.02497600
H	-3.86024800	-1.05790500	-0.42842100
N	1.08789400	2.53898800	1.12484700
N	2.10458200	2.86840400	1.45187100

Ar_{OMe}N₂•

C	-2.63288700	0.10703400	-0.23638800
C	-1.25023400	0.09289600	-0.37593100
C	-0.50957200	1.23934900	-0.12277500
C	-1.13872100	2.42460000	0.27423000
C	-2.50939200	2.44586600	0.41508900
C	-3.26628100	1.28840800	0.16155700
H	-3.20074600	-0.79532100	-0.43777200
H	-0.73114800	-0.81214600	-0.68258300
H	-0.53801600	3.31067500	0.46669900
H	-3.03484200	3.34698600	0.72084000
N	0.91862900	1.14752900	-0.28697200
N	1.68355800	2.03632100	-0.10751400
O	-4.59498300	1.41991000	0.33094700
C	-5.41622700	0.29236000	0.08640700
H	-6.44056300	0.60920300	0.28615100
H	-5.33728000	-0.04026000	-0.95630200
H	-5.15888100	-0.54086000	0.75241100

10''

Au	-0.17864700	-0.95839400	-1.19883500
P	0.45938400	1.17274600	-0.32505700
C	-0.38793600	2.45480800	-1.27991000
C	-0.46898300	3.75452500	-0.76788600
C	-0.88064000	2.16829000	-2.55707500
C	-1.05666400	4.75946400	-1.52525000
H	-0.07233500	3.98873300	0.21775100
C	-1.46823400	3.17477300	-3.30908400

H	-0.79971100	1.16377000	-2.97026500
C	-1.55619300	4.46342800	-2.78873900
H	-1.12294300	5.76867600	-1.13151400
H	-1.85597700	2.96040700	-4.30150100
C	0.04447900	1.38583600	1.42362500
C	0.89059100	0.87993300	2.41275500
C	-1.21035100	1.90786300	1.76963400
C	0.47352500	0.87192600	3.73850500
H	1.85901800	0.45117800	2.17487800
C	-1.61106400	1.91687500	3.09440800
H	-1.89482900	2.27851500	1.01033000
C	-0.77374000	1.38199100	4.07290300
H	1.12117300	0.45208600	4.50210100
H	-2.58480900	2.31829600	3.36561900
C	2.24679100	1.38428500	-0.58204400
C	2.68620200	2.46586900	-1.35468600
C	3.16947800	0.46761400	-0.06479200
C	4.04172400	2.63849700	-1.59031100
H	1.98208700	3.17466400	-1.78091300
C	4.52555000	0.65500200	-0.29765600
H	2.84468400	-0.40718100	0.49237400
C	4.95734900	1.73436800	-1.05986000
H	4.38323500	3.47660700	-2.19280600
H	5.24320000	-0.05259100	0.10575200
C	-1.70557300	-1.27257400	1.38429500
C	-1.77902600	-0.78227500	0.08614700
C	-2.93851200	-0.21358400	-0.42774500
C	-4.07838800	-0.18030600	0.37401100
C	-4.03229200	-0.69606400	1.66726800
C	-2.84886000	-1.22711000	2.17831500
H	-0.77693600	-1.66696900	1.79047400
H	-2.98470800	0.17402700	-1.44461100
H	-5.01315700	0.23261000	0.00023000
H	-2.82320200	-1.59050200	3.20503000
Cl	1.58691900	-0.89062800	-2.94875700
C	-1.28955000	1.28884900	5.47633800
C	6.41181000	1.95398600	-1.35218900
C	-2.24026400	5.51335000	-3.61503000
F	-1.77536100	5.52143100	-4.86885400
F	-2.08135600	6.73890200	-3.11431000
F	-3.55562100	5.27407700	-3.69081400
F	6.81926300	3.14715700	-0.90040600
F	7.19278500	1.02485200	-0.79864900
F	6.64165300	1.94312600	-2.67130800

F	-2.20105700	0.30605400	5.57811800
F	-0.32547900	1.02651100	6.35884100
F	-1.89650200	2.41807500	5.85581800
C	-2.71982400	-3.57145300	-0.93846500
C	-2.10881300	-4.21895900	0.13586400
C	-0.72767700	-4.41428000	0.15912700
C	0.09005900	-3.96281000	-0.87419100
C	-0.53520900	-3.28086700	-1.95667900
C	-1.93344500	-3.11605600	-1.99369700
H	-2.72079200	-4.57515300	0.96022400
H	-0.27345700	-4.93357800	0.99944300
H	0.03383700	-3.07888000	-2.86377500
H	-2.40956500	-2.62998900	-2.84296100
B	1.63753900	-4.31182100	-0.86227400
O	2.60699900	-3.53794100	-1.40792700
H	2.32447300	-2.68124900	-1.76551500
O	1.94631300	-5.54113300	-0.36904300
H	2.89910000	-5.68393100	-0.35837700
C	-4.17762600	-3.28865500	-0.98508900
O	-4.79454600	-3.63249300	0.14702100
O	-4.73900300	-2.78385900	-1.93529300
C	-6.18737700	-3.32173800	0.20849300
H	-6.72678000	-3.80440200	-0.61072000
H	-6.53754200	-3.69573200	1.17028100
H	-6.33275900	-2.23826500	0.15002600
B	1.85010900	-2.36170300	2.11185700
F	2.94653700	-1.60682500	2.52208900
F	2.22245000	-3.65000600	1.76210700
F	1.30890600	-1.72549700	0.95205700
F	0.87240100	-2.37732100	3.09788900
O	-5.17309900	-0.68775000	2.42141400
C	-5.21990300	0.36849100	3.36786200
H	-6.17872100	0.29758800	3.88558300
H	-4.40827100	0.28690400	4.10436800
H	-5.14938300	1.34562800	2.86709600

TS12

Au	0.97560400	-0.45178700	2.17854300
P	1.67449900	1.85651400	2.59012300
C	0.67089000	2.95940600	1.55096400
C	0.57455300	4.32426400	1.84289700
C	0.01506900	2.43780600	0.43062000
C	-0.17118500	5.16055100	1.02204800
H	1.07691700	4.73965800	2.71459200

C	-0.73079600	3.27416000	-0.38757100
H	0.08833900	1.37701200	0.19512700
C	-0.82099100	4.63146100	-0.08771900
H	-0.24760000	6.21952600	1.24757700
H	-1.24403800	2.86921400	-1.25653200
C	1.41484200	2.37401800	4.31525800
C	2.40455900	2.12347400	5.26789700
C	0.16724200	2.86411200	4.71888700
C	2.14798200	2.34632300	6.61597400
H	3.37825600	1.74090900	4.97079600
C	-0.08491400	3.09033500	6.06179900
H	-0.61941400	3.04837900	3.99122900
C	0.90270600	2.82042900	7.00764900
H	2.91424500	2.14410000	7.35804900
H	-1.05879800	3.45688500	6.37856000
C	3.42513200	2.19052500	2.20156500
C	3.79210900	3.33246700	1.48420900
C	4.40514400	1.29084700	2.63205000
C	5.13140000	3.58200700	1.21976300
H	3.04071500	4.02940900	1.12286800
C	5.74571600	1.55073600	2.37651500
H	4.13038000	0.37607600	3.15213500
C	6.10391400	2.69468600	1.67224900
H	5.41893900	4.46825900	0.65917900
H	6.50842700	0.85682100	2.71635200
C	0.02376700	-0.50529900	5.01816300
C	-0.36173400	-0.22291400	3.71383900
C	-1.63715600	0.24393700	3.41477400
C	-2.54594300	0.44047200	4.45538600
C	-2.17725300	0.16508300	5.76879200
C	-0.89809200	-0.30900000	6.04659200
H	1.02326500	-0.86489400	5.24935600
H	-1.93298100	0.44977600	2.38676300
H	-3.54558500	0.80531200	4.23011000
H	-0.60279300	-0.51546200	7.07333000
Cl	2.56831100	-0.44897800	0.24719700
C	0.55171800	2.99542600	8.45235300
C	7.53590400	2.99556100	1.34875600
C	-1.64756100	5.50039100	-0.98851900
F	-1.19888000	5.45507500	-2.24871300
F	-1.64765400	6.77866000	-0.60620600
F	-2.92109200	5.08766900	-1.01779000
F	7.87655800	4.22568500	1.75565300
F	8.38288000	2.13465700	1.91699700

F	7.74940400	2.95725900	0.02637000
F	-0.40929600	2.13112900	8.81230200
F	1.59280200	2.79894800	9.26379900
F	0.07323200	4.22218400	8.69667500
C	-1.96280700	-3.97620800	0.74673200
C	-1.90273500	-3.70306500	2.11664500
C	-0.87830000	-2.91243900	2.62751700
C	0.15221100	-2.42621400	1.78743200
C	0.03882700	-2.66922400	0.39455900
C	-0.99085100	-3.45123600	-0.11406200
H	-0.85314000	-2.74681900	3.70126000
H	0.79488900	-2.29740300	-0.29320500
B	1.59582900	-3.53653300	2.26710900
O	2.76357400	-3.26034700	1.62303900
H	2.91865300	-2.34555200	1.34392800
O	1.15010800	-4.83757100	2.30880000
H	1.78345200	-5.40317700	1.85604900
B	2.94097400	-2.53504100	4.57013300
F	3.94006200	-3.41155600	4.32300900
F	1.68344600	-3.07268200	3.84382700
F	3.14790800	-1.28325600	4.02349900
F	2.55148800	-2.46824700	5.87317200
H	-2.88753800	0.32061800	6.57729300
H	-2.75863100	-4.59823400	0.35063300
O	-2.79961800	-4.16540600	3.01344000
O	-0.98080100	-3.65767400	-1.44794600
C	-3.87133000	-4.96040200	2.54321000
H	-4.47224100	-5.21489600	3.41718000
H	-4.49415300	-4.41008800	1.82603200
H	-3.50894100	-5.88490400	2.07509500
C	-2.01611500	-4.43555400	-2.01836600
H	-3.00108600	-3.98284200	-1.84465300
H	-1.82139200	-4.46513700	-3.09108200
H	-2.01224200	-5.46029000	-1.62514500

TS13

Au	0.95639300	-0.47258500	2.06206400
P	1.71227200	1.81063400	2.56875700
C	0.73038200	2.99410500	1.59752000
C	0.62351600	4.33411300	1.98490900
C	0.09592200	2.55441400	0.43079600
C	-0.11997100	5.22413300	1.21936500
H	1.11477500	4.68888700	2.88891800
C	-0.64690300	3.44372800	-0.33241600

H	0.18206900	1.51552400	0.11569000
C	-0.75469000	4.77368500	0.06747500
H	-0.20514000	6.26303200	1.52201600
H	-1.14571900	3.10238000	-1.23639400
C	1.47273800	2.24014200	4.32137700
C	2.46397900	1.91519900	5.24983000
C	0.23834700	2.72960800	4.76315000
C	2.22092900	2.06159500	6.61074900
H	3.42960000	1.53678100	4.92168900
C	0.00128500	2.88509800	6.11881700
H	-0.55071400	2.97017400	4.05479000
C	0.98850400	2.53842600	7.03936800
H	2.98853400	1.79925000	7.33224000
H	-0.96081100	3.25563100	6.46522000
C	3.46652100	2.14126700	2.19029800
C	3.85117500	3.33712900	1.57725700
C	4.43135700	1.18494000	2.52215000
C	5.19212000	3.58048800	1.31521300
H	3.11140600	4.08194600	1.29613200
C	5.77387800	1.43656300	2.26834000
H	4.14245500	0.23483200	2.96503100
C	6.14886200	2.63200100	1.66549400
H	5.49474300	4.50972800	0.83860600
H	6.52599800	0.69818500	2.52951800
C	-0.08633500	-0.58536100	4.87601700
C	-0.41873600	-0.25774400	3.56681400
C	-1.68118600	0.22531800	3.23800400
C	-2.62906400	0.38803500	4.24953700
C	-2.31411300	0.06009100	5.56564300
C	-1.04569000	-0.42476700	5.87591000
H	0.90178200	-0.95933700	5.13398200
H	-1.93899100	0.46372400	2.20681000
H	-3.61827800	0.76502400	3.99958900
H	-0.78870700	-0.66435700	6.90592700
Cl	2.55584500	-0.44902000	0.13937400
C	0.65005800	2.62417100	8.49498700
C	7.58047000	2.91556400	1.32675200
C	-1.59018900	5.69378200	-0.77179900
F	-1.16766200	5.70724000	-2.04172000
F	-1.57278000	6.95156800	-0.32750000
F	-2.86770500	5.29189700	-0.79554200
F	7.94050700	4.14340200	1.72201600
F	8.42216100	2.04641300	1.89075300
F	7.78038600	2.86538400	0.00223000

F	-0.26101500	1.69469900	8.82316300
F	1.71140200	2.44006900	9.28316300
F	0.11464300	3.81140600	8.80686900
C	-2.10053500	-3.84951600	0.61224400
C	-2.02206100	-3.63321000	2.00395800
C	-0.92287200	-2.89515100	2.46797100
C	0.09799900	-2.41494900	1.61189500
C	-0.06232000	-2.61575200	0.21372800
C	-1.13477300	-3.35193700	-0.25795200
H	-0.80306800	-2.74473800	3.53478500
H	0.68991200	-2.23537400	-0.47309000
B	1.52927700	-3.59789600	2.05286700
O	2.67948600	-3.32591000	1.36973000
H	2.83857400	-2.40358700	1.11834800
O	1.05870000	-4.89323100	2.05466900
H	1.57928800	-5.41857500	1.43999900
B	2.89811200	-2.68063500	4.38324500
F	3.85215400	-3.61839400	4.20669900
F	1.63084400	-3.19026400	3.60086400
F	3.18136400	-1.46468000	3.80824500
F	2.43667600	-2.56730200	5.65647400
H	-2.93016800	-4.41429600	0.19629600
N	-2.97557800	-4.11464000	2.87060500
C	-2.96318100	-3.67240600	4.25067100
H	-3.01043300	-2.57437400	4.33954800
H	-3.82569800	-4.09572500	4.76839600
H	-2.06165300	-4.01374000	4.77727700
C	-4.16232400	-4.75070400	2.34090700
H	-4.79372400	-5.07589300	3.16974000
H	-4.75617600	-4.07783900	1.70227400
H	-3.90900800	-5.64179300	1.75193700
H	-1.24007400	-3.54224500	-1.32353300
H	-3.05620600	0.18642400	6.35023700