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Catalytic enantioselective synthesis of cyclopropanes featuring vicinal all-carbon quaternary stereocenters with a CH_2F group; study of influence of C-F···H-N interactions on reactivity

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Supporting Information

(Part A)

Contents

NMR spectra are provided in Part B

HPLC spectra are provided in Part C

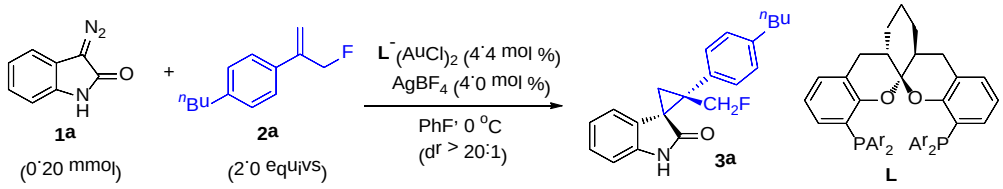
General: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products were carried out by flash chromatography on silica gel. Chemical yields refer to pure isolated substances. The $[\alpha]_D$ was recorded using PolAAr 3005 High Accuracy Polarimeter. Infrared (IR) spectra were obtained using a Bruker tensor 27 infrared spectrometer. ^{1}H, ^{13}C, ^{19}F NMR spectra were obtained using a Bruker DPX-400 spectrometer. Chemical shifts of ^{1}H NMR and ^{13}C NMR spectra are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard while $PhCF_3$ (δ: -63.2 ppm) was used as external standard for ^{19}F NMR spectra. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

All reactions were run in an atmosphere of N_2 except noted. Toluene was prepared by distillation over sodium-benzophenone ketyl prior to use. Anhydrous CH_2Cl_2 was prepared by first distillation over P_2O_5 and then from CaH_2. Fluorobenzene was prepared by first dried in P_2O_5 and then distillation under N_2 atmosphere. α, α, α-Trifluorotoluene was purified by treatment with boiling aqueous Na_2CO_3 several times, dried with K_2CO_3, then with P_2O_5, and fractionally distilled. 1,4-Difluorobenzene was prepared by first dried in P_2O_5 and then distillation under N_2 atmosphere. AgOTf was purchased from TCI Company. $AgBF_4$ and Rh_2(*R*-DOSP)$_4$ were purchased from Strem Chemicals. $AgPF_6$, $NaBAr^F{}_4$ and $AgSbF_6$ were purchased from Alfa-Aesar Company. 3-Diazooxindoles were synthesized according to literature procedures.[1] Chiral spiro bisphosphine Ligands **L1-L6** were synthesized according to the literature method.[2] Alkenes **2a-2i** were synthesized according to the literature methods.[3]

(1) Augusti, R.; Kascheres, C. *J. Org. Chem.* **1993**, *58*, 7079-7083.
(2) (a) Wang, X.-M.; Han, Z.-B.; Wang, Z.; Ding, K.-L. *Angew. Chem.Int. Ed.* **2012**, *51*, 936-940. (b) Wang, X.-M.; Meng, F.-Y.; Wang, Y.; Han, Z.-B.; Chen, Y.-J.; Liu, L.; Wang, Z.; Ding, K.-L. *Angew. Chem.Int. Ed.* **2012**, *51*, 9276-9282.
(3) (a) Walkowiak, J.; del Campo, T. M.; Ameduri, B.; Gouverneur, V. *Synthesis* **2010**, *11*, 1883-1890. (b) Miura, T.; Ito, Y.; Murakami, M. *Chem. Lett.* **2008**, *37*, 1006-1007.

Part I: Condition optimization for Au(I) catalyzed asymmetric cyclopropanation of diazooxindole 1a with 2a

Table S1. Ligand Screen for Au(I) Catalyzed Cyclopropanation of **1a** and **2a**



Entry[a]	Ar	Time (h)	Isolated yield (%)	Ee (%)[b]
1	**L1:** Ph	0.3	58	90
2	**L2:** *o*-MeC_6H_4	25	31	69
3	**L3:** *p*-$MeOC_6H_4$	0.3	60	88
4	**L4:** *p*-MeC_6H_4	3.0	44	90
5	**L5:** *p*-FC_6H_4	0.3	57	90
6	**L6:** 3,5-$Me_2C_6H_3$	1.3	33	88

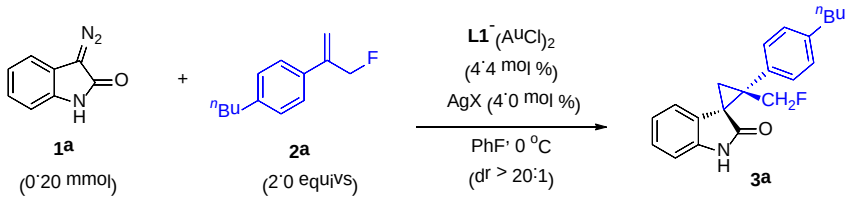
[a]Determined by crude ^{1}H NMR; [b]Determined by chiral HPLC analysis.

We commenced our study first by using the optimal condition established in our previous work,[4] with diazooxindole **1a** and α-CH_2F styrene **2a** as substrate. As shown in Table S1, for ligands bearing different steric and electronic properties, although employing ligands **L1**, **L4** and **L5** can give the same level of enantioselectivity (90%) (entries 1, 4 and 5), we decided to choose **L1** as the best ligand for other condition screen due to its little higher yield and easier availability.

(4) Cao, Z.-Y.; Wang, X.-M.; Tan, C.; Zhao, X.-L.; Zhou, J.; Ding, K.-L. *J. Am. Chem. Soc.*, **2013**, *135*, 8197-8200.

Giving that counteranion of the catalyst often plays a very important role in asymmetric gold catalysis,[5] we continued the study by screening various different silver salts. It's very interesting to note that, of nine different anions we screened; only four of them enabled the reaction to work well (entries 1-4, Table S2). Considering the use of AgOTf was able to induce the best ee, we decided to choose it as the best silver salt for further solvent screen.

Table S2. Counteranion screen



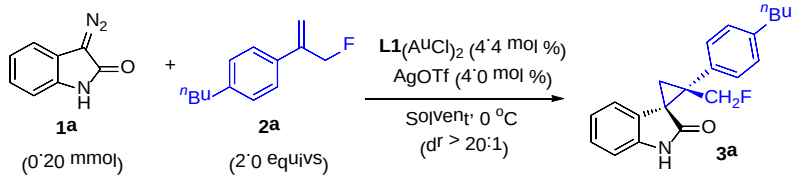
Entry[a]	X	Time (h)	Isolated yield (%)	Ee (%)[b]
1	BF_4	0.3	58	90.5
2	OTf	1.0	47	92
3	SbF_6	10	38	88
4	AsF_6	2.0	38	90
5	PF_6	24	trace	-
6	NTf_2	24	trace	-
7	$MeSO_3$	24	trace	-
8	*p*-$MeC_6H_4SO_3$	24	trace	-
9[c]	BAr^F_4	24	trace	-

[a]Determined by crude ^{1}H NMR; [b]Determined by chiral HPLC analysis; [c]$NaBAr^F_4$ was used as salt (Ar = 3,5-$(CF_3)_2C_6H_3$).

(5) Jia, M.-Q.; Bandini, M. *ACS Catal.*, **2015**, *5*, 1638-1652.

Having identified that AgOTf was the best silver salt for the reaction, we started to evaluate the reactivity in various solvents (Table S3). For these commonly used solvents, the use of aromatic ones could give rise to better yield and enantioselectivity in general (entries 1-5 *vs.* 6-13). And again, PhF was the best one as 92% ee was observed (entry 1). Surprisingly, when 1,2-$F_2C_6H_4$ was employed for the reaction, a dramatic decrease of enantioselectivity was observed (entry 2), which indicated that fluorinated aromatic solvents might play a very important role for the enantioselectivity and promoted us to screen other fluorinated aromatic solvents systematically.

Table S3. Solvent screen



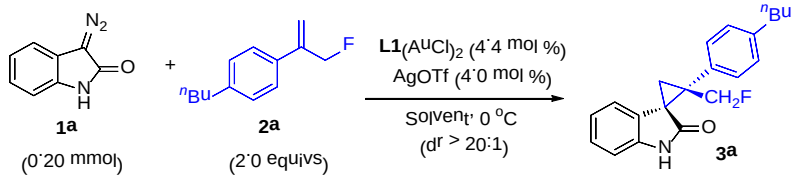
Entry[a]	Solvent	Time (h)	Isolated yield (%)	Ee (%)[b]
1	PhF	1.0	47	92
2	1,2-$F_2C_6H_4$	1.5	54	82
3	PhMe	24	26	92
4	$PhCF_3$	3	52	87
5	PhCl	22	43	90
6	Et_2O	12	26	86
7	THF	0.5	20	87
8	CH_2Cl_2	0.3	55	82
9	$ClCH_2CH_2Cl$	0.3	53	77
10	acetone	0.1	7	63
11	EtOAc	1	15	90
12[c]	DMF	24	0	
13[c]	MeCN	1	0	

[a]Determined by crude ^{1}H NMR; [b]Determined by chiral HPLC analysis;

[c]Full decomposition of **1a** was observed.

Unexpectedly, of thirteen fluorinated aromatic solvents we screened (Table S4), up to 95% ee could be detected when 1,4-$F_2C_6H_4$ or 4-F-C_6H_4Cl was used as solvent (entries 4 and 5). Since a little higher yield was isolated in the presence of 1,4-$F_2C_6H_4$, we decided to use this as the best solvent for the reaction. It should be pointed out that due to the very poor solubility of the catalyst in solvents such as 1,3,5-$F_3C_6H_3$, 1,2,4,5-$F_4C_6H_2$, 1,2,3,5-$F_4C_6H_2$ and C_6F_6, we didn't see any reactivity (entries 10-13).

Table S4. Fluorinated aromatic solvent screen

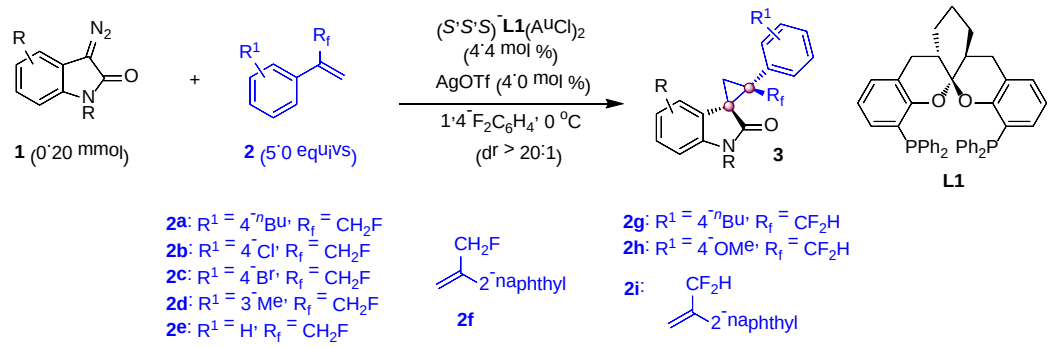


Entry[a]	Solvent	Time (h)	Isolated yield (%)	Ee (%)[b]
1	PhF	1.0	47	92
2	1,2-$F_2C_6H_4$	1.5	54	82
3	1,3-$F_2C_6H_4$	0.3	52	92
4	1,4-$F_2C_6H_4$	9	51	95
5	4-F-C_6H_4Cl	13	42	95
6	4-F-C_6H_4Me	84	12	89
7	1,2,3-$F_3C_6H_3$	1	49	67
8	1,2,4-$F_3C_6H_3$	1	34	92
9	1,2,3,4-$F_4C_6H_2$	3	44	77
10	1,3,5-$F_3C_6H_3$	24	n.r.	-
11	1,2,4,5-$F_4C_6H_2$	24	n.r.	-
12	C_6F_5H	24	n.r.	-
13	C_6F_6	24	n.r.	-

[a]Determined by crude ^{1}H NMR; [b]Determined by chiral HPLC analysis;

n.r. = no reaction.

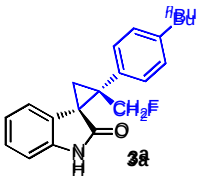
Part II General procedure for Au(I) catalyzed stereoselective cyclopropanation of diazooxindoles 1 and experimental data for products 3



All the racemic compounds were prepared using 5 mol % of PPh_3AuOTf generated *in situ* as catalyst in CH_2Cl_2 at room temperature.

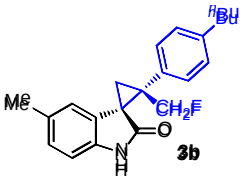
The synthesis of products **3b-3l** were carried out at 0 °C: under N_2 atmosphere, to an over-dried Schlenk tube were added (*S*, *S*, *S*)-**L1**-$(AuCl)_2$ (9.9 mg, 0.088 mmol, 4.4 mol %) and AgOTf (2.0 mg, 0.080 mmol, 4.0 mol %), followed by 4.0 mL of anhydrous 1,4-$F_2C_6H_4$. After the solution was stirred at 25 °C for 0.5 hour, alkene (1.0 mmol) was added. The reaction mixture was cooled to 0 °C and stirred for 0.5 hour, then 3-diazooxindole **1** (0.20 mmol) was added directly. The resulting mixture was stirred at 0 °C till almost full conversion of **1** by TLC analysis and diluted with brine, extracted with EtOAc three times (3×5 mL). The organic layer was dried by Na_2SO_4, concentrated in vacuum. To determine the diastereoselectivity of product, the residue was first dissolved in acetone-d_6, and took some samples for NMR analysis. Then the sample for analysis and the rest of the product were recombined for column chromatographic purification using the indicated solvent mixtures to afford the desired products.

Procedures for the synthesis of products **3a** were the same as the above except alkene (0.6 mmol) was used. Procedures for the synthesis of products **3m-3p** were the same as the above except alkene (2.0 mmol) was used and the reaction was running at 10 °C.

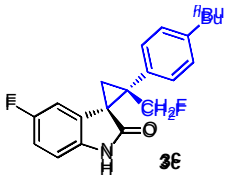


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3a** in 65% yield as red oil. ^1H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.10 min, t_r (major) = 17.35 min) gave the isomeric composition of the product: 95% ee, $[\alpha]^{25}_D$ = +192.4 (c = 4.30, acetone); ^1H NMR (400 MHz, acetone-d_6): δ 9.66 (s, br, 1H), 7.15 (br, 4H), 7.07-7.03 (m, 1H), 6.94-6.92 (m, 1H), 6.51 (t, J = 7.6 Hz, 1H), 5.52 (d, J = 7.6 Hz, 1H), 5.23 (ABd, J_1 = 9.2 Hz, J_2 = 46.8 Hz, 1H), 4.98 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.64-2.60 (m, 2H), 2.20-2.18 (m,

1H), 2.14-2.12 (m, 1H), 1.64-1.56 (m, 2H), 1.38-1.29 (m, 2H), 0.92 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.39, 142.87, 142.48, 134.99, 131.22, 128.75, 128.47, 127.23, 122.62, 120.86, 109.52 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 84.67 (d, $^{1}J_{F\text{-}C}$ = 167 Hz), 43.92 (d, $^{2}J_{F\text{-}C}$ = 22.0 Hz), 35.77 (d, $^{3}J_{F\text{-}C}$ = 6.0 Hz), 35.48, 34.04, 26.84 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz), 22.46, 13.85; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.85; IR (ATR): 3203, 2928, 1697, 1620, 1469, 1358, 1218; GC-MS: 323 (M^+, 16), 132 (100), 246 (19), 303 (17), 147 (14), 260 (8), 275 (7), 217 (4); HRMS (EI): Exact mass calcd for $C_{21}H_{22}NOF$ $[M]^+$: 323.1685, Found: 323.1682.

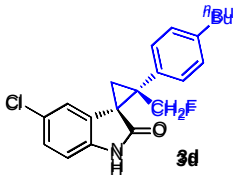


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3b** in 62% yield as white solid (m. p. 129-131 °C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.31 min, t_r (major) = 10.24 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_{D}$ = +132.7 (c = 1.26, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.60 (s, br, 1H), 7.15 (br, 4H), 6.87-6.80 (m, 2H), 5.29 (m, 1H), 5.23 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 4.99 (ABd, J_1 = 9.4 Hz, J_2 = 48.4 Hz, 1H), 2.65-2.61 (m, 2H), 2.16-2.11 (m, 2H), 1.89 (s, 3H), 1.64-1.57 (m, 2H), 1.38-1.29 (m, 2H), 0.92 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.89, 143.20, 140.40, 135.44, 131.61, 130.27, 129.08, 128.93, 127.86, 123.95, 109.56, 85.02 (d, $^{1}J_{F\text{-}C}$ = 167 Hz), 44.21 (d, $^{2}J_{F\text{-}C}$ = 22 Hz), 36.14 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 35.85, 34.60, 27.18 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz), 22.75, 21.05, 14.25; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.81; IR (ATR): 3290, 2927, 1711, 1670, 1492, 1357, 1309, 1217; GC-MS: 337 (M^+, 14), 146 (100), 91 (18), 118 (14), 317 (12), 260 (11), 289 (8), 207 (7); HRMS (EI): Exact mass calcd for $C_{22}H_{24}NOF$ $[M]^+$: 337.1842, Found: 337.1844.

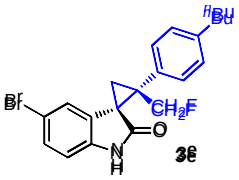


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3c** in 74% yield as white solid (m. p. 96-98 °C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.25 min, t_r (major) = 13.76 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{25}_{D}$ = +123.3 (c = 1.71, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.71 (s, br, 1H), 7.19 (br, 4H), 6.93-6.90 (m, 1H), 6.82 (td, J_1 = 10.2 Hz, J_2 = 2.4 Hz, 1H), 5.25 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 5.25 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 4.99 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.65-2.61 (m, 2H), 2.29-2.26 (m, 1H), 2.18-2.17 (m, 1H), 1.64-1.56 (m, 2H), 1.38-1.28 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.70, 158.58 (d, $^{1}J_{F\text{-}C}$

= 235 Hz), 143.57, 138.92 (d, $^{4}J_{F\text{-}C}$ = 1.0 Hz), 134.91, 131.88, 130.88 (d, $^{3}J_{F\text{-}C}$ = 9.0 Hz), 129.30, 113.72 (d, $^{2}J_{F\text{-}C}$ = 23 Hz), 110.67 (d, $^{2}J_{F\text{-}C}$ = 26.2 Hz), 110.40 (d, $^{3}J_{F\text{-}C}$ = 8.4 Hz), 84.88 (d, $^{1}J_{F\text{-}C}$ = 168 Hz), 44.84 (d, $^{2}J_{F\text{-}C}$ = 22 Hz), 36.62 (dd, $^{3}J_{F\text{-}C}$ = 5.4 Hz, $^{4}J_{F\text{-}C}$ = 2.9 Hz), 35.85, 34.43, 27.58 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz), 22.78, 14.24; ^{19}F NMR (376 MHz, acetone-d_6): δ -124.11, -216.86; IR (ATR): 3196, 2928, 1701, 1466, 1231, 1159; GC-MS: 341 (M^+, 62), 129 (100), 150 (98), 264 (79), 321 (78), 278 (36), 250 (29), 293 (25); HRMS (EI): Exact mass calcd for $C_{21}H_{21}NOF_2$ [M]$^+$: 341.1591, Found: 341.1589.

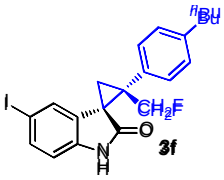


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3d** in 72% yield as white solid (m. p. 95-97 ºC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.96 min, t_r (major) = 10.57 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_{D}$ = +5.4 (c = 2.00, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.78 (s, br, 1H), 7.19 (br, 4H), 7.08-7.06 (m, 1H), 6.94-6.92 (m, 1H), 5.44-5.43 (m, 1H), 5.24 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 4.98 (ABd, J_1 = 9.2 Hz, J_2 = 48.0 Hz, 1H), 2.64 (t, J = 7.6 Hz, 2H), 2.31-2.28 (m, 1H), 2.19-2.17 (m, 1H), 1.65-1.57 (m, 2H), 1.37-1.30 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.41, 143.60, 141.57, 134.87, 131.84, 130.98, 129.31, 127.37, 126.25, 123.23, 111.00, 84.81 (d, $^{1}J_{F\text{-}C}$ = 168.0 Hz), 44.94 (d, $^{2}J_{F\text{-}C}$ = 22.2 Hz), 36.32 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 35.88, 34.51, 27.60 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz), 22.74, 14.30; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.96; IR (ATR): 3318, 1715, 1678, 1484, 1358, 1217, 1134, 1064, 1001; GC-MS: 357, 359 (M^+, 25, 8), 207 (100), 129 (83), 166 (55), 281 (37), 337 (25), 246 (23), 302 (18); HRMS (EI): Exact mass calcd for $C_{21}H_{21}NOF^{35}Cl$ [M]$^+$: 357.1296, Found: 357.1293; Exact mass calcd for $C_{21}H_{21}NOF^{37}Cl$ [M]$^+$: 359.1266, Found: 359.1264;

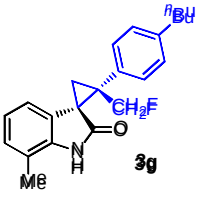


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3e** in 79% yield as white solid (m. p. 94-96 ºC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.08 min, t_r (major) = 10.67 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_{D}$ = -13.6 (c = 1.33, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.76 (s, br, 1H), 7.23-7.20 (m, 5H), 6.90-6.88 (m, 1H), 5.571-5.566 (m, 1H), 5.24 (ABd, J_1 = 9.2 Hz, J_2 = 46.8 Hz, 1H), 4.98 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.64 (t, J = 8.4 Hz, 2H), 2.32-2.30 (m, 1H), 2.18-2.16 (m, 1H), 1.66-1.59 (m, 2H), 1.41-1.31 (m, 2H), 0.92 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz,

acetone-d_6): δ 176.27, 143.62, 141.99, 134.83, 131.94, 131.34, 130.26, 129.29, 126.05, 113.56, 111.50, 84.79 (d, $^1J_{F\text{-}C}$ = 168.0 Hz), 44.97 (d, $^2J_{F\text{-}C}$ = 22.0 Hz), 36.24 (d, $^3J_{F\text{-}C}$ = 5.0 Hz), 35.91, 34.55, 27.62 (d, $^3J_{F\text{-}C}$ = 7.0 Hz), 22.80, 14.34; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.95; IR (ATR): 3202, 2926, 1706, 1617, 1475, 1356, 1219, 1062, 1005; GC-MS: 401, 403 (M^+, 11, 11), 207 (100), 133 (67), 281 (31), 191 (27), 246 (23), 383 (11), 326 (10); HRMS (EI): Exact mass calcd for $C_{21}H_{21}NOF^{79}Br$ [M]$^+$: 401.0791, Found: 401.0789; Exact mass calcd for $C_{21}H_{21}NOF^{81}Br$ [M]$^+$: 403.0770, Found: 403.0767.

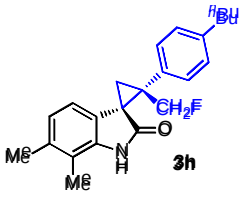


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3f** in 80% yield as white solid (m. p. 280-282 ^oC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.74 min, t_r (major) = 10.98 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{25}_D$ = -62.0 (c = 1.76, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.74 (s, br, 1H), 7.40 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 7.20 (br, 4H), 6.79 (d, J = 8.0 Hz, 1H), 5.75 (d, J = 4.0 Hz, 1H), 5.22 (ABd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 4.97 (ABd, J_1 = 9.2 Hz, J_2 = 48.0 Hz, 1H), 2.65 (t, J = 7.6 Hz, 2H), 2.30-2.27 (m, 1H), 2.17-2.14 (m, 1H), 1.69-1.62 (m, 2H), 1.44-1.34 (m, 2H), 0.93 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.06, 143.63, 142.55, 136.25, 134.83, 131.87, 131.55, 129.21, 112.06, 84.77 (d, $^1J_{F\text{-}C}$ = 168.0 Hz), 83.34, 44.92 (d, $^2J_{F\text{-}C}$ = 22.0 Hz), 36.05 (d, $^3J_{F\text{-}C}$ = 5.0 Hz), 35.96, 34.63, 27.58 (d, $^3J_{F\text{-}C}$ = 7.0 Hz), 22.95, 14.39; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.93; IR (ATR): 3182, 2927, 1704, 1614, 1473, 1355, 1303, 1217,; GC-MS: 449 (M^+, 64), 258 (100), 129 (97), 246 (88), 429 (61), 147 (51), 372 (48), 207 (45); HRMS (EI): Exact mass calcd for $C_{21}H_{21}NOFI$ [M]$^+$: 449.0652, Found: 449.0650.

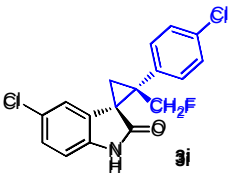


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3g** in 59% yield as white solid (m. p. 75-77^oC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.77 min, t_r (major) = 22.90 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_D$ = +97.1 (c = 1.51, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.64 (s, br, 1H), 7.14 (br, 4H), 6.88 (d, J = 7.6 Hz, 1H), 6.43 (t, J = 7.6 Hz, 1H), 5.36 (d, J = 7.2 Hz, 1H), 5.24 (ABd, J_1 = 9.2 Hz, J_2 = 46.8 Hz, 1H), 4.98 (ABd, J_1 = 9.2 Hz, J_2 = 48.8 Hz, 1H), 2.64-2.60 (m, 2H), 2.30 (s, 3H), 2.17-2.15 (m, 1H), 2.12-2.10 (m, 1H), 1.63-1.55 (m, 2H), 1.38-1.28 (m, 2H), 0.92 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 177.43, 143.19, 141.32, 135.40, 131.71, 129.30,

129.06 (d, $^{3}J_{F\text{-}C}$ = 8.0 Hz), 128.44, 121.32, 120.49, 119.30, 85.10 (d, $^{1}J_{F\text{-}C}$ = 168.0 Hz), 44.38 (d, $^{2}J_{F\text{-}C}$ = 22.0 Hz), 36.40 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 35.86, 34.43, 27.37 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz), 22.84, 16.62, 14.26; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.77; IR (ATR): 3176, 2928, 1694, 1626, 1458, 1358, 1217; GC-MS: 337 (M^+, 18), 146 (100), 91 (21), 118 (20), 317 (17), 260 (16), 289 (10), 207 (5); HRMS (EI): Exact mass calcd for $C_{22}H_{24}NOF$ $[M]^+$: 337.1842, Found: 337.1841.

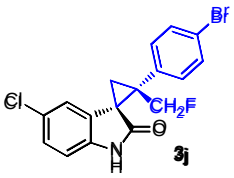


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3h** in 57% yield as white solid (m. p. 199-201 °C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.50 min, t_r (major) = 20.18 min) gave the isomeric composition of the product: 87% ee, $[\alpha]^{25}_{D}$ = +115.0 (c = 0.75, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.64 (s, br, 1H), 7.14 (br, 4H), 6.34 (d, *J* = 7.6 Hz, 1H), 5.25 (d, *J* = 10.0 Hz, 1H), 5.23 (ABd, J_1 = 9.2 Hz, J_2 = 46.8 Hz, 1H), 4.97 (ABd, J_1 = 9.2 Hz, J_2 = 48.4 Hz, 1H), 2.62 (t, *J* = 7.6 Hz, 2H), 2.16 (s, 3H), 2.12 (s, 3H), 2.11-2.08 (m, 2H), 1.63-1.56 (m, 2H), 1.38-1.29 (m, 2H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 177.58, 143.14, 141.49, 136.08, 135.54, 131.65, 129.09, 126.12, 122.76, 120.16, 118.04, 85.18 (d, $^{1}J_{F\text{-}C}$ = 167.0 Hz), 44.05 (d, $^{2}J_{F\text{-}C}$ = 22.0 Hz), 36.46 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 35.89, 34.47, 27.16 (d, $^{3}J_{F\text{-}C}$ = 8.0 Hz), 22.88, 19.80, 14.27, 13.23; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.65; IR (ATR): 3233, 2925, 1700, 1628, 1453, 1355, 1214; GC-MS: 351 (M^+, 12), 160 (100), 207 (55), 133 (34), 281 (18), 191 (12), 331 (10), 253 (9); HRMS (EI): Exact mass calcd for $C_{23}H_{26}NOF$ $[M]^+$: 351.1998, Found: 351.1996.

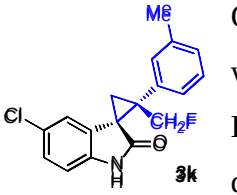


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3i** in 78% yield as white solid (m. p. 194-196 °C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 10.61 min, t_r (major) = 18.37 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{25}_{D}$ = -8.2 (c = 1.22, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.80 (s, br, 1H), 7.41 (br, 4H), 7.12-7.10 (m, 1H), 6.97-6.95 (m, 1H), 5.562-5.557 (m, 1H), 5.24 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 4.97 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.37-2.34 (m, 1H), 2.22-2.20 (m, 1H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.08, 141.77, 136.59, 134.42, 133.64, 130.60, 129.35, 127.69, 126.33, 123.16, 111.26, 84.64 (d, $^{1}J_{F\text{-}C}$ = 168.0 Hz), 44.38 (d, $^{2}J_{F\text{-}C}$ = 22.0 Hz), 36.24 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 27.22 (d, $^{3}J_{F\text{-}C}$ = 7.0 Hz); ^{19}F NMR (376 MHz, acetone-d_6): δ -217.17; IR (ATR): 3313, 1713,

1676, 1473, 1351, 1298, 1219, 1085, 1001; GC-MS: 335, 337 (M^+, 10, 7), 166 (100), 207 (96), 73 (60), 281 (25), 253 (18), 315 (5), 131 (5); HRMS (EI): Exact mass calcd for $C_{17}H_{12}NOF^{35}Cl_2$ $[M]^+$: 335.0280, Found: 335.0281; Exact mass calcd for $C_{17}H_{12}NOF^{35}Cl^{37}Cl$ $[M]^+$: 337.0254, Found: 337.0250.

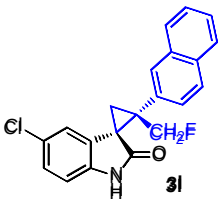


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3j** in 65% yield as white solid (m. p. 188-190 ^oC). ^1H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 11.13 min, t_r (major) = 19.63 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{25}_D$ = +0.2 (c = 0.41, acetone); ^1H NMR (400 MHz, acetone-d_6): δ 9.82 (s, br, 1H), 7.55 (br, 4H), 7.12-7.09 (m, 1H), 6.97-6.95 (m, 1H), 5.56 (d, J = 2.4 Hz, 1H), 5.24 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 4.97 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.36-2.33 (m, 1H), 2.22-2.20 (m, 1H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.09, 141.72, 137.00, 134.00, 132.33, 130.54, 127.68, 126.32, 123.12, 122.56, 111.25, 84.56 (d, $^1J_{F-C}$ = 168.0 Hz), 44.43 (d, $^2J_{F-C}$ = 22.0 Hz), 36.18 (d, $^3J_{F-C}$ = 5.0 Hz), 27.16 (d, $^3J_{F-C}$ = 7.0 Hz); ^{19}F NMR (376 MHz, acetone-d_6): δ -217.11; IR (ATR): 3320, 2920, 1714, 1678, 1484, 1218, 1134, 1000; GC-MS: 379, 381 (M^+, 3, 3), 207 (100), 133 (54), 166 (50), 281 (26), 191 (24), 253 (19), 327 (5); HRMS (EI): Exact mass calcd for $C_{17}H_{12}NOF^{35}Cl^{79}Br$ $[M]^+$: 378.9775, Found: 378.9777; Exact mass calcd for $C_{17}H_{12}NOF^{35}Cl^{81}Br$ $[M]^+$: 380.9754, Found: 378.9753; Exact mass calcd for $C_{17}H_{12}NOF^{37}Cl^{79}Br$ $[M]^+$: 380.9745, Found: 380.9744;

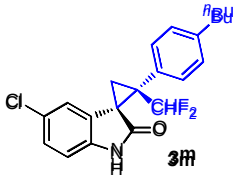


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3k** in 87% yield as white solid (m. p. 163-165 ^oC). ^1H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 6.27 min, t_r (major) = 9.54 min) gave the isomeric composition of the product: 94% ee, $[\alpha]^{25}_D$ = -26.9 (c = 2.00, acetone); ^1H NMR (400 MHz, acetone-d_6): δ 9.78 (s, br, 1H), 7.24-7.17 (m, 4H), 7.11-7.06 (m, 1H), 6.97-6.93 (m, 1H), 5.51-5.49 (m, 1H), 5.32-5.16 (m, 1H), 5.09-4.92 (m, 1H), 2.33-2.16 (m, 5H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.41, 141.60, 138.83, 137.55, 132.29, 130.98, 129.55, 129.11, 127.43, 126.22, 123.30, 110.04, 84.86 (d, $^1J_{F-C}$ = 167.0 Hz), 45.16 (d, $^2J_{F-C}$ = 23.0 Hz), 36.28 (d, $^3J_{F-C}$ = 5.0 Hz), 27.66 (d, $^3J_{F-C}$ = 8.0 Hz), 21.40; ^{19}F NMR (376 MHz, acetone-d_6): δ -216.89; IR (ATR): 3199, 2917, 1704, 1513, 1476, 1297, 1221, 1028; GC-MS: 315, 317 (M^+, 28, 9), 129 (100), 166 (61), 260 (24), 207 (24), 295 (21), 102 (19), 75 (18); HRMS (EI): Exact mass calcd for $C_{18}H_{15}NOF^{35}Cl$ $[M]^+$: 315.0826, Found: 315.0825; Exact mass calcd

for $C_{18}H_{15}NOF^{37}Cl$ $[M]^+$: 317.0797, Found: 317.0799.

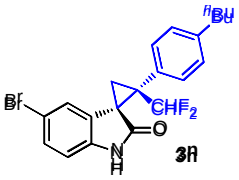


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3l** in 93% yield as white solid (m. p. 197-199 ^oC). ^1H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 14.16 min, t_r (major) = 22.62 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_D$ = +92.3 (c = 0.92, acetone); ^1H NMR (400 MHz, acetone-d_6): δ 9.84 (s, br, 1H), 7.92-7.85 (m, 4H), 7.54-7.52 (m, 3H), 7.06-7.03 (m, 1H), 6.97-6.94 (m, 1H), 5.49 (s, 1H), 5.34 (ABd, J_1 = 9.6 Hz, J_2 = 46.8 Hz, 1H), 5.08 (ABd, J_1 = 9.6 Hz, J_2 = 48.4 Hz, 1H), 2.50 (br, 1H), 2.31-2.29 (m, 1H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.36, 141.71, 135.32, 134.21, 133.99, 130.81, 129.70, 128.89, 128.57, 127.53, 127.32, 127.20, 126.26, 123.08, 111.16, 84.96 (d, $^1J_{F-C}$ = 167.0 Hz), 45.31 (d, $^2J_{F-C}$ = 22.0 Hz), 36.39, 27.64 (d, $^3J_{F-C}$ = 7.0 Hz); ^{19}F NMR (376 MHz, acetone-d_6): δ -216.79; IR (ATR): 3169, 3061, 1702, 1441, 1350, 1298, 1221, 1077; GC-MS: 351, 353 (M^+, 1, 1), 207 (100), 183 (44), 262 (33), 96 (30), 133 (29), 281 (16), 327 (4); HRMS (EI): Exact mass calcd for $C_{21}H_{15}NOF^{35}Cl$ $[M]^+$: 351.0826, Found: 351.0825; Exact mass calcd for $C_{21}H_{15}NOF^{37}Cl$ $[M]^+$: 353.0797, Found: 357.0799.

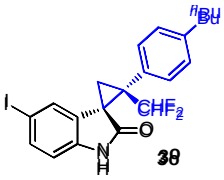


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3m** in 46% yield as white solid (m. p. 140-142 ^oC). ^1H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.34 min, t_r (major) = 8.19 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{25}_D$ = +23.2 (c = 1.00, acetone); ^1H NMR (400 MHz, acetone-d_6): δ 9.92 (s, br, 1H), 7.50 (ABd, J = 7.6 Hz, 1H), 7.36 (ABd, J = 7.2 Hz, 1H), 7.14-7.11 (m, 1H), 7.09 (ABd, J = 7.2 Hz, 1H), 6.98-6.96 (m, 1H), 6.82 (ABd, J = 7.6 Hz, 1H), 6.74 (dd, J_1 = 56.4 Hz, J_2 = 54.8 Hz, 1H), 5.40 (d, J = 5.0 Hz, 1H), 2.68-2.64 (m, 2H), 2.44-2.39 (m, 2H), 1.66-1.58 (m, 2H), 1.39-1.32 (m, 2H), 0.92 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.11, 144.49, 141.76, 134.06, 132.30, 129.77, 129.47, 128.97, 128.90, 128.01, 126.61, 123.66, 115.81 (dd, $^1J_{F-C}$ = 237.0 Hz, $^1J_{F-C}$ = 234.0 Hz), 111.41, 44.86 (dd, $^2J_{F-C}$ = 30.2 Hz, $^2J_{F-C}$ = 25.0 Hz), 36.16 (d, $^3J_{F-C}$ = 5.0 Hz), 35.92, 34.47, 26.60 (d, $^3J_{F-C}$ = 8.0 Hz), 22.77, 14.29; ^{19}F NMR (376 MHz, acetone-d_6): δ -114.93 (ABd, J = 285.8 Hz, 1F), -121.46 (ABd, J = 285.8 Hz, 1F); IR (ATR): 3208, 2927, 1710, 1618, 1478, 1221, 1141, 1091, 1042; GC-MS: 375, 377 (M^+, 11, 4), 207 (100), 133 (43), 281 (33), 292 (32), 355 (29), 335 (22), 253 (22);

HRMS (EI): Exact mass calcd for $C_{21}H_{20}NOF_2{}^{35}Cl$ [M]$^+$: 375.1201, Found: 375.1199; Exact mass calcd for $C_{21}H_{20}NOF_2{}^{37}Cl$ [M]$^+$: 377.1172, Found: 377.1177.

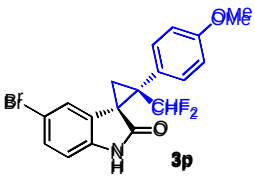


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3n** in 53% yield as white solid (m. p. 149-151 ^{o}C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.24 min, t_r (major) = 8.05 min) gave the isomeric composition of the product: 91% ee, $[\alpha]^{25}_D$ = -3.7 (c = 1.44, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.93 (s, br, 1H), 7.49 (ABd, *J* = 7.2 Hz, 1H), 7.35 (ABd, *J* = 7.2 Hz, 1H), 7.28-7.25 (m, 1H), 7.08 (ABd, *J* = 7.6 Hz, 1H), 6.93-6.91 (m, 1H), 6.81 (ABd, *J* = 6.8 Hz, 1H), 6.74 (dd, J_1 = 56.4 Hz, J_2 = 55.2 Hz, 1H), 5.53 (d, *J* = 2.0 Hz, 1H), 2.67-2.64 (m, 2H), 2.42-2.39 (m, 2H), 1.67-1.61 (m, 2H), 1.59-1.32 (m, 2H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 175.97, 144.51, 142.18, 134.07, 132.29, 130.89, 130.11, 129.46, 128.94, 128.88, 126.48, 115.80 (dd, $^1J_{F\text{-}C}$ = 238.0 Hz, $^2J_{F\text{-}C}$ = 235.0 Hz),113.87, 113.43, 111.91, 44.86 (dd, $^2J_{F\text{-}C}$ = 30.0 Hz, $^2J_{F\text{-}C}$ = 25.0 Hz), 36.07 (d, $^3J_{F\text{-}C}$ = 6.0 Hz), 35.95, 26.62 (d, $^3J_{F\text{-}C}$ = 8.0 Hz), 22.83, 14.33; ^{19}F NMR (376 MHz, acetone-d_6): δ -114.94 (ABd, *J* = 285.76 Hz, 1F), -121.45 (ABd, *J* = 285.76 Hz, 1F); IR (ATR): 3191, 2921, 1705, 1615, 1342, 1224, 1088, 1038; MS (EI): 419, 421 (M$^+$, 50, 50), 399 (100), 401 (98), 356 (57), 358 (57), 381 (51), 342 (48), 344 (43); HRMS (EI): Exact mass calcd for $C_{21}H_{20}NOF_2{}^{79}Br$ [M]$^+$:419.0696, Found: 419.0692; Exact mass calcd for $C_{21}H_{20}NOF_2{}^{81}Br$ [M]$^+$: 421.0676, Found: 421.0677.

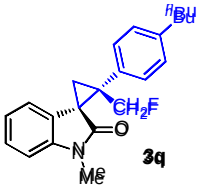


Column chromatography (5% acetone in CH_2Cl_2) afforded product **3o** in 41% yield as white solid (m. p. 165-167 ^{o}C). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 7.72 min, t_r (major) = 14.57 min) gave the isomeric composition of the product: 89% ee, $[\alpha]^{25}_D$ = -37.8 (c = 1.39, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.90 (s, br, 1H), 7.48 (ABd, *J* = 6.8 Hz, 1H), 7.46-7.44 (m, 1H), 7.35 (ABd, *J* = 6.4 Hz, 1H), 7.09 (ABd, *J* = 6.4 Hz, 1H), 6.83-6.81 (m, 2H), 6.73 (dd, J_1 = 56.4 Hz, J_2 = 55.2 Hz, 1H), 5.71 (d, *J* = 1.6 Hz, 1H), 2.68-2.64 (m, 2H), 2.40-2.36 (m, 2H), 1.70-1.62 (m, 2H), 1.44-1.35 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): δ 175.79, 144.53, 142.75, 136.90, 134.12, 132.32, 130.32, 129.40, 128.96, 128.82, 115.78 (dd, $^1J_{F\text{-}C}$ = 238.0 Hz, $^1J_{F\text{-}C}$ = 235.0 Hz), 112.43, 83.63, 44.83 (dd, $^2J_{F\text{-}C}$ = 30.0 Hz, $^2J_{F\text{-}C}$ = 24.9 Hz), 36.01, 34.61, 35.89 (d, $^3J_{F\text{-}C}$ = 5.4 Hz), 26.59 (d, $^3J_{F\text{-}C}$ = 8.0 Hz), 22.99, 14.38;

^{19}F NMR (376 MHz, acetone-d_6): δ -114.92 (ABd, *J* = 285.76 Hz, 1F), -121.43 (ABd, *J* = 285.76 Hz, 1F); IR (ATR): 3250, 2926, 1713, 1614, 1474, 1338, 1222, 1141, 1089, 1037; MS (EI): 467 (M^+, 54), 447 (100), 404 (48), 427 (44), 390 (40), 384 (27), 264 (23), 448 (23); HRMS (EI): Exact mass calcd for $C_{21}H_{20}NOF_2I[M]^+$:467.0558, Found: 467.0555.



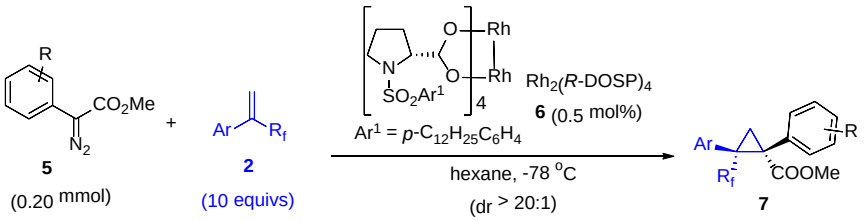
Column chromatography (5% acetone in CH_2Cl_2) afforded product **3p** in 54% yield as white solid (m. p. 103-105 ºC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 8.34 min, t_r (major) = 12.93 min) gave the isomeric composition of the product: 91% ee, $[\alpha]^{25}_D$ = -23.1 (c = 0.83, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.90 (s, br, 1H), 7.51 (ABd, *J* = 7.6 Hz, 1H), 7.29-7.26 (m, 1H), 7.06 (ABd, *J* = 7.2 Hz, 1H), 6.94-6.92 (m, 1H), 6.82 (m, 2H), 6.72 (dd, J_1 = 56.4 Hz, J_2 = 54.8 Hz, 1H), 5.63 (d, *J* = 5.0 Hz, 1H), 3.83 (s, 3H), 2.41-2.36 (m, 2H); ^{13}C NMR (100 MHz, acetone-d_6): δ 176.01, 161.18, 142.23, 135.27, 133.65, 130.90, 130.16, 126.57, 123.47, 115.76 (dd, $^1J_{F-C}$ = 237.0 Hz, $^1J_{F-C}$ = 235.0 Hz), 114.64 (d, $^3J_{F-C}$ =7.0 Hz), 111.93, 55.80, 44.58 (dd, $^2J_{F-C}$ = 30.0 Hz, $^2J_{F-C}$ = 25.2 Hz), 36.26 (d, $^3J_{F-C}$ = 5.0 Hz), 26.77 (d, $^3J_{F-C}$ = 8.0 Hz); ^{19}F NMR (376 MHz, acetone-d_6): δ -115.05 (ABd, *J* = 285.76 Hz, 1F), -121.61 (ABd, *J* = 285.76 Hz, 1F); IR (ATR): 3273, 2841, 1706, 1611, 1514, 1476, 1294, 1220, 1177, 1141, 1091, 1030; MS (EI): 393, 395 (M^+, 26, 26), 373 (100), 375 (91), 43 (90), 44 (54), 59 (46), 355 (38), 353 (36); HRMS (EI): Exact mass calcd for $C_{18}H_{14}NO_2F_2{}^{79}Br$ [M]$^+$: 393.0176, Found: 393.0179; Exact mass calcd for $C_{18}H_{14}NO_2F_2{}^{81}Br$ [M]$^+$: 395.0156, Found: 395.0158.



Column chromatography (20% Et_2O in petroleum ether) afforded product **3q** in 40% yield as red oil. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm; major diastereomer: t_r (minor) = 5.12 min, t_r (major) = 6.44 min) gave the isomeric composition of the product: 80% ee, $[\alpha]^{25}_D$ = +30.3 (c = 1.05, acetone); ^{1}H NMR (300 MHz, acetone-d_6): δ 7.17-7.11 (m, br, 5H), 6.98-6.96 (m, 1H), 6.59-6.6.53 (m, 1H), 5.55-5.53 (m, 1H), 5.24 (ABd, J_1 = 12.8 Hz, J_2 = 46.8 Hz, 1H), 5.00 (ABd, J_1 = 12.8 Hz, J_2 = 48.3 Hz, 1H), 3.28 (s, 3H), 2.62-2.59 (m, 2H), 2.23-2.20 (m, 1H), 2.15-2.13 (m, 1H), 1.64-1.54 (m, 2H), 1.40-1.27 (m, 2H), 0.92 (t, *J* = 9.6 Hz, 3H); ^{13}C NMR (75 MHz, acetone-d_6): δ 175.09, 144.78, 143.28, 135.32, 131.66, 129.14, 128.13, 127.75, 122.63, 121.65, 108.62, 85.12 (d, $^1J_{F-C}$ = 167 Hz), 44.26 (d, $^2J_{F-C}$ = 22.5 Hz), 35.86, 35.78, 34.43, 27.30 (d, $^3J_{F-C}$ = 6.8 Hz), 26.74

(d, $^4J_{F\text{-}C}$ = 2.2 Hz), 22.86, 14.26; ^{19}F NMR (282 MHz, acetone-d_6): δ -216.78; IR (ATR): 3203, 2928, 1697, 1620, 1469, 1358, 1218; GC-MS: 337 (M^+, 26), 146 (100), 317 (22), 91 (15), 207 (11), 260 (10), 274 (5), 184 (2); HRMS (EI): Exact mass calcd for $C_{22}H_{24}NOF$ $[M]^+$: 337.1842, Found: 337.1844.

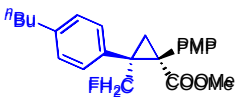
Part III General procedure for Rh(II) catalyzed stereoselective cyclopropanation of aryl diazoacetate and experimental data for products 7



All the racemic compounds were prepared using 0.5 mol% of $Rh_2(OAc)_4$ as catalyst in CH_2Cl_2 at room temperature.

The synthesis of products **7a-7d** were carried out at -78 °C: under N_2 atmosphere, to an over-dried Schlenk tube were added Rh_2(*R*-DOSP)$_4$ **6** (1.9 mg, 0.0010 mmol, 0.5 mol%), followed by 1.0 mL of anhydrous *n*-hexane and alkene **2** (10.0 equivs). After the solution was stirred at -78 °C for 0.5 hour, an *n*-hexane solution of diazo acetate **5** (0.2 mmol, 0.1 M) was added via syringe over half an hour. The resulting mixture was stirred at -78 °C till almost full conversion of **5** by TLC analysis and diluted with brine, extracted with EtOAc three times (3 × 5 mL). The organic layer was dried by Na_2SO_4, concentrated in vacuum. To determine the diastereoselectivity of product, the residue was first dissolved in acetone-d_6, and took some samples for NMR analysis. Then the sample for analysis and the rest of the product were recombined for column chromatographic purification using the indicated solvent mixtures to afford the desired products.

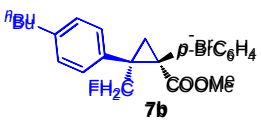
Procedure for the synthesis of product **7e** were the same as the above except the reaction was running at room temperature.



7a

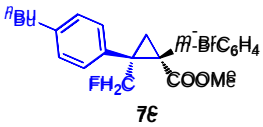
Column chromatography (5% petroleum ether in ethyl acetate) afforded product **7a** in 60% yield as colorless oil. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel OZ-H, ^{i}PrOH/hexane = 1/99, 0.8 mL/min, 230 nm; major diastereomer: t_r (minor) = 15.46 min, t_r (major) = 16.80 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{25}_D$ = -20.4 (c = 1.68, acetone); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09-7.03 (m, 4H),

6.91 (ABd, J = 8.0 Hz, 2H), 6.60-6.57 (m, 2H), 4.96-4.90 (m, 1H), 4.84-4.78 (m, 1H), 3.70 (s, 3H), 3.67 (s, 3H), 2.46 (t, J = 7.6 Hz, 2H), 2.18-2.17 (m, 1H), 2.11-2.08 (m, 1H), 1.52-1.44 (m, 2H), 1.28-1.18 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.12, 158.33, 141.44, 134.39, 132.57, 128.53, 127.92, 127.39, 112.77, 87.49 (d, $^{1}J_{F\text{-}C}$ = 170.0 Hz), 55.01, 52.76, 39.82 (d, $^{3}J_{F\text{-}C}$ = 5.2 Hz), 38.61 (d, $^{2}J_{F\text{-}C}$ = 20.8 Hz), 35.00, 33.27, 22.11, 21.14 (d, $^{3}J_{F\text{-}C}$ = 8.0 Hz), 13.87; ^{19}F NMR (376 MHz, $CDCl_3$): δ -210.07; IR (ATR): 2955, 1718, 1600, 1514, 1436, 1248, 1209, 1163, 1132, 1032; GC-MS: 370 (M^+, 20), 291 (100), 235 (77), 220 (37), 203 (21), 318 (15), 277 (14), 335 (5); HRMS (EI): Exact mass calcd for $C_{23}H_{27}O_3F$ $[M]^+$: 370.1944, Found: 370.1945.



7b

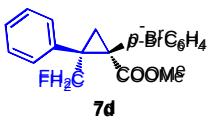
Column chromatography (2% petroleum ether in ethyl acetate) afforded product **7b** in 78% yield as colorless oil. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel OZ-H, ^{i}PrOH/hexane = 1/99, 0.8 mL/min, 230 nm; major diastereomer: t_r (minor) = 8.25 min, t_r (major) = 8.57 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_D$ = -24.1 (c = 0.60, acetone); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (ABd, J = 8.4 Hz, 2H), 7.02-6.93 (m, 4H), 6.92 (ABd, J = 8.4 Hz, 2H), 4.90 (ABd, J_1 = 9.6 Hz, J_2 = 47.6 Hz, 1H), 4.85 (ABd, J_1 = 9.8 Hz, J_2 = 47.6 Hz, 1H), 3.70 (s, 3H), 2.48 (t, J = 8.4 Hz, 2H), 2.22-2.21 (m, 1H), 2.13-2.10 (m, 1H), 1.52-1.45 (m, 2H), 1.29-1.18 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.33, 141.85, 134.52, 133.94, 133.23, 130.49, 128.40 (d, $^{4}J_{F\text{-}C}$ = 1.0 Hz), 128.13, 121.10, 87.21 (d, $^{1}J_{F\text{-}C}$ = 170.0 Hz), 52.86, 39.84 (d, $^{3}J_{F\text{-}C}$ = 5.0 Hz), 38.87 (d, $^{2}J_{F\text{-}C}$ = 21 Hz), 34.99, 33.22, 22.06, 21.05 (d, $^{3}J_{F\text{-}C}$ = 8.0 Hz), 13.90; ^{19}F NMR (376 MHz, $CDCl_3$): δ -210.06; IR (ATR): 2928, 1719, 1435, 1258, 1208, 1133, 1074, 1043, 1010; GC-MS: 418, 420 (M^+, 2, 3), 207 (100), 260 (34), 281 (22), 187 (14), 341 (7), 400 (4), 361 (1); HRMS (EI): Exact mass calcd for $C_{22}H_{24}O_2F^{79}Br$ $[M]^+$: 418.0944, Found: 418.0945; Exact mass calcd for $C_{22}H_{24}O_2F^{81}Br$ $[M]^+$: 420.0923, Found: 420.0925.



7c

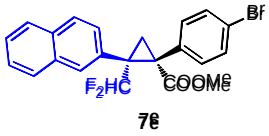
Column chromatography (2% petroleum ether in ethyl acetate) afforded product **7c** in 66% yield as colorless oil. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel OZ-H, ^{i}PrOH/hexane = 1/99, 0.8 mL/min, 230 nm; major diastereomer: t_r (minor) = 8.85 min, t_r (major) = 9.67 min) gave the isomeric composition of the product: 91% ee, $[\alpha]^{25}_D$ = -7.9 (c = 1.61, acetone); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.29 (m, 1H), 7.16-7.14 (m, 1H), 7.08-7.03 (m, 3H), 6.94-6.88 (m, 3H), 4.92 (ABd, J_1 = 10.0 Hz, J_2 = 48.0 Hz, 1H), 4.86 (ABd, J_1 = 9.6 Hz, J_2 = 47.6 Hz, 1H), 3.71 (s, 3H), 2.47 (t, J = 7.6 Hz, 2H), 2.23-2.21 (m, 1H), 2.17-2.12 (m, 1H), 1.52-1.44 (m, 2H), 1.27-1.19 (m, 2H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz,

$CDCl_3$): δ 171.24, 141.89, 137.71, 134.64, 133.83, 130.26, 129.98, 128.75, 128.38 (d, $^4J_{F\text{-}C}$ = 2.0 Hz), 128.08, 121.21, 87.14 (d, $^1J_{F\text{-}C}$ = 170.0 Hz), 52.91, 39.93 (d, $^3J_{F\text{-}C}$ = 5.5 Hz), 38.92 (d, $^2J_{F\text{-}C}$ = 20.8 Hz), 35.00, 33.28, 22.06, 21.11 (d, $^3J_{F\text{-}C}$ = 8.0 Hz), 13.88; ^{19}F NMR (376 MHz, $CDCl_3$): δ -210.08; IR (ATR): 2928, 1723, 1433, 1256, 1208; GC-MS: 418, 420 (M^+, 10, 10), 260 (100), 217 (53), 341 (31), 287 (31), 204 (31), 367 (7), 297 (7); HRMS (EI): Exact mass calcd for $C_{22}H_{24}O_2F^{79}Br$ $[M]^+$: 418.0944, Found: 418.0941; Exact mass calcd for $C_{22}H_{24}O_2F^{81}Br$ $[M]^+$: 420.0923, Found: 420.0920.



7d

Column chromatography (1% petroleum ether in ethyl acetate) afforded product **7d** in 79% yield as white solid (M. P. 35 ºC). ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel OD-H, ^{i}PrOH/hexane = 1/99, 0.8 mL/min, 230 nm; major diastereomer: t_r (major) = 14.68 min, t_r (minor) = 18.69 min) gave the isomeric composition of the product: 95% ee, $[\alpha]^{25}_D$ = -19.8 (c = 4.15, acetone); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20-7.04 (m, 9H), 4.91 (ABd, J_1 = 10.0 Hz, J_2 = 48.0 Hz, 1H), 4.87 (ABd, J_1 = 10.0 Hz, J_2 = 48.0 Hz, 1H), 3.71 (s, 3H), 2.25-2.24 (m, 1H), 2.17-2.14 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.20, 136.84, 134.30, 133.15, 130.56, 128.62 (d, $^4J_{F\text{-}C}$ = 1.0 Hz), 128.08, 127.25, 121.21, 87.14 (d, $^1J_{F\text{-}C}$ = 171.0 Hz), 52.90, 39.85 (d, $^3J_{F\text{-}C}$ = 6.0 Hz), 39.06 (d, $^2J_{F\text{-}C}$ = 20.0 Hz), 20.97 (d, $^3J_{F\text{-}C}$ = 8.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ -210.14; IR (ATR): 2925, 1718, 1430, 1258, 1207, 1071, 1008; GC-MS: 362, 364 (M^+, 9, 9), 204 (100), 237 (17), 191 (15), 283 (8), 248 (7), 344 (4), 312 (2); HRMS (EI): Exact mass calcd for $C_{18}H_{16}O_2F^{79}Br$ $[M]^+$: 362.0318, Found: 362.0320; Exact mass calcd for $C_{18}H_{16}O_2F^{81}Br$ $[M]^+$: 364.0297, Found: 364.0294.

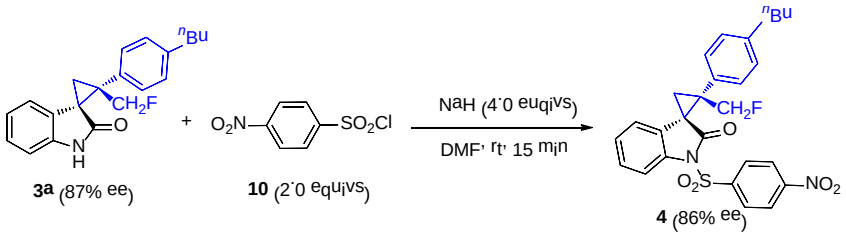


7e

Column chromatography (5% petroleum ether in ethyl acetate) afforded product **7e** in 51% yield as yellow oil. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel OD-H, ^{i}PrOH/hexane = 1/99, 1.0 mL/min, 230 nm; major diastereomer: t_r (major) = 12.91 min, t_r (minor) = 13.80 min) gave the isomeric composition of the product: 87% ee, $[\alpha]^{25}_D$ = +54.4 (c = 0.50, acetone); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73-7.69 (m, 2H), 7.66-7.64 (m, 2H), 7.45-7.41 (m, 3H), 7.16 (s, 4H), 6.23 (t, J = 16.0 Hz, 1H), 3.76 (s, 3H), 2.46-2.44 (m, 1H), 2.35-2.32 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.73, 133.02, 132.80 (d, J = 4.8 Hz), 132.59, 130.82, 130.10, 129.21 (d, J = 1.4 Hz), 128.08 (d, J = 1.4 Hz), 127.85, 127.66, 127.52, 126.35, 126.08, 121.75, 116.40 (d, J = 240 Hz), 53.22, 41.21 (d, J = 25 Hz) , 41.00 (d, J = 237.5 Hz), 39.33, 29.69, 19.40 (d, J = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ -111.30 (d, J = 286 Hz, 1F), -118.00 (d, J = 286 Hz, 1F);

IR (ATR): 2993, 1718, 1591, 1490, 1256, 1205, 1106, 1089, 1009; GC-MS: 431, 429 (M^+, 35, 34), 272 (100), 370 (85), 350 (70), 320 (44), 411 (42), 239 (42), 215 (21); HRMS (EI): Exact mass calcd for $C_{22}H_{17}F_2O_2{}^{79}Br$ $[M]^+$: 430.0380, Found: 430.0380; Exact mass calcd for $C_{22}H_{17}F_2O_2{}^{81}Br$ $[M]^+$: 432.0360, Found: 432.0362.

Part IV: Synthesis of product 4



To a stirred solution of **3a** (180.0 mg, 0.56 mmol) in 3 mL DMF, NaH (89.6 mg, 60% in mineral oil, 4.0 equivs) was added in one portion and stirred at room temperature for 10 minutes. Then sulfonyl chloride **10** (248 mg, 1.12 mmol) was added and stirred for another 15 minutes. The reaction mixture was quenched with saturated NH_4Cl and extracted with ethyl acetate (3 × 5 mL). The organic layer was dried by Na_2SO_4, concentrated in vacuum. To determine the diastereoselectivity of product, the residue was first dissolved in acetone-d_6, and took some samples for NMR analysis. Then the sample for analysis and the rest of the product were recombined for column chromatographic purification to afford the desired product **4** in 67% yield (m. p. 187-189 °C) as red solid. ^{1}H NMR analysis revealed that the dr is above 20:1. HPLC analysis (Chiralcel AD-H, ^{i}PrOH/hexane = 20/80, 1.0 mL/min, 230 nm; major diastereomer: t_r (major) = 9.23 min, t_r (minor) = 14.11 min) gave the isomeric composition of the product: 86% ee, $[\alpha]^{25}_D$ = 100.4 (c = 0.88, acetone); ^{1}H NMR (400 MHz, acetone-d_6): 8.52-8.50 (m, 2H), 8.43-8.40 (m, 2H), 7.94 (d, J = 8.0 Hz, 1H), 7.28-7.24 (m, 1H), 7.13 (br, 4H), 6.76 (t, J = 7.6 Hz, 1H), 5.66 (d, J = 7.6 Hz, 1H), 5.02 (ABdd, J_1 = 9.8 Hz, J_2 = 46.8 Hz, 1H), 4.84 (ABdd, J_1 = 9.6 Hz, J_2 = 48.0 Hz, 1H), 2.60 (t, J = 7.6 Hz, 2H), 2.36-2.34 (m, 1H), 2.28-2.26 (m, 1H), 1.60-1.53 (m, 2H), 1.35-1.28 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6): 173.96, 152.30, 144.08, 143.81, 139.23, 133.76, 131.58, 130.38, 129.32, 128.49, 127.53, 125.51, 124.75, 123.36, 113.68, 84.72 (d, $^1J_{F\text{-}C}$ = 169.0 Hz), 47.66 (d, $^2J_{F\text{-}C}$ = 21.0 Hz), 36.49 (d, $^3J_{F\text{-}C}$ = 5.1 Hz), 35.81, 34.37, 28.71 (d, $^3J_{F\text{-}C}$ = 8.0 Hz), 22.81, 14.23; ^{19}F NMR (376 MHz, acetone-d_6): δ -215.88; IR (ATR): 2928, 1723, 1433, 1256, 1208; MS (EI): 508, (M^+, 16), 302 (100), 246 (33), 303 (28), 122 (24), 92 (22), 156 (21), 115 (18); HRMS (EI): Exact mass calcd for $C_{27}H_{25}N_2O_5FS$ $[M]^+$: 508.1468, Found: 508.1465.

Part V: Determining the solubility of 1a in PhF and PhCl

The detail for measuring the solubility of **1a** in PhF and PhCl was described below. To **1a** (0.20 mmol, 31.8 mg) was added 4.0 mL of the corresponding PhF or PhCl, respectively. After stirring the reaction mixture at 0 ^{o}C for one hour, the solution kept still for another half an hour. And then 50 uL supernate was quickly taken and moved to the NMR tube containing 0.05 mmol trimethoxybenzene as internal standard. The procedure was repeated for three times. By this, the solubility of **1a** in PhF and PhCl was determined to be 5.6 and 6.4 mg/mL respectively.

Part VI: Results of DFT Calculations and Discussion

We conducted density functional theory (DFT) calculations of the Au(I)-catalyzed cyclopropanation of diazooxindole **1a** and alkene **2a** by using Gausssian 09 software package.[6] Molecular geometries of the reactants, intermediates, transition states and products were optimized with M06-2X functionals.[7] The 6-311G(d) basis set was used for the other atoms (C, H, O, N, P, Cl, F) and LANL2DZ effective core potential for Au. All the stationary points were tested by the frequency calculation and the relative free energies (ΔG) with the zero-point energy (ZPE) corrections. The reaction paths connecting the related reactants and the transition geometries and products were confirmed by intrinsic reaction coordinate (IRC) calculations.

The formula of rate constants for calculation:

k (s^{-1}) = $k_b \times T \times \sigma \times \kappa/h \times \exp(-\Delta G^0/(R/1000T))$ (Formula s1)

ΔG^0: The difference between G (T) of reactants and G (T) of transition state (TS) under a standard pressure

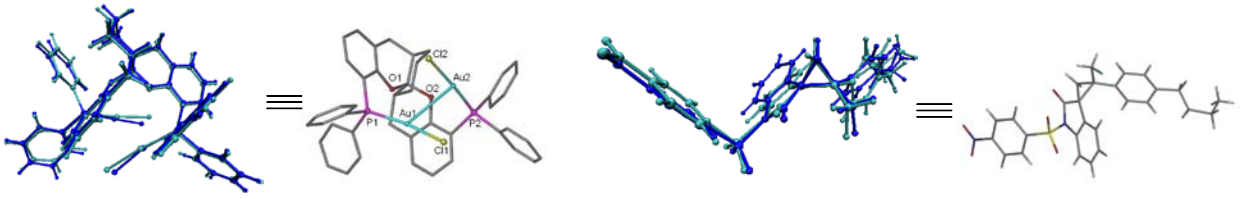
k_b (J/K): Boltzmann constant T(K) : 298 σ: Reaction path degenerac

h(J*s): Planck constant R(J/mol/K): Gas constant

κ: Correction factor of tunnel effect, $\kappa = 1 + (h/k_b/T \times F \times 3 \times 10^{10})^2/24$

F(cm^{-1}): Imaginary frequency size of transition state structure

In order to make sure that we choose the right calculation method, we first calculate the two crystal structures of catalyst precursor and product **4**. As shown in Figure 1, the calculated structures are in in accordance with the experimental data, which indicates the used DFT method is suitable for calculation.



Au precursor (RMSD = 0.30 Å) Product **4** (RMSD = 0.61 Å)

Figure S1. Comparison between the experimental crystal and calculated structures of catalyst precursor and **4**

(6) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A. et al. Gaussian 09, Revision B.01; Gaussian, Inc.: Wallingford CT, **2010**.
(7) (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157-167.

We further optimized the structures of the key intermediates **IM$_2$-Sol**. It is noticed that for each of them, two possible isomers were found (Figure S2), so only the two isomers with lower energy of **IM$_2$-PhF** and **IM$_2$-PhCl** was used for further investigation.

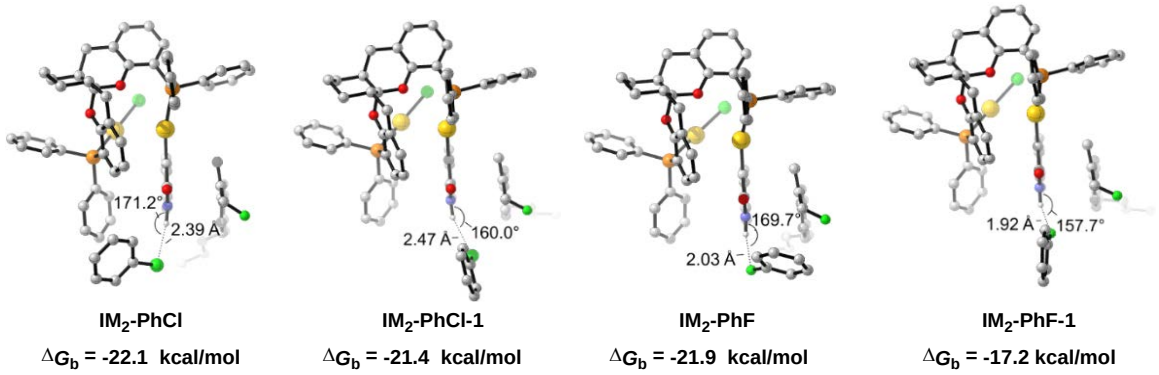


Figure S2. The isomers of **IM$_2$-PhCl** and **IM$_2$-PhF** using M06-2X/6-311G(d)

After this, we checked the presence of H-bonding interaction with solvent on the influence of the key intermediate **IM$_2$**. As demonstrated below, first, it tunes the orientation of dipole moment (Figure S3), which directs straightly from Au atom to the more negatively charged C atom (the influence on charge distribution are descried in Table S5).

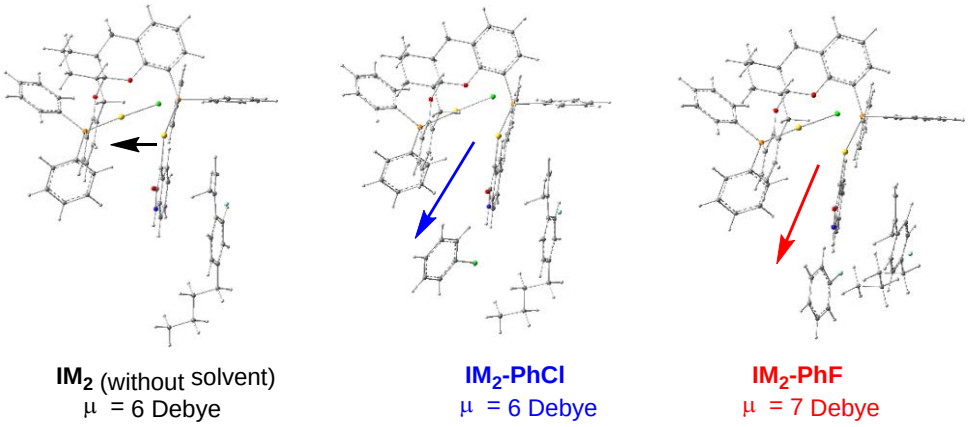
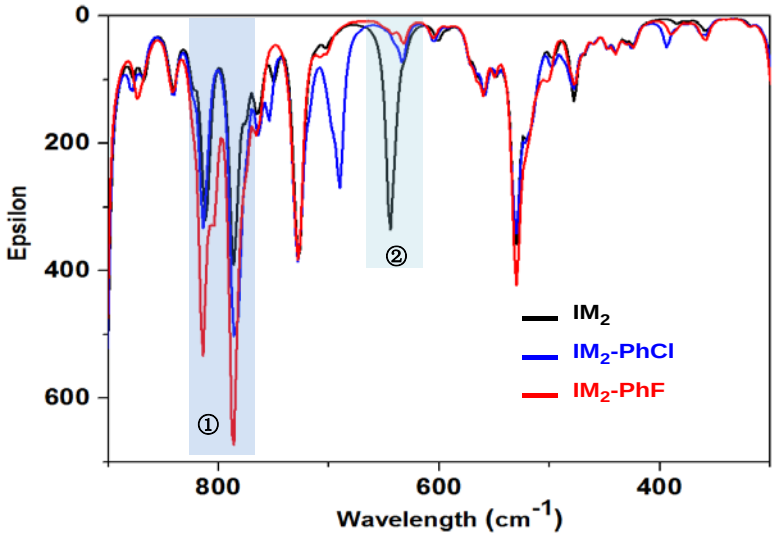


Figure S3. The dipole moments of reactants, **IM$_2$**, **IM$_2$-PhCl** and **IM$_2$-PhF**

We also examined the low-frequency vibrational modes of **IM** (without solvent), **IM$_2$-PhCl** and **IM$_2$-PhF** in the simulated IR spectra (Figure S4). It was noticed, the low-frequency vibrations at about 600 cm^{-1} of N-H vibrations and indole ring breath are depressed by H···Cl (H···F) interaction in gold carbenoid and PhCl (PhF), slightly lowering the entropy during the reaction. In contrast, at about 800 cm^{-1}, the translation motion of indole ring towards the attacking of olefin (i.e. the motion along the reaction coordinate) is significantly promoted by H···Cl (H···F) interaction between gold carbenoid and

PhCl (PhF), especially for H···F interaction with the value of oscillator strength (f) is 77 which is larger than that of H···Cl (f = 48).

(a)



(b)

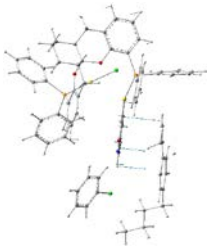
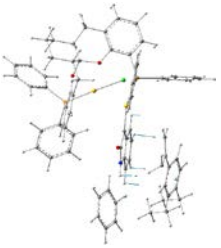
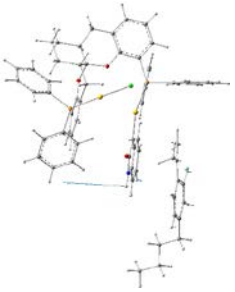
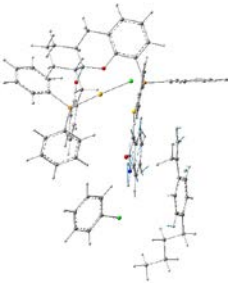
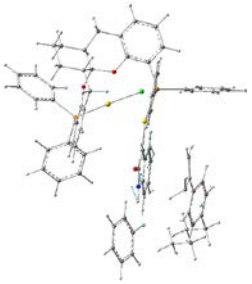
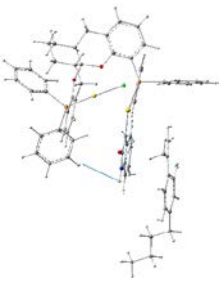
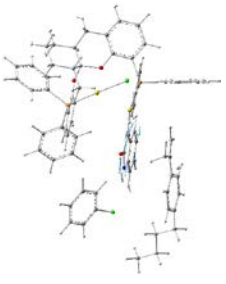
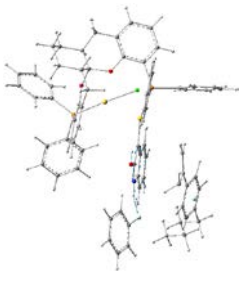
①	 **IM_2** (without solvent) **ν_{148} (813 cm^{-1}) f = 63**	 **IM_2-PhCl** **ν_{163} (813 cm^{-1}) f = 48**	 **IM_2-PhF** **ν_{163} (814 cm^{-1}) f = 77**
②	 **ν_{116} (645 cm^{-1}) f = 86**	 **ν_{124} (633 cm^{-1}) f = 18**	 **ν_{124} (632 cm^{-1}) f = 10**
	 **ν_{113} (631 cm^{-1}) f = 8**	 **ν_{123} (605 cm^{-1}) f = 7**	 **ν_{123} (606 cm^{-1}) f = 6**

Figure S4. The simulated IR spectra and vibrational modes of **IM_2**, **IM_2-PhF** and **IM_2-PhCl** at the B3LYP/6-31G level.

Besides this, the influence of H-bonding interaction on the atomic charge distrubition of Au atom and the adjcent carbon atom of the carbenoid was also calculated and the data was shown in Table S5.

Table S5: The atomic charges of Au and C of reactants, **IM_2, $TS_{2\text{-}3}$, IM_2-Sol** and **$TS_{2\text{-}3}$-Sol**

Reactants/intermediates/transition states		Charge (a.u.)	
		Au	**C**
Reactants	**1a**	-	0.05
	1a + PhCl	-	0.16
	1a + PhF	-	0.16
Without solvent	**IM_2**	-0.02	-0.16
	$TS_{2\text{-}3}$	-0.13	-0.25
PhCl as solvent	**IM_2-PhCl**	-0.02	-0.17
	$TS_{2\text{-}3}$-PhCl	-0.12	-0.21
PhF as solvent	**IM_2-PhF**	-0.04	-0.16
	$TS_{2\text{-}3}$-PhF	-0.11	-0.22

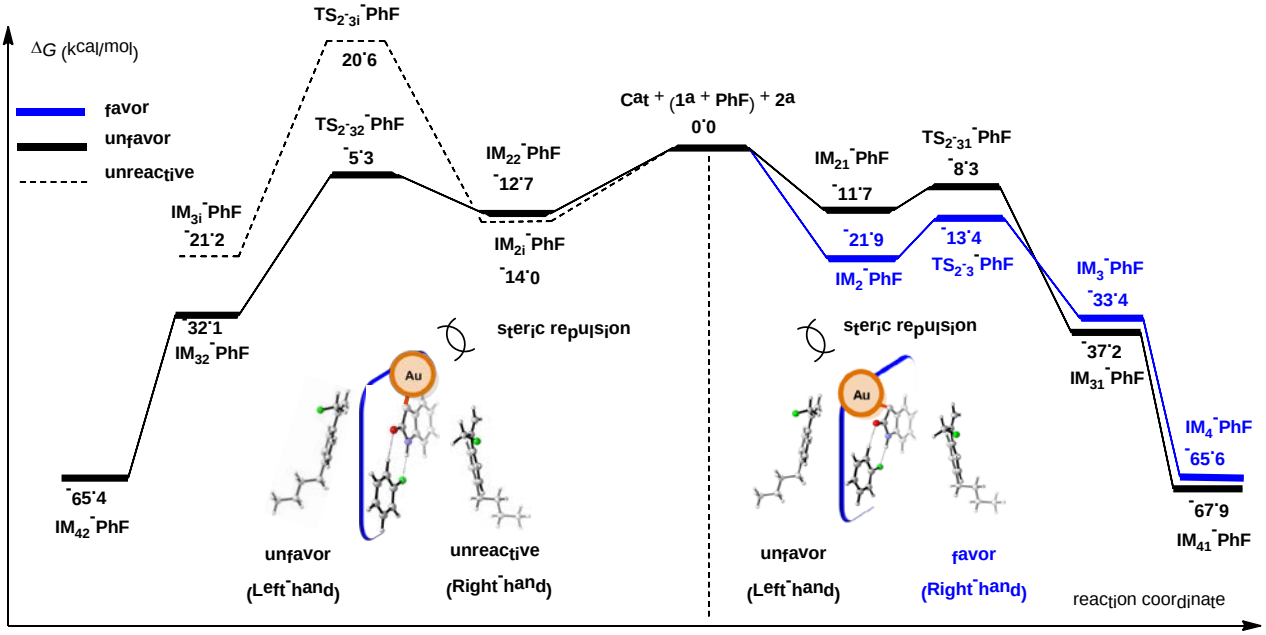
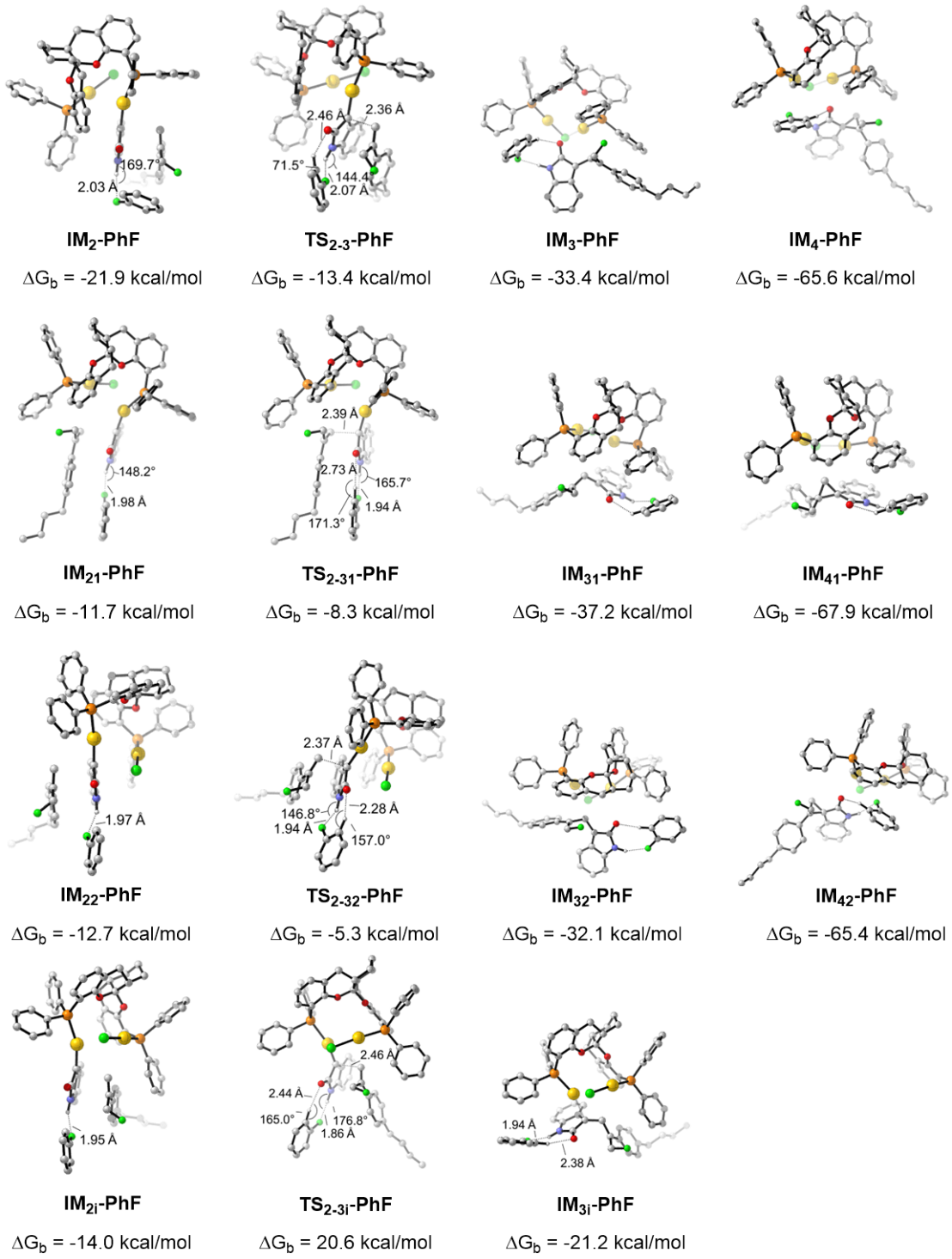


Figure S5. Free energy curves of the possible pathways using PhF as the solvent

For determing the stereo-determining step in PhF, we checked the possible reactions pathways. As presented in Figure S5, four possible pathways that working through intermediates **IM_2-PhF**, **IM_{21}-PhF**, **IM_{22}-PhF**, and **IM_{2i}-PhF**, respectively, were calculated to determine the stereo-determining step in PhF,

and the most favorable path (shown in blue) is benefited from the less steric repulsion in **IM_2-PhF** with the right-hand attacking mode. The difference between **IM_2-PhF**/**IM_{21}-PhF** and **IM_{22}-PhF**/**IM_{2i}-PhF** lies in the different configurations of Au-carbenoid part relative to the molecular plane. The appropriate images of DFT optimized strucutures and transition states are provided in Figure S6.



IM_2-PhF
ΔG_b = -21.9 kcal/mol

$TS_{2\text{-}3}$-PhF
ΔG_b = -13.4 kcal/mol

IM_3-PhF
ΔG_b = -33.4 kcal/mol

IM_4-PhF
ΔG_b = -65.6 kcal/mol

IM_{21}-PhF
ΔG_b = -11.7 kcal/mol

$TS_{2\text{-}31}$-PhF
ΔG_b = -8.3 kcal/mol

IM_{31}-PhF
ΔG_b = -37.2 kcal/mol

IM_{41}-PhF
ΔG_b = -67.9 kcal/mol

IM_{22}-PhF
ΔG_b = -12.7 kcal/mol

$TS_{2\text{-}32}$-PhF
ΔG_b = -5.3 kcal/mol

IM_{32}-PhF
ΔG_b = -32.1 kcal/mol

IM_{42}-PhF
ΔG_b = -65.4 kcal/mol

IM_{2i}-PhF
ΔG_b = -14.0 kcal/mol

$TS_{2\text{-}3i}$-PhF
ΔG_b = 20.6 kcal/mol

IM_{3i}-PhF
ΔG_b = -21.2 kcal/mol

Figure S6. The appropriate images of DFT optimized structures and transition states

Coordinates of DFT optimized structures and transition states shown in Figure S5.

(1) Cat

Zero-point correction =			0.713564 (Hartree/Particle)
Thermal correction to Energy =			0.758118
Thermal correction to Enthalpy =			0.759063
Thermal correction to Gibbs Free Energy =			0.632606
Sum of electronic and zero-point Energies =			-3262.489478
Sum of electronic and thermal Energies =			-3262.444924
Sum of electronic and thermal Enthalpies =			-3262.443979
Sum of electronic and thermal Free Energies =			-3262.570436
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Au	-1.56584400	-1.63812500	-1.07194800
P	3.25943300	-0.18340200	0.32290200
P	-3.14528900	-0.54315800	0.14797400
Cl	0.25077800	-2.86292700	-2.18622400
O	-1.12296500	1.48959900	0.06737600
O	1.10162100	1.62919100	-0.18473300
C	2.85530300	0.26746800	2.03119700
C	3.55988300	1.30540500	2.64939100
H	4.31639900	1.85589700	2.09764400
C	3.28360000	1.63477900	3.97001000
H	3.83044000	2.43664000	4.45248800
C	2.30425900	0.93353500	4.67143000
H	2.09387000	1.18812400	5.70428700
C	1.59772500	-0.09122200	4.05252800
H	0.82716300	-0.62766200	4.59351900
C	1.86805200	-0.42445600	2.72935700
H	1.30710700	-1.21476200	2.23980400
C	4.91929200	-0.92478600	0.32380000
C	5.71543400	-0.97962800	1.46703400
H	5.35483200	-0.58464500	2.40950200
C	6.97687300	-1.56492700	1.40277900
H	7.59057600	-1.61137100	2.29467200
C	7.44496500	-2.08919600	0.20497900
H	8.42730700	-2.54463900	0.15920200
C	6.64864400	-2.04068600	-0.93714500
H	7.00733600	-2.45860200	-1.87037100
C	5.38661300	-1.46871600	-0.87825300
H	4.76250800	-1.44610300	-1.76750800
C	-4.41323300	-1.66269200	0.80783200
C	-4.05291400	-2.97878400	1.10879800
H	-3.05062300	-3.33422900	0.88912700
C	-4.98060300	-3.83766500	1.68405100
H	-4.69977700	-4.85877600	1.91355200
C	-6.27037400	-3.38976800	1.95089600
H	-6.99603300	-4.06402300	2.39075200

C	-6.63418700	-2.08292500	1.64296300
H	-7.64193000	-1.73744000	1.84114900
C	-5.70859000	-1.21550600	1.07416600
H	-6.00135500	-0.20067000	0.82785400
C	-4.00373800	0.81417000	-0.70223900
C	-4.47710200	1.90759800	0.02761000
H	-4.31765300	1.95918400	1.10056400
C	-5.14746000	2.93613900	-0.62484400
H	-5.51475600	3.78389800	-0.05772900
C	-5.34380600	2.87663400	-2.00198400
H	-5.86459100	3.68058600	-2.50938500
C	-4.87196200	1.78842700	-2.72865000
H	-5.02365400	1.74237500	-3.80055400
C	-4.20022900	0.75622100	-2.08151300
H	-3.82648300	-0.08968800	-2.65026400
C	3.39566200	1.36583700	-0.61512900
C	2.20261600	2.06556100	-0.86043700
C	2.16022800	3.10704000	-1.78238600
C	3.35857800	3.50975300	-2.37230300
H	3.33519300	4.32787600	-3.08579400
C	4.56107800	2.88411200	-2.07916700
H	5.48005500	3.22164400	-2.54195900
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C	-2.74287100	-0.09589200	2.90464700
H	-3.49868700	-0.85326300	3.07963300
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H	0.11380100	3.76039900	2.91169600
C	0.83887800	3.72872800	-2.15291400
H	0.78501400	4.74507700	-1.75244400
H	0.78233400	3.82876400	-3.24010100
C	-0.09853700	2.40742700	-0.25055600
C	-0.06084800	3.55368200	0.76466800
H	0.77440900	4.20742400	0.49431600
C	-1.37891500	4.34274300	0.68806100
H	-1.31777800	5.19396500	1.37159400
H	-2.19624200	3.71047900	1.05327300
C	-1.71221400	4.81940600	-0.72716200
H	-2.70919400	5.26751100	-0.73434100
H	-1.02330500	5.61730200	-1.02071400

C	-1.67082900	3.66922000	-1.73785000
H	-2.49263100	2.97893800	-1.53631300
H	-1.81647100	4.04866500	-2.75334400
C	-0.35249300	2.89055700	-1.67453800
H	-0.42196800	1.98649700	-2.29136400

(2) 2a

Zero-point correction =	0.270531 (Hartree/Particle)
Thermal correction to Energy =	0.284867
Thermal correction to Enthalpy =	0.285811
Thermal correction to Gibbs Free Energy =	0.227565
Sum of electronic and zero-point Energies =	-605.046074
Sum of electronic and thermal Energies =	-605.031738
Sum of electronic and thermal Enthalpies =	-605.030794
Sum of electronic and thermal Free Energies =	-605.089041

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H	-5.19077800	-0.24603100	-0.07340700
H	-3.97229800	-0.84999600	-1.23320400
F	-3.99098300	-1.71927500	0.57407100
C	-1.77003600	0.34849000	-0.08813400
C	-1.18551800	-0.91987800	-0.16299500
C	-0.96969900	1.46115900	-0.36587100
C	0.15877400	-1.06101600	-0.48283200
H	-1.78234200	-1.79891500	0.05011000
C	0.37203000	1.31179100	-0.68514100
H	-1.41172700	2.45189400	-0.36186800
C	0.96056200	0.04817100	-0.74685500
H	0.59419500	-2.05512500	-0.52922900
H	0.97125700	2.19008000	-0.90854900
C	-3.67211500	1.55478400	0.93628600
H	-3.01759400	2.33513100	1.30826200
H	-4.72888300	1.65493900	1.15881100
C	2.43059100	-0.10907700	-1.03659200
C	3.27457900	-0.03561700	0.24155300
H	2.75903300	0.67062700	-1.73182500
H	2.60900900	-1.06870900	-1.53275800
C	4.76662300	-0.22108400	-0.02005600
H	3.10098100	0.93015300	0.73058100
H	2.92416600	-0.79928600	0.94554200
C	5.59535300	-0.13936700	1.25864200
H	4.93037400	-1.18972300	-0.50525500
H	5.10845900	0.53896800	-0.73147500
H	6.65938300	-0.28101000	1.05963300
H	5.47304200	0.83308300	1.74269800
H	5.28537300	-0.90488900	1.97470000

(3) N_2

Zero-point correction =			0.005738 (Hartree/Particle)
Thermal correction to Energy =			0.008098
Thermal correction to Enthalpy =			0.009043
Thermal correction to Gibbs Free Energy =			-0.012685
Sum of electronic and zero-point Energies =			-109.513390
Sum of electronic and thermal Energies =			-109.511030
Sum of electronic and thermal Enthalpies =			-109.510086
Sum of electronic and thermal Free Energies =			-109.531813
N	0.00000000	0.00000000	0.54496900
N	0.00000000	0.00000000	-0.54496900

(4) 1a + PhF

Zero-point correction =			0.215769 (Hartree/Particle)
Thermal correction to Energy =			0.231929
Thermal correction to Enthalpy =			0.232873
Thermal correction to Gibbs Free Energy =			0.166568
Sum of electronic and zero-point Energies =			-878.444528
Sum of electronic and thermal Energies =			-878.428369
Sum of electronic and thermal Enthalpies =			-878.427424
Sum of electronic and thermal Free Energies =			-878.493729
C	1.97197500	-0.92926300	0.00002200
C	2.99327800	0.04194200	-0.00002700
C	4.32572600	-0.33829600	-0.00006000
C	4.62854200	-1.69910300	-0.00004300
C	3.61456300	-2.65328900	0.00000600
C	2.27029300	-2.28070300	0.00003900
C	0.83730600	1.08184300	0.00002300
C	2.29462200	1.31157100	-0.00003500
H	5.11646000	0.40395400	-0.00010200
H	5.66463000	-2.01598100	-0.00006900
H	3.87034200	-3.70647300	0.00001900
H	1.48152500	-3.02411500	0.00007900
H	-0.16743100	-0.76024700	0.00007500
O	-0.06583300	1.88854700	0.00003400
F	-2.05321200	-1.44587100	0.00006200
C	-3.21534500	-0.73994000	0.00003900
C	-4.40270400	-1.44724600	0.00002900
C	-3.15343700	0.64043000	0.00002500
C	-5.59332900	-0.72846500	0.00000500
H	-4.38258900	-2.53007700	0.00004000
C	-4.35690100	1.33950000	0.00000200
H	-2.19358300	1.14797800	0.00003100
C	-5.57241300	0.66269100	-0.00000700
H	-6.53740900	-1.26062000	-0.00000300
H	-4.33715600	2.42296900	-0.00000900
H	-6.50255100	1.21845200	-0.00002500
N	0.73053800	-0.29660000	0.00005100
N	2.79568900	2.51595700	-0.00007700

N	3.20809700	3.55758600	-0.00011200

(5) 1a + PhCl

Zero-point correction =	0.214274 (Hartree/Particle)
Thermal correction to Energy =	0.229944
Thermal correction to Enthalpy =	0.230889
Thermal correction to Gibbs Free Energy =	0.166804
Sum of electronic and zero-point Energies =	-1238.804847
Sum of electronic and thermal Energies =	-1238.789176
Sum of electronic and thermal Enthalpies =	-1238.788232
Sum of electronic and thermal Free Energies =	-1238.852316

C	2.25360300	-0.87162600	0.00023900
C	3.22750400	0.14694700	-0.00016000
C	4.57638900	-0.17210200	-0.00070100
C	4.94135200	-1.51753300	-0.00083200
C	3.97289900	-2.51784700	-0.00043800
C	2.61298500	-2.20753600	0.00010100
C	1.02383400	1.08395900	0.00077800
C	2.46866800	1.38227300	0.00011800
H	5.33197300	0.60591100	-0.00103800
H	5.99111500	-1.78567800	-0.00124900
H	4.27747900	-3.55793300	-0.00054400
H	1.86022900	-2.98754000	0.00043600
H	0.10958500	-0.80354000	0.00095000
O	0.08105600	1.84370500	0.00115400
C	-3.41584600	-0.68835600	0.00005700
C	-4.74621400	-1.08130800	-0.00026500
C	-3.03817200	0.64566400	-0.00001600
C	-5.73072600	-0.10009700	-0.00067600
H	-5.00223700	-2.13370900	-0.00019900
C	-4.03926300	1.61215400	-0.00042800
H	-1.99374200	0.93949900	0.00025800
C	-5.38033600	1.24592200	-0.00076600
H	-6.77425100	-0.39378800	-0.00093100
H	-3.75665100	2.65860800	-0.00048400
H	-6.15188500	2.00701300	-0.00111400
N	0.98405300	-0.29794700	0.00080300
N	2.91002900	2.61003900	-0.00007200
N	3.26807100	3.67135800	-0.00022100
Cl	-2.17854100	-1.93798400	0.00053200

(6) IM_2-PhF

Zero-point correction =	1.191813 (Hartree/Particle)
Thermal correction to Energy =	1.268218
Thermal correction to Enthalpy =	1.269162
Thermal correction to Gibbs Free Energy =	1.067194
Sum of electronic and zero-point Energies =	-4636.531596
Sum of electronic and thermal Energies =	-4636.455191

Sum of electronic and thermal Enthalpies = -4636.454247
Sum of electronic and thermal Free Energies = -4636.656215

Au	0.29251700	-1.18743000	-0.15370300
Au	1.26779100	1.65412200	-1.49432000
P	1.96220200	-2.80407300	-0.63696400
P	1.30257000	2.86838800	0.44501200
Cl	1.29529500	0.09375900	-3.32790200
O	3.61744500	1.34417700	0.68152500
O	3.80500900	-0.69675100	-0.23124600
C	2.67680100	-3.52038700	0.87637000
C	3.89185200	-4.21442900	0.84256200
H	4.42778000	-4.32741500	-0.09432200
C	4.41881600	-4.75184100	2.01208700
H	5.35693100	-5.28636000	1.98628700
C	3.73432100	-4.60384700	3.21668800
H	4.14460700	-5.02332400	4.12896700
C	2.52221700	-3.91806600	3.25192200
H	1.99164500	-3.80394400	4.19455900
C	2.00148500	-3.37063600	2.08591700
H	1.06739400	-2.81240100	2.12619700
C	1.07021400	-4.15788600	-1.47759300
C	1.02406300	-5.45823800	-0.98153300
H	1.55807500	-5.71606100	-0.07936200
C	0.26927500	-6.42032700	-1.65389900
H	0.22923400	-7.43105100	-1.26517900
C	-0.41645700	-6.09060700	-2.81237000
H	-0.99374200	-6.84880100	-3.32830200
C	-0.36450800	-4.79114800	-3.31327500
H	-0.89505600	-4.53817300	-4.22156400
C	0.36853300	-3.82094300	-2.64201400
H	0.41791300	-2.80506200	-3.02915700
C	-0.20976200	3.77747700	0.90828800
C	-1.31455900	3.78057700	0.05973900
H	-1.28447400	3.23557300	-0.87829700
C	-2.44832900	4.51561000	0.40757400
H	-3.29806500	4.53367200	-0.26313300
C	-2.48301000	5.22990700	1.59491400
H	-3.36214900	5.80429000	1.86188000
C	-1.37807400	5.22420200	2.44427900
H	-1.39460800	5.78792500	3.37190600
C	-0.23754700	4.50902700	2.10057600
H	0.62555200	4.52238700	2.75149300
C	2.66383100	4.08316000	0.55086100
C	3.35216500	4.29230200	1.74995200
H	3.08868400	3.72477300	2.63714100
C	4.38907700	5.21495100	1.79400800
H	4.92435100	5.37544600	2.72737700
C	4.74885300	5.91923700	0.65143900

H	5.56732900	6.63685200	0.68971100
C	4.06583300	5.70917200	-0.53769100
H	4.35142000	6.25445000	-1.43482200
C	3.02999900	4.78229500	-0.59491600
H	2.50948300	4.60504000	-1.52849300
C	3.38621400	-2.45616500	-1.70222400
C	4.20496100	-1.38085000	-1.34149000
C	5.35170400	-1.06387500	-2.05782400
C	5.65345900	-1.83488300	-3.18017100
H	6.53811600	-1.58960700	-3.76045100
C	4.85139500	-2.90167400	-3.56748400
H	5.10608200	-3.48327100	-4.43989100
C	3.71584600	-3.21168200	-2.82584000
H	3.08655500	-4.04430800	-3.11858200
C	1.60371400	1.69277900	1.80441900
C	2.80744400	0.98530900	1.71573300
C	3.16102000	0.00091100	2.63001800
C	2.24013300	-0.29538900	3.63811900
H	2.48875400	-1.06502400	4.35958100
C	1.02292900	0.37144000	3.72946900
H	0.31689500	0.10892200	4.50620500
C	0.70597500	1.37776400	2.81240100
H	-0.24344000	1.89326200	2.88591800
C	4.47459100	-0.73141700	2.47862500
H	4.26557000	-1.75984500	2.17832800
H	4.97757200	-0.78271000	3.44823200
C	6.20594700	0.10473200	-1.61907800
H	7.04568400	-0.25364000	-1.02027200
H	6.63650300	0.59551400	-2.49822500
C	4.57567100	0.40525500	0.25448700
C	5.40112700	-0.05826900	1.45441600
H	6.11571500	-0.80595000	1.09156700
C	6.17050800	1.13927700	2.02397300
H	6.79864000	0.79649100	2.85389900
H	5.45099600	1.85177200	2.44461800
C	7.01565400	1.82608200	0.95430700
H	7.51767200	2.69710500	1.38234200
H	7.80965500	1.14626800	0.62584700
C	6.16025800	2.26984600	-0.23974300
H	5.46354200	3.04405200	0.08363700
H	6.79180700	2.71222100	-1.01577400
C	5.35916000	1.10676000	-0.84269600
H	4.60050200	1.50939300	-1.53211500
C	-1.44372500	-0.18981500	0.20750100
C	-2.16240000	-0.12532300	1.56228900
C	-2.26937900	0.50594000	-0.65392900
C	-3.41191400	1.01133400	0.06611200
O	-1.81892400	-0.60145100	2.60811200

N	-3.32906400	0.63270200	1.36958400
C	-2.12894000	0.78426300	-2.04807100
C	-4.37341300	1.79360900	-0.56677700
C	-3.07554100	1.56539600	-2.65800200
C	-4.17621900	2.05881800	-1.91234600
H	-4.90704800	2.68555300	-2.42206500
H	-5.23878400	2.16686000	-0.03450200
H	-2.99056100	1.80764800	-3.70553400
H	-1.28166100	0.38234900	-2.58748500
H	-3.98370600	0.88646000	2.09398600
F	-5.55228000	1.28303300	3.31559100
C	-5.50460100	0.06674700	3.91676900
C	-4.37102800	-0.26307000	4.63326900
C	-6.56979100	-0.80670800	3.74446100
C	-4.29908400	-1.54163800	5.18986100
H	-3.56789800	0.45426600	4.74209000
C	-6.47535400	-2.07464100	4.30219600
H	-7.43781200	-0.48532300	3.17900800
C	-5.34336000	-2.44329100	5.02406200
H	-3.41757200	-1.81983000	5.75117100
H	-7.28363800	-2.78052400	4.16302200
H	-5.27310900	-3.43720300	5.44402000
C	-3.81091600	-2.41577400	0.33283400
C	-2.62308700	-2.80887800	-0.14349300
H	-1.92758700	-3.37572600	0.47122500
H	-2.29532300	-2.63029900	-1.16313100
C	-4.81882500	-1.68786400	-0.47050700
C	-5.97865800	-1.17916300	0.13818400
C	-4.66584000	-1.49276900	-1.85392200
C	-6.94152000	-0.52360400	-0.61050000
H	-6.15119500	-1.34571300	1.19186800
C	-5.63528700	-0.83276400	-2.59125600
H	-3.80153100	-1.88929400	-2.36970200
C	-6.79789700	-0.34488800	-1.98542100
H	-5.50725700	-0.72088300	-3.66343700
C	-4.15099500	-2.72384900	1.77340000
H	-3.34581100	-3.29111000	2.24405600
H	-4.32669600	-1.82000400	2.35378500
F	-5.30693300	-3.48549300	1.83963800
H	-7.84157200	-0.16634800	-0.11576100
C	-7.87091000	0.33421600	-2.79899900
C	-7.53129700	1.78739100	-3.13979900
H	-8.81810800	0.30053300	-2.25703100
H	-8.02703600	-0.22464500	-3.72959100
C	-8.64462200	2.49682000	-3.89887300
H	-7.31907200	2.32937600	-2.20960600
H	-6.61195500	1.81152200	-3.73857500
C	-8.28282700	3.94035400	-4.24076100

H	-8.86874100	1.94270400	-4.81698900
H	-9.56329200	2.47878200	-3.29560400
H	-9.09634200	4.44179300	-4.77394400
H	-8.08004900	4.51773400	-3.33813100
H	-7.39582800	3.98280500	-4.87425200

(7) IM$_2$-PhF-1

Zero-point correction = 1.189631 (Hartree/Particle)
Thermal correction to Energy = 1.266014
Thermal correction to Enthalpy = 1.266958
Thermal correction to Gibbs Free Energy = 1.065280
Sum of electronic and zero-point Energies = -4636.524394
Sum of electronic and thermal Energies = -4636.448011
Sum of electronic and thermal Enthalpies = -4636.447066
Sum of electronic and thermal Free Energies = -4636.648745

Au	-0.27338300	1.25079600	0.33592600
Au	-1.29714900	-0.63310300	-2.15731300
P	-1.95484600	2.88036500	0.71945800
P	-1.32943500	-2.65534700	-1.08448500
Cl	-1.33611000	1.62378300	-3.01369500
O	-3.59807200	-1.40808100	-0.07045800
O	-3.82409100	0.82592600	0.13903700
C	-2.67595000	2.75276800	2.38831400
C	-3.91465800	3.31726600	2.68160400
H	-4.47483000	3.84832900	1.91320600
C	-4.44354200	3.21236600	3.96765500
H	-5.41056500	3.65957400	4.18797100
C	-3.72617600	2.53901000	4.94546400
H	-4.13878300	2.46256300	5.94860500
C	-2.49584200	1.96326400	4.65786900
H	-1.93206500	1.44772500	5.43841700
C	-1.96837700	2.06938300	3.38007500
H	-1.00798400	1.61409200	3.14488900
C	-1.11963800	4.49628300	0.63732300
C	-1.20485800	5.44373600	1.66778000
H	-1.78622000	5.21628900	2.55152100
C	-0.54263000	6.65634000	1.54835400
H	-0.61540400	7.38624200	2.35257500
C	0.20247300	6.94145800	0.41460700
H	0.71687500	7.89066300	0.31886100
C	0.29511300	6.00236800	-0.62322600
H	0.85715100	6.22233400	-1.51008900
C	-0.36093800	4.76986900	-0.50827600
H	-0.30559700	4.05158900	-1.31129900
C	0.15978000	-3.69483500	-1.16971000
C	1.23362000	-3.32434100	-1.97273600
H	1.19887600	-2.38382800	-2.52415500
C	2.34239200	-4.15627800	-2.07919600

H	3.16202000	-3.87066700	-2.72658200
C	2.37737600	-5.36592500	-1.38685700
H	3.23832900	-6.02053600	-1.49759400
C	1.30598500	-5.73903300	-0.59189500
H	1.32113700	-6.68934800	-0.06191700
C	0.18652800	-4.91560700	-0.48696600
H	-0.66015500	-5.23083500	0.12206000
C	-2.72036800	-3.71785600	-1.58544600
C	-3.39770400	-4.52081900	-0.66441300
H	-3.11710900	-4.50013900	0.38391400
C	-4.45335200	-5.32386300	-1.09298100
H	-4.98815400	-5.93704100	-0.38233200
C	-4.83468300	-5.32101800	-2.42757200
H	-5.65945100	-5.94259100	-2.76667800
C	-4.16193200	-4.51231700	-3.34435000
H	-4.45446300	-4.51090300	-4.38919800
C	-3.10381400	-3.71093600	-2.92972200
H	-2.59270800	-3.07776200	-3.64289200
C	-3.38718900	3.05492900	-0.38628900
C	-4.22004400	1.94626500	-0.54826200
C	-5.38273800	1.99445200	-1.31156500
C	-5.67299100	3.18873400	-1.96634100
H	-6.55597400	3.24209400	-2.57515600
C	-4.84923200	4.30801200	-1.84810000
H	-5.08829600	5.22285200	-2.37151900
C	-3.69881100	4.23653800	-1.05681500
H	-3.06568500	5.10740600	-0.95259900
C	-1.59370300	-2.31267500	0.68959200
C	-2.78523400	-1.62521300	0.99339900
C	-3.10601900	-1.22534000	2.27597500
C	-2.17934900	-1.50564600	3.29152500
H	-2.41472700	-1.20644400	4.30296400
C	-0.99684300	-2.16247600	3.01383000
H	-0.27539500	-2.35136900	3.81296900
C	-0.68575900	-2.57193700	1.72282100
H	0.23780000	-3.08335300	1.49917400
C	-4.39887800	-0.48896800	2.53705600
H	-4.17474000	0.55817000	2.74591000
H	-4.88337200	-0.89361300	3.42880200
C	-6.23801200	0.77170000	-1.41768300
H	-7.04907000	0.80805400	-0.68278200
H	-6.72507800	0.73773000	-2.40333700
C	-4.57053100	-0.39061500	0.04454600
C	-5.36507300	-0.58103600	1.34498500
H	-6.08391100	0.22391600	1.41239800
C	-6.10308700	-1.91945500	1.26368000
H	-6.70736500	-2.04664400	2.18249700
H	-5.37420900	-2.73983800	1.25659500

C	-6.99265200	-2.00523400	0.02690200
H	-7.48850300	-2.98150600	-0.00732800
H	-7.79176000	-1.26879600	0.09511200
C	-6.18459800	-1.79900200	-1.25690100
H	-5.48365700	-2.62779300	-1.37274800
H	-6.83140500	-1.81164800	-2.13087400
C	-5.38785500	-0.48480600	-1.23546000
H	-4.64800600	-0.49812900	-2.05336700
C	1.42123300	0.12848300	0.13821200
C	2.11489900	-0.64534100	1.27356600
C	2.21812800	-0.11171200	-0.96822800
C	3.29863900	-0.99076900	-0.61364600
O	1.78871100	-0.69864600	2.42718000
N	3.20400600	-1.30495700	0.71419500
C	2.08971100	0.35891000	-2.31295500
C	4.23590600	-1.38740500	-1.55289900
C	3.01505600	-0.05644400	-3.22982000
C	4.08148600	-0.90795800	-2.84276500
H	4.80742000	-1.20434000	-3.58504600
H	5.07398200	-2.04011400	-1.29164900
H	2.94914600	0.27249700	-4.26546500
H	1.26044800	1.02064200	-2.56198900
H	3.85045100	-1.87885300	1.24569100
F	4.95921300	-2.40292700	2.72397700
C	4.76330700	-2.84885200	4.00431800
C	3.68188800	-2.35699800	4.72646300
C	5.66171800	-3.77944700	4.50099600
C	3.51251800	-2.79587800	6.05827300
H	3.00047200	-1.65276500	4.26253400
C	5.47793900	-4.20366500	5.83169200
H	6.47983300	-4.14470000	3.89143600
C	4.42203700	-3.68191000	6.59998200
H	2.69028000	-2.41608400	6.67664300
H	6.15322500	-4.92614600	6.29123400
C	4.01248900	1.71035000	1.34519300
C	2.83583600	2.35020700	1.18002000
H	2.18695900	2.54469500	2.02678900
H	2.52385800	2.77090200	0.23642500
C	4.97240600	1.44960100	0.26381700
C	6.08755500	0.61002300	0.46679000
C	4.81045300	2.00390700	-1.00904500
C	6.97503100	0.34596500	-0.55235800
H	6.28479700	0.21330300	1.46028500
C	5.70318700	1.72198000	-2.03349100
H	3.97901500	2.66935700	-1.21634500
C	6.79257600	0.87189900	-1.83549200
H	5.54615500	2.16844300	-3.00563200
C	4.36879800	1.21509800	2.72816100

H	3.57737100	1.45324000	3.44558800
H	4.54940800	0.12973200	2.74284000
F	5.54205400	1.81399100	3.15235700
H	7.84066000	-0.29415600	-0.35023300
C	7.79506200	0.63193100	-2.92142900
H	7.29359600	0.65644400	-3.90235400
H	8.23978400	-0.37158900	-2.81350000
C	8.92524800	1.67783800	-2.90151100
C	9.95971000	1.44915600	-4.00236200
H	9.41840300	1.66080600	-1.92898400
H	8.47869900	2.66915500	-3.00542800
C	11.06542700	2.49895300	-3.97360300
H	10.38984000	0.45363100	-3.90136600
H	9.44788900	1.47740000	-4.98385100
H	11.78894400	2.34237200	-4.78422700
H	10.65134400	3.50953200	-4.10568200
H	11.59545300	2.48055500	-3.02696100
H	4.30259400	-3.97119100	7.63579100

(8) $TS_{2\text{-}3}$-PhF

Zero-point correction = 1.191356 (Hartree/Particle)
Thermal correction to Energy = 1.265900
Thermal correction to Enthalpy = 1.266844
Thermal correction to Gibbs Free Energy = 1.069084
Sum of electronic and zero-point Energies = -4636.520540
Sum of electronic and thermal Energies = -4636.445996
Sum of electronic and thermal Enthalpies = -4636.445052
Sum of electronic and thermal Free Energies = -4636.642811

Au	0.31109600	-1.27707500	-0.35779100
Au	1.23680600	1.73158700	-1.31657100
P	2.18169100	-2.63760300	-0.89601200
P	1.07985100	2.75507100	0.72925000
Cl	1.44707600	0.40232300	-3.31089900
O	3.46336200	1.36718900	1.01184600
O	3.92014100	-0.56284000	-0.05376000
C	2.88617800	-3.47804300	0.55953400
C	4.16404600	-4.04737900	0.51313400
H	4.74929900	-3.98224000	-0.39438300
C	4.67991800	-4.68749600	1.63645100
H	5.66812200	-5.12560500	1.59323400
C	3.92850900	-4.76714500	2.80075000
H	4.33575900	-5.26675100	3.67224200
C	2.65284100	-4.20396700	2.84872500
H	2.06845600	-4.26566600	3.76053600
C	2.13483200	-3.55559500	1.73432600
H	1.15439200	-3.09993600	1.78271100
C	1.47833400	-3.94684800	-1.95679500
C	1.60718700	-5.30313800	-1.67507300

H	2.15667100	-5.63220500	-0.80147800
C	1.02347800	-6.24199300	-2.52267500
H	1.11975500	-7.30403600	-2.30026800
C	0.31883600	-5.82961900	-3.64893700
H	-0.13211900	-6.56730500	-4.30358300
C	0.19512000	-4.47315400	-3.93192900
H	-0.34423400	-4.14924100	-4.81547600
C	0.76219000	-3.53066900	-3.08863000
H	0.67762700	-2.47048000	-3.31194900
C	-0.49358600	3.56890900	1.14718700
C	-1.48835700	3.70910800	0.18078300
H	-1.34895200	3.27589300	-0.80740700
C	-2.64648600	4.42483700	0.47776700
H	-3.40013400	4.55700200	-0.28597700
C	-2.81900100	4.98178700	1.73724500
H	-3.71411000	5.54685800	1.96161600
C	-1.83042000	4.83261400	2.70818700
H	-1.96279400	5.27377600	3.69113300
C	-0.66723900	4.13802600	2.41439700
H	0.10668900	4.04450800	3.16563500
C	2.35270900	4.02504200	1.03368000
C	2.91951100	4.19309500	2.30059300
H	2.62425600	3.54766600	3.12242700
C	3.87941800	5.17544000	2.50498200
H	4.31626300	5.30742800	3.48396000
C	4.27852800	5.99075700	1.45066700
H	5.03264400	6.75731500	1.61241800
C	3.72381000	5.82006900	0.18691300
H	4.04007200	6.44997300	-0.63895400
C	2.76297200	4.83585700	-0.02531800
H	2.33547500	4.69336300	-1.01543900
C	3.62663700	-2.04499300	-1.82629900
C	4.38087800	-1.01827000	-1.24849500
C	5.54154400	-0.54026000	-1.84451700
C	5.92152500	-1.09631900	-3.06960400
H	6.81674400	-0.71901200	-3.56062500
C	5.17927300	-2.10397500	-3.66922300
H	5.48926800	-2.51624300	-4.62090500
C	4.03612000	-2.58336300	-3.04105600
H	3.45600600	-3.37526900	-3.50780400
C	1.35464100	1.48427900	1.99586600
C	2.60951900	0.85882400	1.94341800
C	2.95404500	-0.18962300	2.78590700
C	1.97951800	-0.63519700	3.68034700
H	2.22164200	-1.46155600	4.34411800
C	0.71567800	-0.05903800	3.72938000
H	-0.03103200	-0.43582300	4.41651700
C	0.40327400	1.01129100	2.89111400

H	-0.58449900	1.46007300	2.93253700
C	4.32689700	-0.81261100	2.67944400
H	4.22350300	-1.81400300	2.24246100
H	4.75073500	-0.94771900	3.67962300
C	6.30729300	0.55911000	-1.16465400
H	7.09840700	0.14180800	-0.52534200
H	6.81168100	1.18387300	-1.90456300
C	4.53148500	0.54271800	0.59875200
C	5.28208700	0.02961400	1.82748800
H	6.08801600	-0.62277100	1.46435500
C	5.89925200	1.21754800	2.57624700
H	6.47624200	0.84317500	3.42536500
H	5.09468000	1.83845900	2.98623600
C	6.78409400	2.05555400	1.65652300
H	7.18713600	2.91018900	2.20195900
H	7.64785100	1.46027500	1.33495600
C	6.00329900	2.55530100	0.43655300
H	5.21957000	3.24618800	0.77454600
H	6.65594200	3.12479100	-0.23542400
C	5.33943700	1.41818300	-0.35002700
H	4.61504800	1.84543900	-1.05301900
C	-1.56677400	-0.48329900	-0.03837200
C	-2.30252000	-0.40974800	1.30150300
C	-2.28483800	0.39678900	-0.88369200
C	-3.39171900	0.93839500	-0.17191700
O	-2.03365300	-0.96999700	2.33325300
N	-3.38109600	0.45253500	1.11503200
C	-2.04576100	0.78140700	-2.21605600
C	-4.26591800	1.83440000	-0.77264000
C	-2.89961300	1.68574800	-2.80882900
C	-4.00292700	2.19085600	-2.08769800
H	-4.67276400	2.89233400	-2.57980100
H	-5.11921900	2.24034600	-0.23702900
H	-2.73448000	2.01000000	-3.82692800
H	-1.18597000	0.38363900	-2.75029800
H	-4.07730600	0.61874400	1.82734900
F	-5.53366300	-0.26924700	2.99309200
C	-5.64645700	-1.12063700	4.05556000
C	-4.49124800	-1.57865100	4.65421500
C	-6.91112200	-1.49499700	4.45502600
C	-4.61473300	-2.46120700	5.72102500
H	-3.52377200	-1.25688400	4.27513600
C	-7.01898800	-2.37969200	5.52780300
H	-7.78379900	-1.10397200	3.94609500
C	-5.87884700	-2.85950700	6.15981600
H	-3.72943200	-2.83608200	6.21102000
H	-8.00005500	-2.68514800	5.86677500
H	-5.96777200	-3.54431500	6.99281200

C	-3.82584700	-2.36117900	-0.13431000
C	-2.54877600	-2.56347400	-0.56914200
H	-1.87254200	-3.18685400	0.00767700
H	-2.24004000	-2.36529600	-1.58414800
C	-4.81417700	-1.62183300	-0.89782500
C	-5.97710400	-1.11815800	-0.27786000
C	-4.62192700	-1.33556600	-2.26136200
C	-6.87376400	-0.33942200	-0.98502800
H	-6.17388100	-1.33523000	0.76298800
C	-5.53000300	-0.55799900	-2.96454500
H	-3.76862800	-1.73749900	-2.79361100
C	-6.66234900	-0.03792300	-2.33902200
H	-5.35387800	-0.35217000	-4.01195400
C	-4.19523300	-2.84961300	1.25305500
H	-3.44944500	-3.54439300	1.62981400
H	-4.28020800	-2.01593100	1.94871100
F	-5.41832700	-3.49365500	1.21967300
H	-7.76214700	0.04634200	-0.48926200
C	-7.68454400	0.82465000	-3.10553900
C	-7.15217000	2.22546600	-3.29134400
H	-8.63765900	0.83751000	-2.53031400
H	-7.87771700	0.34698800	-4.09846700
C	-8.13858400	3.09895700	-4.03429800
H	-6.93386200	2.67933200	-2.28547100
H	-6.19527400	2.18826300	-3.87664500
C	-7.61120900	4.49988900	-4.20803300
H	-8.35687000	2.65014500	-5.03518600
H	-9.10774300	3.13433600	-3.47149000
H	-8.35365900	5.13057100	-4.76083800
H	-7.41096400	4.97734300	-3.22204800
H	-6.65792300	4.49381700	-4.79207400

(9) IM$_3$-PhF

Zero-point correction =	1.193636 (Hartree/Particle)
Thermal correction to Energy =	1.268862
Thermal correction to Enthalpy =	1.269806
Thermal correction to Gibbs Free Energy =	1.072410
Sum of electronic and zero-point Energies =	-4636.553374
Sum of electronic and thermal Energies =	-4636.478148
Sum of electronic and thermal Enthalpies =	-4636.477203
Sum of electronic and thermal Free Energies =	-4636.674599

Au	-0.57938000	-0.79639800	-1.46948400
Au	2.46126100	0.43940400	-1.83579400
P	-1.65884400	-2.02932600	0.12290800
P	4.21230200	0.46331400	-0.37911500
Cl	0.52673800	0.37229100	-3.36235900
O	3.00869600	-1.99059000	0.51196600
O	1.00915600	-3.00572700	0.41693700

C	-1.34364400	-1.54330200	1.84267500
C	-1.80199700	-2.36348200	2.87777300
H	-2.30845400	-3.29704600	2.65049000
C	-1.60282100	-1.98502800	4.19820600
H	-1.96590800	-2.61584800	5.00120200
C	-0.94115200	-0.79374700	4.48660000
H	-0.79723300	-0.49328300	5.51846400
C	-0.46297700	0.00632500	3.45647100
H	0.07166900	0.92222200	3.68141200
C	-0.65417500	-0.36601900	2.12960400
H	-0.26323100	0.25461000	1.32652700
C	-3.46001500	-2.01069700	-0.14162300
C	-4.38097400	-1.85210700	0.89399200
H	-4.05023400	-1.63934400	1.90387300
C	-5.74524900	-1.92186700	0.61923700
H	-6.45995700	-1.78460800	1.42210200
C	-6.19070500	-2.13507100	-0.67782500
H	-7.25426700	-2.18353900	-0.88158300
C	-5.27305900	-2.26442600	-1.71859600
H	-5.61693300	-2.41319200	-2.73559400
C	-3.91283000	-2.19760800	-1.45412200
H	-3.19762400	-2.29867600	-2.26603900
C	5.06448200	2.06883100	-0.30512000
C	4.37196800	3.22191600	-0.67690800
H	3.35111700	3.15283200	-1.03999200
C	4.99283500	4.46368300	-0.59525800
H	4.45061500	5.35216300	-0.89453100
C	6.30445500	4.55752200	-0.14646200
H	6.78982800	5.52509500	-0.09054400
C	6.99959300	3.40957800	0.22161800
H	8.02554200	3.47995100	0.56339900
C	6.38501100	2.16705600	0.14361900
H	6.94272800	1.27866400	0.41637500
C	5.51163000	-0.78149100	-0.65521100
C	6.28636900	-1.23244900	0.41711600
H	6.08199300	-0.88133900	1.42444200
C	7.31795700	-2.13738000	0.19505000
H	7.92141100	-2.48014700	1.02794100
C	7.57126000	-2.60275900	-1.09250000
H	8.37345000	-3.31123400	-1.26379600
C	6.79126900	-2.16557100	-2.15777400
H	6.98211300	-2.53325600	-3.15915700
C	5.76141300	-1.25468400	-1.94212900
H	5.15051500	-0.91729100	-2.77375100
C	-1.16504700	-3.77145300	-0.02456500
C	0.21097800	-4.04299500	0.03421600
C	0.70996400	-5.28883600	-0.33185700
C	-0.20275800	-6.29436200	-0.65116900

H	0.17917100	-7.27141200	-0.93141300
C	-1.57055100	-6.06745300	-0.63326200
H	-2.26047500	-6.86632500	-0.87506200
C	-2.05243600	-4.79387200	-0.34573600
H	-3.11671400	-4.59159000	-0.38698800
C	3.61580900	0.13657400	1.30471800
C	3.03440200	-1.11409200	1.56411100
C	2.58916200	-1.44414000	2.84183100
C	2.73812500	-0.50006500	3.85568900
H	2.41080300	-0.76442200	4.85675600
C	3.29032200	0.74939400	3.61225600
H	3.40333900	1.46719600	4.41639900
C	3.72802100	1.07127200	2.33125400
H	4.16782300	2.04351300	2.13497500
C	2.01364300	-2.81238500	3.08298900
H	0.92465800	-2.77628800	2.97760300
H	2.23137100	-3.13451800	4.10464500
C	2.19773200	-5.50081300	-0.42047700
H	2.52512200	-6.15204300	0.39498000
H	2.43082100	-6.03351100	-1.34623300
C	2.39581400	-3.25611500	0.66286800
C	2.60908500	-3.79926800	2.07961500
H	2.07224600	-4.75033100	2.15247100
C	4.11156700	-4.03324300	2.31489300
H	4.24649400	-4.47478300	3.30627300
H	4.62476800	-3.06513400	2.33464100
C	4.76004300	-4.91541300	1.24608200
H	5.84126900	-4.94212900	1.40461500
H	4.41500600	-5.94771400	1.35842700
C	4.47048400	-4.39718400	-0.16556500
H	4.98616900	-3.44813700	-0.31734900
H	4.85894400	-5.09303000	-0.91503600
C	2.97466800	-4.17874900	-0.40699300
H	2.82228200	-3.66738700	-1.36459300
C	-2.30643700	2.67756900	-0.46749100
C	-0.84522500	2.75910200	-0.59020700
C	-2.82370100	3.94055400	-0.79342400
C	-1.71943400	4.77935500	-1.13650000
O	-0.00529200	1.89396200	-0.34149900
N	-0.55871000	4.04324200	-1.01716200
C	-4.13120800	4.47263000	-0.82953800
C	-1.89340300	6.10030500	-1.50987200
C	-4.30075800	5.78974600	-1.20146000
C	-3.19515600	6.59216600	-1.53811200
H	-3.36117800	7.62359300	-1.82688600
H	-1.04922700	6.72779000	-1.77035100
H	-5.29507800	6.21758200	-1.23557400
H	-4.98207000	3.85610300	-0.56215300

H	0.37784700	4.38556000	-1.16999600
F	2.05623900	5.22994200	-0.46528200
C	2.09454900	5.17626500	0.89594200
C	1.79196100	3.97966400	1.51699000
C	2.44399100	6.32342000	1.58152700
C	1.83023500	3.94946300	2.90839800
H	1.52347500	3.10502000	0.93165400
C	2.48435600	6.26802200	2.97064800
H	2.67167500	7.23033500	1.03460900
C	2.17571200	5.08474500	3.63458200
H	1.59086300	3.02546100	3.42139200
H	2.75371800	7.15433300	3.53266300
H	2.20110200	5.05064400	4.71715300
C	-4.03281300	1.54567400	1.00210900
C	-3.01078400	1.41536000	-0.09194300
H	-2.23642800	0.72437700	0.25499300
H	-3.44308200	0.95075300	-0.98482300
C	-5.43438700	1.36581700	0.79134500
C	-6.31071000	1.18862800	1.88822100
C	-6.01075100	1.33102100	-0.50086600
C	-7.66546600	0.98529000	1.69752100
H	-5.91127800	1.16520200	2.89527300
C	-7.36755400	1.13399100	-0.67462500
H	-5.38884900	1.47443800	-1.37783400
C	-8.22502900	0.95320300	0.41663300
H	-7.77886500	1.12198000	-1.68022200
C	-3.49152700	1.70793800	2.38255100
H	-2.43924600	2.00201700	2.35888900
H	-4.05723200	2.43464800	2.96965800
F	-3.55336000	0.49259300	3.08758400
H	-8.30918700	0.84569000	2.56099800
C	-9.69101600	0.68612200	0.20643100
C	-9.95812300	-0.75873400	-0.23383600
H	-10.08722700	1.36977200	-0.55184600
H	-10.24001500	0.89086700	1.13048500
C	-11.44362700	-1.05911700	-0.41396800
H	-9.43065800	-0.94918900	-1.17677400
H	-9.52898700	-1.44570500	0.50644000
C	-11.69526800	-2.49088000	-0.87650700
H	-11.96551300	-0.87799000	0.53167500
H	-11.86842200	-0.35570400	-1.13818400
H	-12.76105000	-2.69230700	-0.99559100
H	-11.21271700	-2.68303100	-1.83847300
H	-11.29958300	-3.21192600	-0.15646400

(10) IM$_4$-PhF

Zero-point correction = 1.195877 (Hartree/Particle)
Thermal correction to Energy = 1.270500

Thermal correction to Enthalpy =			1.271444
Thermal correction to Gibbs Free Energy =			1.076531
Sum of electronic and zero-point Energies =			-4636.606653
Sum of electronic and thermal Energies =			-4636.532030
Sum of electronic and thermal Enthalpies =			-4636.531086
Sum of electronic and thermal Free Energies =			-4636.725999
Au	-0.08194900	-1.13768700	-1.42168500
Au	2.09524100	1.28102200	-1.49623600
P	-0.45334200	-2.93985300	-0.07765100
P	3.71646100	1.83674000	0.00443300
Cl	0.28118500	0.71059600	-3.05353800
O	3.75174000	-0.95937700	0.58137100
O	2.37561700	-2.69848900	0.23697500
C	-0.40314900	-2.62724200	1.70674700
C	-0.48655600	-3.71080500	2.58685000
H	-0.56521200	-4.72223800	2.19882600
C	-0.46550700	-3.48842200	3.95689700
H	-0.53357800	-4.32553400	4.64180300
C	-0.35842600	-2.18759900	4.44755700
H	-0.34650300	-2.01573400	5.51814300
C	-0.27089500	-1.11328100	3.57020700
H	-0.16997400	-0.10308700	3.95030700
C	-0.28855000	-1.32688400	2.19445700
H	-0.22219400	-0.48933200	1.50684000
C	-2.11129300	-3.58567900	-0.45948800
C	-3.13668200	-3.56455300	0.48245500
H	-2.94848600	-3.26368800	1.50623000
C	-4.43723900	-3.88764500	0.09841800
H	-5.23261000	-3.83490900	0.83182600
C	-4.70823200	-4.24864500	-1.21351600
H	-5.72002200	-4.50415500	-1.50795300
C	-3.68271800	-4.27172500	-2.15952700
H	-3.89469900	-4.54096700	-3.18781100
C	-2.39221900	-3.92694600	-1.79021500
H	-1.60370200	-3.90438300	-2.53754400
C	3.89182600	3.64152700	0.18687400
C	3.37640000	4.46805400	-0.81273000
H	2.79415200	4.04454200	-1.62411700
C	3.60744600	5.83954500	-0.77395900
H	3.21156900	6.47361200	-1.55857000
C	4.34045400	6.39230900	0.26928900
H	4.51813400	7.46111000	0.30055500
C	4.85887800	5.57152900	1.26833400
H	5.44074000	5.99947900	2.07630600
C	4.65037500	4.20013000	1.22076500
H	5.08166400	3.56928600	1.99045600
C	5.40441700	1.28275600	-0.40132200
C	6.36956700	1.19331200	0.60453600

H	6.10073300	1.36971800	1.64190000
C	7.67892300	0.86033700	0.27907000
H	8.42747900	0.79177600	1.06021000
C	8.02688500	0.61167400	-1.04618900
H	9.04928600	0.35405200	-1.29789900
C	7.06326800	0.68799700	-2.04569100
H	7.33029400	0.48778000	-3.07683700
C	5.75110500	1.02435900	-1.72570000
H	4.99879400	1.08609600	-2.50624000
C	0.74362300	-4.26210400	-0.40805500
C	2.10208500	-3.92034600	-0.30332300
C	3.09188000	-4.77992900	-0.76953200
C	2.70507400	-6.03494200	-1.24035000
H	3.47335700	-6.71428900	-1.59719900
C	1.37385400	-6.42193600	-1.27179600
H	1.09817300	-7.40644200	-1.62856900
C	0.38777500	-5.52250000	-0.87821700
H	-0.65876100	-5.79712300	-0.94648600
C	3.34279800	1.10925500	1.62496000
C	3.37597700	-0.29292900	1.71747800
C	3.09153700	-0.93853300	2.91791200
C	2.77887800	-0.15703900	4.02810200
H	2.57849300	-0.65834000	4.97040100
C	2.70580200	1.22544300	3.94724800
H	2.44100600	1.81622700	4.81600000
C	2.97890000	1.85989100	2.74073600
H	2.90352600	2.93913100	2.67353600
C	3.15298100	-2.44018500	2.97470200
H	2.15326600	-2.85325300	2.80353600
H	3.47172000	-2.76439600	3.96873200
C	4.52762000	-4.32666500	-0.79307200
H	5.09986700	-4.88797100	-0.04893300
H	4.96692300	-4.57580700	-1.76271800
C	3.73320900	-2.37290500	0.55384500
C	4.12669000	-2.95397500	1.91549900
H	4.04028300	-4.04347700	1.84623700
C	5.58153900	-2.57079100	2.23464000
H	5.86579300	-3.03521700	3.18297700
H	5.63862600	-1.48735900	2.39006700
C	6.56340400	-2.96568000	1.13100400
H	7.55453600	-2.56917700	1.36581100
H	6.67478500	-4.05380500	1.10462200
C	6.11618400	-2.42942200	-0.23158400
H	6.19163300	-1.34142600	-0.23372700
H	6.77791400	-2.79363800	-1.02307300
C	4.67206300	-2.81754700	-0.56443700
H	4.34270200	-2.28520800	-1.46452600
C	-3.69377600	0.93693400	-0.97455400

C	-2.32062800	1.41500800	-0.59245800
C	-4.26612900	2.03430100	-1.79562100
C	-3.30694100	3.05147400	-1.85805100
O	-1.46978700	0.82237700	0.06239400
N	-2.17766100	2.65790900	-1.12083800
C	-5.47060800	2.18571200	-2.46246000
C	-3.51574600	4.22381900	-2.56034700
C	-5.69852300	3.36318600	-3.17622500
C	-4.73563200	4.36606500	-3.22174200
H	-4.93218300	5.27313700	-3.78120000
H	-2.76080600	5.00032500	-2.60154400
H	-6.63828700	3.49711800	-3.69800000
H	-6.22858500	1.41102900	-2.42452900
H	-1.30867000	3.16856000	-1.04498200
F	0.48769200	3.68930200	-0.04800400
C	0.51155000	3.86722300	1.30068700
C	-0.14567200	2.94919200	2.09871100
C	1.19429800	4.95879700	1.80571700
C	-0.11923900	3.15144500	3.47567500
H	-0.65495200	2.10900000	1.63903400
C	1.21871900	5.13455300	3.18591000
H	1.68877400	5.64805700	1.13220400
C	0.56265200	4.23471200	4.02170100
H	-0.64123700	2.45738600	4.12492200
H	1.74493600	5.98479200	3.60425900
H	0.57204700	4.38654400	5.09466700
C	-4.51638400	0.04074900	-0.03488100
C	-3.92136000	-0.53425000	-1.26883100
H	-3.05777200	-1.18156500	-1.16160600
H	-4.56747300	-0.74331300	-2.11362600
C	-5.99196800	0.28834700	0.03235400
C	-6.48506400	1.48712300	0.54493500
C	-6.89211600	-0.68166600	-0.39885200
C	-7.85264300	1.71437700	0.60966100
H	-5.79056600	2.25945600	0.86353900
C	-8.26137200	-0.44934600	-0.33472000
H	-6.51205700	-1.62110000	-0.79018200
C	-8.76250300	0.75250100	0.16592000
H	-8.95422200	-1.21084200	-0.68077400
C	-3.90379600	-0.33616400	1.29547300
H	-2.86234700	-0.64014400	1.19173300
H	-3.98213000	0.48543700	2.01284500
F	-4.61447300	-1.40768200	1.82093100
H	-8.22359400	2.65898000	0.99633300
C	-10.24669000	0.98350600	0.28279100
C	-10.79185000	0.51254400	1.63677500
H	-10.76909400	0.45553600	-0.52139200
H	-10.46726200	2.04808900	0.15480100

C	-12.29367600	0.74183600	1.78155200
H	-10.56544600	-0.55259900	1.76382700
H	-10.25848500	1.03445300	2.43986300
C	-12.82551500	0.26659200	3.13036500
H	-12.51127200	1.80783200	1.65308300
H	-12.81926600	0.22272700	0.97252800
H	-13.89919400	0.43925000	3.22266000
H	-12.64719000	-0.80303700	3.26725300
H	-12.33227300	0.79111100	3.95280800

(11) IM_2-PhCl

Zero-point correction = 1.190820 (Hartree/Particle)
Thermal correction to Energy = 1.267224
Thermal correction to Enthalpy = 1.268168
Thermal correction to Gibbs Free Energy = 1.068822
Sum of electronic and zero-point Energies = -4996.893238
Sum of electronic and thermal Energies = -4996.816834
Sum of electronic and thermal Enthalpies = -4996.815890
Sum of electronic and thermal Free Energies = -4997.015235

Au	0.60337700	-1.47244900	0.39571500
Au	0.84018800	0.74286400	-2.05303700
P	2.65272100	-2.66010100	0.56631200
P	0.48837500	2.63749200	-0.80973300
Cl	1.44904300	-1.35153300	-3.06478300
O	3.11402300	1.92311700	-0.24593500
O	3.84422800	-0.20289500	-0.21362800
C	3.53572100	-2.38358900	2.13698900
C	4.90240400	-2.65339600	2.24971500
H	5.45609900	-3.01890500	1.39048900
C	5.55422100	-2.44279000	3.45948200
H	6.61455100	-2.65117000	3.54346700
C	4.84634300	-1.96668300	4.56009500
H	5.35589000	-1.80482000	5.50309800
C	3.48540700	-1.70029800	4.45082500
H	2.93202100	-1.33250300	5.30772600
C	2.82983400	-1.90237100	3.24021900
H	1.77238000	-1.66983500	3.15055900
C	2.22457300	-4.43379100	0.53161200
C	2.68611700	-5.33872500	1.48530900
H	3.32113000	-5.00239000	2.29758500
C	2.32565800	-6.68092800	1.39621100
H	2.68351100	-7.38292900	2.14045800
C	1.51550800	-7.11970600	0.35664000
H	1.24024400	-8.16591000	0.28915300
C	1.05604700	-6.21634200	-0.59983000
H	0.42909500	-6.55859000	-1.41511900
C	1.40147500	-4.87464300	-0.51094700
H	1.05120500	-4.16760200	-1.25996100

C	-1.21076300	3.24386200	-0.59526500
C	-2.26585800	2.62960200	-1.26810000
H	-2.06911500	1.79067300	-1.93089000
C	-3.56448800	3.10869000	-1.10575300
H	-4.38057200	2.64063000	-1.64383100
C	-3.80836800	4.19219900	-0.27206800
H	-4.81998100	4.56115300	-0.14154800
C	-2.75344000	4.81777600	0.38946300
H	-2.94463800	5.66450100	1.03814800
C	-1.45883800	4.35145400	0.22422200
H	-0.63846700	4.84752100	0.73452400
C	1.47143100	4.06509900	-1.38345000
C	2.09330000	4.93061000	-0.48245500
H	2.00348700	4.76457700	0.58685600
C	2.85540900	5.99250300	-0.95615400
H	3.34081600	6.66135200	-0.25448200
C	2.99796600	6.19408700	-2.32594000
H	3.59592200	7.02083500	-2.69168500
C	2.37923100	5.33160500	-3.22470900
H	2.49410400	5.48240000	-4.29176700
C	1.62037200	4.26492500	-2.75574800
H	1.15657600	3.57881100	-3.45822400
C	3.92757500	-2.48040300	-0.71487800
C	4.41927200	-1.19264400	-0.95345300
C	5.43613700	-0.96319400	-1.87559800
C	5.93746300	-2.05691900	-2.57816400
H	6.71871200	-1.88871100	-3.31306100
C	5.45625200	-3.34076700	-2.36518000
H	5.85783800	-4.17446500	-2.92762700
C	4.45013400	-3.55402200	-1.42900500
H	4.07088600	-4.55498300	-1.25827000
C	1.10118700	2.28776200	0.86858200
C	2.44633200	1.90327400	0.94065600
C	3.05826100	1.54714800	2.13569000
C	2.26204600	1.54660800	3.28275200
H	2.71535700	1.26289700	4.22795500
C	0.91768800	1.89229200	3.23474200
H	0.31393400	1.85368000	4.13410100
C	0.33536000	2.27604500	2.02859100
H	-0.71405800	2.54671800	1.99187000
C	4.51413800	1.14642500	2.14341500
H	4.57813100	0.07241000	2.33398600
H	5.02884900	1.64561700	2.96979500
C	5.93184800	0.44272900	-2.09383300
H	6.84201800	0.61600200	-1.50924300
H	6.20731500	0.57834500	-3.14254800
C	4.28597700	1.14531200	-0.34471900
C	5.21864100	1.48431600	0.82139500

H	6.10868600	0.85141400	0.72922900
C	5.63297100	2.95703700	0.71846600
H	6.34007400	3.18508300	1.52075500
H	4.75252300	3.59087000	0.88296800
C	6.24884100	3.28038300	-0.64424500
H	6.48814000	4.34525300	-0.69871200
H	7.20091100	2.74874100	-0.74875500
C	5.30278500	2.91298900	-1.79066400
H	4.41947900	3.55774600	-1.74952700
H	5.78252900	3.09529400	-2.75651100
C	4.84379300	1.45091000	-1.73010100
H	4.00637100	1.30157000	-2.42342400
C	-1.32540800	-0.81525400	0.30452000
C	-2.11339600	-0.14041500	1.43650600
C	-2.22058600	-0.86754500	-0.75173400
C	-3.46860500	-0.26425300	-0.36871900
O	-1.74630100	0.11435600	2.55016000
N	-3.38398700	0.14889200	0.92821100
C	-2.04791600	-1.35621200	-2.07777200
C	-4.51627100	-0.13401100	-1.27192000
C	-3.07908800	-1.21230100	-2.96685400
C	-4.29297200	-0.60407900	-2.55576200
H	-5.08495000	-0.49507100	-3.28866500
H	-5.46268200	0.30917900	-0.98716300
H	-2.97584700	-1.55433500	-3.98859000
H	-1.09978500	-1.80169000	-2.36506600
H	-4.08717100	0.68375200	1.42284300
C	-4.54399600	3.45085400	2.98473200
C	-3.25437300	3.08902400	3.34472200
C	-5.00536000	4.75383300	3.10211500
C	-2.40063700	4.07809200	3.82569200
H	-2.91767800	2.06036100	3.26742200
C	-4.14082000	5.72626500	3.59438400
H	-6.02409600	4.99806200	2.82628100
C	-2.83838000	5.39186700	3.95246600
H	-1.38863500	3.81296300	4.11199400
H	-4.49359600	6.74532900	3.70189600
H	-2.16995900	6.15142000	4.34021800
C	-3.32849400	-2.87394400	1.82360800
C	-2.07580300	-3.25348400	1.51582600
H	-1.29576800	-3.26507200	2.26979600
H	-1.78302300	-3.60904100	0.53561200
C	-4.44319000	-2.87715300	0.85817300
C	-5.66820500	-2.26299500	1.17948200
C	-4.33458900	-3.48648200	-0.39916900
C	-6.72317300	-2.26554400	0.28421500
H	-5.81356100	-1.81978200	2.15750400
C	-5.39620500	-3.48407400	-1.29230700

H	-3.42471800	-4.00562800	-0.67699600
C	-6.61255600	-2.88227400	-0.96696100
H	-5.28709900	-3.98358100	-2.25026000
C	-3.60512000	-2.39142800	3.22645000
H	-2.73242400	-2.54256700	3.86253600
H	-3.86874500	-1.32887200	3.24435900
F	-4.66483000	-3.08883500	3.77526800
H	-7.66660900	-1.81036600	0.57198300
Cl	-5.64894400	2.22658500	2.37734400
C	-7.78806500	-2.90160300	-1.90807700
C	-8.04727100	-1.54311700	-2.57020600
H	-8.68393500	-3.20117400	-1.35390800
H	-7.63194700	-3.65904500	-2.68152100
C	-9.28290900	-1.54887500	-3.46659300
H	-8.15966200	-0.77431000	-1.79572200
H	-7.17043800	-1.26052400	-3.16426600
C	-9.52432800	-0.19726600	-4.13144300
H	-9.16976800	-2.32386800	-4.23199500
H	-10.15770300	-1.83104700	-2.87163600
H	-10.41014600	-0.21656800	-4.76799000
H	-9.67069600	0.58744100	-3.38464600
H	-8.67476100	0.09153800	-4.75612600

(12) IM_2-PhCl-1

Zero-point correction = 1.189270 (Hartree/Particle)
Thermal correction to Energy = 1.266226
Thermal correction to Enthalpy = 1.267170
Thermal correction to Gibbs Free Energy = 1.063661
Sum of electronic and zero-point Energies = -4996.888460
Sum of electronic and thermal Energies = -4996.811504
Sum of electronic and thermal Enthalpies = -4996.810560
Sum of electronic and thermal Free Energies = -4997.014069

Au	-0.37540100	1.22824500	0.30110000
Au	-1.45554300	-0.72197600	-2.14225100
P	-2.03423800	2.87975700	0.70227700
P	-1.44025500	-2.70853100	-0.99911200
Cl	-1.57187600	1.50285800	-3.04088600
O	-3.68499600	-1.43386100	0.02503700
O	-3.88849600	0.80079100	0.17430700
C	-2.70062800	2.79541300	2.39663100
C	-3.91767800	3.39964300	2.72167200
H	-4.48201200	3.91666400	1.95137700
C	-4.41050000	3.32867500	4.01710300
H	-5.35253100	3.79063700	4.26156300
C	-3.68022600	2.65494000	5.00262200
H	-4.06658700	2.60623700	6.01318700
C	-2.46639700	2.05589900	4.68731200
H	-1.89835500	1.53695400	5.44569700

C	-1.97225800	2.12698500	3.38549900
H	-1.04082700	1.62966400	3.13598700
C	-1.19499500	4.49389700	0.55437900
C	-1.19584400	5.44105600	1.58030200
H	-1.71621700	5.23858900	2.50876200
C	-0.52180600	6.64443400	1.40222900
H	-0.52716900	7.38301100	2.20491900
C	0.14575900	6.90450400	0.21737600
H	0.66914100	7.84848800	0.08110300
C	0.14800200	5.95952000	-0.80663500
H	0.66480700	6.17044000	-1.73764700
C	-0.51023000	4.75209200	-0.63645500
H	-0.51955300	4.00989200	-1.43691300
C	0.05250800	-3.74923400	-1.09427200
C	1.12355600	-3.37938100	-1.90778800
H	1.07810900	-2.45944500	-2.48302200
C	2.23896500	-4.21493300	-1.99828700
H	3.06238900	-3.93839700	-2.64978400
C	2.28970300	-5.39782200	-1.28417000
H	3.15640400	-6.04461800	-1.36011100
C	1.22043600	-5.76458400	-0.46541800
H	1.25321400	-6.69843100	0.09018200
C	0.10235500	-4.94857100	-0.38155100
H	-0.73408800	-5.25360900	0.23944000
C	-2.83536200	-3.81150200	-1.42173800
C	-3.47882900	-4.56737100	-0.44267300
H	-3.16960700	-4.49930400	0.59273700
C	-4.54264700	-5.38914000	-0.79564700
H	-5.04705100	-5.97580500	-0.03138600
C	-4.96245100	-5.46287200	-2.11769900
H	-5.79601500	-6.09977500	-2.39381200
C	-4.32509200	-4.70134600	-3.09803900
H	-4.65112800	-4.74664600	-4.12569900
C	-3.26244600	-3.87518700	-2.74425100
H	-2.77313100	-3.27353400	-3.50539900
C	-3.49901800	3.03695100	-0.35214100
C	-4.32000400	1.91049700	-0.47882900
C	-5.50492600	1.95261900	-1.20421900
C	-5.84126700	3.14351400	-1.83984800
H	-6.75555600	3.18322900	-2.42436400
C	-5.03794300	4.27352200	-1.74097100
H	-5.31592200	5.18643200	-2.24617400
C	-3.85907500	4.21992500	-0.99354300
H	-3.23371300	5.09918900	-0.91524100
C	-1.65460000	-2.31399000	0.76229000
C	-2.83007200	-1.61719700	1.07340300
C	-3.11687700	-1.17158700	2.35836300
C	-2.15914400	-1.41178800	3.34675600

H	-2.35492400	-1.06945700	4.35014100
C	-0.96958300	-2.07909100	3.05696700
H	-0.23576800	-2.23602400	3.83402700
C	-0.72138300	-2.53758000	1.76964600
H	0.20346100	-3.06000400	1.54361200
C	-4.41345500	-0.43985400	2.62424500
H	-4.18535400	0.61375100	2.80497500
H	-4.86533100	-0.82370700	3.53904100
C	-6.35472400	0.70879900	-1.29695500
H	-7.15405800	0.75369800	-0.54955000
H	-6.85372900	0.67267400	-2.27577000
C	-4.64205900	-0.40923800	0.13522800
C	-5.39924400	-0.56551800	1.45424900
H	-6.12476800	0.25335400	1.52297000
C	-6.15223300	-1.90288300	1.44414200
H	-6.72946600	-1.99443500	2.36754800
H	-5.42537900	-2.72435000	1.43989200
C	-7.06727300	-2.02127700	0.22614700
H	-7.55621800	-2.99847800	0.22402900
H	-7.87204600	-1.27930500	0.29838000
C	-6.28662000	-1.84486400	-1.08126000
H	-5.58378000	-2.67690700	-1.19316200
H	-6.95754400	-1.88534000	-1.94317900
C	-5.49629000	-0.53208600	-1.12124100
H	-4.77894000	-0.57134100	-1.95658500
C	1.31160100	0.11503200	0.06263000
C	2.06335100	-0.61849000	1.18305400
C	2.07467600	-0.11929700	-1.06951000
C	3.19361500	-0.96497900	-0.74130800
O	1.79704900	-0.66172000	2.35149700
N	3.15529500	-1.26555600	0.58362500
C	1.88853900	0.32244100	-2.41208400
C	4.10506900	-1.36268700	-1.71267600
C	2.78911000	-0.07594600	-3.36363100
C	3.89081300	-0.89921700	-3.00511500
H	4.59636200	-1.18715100	-3.77483500
H	4.95975000	-1.98151500	-1.46783500
H	2.67749700	0.24212900	-4.38918800
H	1.04410400	0.95946200	-2.65639600
H	3.86027000	-1.78276800	1.10118700
C	5.46744700	-2.50456600	4.01233500
C	4.18288400	-2.16136400	4.41342900
C	6.40537900	-3.03098400	4.89027400
C	3.83581200	-2.35451400	5.74807600
H	3.46747500	-1.74722700	3.70778500
C	6.03836500	-3.22273800	6.21438200
H	7.39560800	-3.29219000	4.53385100
C	4.75731100	-2.89103100	6.64979800

H	2.83989800	-2.08941600	6.07496900
H	6.75495300	-3.63598200	6.91810800
C	3.91563500	1.81121300	1.15321300
C	2.72962500	2.43162700	1.01573400
H	2.09810600	2.62098600	1.87396800
H	2.36238800	2.81674000	0.07261200
C	4.83027400	1.54776100	0.02433000
C	5.97064200	0.74583100	0.21529900
C	4.60765400	2.06519500	-1.25628400
C	6.82511800	0.45288900	-0.83623500
H	6.21692000	0.37205600	1.20411200
C	5.45854900	1.77076500	-2.30630100
H	3.75746000	2.71140300	-1.44736500
C	6.57478300	0.94655800	-2.12048900
H	5.26306600	2.18741500	-3.29187500
C	4.31501600	1.32267800	2.52210200
H	3.58114300	1.62678800	3.26983500
H	4.41338800	0.23283600	2.54726400
F	5.53911800	1.85338500	2.88242700
H	7.70193200	-0.15819200	-0.66172900
C	7.53476800	0.68374000	-3.25363600
H	6.99166000	0.66404500	-4.20412600
H	7.99242600	-0.30260400	-3.13393800
C	8.63425900	1.74770500	-3.32752000
C	9.62126900	1.50225100	-4.46554900
H	9.17650200	1.77174900	-2.36830700
H	8.17325100	2.73920800	-3.44075700
C	10.70355700	2.57008100	-4.53641700
H	10.07437900	0.51080800	-4.34785300
H	9.07008100	1.47465400	-5.41423900
H	11.40169900	2.38509400	-5.35372200
H	10.27023400	3.56117000	-4.67736000
H	11.28595600	2.59630000	-3.61019400
H	4.47676300	-3.03738200	7.68902400
Cl	5.94487300	-2.26832600	2.32498800

(13) $TS_{2\text{-}3}$-PhCl

Zero-point correction =			1.185613 (Hartree/Particle)
Thermal correction to Energy =			1.262440
Thermal correction to Enthalpy =			1.263384
Thermal correction to Gibbs Free Energy =			1.058914
Sum of electronic and zero-point Energies =			-4996.866958
Sum of electronic and thermal Energies =			-4996.790132
Sum of electronic and thermal Enthalpies =			-4996.789188
Sum of electronic and thermal Free Energies =			-4996.993658
Au	-0.19734600	1.63892400	-0.20950300
Au	-1.31493900	-1.24829600	-2.12150100
P	-2.15379700	3.01273800	-0.01461700

P	-1.45676100	-3.07645000	-0.70418400
Cl	-1.15967400	0.65924000	-3.55389600
O	-3.58692300	-1.51710000	0.47667100
O	-4.01097100	0.72914500	0.40047300
C	-2.53639100	3.36722700	1.74800600
C	-3.75325000	3.94811600	2.12745000
H	-4.50766800	4.16725700	1.38082000
C	-4.00517500	4.24055100	3.46526600
H	-4.95010500	4.69207700	3.74868200
C	-3.04432600	3.96067400	4.43762000
H	-3.24036000	4.19320700	5.47867700
C	-1.83327300	3.38177400	4.06724900
H	-1.08398500	3.15495700	4.81823600
C	-1.58101600	3.08034800	2.73090100
H	-0.64117800	2.60936500	2.45365700
C	-1.56194700	4.60680400	-0.72472800
C	-1.61366200	5.81657000	-0.02576400
H	-2.02799300	5.85409000	0.97390800
C	-1.12367400	6.98434900	-0.61065100
H	-1.16588900	7.91801700	-0.05964500
C	-0.58794800	6.95237700	-1.89522300
H	-0.21244200	7.86343700	-2.35108200
C	-0.53278900	5.74794100	-2.59768000
H	-0.12051200	5.72130400	-3.60088700
C	-1.00821600	4.57688600	-2.01557800
H	-0.96146100	3.64213100	-2.56676900
C	-0.01196100	-4.20429200	-0.81686300
C	1.11557200	-3.81958100	-1.54820900
H	1.13840700	-2.85246400	-2.03796200
C	2.20242500	-4.68425500	-1.66737600
H	3.06646100	-4.37963900	-2.24926000
C	2.17190500	-5.93609000	-1.06061600
H	3.01492000	-6.61155000	-1.16177900
C	1.05100800	-6.32655800	-0.32999100
H	1.01664300	-7.30375000	0.13920200
C	-0.03746200	-5.46901700	-0.21017400
H	-0.91074700	-5.79525200	0.34168500
C	-2.89737200	-4.16516400	-1.01843500
C	-3.49321000	-4.90760700	0.01053400
H	-3.15629400	-4.78800200	1.03406900
C	-4.53292800	-5.79033000	-0.27685700
H	-4.98867200	-6.36142500	0.52276600
C	-4.98532800	-5.93527800	-1.58547500
H	-5.79465500	-6.62424700	-1.80881800
C	-4.40347000	-5.19091100	-2.60936700
H	-4.75644300	-5.29512500	-3.62995600
C	-3.36302800	-4.30779100	-2.32900300
H	-2.91683100	-3.72635800	-3.13034800

C	-3.78846300	2.75116200	-0.80586100
C	-4.56239100	1.61979100	-0.48023400
C	-5.85261300	1.46084100	-0.99413000
C	-6.34670200	2.41924000	-1.87728200
H	-7.34251000	2.28786500	-2.29034000
C	-5.59239200	3.53264700	-2.22971100
H	-5.98582100	4.27130700	-2.91864000
C	-4.32316600	3.69754200	-1.68612000
H	-3.74358900	4.57111200	-1.94941100
C	-1.54683200	-2.53335800	1.04224500
C	-2.62032300	-1.71208700	1.42880100
C	-2.70241400	-1.16576300	2.70994100
C	-1.67887100	-1.45969200	3.61269900
H	-1.73456300	-1.04753100	4.61495400
C	-0.60291300	-2.26597900	3.25469000
H	0.18262400	-2.48009200	3.97005600
C	-0.53528700	-2.79906800	1.97042200
H	0.30628300	-3.42071500	1.68921700
C	-3.86626800	-0.27126400	3.05914000
H	-3.55912300	0.77551900	2.96343800
H	-4.15341100	-0.41733900	4.10474500
C	-6.64774400	0.25326700	-0.58255900
H	-7.25062000	0.48184300	0.30429100
H	-7.35772600	-0.01486800	-1.37006700
C	-4.61954700	-0.55519300	0.67975900
C	-5.07647100	-0.53869000	2.14973500
H	-5.77673900	0.29818700	2.25057000
C	-5.81427000	-1.83974400	2.52092500
H	-6.19008400	-1.74701500	3.54407500
H	-5.10452400	-2.67592800	2.52983600
C	-6.96009900	-2.14848600	1.55475700
H	-7.42830100	-3.10340600	1.82065600
H	-7.74505100	-1.39160400	1.65640800
C	-6.45522600	-2.21065600	0.10856800
H	-5.77882000	-3.06404100	-0.00052800
H	-7.28467900	-2.38757500	-0.58210200
C	-5.71400500	-0.93488700	-0.32822200
H	-5.18992600	-1.14234800	-1.26708400
C	1.74843200	0.93059300	-0.15254400
C	2.37859000	0.50536200	1.17698500
C	2.49143000	0.20744000	-1.14126100
C	3.50259600	-0.56196500	-0.50226600
O	2.05723700	0.83105200	2.30250800
N	3.41951100	-0.35669800	0.86730200
C	2.34059700	0.12868800	-2.53825400
C	4.35707100	-1.39029100	-1.21755800
C	3.19822100	-0.69147700	-3.25922200
C	4.19392700	-1.43146000	-2.60217100

H	4.84984900	-2.06742400	-3.18801800
H	5.12030200	-1.98312200	-0.72593800
H	3.09010800	-0.77011300	-4.33592900
H	1.54516600	0.67793500	-3.02986500
H	4.00361000	-0.78981000	1.57121500
C	4.60693600	-1.66162600	4.92526700
C	3.38004100	-1.02506900	5.07197700
C	5.10604400	-2.54045000	5.87939600
C	2.63445500	-1.28923000	6.22226200
H	3.00913900	-0.34423800	4.31513000
C	4.34502300	-2.78731300	7.02061500
H	6.06816300	-3.01740700	5.73764000
C	3.11136900	-2.16489600	7.19453200
H	1.67838600	-0.79152900	6.35604700
H	4.72461000	-3.46946800	7.77457000
H	2.52677300	-2.35680300	8.08785200
C	3.89509300	2.87294200	0.34249400
C	2.65361200	2.97701700	-0.26391000
H	1.86917400	3.51181100	0.25047800
H	2.53959500	2.93399100	-1.33558700
C	5.07551400	2.39597200	-0.34944200
C	6.22941100	1.97118900	0.35963000
C	5.12277200	2.32708200	-1.75922500
C	7.34190800	1.50024800	-0.30968100
H	6.25328000	2.02939800	1.43896300
C	6.24794600	1.85969900	-2.42021500
H	4.28998600	2.68762900	-2.35135000
C	7.37957700	1.43642700	-1.71252300
H	6.25701500	1.84253300	-3.50537900
C	3.95751700	3.23915300	1.80964700
H	3.13264600	3.90078200	2.07012300
H	3.89133400	2.35078600	2.44747400
F	5.14017900	3.90423600	2.12691400
H	8.21288400	1.18785300	0.25942100
Cl	5.58811700	-1.33903400	3.48150100
C	8.60250700	0.92188900	-2.43018500
C	8.59825700	-0.61238700	-2.59540700
H	9.49813600	1.21722100	-1.87967700
H	8.67241200	1.38937700	-3.41841800
C	9.84811100	-1.13633200	-3.31132600
H	8.51576800	-1.08442900	-1.61082800
H	7.70014300	-0.91129500	-3.15111300
C	9.84806500	-2.65686500	-3.47905400
H	9.92941600	-0.65952800	-4.29429100
H	10.73938400	-0.82899800	-2.75145500
H	10.75102500	-2.99950000	-3.99124400
H	9.80833900	-3.16770200	-2.51208100
H	8.99017400	-2.99700900	-4.06854300

(14) IM_3-PhCl

Zero-point correction =	1.191562 (Hartree/Particle)
Thermal correction to Energy =	1.267523
Thermal correction to Enthalpy =	1.268467
Thermal correction to Gibbs Free Energy =	1.067528
Sum of electronic and zero-point Energies =	-4996.911816
Sum of electronic and thermal Energies =	-4996.835855
Sum of electronic and thermal Enthalpies =	-4996.834911
Sum of electronic and thermal Free Energies =	-4997.035850

Au	0.14602600	-1.26670300	-1.34906500
Au	1.98202900	1.40677000	-1.09288800
P	0.02628300	-3.07990000	0.03141800
P	3.38911700	2.07753300	0.57247100
Cl	0.53039500	0.61281200	-2.93926100
O	3.99707300	-0.70668000	0.64154900
O	2.82106500	-2.54100600	0.17357600
C	0.17514000	-2.65633800	1.78663100
C	0.35602700	-3.66614400	2.73353100
H	0.47600500	-4.69748500	2.41352700
C	0.37246700	-3.34647200	4.08654700
H	0.50555900	-4.12904200	4.82466200
C	0.19967900	-2.02506500	4.48961000
H	0.19922100	-1.77989600	5.54607200
C	0.02948400	-1.01859100	3.54490900
H	-0.08809300	0.01148300	3.86048900
C	0.02556500	-1.32798200	2.19004300
H	-0.11715100	-0.54312600	1.45142400
C	-1.56861400	-3.92680700	-0.17994300
C	-2.46568600	-4.05817300	0.87802400
H	-2.19580300	-3.75041900	1.88076900
C	-3.75596000	-4.52605300	0.63764000
H	-4.45872600	-4.58144200	1.46015100
C	-4.13673000	-4.89524300	-0.64518200
H	-5.14054400	-5.26134100	-0.82791700
C	-3.23492900	-4.78034300	-1.70368700
H	-3.53343000	-5.05887500	-2.70765300
C	-1.96145700	-4.28054400	-1.47820100
H	-1.27784800	-4.14274500	-2.31148400
C	3.01414700	3.75243500	1.15907400
C	1.67359300	4.07169800	1.38849700
H	0.89549700	3.34334600	1.17556700
C	1.33167900	5.31889800	1.89297300
H	0.28883900	5.55920300	2.07246700
C	2.32917300	6.25587400	2.15137900
H	2.06348700	7.23433400	2.53481000
C	3.66294300	5.94433200	1.91154500
H	4.43618700	6.67878800	2.10446100

C	4.01258900	4.69014000	1.42041200
H	5.05388800	4.45138500	1.23332700
C	5.14639800	2.03426400	0.10051200
C	6.12769700	1.81628200	1.07078200
H	5.84652700	1.67223200	2.10960600
C	7.46734400	1.77309400	0.70213900
H	8.22760200	1.60435600	1.45635600
C	7.83020600	1.94872800	-0.63053900
H	8.87531300	1.91319300	-0.91620200
C	6.85366300	2.16934600	-1.59643700
H	7.13433900	2.30484500	-2.63423900
C	5.51121400	2.20953300	-1.23396700
H	4.74922900	2.36821000	-1.99098600
C	1.33750500	-4.24892600	-0.43144000
C	2.64264700	-3.73189900	-0.45723800
C	3.66469800	-4.37775800	-1.14579200
C	3.38926300	-5.63548000	-1.68388100
H	4.18008700	-6.15903900	-2.21279800
C	2.13395700	-6.21655500	-1.57077700
H	1.95077300	-7.20115900	-1.98289000
C	1.09467400	-5.50698800	-0.97473800
H	0.09424700	-5.92384700	-0.94822100
C	3.28128100	1.02343300	2.04865300
C	3.60119900	-0.33128400	1.89725200
C	3.59254700	-1.20038500	2.98679700
C	3.26908000	-0.67903400	4.23653600
H	3.27678900	-1.34705900	5.09249800
C	2.94501700	0.66005900	4.40686700
H	2.70236700	1.04335300	5.39070700
C	2.94991400	1.51454500	3.31040600
H	2.71562100	2.56526400	3.43723800
C	3.96315600	-2.64477600	2.78342700
H	3.05155900	-3.24029200	2.67274500
H	4.49178300	-3.02204500	3.66293100
C	4.99276900	-3.68717600	-1.34374700
H	5.77370100	-4.22686500	-0.80093100
H	5.26593400	-3.74396800	-2.40090000
C	4.15751500	-2.07760500	0.36550600
C	4.83818500	-2.78875200	1.54127200
H	4.92738300	-3.85004800	1.29021700
C	6.24067600	-2.18802500	1.73535200
H	6.74383700	-2.72416100	2.54471000
H	6.14142900	-1.14788300	2.06641300
C	7.08952100	-2.23167200	0.46222500
H	8.02541300	-1.69263500	0.62969500
H	7.37353500	-3.26624700	0.24589500
C	6.35661200	-1.61275800	-0.73267100
H	6.25510800	-0.53507500	-0.57715500

H	6.93683100	-1.74934500	-1.64978800
C	4.95740700	-2.20823600	-0.92481400
H	4.40773200	-1.63628300	-1.68179500
C	-3.58932600	-0.03231100	-1.57496100
C	-2.50048200	0.86345300	-1.16683100
C	-4.08221700	0.44551600	-2.79893900
C	-3.34202100	1.61896400	-3.13295700
O	-1.75863800	0.76883300	-0.18842700
N	-2.43636000	1.86592000	-2.12109800
C	-5.09531200	-0.00382800	-3.67099700
C	-3.58092500	2.32193700	-4.30128900
C	-5.33585200	0.70094500	-4.83163000
C	-4.58351500	1.84868400	-5.14289700
H	-4.79121100	2.38069600	-6.06396700
H	-3.00984800	3.20821100	-4.55126400
H	-6.10716700	0.37054000	-5.51641700
H	-5.66669700	-0.89544600	-3.43445200
H	-1.65184000	2.49938400	-2.18568500
C	-0.94277900	4.94618300	-0.51454700
C	-1.60097400	4.10819100	0.37513500
C	-1.05047900	6.32737400	-0.44721800
C	-2.38840800	4.68513100	1.36767400
H	-1.50133000	3.02927100	0.29932700
C	-1.84225600	6.88537800	0.55096200
H	-0.52029900	6.94903800	-1.15789800
C	-2.50870200	6.06835800	1.45932200
H	-2.91498500	4.04397100	2.06510300
H	-1.93832100	7.96311100	0.61407300
H	-3.12767200	6.50894800	2.23182800
C	-4.40210800	-0.90203700	0.64395200
C	-4.00900300	-1.22442700	-0.77651800
H	-3.17221400	-1.93140600	-0.75177000
H	-4.82522700	-1.73685600	-1.29436200
C	-5.69980400	-0.38893000	0.95337800
C	-6.12516500	-0.24220000	2.29486900
C	-6.60778800	0.00472700	-0.05761600
C	-7.37591900	0.26509000	2.59462100
H	-5.47491100	-0.56517100	3.09932500
C	-7.85190600	0.51586500	0.25952700
H	-6.31929100	-0.05998400	-1.10077200
C	-8.26470800	0.65657200	1.58877000
H	-8.52103000	0.82452200	-0.53868600
C	-3.37196400	-1.03998700	1.71087400
H	-2.40581700	-1.30150100	1.28434200
H	-3.25871100	-0.12008900	2.29223900
F	-3.70631700	-2.04558800	2.63743800
H	-7.67867800	0.35700600	3.63345600
Cl	0.08035500	4.23899300	-1.75250300

C	-9.64615800	1.15636800	1.91423900
C	-10.70525200	0.05604000	1.76373000
H	-9.90287400	1.99309200	1.25569100
H	-9.66928800	1.54308800	2.93784100
C	-12.11185000	0.53993300	2.10479800
H	-10.68435000	-0.32420200	0.73565700
H	-10.43773000	-0.79040800	2.40666100
C	-13.16020000	-0.55479900	1.92924600
H	-12.12796400	0.90520900	3.13746100
H	-12.36405800	1.39862900	1.47282300
H	-14.15942800	-0.20003800	2.18762900
H	-13.18936100	-0.90717900	0.89500100
H	-12.93773500	-1.41561700	2.56506800

(15) IM_4-PhCl

Zero-point correction = 1.194531 (Hartree/Particle)
Thermal correction to Energy = 1.269742
Thermal correction to Enthalpy = 1.270686
Thermal correction to Gibbs Free Energy = 1.073754
Sum of electronic and zero-point Energies = -4996.966156
Sum of electronic and thermal Energies = -4996.890946
Sum of electronic and thermal Enthalpies = -4996.890002
Sum of electronic and thermal Free Energies = -4997.086933

Au	0.20455700	-1.24228000	-1.42606400
Au	2.07785500	1.39283600	-1.08382300
P	-0.00897200	-3.05432200	-0.05373500
P	3.52099900	1.97271000	0.58657400
Cl	0.59789700	0.69687300	-2.94803600
O	4.02718300	-0.83304100	0.63381300
O	2.79644500	-2.62442000	0.14356100
C	0.11140600	-2.62582000	1.70319000
C	0.27061000	-3.63211100	2.65722900
H	0.38757400	-4.66597300	2.34436600
C	0.27248900	-3.30536100	4.00885500
H	0.39221900	-4.08500800	4.75247200
C	0.10696800	-1.98035100	4.40317200
H	0.10037000	-1.72892100	5.45818900
C	-0.04646500	-0.97829700	3.45095200
H	-0.15859500	0.05435700	3.76028500
C	-0.03940100	-1.29466900	2.09700400
H	-0.16411400	-0.51309300	1.35251100
C	-1.63598200	-3.83427800	-0.28345100
C	-2.57707700	-3.85735700	0.74369400
H	-2.32986400	-3.49689800	1.73504000
C	-3.87378300	-4.29661300	0.48386600
H	-4.60625900	-4.27989200	1.28209800
C	-4.22414300	-4.72640400	-0.78836800
H	-5.23293000	-5.07131500	-0.98645300

C	-3.28461800	-4.70043400	-1.81962100
H	-3.56106400	-5.02030600	-2.81751400
C	-1.99986400	-4.24169200	-1.57439400
H	-1.28345300	-4.17872300	-2.38881500
C	3.23436700	3.65794600	1.19528800
C	1.91345300	4.03221500	1.45210100
H	1.10451300	3.33507700	1.25327200
C	1.63153300	5.28964100	1.96738600
H	0.60312700	5.57066900	2.16991500
C	2.67164000	6.18375800	2.20962700
H	2.45553900	7.17029200	2.60345000
C	3.98621000	5.81834300	1.94219600
H	4.79227100	6.51948800	2.12402700
C	4.27517300	4.55304800	1.43971500
H	5.30229800	4.27361800	1.23179500
C	5.27405700	1.85370200	0.11522300
C	6.24486000	1.59756700	1.08654900
H	5.95590000	1.46151400	2.12436000
C	7.58281500	1.50789100	0.72027100
H	8.33540300	1.31075000	1.47529600
C	7.95406400	1.67479600	-0.61135100
H	8.99780200	1.60389800	-0.89514100
C	6.98777600	1.93134200	-1.57842300
H	7.27511300	2.05871300	-2.61543000
C	5.64684600	2.01830300	-1.21824000
H	4.89185400	2.20407500	-1.97612000
C	1.26271800	-4.28177000	-0.47612000
C	2.58500500	-3.80894400	-0.48799200
C	3.59252500	-4.48847200	-1.16497200
C	3.28389900	-5.74055700	-1.69799000
H	4.06275300	-6.29064200	-2.21758900
C	2.01069800	-6.28261300	-1.59090200
H	1.80124100	-7.26472000	-1.99634200
C	0.98758400	-5.53646200	-1.01151000
H	-0.02502300	-5.92263500	-0.99257000
C	3.35645500	0.90769600	2.05033200
C	3.62722500	-0.45653700	1.88797200
C	3.57099600	-1.33653200	2.96780000
C	3.23924700	-0.81876000	4.21689600
H	3.20947600	-1.49601100	5.06504800
C	2.95935100	0.52897100	4.39704800
H	2.71097800	0.90944200	5.38055200
C	3.01975500	1.39554600	3.31201600
H	2.82443300	2.45292700	3.44858100
C	3.90546600	-2.78883900	2.75833200
H	2.98019800	-3.35902100	2.63084900
H	4.41226000	-3.18620300	3.64176200
C	4.94143000	-3.83756100	-1.35738600

H	5.70443400	-4.40242800	-0.81472200
H	5.21484500	-3.89956900	-2.41418400
C	4.14551100	-2.20676500	0.34961600
C	4.79168300	-2.94753400	1.52639000
H	4.85249900	-4.00870600	1.26674700
C	6.20949800	-2.39116100	1.73890200
H	6.68746100	-2.94560200	2.55122100
H	6.13925300	-1.34951500	2.07241500
C	7.06884300	-2.45813600	0.47371500
H	8.02001600	-1.94997300	0.65151500
H	7.32151500	-3.50079400	0.25722100
C	6.36870300	-1.81249300	-0.72674400
H	6.30305300	-0.73246700	-0.57030500
H	6.95299900	-1.96758100	-1.63839800
C	4.95171300	-2.35885300	-0.93402600
H	4.42906800	-1.76535200	-1.69352300
C	-3.75414500	0.37700700	-1.09579700
C	-2.41099400	1.04669200	-0.97021800
C	-4.48715400	1.17293300	-2.11628400
C	-3.61541700	2.16919800	-2.56861600
O	-1.47666500	0.75545000	-0.22978900
N	-2.40499300	2.06820500	-1.86554100
C	-5.74728900	1.05909000	-2.68145700
C	-3.96309700	3.06741200	-3.56029500
C	-6.11675800	1.95868100	-3.68251200
C	-5.23794500	2.94784500	-4.11303200
H	-5.54410600	3.63481300	-4.89322900
H	-3.27021000	3.82974800	-3.89728800
H	-7.10092500	1.88321600	-4.12902200
H	-6.43896800	0.29163400	-2.35258400
H	-1.56181900	2.58848500	-2.07078200
C	-0.76368800	4.95256000	-0.35308700
C	-1.35099000	4.08441800	0.55796100
C	-0.92688200	6.32735000	-0.27051300
C	-2.11945000	4.62168000	1.58634900
H	-1.20438700	3.01240200	0.46815600
C	-1.70077000	6.84653600	0.76228700
H	-0.45362100	6.97532900	-0.99778000
C	-2.29481000	5.99823300	1.69165400
H	-2.58307800	3.95613900	2.30578100
H	-1.83901000	7.91887100	0.83653900
H	-2.89772100	6.40905300	2.49270000
C	-4.40699800	-0.40050200	0.05048400
C	-3.81486900	-1.14273700	-1.09220700
H	-2.87589700	-1.65872400	-0.93153500
H	-4.47503600	-1.57824300	-1.83328800
C	-5.89538700	-0.31158300	0.19135000
C	-6.50656800	0.90989100	0.46952200

C	-6.68592200	-1.45109200	0.07732200
C	-7.88425000	0.98926000	0.61672600
H	-5.89909500	1.80856600	0.53293400
C	-8.06592900	-1.36765400	0.22543000
H	-6.21043700	-2.40510700	-0.13068800
C	-8.68613000	-0.14760200	0.49384400
H	-8.67322900	-2.26335100	0.13308300
C	-3.68202700	-0.48188800	1.37332300
H	-2.60379100	-0.55802300	1.24447900
H	-3.92589000	0.37417300	2.00817300
F	-4.11808100	-1.62439700	2.03536900
H	-8.35042400	1.94980200	0.81548000
Cl	0.23717100	4.29423400	-1.63343600
C	-10.17442800	-0.06678200	0.71379200
C	-10.53403800	-0.20832500	2.19787700
H	-10.67828600	-0.85277900	0.14245000
H	-10.55438800	0.88882400	0.33828600
C	-12.03678200	-0.13646500	2.45524600
H	-10.13897100	-1.15976000	2.57301900
H	-10.02332400	0.57778900	2.76644700
C	-12.37711700	-0.27164900	3.93631700
H	-12.42601400	0.81290600	2.07122100
H	-12.54038700	-0.92614500	1.88688600
H	-13.45365700	-0.22039200	4.10789300
H	-12.02148800	-1.22547400	4.33448800
H	-11.90858500	0.52507500	4.51979000

(16) IM_{21}-PhF

Zero-point correction = 1.192228 (Hartree/Particle)
Thermal correction to Energy = 1.268522
Thermal correction to Enthalpy = 1.269466
Thermal correction to Gibbs Free Energy = 1.068932
Sum of electronic and zero-point Energies = -4636.516686
Sum of electronic and thermal Energies = -4636.440392
Sum of electronic and thermal Enthalpies = -4636.439447
Sum of electronic and thermal Free Energies = -4636.639982

Au	0.32127900	-1.80168700	-0.38832500
Au	1.67607500	1.27811200	-1.70842300
P	2.22571500	-2.97388200	0.49894900
P	1.65777300	3.10957900	-0.32289200
Cl	1.83248400	-0.76181100	-2.98227000
O	3.69031400	1.53311900	0.72363500
O	3.99370000	-0.69001600	0.58954900
C	2.45210400	-2.85418600	2.30278100
C	3.56949100	-3.42941900	2.91658400
H	4.32644000	-3.92142400	2.31329700
C	3.71086700	-3.36819900	4.29719200
H	4.57628500	-3.81689400	4.77106300

C	2.74101000	-2.73171900	5.06968700
H	2.85215200	-2.68761800	6.14727200
C	1.63206700	-2.15581200	4.46033200
H	0.87591400	-1.65975000	5.05809200
C	1.48667900	-2.21217400	3.07648700
H	0.62639200	-1.74978800	2.60093100
C	1.71776300	-4.70607400	0.18662000
C	1.67184700	-5.67864000	1.18291500
H	1.94051000	-5.43278500	2.20411300
C	1.26598100	-6.97405100	0.87029100
H	1.22552100	-7.72530200	1.65058000
C	0.91444400	-7.30329100	-0.43207500
H	0.60323700	-8.31361700	-0.67127300
C	0.95832400	-6.33309300	-1.43089400
H	0.68465700	-6.58576800	-2.44887700
C	1.34867100	-5.03769000	-1.12287200
H	1.38383700	-4.28200500	-1.90447200
C	0.25703100	4.25619500	-0.44914100
C	-0.68287100	4.09961100	-1.46548100
H	-0.56479400	3.30492000	-2.19430600
C	-1.77334400	4.95847600	-1.54316400
H	-2.51107400	4.82125100	-2.32512100
C	-1.91618800	5.98277500	-0.61665600
H	-2.76912500	6.64907200	-0.67322200
C	-0.96253500	6.16156100	0.38268700
H	-1.06829400	6.96887100	1.09773500
C	0.12368800	5.30380900	0.46683600
H	0.86588000	5.44819000	1.24566800
C	3.15081700	4.15215800	-0.44556400
C	3.67752600	4.78338800	0.68247100
H	3.22871200	4.62552200	1.65874600
C	4.79595500	5.59987500	0.56014500
H	5.20425000	6.08778700	1.43789000
C	5.39176100	5.78671200	-0.68418600
H	6.26403500	6.42358200	-0.77598700
C	4.87083500	5.15323300	-1.80742300
H	5.33600700	5.29204100	-2.77649800
C	3.75274500	4.33400400	-1.69020500
H	3.35320900	3.83206500	-2.56630200
C	3.91408000	-2.90224100	-0.18431000
C	4.63697500	-1.70904900	-0.04854500
C	5.94015300	-1.60115100	-0.53252200
C	6.50993200	-2.70974900	-1.15397600
H	7.52042400	-2.62367200	-1.54162400
C	5.81530200	-3.90137700	-1.28901600
H	6.27642300	-4.75339900	-1.77291000
C	4.51625300	-3.99602500	-0.80356900
H	3.97295400	-4.92734600	-0.90593600

C	1.66587000	2.47689000	1.38591400
C	2.76105300	1.66689300	1.71217900
C	2.90630200	1.08800300	2.96778200
C	1.89587000	1.31829900	3.90050400
H	1.99677900	0.88235500	4.89003200
C	0.78263000	2.08991200	3.59101600
H	0.00797400	2.24888200	4.33159100
C	0.66480700	2.67705600	2.33306800
H	-0.20819900	3.27131300	2.08971700
C	4.12524800	0.25171100	3.26101200
H	3.85108800	-0.80407600	3.21812200
H	4.47389800	0.44922500	4.27886100
C	6.68046200	-0.29895100	-0.39601800
H	7.36894400	-0.34726200	0.45398000
H	7.29686600	-0.13145100	-1.28290200
C	4.67965700	0.53962200	0.84173300
C	5.25151000	0.54049300	2.26340100
H	5.99103600	-0.26577000	2.32370700
C	5.93741900	1.88761700	2.53270200
H	6.38975700	1.85947500	3.52792400
H	5.17660900	2.67746500	2.55658000
C	6.98917000	2.23149000	1.47716200
H	7.39535900	3.22733600	1.67216100
H	7.83274700	1.53804500	1.56003100
C	6.39579900	2.19418300	0.06672300
H	5.66651300	3.00046900	-0.03856200
H	7.17351200	2.37197800	-0.68183300
C	5.70348800	0.86268800	-0.24246400
H	5.13057400	0.95329300	-1.17383400
C	-1.60210300	-1.65033000	-1.00277400
C	-2.81820300	-1.49255300	-0.06840500
C	-2.16054100	-1.95951800	-2.23283700
C	-3.59782600	-1.94624800	-2.13235700
O	-2.81452800	-1.27814600	1.10885700
N	-3.96120800	-1.68886200	-0.84970900
C	-1.53850500	-2.17891600	-3.49186100
C	-4.40070200	-2.14716100	-3.24987400
C	-2.33542000	-2.37767900	-4.58855800
C	-3.74669600	-2.36182000	-4.45375100
H	-4.34771900	-2.52224800	-5.34309100
H	-5.48096000	-2.13528000	-3.17793400
H	-1.89957000	-2.53816100	-5.56614500
H	-0.45535300	-2.14863700	-3.55727800
H	-4.90855400	-1.52169200	-0.53417500
C	-2.84879800	1.42797800	-0.67528400
C	-4.29370200	1.43679800	-0.35414700
C	-4.72596900	1.33914400	0.97441000
C	-5.26854000	1.48539800	-1.35810500

C	-6.07793700	1.26388400	1.27747100
H	-4.00660200	1.32390200	1.78355900
C	-6.61887200	1.41012300	-1.04638900
H	-4.97189600	1.60694400	-2.39453100
C	-7.04919100	1.29120000	0.27655200
H	-7.35524100	1.45525800	-1.84326900
H	-6.38994300	1.17693700	2.31446900
C	-2.35834500	1.08560700	-1.87352100
H	-2.99261900	0.77118000	-2.69595600
H	-1.29054100	1.08777100	-2.07152600
C	-8.99476300	-2.15608800	0.15436900
C	-7.63737700	-1.99139000	0.34401500
C	-7.05155000	-1.91732900	1.59361900
C	-7.87894700	-2.00658000	2.70833600
C	-9.25325100	-2.16734300	2.55463200
C	-9.80705400	-2.24560600	1.28062900
H	-9.39585300	-2.20869700	-0.85040400
H	-5.97978400	-1.78067400	1.69237500
H	-7.44458200	-1.94917400	3.69946700
H	-9.89118300	-2.23483500	3.42753300
H	-10.87584500	-2.37470500	1.15783200
F	-6.84062700	-1.87925000	-0.75381100
C	-1.88119800	1.72150100	0.43645500
H	-1.92395500	0.95910700	1.21949800
H	-0.86117100	1.76058300	0.05106600
F	-2.17624700	2.94376700	1.02604400
C	-8.51163100	1.25824600	0.63242300
C	-9.02348700	2.62391900	1.10647200
H	-8.67984100	0.51899700	1.42376700
H	-9.09689600	0.92942000	-0.23249300
C	-10.50161200	2.59094400	1.48567100
H	-8.42904600	2.95095400	1.96760900
H	-8.85692200	3.36856300	0.31976200
C	-11.00239400	3.94021700	1.99244000
H	-11.09134600	2.28016600	0.61621800
H	-10.65919200	1.82435900	2.25281400
H	-12.06081200	3.90312000	2.25611400
H	-10.44889300	4.25423300	2.88102800
H	-10.87595700	4.71594400	1.23304000

(17) $TS_{2\text{-}31}$-PhF

Zero-point correction =	1.191921 (Hartree/Particle)
Thermal correction to Energy =	1.267227
Thermal correction to Enthalpy =	1.268171
Thermal correction to Gibbs Free Energy =	1.071461
Sum of electronic and zero-point Energies =	-4636.514193
Sum of electronic and thermal Energies =	-4636.438887
Sum of electronic and thermal Enthalpies =	-4636.437943

Sum of electronic and thermal Free Energies = -4636.634654

Au	0.12193700	-1.69413500	-0.33869000
Au	1.74070700	1.29771400	-1.63502300
P	1.96281800	-2.95650900	0.54096600
P	1.75154500	3.10634200	-0.21970100
Cl	1.87694300	-0.72757200	-2.92034500
O	3.77561400	1.43408600	0.63798700
O	3.90080000	-0.80259000	0.47305800
C	2.32211600	-2.81634500	2.31999900
C	3.42872900	-3.47158900	2.87032500
H	4.10430800	-4.02750400	2.22708800
C	3.66118200	-3.41012700	4.23820400
H	4.51752300	-3.92012600	4.66419100
C	2.79396400	-2.69307700	5.06095100
H	2.97474700	-2.65016500	6.12903900
C	1.69789100	-2.03604700	4.51408900
H	1.02247400	-1.47673800	5.15147800
C	1.46119200	-2.09343200	3.14303100
H	0.60837200	-1.57431600	2.71484000
C	1.32053900	-4.65839000	0.31757800
C	1.27909200	-5.59803900	1.34529900
H	1.63162100	-5.34332500	2.33812300
C	0.76931400	-6.87147600	1.10250700
H	0.73376800	-7.59585200	1.90796500
C	0.30874100	-7.21286900	-0.16206600
H	-0.08484200	-8.20589100	-0.34618000
C	0.34677100	-6.27580200	-1.19216600
H	-0.01351100	-6.53640100	-2.18057700
C	0.84080000	-5.00151200	-0.95267500
H	0.86939300	-4.27256400	-1.75938500
C	0.32434600	4.22381400	-0.26484700
C	-0.67937600	4.01673000	-1.20888400
H	-0.57956600	3.21665000	-1.93439600
C	-1.80130600	4.83802400	-1.22572900
H	-2.58416800	4.66701500	-1.95576000
C	-1.91316800	5.87464100	-0.30823200
H	-2.78893800	6.51320900	-0.31726800
C	-0.89689600	6.10535900	0.61632000
H	-0.97809700	6.92571900	1.31969700
C	0.22232800	5.28584000	0.63834700
H	1.01599800	5.47233100	1.35555700
C	3.23982500	4.14667600	-0.40556400
C	3.88733200	4.68682500	0.70637100
H	3.51696500	4.48611500	1.70712100
C	5.02571500	5.46631000	0.53314000
H	5.52859900	5.88312200	1.39833500
C	5.51803300	5.70912500	-0.74565300
H	6.40731600	6.31467800	-0.87752800

C	4.87241200	5.17160900	-1.85451200
H	5.25752300	5.35446100	-2.85087600
C	3.73640000	4.38783500	-1.68664700
H	3.24385200	3.95402500	-2.55171800
C	3.59860200	-3.01098600	-0.26320600
C	4.40900100	-1.86718100	-0.21309100
C	5.65933900	-1.84774700	-0.82817900
C	6.09394900	-2.99824400	-1.48241300
H	7.06349600	-2.98089100	-1.97080200
C	5.31730100	-4.14515100	-1.52463000
H	5.67424800	-5.03173700	-2.03383300
C	4.06748700	-4.14827800	-0.91705000
H	3.45782400	-5.04259500	-0.95216700
C	1.85889900	2.45357400	1.47748700
C	2.94626000	1.60072200	1.70624900
C	3.18430600	1.01367400	2.94275500
C	2.27744200	1.29002100	3.96559100
H	2.44969700	0.84969900	4.94323000
C	1.17289800	2.10661700	3.75730000
H	0.47846600	2.29898400	4.56632000
C	0.95940800	2.69501800	2.51214800
H	0.09086400	3.32075400	2.34680800
C	4.37846600	0.10936500	3.11394000
H	4.03654300	-0.92767100	3.10317000
H	4.84056000	0.28302400	4.09008900
C	6.49015800	-0.59258600	-0.79829300
H	7.27604800	-0.68258200	-0.04111600
H	6.99900600	-0.46887000	-1.75751900
C	4.69704000	0.37062400	0.64968600
C	5.41276300	0.32799100	2.00392100
H	6.10169900	-0.52365900	1.99095200
C	6.20791700	1.62840600	2.19211400
H	6.76152000	1.57101500	3.13334600
H	5.50433400	2.46426200	2.29178700
C	7.15968600	1.90567900	1.02753000
H	7.65108400	2.87057000	1.17574400
H	7.95754900	1.15541800	1.01926700
C	6.41682700	1.91513900	-0.31135200
H	5.73123800	2.76670600	-0.33674100
H	7.12016200	2.04933400	-1.13824700
C	5.61407100	0.62941800	-0.54068400
H	4.94618200	0.75751500	-1.40241700
C	-1.77118200	-1.43147200	-1.06952500
C	-3.03919800	-1.47744100	-0.19304400
C	-2.22558100	-1.86861900	-2.34415200
C	-3.63598500	-2.05263400	-2.30496700
O	-3.11539400	-1.31174000	0.99697900
N	-4.09330900	-1.78636800	-1.03245100

C	-1.51786300	-2.08233100	-3.53963600
C	-4.34573300	-2.44534300	-3.42750400
C	-2.22201900	-2.47727700	-4.66092100
C	-3.61482000	-2.65193100	-4.59542000
H	-4.14527300	-2.96023300	-5.48994400
H	-5.41877100	-2.59049600	-3.39730100
H	-1.70663100	-2.64930200	-5.59716600
H	-0.44547300	-1.91289800	-3.56425100
H	-5.06077500	-1.82717500	-0.73856000
C	-2.58852300	1.29391200	-0.51364600
C	-4.02555400	1.43893600	-0.28024700
C	-4.53116500	1.46594200	1.02999200
C	-4.94596500	1.46013500	-1.34272900
C	-5.89694300	1.46884300	1.26047900
H	-3.85526000	1.47281000	1.87453000
C	-6.30791900	1.45517000	-1.10117400
H	-4.59485300	1.48069200	-2.36825900
C	-6.80912900	1.44238000	0.20526500
H	-7.00138200	1.45770900	-1.93639100
H	-6.26882500	1.46406900	2.28051000
C	-2.06023300	0.85720100	-1.68819600
H	-2.68062800	0.65767500	-2.55213300
H	-0.99095300	0.86679600	-1.86545500
C	-8.98917700	-1.98024700	0.59952500
C	-7.61451000	-1.85050900	0.56036000
C	-6.84012900	-1.63907000	1.68500400
C	-7.49017800	-1.54389400	2.91196600
C	-8.87496800	-1.66127700	2.98894200
C	-9.62087800	-1.88309700	1.83496200
H	-9.53906100	-2.15047700	-0.31799600
H	-5.76174000	-1.53982100	1.60581000
H	-6.90721600	-1.37887400	3.81058200
H	-9.37193200	-1.58703600	3.94871600
H	-10.69837100	-1.98193100	1.89238700
F	-6.99651700	-1.92123200	-0.65057400
C	-1.65116500	1.46323300	0.65193600
H	-1.78579200	0.64001100	1.36215300
H	-0.61245700	1.47070800	0.31632200
F	-1.90435800	2.65320500	1.31575700
C	-8.28834900	1.45424900	0.47158400
C	-8.83180600	2.88119400	0.62323700
H	-8.50138500	0.88305700	1.38216000
H	-8.81410100	0.95027200	-0.34598400
C	-10.33414700	2.90619600	0.89196400
H	-8.30109500	3.38494000	1.43942100
H	-8.60786300	3.45233000	-0.28528400
C	-10.87210100	4.32590200	1.04220400
H	-10.85590600	2.39718600	0.07410500

H	-10.54893000	2.32937400	1.79836500
H	-11.94662800	4.32991900	1.23206500
H	-10.38544200	4.84388200	1.87246900
H	-10.69196200	4.91046900	0.13648700

(18) IM$_{31}$-PhF

Zero-point correction = 1.193177 (Hartree/Particle)
Thermal correction to Energy = 1.268276
Thermal correction to Enthalpy = 1.269221
Thermal correction to Gibbs Free Energy = 1.073724
Sum of electronic and zero-point Energies = -4636.561168
Sum of electronic and thermal Energies = -4636.486069
Sum of electronic and thermal Enthalpies = -4636.485125
Sum of electronic and thermal Free Energies = -4636.680621

Au	1.26460900	0.09538900	-2.06901400
Au	-1.59613600	1.65381600	-1.48059800
P	3.27095700	-0.19275400	-1.00307300
P	-2.42256900	2.25523200	0.55383800
Cl	-0.57771100	0.90394000	-3.58060800
O	0.35730200	2.93241600	0.86394600
O	2.34608100	2.27281800	0.04916800
C	3.38682000	-0.57536200	0.76244400
C	4.61062800	-0.37951600	1.41309700
H	5.45426900	0.04270400	0.87539700
C	4.73689400	-0.72358400	2.75168200
H	5.68327900	-0.57771500	3.25986300
C	3.65281100	-1.26982000	3.43774800
H	3.76534800	-1.56285300	4.47539000
C	2.44223400	-1.47282400	2.78723100
H	1.60538200	-1.92863500	3.30337000
C	2.30539600	-1.11237800	1.44926200
H	1.35847300	-1.24183100	0.93736800
C	4.23781600	-1.48092100	-1.85198400
C	4.75086000	-2.57431600	-1.15450200
H	4.63475200	-2.64959800	-0.08006600
C	5.39310500	-3.59749400	-1.84710400
H	5.77974400	-4.44985600	-1.29966900
C	5.53150200	-3.52809600	-3.22806900
H	6.03711700	-4.32377900	-3.76341700
C	5.01373400	-2.43894400	-3.92683000
H	5.11326800	-2.38601700	-5.00491100
C	4.35758400	-1.42382100	-3.24449300
H	3.92632100	-0.59199600	-3.79519500
C	-4.05815900	1.55769600	0.90753300
C	-4.43852800	0.37282600	0.27535400
H	-3.80136400	-0.07682900	-0.48040500
C	-5.64408500	-0.23687600	0.60121300
H	-5.92930500	-1.16031100	0.10925000

C	-6.47402400	0.34217000	1.55373200
H	-7.41535200	-0.13234000	1.80679700
C	-6.10403200	1.53001300	2.17875500
H	-6.75754500	1.98342000	2.91481900
C	-4.89697500	2.13996800	1.86161800
H	-4.61439800	3.06654500	2.34993800
C	-2.50288800	4.05222600	0.82506700
C	-2.31379900	4.58315300	2.10366900
H	-2.10588400	3.92653000	2.94322500
C	-2.37920500	5.95848300	2.29789200
H	-2.23349700	6.36940700	3.29051200
C	-2.63078300	6.80405100	1.22114400
H	-2.67903700	7.87591700	1.37475300
C	-2.81969700	6.27583900	-0.05211800
H	-3.01490500	6.93337600	-0.89107900
C	-2.75429700	4.90137100	-0.25260500
H	-2.89276200	4.49095800	-1.24827700
C	4.13104500	1.39536900	-1.20141500
C	3.47086900	2.52207100	-0.68029800
C	3.93295400	3.80770100	-0.94347100
C	5.11822300	3.94316400	-1.66683400
H	5.48905000	4.94293500	-1.87144400
C	5.81718100	2.84006500	-2.13453300
H	6.73985100	2.97202500	-2.68580700
C	5.31082800	1.56155900	-1.91882700
H	5.82767900	0.69472500	-2.31607200
C	-1.32991700	1.63691900	1.86211200
C	0.00574900	2.06820300	1.86723400
C	0.87708100	1.68607000	2.88280300
C	0.39098900	0.83825900	3.87846100
H	1.06404200	0.54886700	4.67999600
C	-0.91460500	0.36846400	3.86638400
H	-1.27697400	-0.29792900	4.63972800
C	-1.78295400	0.77553900	2.85716800
H	-2.80374800	0.41075000	2.84745500
C	2.27938400	2.23255700	2.89331400
H	2.96171100	1.50298800	2.44774800
H	2.60731000	2.39084000	3.92433600
C	3.13218200	4.99767200	-0.48230400
H	3.63930200	5.47868100	0.35938000
H	3.09911800	5.74191600	-1.28231000
C	1.70074500	3.34839200	0.74024500
C	2.33458500	3.55133200	2.11969300
H	3.38255500	3.82917500	1.96428700
C	1.60191700	4.68935900	2.84920200
H	2.09440300	4.86570500	3.80939200
H	0.57960600	4.36675200	3.07901500
C	1.54744000	5.98240300	2.03332800

H	0.93207600	6.71879000	2.55658400
H	2.54884700	6.41915400	1.96785100
C	0.96973300	5.74485700	0.63488700
H	-0.08850200	5.48641100	0.71904200
H	1.02420200	6.66030600	0.03846600
C	1.69510900	4.61695700	-0.10783700
H	1.14692300	4.36411300	-1.02339000
C	-0.41877700	-2.80059300	-0.07532900
C	0.49165000	-3.62046400	0.73667200
C	-0.01405300	-2.92864200	-1.41244900
C	1.15127500	-3.75920200	-1.43458800
O	0.48533300	-3.77389300	1.94809300
N	1.41631900	-4.16940500	-0.14629600
C	-0.49996900	-2.38959600	-2.62216400
C	1.83457300	-4.01746100	-2.61163900
C	0.18178100	-2.65249900	-3.79456600
C	1.33942600	-3.45208100	-3.78420600
H	1.85967900	-3.64035000	-4.71639000
H	2.72783000	-4.63099500	-2.62141200
H	-0.17523500	-2.23545600	-4.72853600
H	-1.38785300	-1.76569700	-2.63247200
H	2.22417600	-4.69131200	0.16043000
C	-2.45237700	-2.48532900	1.42201300
C	-3.67498500	-2.98493500	0.87422100
C	-4.74204100	-3.38407200	1.71448600
C	-3.87955400	-3.08905200	-0.52107900
C	-5.93263100	-3.84217600	1.18333400
H	-4.63900700	-3.29446300	2.78918300
C	-5.07851200	-3.54986700	-1.03771100
H	-3.07619700	-2.84133800	-1.20655800
C	-6.13125100	-3.93121300	-0.19968200
H	-5.20174600	-3.62894900	-2.11393000
H	-6.73606800	-4.13657500	1.85240300
C	-1.40639500	-1.85815900	0.53721600
H	-1.87444700	-1.27298200	-0.26216600
H	-0.84310400	-1.13571800	1.14646400
C	3.28456600	-4.67275800	3.44415500
C	4.29691800	-4.46812200	2.52659500
C	5.58386500	-4.11518700	2.88210400
C	5.87392400	-3.97109200	4.23557600
C	4.88363300	-4.18091100	5.19084100
C	3.59522400	-4.52892300	4.79294400
H	2.28210300	-4.90541500	3.10419600
H	6.33538800	-3.96659500	2.11533900
H	6.87920300	-3.70510600	4.54099600
H	5.11722900	-4.08067900	6.24416200
H	2.82273600	-4.69188900	5.53568000
F	4.01469000	-4.60755800	1.20266400

C	-2.17083900	-2.61395500	2.88240700
H	-2.31024000	-3.63983800	3.23216800
H	-1.15864100	-2.29368800	3.12049400
F	-3.04899500	-1.81807200	3.64510700
C	-7.45955900	-4.36054200	-0.75892700
C	-8.43268700	-3.17989600	-0.88401700
H	-7.90274500	-5.12484800	-0.11258000
H	-7.32024300	-4.81999400	-1.74240900
C	-9.79919300	-3.59612100	-1.42118300
H	-8.55235100	-2.70752400	0.09912100
H	-7.99297600	-2.41841800	-1.53990100
C	-10.75981300	-2.41749400	-1.54632900
H	-9.67244300	-4.07585200	-2.39761500
H	-10.22956300	-4.35578400	-0.75982900
H	-11.73331200	-2.73321700	-1.92502200
H	-10.92044200	-1.93759500	-0.57731200
H	-10.36631100	-1.66109000	-2.23016500

(19) IM$_{41}$-PhF

Zero-point correction = 1.196334 (Hartree/Particle)
Thermal correction to Energy = 1.270349
Thermal correction to Enthalpy = 1.271294
Thermal correction to Gibbs Free Energy = 1.080338
Sum of electronic and zero-point Energies = -4636.613620
Sum of electronic and thermal Energies = -4636.539605
Sum of electronic and thermal Enthalpies = -4636.538661
Sum of electronic and thermal Free Energies = -4636.729616

Au	0.29972200	-0.65018700	-2.01171400
Au	-1.98138000	1.62824100	-0.87397500
P	2.55752100	-0.97087100	-1.83435700
P	-1.81581700	3.02594800	0.91709900
Cl	-2.06578800	-0.13275500	-2.59581600
O	0.91674300	3.05562500	0.05072500
O	2.31682100	1.83488900	-1.21512000
C	3.29049000	-1.00813800	-0.17858200
C	4.68084100	-0.92450800	-0.03994200
H	5.31142100	-0.81917900	-0.91860800
C	5.25002600	-0.95397300	1.22601300
H	6.32669000	-0.89120000	1.33602700
C	4.43710500	-1.07211100	2.35372800
H	4.88790500	-1.09916800	3.34285700
C	3.05552800	-1.14384900	2.21584800
H	2.42372600	-1.22611100	3.09047500
C	2.47964700	-1.10571900	0.94856800
H	1.39974800	-1.13160400	0.83362200
C	3.04512200	-2.49612400	-2.70056700
C	3.94449800	-3.41408400	-2.16193400
H	4.39052700	-3.23954400	-1.18620800

C	4.26463200	-4.56617600	-2.86975900
H	4.96259400	-5.27991800	-2.44723100
C	3.68472300	-4.81122100	-4.11206400
H	3.94017300	-5.71176200	-4.66081300
C	2.78120700	-3.89710400	-4.64995900
H	2.32411400	-4.08362300	-5.61479900
C	2.45537500	-2.74800400	-3.94320900
H	1.73684100	-2.04572100	-4.35720000
C	-3.28003600	2.92318800	1.99360600
C	-3.71008000	1.65930000	2.40170300
H	-3.17138500	0.76292600	2.11212700
C	-4.82900800	1.53803900	3.21270200
H	-5.13982500	0.54863600	3.53410700
C	-5.52728500	2.67795400	3.60550600
H	-6.40701500	2.58025700	4.23182200
C	-5.10574700	3.93409300	3.19690700
H	-5.65067700	4.81969500	3.49828200
C	-3.97723500	4.06392200	2.38781900
H	-3.65197400	5.04702700	2.06712900
C	-1.55929900	4.78201400	0.54295900
C	-0.96383200	5.61100500	1.50016400
H	-0.63109600	5.19931000	2.44849700
C	-0.80240000	6.96566400	1.23373100
H	-0.34688700	7.61050000	1.97643900
C	-1.23362600	7.49266100	0.02190100
H	-1.10732000	8.54956400	-0.18270800
C	-1.82000000	6.66647800	-0.93106300
H	-2.15147700	7.07592500	-1.87812800
C	-1.98237000	5.30920300	-0.67588200
H	-2.43453700	4.66138400	-1.42052100
C	3.40142900	0.37959200	-2.71423700
C	3.10862400	1.69566200	-2.31777800
C	3.58383800	2.78095100	-3.04894000
C	4.41798500	2.53109500	-4.13839800
H	4.79339400	3.38160300	-4.70690900
C	4.76217800	1.24583500	-4.50995600
H	5.41714000	1.07480400	-5.35521100
C	4.23660400	0.16200700	-3.80660300
H	4.46932600	-0.85117400	-4.11441900
C	-0.39577000	2.50953000	1.92176400
C	0.87744300	2.55328000	1.32287000
C	2.01489900	2.17900600	2.02688000
C	1.85789100	1.71898000	3.33308900
H	2.74543500	1.42823400	3.88733500
C	0.60974400	1.64494000	3.93575300
H	0.51237900	1.27868900	4.95202800
C	-0.51831000	2.05705100	3.23465000
H	-1.49274500	2.01677800	3.70302500

C	3.36767900	2.34855000	1.37876300
H	3.68433800	1.40864800	0.91910300
H	4.10781300	2.60257200	2.13738500
C	3.17209100	4.17915500	-2.67334800
H	4.02435400	4.70344700	-2.23098100
H	2.91157900	4.73502400	-3.57787800
C	2.14578600	3.13655000	-0.64106400
C	3.29510600	3.45058500	0.32197500
H	4.22177700	3.44790500	-0.26192500
C	3.07605100	4.84224800	0.94058000
H	3.93064500	5.07584200	1.58160900
H	2.19641500	4.81513300	1.59430300
C	2.88150600	5.93722900	-0.10877100
H	2.63714700	6.87960700	0.38802800
H	3.82207000	6.11233000	-0.63980500
C	1.76077000	5.57668300	-1.08809300
H	0.80650200	5.57946200	-0.55824600
H	1.68468100	6.32818300	-1.87960800
C	1.97070300	4.19729600	-1.72412000
H	1.07270900	3.90956700	-2.28376500
C	-0.80560300	-2.53687500	1.57514200
C	0.25321300	-2.92652200	2.58157300
C	-0.45045300	-3.27331700	0.33314600
C	0.70762900	-4.01356800	0.60863000
O	0.41014500	-2.49805900	3.70953300
N	1.06758700	-3.82390500	1.94793800
C	-0.99825600	-3.30922600	-0.94113300
C	1.35197500	-4.76409000	-0.35457200
C	-0.35766300	-4.06442200	-1.92940500
C	0.80104100	-4.77853200	-1.63593600
H	1.29140600	-5.34770500	-2.41818900
H	2.25372300	-5.32071700	-0.12510300
H	-0.77452400	-4.09942800	-2.92964200
H	-1.91015400	-2.76192200	-1.17575000
H	1.90054500	-4.19828100	2.38778700
C	-2.22503100	-2.13020600	1.97548800
C	-3.32641300	-2.52355800	1.03322200
C	-3.67738200	-3.86625500	0.91335400
C	-3.99910100	-1.58359200	0.26232100
C	-4.67014200	-4.25997600	0.03340500
H	-3.14198100	-4.61670900	1.49181200
C	-4.99208500	-1.97697500	-0.62789700
H	-3.73819800	-0.52828100	0.33578000
C	-5.34083000	-3.32140700	-0.75904200
H	-5.49152900	-1.23175600	-1.23797600
H	-4.92501100	-5.31038800	-0.06145100
C	-1.24663700	-1.08361300	1.56279500
H	-1.34753900	-0.64018100	0.57965800

H	-0.80971600	-0.45399400	2.33618000
C	3.48862500	-3.13139700	4.93554700
C	4.24706100	-3.91540000	4.08607500
C	5.62872500	-3.90510400	4.07679700
C	6.28443000	-3.06249400	4.96884000
C	5.55509600	-2.25548800	5.83793500
C	4.16300900	-2.29345200	5.81936300
H	2.40499000	-3.16486000	4.88955600
H	6.16626800	-4.54693700	3.38966400
H	7.36763700	-3.03857300	4.98739700
H	6.07109700	-1.60788000	6.53657400
H	3.59207600	-1.67406000	6.50147400
F	3.60760900	-4.72402000	3.20347500
C	-2.60090100	-2.16880800	3.43448800
H	-3.07982000	-3.11407900	3.69297100
H	-1.74980900	-1.97759200	4.08734600
F	-3.53689300	-1.15396900	3.64899500
C	-6.45487700	-3.74715100	-1.67862700
C	-7.80537600	-3.80873300	-0.94630000
H	-6.22319500	-4.73844600	-2.10155300
H	-6.52748300	-3.05399800	-2.52364600
C	-8.94316100	-4.26347400	-1.85431400
H	-7.71811400	-4.49525200	-0.09256600
H	-8.03106200	-2.81634200	-0.52765400
C	-10.28116800	-4.31310600	-1.11141800
H	-9.02310900	-3.57723500	-2.71233300
H	-8.70666300	-5.25561900	-2.26768800
H	-11.08957900	-4.65189800	-1.76867200
H	-10.23365500	-5.00784600	-0.25576300
H	-10.56000100	-3.32200300	-0.72531800

(20) IM$_{22}$-PhF

Zero-point correction = 1.192947 (Hartree/Particle)
Thermal correction to Energy = 1.268929
Thermal correction to Enthalpy = 1.269873
Thermal correction to Gibbs Free Energy = 1.070686
Sum of electronic and zero-point Energies = -4636.519295
Sum of electronic and thermal Energies = -4636.443314
Sum of electronic and thermal Enthalpies = -4636.442369
Sum of electronic and thermal Free Energies = -4636.641556

Au	-0.27634000	-1.65054700	-0.41198900
Au	-0.74747100	1.48513400	1.86040300
P	-2.01554100	-3.12001000	-1.04890100
P	-1.60729300	3.20522700	0.63852400
Cl	0.27101300	-0.33184700	3.02583800
O	-3.56952800	1.24327800	0.11296500
O	-3.69474800	-1.00438600	-0.03415600
C	-2.87574300	-2.78392600	-2.61962700

C	-4.15245200	-3.30220200	-2.85549000
H	-4.64967200	-3.88988300	-2.08991800
C	-4.79067700	-3.05473700	-4.06519000
H	-5.77974700	-3.46020000	-4.24494200
C	-4.16059500	-2.28679300	-5.04124300
H	-4.65934800	-2.09541500	-5.98452900
C	-2.89041600	-1.76985800	-4.80874400
H	-2.39689900	-1.17556000	-5.56938800
C	-2.24686300	-2.01627700	-3.59948500
H	-1.25896100	-1.60455800	-3.41605100
C	-1.29429500	-4.78723100	-1.22822400
C	-1.74173900	-5.69159800	-2.19210900
H	-2.51775700	-5.40669100	-2.89372800
C	-1.18182500	-6.96269200	-2.26394700
H	-1.52912100	-7.66003100	-3.01745500
C	-0.17977300	-7.33617700	-1.37582800
H	0.25504200	-8.32720500	-1.43638300
C	0.27062900	-6.43597800	-0.41446200
H	1.05553000	-6.72242500	0.27570900
C	-0.27869800	-5.16170000	-0.34202400
H	0.08552400	-4.45980300	0.40393800
C	-0.45468000	4.59949700	0.43122700
C	0.77211300	4.57233400	1.09305100
H	1.04874200	3.70562400	1.68587600
C	1.64308800	5.65317700	0.99387500
H	2.58809100	5.63124600	1.52494000
C	1.29483200	6.75898000	0.22802600
H	1.97151300	7.60265300	0.15425500
C	0.06640800	6.79478500	-0.42909100
H	-0.21268600	7.66389000	-1.01336100
C	-0.81131800	5.72515300	-0.31952000
H	-1.77794800	5.77094000	-0.81167300
C	-3.12836100	3.96305100	1.30218800
C	-4.10067700	4.49575500	0.45372200
H	-3.98145800	4.43216800	-0.62397600
C	-5.23848400	5.08916600	0.98913300
H	-5.99361500	5.49791400	0.32710500
C	-5.40720100	5.15535000	2.36926600
H	-6.29547900	5.61671500	2.78503600
C	-4.43787700	4.62636600	3.21538900
H	-4.56944200	4.67223900	4.29010600
C	-3.30043300	4.02706400	2.68477600
H	-2.55249800	3.60082000	3.34655100
C	-3.35609700	-3.32264600	0.16265900
C	-4.08447100	-2.18281400	0.53742400
C	-5.13816100	-2.27766200	1.44349200
C	-5.44479800	-3.53010200	1.97358500
H	-6.25993100	-3.60414300	2.68697600

C	-4.73147200	-4.66499600	1.62007000
H	-4.98245200	-5.62650500	2.05031900
C	-3.68333500	-4.55907800	0.71247200
H	-3.11613200	-5.43980100	0.43294600
C	-2.07898100	2.64126600	-1.02681500
C	-3.08398700	1.66382000	-1.08848300
C	-3.59178900	1.21503200	-2.30568000
C	-3.00668200	1.70296700	-3.47283300
H	-3.39453500	1.35990800	-4.42741700
C	-1.96674300	2.62384100	-3.43643700
H	-1.53038000	2.99050600	-4.35779600
C	-1.51591100	3.10870700	-2.21202800
H	-0.73120000	3.85661800	-2.17797300
C	-4.76254100	0.26639200	-2.31591000
H	-4.40906600	-0.74442400	-2.52113100
H	-5.44505300	0.53707600	-3.12654100
C	-5.90510000	-1.04291600	1.83121400
H	-6.86053900	-1.02353800	1.29672000
H	-6.15049900	-1.08079200	2.89553600
C	-4.48795800	0.17088300	0.15879500
C	-5.50651900	0.29575500	-0.97778700
H	-6.16795100	-0.57634100	-0.92290700
C	-6.33351500	1.57520100	-0.78927300
H	-7.09418300	1.62282100	-1.57355900
H	-5.68310300	2.44671100	-0.93172100
C	-6.98339900	1.65306700	0.59276900
H	-7.49050900	2.61474700	0.70674700
H	-7.76131800	0.88716900	0.67780300
C	-5.94569300	1.49764500	1.70772600
H	-5.28007900	2.36199000	1.69953800
H	-6.43465800	1.48422900	2.68624500
C	-5.10229500	0.22647400	1.55452800
H	-4.25350700	0.26109000	2.24801800
C	1.41613900	-0.67449900	0.13799600
C	2.42388100	-1.29249100	1.12147500
C	1.93888200	0.56798900	-0.16526300
C	3.13345500	0.79071300	0.60252000
O	2.45338800	-2.40646100	1.55270600
N	3.39422100	-0.30072200	1.36173900
C	1.46331900	1.57062800	-1.05408800
C	3.83083900	1.99760900	0.50471200
C	2.16817700	2.73400600	-1.16704800
C	3.34352700	2.93089300	-0.38668700
H	3.87763200	3.86963400	-0.49660600
H	4.73301300	2.17765600	1.07481400
H	1.84170600	3.52710600	-1.82936600
H	0.55267500	1.38508000	-1.61671700
H	4.20775900	-0.44249400	1.94756200

C	4.17651300	-1.86314200	-1.28732400
C	4.86771100	-0.58459000	-1.55102600
C	6.00763500	-0.22150200	-0.81322800
C	4.40956400	0.31531800	-2.52207700
C	6.64532600	0.98915700	-1.03701000
H	6.41385900	-0.89804100	-0.07122100
C	5.05217700	1.52317700	-2.74031000
H	3.55378900	0.06341200	-3.13768900
C	6.17808400	1.88770400	-1.99850100
H	4.67803400	2.19710000	-3.50600000
H	7.52844200	1.24154200	-0.45686000
C	6.91470500	3.16917700	-2.28264800
H	7.33426200	3.57257600	-1.35481600
H	6.21880000	3.92052300	-2.67137700
C	2.96236400	-2.16220100	-1.77418400
H	2.39928300	-1.49188700	-2.41167200
H	2.49603200	-3.11901700	-1.56303600
C	7.41133800	-2.31429000	3.93560200
C	6.16574000	-2.21135100	3.35027100
C	5.12197700	-3.07525500	3.61496300
C	5.35039500	-4.10170000	4.52691400
C	6.59154800	-4.23903100	5.13947600
C	7.61801900	-3.34784600	4.84337100
H	8.18930200	-1.60433200	3.68378000
H	4.16222700	-2.94804200	3.12535700
H	4.54885100	-4.79312100	4.75770300
H	6.75917700	-5.03963900	5.84960300
H	8.58603400	-3.45406200	5.31846800
F	5.95628000	-1.19641300	2.45546700
C	4.86037700	-2.86140100	-0.38662900
H	4.97180000	-2.47419500	0.62986000
H	4.29557500	-3.79315200	-0.34559200
F	6.12951200	-3.14226300	-0.86036100
C	8.04697800	2.95759500	-3.29705500
C	8.81032200	4.24241000	-3.60766200
H	7.62696200	2.54220200	-4.22011300
H	8.73781500	2.20036700	-2.90938600
C	9.93571900	4.01639800	-4.61275000
H	8.11307600	4.99356300	-3.99515400
H	9.22090700	4.65396800	-2.67903600
H	10.47095400	4.94208100	-4.83026000
H	10.66172400	3.29388300	-4.23181000
H	9.54609600	3.62702300	-5.55665400

(21) $TS_{2\text{-}32}$-PhF

Zero-point correction = 1.188696 (Hartree/Particle)
Thermal correction to Energy = 1.264211
Thermal correction to Enthalpy = 1.265155

Thermal correction to Gibbs Free Energy = 1.067660
Sum of electronic and zero-point Energies = -4636.508538
Sum of electronic and thermal Energies = -4636.433023
Sum of electronic and thermal Enthalpies = -4636.432079
Sum of electronic and thermal Free Energies = -4636.629575

Au	0.18088000	-1.69037200	0.48231200
Au	0.68092400	1.33741600	-1.83790900
P	2.08153300	-3.07785600	1.02770200
P	1.53734200	3.22006400	-0.71995200
Cl	-0.28331300	-0.63907300	-2.85659700
O	3.55742200	1.34506200	-0.10904700
O	3.77646200	-0.93378700	0.09158500
C	2.96874000	-2.71588100	2.61778100
C	4.27188800	-3.17709200	2.82403900
H	4.77854200	-3.73298900	2.04559600
C	4.92101100	-2.90609400	4.02812700
H	5.92677400	-3.26671600	4.18828200
C	4.27145600	-2.17401500	5.02334000
H	4.77484200	-1.96740200	5.95671400
C	2.97163300	-1.71383500	4.81504800
H	2.46498400	-1.15028100	5.58550800
C	2.31771000	-1.98490800	3.61250200
H	1.31286900	-1.61949600	3.44503200
C	1.42352300	-4.80840200	1.21640200
C	1.94534400	-5.69881100	2.15643600
H	2.73620500	-5.38775300	2.82473200
C	1.43273200	-6.99307300	2.24305300
H	1.83370800	-7.67931800	2.97481300
C	0.40627600	-7.39834900	1.39179800
H	0.01141800	-8.40134000	1.46225500
C	-0.11511400	-6.50749700	0.45323100
H	-0.91360000	-6.81640200	-0.20522000
C	0.38768700	-5.21048100	0.36574300
H	-0.02853000	-4.51842600	-0.35743700
C	0.36698500	4.65425400	-0.59831200
C	-0.80670400	4.62674200	-1.35105900
H	-1.05077900	3.75118000	-1.93913000
C	-1.66871600	5.72365100	-1.33462900
H	-2.57025500	5.70387700	-1.93017300
C	-1.36219000	6.84047000	-0.56029000
H	-2.02816100	7.69113200	-0.55020600
C	-0.18437700	6.87016200	0.18913400
H	0.06207700	7.74170700	0.77786800
C	0.68624400	5.78345700	0.16281700
H	1.61166200	5.82207800	0.72235300
C	3.07454100	3.98468200	-1.43091000
C	4.00636200	4.61136500	-0.60227800
H	3.86667200	4.61491200	0.47152100

C	5.13289300	5.21374000	-1.16162600
H	5.85576400	5.69812200	-0.52069000
C	5.32422900	5.19130000	-2.54364100
H	6.19641700	5.65982900	-2.97565100
C	4.39170000	4.56151800	-3.36716000
H	4.53998100	4.53825000	-4.43681800
C	3.26459300	3.95521900	-2.81196700
H	2.54631700	3.45397800	-3.44793100
C	3.44993000	-3.25912100	-0.20236800
C	4.17570700	-2.11346700	-0.53833500
C	5.24016700	-2.16799800	-1.43625000
C	5.55405600	-3.40329600	-2.00981700
H	6.37146500	-3.45317700	-2.71693900
C	4.83681400	-4.55156900	-1.69350400
H	5.09094500	-5.49564900	-2.15069400
C	3.78089900	-4.47955800	-0.78458200
H	3.21758600	-5.36647700	-0.53121700
C	2.02395100	2.74763500	1.00238700
C	3.04598900	1.79853700	1.10179800
C	3.55515900	1.38477400	2.33145200
C	2.95324900	1.89546400	3.48470700
H	3.33426800	1.58310800	4.44842400
C	1.89674200	2.80116500	3.41065900
H	1.44755400	3.18514000	4.31454800
C	1.43975500	3.24160300	2.16642800
H	0.64067100	3.96713700	2.10378400
C	4.73212100	0.44157300	2.36675300
H	4.37931100	-0.57189500	2.55132200
H	5.39602200	0.71340800	3.18978500
C	6.00424700	-0.91237500	-1.76622100
H	6.93001500	-0.87873100	-1.18506000
H	6.29713600	-0.92595200	-2.81722800
C	4.53385700	0.29098900	-0.12028800
C	5.51345900	0.47243200	1.04315300
H	6.20177000	-0.37766800	1.02493300
C	6.30944800	1.77422900	0.84739000
H	7.04496200	1.86066700	1.64930700
H	5.62969200	2.62736300	0.94312700
C	6.99618500	1.83126800	-0.52318100
H	7.49085900	2.79613700	-0.64640300
H	7.78134000	1.07175900	-0.57279600
C	5.98248600	1.63725100	-1.66016700
H	5.29300100	2.47977100	-1.66789700
H	6.48966600	1.62583800	-2.62717700
C	5.16553200	0.34461400	-1.50909300
H	4.32829100	0.35733400	-2.21405000
C	-1.61525700	-0.81936800	0.06822800
C	-2.58826800	-1.42963400	-0.94756900

C	-2.04472100	0.52385600	0.21129900
C	-3.19076600	0.74575400	-0.60985500
O	-2.63017300	-2.59140200	-1.34875600
N	-3.49807900	-0.42552700	-1.27618400
C	-1.52307200	1.57378600	0.99478100
C	-3.81633700	1.98896000	-0.65513700
C	-2.15177800	2.80209100	0.96162100
C	-3.29199800	2.99570200	0.14720000
H	-3.76465600	3.96863200	0.14120200
H	-4.68795700	2.15821800	-1.26879600
H	-1.77632700	3.63141700	1.54333200
H	-0.63922200	1.39894400	1.59703400
H	-4.27795200	-0.57707600	-1.89974100
C	-4.08978600	-1.69866900	1.44586900
C	-4.82395000	-0.45445300	1.64492800
C	-5.99555600	-0.18217900	0.90129600
C	-4.36339100	0.53500200	2.53442700
C	-6.64686600	1.03352800	1.02966200
H	-6.38956700	-0.92598500	0.22419800
C	-5.02297500	1.74796400	2.65727900
H	-3.49710000	0.34680100	3.15186800
C	-6.16736800	2.02565400	1.89938300
H	-4.65025500	2.49424200	3.34698400
H	-7.53941500	1.22695300	0.44876500
C	-6.91103300	3.32389900	2.06702000
H	-7.31271300	3.65154300	1.10443100
H	-6.22630100	4.10204800	2.41378300
C	-2.79191700	-1.87038900	1.84226700
H	-2.27739400	-1.15884500	2.46881200
H	-2.31353900	-2.83326300	1.72581100
C	-7.31820800	-2.76943500	-3.79353300
C	-6.07366700	-2.65188000	-3.20898300
C	-5.00481400	-3.48523100	-3.46913500
C	-5.20891500	-4.51190200	-4.39315500
C	-6.44903300	-4.67054100	-5.01204400
C	-7.50020300	-3.80314800	-4.71326300
H	-8.10893500	-2.08131900	-3.53828900
H	-4.05782600	-3.33534000	-2.96958300
H	-4.39503700	-5.18162400	-4.62667400
H	-6.59614500	-5.46690500	-5.72619700
H	-8.46038800	-3.92745000	-5.19114500
F	-5.88142900	-1.60405300	-2.27319200
C	-4.77693900	-2.82601400	0.71511600
H	-4.96714900	-2.58886600	-0.33122900
H	-4.20264200	-3.74474800	0.78042300
F	-6.05437200	-3.06192500	1.32479500
C	-8.07154500	3.19193200	3.07317500
C	-8.82845200	4.50835400	3.26979400

H	-7.67570100	2.84636100	4.03265700
H	-8.76199400	2.41788200	2.72530900
C	-9.98524500	4.36772200	4.26184600
H	-8.13133900	5.27479400	3.62052800
H	-9.20972400	4.85240100	2.30408900
H	-10.51067600	5.31244100	4.39549700
H	-10.70699600	3.62814000	3.91226800
H	-9.62150500	4.04387700	5.23808200

(22) IM_{32}-PhF

Zero-point correction =	1.193097 (Hartree/Particle)
Thermal correction to Energy =	1.268669
Thermal correction to Enthalpy =	1.269613
Thermal correction to Gibbs Free Energy =	1.069027
Sum of electronic and zero-point Energies =	-4636.548441
Sum of electronic and thermal Energies =	-4636.472870
Sum of electronic and thermal Enthalpies =	-4636.471925
Sum of electronic and thermal Free Energies =	-4636.672511

Au	1.82342200	-0.94101400	-0.85795200
Au	-1.36192400	-0.66847100	-2.12826400
P	2.70668600	-1.81967600	1.05673400
P	-3.24765700	-1.78444200	-1.51697400
Cl	0.83996500	0.19195200	-2.84595500
O	-2.00183000	-1.44297100	1.01237200
O	0.04766400	-1.09347600	1.84802800
C	2.12020900	-3.47192800	1.53035200
C	2.42711400	-3.94330900	2.81137500
H	2.96946600	-3.31772300	3.50746800
C	2.03094200	-5.21956500	3.18389000
H	2.27078500	-5.59179500	4.17538200
C	1.32571000	-6.02502900	2.28772300
H	1.02356500	-7.02410600	2.58145800
C	1.01741800	-5.54833200	1.01741900
H	0.46368200	-6.16565300	0.32291800
C	1.40598400	-4.26772200	0.63972200
H	1.14932300	-3.88636900	-0.34642000
C	4.52128700	-1.91046600	1.02509000
C	5.21859400	-3.09913400	1.22832200
H	4.68212300	-4.02924800	1.39047500
C	6.61088000	-3.09804000	1.22497100
H	7.14401200	-4.02477900	1.38065400
C	7.30465500	-1.91020100	1.03984000
H	8.38880500	-1.90522200	1.05552700
C	6.60698300	-0.71772700	0.82850600
H	7.14216000	0.21440800	0.68988100
C	5.22090000	-0.71998900	0.79284100
H	4.69285800	0.20797100	0.61211900
C	-4.06100200	-2.58788800	-2.93491900

C	-3.26710600	-3.05871000	-3.97914300
H	-2.19348500	-2.89643700	-3.97305900
C	-3.85133100	-3.74110200	-5.04413900
H	-3.23103900	-4.10653700	-5.85255900
C	-5.22912900	-3.93410800	-5.06543000
H	-5.68424600	-4.46029800	-5.90277600
C	-6.02207000	-3.45045900	-4.03380800
H	-7.09591500	-3.59809900	-4.05594500
C	-5.43976200	-2.77987500	-2.96132700
H	-6.06514400	-2.40209300	-2.16400800
C	-4.53855900	-0.88726100	-0.60328400
C	-5.30919500	-1.57240500	0.33696000
H	-5.12455300	-2.62422100	0.53718500
C	-6.32265700	-0.90836800	1.01433400
H	-6.92386000	-1.43941900	1.74068700
C	-6.56926100	0.43760900	0.75749800
H	-7.35710500	0.95143500	1.29201700
C	-5.79156700	1.12622900	-0.17313800
H	-5.97382900	2.17654200	-0.36082900
C	-4.77290600	0.46715600	-0.85519800
H	-4.16086000	1.00187400	-1.57187700
C	2.29450800	-0.71026200	2.43374400
C	0.93658000	-0.38939300	2.59987800
C	0.54247500	0.63258400	3.45807800
C	1.52196200	1.23226500	4.25525900
H	1.21830300	2.02508900	4.93577700
C	2.85413900	0.85242000	4.17659400
H	3.59311500	1.31532900	4.82268200
C	3.24573500	-0.09582000	3.23883000
H	4.29397100	-0.34990400	3.13398200
C	-2.77016500	-3.14015900	-0.40888500
C	-2.17445200	-2.78439000	0.81191400
C	-1.87023500	-3.74383000	1.77399900
C	-2.15400000	-5.07628400	1.47557400
H	-1.93646700	-5.83315000	2.22834000
C	-2.71120300	-5.45672000	0.25823300
H	-2.92104100	-6.49452800	0.05516600
C	-3.02829300	-4.48107100	-0.68297800
H	-3.48667600	-4.76322400	-1.62544900
C	-1.29649400	-3.30481800	3.09123400
H	-0.20585300	-3.38787600	3.05514200
H	-1.64884000	-3.96088200	3.88700400
C	-0.88401000	1.11036200	3.46828100
H	-1.32114700	0.92964900	4.45585800
H	-0.89593100	2.19403100	3.31300900
C	-1.34542100	-0.98562700	2.17496700
C	-1.70637200	-1.85821100	3.37649400
H	-1.14069900	-1.48887700	4.23550600

C	-3.21222900	-1.72948600	3.66439100
H	-3.45347700	-2.31601700	4.55736700
H	-3.77350800	-2.17428000	2.83804500
C	-3.66749800	-0.27897200	3.84208300
H	-4.75673500	-0.24548500	3.94045500
H	-3.26310400	0.11504800	4.78345700
C	-3.23587400	0.59891800	2.66225200
H	-3.80198600	0.32040600	1.77023600
H	-3.44846600	1.65557600	2.85275200
C	-1.73856000	0.47150500	2.36363600
H	-1.52658400	0.97859800	1.41794000
C	0.22998000	3.81006900	0.05701800
C	-1.13415100	4.06475900	0.54137600
C	0.60694500	4.90287900	-0.73529100
C	-0.49343000	5.81478700	-0.75292900
O	-1.82404200	3.35915700	1.26114800
N	-1.50906400	5.29119400	0.01316700
C	1.78224700	5.23201100	-1.45028900
C	-0.44369200	7.00730300	-1.45959200
C	1.82894000	6.41696800	-2.15164300
C	0.72626100	7.29887600	-2.15290900
H	0.79021800	8.22130000	-2.70982700
H	-1.28345700	7.69299800	-1.46543900
H	2.71850600	6.68565500	-2.70376300
H	2.62949900	4.55538200	-1.45733100
H	-2.43806200	5.67435000	0.11994600
C	2.36881400	2.84789600	0.93740200
C	3.55263300	2.58787300	0.18554100
C	4.84187900	2.90848900	0.69416600
C	3.51572100	2.06746100	-1.12922500
C	5.97903400	2.73752900	-0.07642300
H	4.95179500	3.31995500	1.69081100
C	4.66547200	1.88586300	-1.88004600
H	2.56468000	1.86459700	-1.60303600
C	5.92610000	2.23389400	-1.38110000
H	4.57520500	1.50660500	-2.89146700
H	6.94042700	3.03504700	0.33517200
C	7.16421000	2.12773000	-2.23340200
H	6.87452500	1.89987100	-3.26095200
H	7.66355200	3.10492800	-2.26353200
C	0.97577300	2.57030900	0.43690800
H	0.99235100	1.87105500	-0.40469900
H	0.40574300	2.08510100	1.23140300
C	-6.73412000	4.97511700	0.31112300
C	-5.39979200	4.84633700	0.65166900
C	-4.96189200	4.04320000	1.68940800
C	-5.91002200	3.34982200	2.43407200
C	-7.24783900	3.48810300	2.11436300

C	-7.68277600	4.27235100	1.05554400
H	-7.02477300	5.60683300	-0.51764200
H	-3.89505900	3.94730300	1.88197600
H	-5.62843800	2.70226700	3.26110400
H	-8.73851900	4.33470200	0.83223600
F	-4.48437900	5.54178500	-0.07471800
C	2.44972900	3.68047700	2.18169000
H	3.16980000	3.28397200	2.89641700
H	2.72219400	4.71830700	1.94346300
F	1.21753000	3.72348500	2.82253500
C	8.16283500	1.07336600	-1.74870300
C	9.39968800	0.97332200	-2.64027800
H	7.66728200	0.09811600	-1.69431000
H	8.48454600	1.31870100	-0.72545400
C	10.39982600	-0.06203900	-2.12813200
H	9.09360900	0.72151900	-3.66015500
H	9.88257800	1.95943200	-2.70106900
H	11.27733800	-0.11899800	-2.76586800
H	10.73422900	0.18756100	-1.11754300
H	9.94075900	-1.05706500	-2.08782000
H	-7.97518100	2.93840500	2.68866900

(23) IM$_{42}$-PhF

Zero-point correction =	1.196117 (Hartree/Particle)
Thermal correction to Energy =	1.271065
Thermal correction to Enthalpy =	1.272009
Thermal correction to Gibbs Free Energy =	1.074075
Sum of electronic and zero-point Energies =	-4636.603536
Sum of electronic and thermal Energies =	-4636.528589
Sum of electronic and thermal Enthalpies =	-4636.527644
Sum of electronic and thermal Free Energies =	-4636.725579

Au	-0.05065100	0.64352200	-1.12600100
Au	2.08000900	-1.93769200	-0.91921600
P	0.20786100	2.89011000	-0.80524200
P	4.34045100	-2.01450700	-0.65171700
Cl	-0.30587600	-1.81311600	-1.48717900
O	3.82233200	0.32438000	0.89021900
O	2.16624400	1.82828500	1.03525000
C	1.70724400	3.65601700	-1.48218800
C	2.04443500	4.95728300	-1.09556100
H	1.43477000	5.48425500	-0.36733100
C	3.16289800	5.57232500	-1.64294500
H	3.42263900	6.58233800	-1.34751100
C	3.94760300	4.88987300	-2.57080400
H	4.81699100	5.37351500	-3.00210000
C	3.61700500	3.59334300	-2.94781200
H	4.23320200	3.05760500	-3.66027800
C	2.49790700	2.97216500	-2.40214600

H	2.24234300	1.95615200	-2.68684700
C	-1.20379900	3.83784500	-1.45489800
C	-1.05400300	4.95791300	-2.27123200
H	-0.06997300	5.30647900	-2.56144300
C	-2.18416200	5.62628700	-2.73522500
H	-2.06688600	6.49267500	-3.37572100
C	-3.45393600	5.18598800	-2.38391200
H	-4.32903800	5.71369300	-2.74535700
C	-3.60664500	4.06190700	-1.57471500
H	-4.59644600	3.71174500	-1.30081000
C	-2.48413200	3.38305300	-1.11909300
H	-2.59162800	2.49348700	-0.50506300
C	5.12412300	-3.12889500	-1.85544600
C	4.53021100	-3.27901100	-3.11166600
H	3.58733400	-2.78710000	-3.33165800
C	5.14229900	-4.06502900	-4.07951500
H	4.67754300	-4.18163700	-5.05150000
C	6.34100700	-4.71126400	-3.79450800
H	6.81300100	-5.33146800	-4.54762000
C	6.92843500	-4.57218300	-2.54154700
H	7.85625800	-5.08449800	-2.31612800
C	6.32556700	-3.78008100	-1.57099800
H	6.78537200	-3.68266200	-0.59372400
C	4.94016600	-2.49421500	0.99490300
C	6.18378500	-2.04706600	1.44819200
H	6.78263200	-1.38277200	0.83200800
C	6.65120900	-2.44937600	2.69429600
H	7.61755000	-2.10446200	3.04382900
C	5.87846000	-3.29028400	3.49066400
H	6.24465200	-3.60363100	4.46144500
C	4.63604100	-3.72822000	3.04322900
H	4.03414200	-4.38239700	3.66344800
C	4.16460700	-3.33118200	1.79636700
H	3.19514900	-3.67232900	1.44593300
C	0.24437800	3.19321500	0.98765300
C	1.21432100	2.50672300	1.73932100
C	1.16284900	2.49542700	3.12877000
C	0.20215600	3.28495000	3.76061200
H	0.16838400	3.28612300	4.84621900
C	-0.71685400	4.02780600	3.03703000
H	-1.45229900	4.63836500	3.54646600
C	-0.71534500	3.95595400	1.64611100
H	-1.46655100	4.48873100	1.07462600
C	5.05943500	-0.37906700	-0.96910700
C	4.66842500	0.66996900	-0.12697200
C	5.17363800	1.95623700	-0.29797100
C	6.08370800	2.16939500	-1.33100800
H	6.49290600	3.16700500	-1.45954700

C	6.47165800	1.14593000	-2.18555000
H	7.18286000	1.33621800	-2.98015400
C	5.95793300	-0.13373800	-2.00516700
H	6.26202700	-0.94261600	-2.66012200
C	4.73356800	3.04081000	0.64684500
H	3.88358100	3.57497900	0.21215500
H	5.53747900	3.76830500	0.78625400
C	2.07269300	1.58887600	3.91304700
H	2.74447900	2.19155400	4.53116400
H	1.46335700	0.99806800	4.60622800
C	3.30205900	1.32180300	1.74400700
C	4.33610000	2.42486900	1.98839100
H	3.86003900	3.19065400	2.61009500
C	5.54456900	1.83601000	2.73555300
H	6.24885100	2.64376500	2.95343600
H	6.06989900	1.13798800	2.07339400
C	5.15636000	1.10599200	4.02227300
H	6.04072400	0.62911700	4.45261700
H	4.81343900	1.83049000	4.76709900
C	4.08140300	0.04618500	3.76305300
H	4.50564700	-0.76236500	3.16383500
H	3.74590600	-0.39918400	4.70511700
C	2.86816600	0.62242800	3.02701100
H	2.21353500	-0.19248600	2.70435300
C	-4.47436200	-0.72011600	-0.53252500
C	-3.17876500	-0.51113900	0.20254400
C	-4.64243600	-2.19480900	-0.59596100
C	-3.56803400	-2.76395500	0.09567800
O	-2.57477500	0.53953800	0.38420100
N	-2.75148900	-1.73847300	0.60198300
C	-5.57983100	-3.01625100	-1.20071800
C	-3.39820500	-4.13111300	0.20674100
C	-5.42483300	-4.39951500	-1.09795400
C	-4.35015700	-4.94674600	-0.40430400
H	-4.24589800	-6.02360600	-0.33934500
H	-2.55403300	-4.55241600	0.74016900
H	-6.15040900	-5.05387400	-1.56575600
H	-6.42095600	-2.59758600	-1.74219100
H	-1.80666100	-1.86903500	0.93686100
C	-5.64352700	0.27320700	-0.43614200
C	-7.02846100	-0.29850200	-0.44423400
C	-7.45415600	-1.11430700	0.60430000
C	-7.91725800	-0.00552300	-1.47363900
C	-8.73653100	-1.64173600	0.60884100
H	-6.76147400	-1.36338800	1.40346100
C	-9.20282400	-0.53778700	-1.46576300
H	-7.60012700	0.64360400	-2.28348900
C	-9.62955100	-1.36790000	-0.43028800

H	-9.88513600	-0.30583700	-2.27805000
H	-9.04919100	-2.28965100	1.42240900
C	-11.03296400	-1.91486000	-0.39394900
H	-11.42367100	-2.00698400	-1.41212700
H	-11.02265500	-2.92387800	0.03131600
C	-4.81673900	0.21870300	-1.67075100
H	-5.23411200	-0.25157600	-2.55308400
H	-4.11034700	1.02316700	-1.84957600
C	0.24954300	-1.61473400	3.99054300
C	-0.30919800	-0.82079100	3.00378100
C	-1.16915300	0.22595600	3.26839300
C	-1.48431700	0.48214700	4.60102000
C	-0.94159500	-0.29298400	5.62081200
C	-0.07553400	-1.34094600	5.31476000
H	0.91880800	-2.42268800	3.71772200
H	-1.57368000	0.80701800	2.44639000
H	-2.15831900	1.29773900	4.83668100
H	-1.19643900	-0.08717600	6.65367000
H	0.34449500	-1.95031800	6.10627300
F	0.01464300	-1.08464500	1.70885000
C	-5.49656700	1.48718100	0.44621800
H	-5.94155500	1.31356900	1.42831100
H	-4.45864600	1.79860800	0.55428600
F	-6.19716500	2.53363400	-0.14569400
C	-11.97312000	-1.02946100	0.43309100
C	-13.38743900	-1.59587400	0.52404300
H	-12.00102900	-0.02553900	-0.00624500
H	-11.55878100	-0.90913900	1.44088300
C	-14.31561300	-0.71132800	1.35107400
H	-13.79582300	-1.71926600	-0.48494700
H	-13.34585400	-2.59931600	0.96199200
H	-15.31830700	-1.13651400	1.42216700
H	-13.93412300	-0.58717600	2.36785000
H	-14.40682100	0.28397300	0.90886900

(24) IM$_{2i}$-PhF

Zero-point correction = 1.191491 (Hartree/Particle)
Thermal correction to Energy = 1.267807
Thermal correction to Enthalpy = 1.268751
Thermal correction to Gibbs Free Energy = 1.067446
Sum of electronic and zero-point Energies = -4636.519720
Sum of electronic and thermal Energies = -4636.443404
Sum of electronic and thermal Enthalpies = -4636.442459
Sum of electronic and thermal Free Energies = -4636.643765

Au	-0.51706600	1.89080500	0.58948500
Au	-0.91916400	-0.73962600	-1.96788300
P	-2.82362800	2.55700400	0.65024100
P	-0.47974300	-2.80507000	-1.05860000

Cl	-1.28179300	1.53931700	-2.61416100
O	-2.95022900	-2.12351600	-0.06102100
O	-3.90404700	-0.08114500	0.12929000
C	-3.60192200	2.16839300	2.26051500
C	-4.99054000	2.12387200	2.40811700
H	-5.63419900	2.32260900	1.55696600
C	-5.55101700	1.82202300	3.64457900
H	-6.62920000	1.79015400	3.75295500
C	-4.73204100	1.56798000	4.74121500
H	-5.17240500	1.33594400	5.70425000
C	-3.34912500	1.61946400	4.60091200
H	-2.70776000	1.42821700	5.45387700
C	-2.78501700	1.91541600	3.36411300
H	-1.70494200	1.94685400	3.25495000
C	-2.72979300	4.37980700	0.58060100
C	-3.45347100	5.20520200	1.44019900
H	-4.08499700	4.77547500	2.21029600
C	-3.35996600	6.58762900	1.31241700
H	-3.91966300	7.22800000	1.98436600
C	-2.55605300	7.14553700	0.32486300
H	-2.48847200	8.22305600	0.22683000
C	-1.83505400	6.32268700	-0.53583100
H	-1.20504800	6.75458700	-1.30451500
C	-1.91290800	4.94198800	-0.40616600
H	-1.34866800	4.30040400	-1.07875600
C	1.23004400	-3.40006800	-1.22518800
C	2.10322500	-2.72353600	-2.07665300
H	1.75616200	-1.86077300	-2.63519700
C	3.42606300	-3.13871100	-2.20022100
H	4.10334300	-2.57926300	-2.83598100
C	3.87323500	-4.24404700	-1.48853100
H	4.90549800	-4.56415500	-1.57508800
C	2.99378400	-4.95127300	-0.66927500
H	3.33584500	-5.83101500	-0.13562900
C	1.67627900	-4.53527500	-0.53750900
H	0.99398000	-5.09878600	0.09166000
C	-1.54747000	-4.17153100	-1.62146900
C	-1.91453600	-5.20631600	-0.75959100
H	-1.59501700	-5.19515900	0.27841200
C	-2.71497600	-6.24324300	-1.22590000
H	-3.00125800	-7.04603500	-0.55613100
C	-3.15141600	-6.24841400	-2.54769000
H	-3.77711600	-7.05704900	-2.90733600
C	-2.79070200	-5.21413400	-3.40500400
H	-3.13453800	-5.21298500	-4.43276800
C	-1.99163300	-4.17365700	-2.94336900
H	-1.71965000	-3.35948900	-3.60843300
C	-4.11906800	2.15094200	-0.56290700

C	-4.56010900	0.82644700	-0.65664800
C	-5.64344400	0.48474900	-1.46284300
C	-6.23879800	1.48291100	-2.22995800
H	-7.07087800	1.21654200	-2.87429800
C	-5.79013000	2.79406900	-2.18141800
H	-6.25947900	3.55680300	-2.79013400
C	-4.73911600	3.12929800	-1.33633100
H	-4.40101400	4.15681400	-1.27935900
C	-0.83082000	-2.64500100	0.72881000
C	-2.13737200	-2.22410200	1.01998700
C	-2.57521700	-1.97915300	2.31748300
C	-1.66006600	-2.18716600	3.34916400
H	-1.98316700	-2.02210400	4.37271200
C	-0.36297100	-2.61780400	3.09196000
H	0.32316800	-2.79335900	3.91256600
C	0.05896000	-2.83875000	1.78195600
H	1.07351600	-3.16905300	1.58749900
C	-3.99622300	-1.52200200	2.53698700
H	-4.00275700	-0.43876500	2.67731100
H	-4.39313100	-1.96657600	3.45384700
C	-6.11165700	-0.94415700	-1.48300200
H	-6.89549800	-1.09670900	-0.73251200
H	-6.55901400	-1.17798500	-2.45206400
C	-4.20065500	-1.47323700	0.04926100
C	-4.89361400	-1.89390100	1.34947100
H	-5.82217400	-1.31632800	1.41954000
C	-5.22781300	-3.38933400	1.30823400
H	-5.77176700	-3.65587300	2.21857200
H	-4.29663100	-3.96989800	1.31552300
C	-6.04025400	-3.75464000	0.06630800
H	-6.23754000	-4.82925000	0.05294700
H	-7.01840300	-3.26280700	0.10886300
C	-5.28847400	-3.35690700	-1.20439100
H	-4.36638500	-3.94088000	-1.26696100
H	-5.87563900	-3.59741400	-2.09526400
C	-4.92534600	-1.86850900	-1.23639800
H	-4.19823400	-1.69810400	-2.04079600
C	1.46846200	1.80526300	1.02357800
C	2.53640800	2.73407300	0.42167100
C	2.14012200	1.11953100	2.02284500
C	3.52884800	1.49959700	2.03879800
O	2.40717600	3.57845300	-0.41427600
N	3.74690300	2.43652200	1.08284600
C	1.65933000	0.17334800	2.96969800
C	4.42173600	0.94094700	2.95352200
C	2.53656100	-0.35780000	3.87300100
C	3.90718800	0.02325300	3.84733500
H	4.58068600	-0.42326300	4.57183600

H	5.47081500	1.20888500	2.95578600
H	2.20289400	-1.06914400	4.61835100
H	0.60837400	-0.09813300	2.95379700
H	4.63231800	2.87826800	0.86631400
C	3.43966600	0.30325800	-1.07273400
C	4.14417600	-0.56772000	-0.12090700
C	5.54254200	-0.51135900	0.01054500
C	3.44978600	-1.46981800	0.70032000
C	6.20582800	-1.32872100	0.91252900
H	6.12147500	0.15416900	-0.61860800
C	4.11843900	-2.28526400	1.59375000
H	2.37229300	-1.55131500	0.62930500
C	5.50905500	-2.23458500	1.71673500
H	3.55554400	-2.98337100	2.20883100
C	4.26110400	1.17001100	-1.99021800
H	3.62125900	1.73680800	-2.66686500
H	4.89497200	1.86276900	-1.43019700
F	5.09975900	0.36973200	-2.75390500
C	2.09831700	0.37068600	-1.14838300
H	1.45521700	-0.25629100	-0.54470900
H	1.59240200	1.02497100	-1.85329400
H	7.28802200	-1.27544400	0.98567700
C	6.23532800	-3.20653000	2.60511500
H	5.63678800	-3.42140600	3.49696100
H	7.17961300	-2.77370300	2.94965500
C	6.51877400	-4.51946400	1.86012000
C	7.23249900	-5.55444500	2.72430700
H	7.11964900	-4.29957900	0.96984800
H	5.57003500	-4.93031900	1.49291800
C	7.51403200	-6.84609900	1.96237400
H	8.17252200	-5.13206000	3.09521400
H	6.62385200	-5.77169600	3.60901200
H	8.02025000	-7.58029500	2.59088500
H	6.58690900	-7.30023800	1.60257900
H	8.14978900	-6.65799900	1.09357500
F	6.32989400	3.20424800	-0.02727900
C	6.56798100	4.09231400	-1.04232800
C	7.87733300	4.30889600	-1.42026200
C	5.48666700	4.71022000	-1.63923800
C	8.11272500	5.20183900	-2.46054400
H	8.68078200	3.79206800	-0.90995700
C	5.74472100	5.59909800	-2.67898900
H	4.47560000	4.50754300	-1.30106700
C	7.05067300	5.84433700	-3.08942700
H	9.13064400	5.39293300	-2.77854600
H	4.91683100	6.09932200	-3.16712600
H	7.24181900	6.53804900	-3.89900500

(25) $TS_{2\text{-}3i}$-PhF

Zero-point correction = 1.180210 (Hartree/Particle)
Thermal correction to Energy = 1.255205
Thermal correction to Enthalpy = 1.256149
Thermal correction to Gibbs Free Energy = 1.061062
Sum of electronic and zero-point Energies = -4636.469464
Sum of electronic and thermal Energies = -4636.394469
Sum of electronic and thermal Enthalpies = -4636.393525
Sum of electronic and thermal Free Energies = -4636.588612

Au	0.26818300	-1.86675300	0.51254200
Au	1.16992300	1.40975600	-1.91528900
P	2.39177700	-3.03654900	0.11546300
P	1.42991500	3.38010100	-0.60446500
Cl	0.67803000	-0.68962500	-2.98764700
O	3.55759800	1.68940300	0.44992400
O	4.16611800	-0.58710400	0.41161000
C	3.21138000	-3.53027200	1.73821800
C	4.56401000	-3.90443100	1.78798800
H	5.16933000	-3.88563700	0.89028300
C	5.13586700	-4.30474500	3.00178400
H	6.18004400	-4.59430400	3.03237400
C	4.36238700	-4.33663700	4.16943400
H	4.80781000	-4.65101300	5.10650100
C	3.01265700	-3.96644900	4.12014100
H	2.40855200	-3.99194300	5.02152900
C	2.43812200	-3.56249900	2.90931300
H	1.39269500	-3.27544600	2.87604400
C	1.80858000	-4.65672800	-0.65278600
C	2.28351300	-5.90218100	-0.21418800
H	3.01131300	-5.96128800	0.58550400
C	1.81038600	-7.07769000	-0.81252100
H	2.17612100	-8.03785800	-0.46833400
C	0.87253800	-7.01121900	-1.84729700
H	0.50669200	-7.92302700	-2.30896800
C	0.39939900	-5.76783800	-2.28707900
H	-0.32784200	-5.71194000	-3.09005900
C	0.86067200	-4.58860900	-1.68969000
H	0.48794500	-3.62966200	-2.03177200
C	-0.09184400	4.47753400	-0.67139300
C	-1.22769900	4.01742200	-1.35375900
H	-1.22480100	3.05153000	-1.84624400
C	-2.37685000	4.81461000	-1.42375500
H	-3.24421800	4.43626200	-1.95017900
C	-2.38956500	6.07769200	-0.82308100
H	-3.27636100	6.70057600	-0.88380800
C	-1.25117200	6.54646200	-0.15316500
H	-1.25344600	7.53178300	0.30161600
C	-0.10237800	5.75131000	-0.07629500
H	0.78001900	6.13059400	0.42790500

C	2.87062100	4.51195500	-0.99831500
C	3.48810900	5.27574400	0.00252500
H	3.17912900	5.17740700	1.03824700
C	4.51755700	6.16429700	-0.33610100
H	4.99180800	6.75879700	0.43799400
C	4.93007600	6.28709300	-1.66856900
H	5.72476600	6.97829400	-1.92876200
C	4.31522800	5.51825800	-2.66480600
H	4.63656100	5.60886000	-3.69753200
C	3.28688600	4.62993100	-2.33256600
H	2.81549600	4.03168500	-3.10526500
C	3.82968900	-2.51813700	-0.97343300
C	4.59366800	-1.38051000	-0.66042700
C	5.79138700	-1.10320500	-1.33774400
C	6.16670900	-1.92487400	-2.40761800
H	7.08103900	-1.69992100	-2.94838400
C	5.38672800	-3.02244000	-2.77562500
H	5.67789600	-3.64718700	-3.61126400
C	4.23287900	-3.32660800	-2.04747500
H	3.64620300	-4.19685500	-2.31116300
C	1.62706700	2.84968100	1.18537600
C	2.68726000	1.97818000	1.49732200
C	2.87092400	1.46291100	2.79016800
C	1.95793900	1.84840800	3.78225700
H	2.09763600	1.47697300	4.79365600
C	0.89254600	2.70951100	3.49537200
H	0.20634900	3.00681300	4.27939300
C	0.72532200	3.20924400	2.19669600
H	-0.09514600	3.88038500	1.97265800
C	4.03162600	0.52756700	3.04398900
H	3.70486300	-0.51172600	2.91802700
H	4.38193100	0.63352600	4.07807600
C	6.61133700	0.07319000	-0.87517700
H	7.25852300	-0.21764300	-0.03333900
H	7.27511300	0.41370400	-1.67523200
C	4.68621100	0.77936300	0.62127300
C	5.20460000	0.80645700	2.07482300
H	5.92009800	-0.02056700	2.15748500
C	5.94569000	2.12293400	2.39566400
H	6.37821200	2.04238800	3.40115700
H	5.22981500	2.95580300	2.42769400
C	7.03771900	2.43139200	1.35731600
H	7.53427500	3.37733500	1.60454500
H	7.81628100	1.65491500	1.39883900
C	6.43078000	2.51292800	-0.05269700
H	5.73516000	3.35890000	-0.09330900
H	7.21155800	2.71432800	-0.79871100
C	5.67797200	1.22832200	-0.46925400

H	5.05736400	1.46429300	-1.34516700
C	-1.65798100	-1.49876200	1.04412900
C	-2.81598900	-2.05185600	0.19119600
C	-2.22657100	-1.35048900	2.34674100
C	-3.60459000	-1.75863300	2.31894500
O	-2.78646600	-2.39962800	-0.99899700
N	-3.92900300	-2.15314100	1.02754400
C	-1.64974900	-0.93242200	3.56699900
C	-4.38726200	-1.76485300	3.47117500
C	-2.43182500	-0.92865700	4.71700700
C	-3.78456600	-1.34766700	4.66203500
H	-4.37105100	-1.34828800	5.57534400
H	-5.42096600	-2.08870000	3.45161500
H	-2.01157300	-0.61637500	5.66487000
H	-0.61189900	-0.61622000	3.59099000
H	-4.82825000	-2.50710600	0.71172800
F	-6.42978000	-3.17914300	0.04284500
C	-6.75488500	-3.72975100	-1.22480600
C	-5.77233000	-3.76956200	-2.20252000
C	-8.05029100	-4.19432500	-1.40505600
C	-6.12191300	-4.31535800	-3.44554100
H	-4.77178000	-3.39540000	-2.00445100
C	-8.37936800	-4.73676600	-2.65460600
H	-8.77062100	-4.13607800	-0.59853000
C	-7.41800300	-4.79547500	-3.67212400
H	-5.37747400	-4.36168400	-4.23285700
H	-9.38282300	-5.10913600	-2.82851900
H	-7.67846100	-5.21422400	-4.63733500
C	-3.02925600	0.90082400	-0.40687500
C	-4.31686800	1.30382700	0.15947500
C	-5.45132100	1.48739300	-0.67679200
C	-4.48979300	1.53307200	1.54753800
C	-6.68044500	1.85843900	-0.14489500
H	-5.35131200	1.37650200	-1.74831900
C	-5.72672700	1.89784600	2.07108700
H	-3.65075100	1.42423700	2.22610300
C	-6.84793400	2.06624800	1.23864800
H	-5.82663300	2.06637300	3.13882000
C	-2.95134200	0.55158500	-1.87596500
H	-1.95866800	0.21250500	-2.17043000
H	-3.69439600	-0.19229900	-2.17157600
F	-3.24130100	1.76114800	-2.64755900
C	-1.85786600	0.84371600	0.31084000
H	-1.77992100	1.18183700	1.33418300
H	-0.91964300	0.69727700	-0.21018300
H	-7.52767400	1.99966400	-0.81086300
C	-8.19208600	2.45490100	1.80400000
H	-8.11964600	2.74741800	2.85530900

H	-8.90209700	1.61896400	1.73995900
C	-8.81224100	3.62689700	1.02078000
C	-10.11536800	4.04887800	1.64950400
H	-8.97237200	3.30018000	-0.03519000
H	-8.08420000	4.47387800	1.01770600
C	-10.74997900	5.19603300	0.90603900
H	-10.82214600	3.17717400	1.66635900
H	-9.93654700	4.34765500	2.71647600
H	-11.71230700	5.48971100	1.39023800
H	-10.07245800	6.08396900	0.90008700
H	-10.96052500	4.91021400	-0.15296100

(26) IM_{3i}-PhF

Zero-point correction = 1.193427 (Hartree/Particle)
Thermal correction to Energy = 1.268851
Thermal correction to Enthalpy = 1.269795
Thermal correction to Gibbs Free Energy = 1.072891
Sum of electronic and zero-point Energies = -4636.534613
Sum of electronic and thermal Energies = -4636.459189
Sum of electronic and thermal Enthalpies = -4636.458245
Sum of electronic and thermal Free Energies = -4636.655149

Au	1.63042700	-0.40713300	-0.03699500
Au	-0.94318600	0.75614500	-2.07175800
P	3.31151200	1.07575100	0.58911900
P	-2.91541600	1.21476800	-0.99769200
Cl	1.21698100	-0.01204700	-2.83712800
O	-1.00597800	2.93785000	0.13006800
O	1.24786700	3.05343400	0.30298900
C	3.19034600	1.64593100	2.31661900
C	3.60922500	2.92215900	2.70132700
H	4.02451500	3.60852900	1.97178300
C	3.47781200	3.31760200	4.03000400
H	3.80498500	4.30517200	4.32975800
C	2.93734000	2.44550200	4.97330400
H	2.83876000	2.75686600	6.00194400
C	2.52692200	1.17147800	4.58509200
H	2.11068900	0.48688100	5.31623500
C	2.65502700	0.77227100	3.25844900
H	2.32466400	-0.21819300	2.95822000
C	4.92290100	0.24510200	0.43256700
C	5.97661000	0.54383300	1.29833300
H	5.83996000	1.25385400	2.10986500
C	7.20640300	-0.09108200	1.13521300
H	8.02431700	0.13298200	1.80868300
C	7.38178200	-1.00965800	0.10432500
H	8.34024400	-1.50197400	-0.02234900
C	6.33332800	-1.30234800	-0.76137100
H	6.47181000	-2.01897100	-1.56566100

C	5.10411700	-0.67907600	-0.59850500
H	4.28244700	-0.91621100	-1.27368900
C	-4.19021900	-0.05680900	-1.19427500
C	-3.91075600	-1.20342900	-1.93516700
H	-2.94979700	-1.32351700	-2.42540800
C	-4.86106100	-2.21373500	-2.05431500
H	-4.61865300	-3.10329900	-2.61939800
C	-6.09404400	-2.07258500	-1.43024400
H	-6.83552300	-2.85847300	-1.52210100
C	-6.39332500	-0.91938000	-0.70596400
H	-7.36612300	-0.80581200	-0.24151300
C	-5.44692700	0.09341300	-0.58949100
H	-5.69218600	0.99596300	-0.03906200
C	-3.68557200	2.83043700	-1.34487600
C	-4.36614300	3.53218800	-0.34104800
H	-4.42108800	3.13042800	0.66335500
C	-4.95653800	4.75479300	-0.63031400
H	-5.47927500	5.29584600	0.14503500
C	-4.86622600	5.28513100	-1.91666200
H	-5.32765300	6.24269700	-2.13925100
C	-4.18921800	4.59362700	-2.91116800
H	-4.11698500	5.00830700	-3.91219400
C	-3.59663600	3.36563400	-2.62754000
H	-3.05775700	2.82834000	-3.40543600
C	3.44900900	2.59990500	-0.38293800
C	2.35048700	3.46998300	-0.39041900
C	2.43156700	4.70443400	-1.02934300
C	3.60402400	5.02879000	-1.70783500
H	3.66334100	5.97929300	-2.22477300
C	4.68976800	4.16186000	-1.73534900
H	5.58951500	4.42779900	-2.27872200
C	4.61371900	2.94468800	-1.06396900
H	5.45917600	2.26736300	-1.06750700
C	-2.52417100	1.29364600	0.78697800
C	-1.51395800	2.19751200	1.15441200
C	-1.11998100	2.36316800	2.47928200
C	-1.77689900	1.60481500	3.44643600
H	-1.50253800	1.74456900	4.48661700
C	-2.78851400	0.71023900	3.10877700
H	-3.29113500	0.14354100	3.88423700
C	-3.16531200	0.55352500	1.77698500
H	-3.94540300	-0.15227800	1.51276700
C	-0.05803300	3.38574300	2.79014600
H	0.91717800	2.89589500	2.82582500
H	-0.23902700	3.82005000	3.77983100
C	1.24411000	5.62790500	-0.97805100
H	1.36328000	6.33721100	-0.14801700
H	1.19391400	6.22489100	-1.88887400

C	0.05938800	3.84539800	0.33956700
C	-0.05120900	4.49115600	1.72676000
H	0.84645000	5.10527100	1.86379100
C	-1.29864500	5.38206000	1.80863700
H	-1.30777900	5.88354900	2.77772800
H	-2.19592800	4.75204200	1.76833000
C	-1.35869100	6.40278800	0.67321700
H	-2.28574100	6.97520500	0.73834800
H	-0.54485600	7.12808700	0.78216700
C	-1.28867100	5.70566400	-0.68801700
H	-2.17630500	5.08317600	-0.81609100
H	-1.29228000	6.44061000	-1.49759200
C	-0.04268000	4.82414400	-0.83097400
H	-0.14896600	4.19352500	-1.72391700
C	0.31674900	-2.52165800	0.10776000
C	1.39711500	-3.46493100	-0.28161100
C	0.48420100	-2.28240600	1.49643700
C	1.62918100	-3.04055200	1.93865900
O	1.59874700	-3.96591400	-1.36792000
N	2.15689400	-3.70035600	0.86578400
C	-0.24900900	-1.52053500	2.44173500
C	2.01330400	-3.04729200	3.27158000
C	0.13144100	-1.55604000	3.76028500
C	1.24837100	-2.32303200	4.17504200
H	1.51748800	-2.34141800	5.22403400
H	2.87013600	-3.62857600	3.60065600
H	-0.42396800	-0.98397100	4.49353400
H	-1.07684100	-0.90196800	2.11396000
H	2.99673400	-4.26244700	0.87016400
F	4.87706200	-4.73684000	0.77431900
C	5.62894100	-4.64134300	-0.35781000
C	4.98011800	-4.52578600	-1.57497400
C	7.00427800	-4.66805600	-0.22696500
C	5.76964400	-4.43647800	-2.72129500
H	3.89590400	-4.51900000	-1.62964600
C	7.77014900	-4.57320900	-1.38365100
H	7.44603200	-4.76375000	0.75802700
C	7.15860700	-4.45685800	-2.62930100
H	5.28668200	-4.35147100	-3.69061200
H	8.85104800	-4.60630000	-1.30856300
H	7.75959900	-4.39470300	-3.52783500
C	-1.73781400	-3.59575200	-0.91769000
C	-2.87817400	-3.86389100	-0.10090000
C	-3.77396600	-4.91709100	-0.42270100
C	-3.21988600	-3.05682500	1.00588900
C	-4.92702000	-5.12315900	0.31025900
H	-3.57212200	-5.55029700	-1.27428000
C	-4.38373800	-3.26844300	1.72296800

H	-2.56432000	-2.25304600	1.31703100
C	-5.26392500	-4.30497300	1.39224500
H	-4.61582600	-2.63001100	2.57229500
C	-1.48223500	-4.42407900	-2.13726000
H	-0.54280800	-4.15628800	-2.61516400
H	-1.48201100	-5.49057900	-1.92173200
F	-2.50700700	-4.19397000	-3.07438700
C	-0.90171500	-2.34551600	-0.75029300
H	-1.50948400	-1.53164200	-0.34963700
H	-0.56615600	-2.04057500	-1.74690000
H	-5.59266800	-5.93385900	0.02949600
C	-6.55589500	-4.47068000	2.14537900
H	-6.37251800	-4.36913900	3.22064500
H	-6.95701800	-5.47614600	1.98830400
C	-7.59735400	-3.42934900	1.72027200
C	-8.90171700	-3.52373200	2.50603100
H	-7.80281800	-3.55351400	0.65029100
H	-7.17052900	-2.42695900	1.83205700
C	-9.91335900	-2.47237500	2.05906700
H	-9.33076700	-4.52432300	2.38301200
H	-8.69120200	-3.40441500	3.57436800
H	-10.84218100	-2.53742500	2.62799200
H	-9.51845600	-1.46317400	2.19755700
H	-10.16869300	-2.58860800	1.00177700

The calculated structures using B3LYP/6-31G

(27) IM_2

Zero-point correction = 1.097763 (Hartree/Particle)
Thermal correction to Energy = 1.168432
Thermal correction to Enthalpy = 1.169376
Thermal correction to Gibbs Free Energy = 0.972083
Sum of electronic and zero-point Energies = -4305.207477
Sum of electronic and thermal Energies = -4305.136808
Sum of electronic and thermal Enthalpies = -4305.135864
Sum of electronic and thermal Free Energies = -4305.333157

Au	-0.36937200	-1.09945300	-0.24659300
Au	1.41074900	1.51537600	-1.69074200
P	1.14457000	-3.03633300	-0.32899800
P	1.85598700	3.07033700	0.06100600
Cl	0.87271400	-0.05003900	-3.46244100
O	3.55743000	0.87768400	0.94877700
O	3.50432600	-1.41484300	0.52635300
C	1.35389600	-3.82949200	1.36056100
C	2.32754900	-4.81794000	1.57668700
H	2.99263900	-5.11437900	0.77223400

C	2.44606500	-5.41927800	2.83512800
H	3.19854600	-6.18409900	2.99679700
C	1.59637000	-5.03679300	3.88062700
H	1.68869800	-5.50653000	4.85430000
C	0.62930900	-4.04725600	3.66814700
H	-0.02822900	-3.74469900	4.47651400
C	0.50706700	-3.44103700	2.41140800
H	-0.23389100	-2.66203800	2.25667000
C	0.17357800	-4.27678800	-1.36331900
C	-0.13157000	-5.56435300	-0.89953700
H	0.20968600	-5.89280900	0.07558000
C	-0.88450400	-6.43373500	-1.70064600
H	-1.12100700	-7.42818800	-1.33689800
C	-1.32644200	-6.02334000	-2.96293400
H	-1.90659800	-6.69995300	-3.58155900
C	-1.01956400	-4.73718900	-3.42711500
H	-1.35682600	-4.41618400	-4.40716100
C	-0.27709700	-3.85924600	-2.63003300
H	-0.04405900	-2.86151200	-2.99267500
C	0.58518800	4.45288800	0.13946700
C	-0.65646700	4.27811800	-0.49082200
H	-0.86089600	3.36178200	-1.03483900
C	-1.61896700	5.29324600	-0.43636600
H	-2.57450300	5.15435300	-0.93107700
C	-1.34402300	6.48584300	0.24216400
H	-2.08752900	7.27510100	0.27842700
C	-0.10275900	6.66490300	0.86505500
H	0.11798400	7.59219200	1.38301800
C	0.86241700	5.65303300	0.81417400
H	1.82706600	5.80777400	1.28492000
C	3.51074800	3.94214600	-0.05841500
C	4.20465800	4.34062500	1.09397300
H	3.81332300	4.10381100	2.07824800
C	5.41359700	5.03716100	0.97178500
H	5.94882300	5.34660500	1.86354800
C	5.92916100	5.33350500	-0.29592300
H	6.86557600	5.87352200	-0.38796900
C	5.23744600	4.93042800	-1.44466200
H	5.63615900	5.15445200	-2.42832000
C	4.02908200	4.23380200	-1.32889900
H	3.49855700	3.91454700	-2.22081800
C	2.85736300	-3.05337000	-1.08775000
C	3.85988300	-2.22433400	-0.55839500
C	5.17081800	-2.25552800	-1.05692500
C	5.46021900	-3.11386700	-2.12476500
H	6.46892300	-3.13172500	-2.52634400
C	4.47431500	-3.93817800	-2.67191100
H	4.70952500	-4.59772200	-3.49936800

C	3.17738600	-3.91093600	-2.14957700
H	2.41478000	-4.55219200	-2.57315600
C	1.78503200	2.23977300	1.73682000
C	2.63714800	1.14622800	1.96534300
C	2.58662900	0.40073600	3.15102300
C	1.65636900	0.78904600	4.12624500
H	1.60868700	0.22895900	5.05555400
C	0.80059200	1.87587800	3.92265600
H	0.08595200	2.15937900	4.68742900
C	0.86190300	2.60085800	2.72623800
H	0.19413500	3.43896200	2.56489000
C	3.50678200	-0.78916500	3.31946700
H	2.97083600	-1.70458900	3.04104600
H	3.79795400	-0.89429400	4.37130000
C	6.20016900	-1.34797400	-0.42894500
H	6.69291300	-1.85218100	0.41497400
H	6.98872200	-1.11581900	-1.15306900
C	4.37648800	-0.32176000	0.99586200
C	4.77540000	-0.65930900	2.44705200
H	5.27190300	-1.63702400	2.41430000
C	5.77781800	0.37726400	3.00410700
H	6.09850200	0.04958400	4.00088900
H	5.27291800	1.34384500	3.13704100
C	6.99375200	0.55750300	2.07779200
H	7.66467100	1.32326600	2.48541100
H	7.57489800	-0.37508300	2.04536500
C	6.54566700	0.96368600	0.66140200
H	6.07682600	1.95339200	0.70436200
H	7.41213400	1.05162900	-0.00587500
C	5.54257000	-0.03296600	0.03398500
H	5.08980400	0.43939500	-0.84753900
C	-1.99154300	0.07138900	-0.10054500
C	-2.74283500	0.27355200	1.22351000
C	-2.72584300	0.81864700	-1.03832900
C	-3.84959500	1.45514700	-0.38115500
O	-2.45778300	-0.20098300	2.33431900
N	-3.82169200	1.12197400	0.96400300
C	-2.51827600	1.01857100	-2.43238300
C	-4.73868000	2.25968400	-1.08397800
C	-3.40926500	1.82260000	-3.12775700
C	-4.50152200	2.42812400	-2.45722900
H	-5.18479000	3.04886700	-3.02843200
H	-5.58757200	2.72913200	-0.60211200
H	-3.27484000	1.99438100	-4.18880300
H	-1.66573000	0.55528000	-2.92072100
H	-4.49353000	1.40426400	1.66867600
C	-4.54586600	-2.47456100	0.56036900
C	-3.73025300	-2.58303600	-0.51890400

H	-2.81170500	-3.15690300	-0.47362900
H	-3.96439700	-2.14893700	-1.48329000
C	-5.84470500	-1.76555900	0.54341300
C	-6.55139000	-1.50528300	1.73998400
C	-6.42578800	-1.31499700	-0.66531700
C	-7.75232200	-0.79650800	1.72632800
H	-6.18032000	-1.88843600	2.68109700
C	-7.62862300	-0.61249900	-0.67170700
H	-5.94990500	-1.53919400	-1.61342700
C	-8.31345500	-0.32847100	0.52479400
H	-8.05567600	-0.29373000	-1.61848300
C	-4.04350300	-3.04268500	1.86521700
H	-3.15418600	-3.65567900	1.70664100
H	-3.80932600	-2.24620800	2.58045500
F	-5.03664800	-3.88352000	2.49680100
H	-8.27121300	-0.61511900	2.66279200
C	-9.59493600	0.47549600	0.52162400
C	-9.35057300	2.00077800	0.65280500
H	-10.23824200	0.14963800	1.34930300
H	-10.15165300	0.28459300	-0.40539800
C	-10.65419200	2.81881200	0.66560600
H	-8.78405600	2.19625100	1.57539700
H	-8.71518200	2.33597700	-0.18152400
C	-10.41117700	4.33108000	0.79226100
H	-11.22041600	2.61234500	-0.25421100
H	-11.28546200	2.47697300	1.49833800
H	-11.35580900	4.88580300	0.79986200
H	-9.87641000	4.56906800	1.72030500
H	-9.81075500	4.70709100	-0.04600400

(28) $TS_{2\text{-}3}$

Zero-point correction =	1.098947 (Hartree/Particle)
Thermal correction to Energy =	1.168025
Thermal correction to Enthalpy =	1.168970
Thermal correction to Gibbs Free Energy =	0.980864
Sum of electronic and zero-point Energies =	-4305.205435
Sum of electronic and thermal Energies =	-4305.136357
Sum of electronic and thermal Enthalpies =	-4305.135412
Sum of electronic and thermal Free Energies =	-4305.323518

Au	-0.49845000	-1.19449800	0.27434900
Au	0.98206500	1.42379800	-1.58387100
P	0.97911500	-3.07901900	-0.27913700
P	2.03458300	2.92481200	-0.05659800
Cl	-0.12356900	-0.10185200	-3.11282000
O	3.82705700	0.66429000	0.33670500
O	3.58224800	-1.62291000	-0.06354100
C	1.64170900	-3.90631800	1.27372200
C	2.62611900	-4.90473900	1.19640700

H	3.03741700	-5.19197500	0.23427700
C	3.08483600	-5.52711100	2.36328300
H	3.84476200	-6.29897800	2.29804100
C	2.56511300	-5.15555200	3.60963500
H	2.92191700	-5.63998400	4.51265300
C	1.58747200	-4.15677800	3.68858200
H	1.18608700	-3.86045200	4.65216500
C	1.12580100	-3.52962100	2.52427100
H	0.37948000	-2.74348100	2.59435100
C	-0.26344000	-4.30188400	-1.00552600
C	-0.42084200	-5.60113100	-0.50312300
H	0.19678700	-5.95128100	0.31611300
C	-1.38314900	-6.45421300	-1.06077500
H	-1.50159100	-7.45856000	-0.66731600
C	-2.18249400	-6.01652600	-2.12213800
H	-2.92256600	-6.68145800	-2.55528300
C	-2.02269000	-4.71925200	-2.62762600
H	-2.63368000	-4.37812600	-3.45715500
C	-1.07149200	-3.85788800	-2.06959100
H	-0.95034600	-2.85243500	-2.46435900
C	0.98206900	4.42374900	0.36720800
C	-0.37518100	4.43927800	0.01354200
H	-0.81271500	3.58878300	-0.49914500
C	-1.15991300	5.56220400	0.30548100
H	-2.20608800	5.57096200	0.02083500
C	-0.59570000	6.66768800	0.95040700
H	-1.20378800	7.53920100	1.16956900
C	0.75938300	6.65342600	1.30391100
H	1.20352000	7.51155600	1.79720500
C	1.54895100	5.53696800	1.01099300
H	2.60201900	5.54465000	1.26930700
C	3.64900100	3.66142000	-0.66498200
C	4.66629400	4.02000200	0.23192300
H	4.55827900	3.81580500	1.29247800
C	5.83189100	4.63180600	-0.24594300
H	6.61670000	4.91150200	0.44936700
C	5.98435000	4.88114900	-1.61546800
H	6.88794100	5.35584100	-1.98319500
C	4.97161500	4.51461600	-2.50992400
H	5.08815200	4.70102200	-3.57224800
C	3.80352600	3.90473100	-2.03747300
H	3.02190500	3.61527800	-2.73331800
C	2.40630400	-3.13167000	-1.49461800
C	3.56524600	-2.38239200	-1.23787600
C	4.68273200	-2.45072000	-2.08342700
C	4.61010300	-3.25803700	-3.22471900
H	5.46484100	-3.30301500	-3.89295000
C	3.46024600	-3.99974700	-3.50632000

H	3.41348600	-4.62095300	-4.39347800
C	2.36498900	-3.94112000	-2.63884200
H	1.47790300	-4.52211700	-2.85601100
C	2.38437900	2.07892100	1.57515300
C	3.22335700	0.95220100	1.56384100
C	3.46126100	0.19223000	2.71667100
C	2.83789200	0.59839900	3.90551800
H	3.01379100	0.02618500	4.81153900
C	2.00102100	1.71779400	3.94133700
H	1.52812000	2.01333500	4.87102200
C	1.77072300	2.45818400	2.77545800
H	1.11740700	3.32232800	2.80020400
C	4.34545700	-1.03298200	2.62890900
H	3.71899600	-1.92374500	2.50083000
H	4.90236700	-1.16337000	3.56438600
C	5.89749300	-1.63028800	-1.72548800
H	6.55756100	-2.19334800	-1.04944700
H	6.48562500	-1.41460400	-2.62414200
C	4.58423100	-0.56361200	0.15900200
C	5.33989900	-0.94013400	1.45023400
H	5.76481500	-1.93721500	1.28020100
C	6.50173000	0.04132600	1.72404200
H	7.05785200	-0.31466400	2.60031300
H	6.09771900	1.02871000	1.98656100
C	7.43549100	0.17498700	0.50861700
H	8.23296100	0.89611400	0.72498800
H	7.93276900	-0.78678000	0.31752000
C	6.64809500	0.63140000	-0.73324100
H	6.26027100	1.64137700	-0.55916000
H	7.30836500	0.69189300	-1.60754500
C	5.46255800	-0.30016000	-1.07794400
H	4.81445000	0.21817400	-1.79641100
C	-2.08933500	-0.07052300	0.94946400
C	-2.21382000	0.28373200	2.43304900
C	-2.77301500	1.00557100	0.26674400
C	-3.34686500	1.89220000	1.23470400
O	-1.72402000	-0.31249200	3.40440700
N	-3.02481400	1.42290800	2.50855400
C	-2.90554200	1.29802500	-1.10573500
C	-4.06009700	3.02711700	0.85866900
C	-3.61110000	2.44105400	-1.48645000
C	-4.18904700	3.28310300	-0.51474200
H	-4.74113300	4.16110400	-0.83505800
H	-4.49482200	3.69468200	1.59386500
H	-3.71242800	2.68662900	-2.53735000
H	-2.43093700	0.66097500	-1.84547400
H	-3.35565300	1.79626600	3.38491900
C	-4.59802700	-1.23063100	1.74063300

C	-3.46821900	-1.71177900	1.05922000
H	-2.79015300	-2.36472000	1.59605300
H	-3.48997000	-1.87609600	-0.00942400
C	-5.69262000	-0.55415300	1.07901800
C	-6.77622100	0.01185200	1.81404900
C	-5.74223000	-0.44297300	-0.34019700
C	-7.83026100	0.63729800	1.16496100
H	-6.76416600	-0.02447400	2.89402300
C	-6.79976000	0.19254000	-0.97661500
H	-4.95840200	-0.87355300	-0.94885600
C	-7.86742200	0.74613700	-0.24206400
H	-6.80901900	0.25922900	-2.05985000
C	-4.63707100	-1.49017100	3.22970400
H	-5.40415800	-2.23299100	3.47400900
H	-3.66637000	-1.82071000	3.59880200
F	-4.96866300	-0.29438400	3.98688300
H	-8.64081600	1.05996200	1.75047100
C	-9.04235700	1.38567700	-0.93937400
H	-9.44200400	2.20044200	-0.32181600
H	-8.71530800	1.83051100	-1.88782000
C	-10.18636800	0.37496600	-1.23012200
C	-11.38581900	1.02947900	-1.93923000
H	-10.51779700	-0.07714300	-0.28460900
H	-9.79447000	-0.44566200	-1.84755400
C	-12.51948100	0.03281500	-2.22816900
H	-11.76811300	1.85291900	-1.31871100
H	-11.04584300	1.48430500	-2.88093700
H	-13.35852100	0.52456200	-2.73210000
H	-12.17392700	-0.78368800	-2.87399200
H	-12.90103700	-0.41250200	-1.30121600

(29) IM$_2$-PhF

Zero-point correction = 1.192834 (Hartree/Particle)
Thermal correction to Energy = 1.270417
Thermal correction to Enthalpy = 1.271361
Thermal correction to Gibbs Free Energy = 1.059830
Sum of electronic and zero-point Energies = -4636.541577
Sum of electronic and thermal Energies = -4636.463994
Sum of electronic and thermal Enthalpies = -4636.463049
Sum of electronic and thermal Free Energies = -4636.674581

Au	-0.06072600	1.23453100	-0.24238800
Au	-1.62105000	-1.45124800	-1.84925700
P	-1.69016700	3.07338000	-0.36888700
P	-2.01930200	-3.07495600	-0.15098200
Cl	-1.12388500	0.20947400	-3.54214400
O	-3.89540400	-1.01348900	0.69093800
O	-3.97753900	1.28773700	0.32076100
C	-2.05100300	3.80229600	1.32451100

C	-3.11306900	4.70104200	1.51371700
H	-3.75904300	4.96533100	0.68298700
C	-3.34402000	5.25427600	2.77864200
H	-4.16521400	5.94937000	2.91963800
C	-2.51826700	4.91336900	3.85719100
H	-2.69866100	5.34490000	4.83625100
C	-1.46129300	4.01469700	3.67048600
H	-0.82091500	3.74469400	4.50381100
C	-1.22662800	3.45672800	2.40750800
H	-0.41433400	2.74865400	2.27138400
C	-0.75118000	4.40951400	-1.31004300
C	-0.58502900	5.70613600	-0.80341100
H	-1.02015700	5.98394100	0.14989600
C	0.15159500	6.65027800	-1.53142000
H	0.28018400	7.65182100	-1.13432700
C	0.71617000	6.30521100	-2.76390000
H	1.28352900	7.03961300	-3.32600000
C	0.54771600	5.01001300	-3.27163100
H	0.97852200	4.73966200	-4.23016300
C	-0.17830600	4.05846100	-2.54699100
H	-0.30575600	3.05482700	-2.94395200
C	-0.65582400	-4.36389800	-0.04677000
C	0.59596500	-4.08138300	-0.61493200
H	0.75699100	-3.13557500	-1.12172600
C	1.62575800	-5.02721500	-0.54681800
H	2.58890400	-4.80526000	-0.99434400
C	1.40879000	-6.25720300	0.08445500
H	2.20469300	-6.99310700	0.13048300
C	0.15867300	-6.54293600	0.64691500
H	-0.01645500	-7.49936400	1.12805100
C	-0.87397100	-5.60078400	0.58184100
H	-1.84405300	-5.83798300	1.00490700
C	-3.59836200	-4.06187000	-0.36132100
C	-4.32215300	-4.52145700	0.74894000
H	-4.00118900	-4.26935900	1.75462000
C	-5.46983300	-5.30101800	0.55625000
H	-6.02838500	-5.65797600	1.41537400
C	-5.89440100	-5.61913800	-0.73957700
H	-6.78362700	-6.22317000	-0.88591000
C	-5.17288600	-5.15536700	-1.84640200
H	-5.50146700	-5.39620300	-2.85178600
C	-4.02559900	-4.37594200	-1.66018100
H	-3.47174700	-4.00994100	-2.51946700
C	-3.35342700	2.99414900	-1.22757400
C	-4.32630500	2.09086100	-0.77021300
C	-5.60684300	2.04513400	-1.34077800
C	-5.89178400	2.90127400	-2.41160100
H	-6.87557700	2.86069700	-2.86944400

C	-4.93291900	3.79705800	-2.89065300
H	-5.16414700	4.45310700	-3.72201100
C	-3.66852300	3.84636400	-2.29496500
H	-2.92663700	4.54261100	-2.66522800
C	-2.07975200	-2.27726800	1.54055100
C	-3.01044300	-1.24514600	1.74681000
C	-3.06793500	-0.52700900	2.94876100
C	-2.16569800	-0.87993800	3.96281500
H	-2.20053500	-0.34121200	4.90514300
C	-1.23421100	-1.90672000	3.78189700
H	-0.54727700	-2.16536200	4.57982400
C	-1.18821300	-2.60533700	2.56935500
H	-0.46413700	-3.39861300	2.42601300
C	-4.07364200	0.59426800	3.09760700
H	-3.58905700	1.55188900	2.87271000
H	-4.42430200	0.64882400	4.13515100
C	-6.60770100	1.06336000	-0.78132900
H	-7.17497500	1.52061000	0.04231700
H	-7.34104100	0.79417000	-1.54937800
C	-4.79530900	0.12831900	0.72172700
C	-5.28594500	0.40448900	2.15830100
H	-5.84277800	1.34910800	2.12048700
C	-6.24495500	-0.70608300	2.64339700
H	-6.63295900	-0.42333100	3.62996200
H	-5.68562700	-1.64166200	2.78061100
C	-7.40075700	-0.93877700	1.65480400
H	-8.04357900	-1.75190400	2.01297200
H	-8.03439500	-0.04155600	1.61004800
C	-6.85905500	-1.28553900	0.25554100
H	-6.33135800	-2.24491600	0.30360800
H	-7.68465200	-1.41339100	-0.45577900
C	-5.89191500	-0.21581600	-0.30325300
H	-5.36686000	-0.64179400	-1.16793300
C	1.62628700	0.16335600	-0.05106700
C	2.35185400	-0.01627200	1.28968700
C	2.43920400	-0.50030500	-0.98255100
C	3.59281100	-1.06609300	-0.30930000
O	2.00409700	0.40084500	2.40398200
N	3.50697200	-0.77004000	1.03971000
C	2.28575100	-0.67993800	-2.38810900
C	4.55425100	-1.79019900	-1.00548800
C	3.25014900	-1.39950400	-3.07436600
C	4.36758100	-1.94046400	-2.38654800
H	5.10982000	-2.49528900	-2.95131400
H	5.42416500	-2.20455000	-0.51190800
H	3.15750100	-1.55467500	-4.14250700
H	1.41494800	-0.26788900	-2.88994100
H	4.21097000	-0.95225300	1.74713600

F	5.43553200	-0.59820800	3.14929200
C	5.30788600	-0.76736500	4.55849200
C	4.07631900	-0.49949300	5.13834300
C	6.42882200	-1.18565300	5.26001900
C	3.97087600	-0.66832000	6.52572600
H	3.24103400	-0.16928900	4.53112600
C	6.30029500	-1.34793100	6.64570200
H	7.36300100	-1.37120600	4.74485700
C	5.07590600	-1.09075700	7.27613500
H	3.02520300	-0.46539500	7.01642200
H	7.15650700	-1.67166200	7.22692000
H	4.98486100	-1.21633000	8.34933100
C	4.39167000	2.50114200	0.45520400
C	3.20858900	2.89906000	-0.07494200
H	2.46376300	3.40451600	0.53005000
H	2.95599300	2.77398800	-1.12056600
C	5.46793500	1.86905400	-0.33726400
C	6.52657200	1.16790700	0.28861000
C	5.48893400	1.95655600	-1.74832300
C	7.53777100	0.57391000	-0.46541200
H	6.57334100	1.10548700	1.36825000
C	6.50220400	1.36083800	-2.49436100
H	4.72716700	2.52997900	-2.26432000
C	7.55015000	0.65677500	-1.86989000
H	6.50192500	1.46657500	-3.57545300
C	4.59872400	2.67166400	1.94102000
H	3.81953900	3.30087600	2.37495400
H	4.61935800	1.71056100	2.46278800
F	5.87027700	3.30427100	2.21047400
H	8.34670900	0.05742400	0.04363500
C	8.65174800	0.01047700	-2.68164700
C	8.34282900	-1.45413400	-3.08405900
H	9.58848600	0.02684100	-2.10919800
H	8.82976000	0.59530600	-3.59354500
C	9.47566700	-2.10591600	-3.89696100
H	8.15691600	-2.04548400	-2.17455500
H	7.41133800	-1.47544300	-3.66979500
C	9.16950800	-3.55884800	-4.29337600
H	9.66076100	-1.50885900	-4.80144300
H	10.40527200	-2.07242400	-3.31090000
H	9.99218400	-3.99435300	-4.87071400
H	9.01573700	-4.18731400	-3.40696900
H	8.26307400	-3.61904300	-4.90921700

(30) $TS_{2\text{-}3}$-PhF

Zero-point correction = 1.193025 (Hartree/Particle)
Thermal correction to Energy = 1.269423
Thermal correction to Enthalpy = 1.270367

Thermal correction to Gibbs Free Energy = 1.063459
Sum of electronic and zero-point Energies = -4636.534843
Sum of electronic and thermal Energies = -4636.458445
Sum of electronic and thermal Enthalpies = -4636.457501
Sum of electronic and thermal Free Energies = -4636.664409

Au	0.30667800	-1.59464900	-0.43981600
Au	1.19095500	1.58525900	-2.02880300
P	2.39542300	-2.86605000	-0.53626500
P	1.12615700	3.22065400	-0.29560500
Cl	1.13522100	-0.12816800	-3.73623100
O	3.19668000	1.58272600	0.97518000
O	3.95988400	-0.61569900	0.67275800
C	2.74857300	-3.68558700	1.12021600
C	3.97499800	-4.32914600	1.35580400
H	4.74418200	-4.33611000	0.58979800
C	4.21130300	-4.95870600	2.58363700
H	5.16003300	-5.45605000	2.75911600
C	3.22816500	-4.94611400	3.58166700
H	3.41369100	-5.43498300	4.53272900
C	2.00828400	-4.29875500	3.35153300
H	1.24628600	-4.27958200	4.12465500
C	1.76620300	-3.66719200	2.12437500
H	0.82473500	-3.15063700	1.95907800
C	2.01630400	-4.27271200	-1.73227800
C	2.19207100	-5.62054600	-1.38686300
H	2.57692300	-5.89321300	-0.41033100
C	1.86553600	-6.62426800	-2.30824400
H	2.00082000	-7.66600100	-2.03585100
C	1.37105500	-6.28595600	-3.57302200
H	1.12287700	-7.06558800	-4.28533200
C	1.19796700	-4.93911400	-3.91868900
H	0.81963500	-4.67084100	-4.90002300
C	1.51224400	-3.93049600	-3.00151500
H	1.37243400	-2.88770700	-3.27410000
C	-0.36863500	4.35620100	-0.41751400
C	-1.31635500	4.14552600	-1.42916700
H	-1.20540600	3.30898800	-2.11087400
C	-2.39956400	5.02267800	-1.56643600
H	-3.12124400	4.86202500	-2.36012700
C	-2.54339400	6.10516000	-0.69339100
H	-3.37878300	6.78786100	-0.80575600
C	-1.60047200	6.31408400	0.32133100
H	-1.70451900	7.15595300	0.99741000
C	-0.51316600	5.44652200	0.45753300
H	0.22233000	5.63125400	1.23240900
C	2.57017300	4.41696500	-0.23251200
C	2.95509300	5.02565900	0.97110400
H	2.47563200	4.74675500	1.90411700

C	3.97359600	5.98648500	0.97035300
H	4.26762800	6.46001100	1.90145100
C	4.61111600	6.33461200	-0.22712400
H	5.39865400	7.08085900	-0.22537100
C	4.23393600	5.71670600	-1.42520200
H	4.72952100	5.97871800	-2.35395400
C	3.21367800	4.75775800	-1.43065000
H	2.92399900	4.27663300	-2.35988700
C	4.06963500	-2.23365800	-1.08965800
C	4.67925700	-1.18269300	-0.38667300
C	5.99034400	-0.77613500	-0.67667100
C	6.66744000	-1.39625700	-1.73365300
H	7.67598500	-1.07369600	-1.97514100
C	6.06360500	-2.41993900	-2.46865900
H	6.59407100	-2.89120400	-3.28845900
C	4.77270200	-2.84509900	-2.13783600
H	4.31285100	-3.65144000	-2.69556300
C	0.99558600	2.37746400	1.36953900
C	2.06372700	1.56797000	1.79337800
C	1.99987800	0.81699500	2.97534200
C	0.82109200	0.88706600	3.73234300
H	0.75196300	0.30918600	4.64909600
C	-0.25989900	1.67431800	3.32350500
H	-1.17403200	1.69985300	3.90574600
C	-0.17245900	2.42042100	2.14244100
H	-1.01107100	3.02765400	1.82260200
C	3.17607500	-0.05353600	3.36216700
H	3.00063300	-1.07800700	3.01207600
H	3.26903600	-0.09792500	4.45385000
C	6.58874400	0.32086400	0.16766900
H	7.03058200	-0.09821700	1.08391600
H	7.40293900	0.81570300	-0.37263100
C	4.32189700	0.69740500	1.24203400
C	4.49999800	0.46512700	2.75643400
H	5.25576700	-0.32333900	2.85830600
C	5.02868900	1.73351600	3.46253200
H	5.21635700	1.49186100	4.51596800
H	4.25676700	2.51496600	3.45059500
C	6.30732400	2.26378800	2.79179000
H	6.65274000	3.17039500	3.30329200
H	7.11326200	1.52340300	2.89686200
C	6.04876300	2.57426900	1.30632600
H	5.32432200	3.39273500	1.23468100
H	6.96821800	2.92295900	0.81967900
C	5.50527200	1.36226100	0.51282800
H	5.09428400	1.72998300	-0.43635400
C	-1.61855700	-0.94892100	-0.19872200
C	-2.18685900	-0.77198900	1.20778500

C	-2.41881400	-0.08063500	-1.01981700
C	-3.38864200	0.58205800	-0.19897100
O	-1.82275900	-1.34033900	2.25825500
N	-3.22093200	0.15361900	1.12193100
C	-2.35694300	0.21175400	-2.39845200
C	-4.28343400	1.50664200	-0.72415500
C	-3.26347200	1.12849300	-2.93187100
C	-4.21417800	1.75913500	-2.10316500
H	-4.90820800	2.47041400	-2.53939500
H	-5.00956200	2.01392100	-0.09999500
H	-3.23288300	1.36432300	-3.98944400
H	-1.59640000	-0.25077600	-3.01970900
H	-3.68410200	0.53268200	1.94111900
F	-3.94474800	1.28246000	3.68924200
C	-4.30212900	0.55913800	4.85879600
C	-3.64700700	-0.63838800	5.11102400
C	-5.28615100	1.09667500	5.67653500
C	-4.01226300	-1.33976300	6.26832100
H	-2.88699500	-1.00141100	4.42791000
C	-5.63480600	0.37921300	6.82834500
H	-5.75591700	2.03911700	5.42380400
C	-5.00099600	-0.83491200	7.12298400
H	-3.52264800	-2.27973400	6.49852600
H	-6.39902100	0.77083800	7.49060400
H	-5.27660900	-1.38471900	8.01601500
C	-3.77095300	-3.01831700	0.03406300
C	-2.54007500	-3.03487600	-0.61006300
H	-1.72835100	-3.61146500	-0.18485600
H	-2.43462400	-2.80241500	-1.65986400
C	-4.96327900	-2.43108300	-0.55742300
C	-6.10012200	-2.09135100	0.22824000
C	-5.03162500	-2.16714700	-1.95196300
C	-7.21444600	-1.49749300	-0.34976400
H	-6.10614900	-2.31240100	1.28598900
C	-6.15595200	-1.58117500	-2.52018800
H	-4.21579400	-2.46049400	-2.60071100
C	-7.26973100	-1.22859200	-1.73312700
H	-6.18551600	-1.41002700	-3.59160900
C	-3.78566100	-3.58196400	1.43929400
H	-3.02514500	-4.35858200	1.54346300
H	-3.58920300	-2.80680400	2.19076100
F	-5.05102200	-4.18567800	1.76486600
H	-8.06878300	-1.25071700	0.27310800
C	-8.48074200	-0.56754600	-2.34717600
C	-8.40620800	0.98238000	-2.30930100
H	-9.38623800	-0.88886900	-1.81638600
H	-8.59070100	-0.89040500	-3.39019600
C	-9.64559400	1.65236200	-2.92924100

H	-8.29141700	1.31255100	-1.26650800
H	-7.50201100	1.31045500	-2.84270900
C	-9.57380100	3.18716400	-2.89326000
H	-9.75884200	1.31304800	-3.96879400
H	-10.54466500	1.31359500	-2.39486700
H	-10.46918900	3.63578500	-3.33673100
H	-9.49147000	3.55557300	-1.86302900
H	-8.70479900	3.55634200	-3.45250000

(31) IM_2-PhCl

Zero-point correction = 1.190978 (Hartree/Particle)
Thermal correction to Energy = 1.269282
Thermal correction to Enthalpy = 1.270226
Thermal correction to Gibbs Free Energy = 1.053885
Sum of electronic and zero-point Energies = -4996.898621
Sum of electronic and thermal Energies = -4996.820317
Sum of electronic and thermal Enthalpies = -4996.819372
Sum of electronic and thermal Free Energies = -4997.035713

Au	-0.22042800	1.38104200	-0.36032200
Au	-1.90499200	-1.09643000	-2.12557100
P	-1.93137100	3.06007000	0.19090700
P	-1.90340100	-3.03073400	-0.73157400
Cl	-1.81965500	0.86519600	-3.54812700
O	-3.67738700	-1.33384900	0.83824400
O	-3.94042200	0.98053500	0.94493400
C	-1.96401800	3.44410600	2.02910700
C	-2.99494700	4.21863700	2.58500900
H	-3.80405400	4.58073600	1.95923400
C	-2.98369000	4.52015400	3.95186300
H	-3.78135800	5.12074500	4.37651600
C	-1.94686500	4.05018400	4.76762400
H	-1.93926300	4.28771200	5.82627400
C	-0.92173100	3.27290900	4.21582300
H	-0.11877200	2.90301000	4.84493700
C	-0.92853500	2.96683600	2.84903500
H	-0.13957000	2.34945500	2.42930000
C	-1.27209000	4.61347300	-0.64793700
C	-1.04174800	5.80503700	0.05431100
H	-1.26296600	5.87061000	1.11353400
C	-0.52028000	6.91988300	-0.61628500
H	-0.34071600	7.83914300	-0.06865100
C	-0.23534800	6.84933700	-1.98410800
H	0.16551400	7.71515200	-2.50059200
C	-0.46760500	5.65898200	-2.68620200
H	-0.25188000	5.60109100	-3.74798900
C	-0.97847700	4.53816500	-2.02275800
H	-1.15411000	3.61598500	-2.57050600
C	-0.49237200	-4.20665700	-1.12998900

C	0.61113700	-3.73116600	-1.85503600
H	0.62829200	-2.70175200	-2.19771500
C	1.67558800	-4.58978900	-2.15431500
H	2.52284800	-4.21758800	-2.72061700
C	1.64000600	-5.92462000	-1.73569200
H	2.46193200	-6.59160000	-1.97364000
C	0.53621300	-6.40265600	-1.01881400
H	0.50023000	-7.43949900	-0.70173300
C	-0.52996200	-5.54831100	-0.71648700
H	-1.38812200	-5.93210400	-0.17578500
C	-3.45167100	-4.08158400	-0.83703000
C	-3.91262700	-4.80609100	0.27243100
H	-3.40296900	-4.72829000	1.22753200
C	-5.04262400	-5.62418100	0.14809200
H	-5.39749400	-6.18563700	1.00617100
C	-5.71132300	-5.71762200	-1.07861900
H	-6.58613800	-6.35232000	-1.17253300
C	-5.25246400	-4.98973900	-2.18323500
H	-5.77066900	-5.05632800	-3.13390400
C	-4.12402800	-4.17029600	-2.06500800
H	-3.77486900	-3.59997300	-2.92041400
C	-3.73188300	2.99516900	-0.32251300
C	-4.54461300	1.94128600	0.12622500
C	-5.91204100	1.89195200	-0.18322900
C	-6.45399800	2.90571400	-0.98282400
H	-7.50826200	2.86557700	-1.23969600
C	-5.65980300	3.95642100	-1.44772600
H	-6.08991100	4.73504300	-2.06721200
C	-4.30290500	4.00262500	-1.11262600
H	-3.68904100	4.81895700	-1.47174800
C	-1.66698400	-2.56828100	1.06661100
C	-2.58812400	-1.67759100	1.64309800
C	-2.43777600	-1.19760600	2.95121000
C	-1.33198900	-1.64717700	3.68765200
H	-1.20356500	-1.29327100	4.70639800
C	-0.40415700	-2.53608300	3.13630900
H	0.44610500	-2.87039200	3.72047800
C	-0.56899200	-2.99548300	1.82384800
H	0.15353200	-3.67894500	1.39349500
C	-3.44548200	-0.21063400	3.50014800
H	-3.06185400	0.80876600	3.37204300
H	-3.58134700	-0.37021400	4.57637300
C	-6.72739900	0.73765500	0.34626600
H	-7.13673300	0.97953000	1.33781200
H	-7.58770500	0.55408700	-0.30660700
C	-4.60549300	-0.29801800	1.25944800
C	-4.81119900	-0.33151200	2.78771000
H	-5.41058500	0.55176400	3.04083800

C	-5.59691500	-1.59201300	3.21599300
H	-5.79451700	-1.52884300	4.29337300
H	-4.97511000	-2.48433300	3.06108100
C	-6.91367000	-1.74295400	2.43342500
H	-7.42634800	-2.66355400	2.73729300
H	-7.59120500	-0.91529600	2.68724900
C	-6.64683300	-1.77626600	0.91697700
H	-6.07173600	-2.67716800	0.67445900
H	-7.59067000	-1.84313400	0.36158800
C	-5.86690000	-0.53955400	0.41158600
H	-5.50608100	-0.74834300	-0.60400400
C	1.52294400	0.44513500	-0.68952000
C	2.48623000	0.07746500	0.44860600
C	2.18162400	0.02164400	-1.85735000
C	3.45568000	-0.57427700	-1.50879800
O	2.32510200	0.26384500	1.66500900
N	3.59852500	-0.53771000	-0.13057800
C	1.78546900	0.09121500	-3.22287600
C	4.30871700	-1.08071200	-2.48222700
C	2.64146500	-0.41602300	-4.18923500
C	3.88325900	-0.98918900	-3.81678500
H	4.53431700	-1.37424600	-4.59544000
H	5.26767100	-1.51682100	-2.23041200
H	2.36522000	-0.37874500	-5.23599100
H	0.82260500	0.52220900	-3.48188100
H	4.39738800	-0.86425900	0.40121400
C	5.28910800	-2.41368700	3.50225900
C	4.10551400	-1.80584000	3.90932800
C	5.90433500	-3.43671400	4.21688200
C	3.51525300	-2.25511100	5.09967500
H	3.65061400	-1.01137300	3.32892600
C	5.29732900	-3.87159400	5.40266500
H	6.82822800	-3.88017500	3.86688300
C	4.10638700	-3.28277400	5.84421700
H	2.59778700	-1.78848300	5.44318700
H	5.76121000	-4.66611500	5.97709500
H	3.64525900	-3.62012500	6.76613500
C	3.85504900	3.12877000	0.20637400
C	2.87642400	3.34545200	-0.70859200
H	1.91863400	3.76234800	-0.41887100
H	3.00563300	3.16036800	-1.76800500
C	5.20542100	2.62854900	-0.13455300
C	6.11166100	2.22510200	0.87286400
C	5.63961600	2.52744000	-1.47729000
C	7.36636100	1.71066800	0.54748800
H	5.84996700	2.34654600	1.91543800
C	6.89661700	2.01782400	-1.79446200
H	5.00214700	2.87629700	-2.28200900

C	7.78397800	1.58834000	-0.78976500
H	7.20539100	1.96772700	-2.83490500
C	3.50009200	3.33454400	1.65876000
H	2.53542400	3.83612900	1.75685300
H	3.46693600	2.38105400	2.19777400
F	4.48065300	4.15522100	2.33494600
H	8.03960600	1.41171200	1.34528600
Cl	6.10398200	-1.82947900	1.95061700
C	9.12978800	0.99090000	-1.13679000
C	9.07648600	-0.54685300	-1.32620900
H	9.85312600	1.22305100	-0.34434700
H	9.51329100	1.44805400	-2.05857300
C	10.44802600	-1.15814600	-1.66379400
H	8.68317700	-1.00887700	-0.40851000
H	8.36091900	-0.78553900	-2.12819300
C	10.39393200	-2.68216900	-1.85479300
H	10.84027300	-0.68610600	-2.57627600
H	11.15857600	-0.91327900	-0.86132400
H	11.38337100	-3.08796100	-2.09238200
H	10.03728400	-3.18201900	-0.94549000
H	9.71655900	-2.95461300	-2.67425600

(32) $TS_{2\text{-}3}$-PhCl

Zero-point correction = 1.191516 (Hartree/Particle)
Thermal correction to Energy = 1.268434
Thermal correction to Enthalpy = 1.269378
Thermal correction to Gibbs Free Energy = 1.059501
Sum of electronic and zero-point Energies = -4996.894209
Sum of electronic and thermal Energies = -4996.817291
Sum of electronic and thermal Enthalpies = -4996.816347
Sum of electronic and thermal Free Energies = -4997.026224

Au	-0.15328500	1.59810100	-0.19100200
Au	-1.23606100	-1.12705700	-2.20747100
P	-2.17515600	2.98843900	-0.09448800
P	-1.36665100	-3.04818200	-0.79862700
Cl	-1.00736100	0.82167400	-3.63245600
O	-3.50784200	-1.53655700	0.46390800
O	-4.06580200	0.73496800	0.47679100
C	-2.60371200	3.43555500	1.68106400
C	-3.81475200	4.07497400	1.99199200
H	-4.53340200	4.29269800	1.20908700
C	-4.10149400	4.42513300	3.31678700
H	-5.03809100	4.91990700	3.55120900
C	-3.18230100	4.14002400	4.33391800
H	-3.40549000	4.41413900	5.35981600
C	-1.97690100	3.49790800	4.02607100
H	-1.26360500	3.27055800	4.81130700
C	-1.68539800	3.14395400	2.70232400

H	-0.75593300	2.63138000	2.47200100
C	-1.58093300	4.59501700	-0.88772400
C	-1.68042300	5.83251100	-0.23578200
H	-2.12744400	5.90030000	0.74894900
C	-1.19472000	6.99012200	-0.85964600
H	-1.27157000	7.94540300	-0.35070400
C	-0.61807400	6.91523500	-2.13217500
H	-0.24722900	7.81422000	-2.61449000
C	-0.52219600	5.67900500	-2.78411900
H	-0.08217700	5.61765300	-3.77414000
C	-0.99451600	4.51663500	-2.16517900
H	-0.91785900	3.55963900	-2.67369200
C	0.12265100	-4.18250300	-0.96114800
C	1.22714700	-3.77032300	-1.72078100
H	1.22454700	-2.79444900	-2.19700400
C	2.32401800	-4.62567700	-1.88084900
H	3.16989000	-4.30486700	-2.47890700
C	2.32454700	-5.88991500	-1.28286100
H	3.17219700	-6.55448300	-1.41360300
C	1.22253800	-6.30362100	-0.52305600
H	1.21442200	-7.28617300	-0.06433100
C	0.12239900	-5.45516000	-0.36477600
H	-0.73649200	-5.79439700	0.20458300
C	-2.82852300	-4.17936200	-1.12229500
C	-3.38536200	-4.95693800	-0.09548400
H	-3.02174900	-4.86176400	0.92298400
C	-4.42630100	-5.84875600	-0.38395700
H	-4.85374200	-6.45109900	0.40981000
C	-4.91293900	-5.96134400	-1.69232000
H	-5.71884100	-6.65292800	-1.91325900
C	-4.36192700	-5.17792400	-2.71379700
H	-4.73962500	-5.25839700	-3.72664500
C	-3.31966800	-4.28634200	-2.43055900
H	-2.89766400	-3.67565700	-3.22345400
C	-3.83112300	2.66894100	-0.91223300
C	-4.60188400	1.56371000	-0.51504200
C	-5.88770500	1.34591800	-1.03309700
C	-6.37837800	2.23013000	-2.00189600
H	-7.36570700	2.05748500	-2.41995500
C	-5.61831800	3.32228700	-2.42610000
H	-6.00588100	4.00030500	-3.17789100
C	-4.35236200	3.54486900	-1.87489500
H	-3.76912800	4.39809200	-2.19802500
C	-1.43136300	-2.54490600	1.00285100
C	-2.51342800	-1.75174200	1.42148300
C	-2.59535800	-1.23583200	2.72214400
C	-1.55720200	-1.54404500	3.61259400
H	-1.60636500	-1.15849200	4.62609500

C	-0.46946300	-2.32931700	3.21848400
H	0.32575300	-2.54859500	3.92183200
C	-0.40462500	-2.82955800	1.91173500
H	0.43974000	-3.43378100	1.60339900
C	-3.77041600	-0.36042000	3.09991900
H	-3.48882800	0.69350700	2.99121000
H	-4.03208700	-0.51583700	4.15336500
C	-6.66231600	0.15507100	-0.52610500
H	-7.21076600	0.41630300	0.39065000
H	-7.41450300	-0.14890300	-1.26199000
C	-4.60340800	-0.61543700	0.72977100
C	-5.00636600	-0.64763000	2.21845300
H	-5.72541200	0.16847400	2.36062500
C	-5.70358600	-1.97682800	2.58312300
H	-6.04304800	-1.91716400	3.62479100
H	-4.97866800	-2.80094200	2.53424600
C	-6.88582900	-2.27611000	1.64490400
H	-7.34449300	-3.23523300	1.91231500
H	-7.66506400	-1.51206000	1.77925700
C	-6.41631500	-2.31798700	0.17933100
H	-5.72580500	-3.15985800	0.04957000
H	-7.26501900	-2.49787300	-0.49263500
C	-5.70079000	-1.02253100	-0.26956400
H	-5.18119800	-1.22747800	-1.21413100
C	1.78304800	0.90233300	-0.07121000
C	2.38734400	0.48322100	1.26694100
C	2.57254100	0.20486100	-1.05335000
C	3.58360700	-0.56051300	-0.39093300
O	2.03027000	0.82856100	2.41241100
N	3.44908800	-0.37154600	0.98850300
C	2.46791300	0.15092500	-2.45870100
C	4.48004800	-1.35758000	-1.09323600
C	3.37036900	-0.64128200	-3.16920900
C	4.36480300	-1.37752200	-2.49200200
H	5.05762900	-1.98443700	-3.06616600
H	5.24001800	-1.94180700	-0.58768400
H	3.30377600	-0.69831700	-4.24955100
H	1.67594200	0.69170100	-2.96753900
H	4.02530400	-0.80040000	1.70375500
C	4.11997300	-1.76526200	5.20301100
C	2.99231200	-0.95134400	5.21154600
C	4.48507900	-2.57812800	6.27228700
C	2.19170500	-0.96030100	6.36393400
H	2.74261300	-0.32694100	4.36150400
C	3.67101300	-2.57157200	7.41251200
H	5.37436800	-3.19361500	6.22252400
C	2.52679500	-1.76550000	7.45859400
H	1.30952500	-0.32832200	6.39927500

H	3.93638300	-3.19397400	8.25967300
H	1.90245300	-1.76192300	8.34624900
C	3.93291900	2.90237300	0.52576800
C	2.70310600	3.01611600	-0.11547900
H	1.88720100	3.52033700	0.38891400
H	2.61104700	2.96725100	-1.19037800
C	5.12914800	2.42671600	-0.15080700
C	6.25370900	1.92836300	0.56528500
C	5.21088900	2.43543900	-1.57024200
C	7.36795200	1.44261800	-0.10740000
H	6.24747200	1.93610100	1.64563100
C	6.33562700	1.95901400	-2.23048500
H	4.40512100	2.85767300	-2.15769000
C	7.43802100	1.44850500	-1.51566100
H	6.37637300	1.99959100	-3.31443700
C	3.92855700	3.23565600	2.00317100
H	3.22760400	4.05063700	2.20022200
H	3.62771000	2.37286300	2.61355300
F	5.21615400	3.66975500	2.47111100
H	8.21094300	1.06646000	0.46459300
Cl	5.20315000	-1.77056700	3.70511600
C	8.64820700	0.90646600	-2.23654200
C	8.49422900	-0.58292300	-2.64324400
H	9.53596800	1.00881200	-1.59958900
H	8.83583300	1.49959400	-3.14170000
C	9.73521200	-1.13288100	-3.36988800
H	8.29672300	-1.18444400	-1.74323900
H	7.61093500	-0.68800600	-3.29012600
C	9.57880600	-2.60381700	-3.78673000
H	9.93583400	-0.51672600	-4.25857400
H	10.61266900	-1.02678000	-2.71618600
H	10.47618800	-2.96629700	-4.29980100
H	9.41032800	-3.24743400	-2.91540000
H	8.73022900	-2.73366700	-4.47029800

Part VII: Single-Crystal X-ray Crystallography of 4 (CCDC: 1832272)

Data intensity of **4** was collected using a Bruker SMART APEX II (Mo radiation) at 296 K in a nitrogen stream. The X-ray condition of was 50 kV × 30 mA. Data collection and reduction were done by using the Bruker ApexII software package. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **4**: $C_{27}H_{25}FN_2O_5S$, T = 296(2) K, monoclinic, space group $P2(1)$, a = 13.420(2) Å, b = 5.3749(8) Å, c = 17.821(3) Å, α = 90 deg, β = 105.381(5) deg, γ = 90 deg, V = 1239.5(3) Å^3. Z = 2, d_{calc} = 1.363 mg/m^3. Total number of reflections 14532 (R_{int} = 0.0688), R_1 = 0.1349, wR_2 = 0.1967 (all data), GOF = 1.024, and 325 parameters.

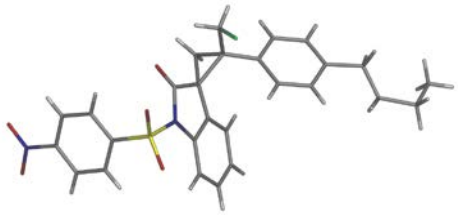

Table S6. Crystal data and structure refinement for z.

Identification code	z
Empirical formula	$C_{27}H_{25}FN_2O_5S$
Formula weight	508.55
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2(1)$
Unit cell dimensions	a = 13.420(2) Å alpha = 90 deg.
	b = 5.3749(8) Å beta = 105.381(5) deg.
	c = 17.821(3) Å gamma = 90 deg.
Volume	1239.5(3) Å^3
Z, Calculated density	2, 1.363 mg/m^3
Absorption coefficient	0.179 mm^{-1}
F(000)	532
Crystal size	0.39 × 0.17 × 0.09 mm
Theta range for data collection	1.57 to 25.00 deg.

Limiting indices	-14<=h<=15, -6<=k<=6, -21<=l<=21
Reflections collected/unique	14532 / 4154 [$R_{(int)}$ = 0.0688]
Completeness to theta = 25.00	99.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9840 and 0.9334
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4154 / 22 / 325
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R_1 = 0.0661, wR_2 = 0.1551
R indices (all data)	R_1 = 0.1349, wR_2 = 0.1967
Absolute structure parameter	-0.02(18)
Largest diff. peak and hole	0.392 and -0.300 e.Å^{-3}

Table S7. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (A^2 × 10^3) for z.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	4256(1)	4336(3)	1449(1)	68(1)
O(1)	3690(3)	5947(9)	1818(2)	82(1)
O(2)	4952(3)	5321(8)	1043(2)	77(1)
O(3)	1752(5)	-4349(17)	-928(4)	153(3)
O(4)	692(5)	-3673(16)	-278(4)	144(3)
O(5)	6026(3)	833(9)	1459(2)	74(1)
F(1)	8168(3)	2829(8)	2859(2)	98(1)
N(1)	4942(3)	2511(10)	2153(2)	62(1)
C(1)	7532(4)	1408(12)	4427(3)	67(2)
C(2)	7997(5)	1584(16)	5209(3)	89(2)
C(3)	8703(5)	-162(16)	5594(4)	82(2)
C(4)	8907(5)	-2073(17)	5172(4)	90(2)
C(5)	8434(4)	-2369(13)	4392(3)	73(2)
C(6)	7747(4)	-632(13)	4006(3)	57(1)
C(7)	7313(4)	-775(13)	3136(3)	57(1)

C(8)	6700(4)	-2940(12)	2765(3)	71(2)
C(9)	6119(4)	-490(13)	2770(3)	56(1)
C(10)	5747(4)	930(12)	2045(3)	55(1)
C(11)	4690(4)	1776(12)	2867(3)	60(2)
C(12)	5372(4)	-61(12)	3229(3)	60(2)
C(13)	5264(5)	-1135(13)	3903(3)	71(2)
C(14)	4465(6)	-308(19)	4205(4)	90(2)
C(15)	3817(5)	1570(19)	3844(4)	96(3)
C(16)	3910(5)	2601(15)	3168(4)	82(2)
C(17)	3411(4)	2241(12)	851(3)	59(2)
C(18)	3702(4)	994(14)	269(3)	67(2)
C(19)	3067(5)	-787(16)	-168(3)	74(2)
C(20)	2134(5)	-1253(13)	-9(4)	69(2)
C(21)	1817(5)	1(16)	553(4)	82(2)
C(22)	2463(5)	1745(15)	990(3)	75(2)
C(23)	8015(5)	331(14)	2691(4)	72(2)
C(24)	9270(7)	120(30)	6464(5)	170(6)
C(25)	8737(11)	1320(40)	6959(6)	267(9)
C(26)	9202(13)	2150(50)	7815(7)	275(10)
C(27)	9830(14)	40(50)	8186(9)	305(13)
N(2)	1480(5)	-3221(16)	-447(4)	98(2)

Table S8. Bond lengths [Å] and angles [deg] for z.

S(1)-O(1)	1.422(5)
S(1)-O(2)	1.427(4)
S(1)-N(1)	1.664(5)
S(1)-C(17)	1.747(6)
O(3)-N(2)	1.185(8)
O(4)-N(2)	1.198(7)
O(5)-C(10)	1.200(6)
F(1)-C(23)	1.379(8)
N(1)-C(10)	1.427(7)
N(1)-C(11)	1.455(7)
C(1)-C(2)	1.370(7)
C(1)-C(6)	1.402(8)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.381(10)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.343(10)
C(3)-C(24)	1.542(9)
C(4)-C(5)	1.376(9)
C(4)-H(4A)	0.9300

C(5)-C(6)	1.363(8)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.507(7)
C(7)-C(8)	1.477(8)
C(7)-C(23)	1.505(9)
C(7)-C(9)	1.570(7)
C(8)-C(9)	1.532(9)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.470(7)
C(9)-C(12)	1.470(7)
C(11)-C(16)	1.370(8)
C(11)-C(12)	1.385(8)
C(12)-C(13)	1.374(8)
C(13)-C(14)	1.394(9)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.376(11)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.362(9)
C(15)-H(15A)	0.9300
C(16)-H(16A)	0.9300
C(17)-C(18)	1.375(8)
C(17)-C(22)	1.384(7)
C(18)-C(19)	1.378(9)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.378(8)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.367(9)
C(20)-N(2)	1.460(9)
C(21)-C(22)	1.371(9)
C(21)-H(21A)	0.9300
C(22)-H(22A)	0.9300
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-C(25)	1.428(9)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(26)	1.553(9)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(27)	1.463(10)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
O(1)-S(1)-O(2)	120.7(3)
O(1)-S(1)-N(1)	105.5(2)

O(2)-S(1)-N(1)	107.2(2)
O(1)-S(1)-C(17)	109.6(3)
O(2)-S(1)-C(17)	109.7(3)
N(1)-S(1)-C(17)	102.7(3)
C(10)-N(1)-C(11)	108.5(5)
C(10)-N(1)-S(1)	122.4(4)
C(11)-N(1)-S(1)	127.5(4)
C(2)-C(1)-C(6)	119.6(6)
C(2)-C(1)-H(1A)	120.2
C(6)-C(1)-H(1A)	120.2
C(1)-C(2)-C(3)	121.8(7)
C(1)-C(2)-H(2A)	119.1
C(3)-C(2)-H(2A)	119.1
C(4)-C(3)-C(2)	117.1(6)
C(4)-C(3)-C(24)	121.2(8)
C(2)-C(3)-C(24)	121.7(9)
C(3)-C(4)-C(5)	123.1(7)
C(3)-C(4)-H(4A)	118.4
C(5)-C(4)-H(4A)	118.4
C(6)-C(5)-C(4)	120.0(7)
C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(6)-C(1)	118.3(5)
C(5)-C(6)-C(7)	120.6(6)
C(1)-C(6)-C(7)	120.8(5)
C(8)-C(7)-C(23)	115.3(5)
C(8)-C(7)-C(6)	121.2(5)
C(23)-C(7)-C(6)	113.4(5)
C(8)-C(7)-C(9)	60.3(4)
C(23)-C(7)-C(9)	117.1(5)
C(6)-C(7)-C(9)	119.7(4)
C(7)-C(8)-C(9)	62.9(4)
C(7)-C(8)-H(8A)	117.5
C(9)-C(8)-H(8A)	117.5
C(7)-C(8)-H(8B)	117.5
C(9)-C(8)-H(8B)	117.5
H(8A)-C(8)-H(8B)	114.5
C(10)-C(9)-C(12)	106.6(5)
C(10)-C(9)-C(8)	119.7(5)
C(12)-C(9)-C(8)	124.1(5)
C(10)-C(9)-C(7)	119.1(5)
C(12)-C(9)-C(7)	123.8(4)
C(8)-C(9)-C(7)	56.9(4)
O(5)-C(10)-N(1)	124.5(5)
O(5)-C(10)-C(9)	129.1(6)
N(1)-C(10)-C(9)	106.4(4)
C(16)-C(11)-C(12)	121.8(6)
C(16)-C(11)-N(1)	129.3(6)

C(12)-C(11)-N(1)	108.8(5)
C(13)-C(12)-C(11)	119.8(6)
C(13)-C(12)-C(9)	131.7(6)
C(11)-C(12)-C(9)	108.5(5)
C(12)-C(13)-C(14)	118.3(7)
C(12)-C(13)-H(13A)	120.9
C(14)-C(13)-H(13A)	120.9
C(15)-C(14)-C(13)	120.6(7)
C(15)-C(14)-H(14A)	119.7
C(13)-C(14)-H(14A)	119.7
C(16)-C(15)-C(14)	121.1(7)
C(16)-C(15)-H(15A)	119.4
C(14)-C(15)-H(15A)	119.4
C(15)-C(16)-C(11)	118.3(7)
C(15)-C(16)-H(16A)	120.8
C(11)-C(16)-H(16A)	120.8
C(18)-C(17)-C(22)	119.9(6)
C(18)-C(17)-S(1)	120.4(5)
C(22)-C(17)-S(1)	119.6(5)
C(17)-C(18)-C(19)	120.6(6)
C(17)-C(18)-H(18A)	119.7
C(19)-C(18)-H(18A)	119.7
C(18)-C(19)-C(20)	118.0(6)
C(18)-C(19)-H(19A)	121.0
C(20)-C(19)-H(19A)	121.0
C(21)-C(20)-C(19)	122.5(6)
C(21)-C(20)-N(2)	119.3(6)
C(19)-C(20)-N(2)	118.2(6)
C(20)-C(21)-C(22)	118.7(6)
C(20)-C(21)-H(21A)	120.6
C(22)-C(21)-H(21A)	120.6
C(21)-C(22)-C(17)	120.2(6)
C(21)-C(22)-H(22A)	119.9
C(17)-C(22)-H(22A)	119.9
F(1)-C(23)-C(7)	110.3(5)
F(1)-C(23)-H(23A)	109.6
C(7)-C(23)-H(23A)	109.6
F(1)-C(23)-H(23B)	109.6
C(7)-C(23)-H(23B)	109.6
H(23A)-C(23)-H(23B)	108.1
C(25)-C(24)-C(3)	118.0(8)
C(25)-C(24)-H(24A)	107.8
C(3)-C(24)-H(24A)	107.8
C(25)-C(24)-H(24B)	107.8
C(3)-C(24)-H(24B)	107.8
H(24A)-C(24)-H(24B)	107.1
C(24)-C(25)-C(26)	126.9(12)
C(24)-C(25)-H(25A)	105.6

C(26)-C(25)-H(25A)	105.6
C(24)-C(25)-H(25B)	105.6
C(26)-C(25)-H(25B)	105.6
H(25A)-C(25)-H(25B)	106.1
C(27)-C(26)-C(25)	104.7(13)
C(27)-C(26)-H(26A)	110.8
C(25)-C(26)-H(26A)	110.8
C(27)-C(26)-H(26B)	110.8
C(25)-C(26)-H(26B)	110.8
H(26A)-C(26)-H(26B)	108.9
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(3)-N(2)-O(4)	122.7(8)
O(3)-N(2)-C(20)	120.0(6)
O(4)-N(2)-C(20)	117.3(7)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for z.

The anisotropic displacement factor exponent takes the form:

$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
S(1)	69(1)	63(1)	63(1)	7(1)	4(1)	9(1)
O(1)	93(3)	69(3)	76(3)	-3(2)	8(2)	23(3)
O(2)	74(3)	73(3)	80(3)	25(2)	15(2)	-12(2)
O(3)	134(5)	206(8)	134(5)	-88(5)	64(4)	-62(5)
O(4)	93(4)	188(8)	156(5)	-59(5)	40(4)	-47(5)
O(5)	73(3)	89(3)	60(2)	11(2)	17(2)	9(2)
F(1)	97(3)	86(3)	120(3)	5(2)	45(2)	-11(2)
N(1)	55(3)	68(3)	57(3)	7(2)	4(2)	7(3)
C(1)	69(4)	66(4)	57(3)	-2(3)	3(3)	2(3)
C(2)	89(5)	106(6)	63(4)	-10(4)	4(4)	11(5)
C(3)	74(4)	104(7)	60(4)	-3(4)	2(3)	6(4)
C(4)	79(5)	101(6)	79(5)	29(4)	-1(4)	26(5)
C(5)	69(4)	66(4)	73(4)	13(3)	0(3)	14(4)
C(6)	58(3)	55(3)	54(3)	-1(3)	9(2)	-12(3)

C(7)	55(3)	57(3)	54(3)	-5(3)	6(3)	3(3)
C(8)	83(4)	57(4)	62(3)	0(3)	2(3)	9(4)
C(9)	54(3)	57(3)	51(3)	-4(3)	3(2)	2(3)
C(10)	52(3)	62(4)	46(3)	0(3)	4(3)	-1(3)
C(11)	52(3)	69(4)	55(3)	1(3)	7(3)	-4(3)
C(12)	58(3)	71(5)	47(3)	4(3)	4(3)	-9(3)
C(13)	74(4)	71(5)	63(3)	14(3)	12(3)	-10(4)
C(14)	85(5)	123(7)	68(4)	9(5)	29(4)	-8(5)
C(15)	75(5)	146(8)	73(4)	5(5)	30(4)	14(6)
C(16)	63(4)	106(6)	79(4)	9(4)	22(3)	18(4)
C(17)	52(3)	65(4)	52(3)	6(3)	1(3)	13(3)
C(18)	56(4)	91(5)	54(3)	2(3)	13(3)	-11(4)
C(19)	59(4)	105(5)	58(3)	-16(4)	16(3)	9(4)
C(20)	51(4)	86(5)	66(4)	-3(3)	7(3)	-2(3)
C(21)	50(4)	119(7)	82(4)	-17(4)	26(3)	-5(4)
C(22)	53(4)	106(6)	69(4)	-14(4)	20(3)	6(4)
C(23)	60(4)	79(5)	76(4)	-5(3)	15(3)	18(3)
C(24)	124(7)	300(18)	69(5)	6(8)	-3(5)	57(10)
C(25)	245(13)	450(20)	84(7)	-4(13)	-5(8)	64(17)
C(26)	250(17)	420(30)	126(10)	-23(15)	-3(11)	40(20)
C(27)	290(20)	420(40)	182(15)	30(20)	23(13)	40(30)
N(2)	64(4)	149(7)	84(4)	-12(5)	24(3)	-21(4)

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for z.

	x	y	z	U(eq)
H(1A)	7075	2637	4177	80
H(2A)	7833	2916	5487	107
H(4A)	9390	-3252	5419	109
H(5A)	8582	-3754	4128	88
H(8A)	6584	-4263	3103	85
H(8B)	6792	-3502	2271	85
H(13A)	5713	-2381	4151	85
H(14A)	4370	-1032	4655	108
H(15A)	3306	2146	4065	115
H(16A)	3456	3832	2917	99
H(18A)	4333	1357	171	81
H(19A)	3262	-1649	-559	89

H(21A)	1175	-322	638	98
H(22A)	2265	2598	1381	90
H(23A)	8674	-528	2828	87
H(23B)	7710	116	2137	87
H(24A)	9465	-1534	6672	204
H(24B)	9905	1030	6500	204
H(25A)	8165	227	6969	321
H(25B)	8433	2800	6681	321
H(26A)	9625	3625	7838	330
H(26B)	8659	2500	8066	330
H(27A)	10137	410	8725	457
H(27B)	10364	-274	7930	457
H(27C)	9400	-1412	8147	457

Table S11. Torsion angles [deg] for z.

O(1)-S(1)-N(1)-C(10)	-168.7(4)
O(2)-S(1)-N(1)-C(10)	-39.0(5)
C(17)-S(1)-N(1)-C(10)	76.5(5)
O(1)-S(1)-N(1)-C(11)	27.6(5)
O(2)-S(1)-N(1)-C(11)	157.4(5)
C(17)-S(1)-N(1)-C(11)	-87.1(5)
C(6)-C(1)-C(2)-C(3)	2.0(10)
C(1)-C(2)-C(3)-C(4)	-0.9(11)
C(1)-C(2)-C(3)-C(24)	176.6(8)
C(2)-C(3)-C(4)-C(5)	-1.2(12)
C(24)-C(3)-C(4)-C(5)	-178.7(8)
C(3)-C(4)-C(5)-C(6)	2.2(11)
C(4)-C(5)-C(6)-C(1)	-1.0(9)
C(4)-C(5)-C(6)-C(7)	173.1(6)
C(2)-C(1)-C(6)-C(5)	-1.0(9)
C(2)-C(1)-C(6)-C(7)	-175.1(6)
C(5)-C(6)-C(7)-C(8)	61.1(7)
C(1)-C(6)-C(7)-C(8)	-124.9(6)
C(5)-C(6)-C(7)-C(23)	-82.8(7)
C(1)-C(6)-C(7)-C(23)	91.2(7)
C(5)-C(6)-C(7)-C(9)	132.3(6)
C(1)-C(6)-C(7)-C(9)	-53.7(8)
C(23)-C(7)-C(8)-C(9)	-108.0(5)
C(6)-C(7)-C(8)-C(9)	108.7(6)
C(7)-C(8)-C(9)-C(10)	107.3(6)
C(7)-C(8)-C(9)-C(12)	-111.1(5)
C(8)-C(7)-C(9)-C(10)	-108.3(6)
C(23)-C(7)-C(9)-C(10)	-3.2(8)
C(6)-C(7)-C(9)-C(10)	140.5(6)

C(8)-C(7)-C(9)-C(12)	111.7(7)
C(23)-C(7)-C(9)-C(12)	-143.2(6)
C(6)-C(7)-C(9)-C(12)	0.5(10)
C(23)-C(7)-C(9)-C(8)	105.1(6)
C(6)-C(7)-C(9)-C(8)	-111.2(7)
C(11)-N(1)-C(10)-O(5)	169.1(6)
S(1)-N(1)-C(10)-O(5)	2.8(8)
C(11)-N(1)-C(10)-C(9)	-10.0(6)
S(1)-N(1)-C(10)-C(9)	-176.4(4)
C(12)-C(9)-C(10)-O(5)	-167.8(6)
C(8)-C(9)-C(10)-O(5)	-20.2(9)
C(7)-C(9)-C(10)-O(5)	46.1(9)
C(12)-C(9)-C(10)-N(1)	11.3(6)
C(8)-C(9)-C(10)-N(1)	158.9(5)
C(7)-C(9)-C(10)-N(1)	-134.8(5)
C(10)-N(1)-C(11)-C(16)	-173.5(6)
S(1)-N(1)-C(11)-C(16)	-8.0(9)
C(10)-N(1)-C(11)-C(12)	4.9(6)
S(1)-N(1)-C(11)-C(12)	170.4(4)
C(16)-C(11)-C(12)-C(13)	1.1(9)
N(1)-C(11)-C(12)-C(13)	-177.4(5)
C(16)-C(11)-C(12)-C(9)	-179.1(6)
N(1)-C(11)-C(12)-C(9)	2.4(6)
C(10)-C(9)-C(12)-C(13)	171.2(6)
C(8)-C(9)-C(12)-C(13)	25.5(9)
C(7)-C(9)-C(12)-C(13)	-44.6(10)
C(10)-C(9)-C(12)-C(11)	-8.5(6)
C(8)-C(9)-C(12)-C(11)	-154.3(5)
C(7)-C(9)-C(12)-C(11)	135.6(6)
C(11)-C(12)-C(13)-C(14)	-0.5(9)
C(9)-C(12)-C(13)-C(14)	179.7(6)
C(12)-C(13)-C(14)-C(15)	-1.3(11)
C(13)-C(14)-C(15)-C(16)	2.6(12)
C(14)-C(15)-C(16)-C(11)	-2.1(12)
C(12)-C(11)-C(16)-C(15)	0.2(10)
N(1)-C(11)-C(16)-C(15)	178.4(6)
O(1)-S(1)-C(17)-C(18)	161.1(5)
O(2)-S(1)-C(17)-C(18)	26.5(6)
N(1)-S(1)-C(17)-C(18)	-87.2(5)
O(1)-S(1)-C(17)-C(22)	-22.2(6)
O(2)-S(1)-C(17)-C(22)	-156.7(5)
N(1)-S(1)-C(17)-C(22)	89.6(5)
C(22)-C(17)-C(18)-C(19)	-1.3(9)
S(1)-C(17)-C(18)-C(19)	175.4(5)
C(17)-C(18)-C(19)-C(20)	0.6(10)
C(18)-C(19)-C(20)-C(21)	0.9(10)
C(18)-C(19)-C(20)-N(2)	-177.2(6)
C(19)-C(20)-C(21)-C(22)	-1.7(11)

N(2)-C(20)-C(21)-C(22)	176.3(6)
C(20)-C(21)-C(22)-C(17)	1.0(11)
C(18)-C(17)-C(22)-C(21)	0.5(9)
S(1)-C(17)-C(22)-C(21)	-176.3(5)
C(8)-C(7)-C(23)-F(1)	152.1(5)
C(6)-C(7)-C(23)-F(1)	-61.8(7)
C(9)-C(7)-C(23)-F(1)	84.1(7)
C(4)-C(3)-C(24)-C(25)	-150.5(13)
C(2)-C(3)-C(24)-C(25)	32.1(18)
C(3)-C(24)-C(25)-C(26)	-170.2(19)
C(24)-C(25)-C(26)-C(27)	-45(3)
C(21)-C(20)-N(2)-O(3)	-178.9(8)
C(19)-C(20)-N(2)-O(3)	-0.8(11)
C(21)-C(20)-N(2)-O(4)	-1.2(10)
C(19)-C(20)-N(2)-O(4)	176.9(7)

Symmetry transformations used to generate equivalent atoms:

Table S12. Hydrogen bonds for z [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Part VIII Single-Crystal X-ray Crystallography of 7d (CCDC: 1832274)

Data intensity of **7d** was collected using a Bruker SMART APEX II (Mo radiation) at 296 K in a nitrogen stream. The X-ray condition of was 50 kV × 30 mA. Data collection and reduction were done by using the Bruker ApexII software package. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **7d**: $C_{18}H_{16}BrFO_2$, T = 296(2) K, monoclinic, space group $P1$, a = 6.6841(6) Å, b = 8.7074(8) Å, c = 14.4482(13) Å, α = 87.391(3) deg, β = 81.591(2) deg, γ = 78.532(3) deg, V = 815.14(13) Å^3. Z = 2, d_{calc} = 1.480 mg/m^3. Total number of reflections 9422 (R_{int} = 0.0302), R_1 = 0.0577, wR_2 = 0.1463 (all data), GOF = 1.065, and 398 parameters.

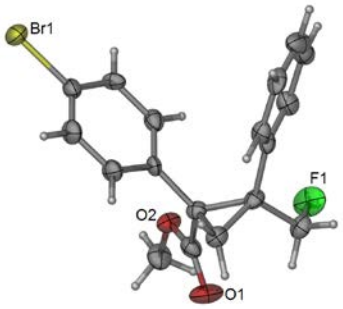

Table S13. Crystal data and structure refinement for z.

Identification code	z	
Empirical formula	$C_{18}H_{16}BrFO_2$	
Formula weight	363.22	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, $P1$	
Unit cell dimensions	a = 6.6841(6) Å	alpha = 87.391(3) deg.
	b = 8.7074(8) Å	beta = 81.591(2) deg.
	c = 14.4482(13) Å	gamma = 78.532(3) deg.
Volume	815.14(13) Å^3	
Z, Calculated density	2, 1.480 mg/m^3	
Absorption coefficient	2.535 mm^{-1}	
F(000)	368	

Crystal size	0.31 × 0.23 × 0.12 mm
Theta range for data collection	1.42 to 25.01 deg.
Limiting indices	-7<=h<=7, -10<=k<=10, -17<=l<=17
Reflections collected / unique	9422/4504 [$R_{(int)}$ = 0.0302]
Completeness to theta = 25.01	99.2%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7507 and 0.5070
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4504 / 3 / 398
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R_1 = 0.0518, wR_2 = 0.1409
R indices (all data)	R_1 = 0.0577, wR_2 = 0.1463
Absolute structure parameter	0.041(15)
Largest diff. peak and hole	1.594 and -0.535 e.A^{-3}

Table S14. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for z.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(2)	8680(1)	6004(1)	4650(1)	38(1)
O(3)	-1148(9)	7000(8)	8701(5)	56(2)
O(4)	2241(9)	5992(6)	8523(3)	35(1)
F(2)	-1350(8)	11884(5)	8997(3)	44(1)
C(19)	2710(12)	7549(9)	5971(5)	31(2)
C(20)	4418(12)	7052(8)	5303(5)	29(2)
C(21)	6358(13)	6734(9)	5585(5)	29(2)
C(22)	6670(12)	6880(8)	6483(5)	29(2)
C(23)	4971(11)	7382(8)	7147(5)	24(2)
C(24)	3019(11)	7742(8)	6900(5)	25(2)
C(25)	1124(10)	8266(8)	7622(4)	25(1)
C(26)	-695(10)	9384(8)	7355(5)	28(1)

C(27)	635(10)	9997(8)	7923(5)	26(1)
C(29)	3762(11)	11208(9)	7804(5)	28(2)
C(30)	4969(13)	12281(9)	7429(6)	36(2)
C(31)	4378(16)	13280(11)	6724(7)	41(2)
C(32)	2504(15)	13189(11)	6369(7)	45(2)
C(33)	1337(13)	12119(9)	6752(5)	33(2)
C(34)	-232(15)	10365(11)	8939(6)	35(2)
C(35)	591(12)	7051(9)	8335(5)	30(2)
C(36)	1781(16)	4694(9)	9136(5)	47(2)
C(38)	1946(13)	11112(9)	7485(5)	29(2)
Br(1)	-2689(1)	10961(1)	4993(1)	41(1)
F(1)	7554(7)	6752(7)	1124(4)	57(1)
O(1)	4673(10)	9784(7)	39(3)	46(1)
O(2)	4625(9)	10662(6)	1469(3)	29(1)
C(1)	-541(11)	9512(9)	2278(5)	32(2)
C(2)	-1778(12)	10078(9)	3087(5)	33(2)
C(3)	-970(12)	10207(9)	3874(5)	29(2)
C(4)	1185(11)	9765(9)	3895(5)	27(2)
C(5)	2398(12)	9208(9)	3081(6)	32(2)
C(6)	1590(11)	9080(8)	2258(5)	21(1)
C(7)	2956(10)	8549(8)	1354(4)	25(1)
C(8)	2203(11)	7546(8)	719(5)	29(2)
C(9)	3914(11)	6793(8)	1236(5)	28(2)
C(10)	3599(12)	5690(9)	2062(5)	25(2)
C(11)	1908(12)	4894(9)	2137(5)	28(2)
C(12)	1740(14)	3795(10)	2864(7)	36(2)
C(13)	3116(15)	3471(10)	3473(5)	41(2)
C(14)	4724(13)	4257(9)	3402(5)	37(2)
C(15)	4946(13)	5363(9)	2690(5)	33(2)
C(16)	5995(12)	6396(10)	639(6)	30(2)
C(17)	4136(11)	9713(8)	867(5)	29(2)
C(18)	5677(14)	11884(9)	1046(6)	40(2)

Table S15. Bond lengths [Å] and angles [deg] for z.

Br(2)-C(21)	1.926(7)
O(3)-C(35)	1.213(9)
O(4)-C(35)	1.342(10)
O(4)-C(36)	1.457(9)
F(2)-C(34)	1.383(11)
C(19)-C(20)	1.393(10)
C(19)-C(24)	1.410(10)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.388(12)
C(20)-H(20A)	0.9300
C(21)-C(22)	1.359(11)

C(22)-C(23)	1.387(10)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.375(11)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.526(10)
C(25)-C(26)	1.486(10)
C(25)-C(35)	1.500(10)
C(25)-C(27)	1.546(10)
C(26)-C(27)	1.480(10)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(38)	1.494(9)
C(27)-C(34)	1.521(11)
C(29)-C(38)	1.379(11)
C(29)-C(30)	1.394(10)
C(29)-H(29A)	0.9300
C(30)-C(31)	1.360(13)
C(30)-H(30A)	0.9300
C(31)-C(32)	1.439(15)
C(31)-H(31A)	0.9300
C(32)-C(33)	1.377(12)
C(32)-H(32A)	0.9300
C(33)-C(38)	1.399(11)
C(33)-H(33A)	0.9300
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
Br(1)-C(3)	1.902(8)
F(1)-C(16)	1.427(9)
O(1)-C(17)	1.200(8)
O(2)-C(17)	1.343(9)
O(2)-C(18)	1.453(9)
C(1)-C(2)	1.379(10)
C(1)-C(6)	1.395(10)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.347(11)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.419(11)
C(4)-C(5)	1.375(11)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.395(11)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.514(9)
C(7)-C(17)	1.496(9)
C(7)-C(8)	1.497(10)
C(7)-C(9)	1.543(10)

C(8)-C(9)	1.484(10)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(16)	1.510(11)
C(9)-C(10)	1.515(10)
C(10)-C(15)	1.352(11)
C(10)-C(11)	1.428(11)
C(11)-C(12)	1.395(12)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.346(13)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.374(12)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.389(11)
C(14)-H(14A)	0.9300
C(15)-H(15A)	0.9300
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600

C(35)-O(4)-C(36)	115.1(6)
C(20)-C(19)-C(24)	118.9(7)
C(20)-C(19)-H(19A)	120.5
C(24)-C(19)-H(19A)	120.5
C(21)-C(20)-C(19)	118.5(7)
C(21)-C(20)-H(20A)	120.8
C(19)-C(20)-H(20A)	120.8
C(22)-C(21)-C(20)	123.0(7)
C(22)-C(21)-Br(2)	119.5(6)
C(20)-C(21)-Br(2)	117.4(6)
C(21)-C(22)-C(23)	118.5(8)
C(21)-C(22)-H(22A)	120.7
C(23)-C(22)-H(22A)	120.7
C(24)-C(23)-C(22)	120.7(7)
C(24)-C(23)-H(23A)	119.7
C(22)-C(23)-H(23A)	119.7
C(23)-C(24)-C(19)	120.3(7)
C(23)-C(24)-C(25)	121.6(6)
C(19)-C(24)-C(25)	118.0(7)
C(26)-C(25)-C(35)	114.0(6)
C(26)-C(25)-C(24)	120.5(6)
C(35)-C(25)-C(24)	116.0(6)
C(26)-C(25)-C(27)	58.4(5)
C(35)-C(25)-C(27)	118.1(6)
C(24)-C(25)-C(27)	117.7(5)
C(27)-C(26)-C(25)	62.8(4)

C(27)-C(26)-H(26A)	117.5
C(25)-C(26)-H(26A)	117.5
C(27)-C(26)-H(26B)	117.5
C(25)-C(26)-H(26B)	117.5
H(26A)-C(26)-H(26B)	114.6
C(26)-C(27)-C(38)	119.4(6)
C(26)-C(27)-C(34)	117.1(6)
C(38)-C(27)-C(34)	112.9(6)
C(26)-C(27)-C(25)	58.8(4)
C(38)-C(27)-C(25)	120.2(6)
C(34)-C(27)-C(25)	118.3(6)
C(38)-C(29)-C(30)	122.1(7)
C(38)-C(29)-H(29A)	119.0
C(30)-C(29)-H(29A)	119.0
C(31)-C(30)-C(29)	120.4(8)
C(31)-C(30)-H(30A)	119.8
C(29)-C(30)-H(30A)	119.8
C(30)-C(31)-C(32)	118.6(8)
C(30)-C(31)-H(31A)	120.7
C(32)-C(31)-H(31A)	120.7
C(33)-C(32)-C(31)	119.9(8)
C(33)-C(32)-H(32A)	120.0
C(31)-C(32)-H(32A)	120.0
C(32)-C(33)-C(38)	120.9(8)
C(32)-C(33)-H(33A)	119.5
C(38)-C(33)-H(33A)	119.5
F(2)-C(34)-C(27)	109.4(7)
F(2)-C(34)-H(34A)	109.8
C(27)-C(34)-H(34A)	109.8
F(2)-C(34)-H(34B)	109.8
C(27)-C(34)-H(34B)	109.8
H(34A)-C(34)-H(34B)	108.2
O(3)-C(35)-O(4)	122.6(7)
O(3)-C(35)-C(25)	124.2(8)
O(4)-C(35)-C(25)	113.1(6)
O(4)-C(36)-H(36A)	109.5
O(4)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
O(4)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(29)-C(38)-C(33)	118.1(7)
C(29)-C(38)-C(27)	121.2(7)
C(33)-C(38)-C(27)	120.8(7)
C(17)-O(2)-C(18)	115.5(6)
C(2)-C(1)-C(6)	120.2(7)
C(2)-C(1)-H(1A)	119.9
C(6)-C(1)-H(1A)	119.9

C(3)-C(2)-C(1)	121.1(7)
C(3)-C(2)-H(2A)	119.4
C(1)-C(2)-H(2A)	119.4
C(2)-C(3)-C(4)	120.9(7)
C(2)-C(3)-Br(1)	120.9(6)
C(4)-C(3)-Br(1)	118.2(6)
C(5)-C(4)-C(3)	117.3(7)
C(5)-C(4)-H(4A)	121.4
C(3)-C(4)-H(4A)	121.4
C(4)-C(5)-C(6)	122.6(7)
C(4)-C(5)-H(5A)	118.7
C(6)-C(5)-H(5A)	118.7
C(5)-C(6)-C(1)	117.9(7)
C(5)-C(6)-C(7)	121.9(6)
C(1)-C(6)-C(7)	120.1(6)
C(17)-C(7)-C(8)	114.9(6)
C(17)-C(7)-C(6)	116.0(6)
C(8)-C(7)-C(6)	118.3(6)
C(17)-C(7)-C(9)	117.9(6)
C(8)-C(7)-C(9)	58.4(5)
C(6)-C(7)-C(9)	118.9(5)
C(9)-C(8)-C(7)	62.3(5)
C(9)-C(8)-H(8A)	117.5
C(7)-C(8)-H(8A)	117.5
C(9)-C(8)-H(8B)	117.5
C(7)-C(8)-H(8B)	117.5
H(8A)-C(8)-H(8B)	114.6
C(8)-C(9)-C(16)	114.7(6)
C(8)-C(9)-C(10)	122.2(6)
C(16)-C(9)-C(10)	114.6(7)
C(8)-C(9)-C(7)	59.2(5)
C(16)-C(9)-C(7)	116.7(6)
C(10)-C(9)-C(7)	118.4(6)
C(15)-C(10)-C(11)	119.4(7)
C(15)-C(10)-C(9)	121.9(7)
C(11)-C(10)-C(9)	118.6(7)
C(12)-C(11)-C(10)	117.6(7)
C(12)-C(11)-H(11A)	121.2
C(10)-C(11)-H(11A)	121.2
C(13)-C(12)-C(11)	122.1(8)
C(13)-C(12)-H(12A)	119.0
C(11)-C(12)-H(12A)	119.0
C(12)-C(13)-C(14)	120.0(7)
C(12)-C(13)-H(13A)	120.0
C(14)-C(13)-H(13A)	120.0
C(13)-C(14)-C(15)	119.8(8)
C(13)-C(14)-H(14A)	120.1
C(15)-C(14)-H(14A)	120.1

C(10)-C(15)-C(14)	121.2(8)
C(10)-C(15)-H(15A)	119.4
C(14)-C(15)-H(15A)	119.4
F(1)-C(16)-C(9)	110.1(6)
F(1)-C(16)-H(16A)	109.6
C(9)-C(16)-H(16A)	109.6
F(1)-C(16)-H(16B)	109.6
C(9)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.2
O(1)-C(17)-O(2)	122.4(6)
O(1)-C(17)-C(7)	125.3(7)
O(2)-C(17)-C(7)	112.2(6)
O(2)-C(18)-H(18A)	109.5
O(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 \times 10^3$) for z.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(2)	25(1)	49(1)	38(1)	-10(1)	7(1)	-7(1)
O(3)	32(4)	58(4)	72(4)	12(3)	16(3)	-13(3)
O(4)	38(3)	35(3)	31(3)	8(2)	0(2)	-9(2)
F(2)	45(3)	42(3)	40(2)	-11(2)	6(2)	-1(2)
C(19)	28(4)	37(4)	27(3)	0(3)	-4(3)	-8(3)
C(20)	31(4)	32(4)	23(3)	-1(3)	-4(3)	-5(3)
C(21)	32(5)	23(4)	30(4)	-1(3)	8(3)	-9(3)
C(22)	18(4)	30(4)	39(4)	-2(3)	-2(3)	-8(3)
C(23)	20(4)	23(4)	30(4)	-3(3)	-2(3)	-6(3)
C(24)	23(4)	23(3)	28(4)	-5(3)	0(3)	-5(3)
C(25)	19(4)	32(4)	26(3)	-3(3)	-2(3)	-7(3)
C(26)	17(4)	35(4)	31(3)	-4(3)	-5(3)	-4(3)
C(27)	12(3)	26(3)	38(4)	5(3)	0(3)	0(3)
C(29)	22(4)	31(4)	31(3)	-2(3)	-3(3)	-10(3)
C(30)	21(4)	32(4)	52(5)	-11(3)	2(4)	-7(3)

C(31)	45(6)	39(5)	40(5)	-3(4)	8(4)	-19(4)
C(32)	47(6)	37(5)	50(5)	13(4)	-5(4)	-8(4)
C(33)	36(5)	34(4)	31(4)	1(3)	-9(3)	-10(3)
C(34)	35(5)	39(5)	31(4)	0(3)	4(4)	-14(4)
C(35)	29(5)	33(4)	30(3)	-8(3)	4(3)	-13(3)
C(36)	76(7)	28(4)	34(4)	3(3)	2(4)	-11(4)
C(38)	29(4)	28(4)	31(4)	-2(3)	6(3)	-10(3)
Br(1)	38(1)	50(1)	29(1)	0(1)	3(1)	3(1)
F(1)	11(2)	103(5)	58(3)	2(3)	-5(2)	-17(2)
O(1)	63(4)	59(4)	25(3)	4(2)	-5(2)	-34(3)
O(2)	34(3)	32(3)	26(2)	-1(2)	-1(2)	-18(2)
C(1)	22(4)	38(4)	34(4)	2(3)	-7(3)	-2(3)
C(2)	19(4)	40(4)	40(4)	0(3)	-5(3)	-2(3)
C(3)	24(4)	29(4)	31(4)	5(3)	-2(3)	-1(3)
C(4)	19(4)	43(4)	22(3)	7(3)	-7(3)	-10(3)
C(5)	25(4)	29(4)	39(4)	5(3)	0(3)	-3(3)
C(6)	16(4)	19(3)	28(3)	-1(3)	-5(3)	0(3)
C(7)	19(4)	33(4)	24(3)	3(3)	1(3)	-8(3)
C(8)	28(4)	33(4)	29(3)	-3(3)	-3(3)	-11(3)
C(9)	25(4)	31(4)	26(3)	-1(3)	5(3)	-10(3)
C(10)	18(4)	22(4)	33(4)	-1(3)	1(3)	-4(3)
C(11)	17(4)	34(4)	33(4)	-6(3)	-3(3)	-6(3)
C(12)	20(5)	34(5)	49(5)	-2(4)	13(4)	-7(4)
C(13)	62(6)	28(4)	32(4)	1(3)	-3(4)	-12(4)
C(14)	43(5)	31(4)	36(4)	-1(3)	-11(3)	-5(3)
C(15)	31(4)	32(4)	40(4)	-2(3)	-11(3)	-9(3)
C(16)	19(4)	38(5)	35(4)	-6(3)	1(3)	-9(3)
C(17)	23(4)	31(4)	35(4)	7(3)	-7(3)	-6(3)
C(18)	39(5)	31(4)	50(5)	4(3)	1(4)	-12(3)

Table S17. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for z.

	x	y	z	U(eq)
H(19A)	1387	7751	5807	37
H(20A)	4261	6936	4683	35
H(22A)	7992	6648	6648	35
H(23A)	5154	7476	7766	29

H(26A)	-649	9722	6705	33
H(26B)	-2046	9255	7660	33
H(29A)	4196	10535	8286	33
H(30A)	6186	12313	7661	43
H(31A)	5169	14007	6476	49
H(32A)	2080	13851	5882	54
H(33A)	126	12066	6520	39
H(34A)	-1115	9638	9184	42
H(34B)	886	10248	9312	42
H(36A)	3044	3999	9231	70
H(36B)	933	4135	8853	70
H(36C)	1064	5094	9727	70
H(1A)	-1130	9416	1743	38
H(2A)	-3194	10377	3089	40
H(4A)	1753	9849	4436	33
H(5A)	3814	8904	3081	38
H(8A)	861	7280	914	35
H(8B)	2532	7713	50	35
H(11A)	954	5100	1717	33
H(12A)	643	3270	2929	43
H(13A)	2979	2716	3942	49
H(14A)	5661	4049	3830	44
H(15A)	6041	5888	2645	40
H(16A)	6302	5290	492	36
H(16B)	5971	6992	56	36
H(18A)	5952	12503	1528	60
H(18B)	4819	12542	648	60
H(18C)	6952	11414	681	60

Table S18. Torsion angles [deg] for z.

C(24)-C(19)-C(20)-C(21)	1.3(10)
C(19)-C(20)-C(21)-C(22)	0.2(11)
C(19)-C(20)-C(21)-Br(2)	178.6(5)
C(20)-C(21)-C(22)-C(23)	-0.5(11)
Br(2)-C(21)-C(22)-C(23)	-178.9(5)
C(21)-C(22)-C(23)-C(24)	-0.8(10)
C(22)-C(23)-C(24)-C(19)	2.4(11)
C(22)-C(23)-C(24)-C(25)	178.8(6)
C(20)-C(19)-C(24)-C(23)	-2.6(10)
C(20)-C(19)-C(24)-C(25)	-179.2(6)
C(23)-C(24)-C(25)-C(26)	148.1(7)
C(19)-C(24)-C(25)-C(26)	-35.4(9)
C(23)-C(24)-C(25)-C(35)	-67.6(9)
C(19)-C(24)-C(25)-C(35)	108.9(8)

C(23)-C(24)-C(25)-C(27)	80.3(9)
C(19)-C(24)-C(25)-C(27)	-103.2(8)
C(35)-C(25)-C(26)-C(27)	109.3(6)
C(24)-C(25)-C(26)-C(27)	-105.7(7)
C(25)-C(26)-C(27)-C(38)	109.5(7)
C(25)-C(26)-C(27)-C(34)	-108.3(7)
C(35)-C(25)-C(27)-C(26)	-102.3(7)
C(24)-C(25)-C(27)-C(26)	110.5(7)
C(26)-C(25)-C(27)-C(38)	-108.1(7)
C(35)-C(25)-C(27)-C(38)	149.6(7)
C(24)-C(25)-C(27)-C(38)	2.3(10)
C(26)-C(25)-C(27)-C(34)	106.1(7)
C(35)-C(25)-C(27)-C(34)	3.8(10)
C(24)-C(25)-C(27)-C(34)	-143.4(7)
C(38)-C(29)-C(30)-C(31)	0.0(12)
C(29)-C(30)-C(31)-C(32)	-0.8(13)
C(30)-C(31)-C(32)-C(33)	0.9(14)
C(31)-C(32)-C(33)-C(38)	0.0(14)
C(26)-C(27)-C(34)-F(2)	-87.5(8)
C(38)-C(27)-C(34)-F(2)	57.0(9)
C(25)-C(27)-C(34)-F(2)	-154.8(6)
C(36)-O(4)-C(35)-O(3)	5.2(11)
C(36)-O(4)-C(35)-C(25)	-173.8(6)
C(26)-C(25)-C(35)-O(3)	-3.0(10)
C(24)-C(25)-C(35)-O(3)	-149.6(8)
C(27)-C(25)-C(35)-O(3)	62.6(10)
C(26)-C(25)-C(35)-O(4)	176.0(6)
C(24)-C(25)-C(35)-O(4)	29.4(9)
C(27)-C(25)-C(35)-O(4)	-118.4(7)
C(30)-C(29)-C(38)-C(33)	0.9(11)
C(30)-C(29)-C(38)-C(27)	-177.6(7)
C(32)-C(33)-C(38)-C(29)	-0.9(12)
C(32)-C(33)-C(38)-C(27)	177.6(8)
C(26)-C(27)-C(38)-C(29)	-152.3(7)
C(34)-C(27)-C(38)-C(29)	64.0(10)
C(25)-C(27)-C(38)-C(29)	-83.5(9)
C(26)-C(27)-C(38)-C(33)	29.3(10)
C(34)-C(27)-C(38)-C(33)	-114.4(8)
C(25)-C(27)-C(38)-C(33)	98.1(9)
C(6)-C(1)-C(2)-C(3)	-1.0(11)
C(1)-C(2)-C(3)-C(4)	0.2(11)
C(1)-C(2)-C(3)-Br(1)	-179.1(5)
C(2)-C(3)-C(4)-C(5)	0.1(11)
Br(1)-C(3)-C(4)-C(5)	179.3(5)
C(3)-C(4)-C(5)-C(6)	0.5(11)
C(4)-C(5)-C(6)-C(1)	-1.3(10)
C(4)-C(5)-C(6)-C(7)	176.6(6)
C(2)-C(1)-C(6)-C(5)	1.5(10)

C(2)-C(1)-C(6)-C(7)	-176.4(6)
C(5)-C(6)-C(7)-C(17)	-73.8(8)
C(1)-C(6)-C(7)-C(17)	104.0(7)
C(5)-C(6)-C(7)-C(8)	143.6(7)
C(1)-C(6)-C(7)-C(8)	-38.6(9)
C(5)-C(6)-C(7)-C(9)	76.0(8)
C(1)-C(6)-C(7)-C(9)	-106.2(8)
C(17)-C(7)-C(8)-C(9)	108.7(6)
C(6)-C(7)-C(8)-C(9)	-108.3(6)
C(7)-C(8)-C(9)-C(16)	-107.6(6)
C(7)-C(8)-C(9)-C(10)	106.2(7)
C(17)-C(7)-C(9)-C(8)	-103.5(7)
C(6)-C(7)-C(9)-C(8)	107.3(7)
C(17)-C(7)-C(9)-C(16)	0.6(10)
C(8)-C(7)-C(9)-C(16)	104.1(7)
C(6)-C(7)-C(9)-C(16)	-148.6(7)
C(17)-C(7)-C(9)-C(10)	143.9(7)
C(8)-C(7)-C(9)-C(10)	-112.5(7)
C(6)-C(7)-C(9)-C(10)	-5.3(10)
C(8)-C(9)-C(10)-C(15)	-160.6(7)
C(16)-C(9)-C(10)-C(15)	53.2(10)
C(7)-C(9)-C(10)-C(15)	-90.9(9)
C(8)-C(9)-C(10)-C(11)	23.9(10)
C(16)-C(9)-C(10)-C(11)	-122.3(8)
C(7)-C(9)-C(10)-C(11)	93.6(8)
C(15)-C(10)-C(11)-C(12)	-0.4(11)
C(9)-C(10)-C(11)-C(12)	175.2(7)
C(10)-C(11)-C(12)-C(13)	-0.6(12)
C(11)-C(12)-C(13)-C(14)	1.4(13)
C(12)-C(13)-C(14)-C(15)	-1.2(13)
C(11)-C(10)-C(15)-C(14)	0.6(12)
C(9)-C(10)-C(15)-C(14)	-174.9(7)
C(13)-C(14)-C(15)-C(10)	0.2(13)
C(8)-C(9)-C(16)-F(1)	139.0(7)
C(10)-C(9)-C(16)-F(1)	-72.2(8)
C(7)-C(9)-C(16)-F(1)	72.5(9)
C(18)-O(2)-C(17)-O(1)	5.8(11)
C(18)-O(2)-C(17)-C(7)	-176.8(6)
C(8)-C(7)-C(17)-O(1)	-7.7(11)
C(6)-C(7)-C(17)-O(1)	-151.7(7)
C(9)-C(7)-C(17)-O(1)	58.2(10)
C(8)-C(7)-C(17)-O(2)	174.9(6)
C(6)-C(7)-C(17)-O(2)	31.0(9)
C(9)-C(7)-C(17)-O(2)	-119.1(7)

Symmetry transformations used to generate equivalent atoms:

Table S19. Hydrogen bonds for z [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)