Supporting Information for

Cobalt-catalyzed nucleophilic fluorination in organic carbonates

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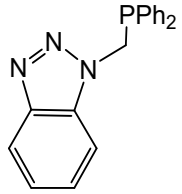
1. NMR Spectra

NMR spectra of 1-((diphenylphosphanyl)methyl)- 1*H*-benzo-1,2,3-triazole (1)



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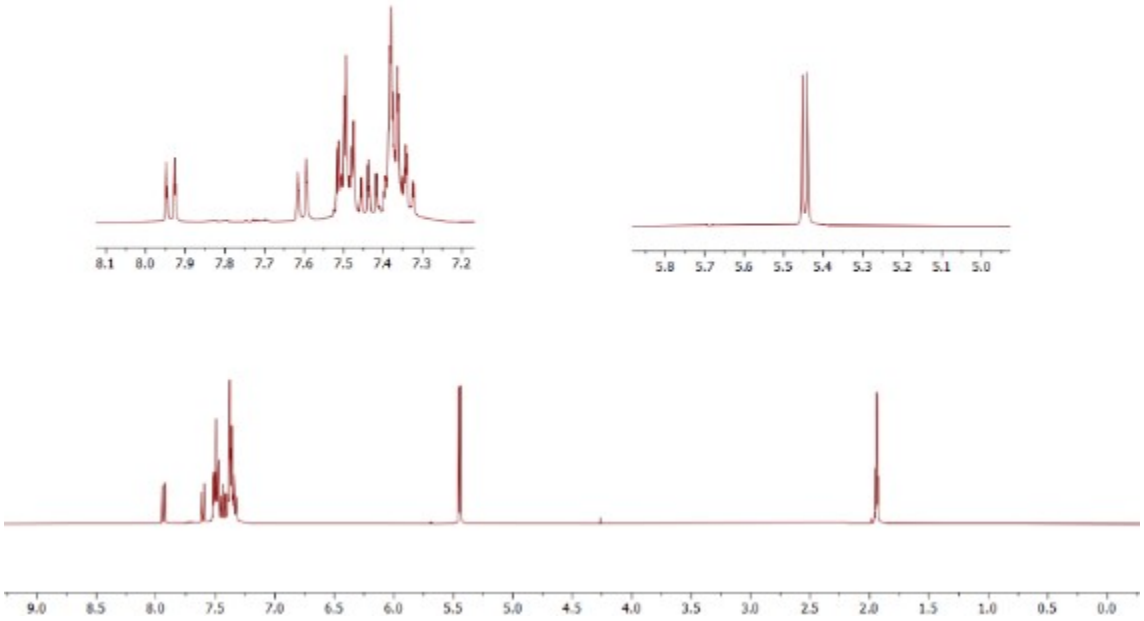


Figure S1. ^{1}H NMR of **1** in CD_3CN.

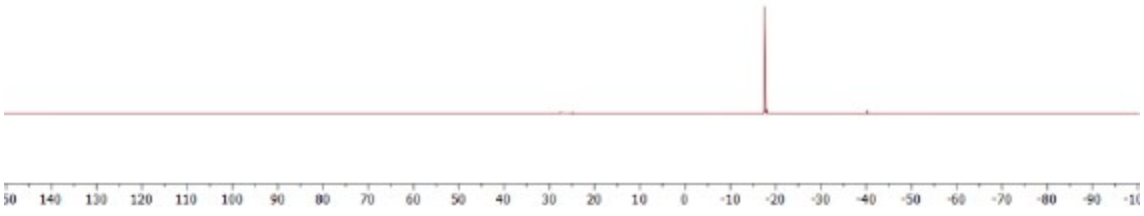


Figure S2. $^{31}P\{^{1}H\}$ NMR of **1** in CD_3CN.

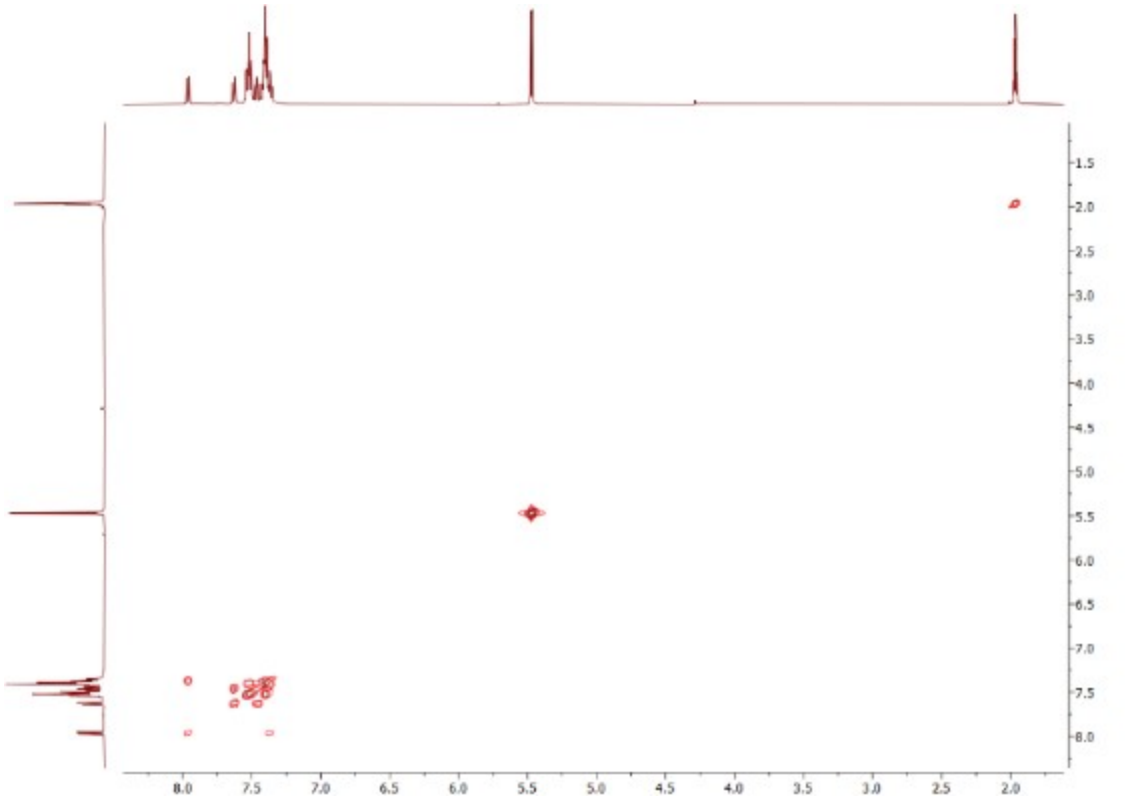


Figure S3. ^{1}H-^{1}H COSY of **1** in CD_3CN.

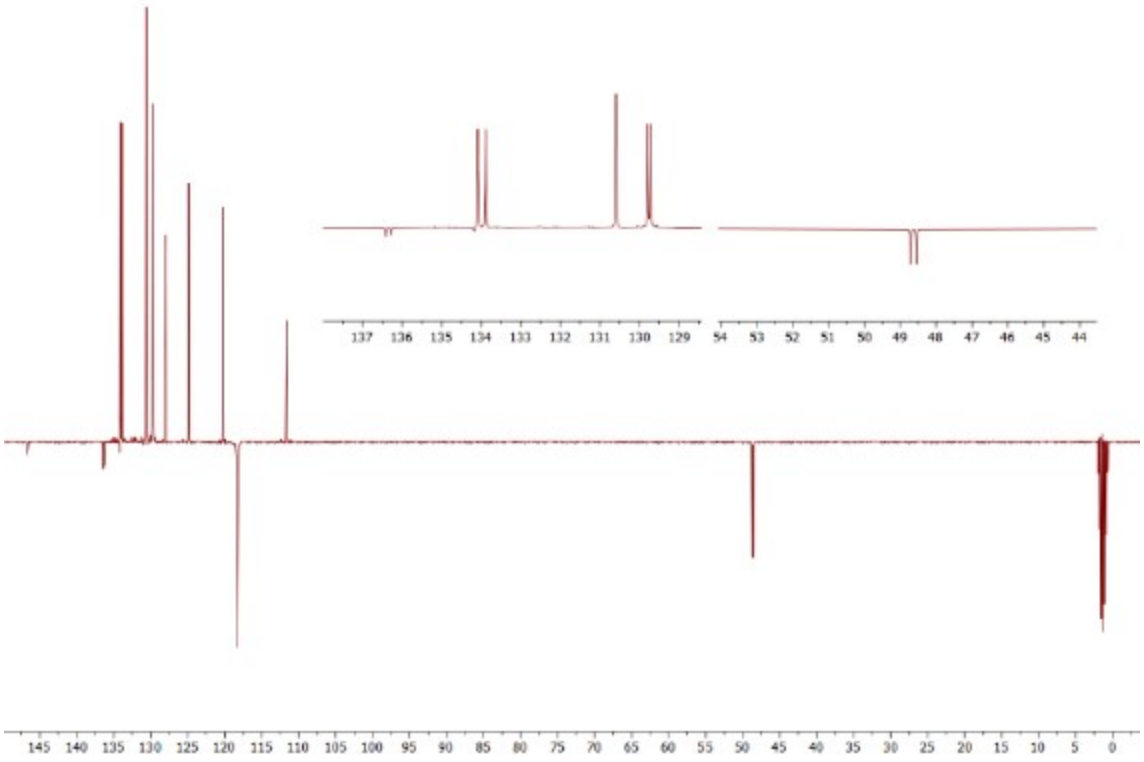


Figure S4. APT NMR of **1** in CD_3CN.

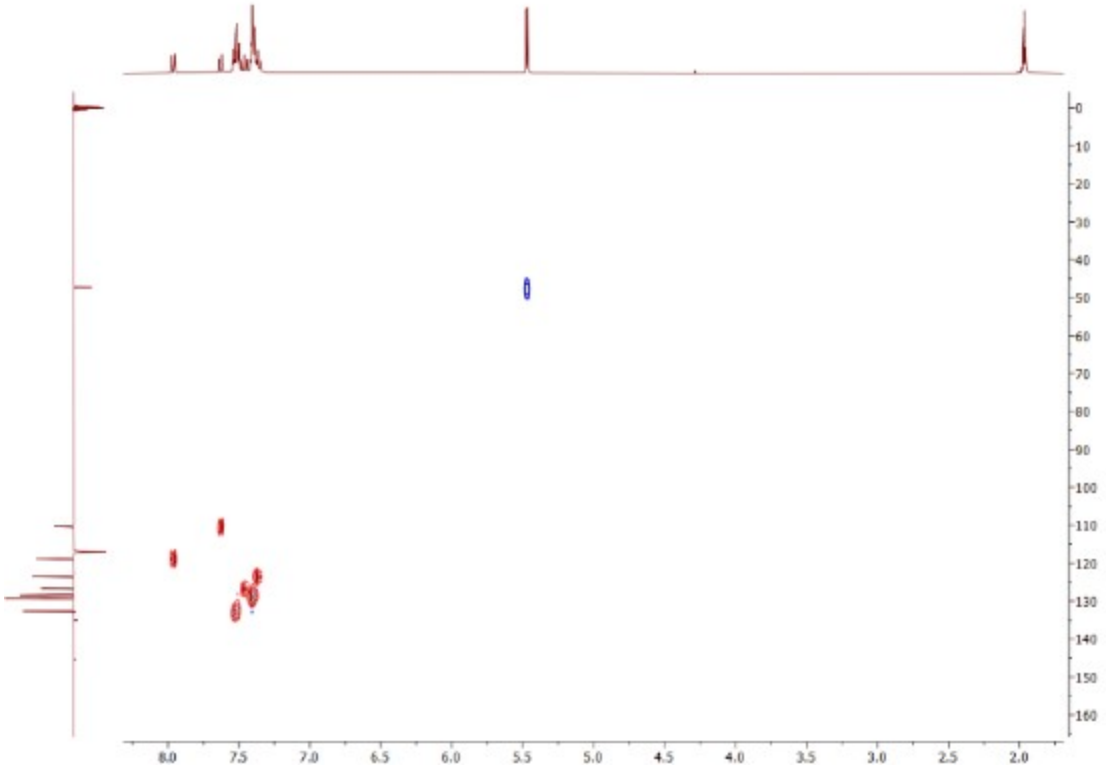


Figure S5. ^{1}H-^{13}C HSQC of **1** in CD_3CN.

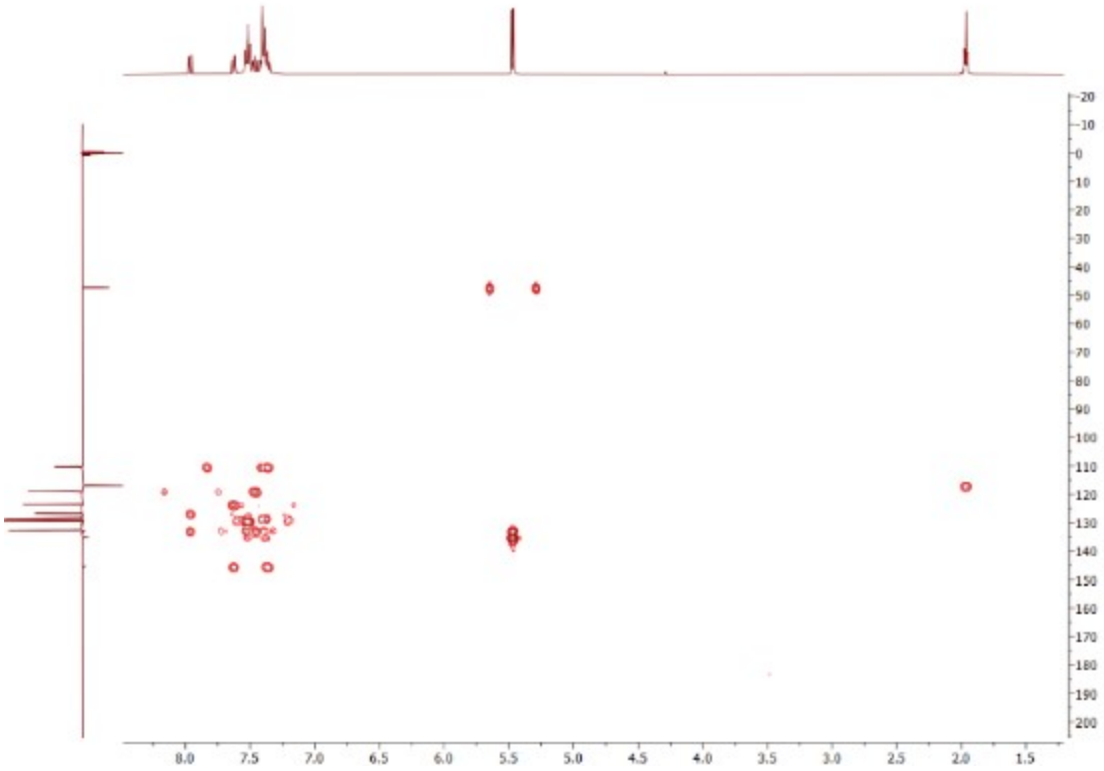
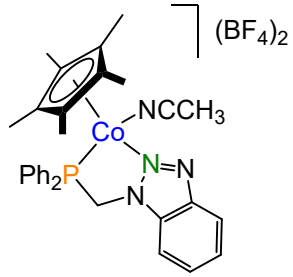


Figure S6. ^{1}H-^{13}C HMBC of **1** in CD_3CN.

NMR spectra of cobalt complex 2



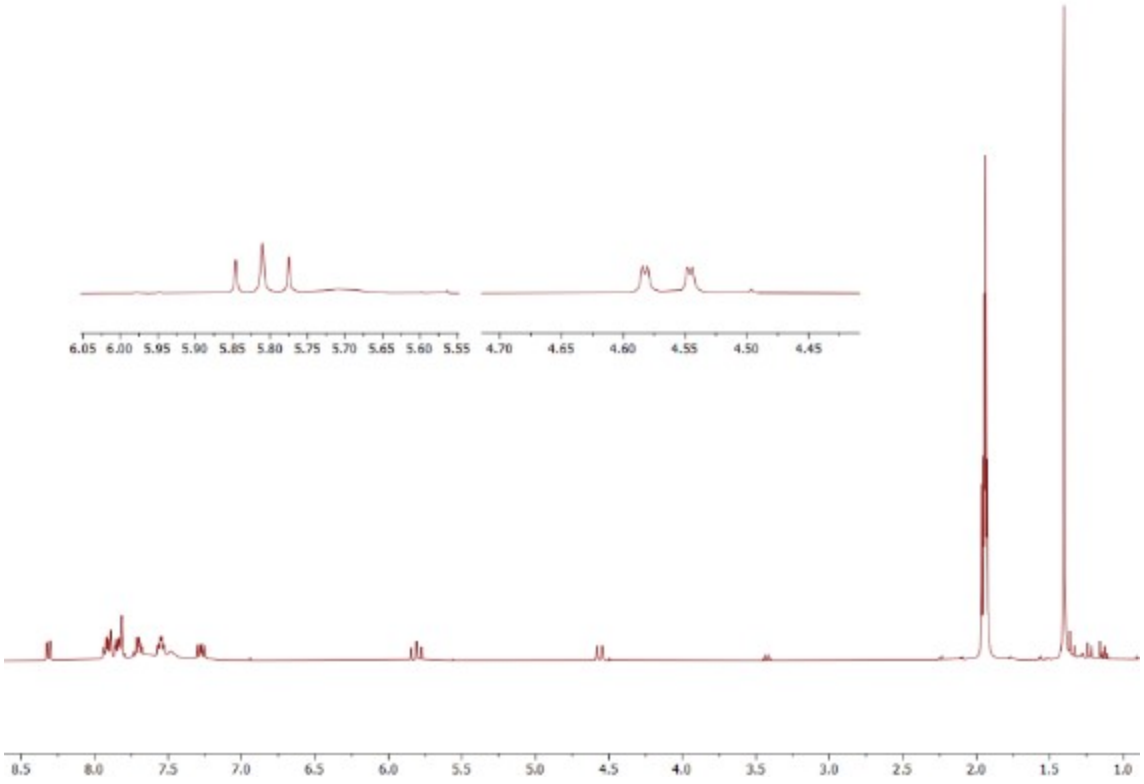


Figure S7. ^{1}H NMR of **2** in CD_3CN.

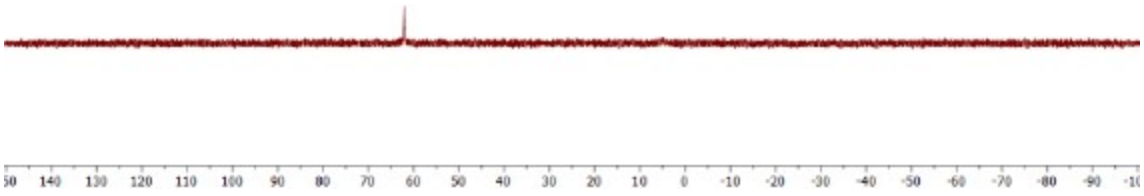


Figure S8. $^{31}P\{^{1}H\}$ NMR of **2** in CD_3CN.

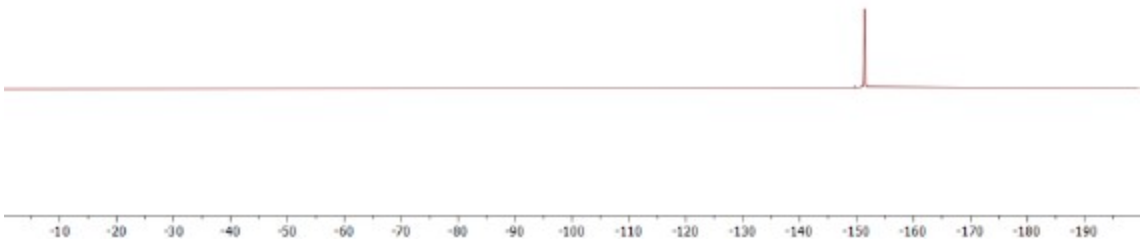


Figure S9. $^{19}F\{^{1}H\}$ NMR of **2** in CD_3CN.

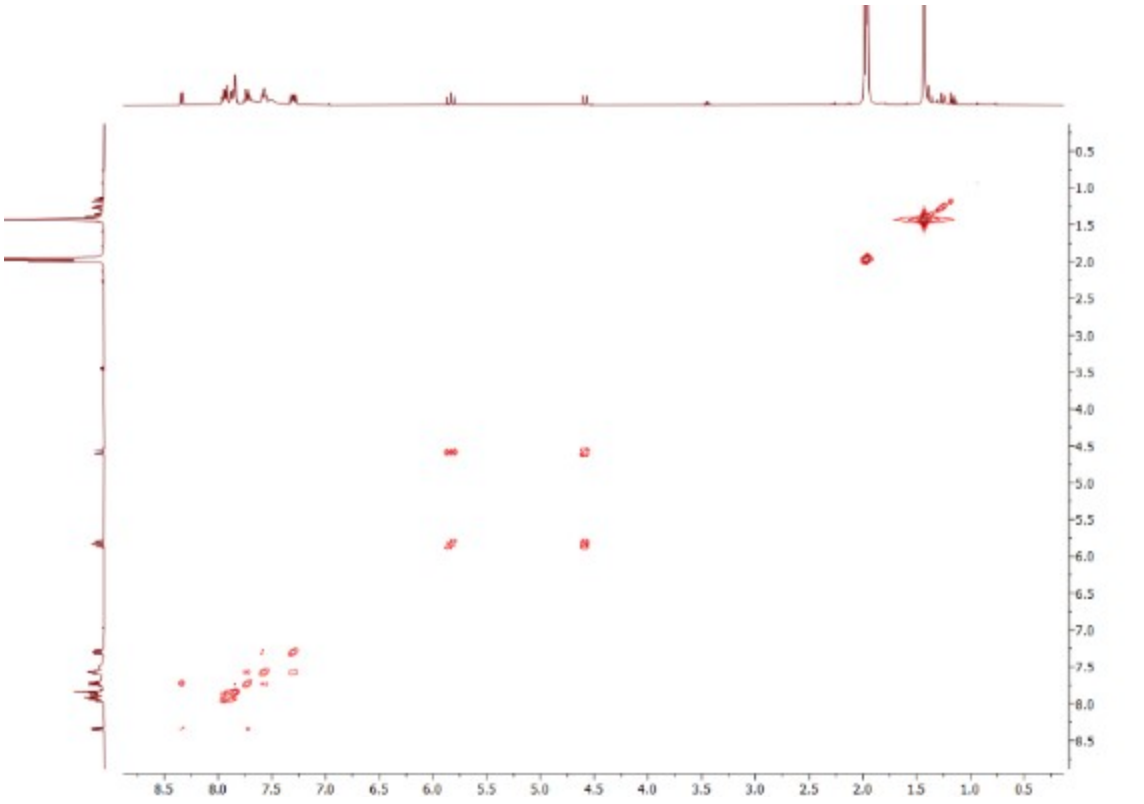


Figure S10. ^{1}H-^{1}H COSY of **2** in CD_3CN.

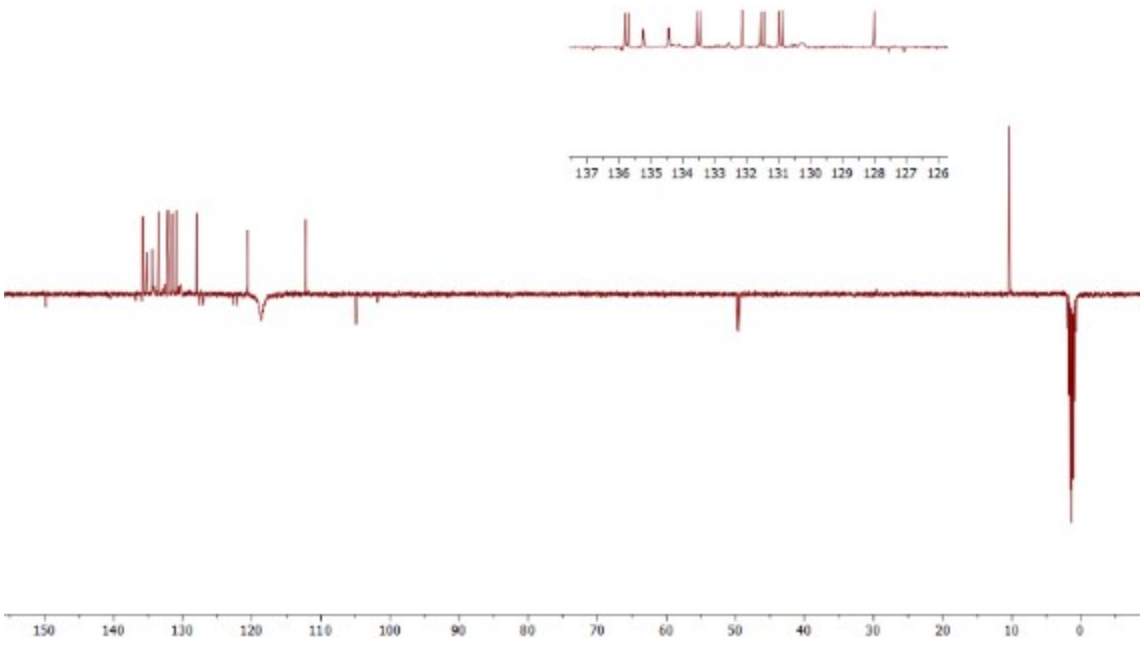


Figure S11. APT NMR of **2** in CD_3CN.

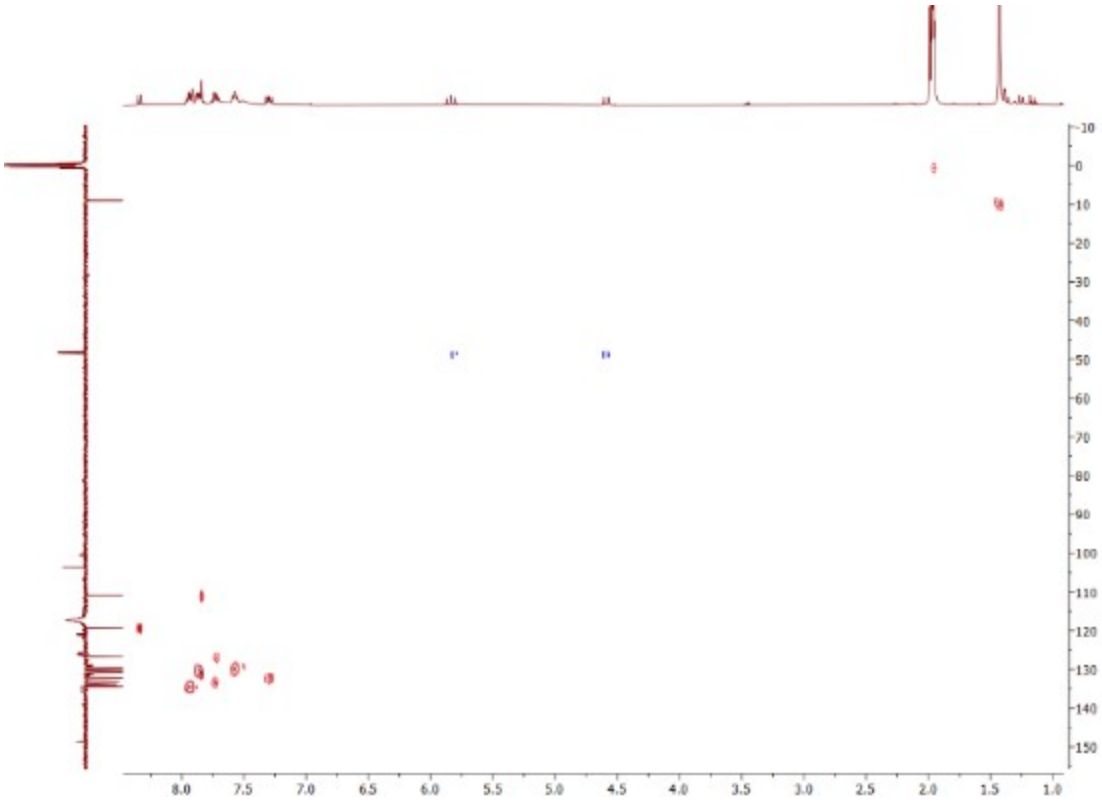


Figure S12. ^{1}H-^{13}C HSQC of **2** in CD_3CN.

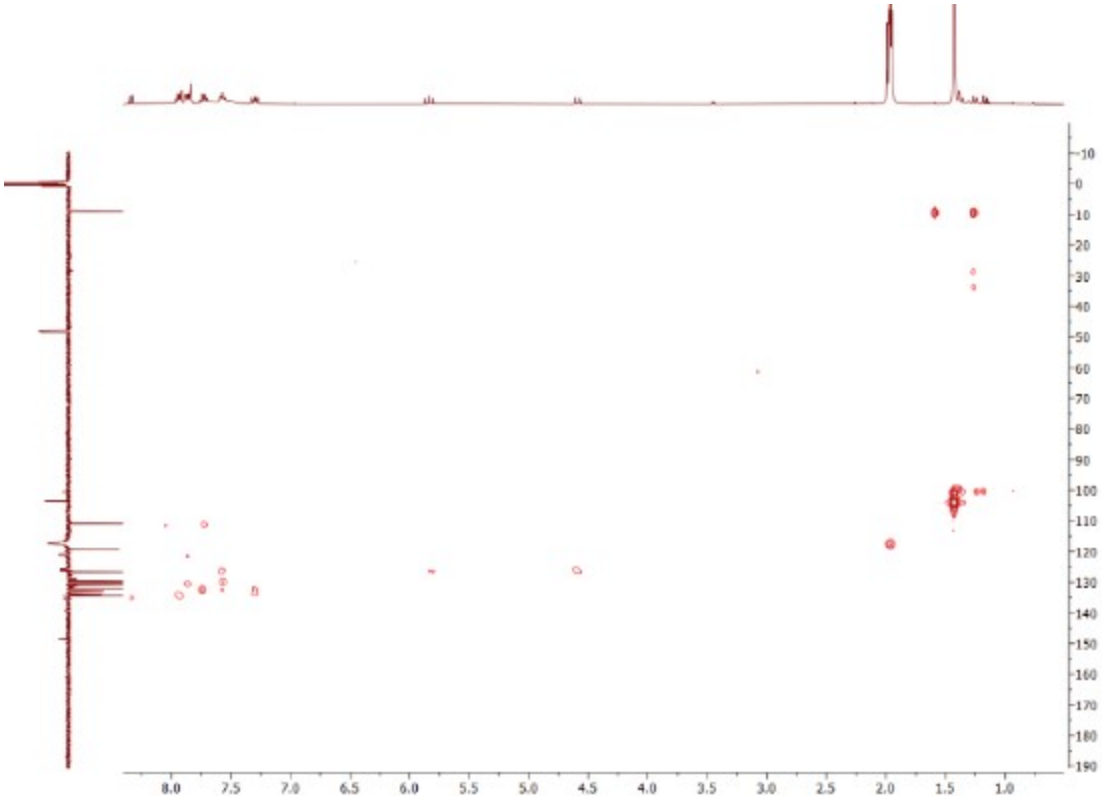


Figure S13. ^{1}H-^{13}C HMBC of **2** in CD_3CN.

NMR spectra of cobalt complex 3

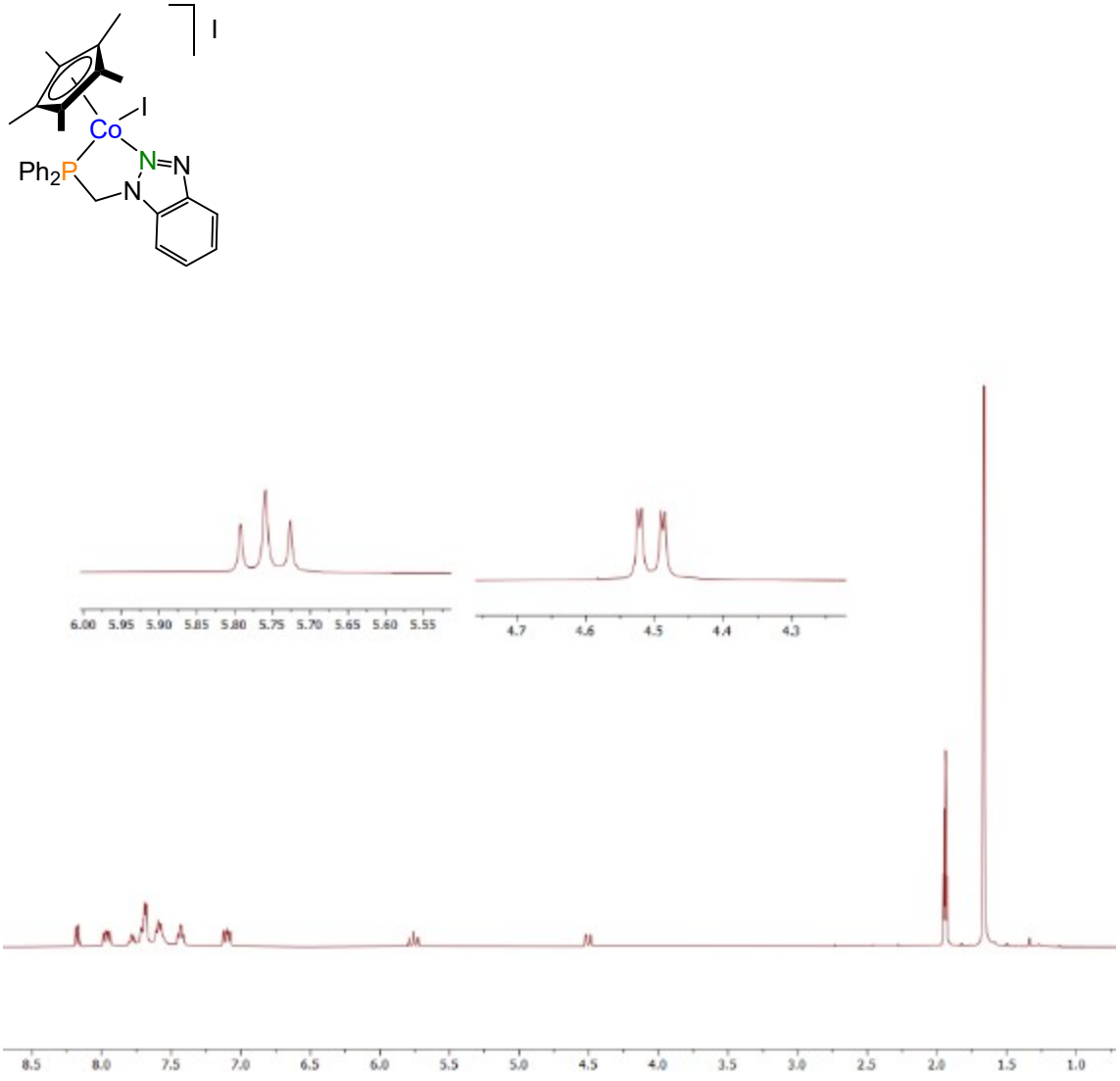


Figure S14. ^{1}H NMR of **3** in CD_3CN.

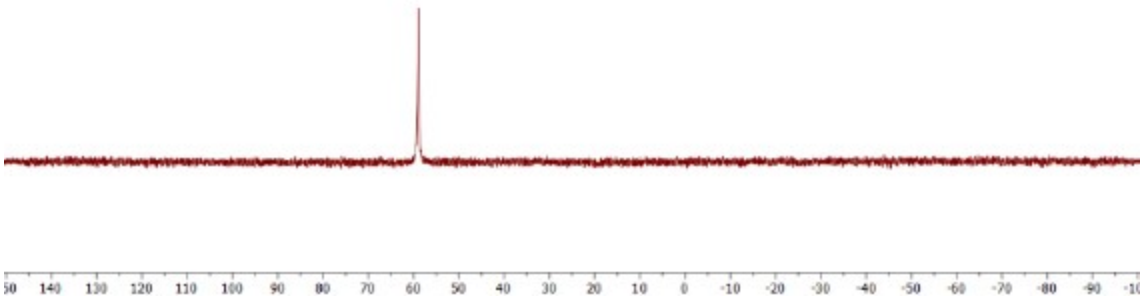


Figure S15. $^{31}P\{^{1}H\}$ NMR of **3** in CD_3CN.

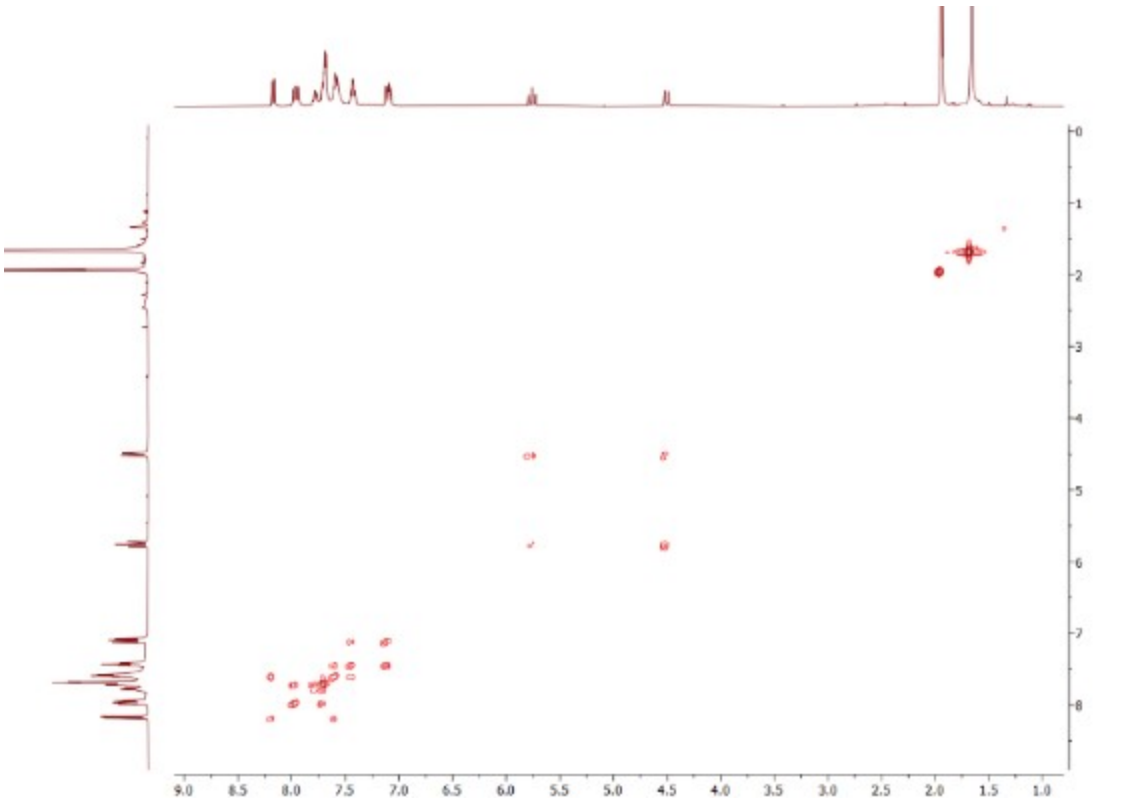


Figure S16. ^{1}H-^{1}H COSY of **3** in CD_3CN.

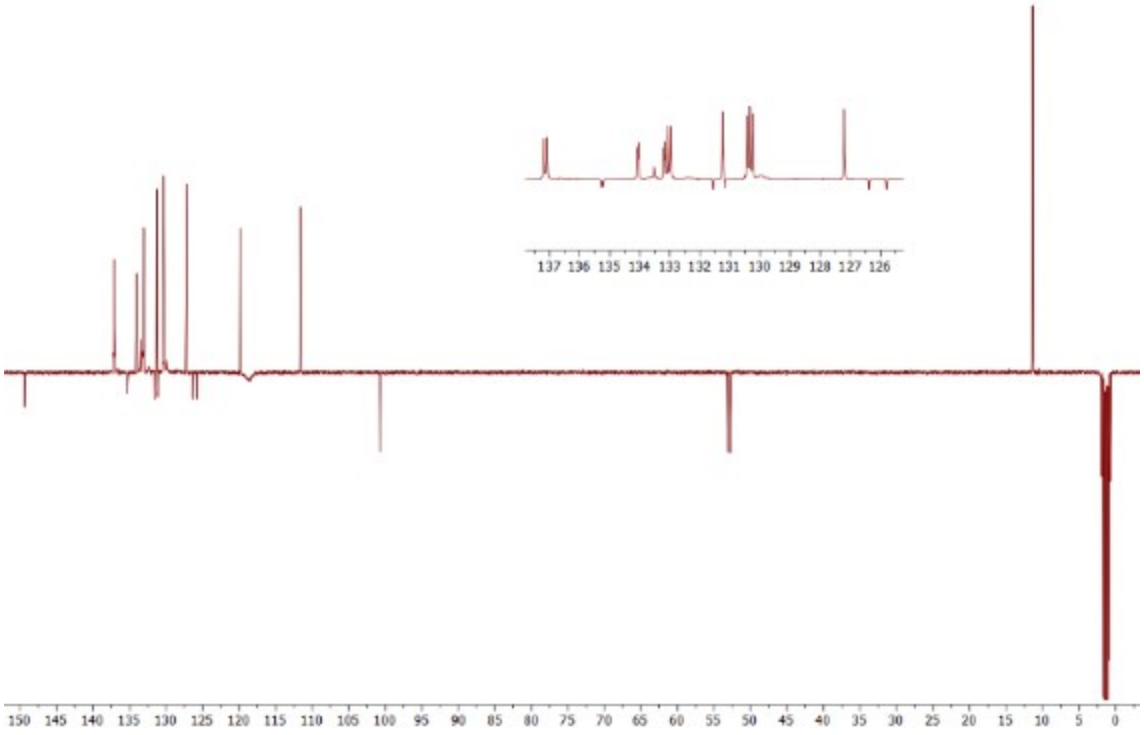


Figure S17. APT NMR of **3** in CD_3CN.

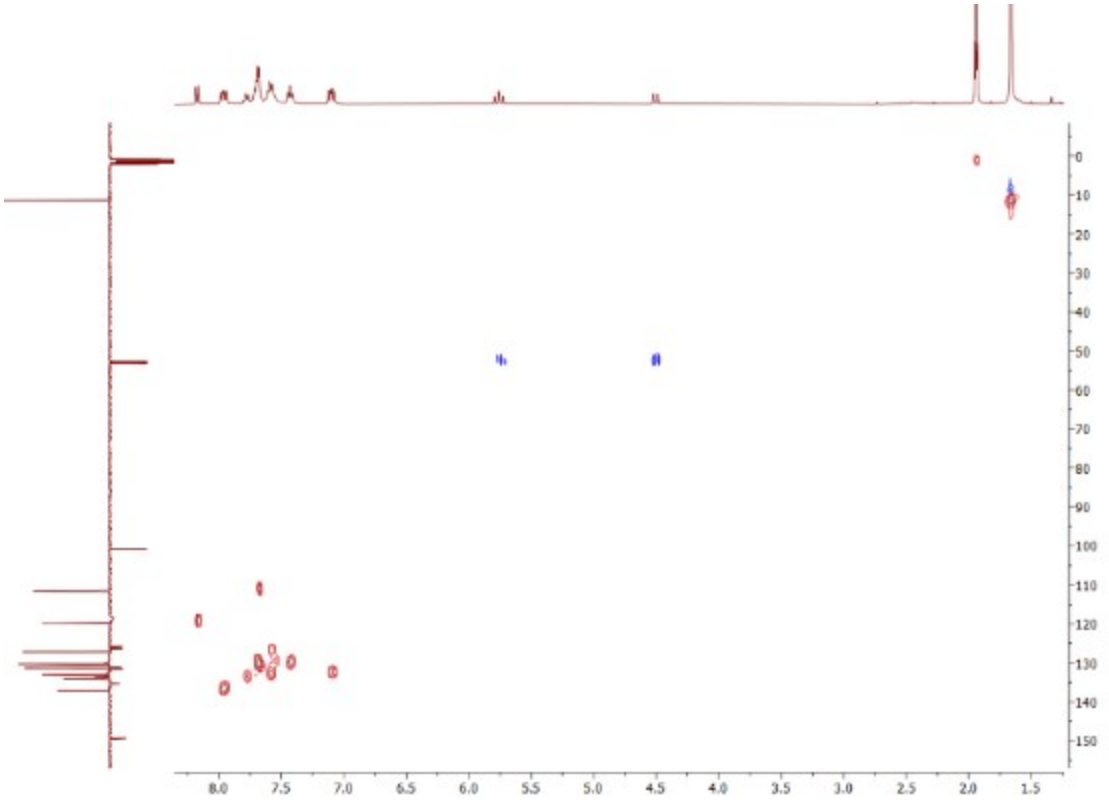


Figure S18. ^{1}H-^{13}C HSQC of **3** in CD_3CN.

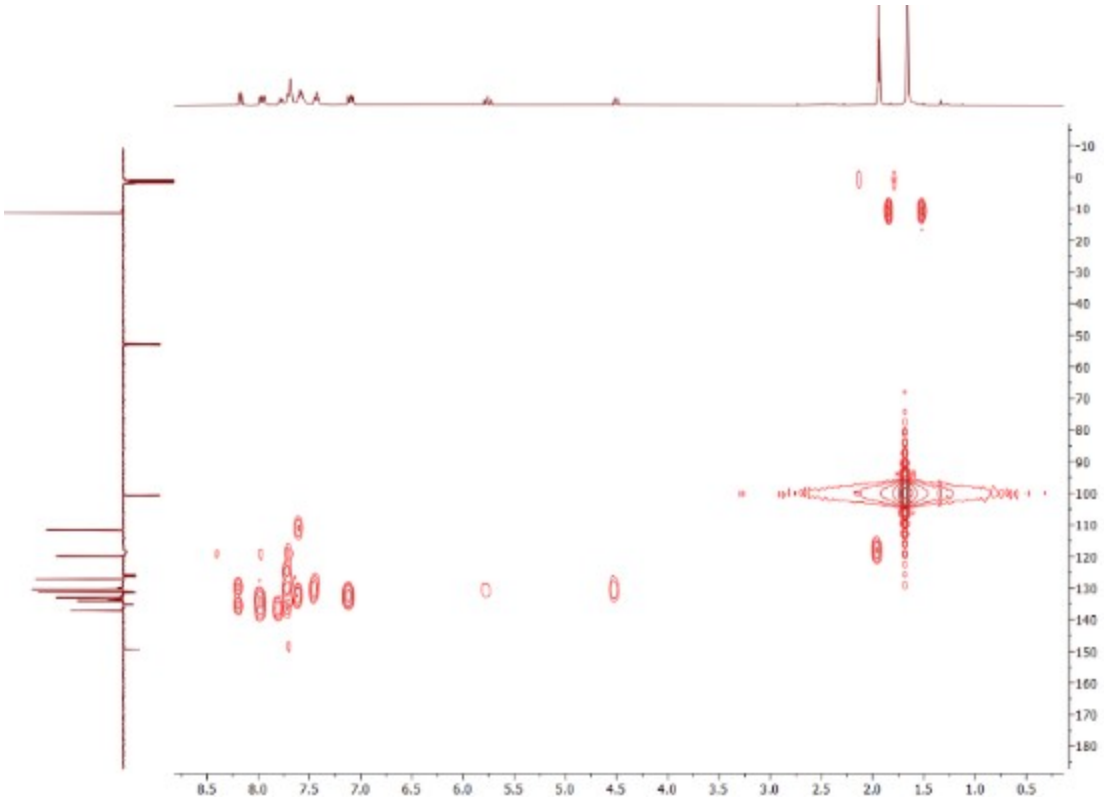


Figure S19. ^{1}H-^{13}C HMBC of **3** in CD_3CN.

2. ^{19}F NMR Spectra of the fluorination reactions

Table 1

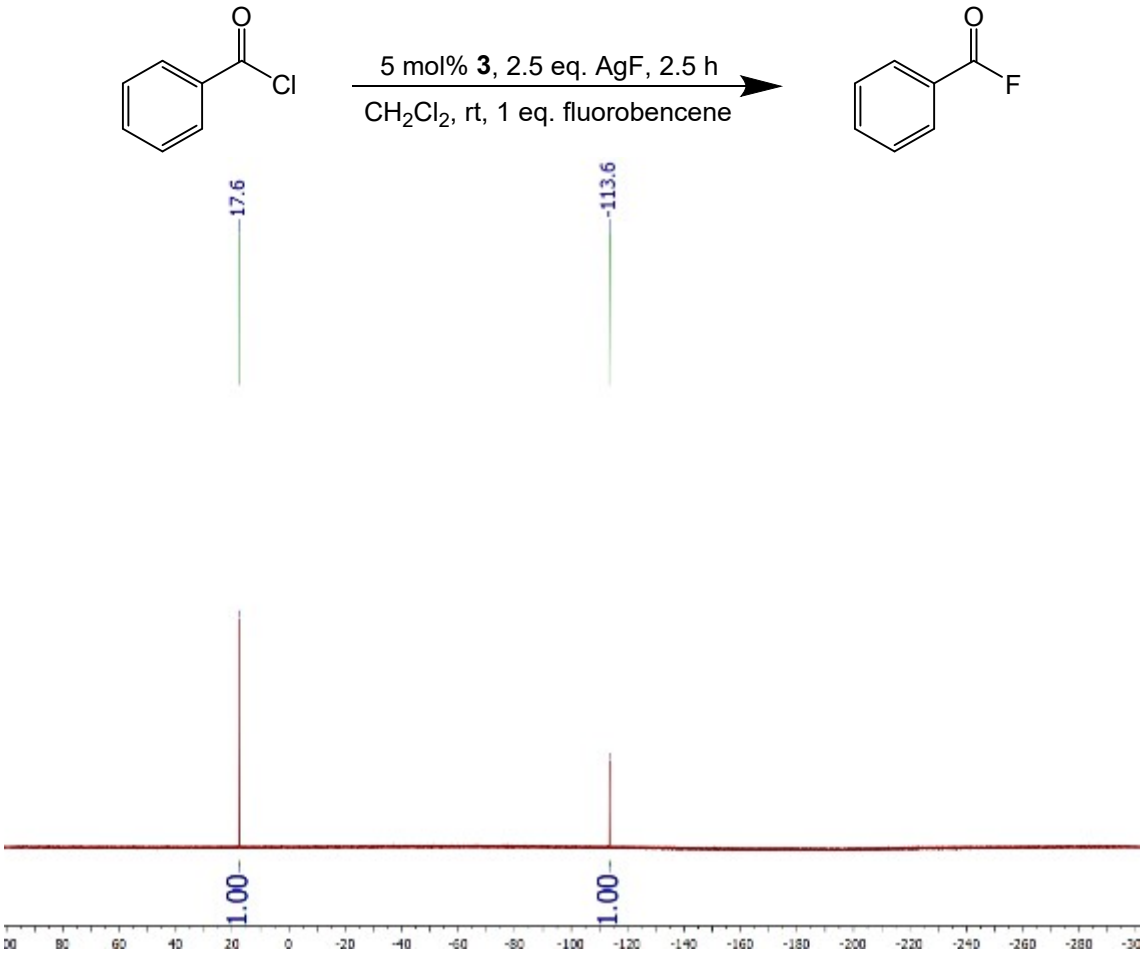


Figure S20. Crude ^{19}F NMR in $CDCl_3$.

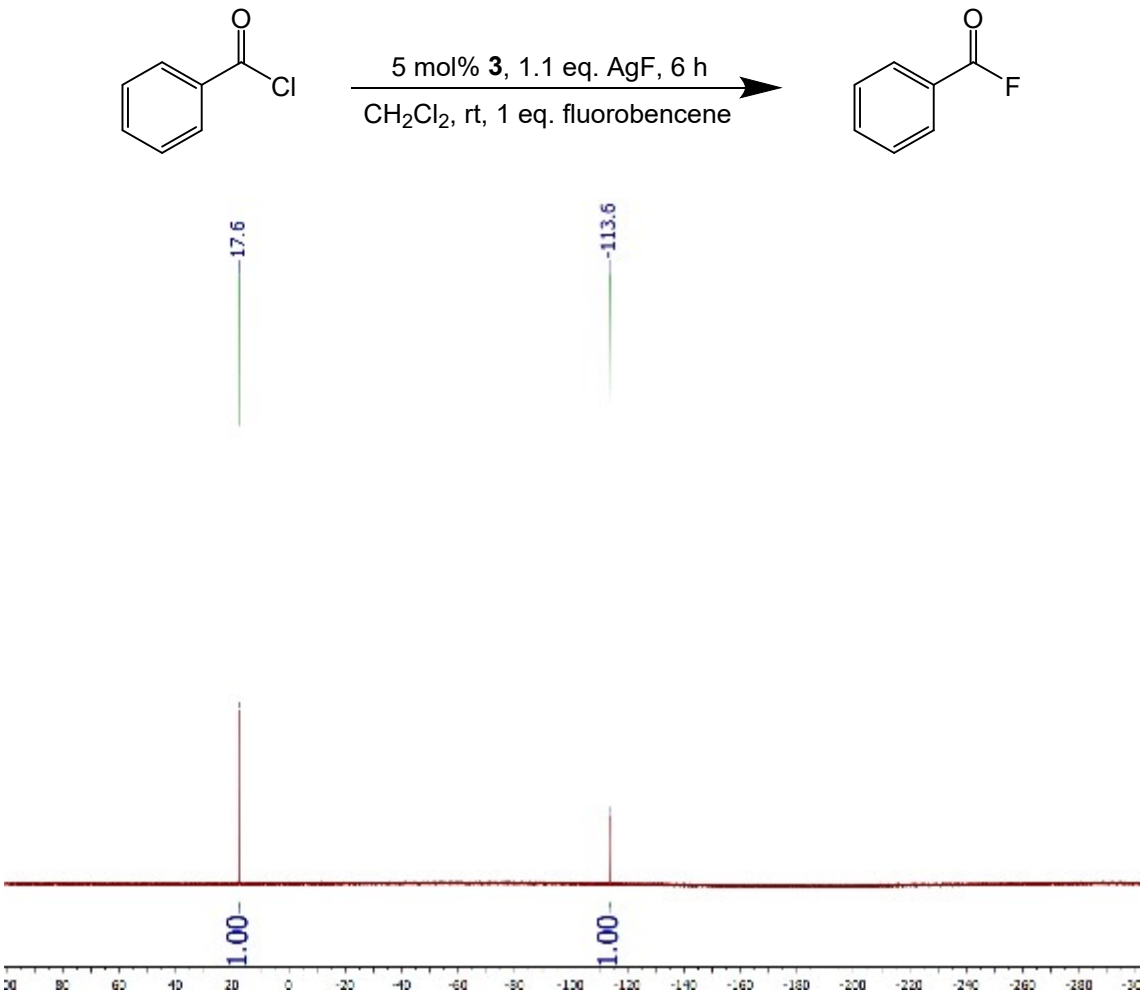


Figure S21. Crude ^{19}F NMR in $CDCl_3$.

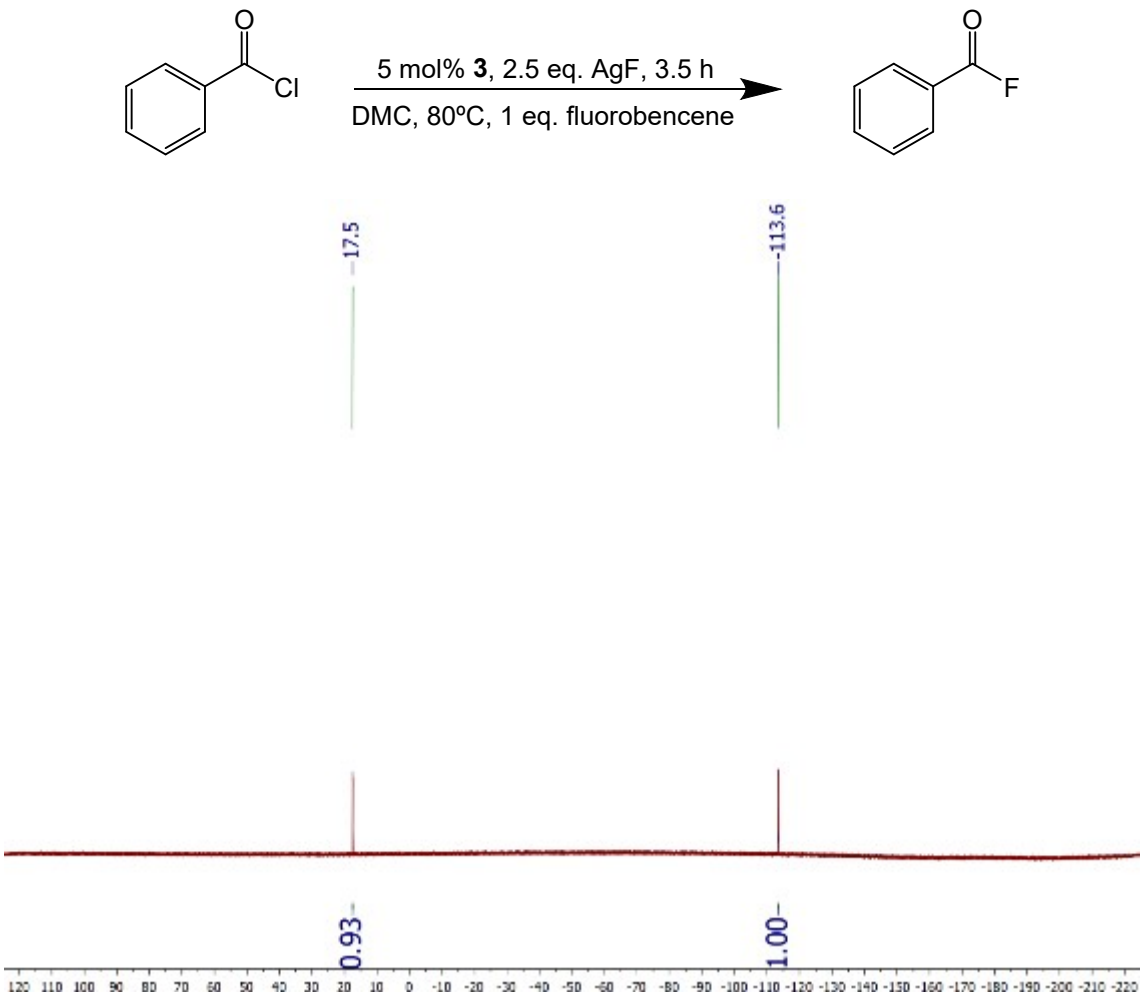


Figure S22. Crude ^{19}F NMR in $CDCl_3$.

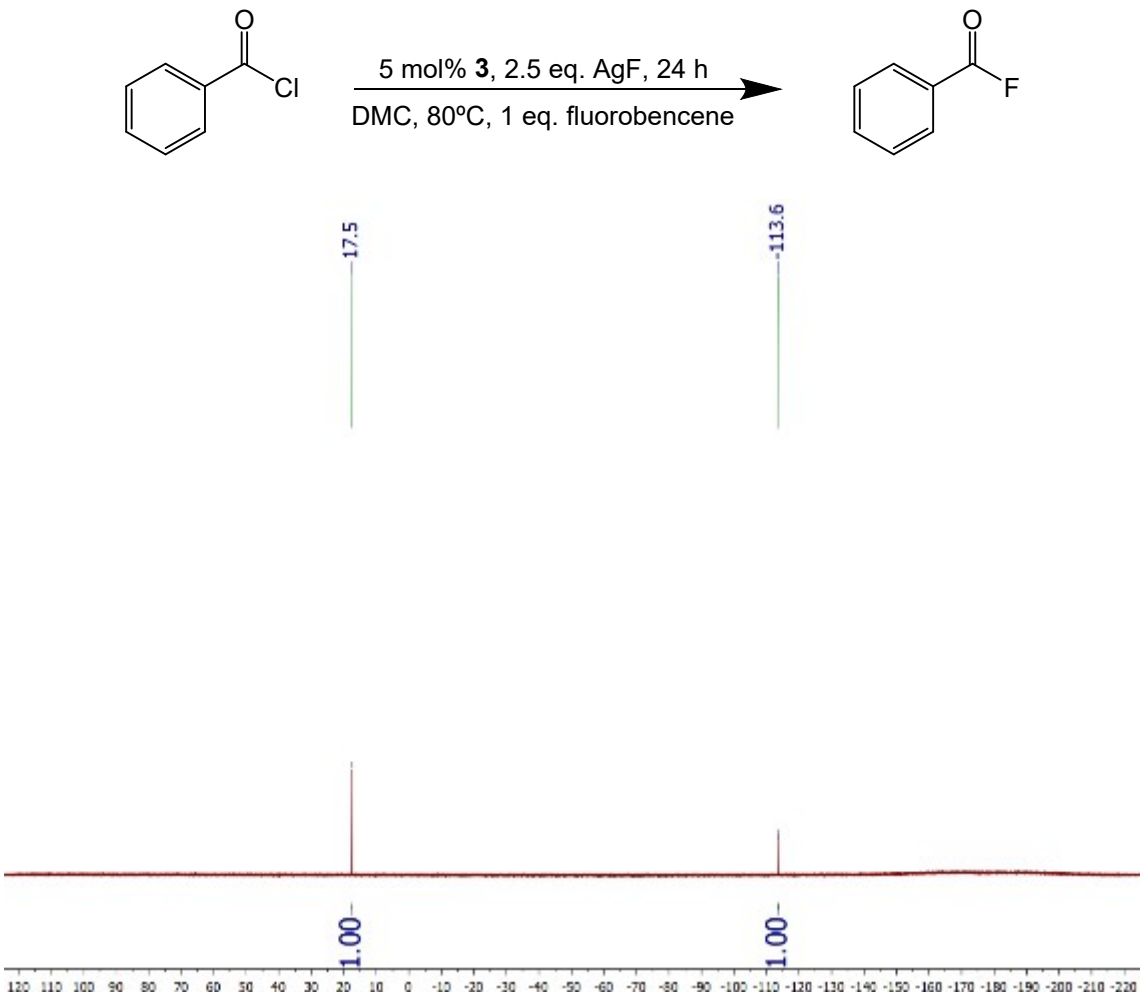


Figure S23. Crude ^{19}F NMR in $CDCl_3$.

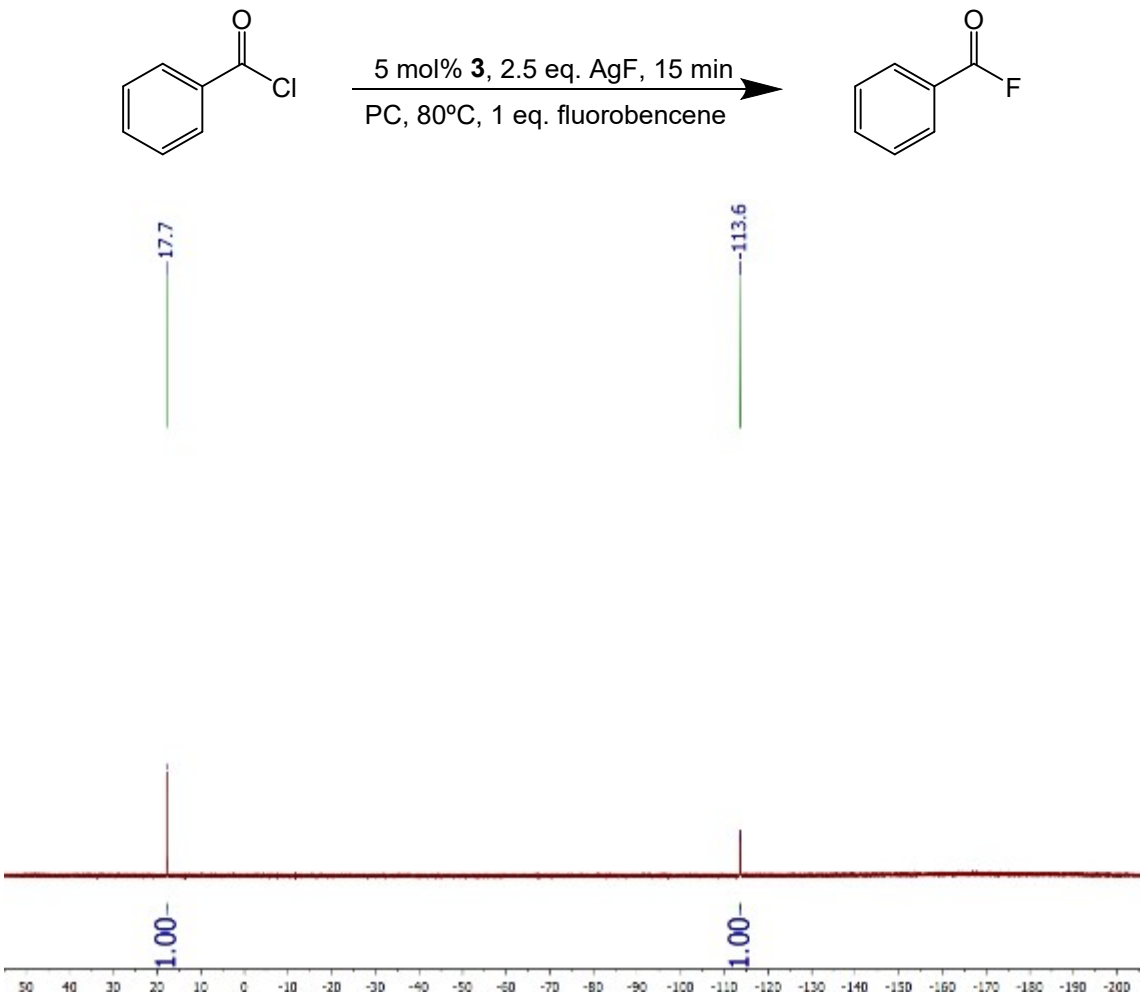


Figure S24. Crude ^{19}F NMR in $CDCl_3$.

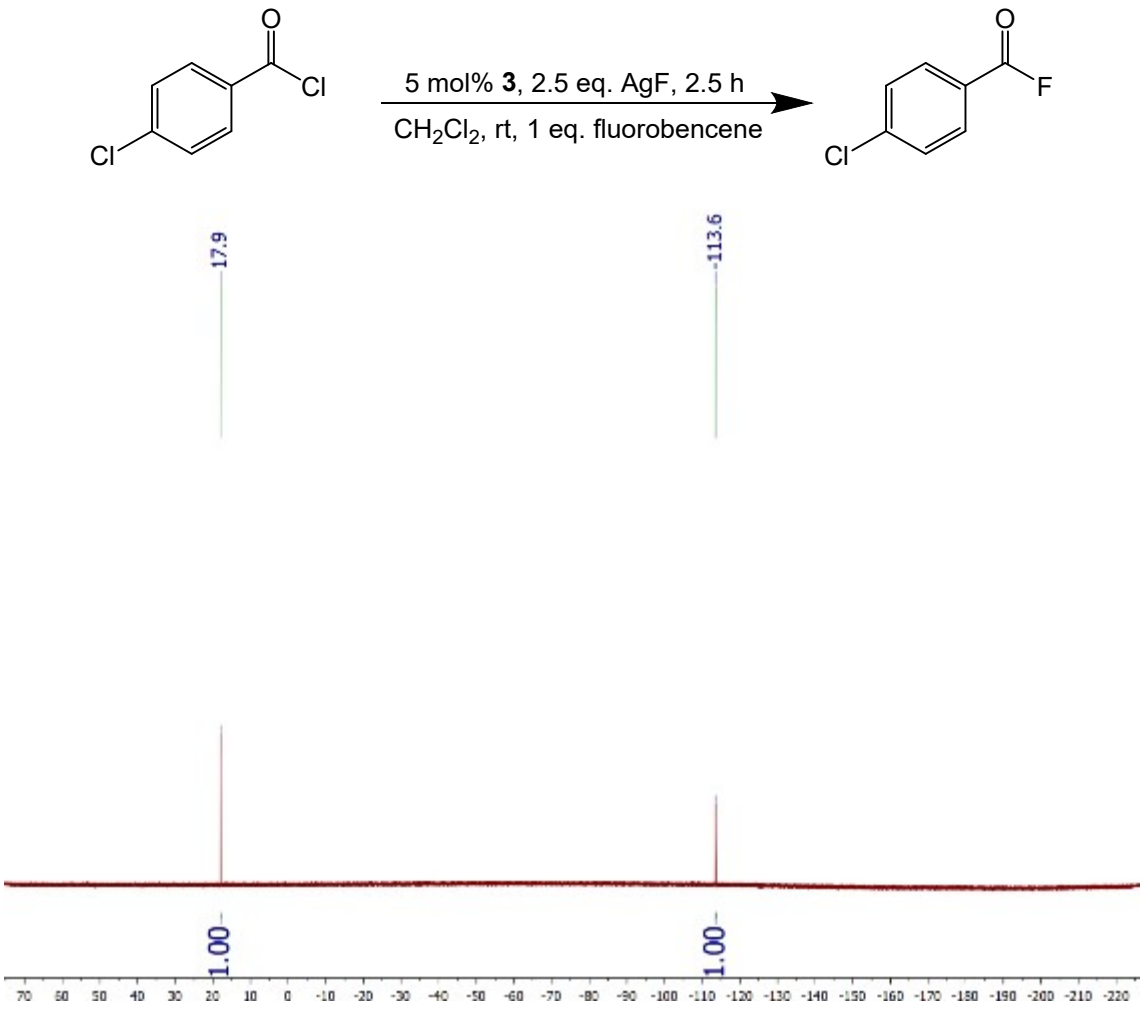


Figure S25. Crude ^{19}F NMR in $CDCl_3$.

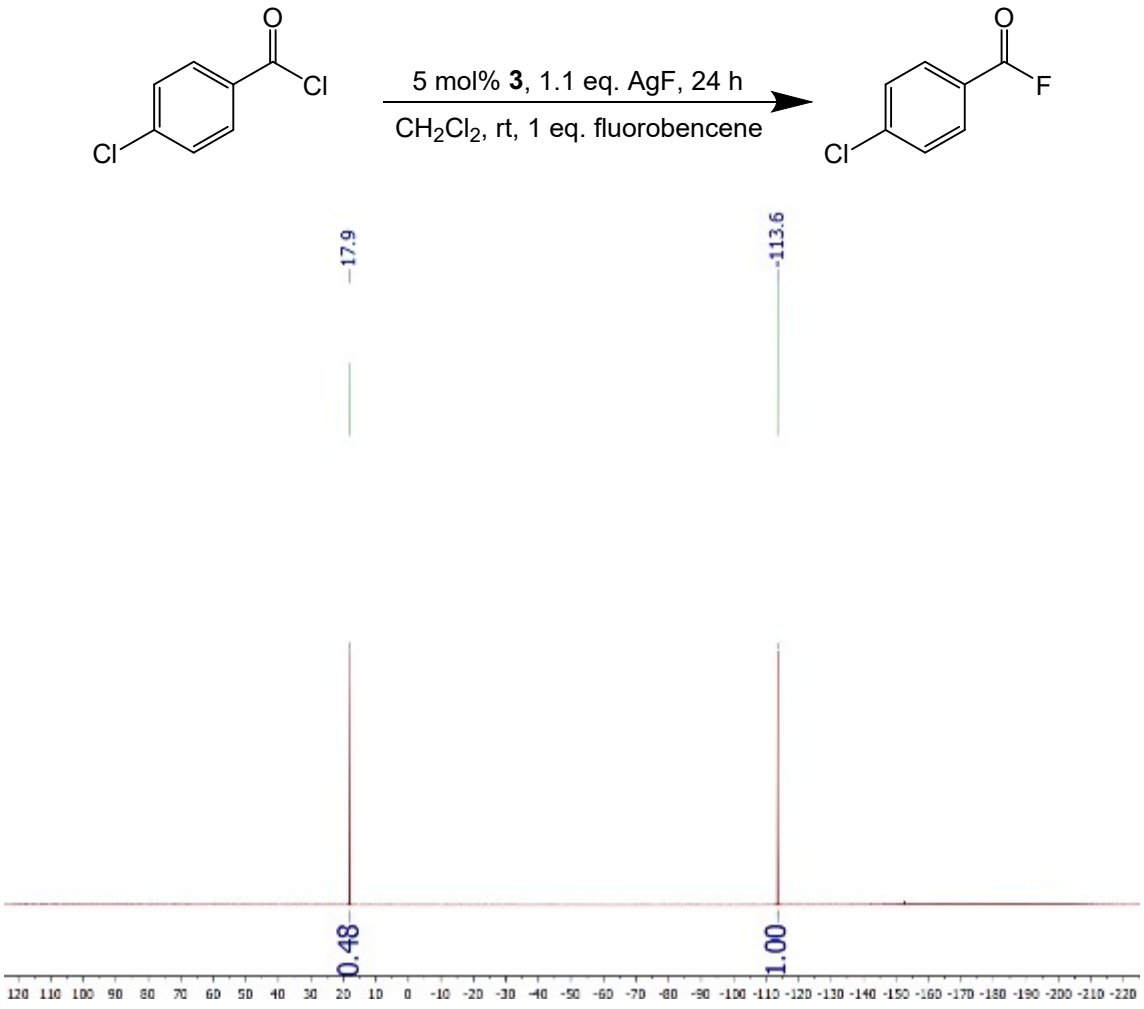


Figure S26. Crude ^{19}F NMR in $CDCl_3$.

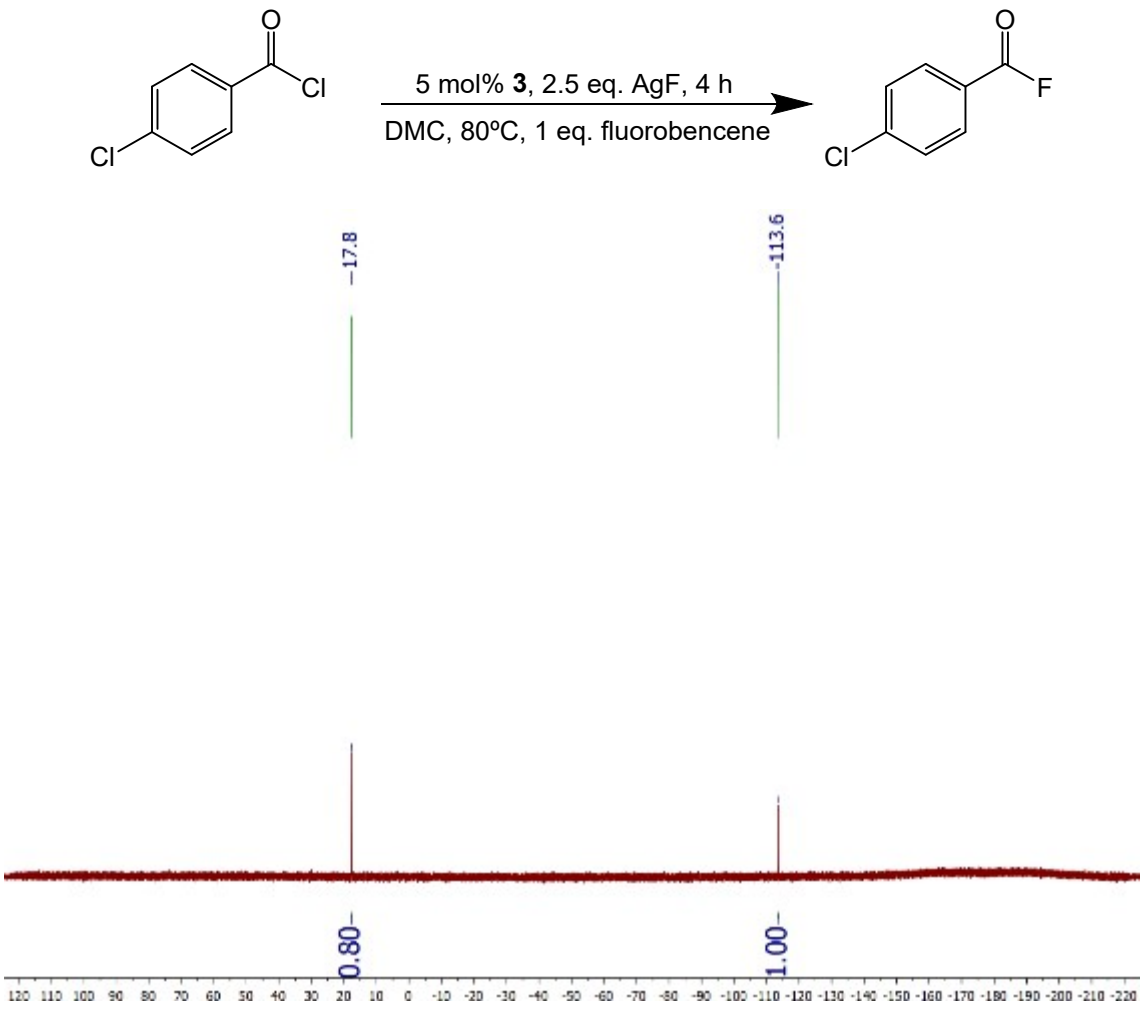


Figure S27. Crude ^{19}F NMR in $CDCl_3$.

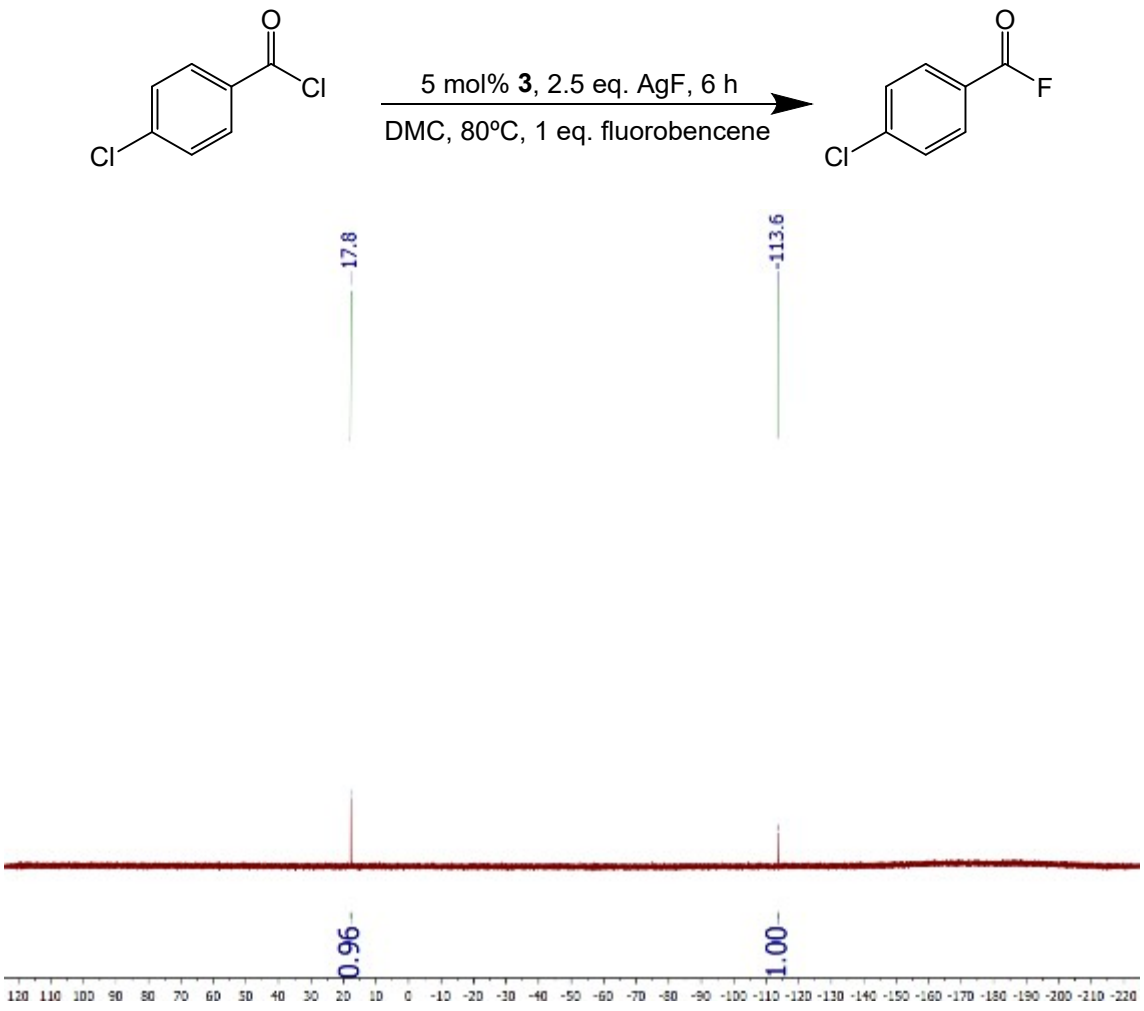


Figure S28. Crude ^{19}F NMR in $CDCl_3$.

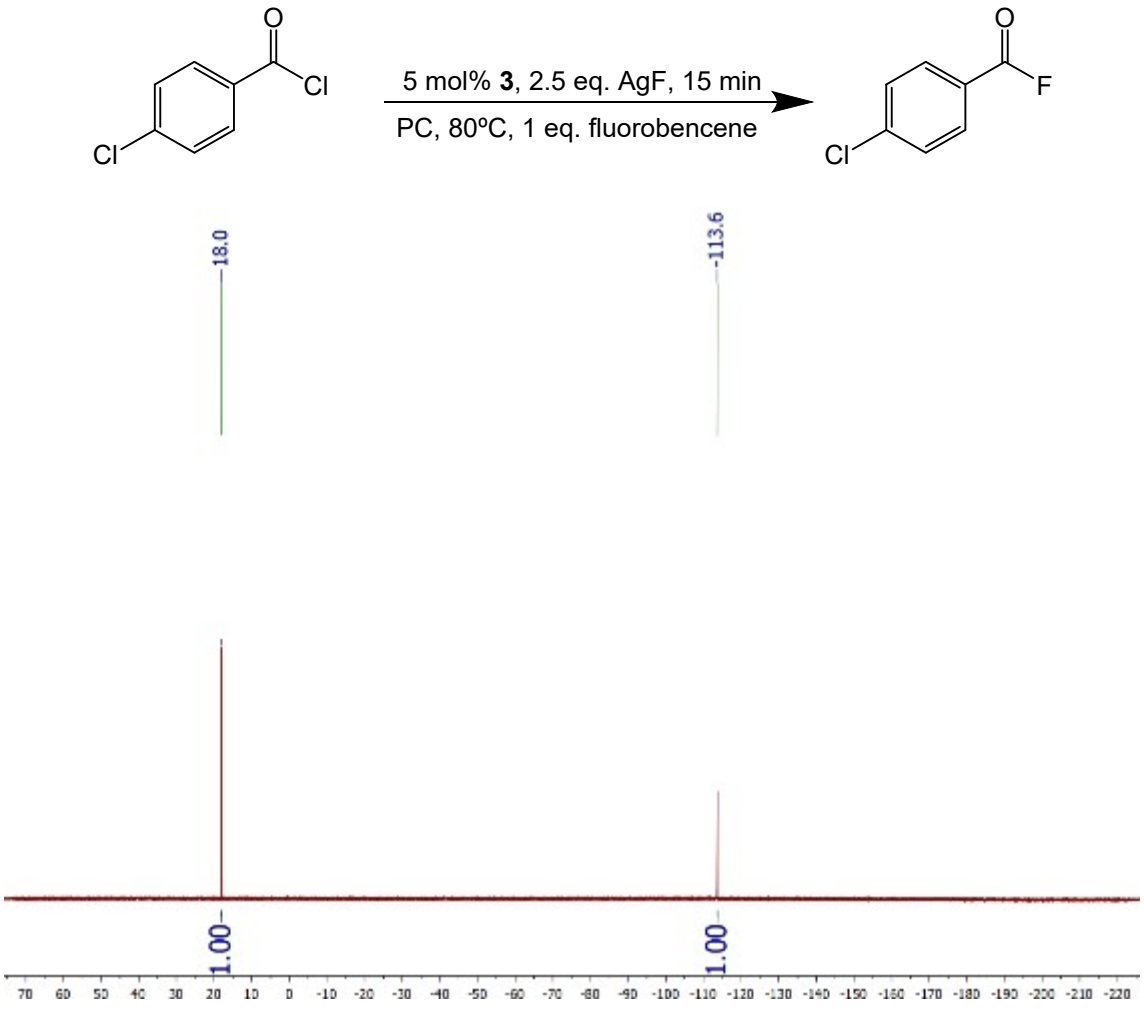


Figure S29. Crude ^{19}F NMR in $CDCl_3$.

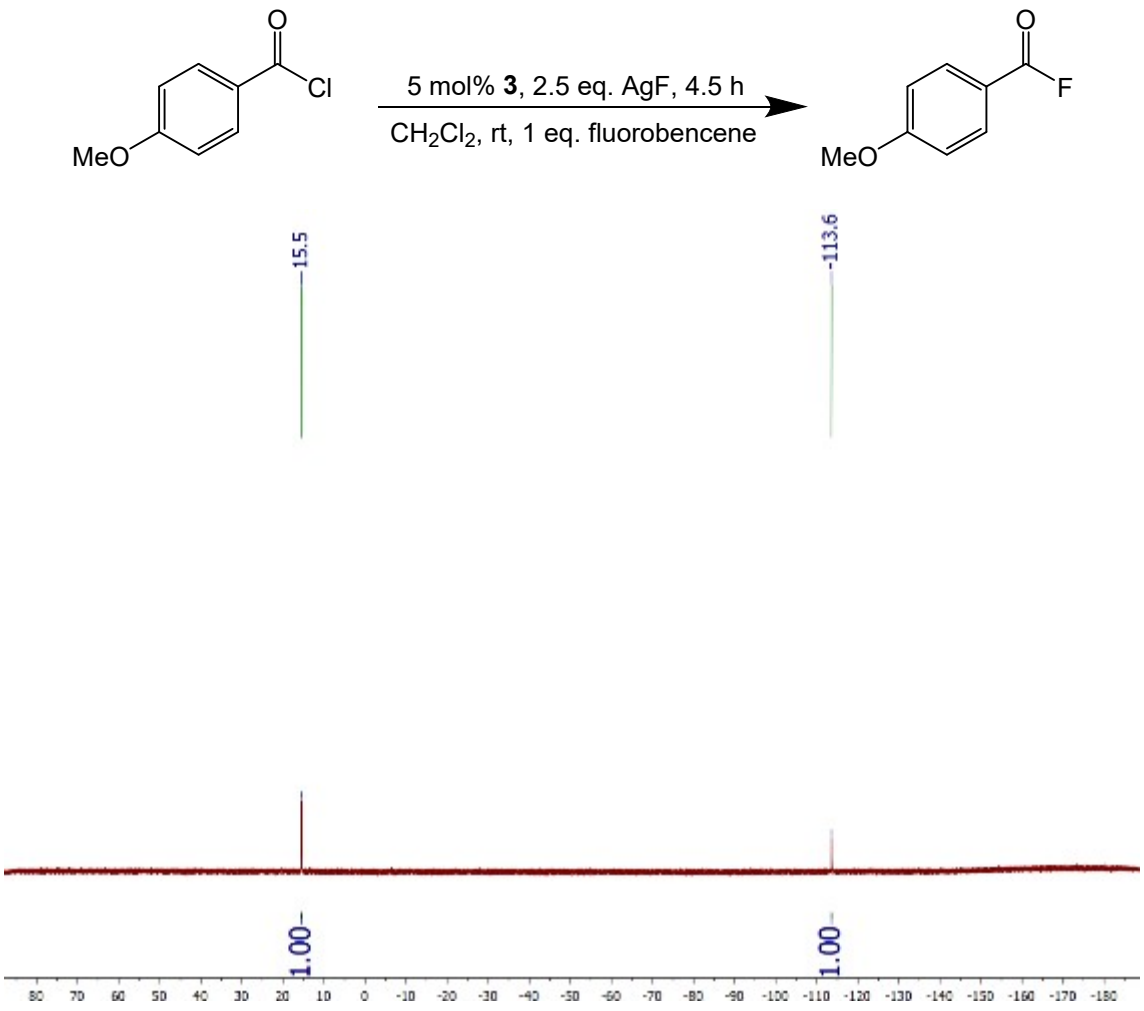


Figure S30. Crude ^{19}F NMR in $CDCl_3$.

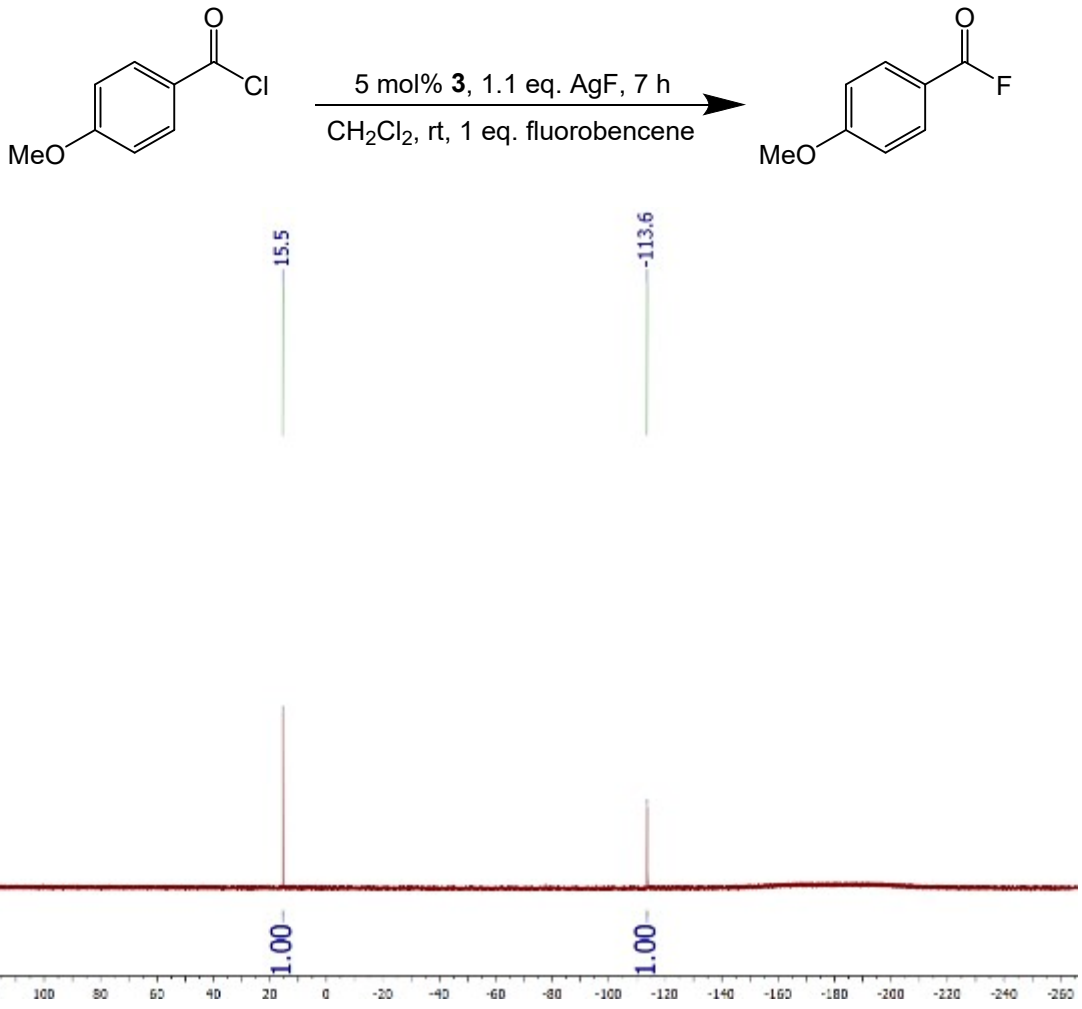


Figure S31. Crude ^{19}F NMR in $CDCl_3$.

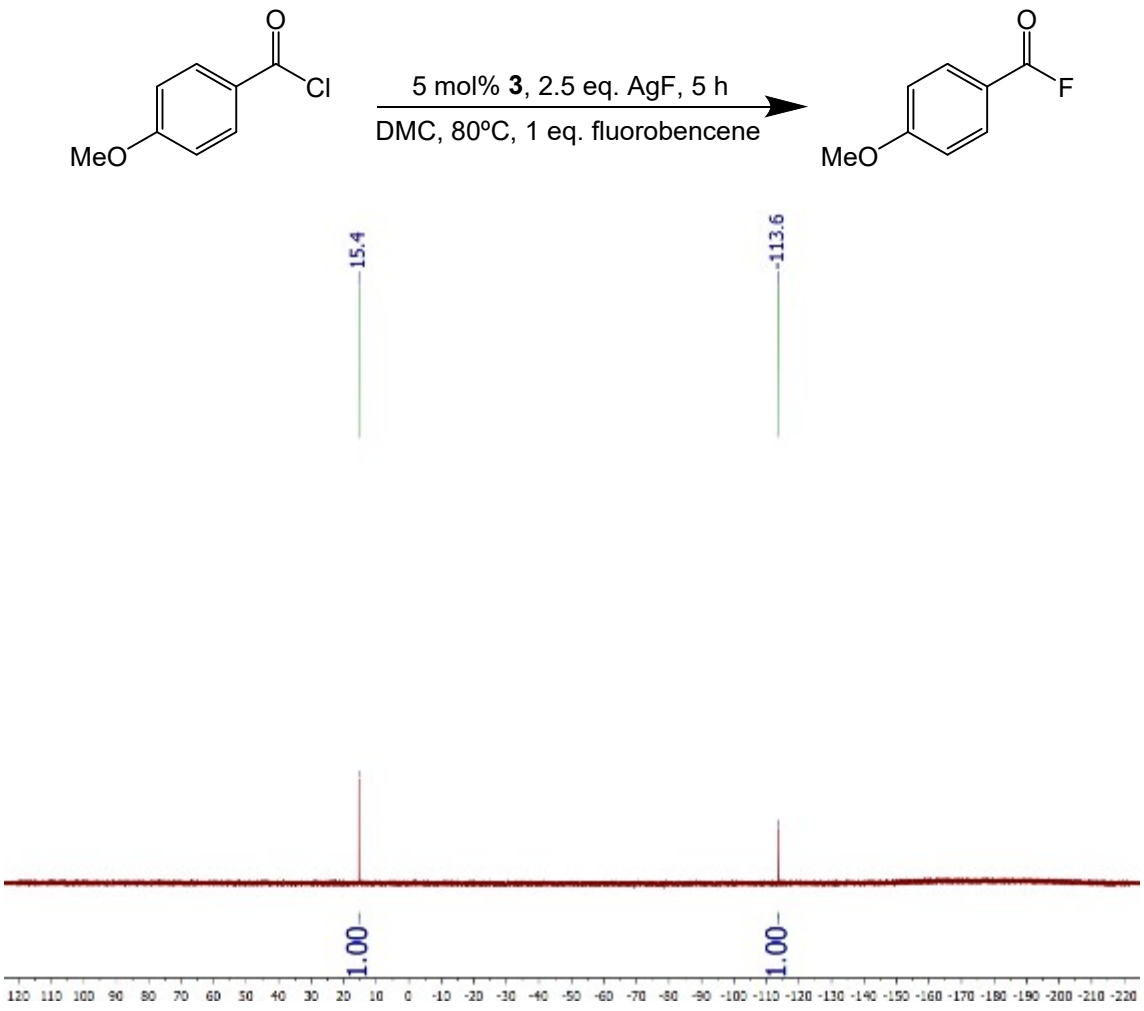


Figure S32. Crude ^{19}F NMR in $CDCl_3$.

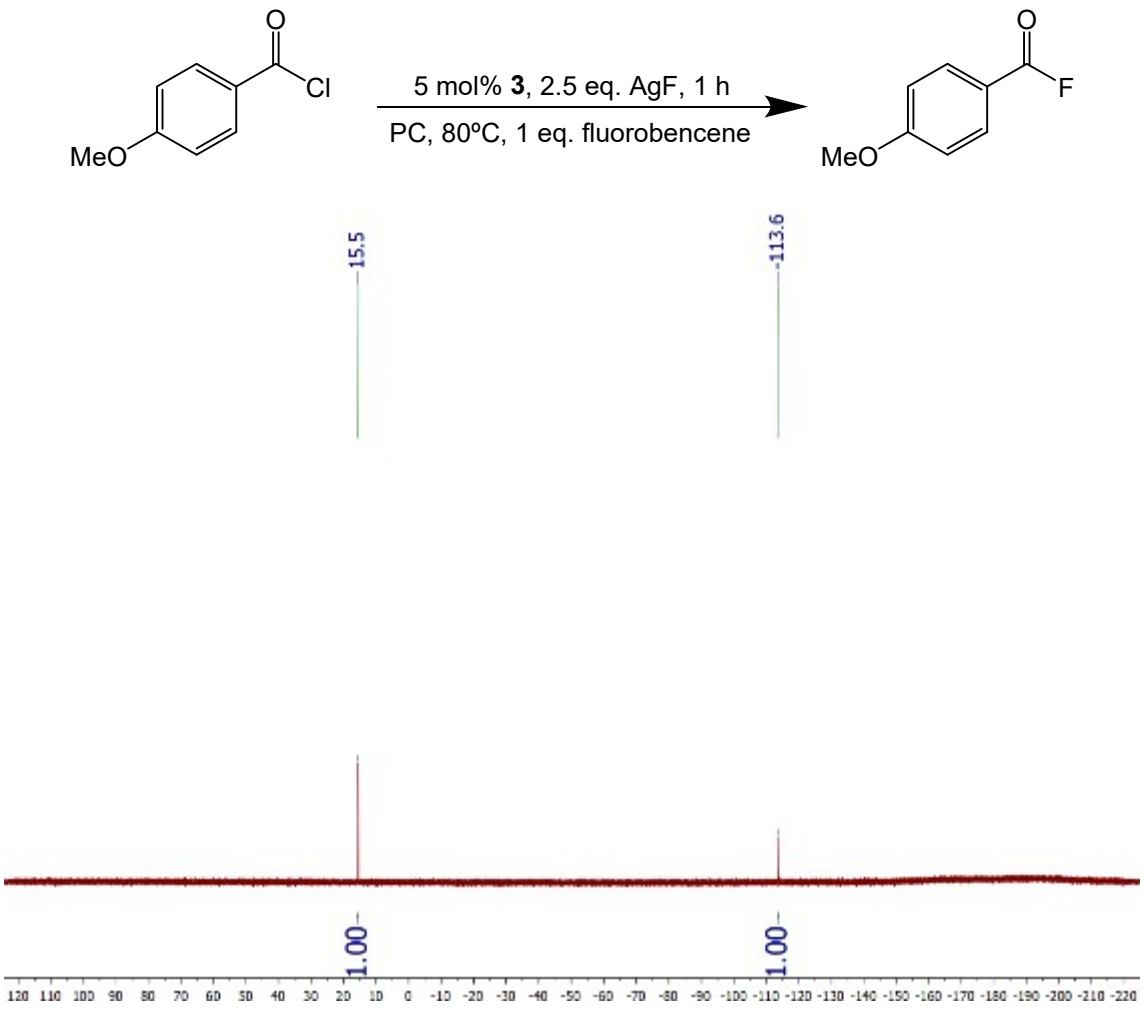


Figure S33. Crude ^{19}F NMR in $CDCl_3$.

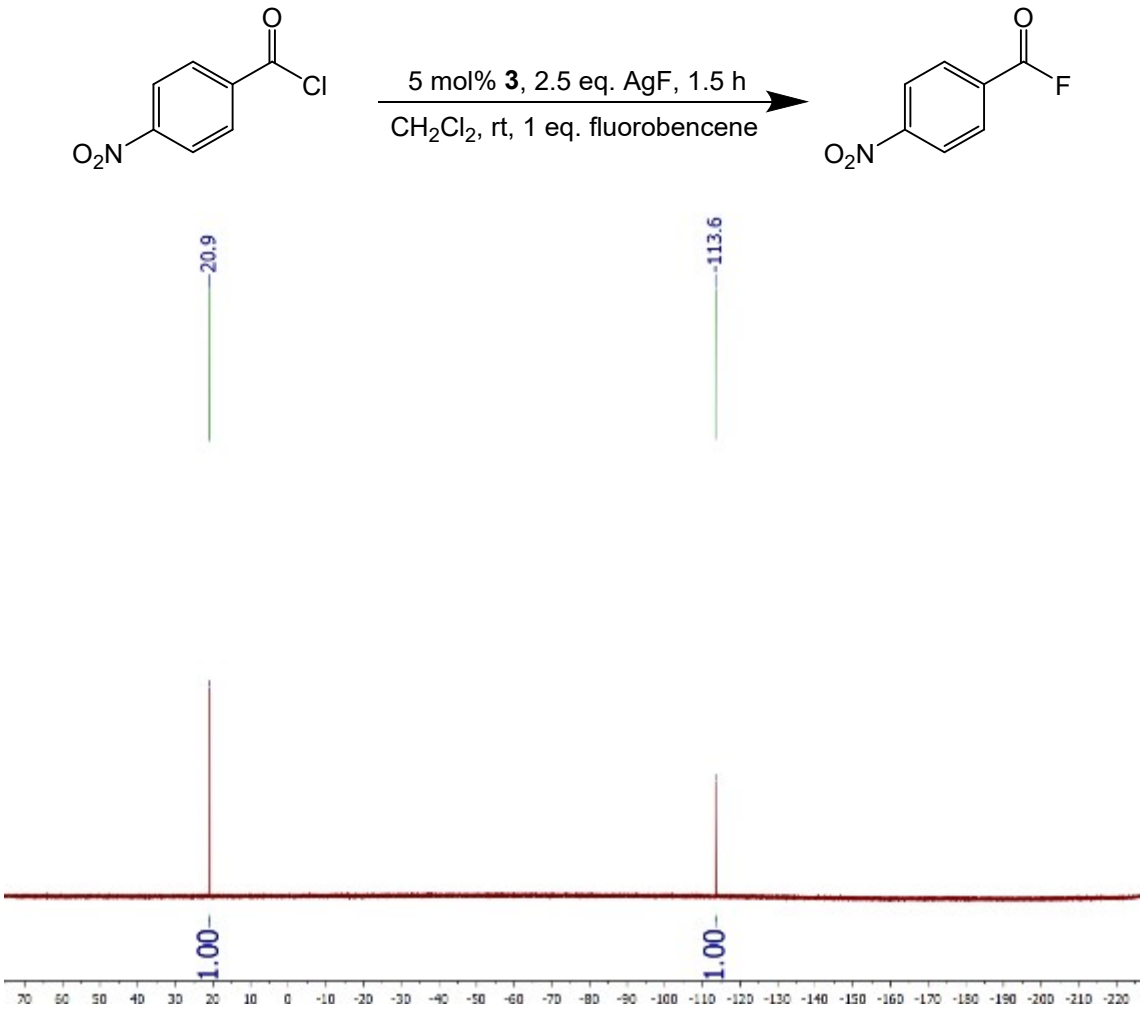


Figure S34. Crude ^{19}F NMR in $CDCl_3$.

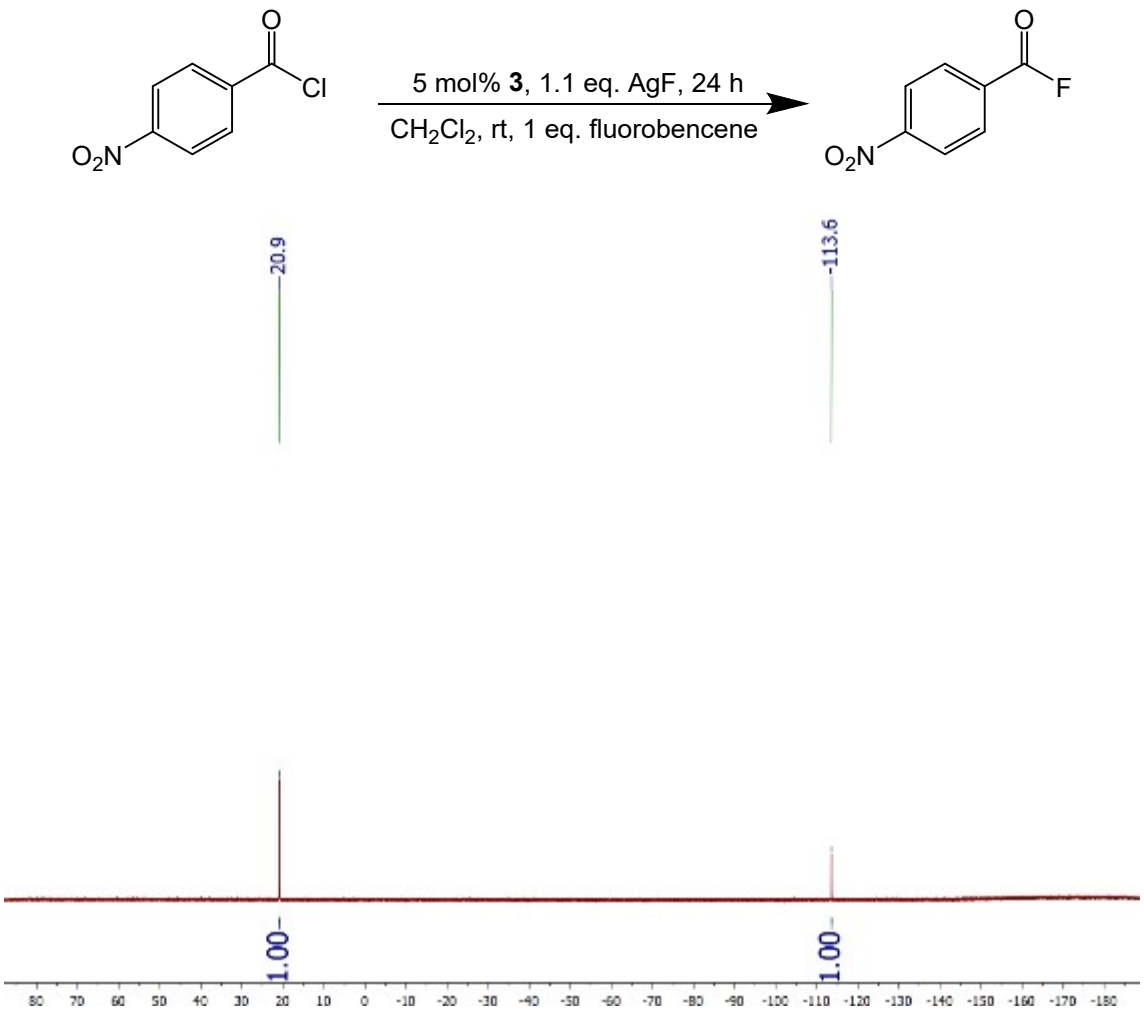


Figure S35. Crude ^{19}F NMR in $CDCl_3$.

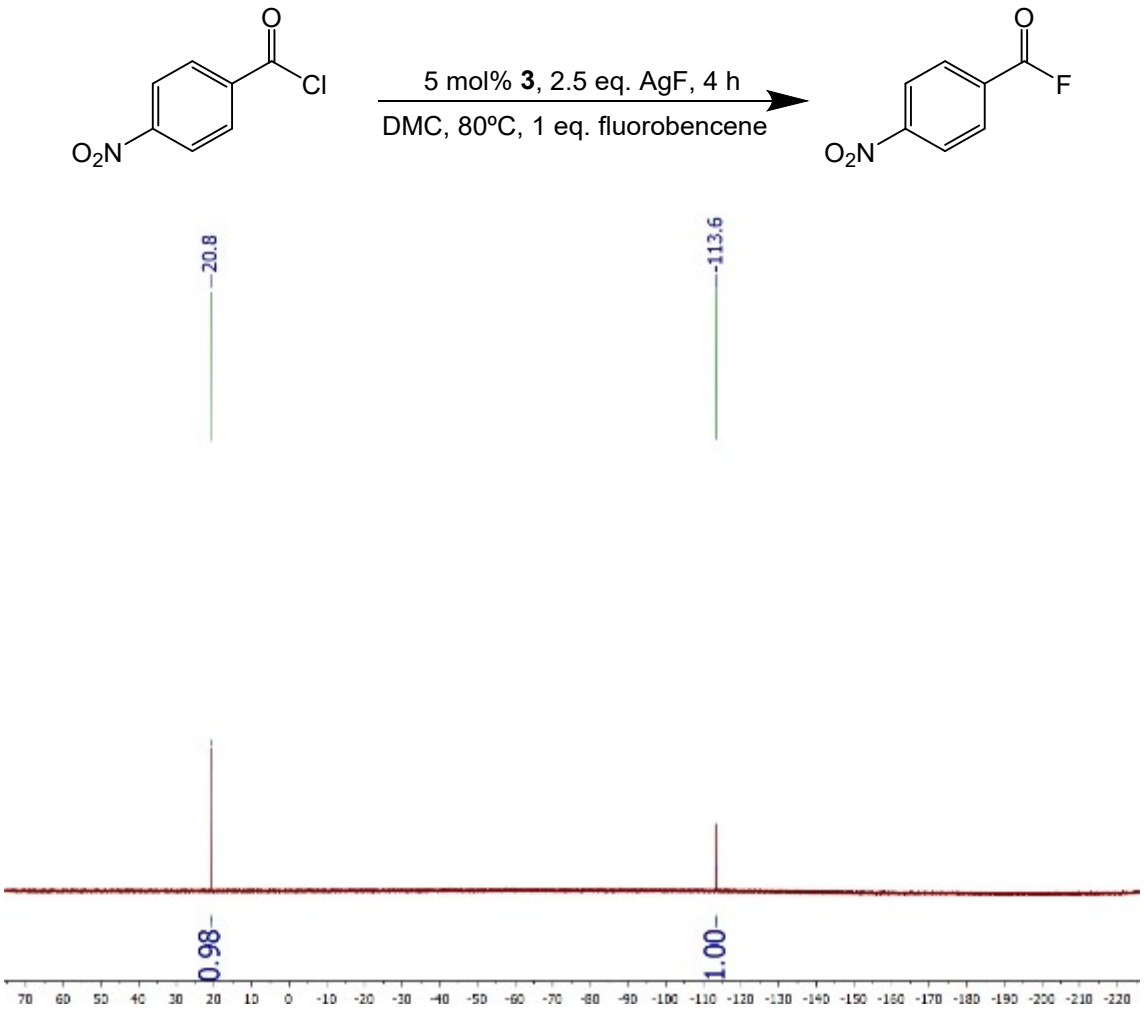


Figure S36. Crude ^{19}F NMR in $CDCl_3$.

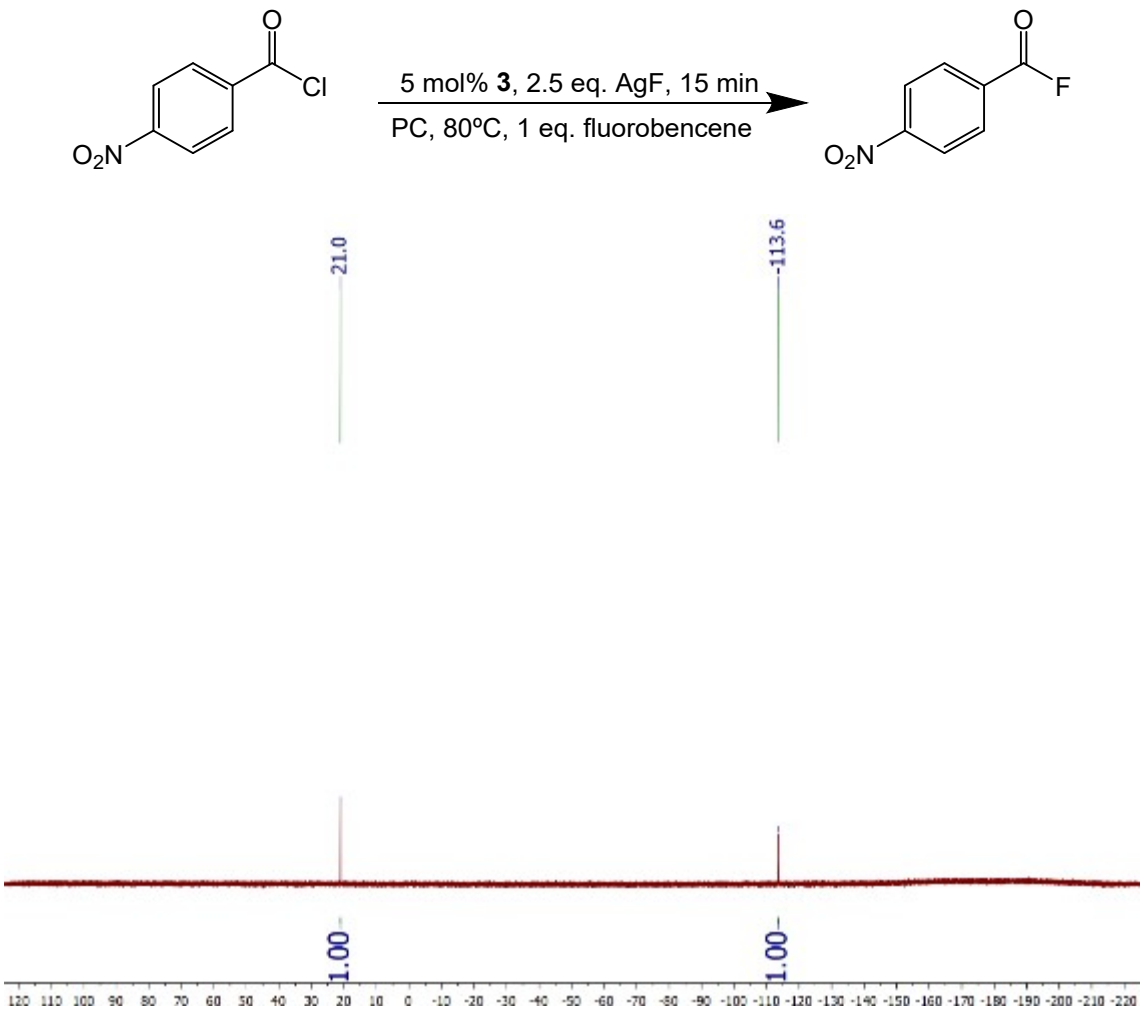


Figure S37. Crude ^{19}F NMR in $CDCl_3$.

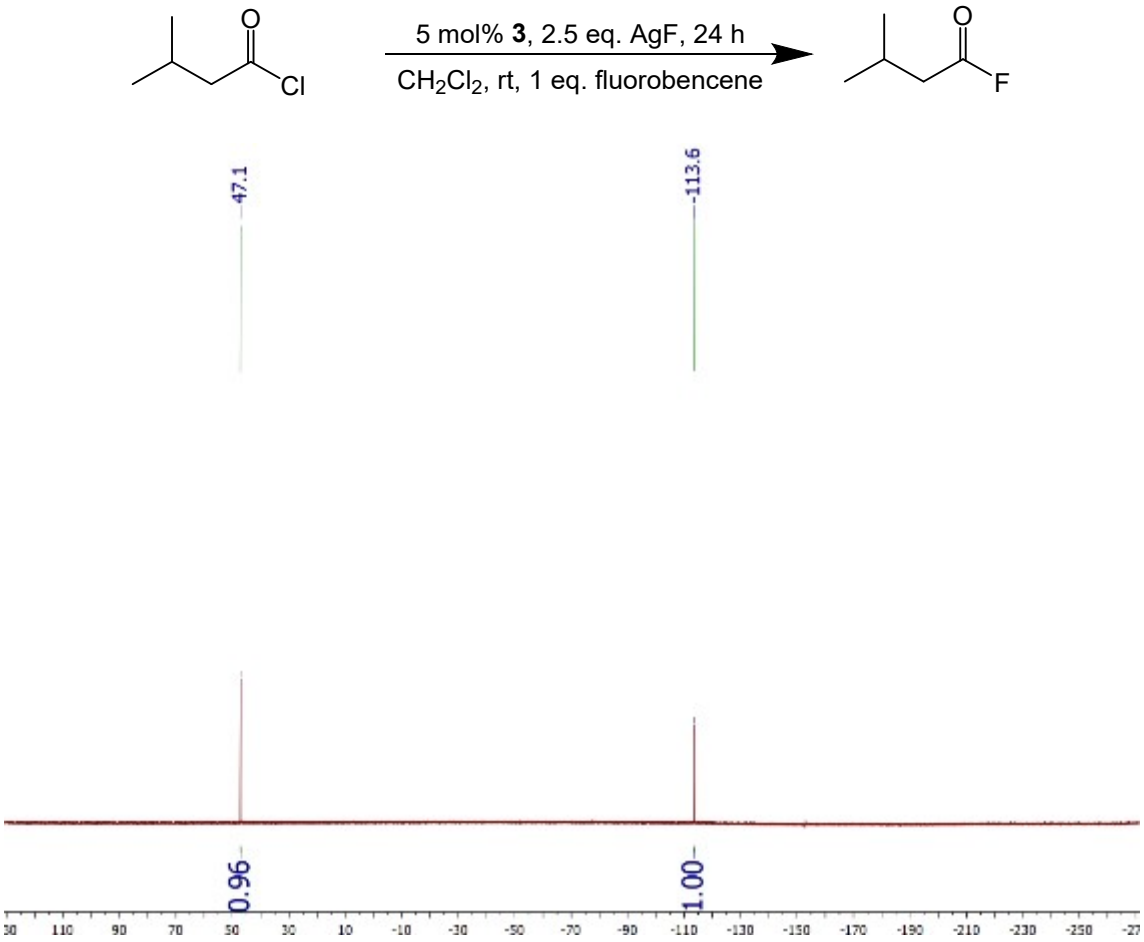


Figure S38. Crude ^{19}F NMR in $CDCl_3$.

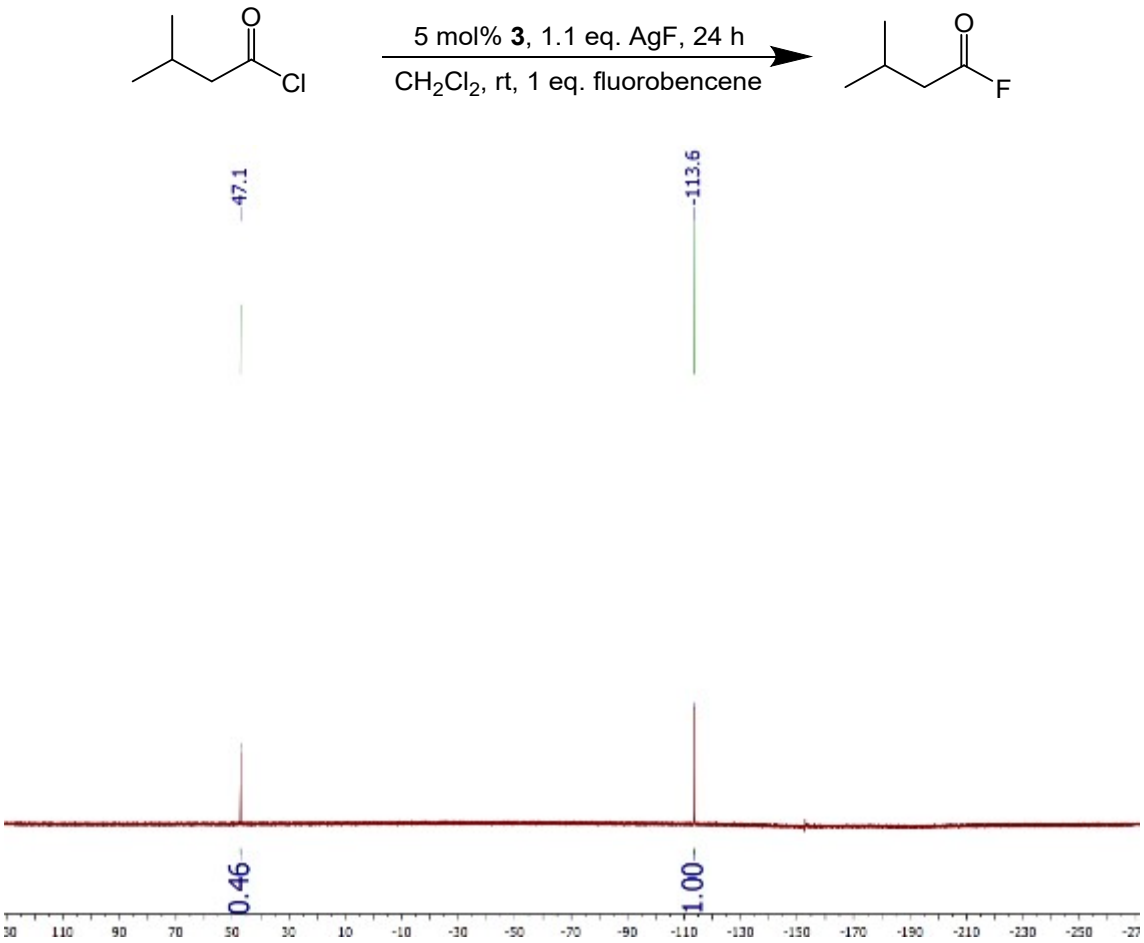


Figure S39. Crude ^{19}F NMR in $CDCl_3$.

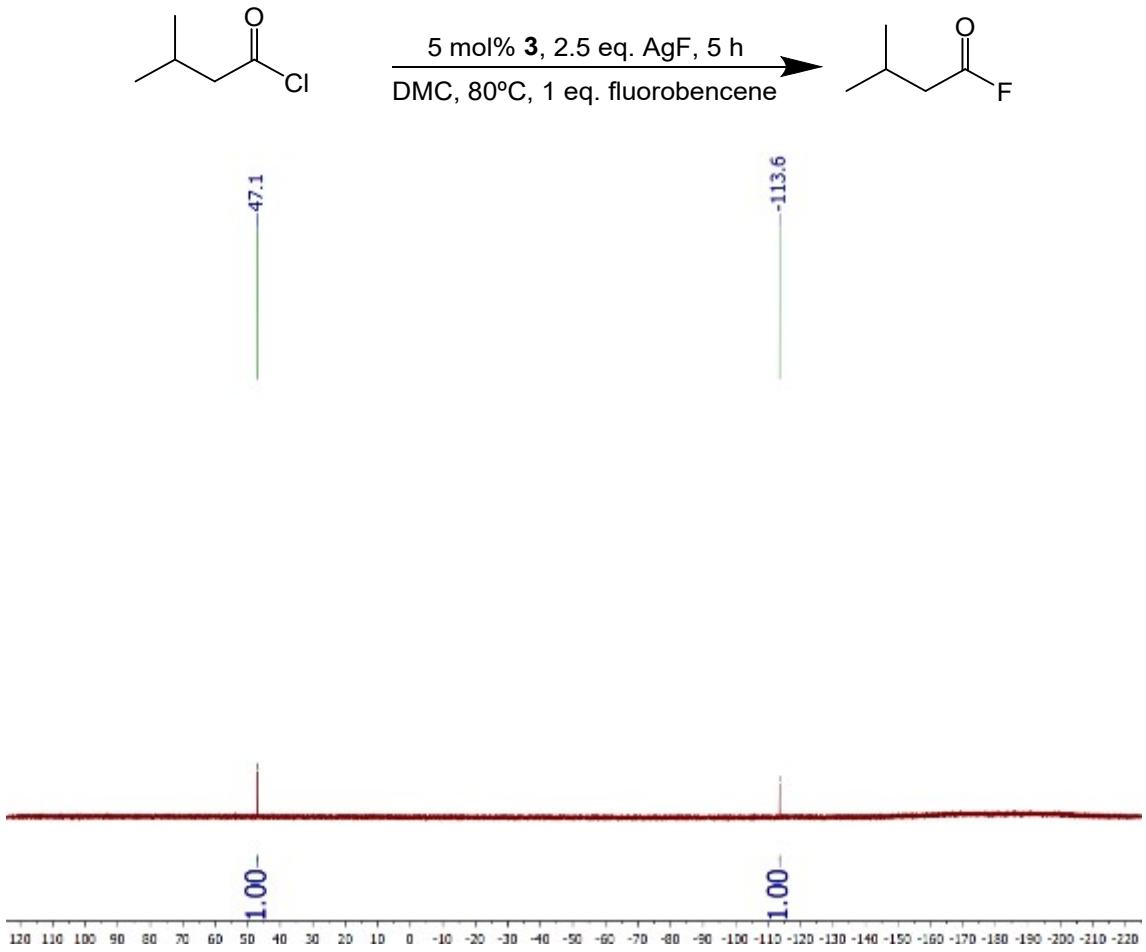


Figure S40. Crude ^{19}F NMR in $CDCl_3$.

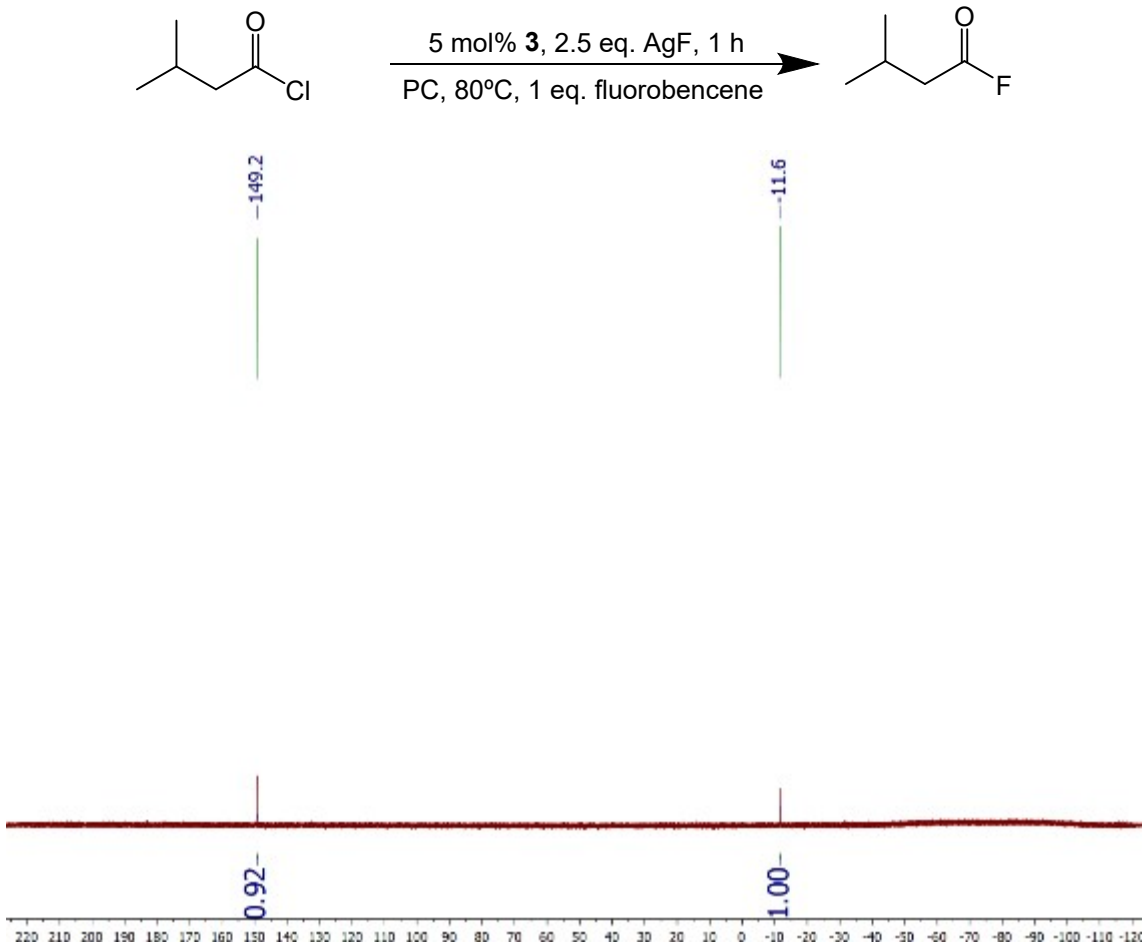


Figure S41. Crude ^{19}F NMR in $CDCl_3$.

Table 2

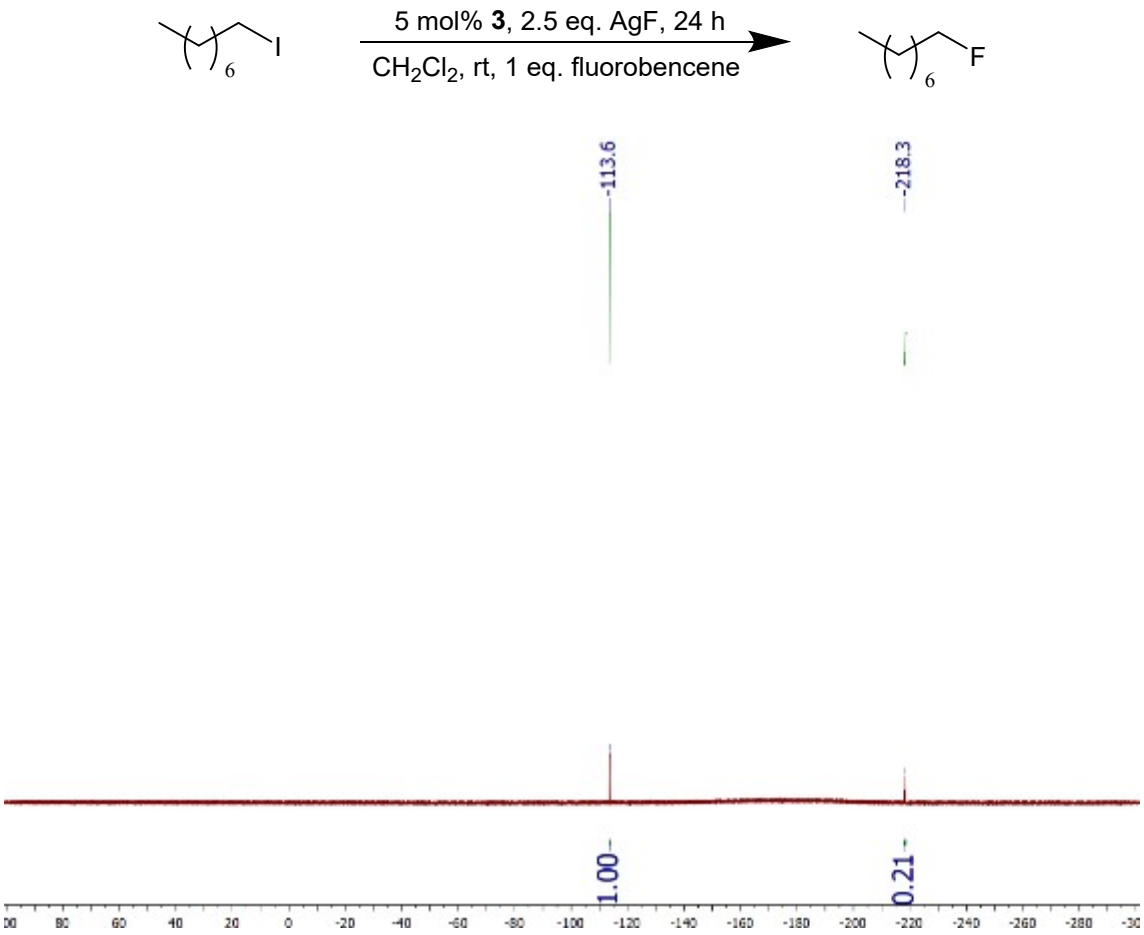


Figure S42. Crude ^{19}F NMR in $CDCl_3$.

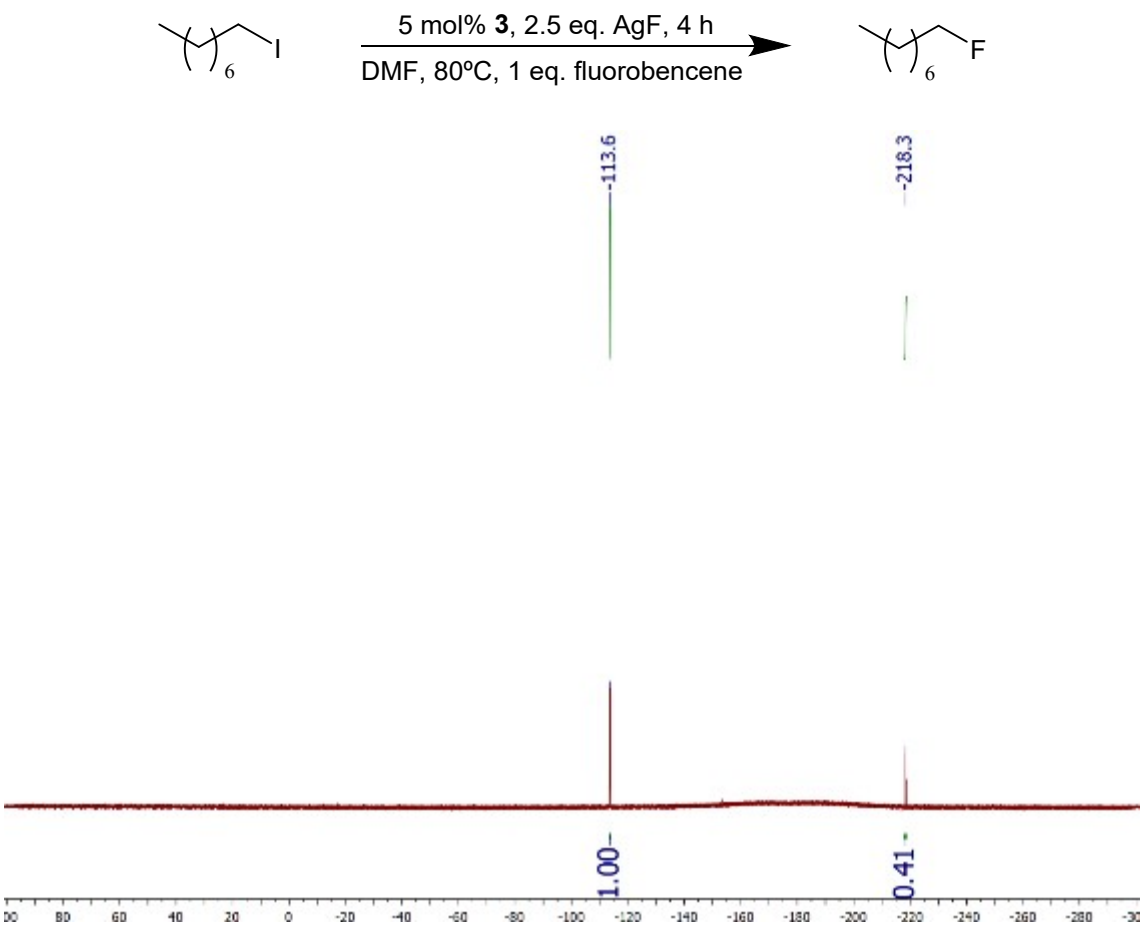


Figure S43. Crude ^{19}F NMR in $CDCl_3$.

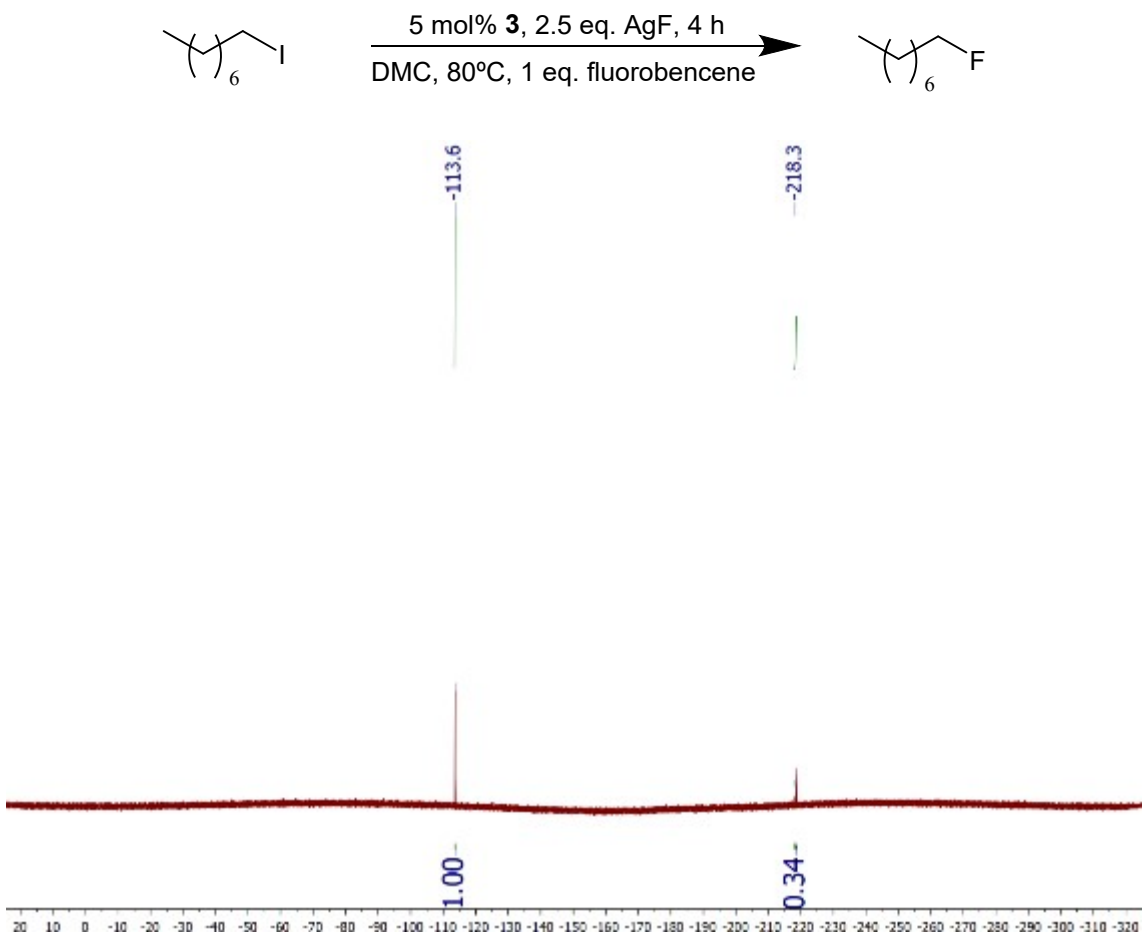


Figure S44. Crude ^{19}F NMR in $CDCl_3$.

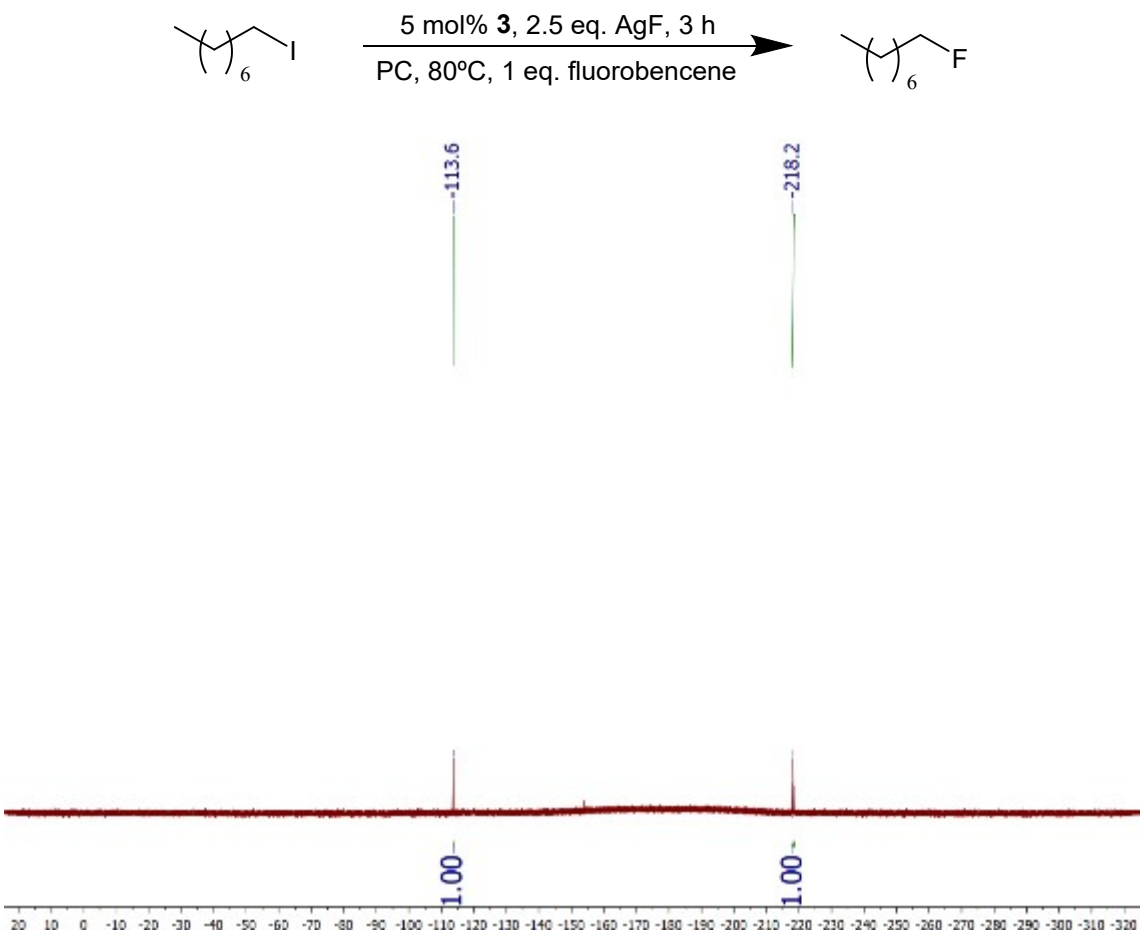


Figure S45. Crude ^{19}F NMR in $CDCl_3$.

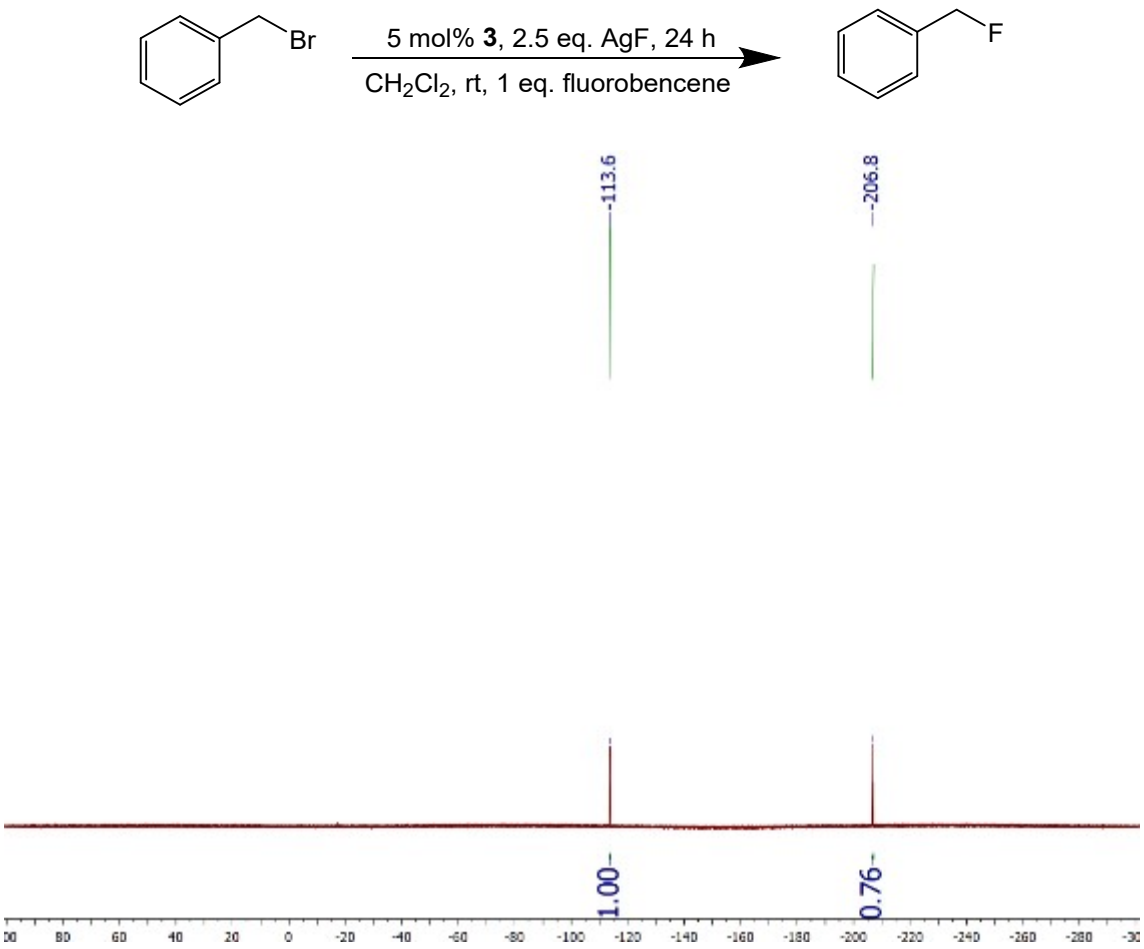


Figure S46. Crude ^{19}F NMR in $CDCl_3$.

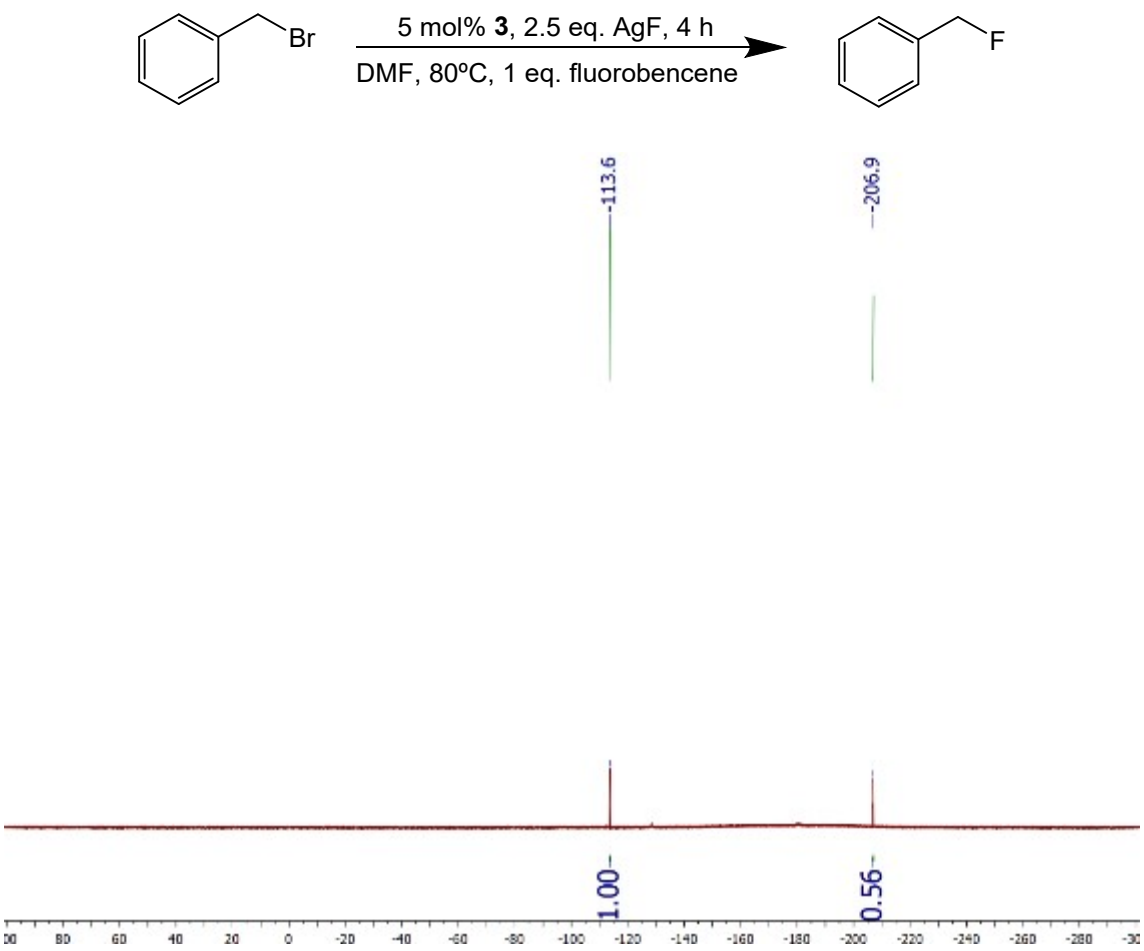


Figure S47. Crude ^{19}F NMR in $CDCl_3$.

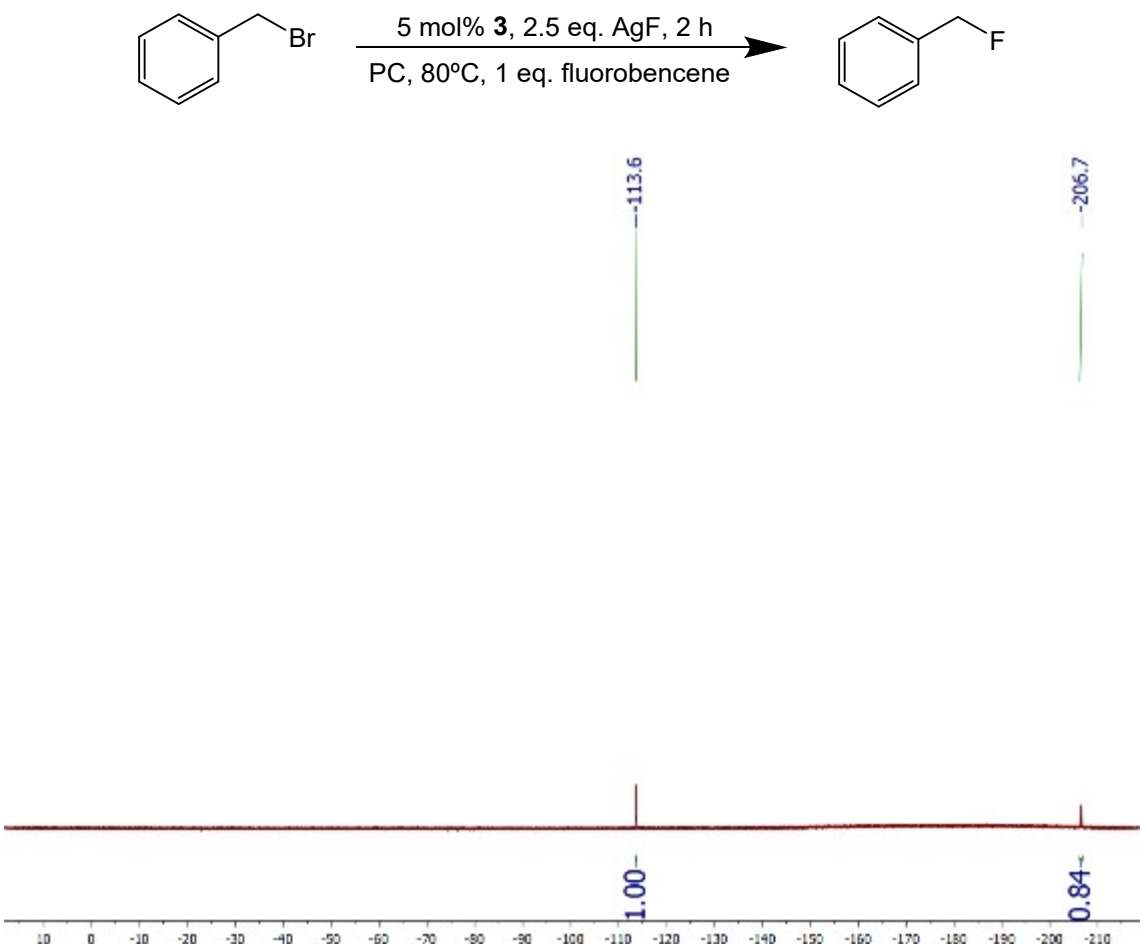


Figure S48. Crude ^{19}F NMR in $CDCl_3$.

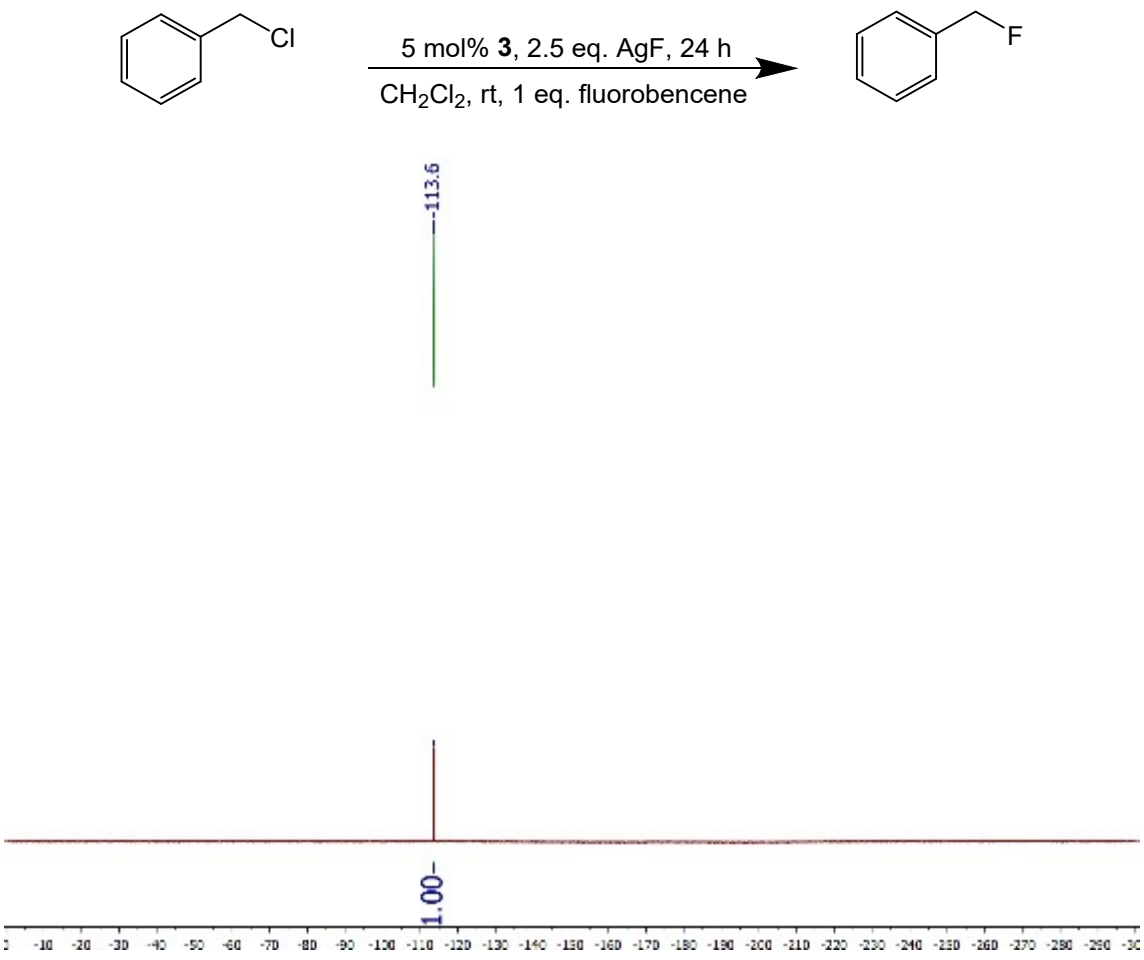


Figure S49. Crude ^{19}F NMR in $CDCl_3$.

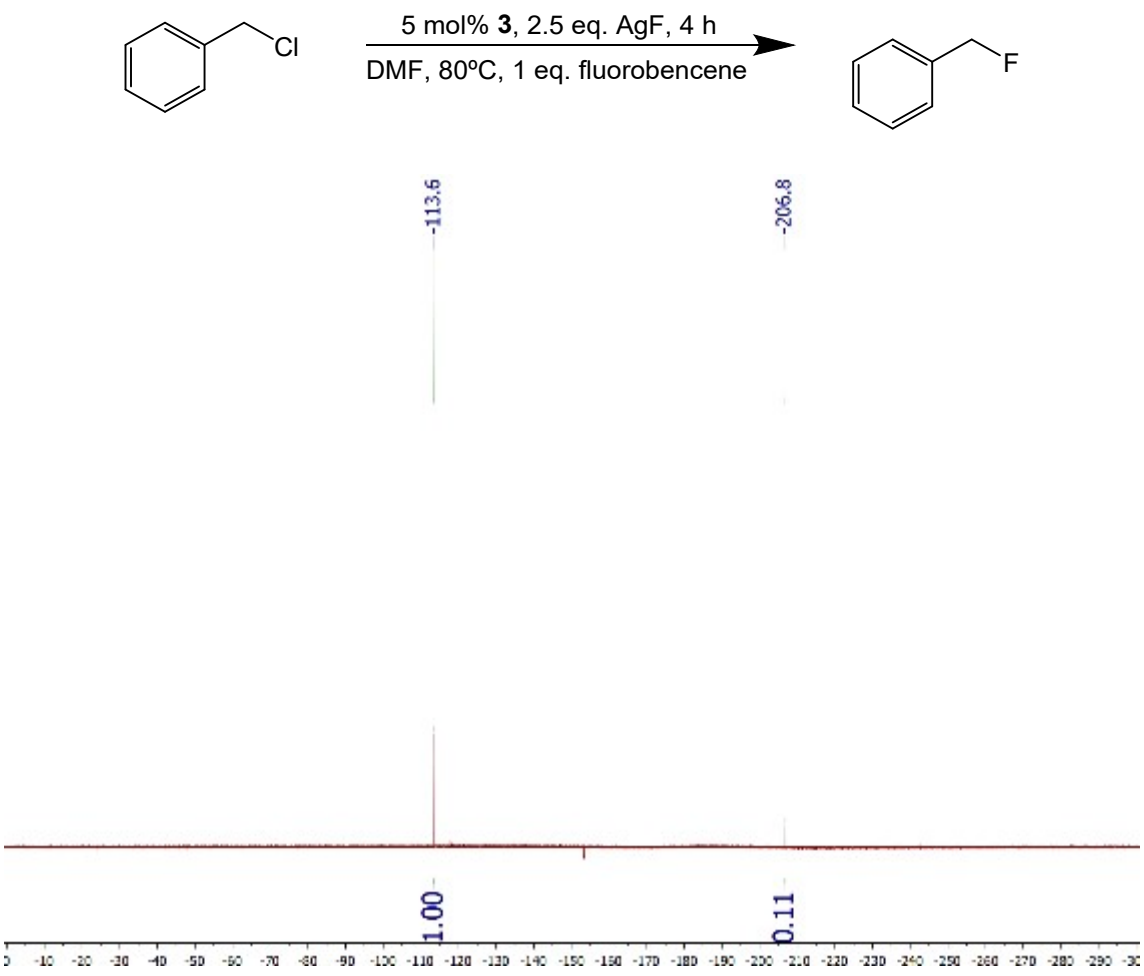


Figure S50. Crude ^{19}F NMR in $CDCl_3$.

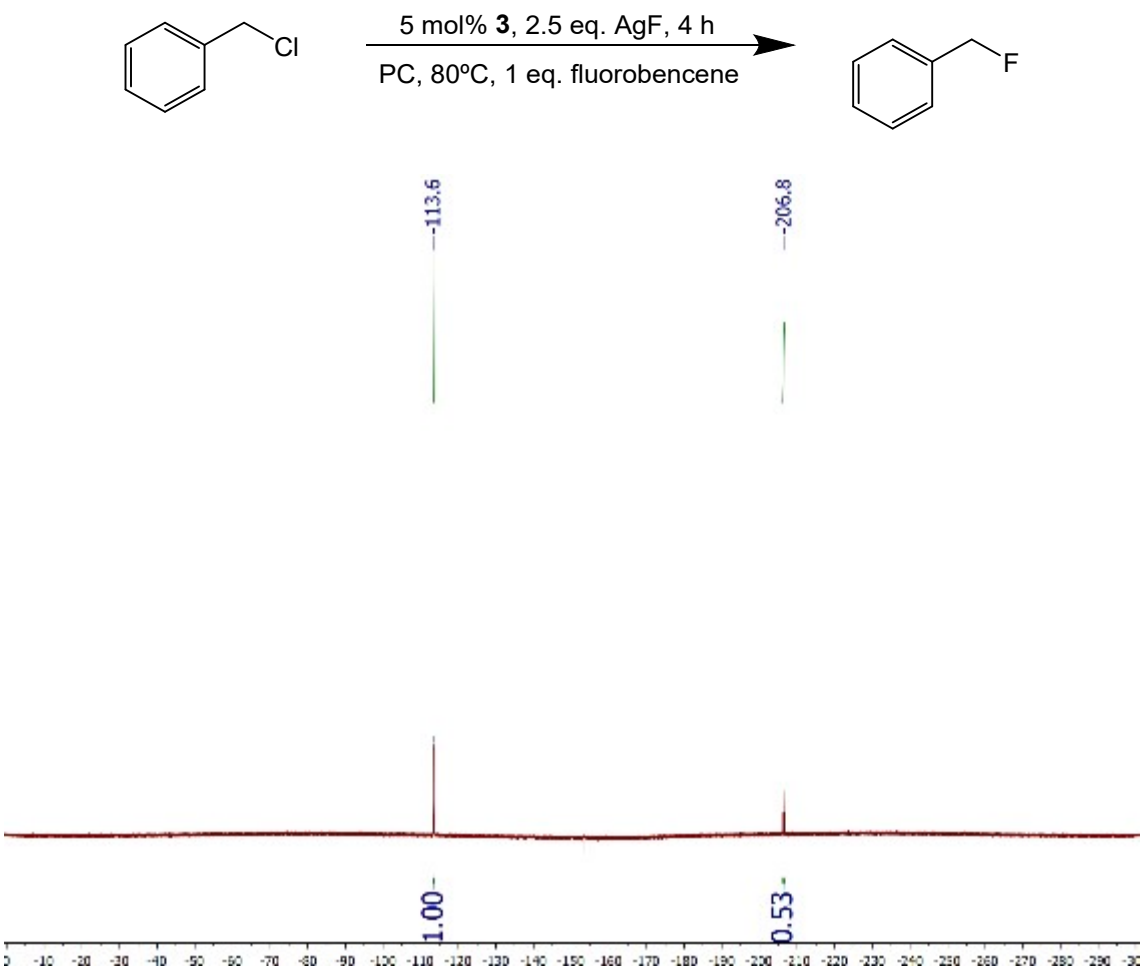


Figure S51. Crude ^{19}F NMR in $CDCl_3$.

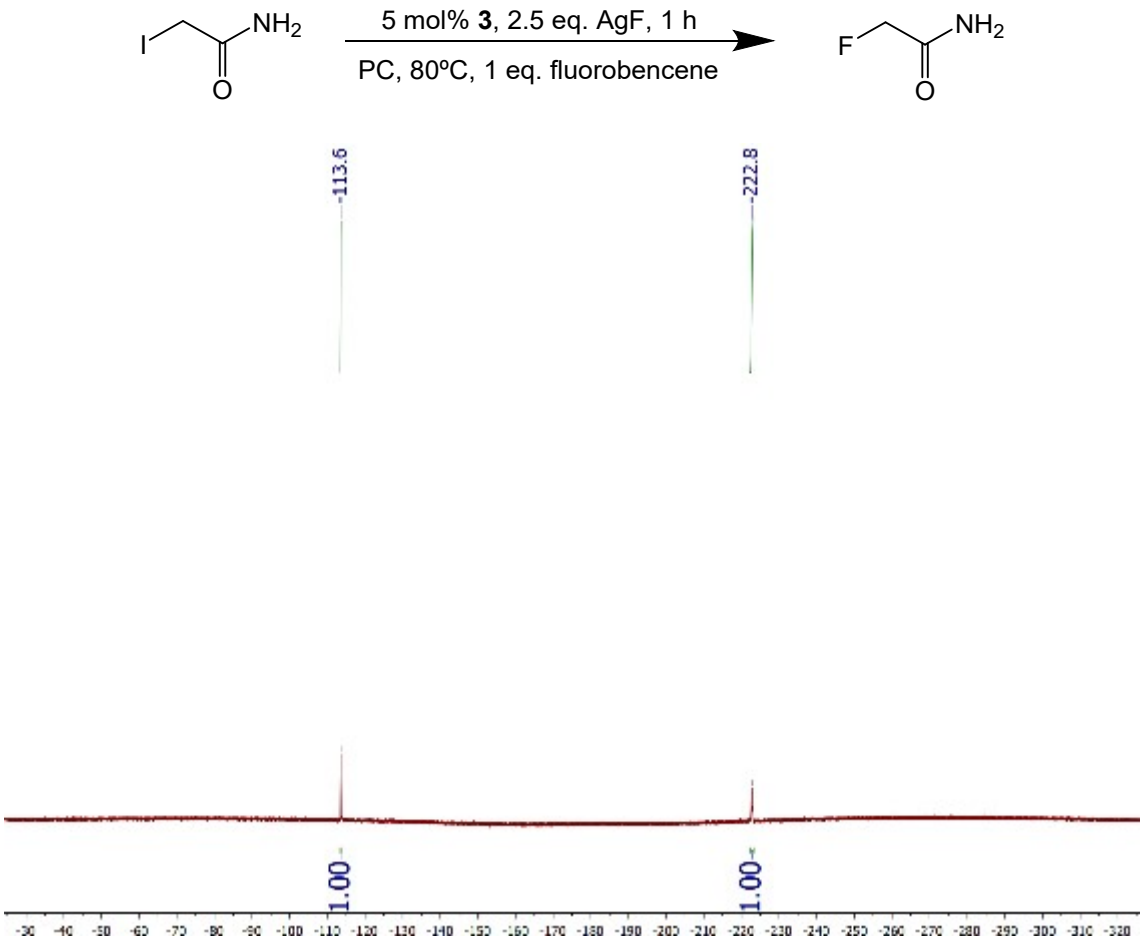


Figure S52. Crude ^{19}F NMR in $CDCl_3$.

Table 3

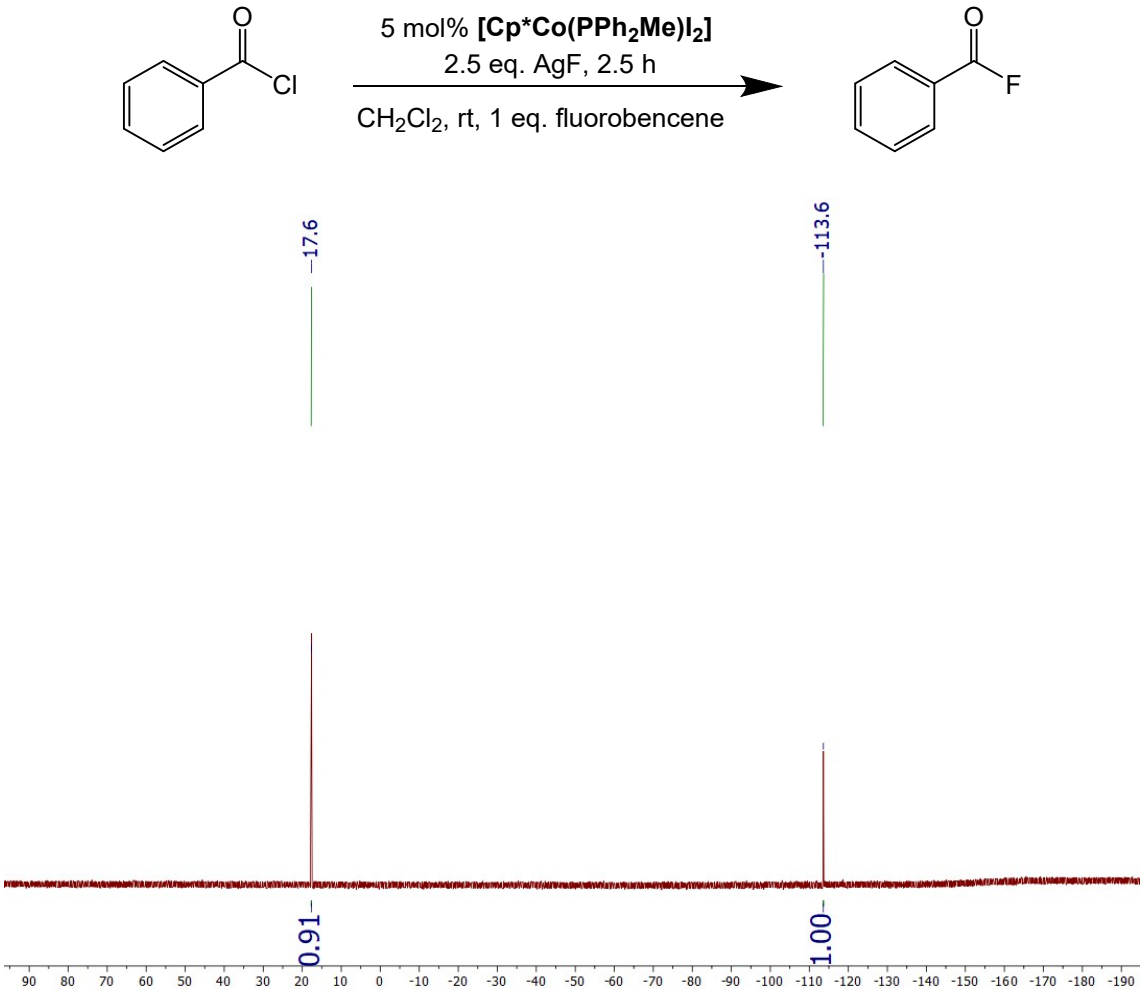


Figure S53. $^{19}F\{^{1}H\}$ NMR in $CDCl_3$.

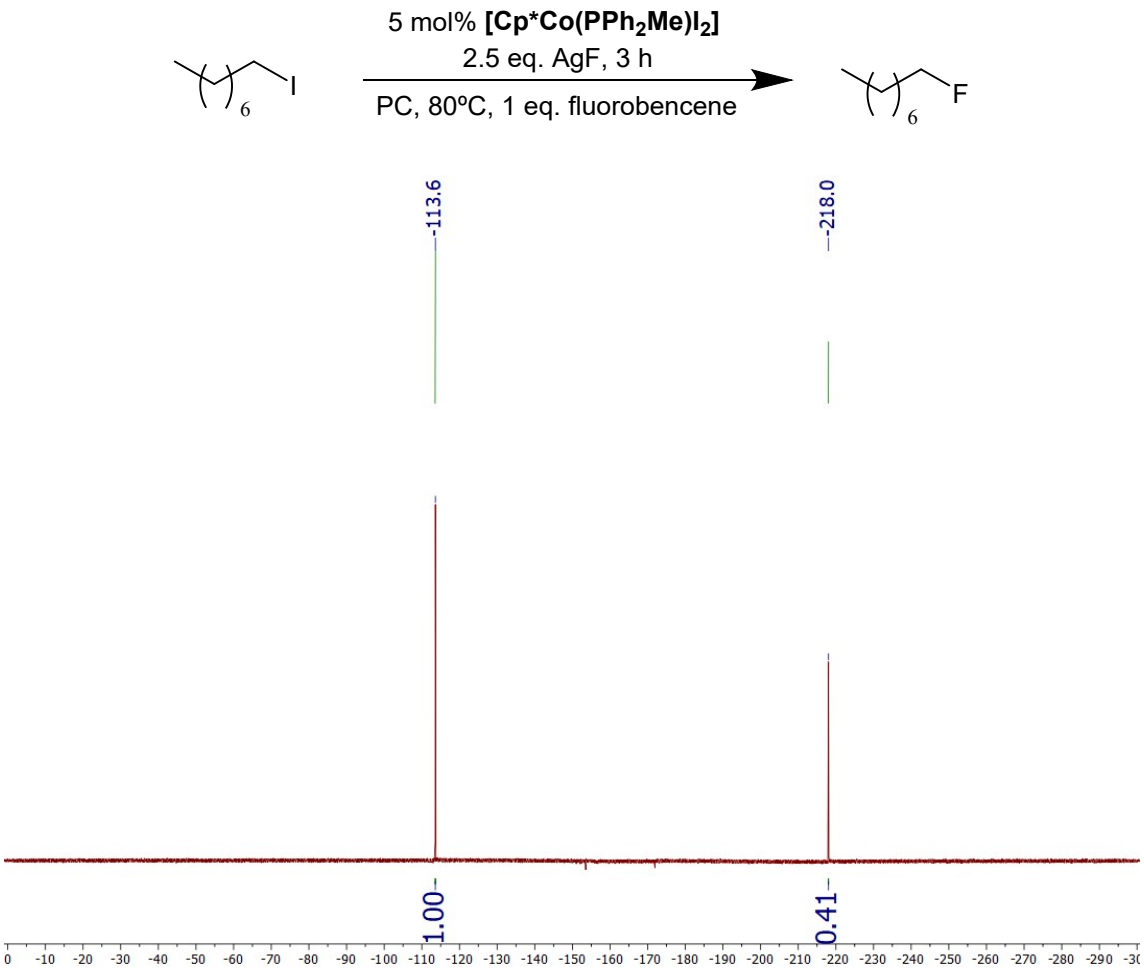


Figure S54. $^{19}F\{^{1}H\}$ NMR in $CDCl_3$.

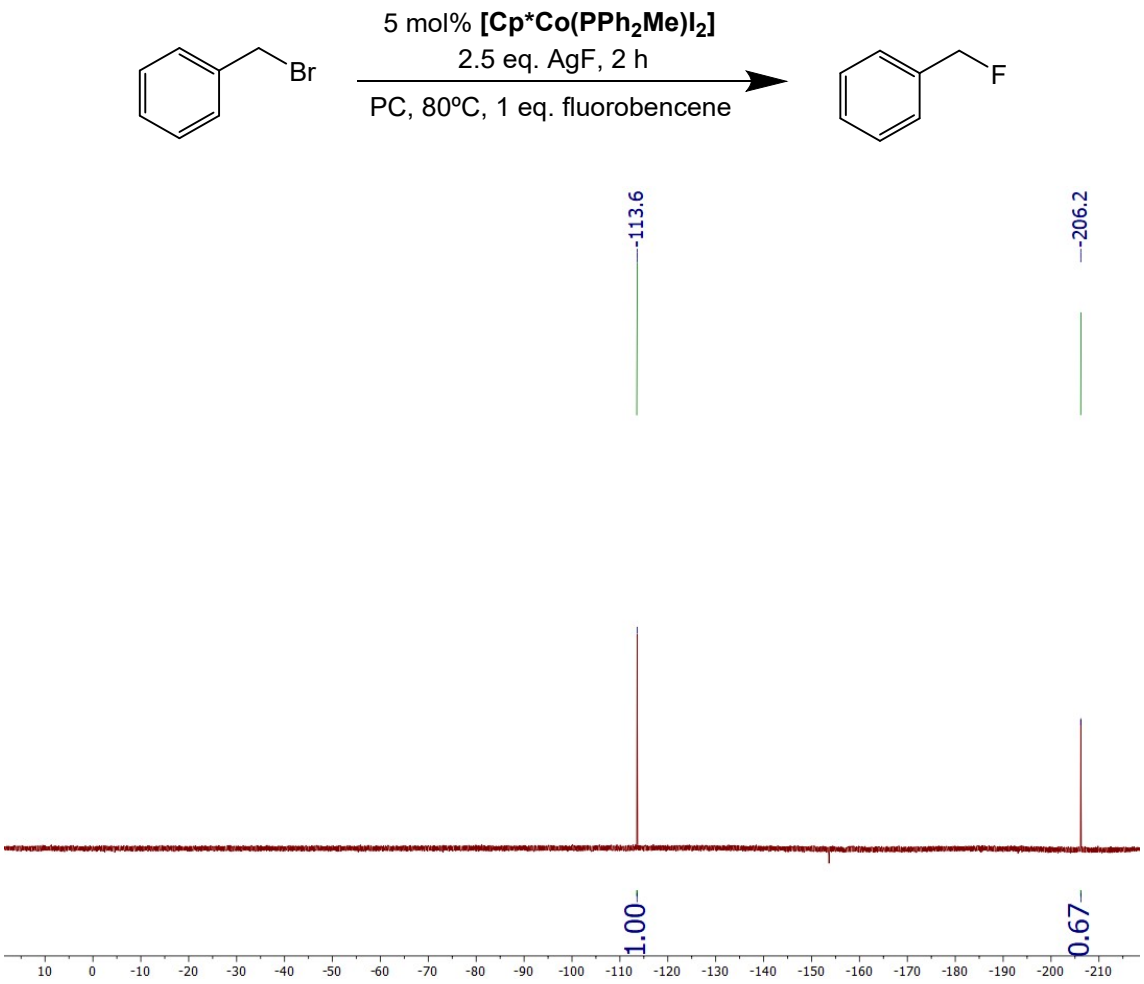
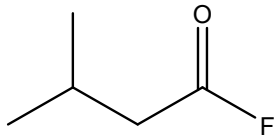


Figure S55. $^{19}F\{^{1}H\}$ NMR in $CDCl_3$.

3. Synthesis and characterization of isovaleryl fluoride

Synthesis of isovaleryl fluoride. A glass vial was charged with **3** (38.2 mg, 0.05 mmol), isovaleryl chloride (122 μL, 1.00 mmol), AgF (317.2 mg, 2.5 mmol) and 1 mL of PC. The mixture thus obtained was capped, covered with aluminium foil and heated to 80 °C. After 1 hour, the reaction was allowed to cool down to room temperature and the title compound was purified by vacuum distillation to obtain 91 mg of a colourless oil (0.87 mmol, 87% yield).



^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.32 (dd, 2H, CH_2), 2.08 (hept, $^{3}J_{H\text{-}H}$ = 6.7, 1H, C*H*), 0.96 (d, $^{3}J_{H\text{-}H}$ = 6.7, 6H, CH_3). APT NMR, ^{1}H-^{13}C HSQC, ^{1}H-^{13}C HMBC ($CDCl_3$, 101 MHz): δ 162.7 (d, $^{1}J_{F\text{-}C}$ = 361.4, *C*O), 40.9 (d, $^{2}J_{F\text{-}C}$ =47.9, *C*H_2), 25.0 (s, *C*H), 22.0 (s, *C*H_3). ^{19}F{^{1}H} NMR ($CDCl_3$, 376 MHz): δ 47.7 (s, *F*).

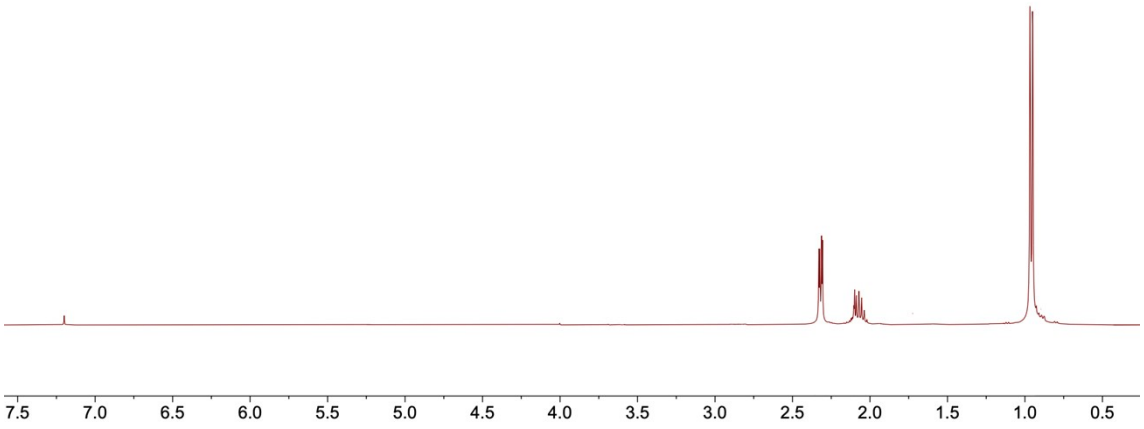


Figure S56. ^{1}H NMR of isovaleryl fluoride in $CDCl_3$.

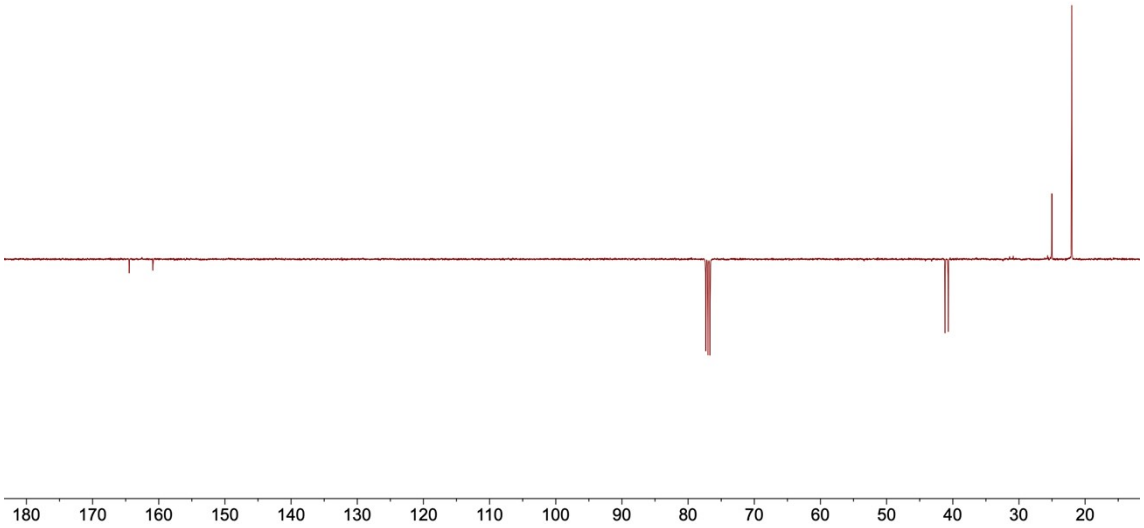


Figure S57. APT NMR of isovaleryl fluoride in $CDCl_3$.

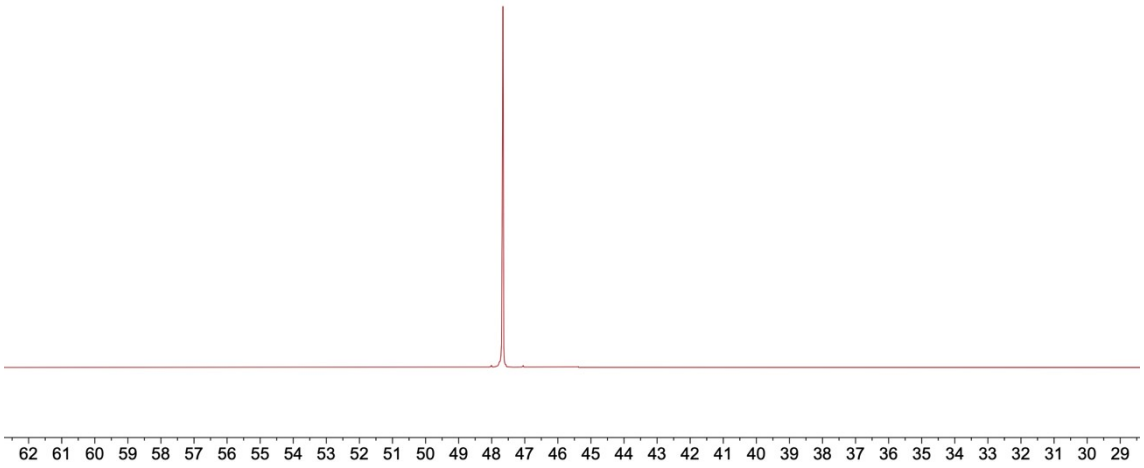


Figure S58. $^{19}F\{^{1}H\}$ NMR of isovaleryl fluoride in $CDCl_3$.

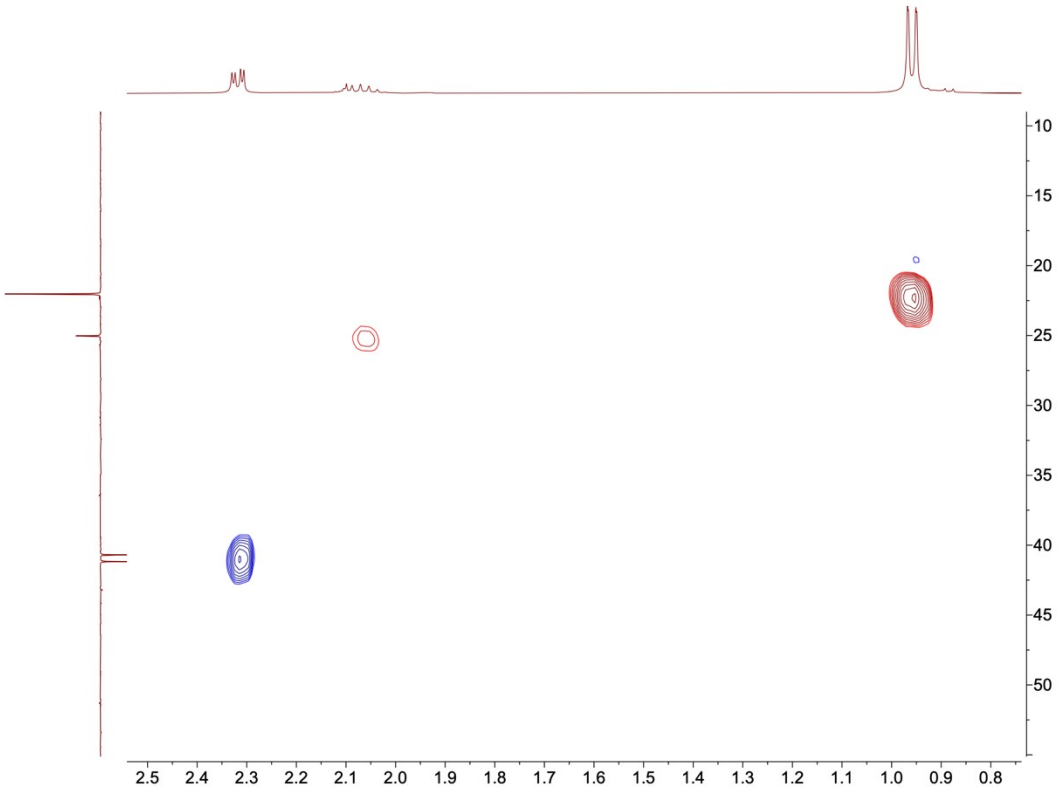


Figure S59. ^{1}H-^{13}C HSQC NMR of isovaleryl fluoride in $CDCl_3$.

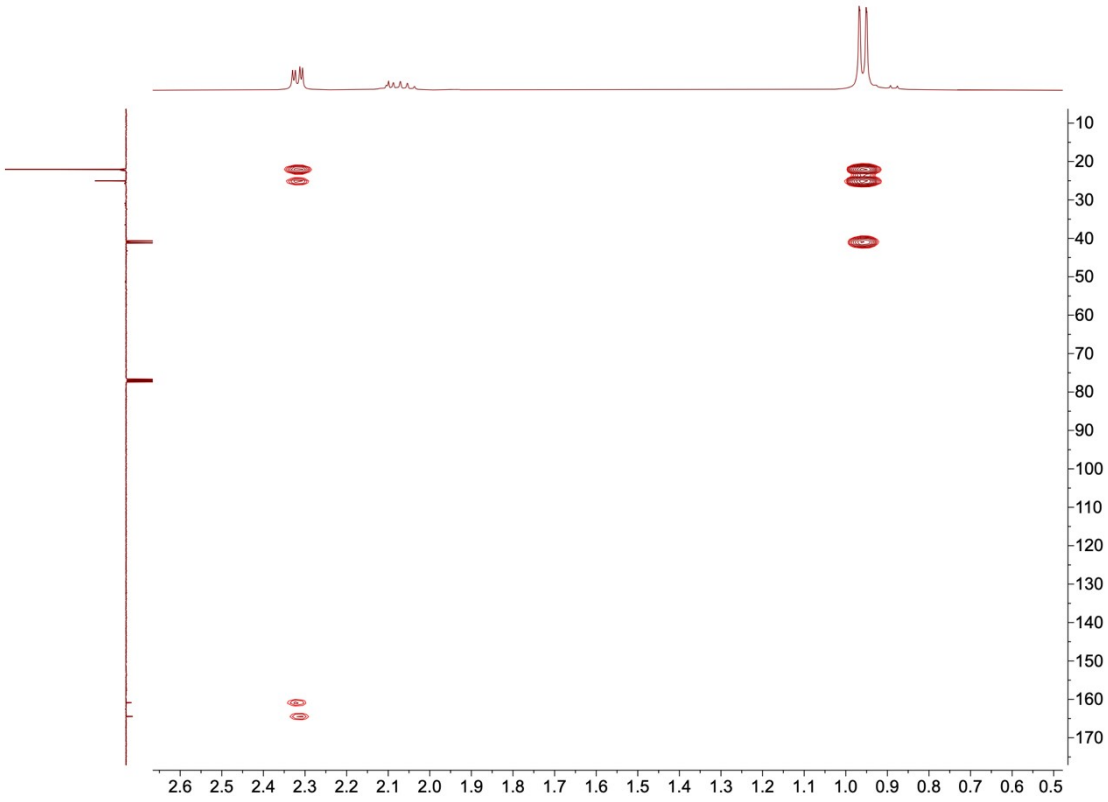


Figure S60. ^{1}H-^{13}C HMBC NMR of isovaleryl fluoride in $CDCl_3$.

4. DFT calculations

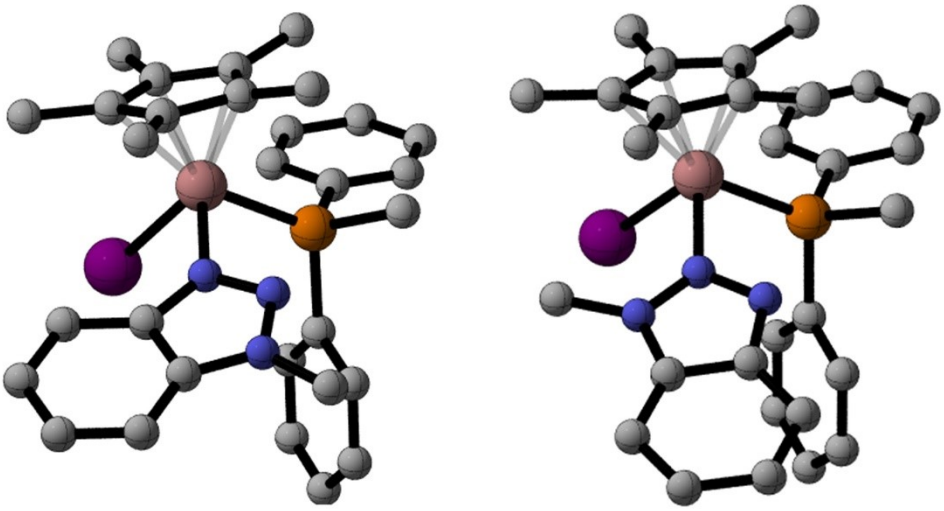


Figure S61. Model for the coordination of the benzotriazole scaffold to the Co center. Hydrogen atoms have been omitted for clarity.

Table S1. Comparison of the relative Gibbs energy for the two possible coordination modes of the model for the benzotriazole-based ligand. Geometrical optimizations and thermochemistry corrections with def2-SVP basis set, E(DZ), and further refinement by single point calculations with def2-TZVP, E(TZ). Corr. G(1M) corresponds to the correction to be added to E(TZ) to calculate the Gibbs energy (reference concentration of 1 mol·L^{-1}), G (1M, TZ). Energies are expressed in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
N3-coordinated	-3349.1200	-3348.6045	-3350.8333	-3350.3148
N2-coordinated	-3349.1126	-3348.5968	-3350.8259	-3350.3070

Table S2. Comparison of the activation barrier ($\Delta G^{\ddagger}$) and reaction Gibbs energy (ΔG_{react}) – in kcal·mol^{-1}, calculated as explained in the Experimental Section – for the nucleophilic fluorination of benzoyl chloride as a function of the exchange-correlation functional.

	M06-L	M06	B3LYP	TPSSh	TPSS
$\Delta G^{\ddagger}$	16.6	23.7	15.3	30.7	29.1
ΔG_{react}	-16.8	-18.5	-19.4	-15.9	-15.2

Table S3. Electronic energy and Gibbs energy difference – in kcal·mol^{-1}, calculated as explained in the Experimental Section – for the nucleophilic fluorination of benzoyl chloride as a function of the exchange-correlation functional.

		M06-L	M06	B3LYP	TPSSh	TPSS
ΔE_{T-S}[a]	$\mathbf{A_{Co-F}}$	12.6	4.1	5.1	10.4	15.2
	$\mathbf{TS_{A-B}}$	12.7	3.3	5.4	7.0	12.6
	$\mathbf{B_{Co-Cl}}$	13.4	5.7	6.2	10.6	15.6
ΔG_{T-S}[a]	$\mathbf{A_{Co-F}}$	9.6	1.1	0.1	7.6	12.7
	$\mathbf{TS_{A-B}}$	9.8	0.3	0.2	1.8	7.4
	$\mathbf{B_{Co-Cl}}$	10.4	2.7	2.2	7.1	12.1

[a] ΔE_{T-S} and ΔG_{T-S} correspond to the electronic energy and Gibbs energy difference between the optimized triplet and singlet state of the same structure, that is, positive values correspond to situations in which the most stable structure is the singlet state.

Table S4. Electronic energy and Gibbs energy difference – in kcal·mol^{-1}, calculated as explained in the Experimental Section – for the Co–F assisted S_N2 fluorination reaction of benzyl bromide and 1-iodooctane for M06-L functional.

	ΔG_{T-S}	M06-L
ΔE_{T-S}[a]	$\mathbf{A_{Co-F}}$	12.6
	$\mathbf{TS_{A-B'}}$**- $\mathbf{S_N2}$ (BnBr)**[b]	11.4
	$\mathbf{TS_{A-B'}}$**- $\mathbf{S_N2}$ (1-I)**[b]	12.3
	$\mathbf{B'_{Co-Br}}$	13.2
	$\mathbf{B'_{Co-I}}$	10.9
ΔG_{T-S}[a]	A_{Co-F}	9.6
	$TS_{A-B'}$- S_N2 (BnBr)	8.6
	$TS_{A-B'}$- S_N2 (1-I)	8.2
	$\mathbf{B'_{Co-Br}}$	10.7
	$\mathbf{B'_{Co-I}}$	7.3

[a] ΔE_{T-S} and ΔG_{T-S} correspond to the electronic energy and Gibbs energy difference between the optimized triplet and singlet state of the same structure, that is, positive values correspond to situations in which the most stable structure is the singlet state. [b] *BnBr* corresponds to benzyl bromide, and *1-I* to 1-iodooctane.

Table S5. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the M06-L (SMD =

dichloromethane)/def2-TZVP//def2-SVP level of theory in the singlet electronic state. Geometrical optimizations and thermochemistry corrections with def2-SVP basis set, E(DZ), and further refinement by single point calculations with def2-TZVP, E(TZ). Corr. G(1M) corresponds to the correction to be added to E(TZ) to calculate the Gibbs energy (reference concentration of 1 mol·L^{-1}), G (1M.). Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A_{Co\text{-}F}}$ and benzyl chloride) in kcal·mol^{-1}.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)	**ΔG (1M, TZ)**
$A_{Co\text{-}F}$	-3210.3869	0.4727	-3212.2876	-3211.8149	**0.0**
$TS_{A\text{-}B}$	-4015.1552	0.5643	-4017.5640	-4016.9996	**16.6**
$TS_{A\text{-}B}$-meta	-4015.1089	0.5643	-4017.5158	-4016.9514	**46.8**
$B_{Co\text{-}Cl}$	-3570.7209	0.4714	-3572.6469	-3572.1755	**-16.8**
Benzoyl chloride	-804.7638	0.0707	-805.2819	-805.2112	
Benzoyl fluoride	-444.4625	0.0739	-444.9513	-444.8774	

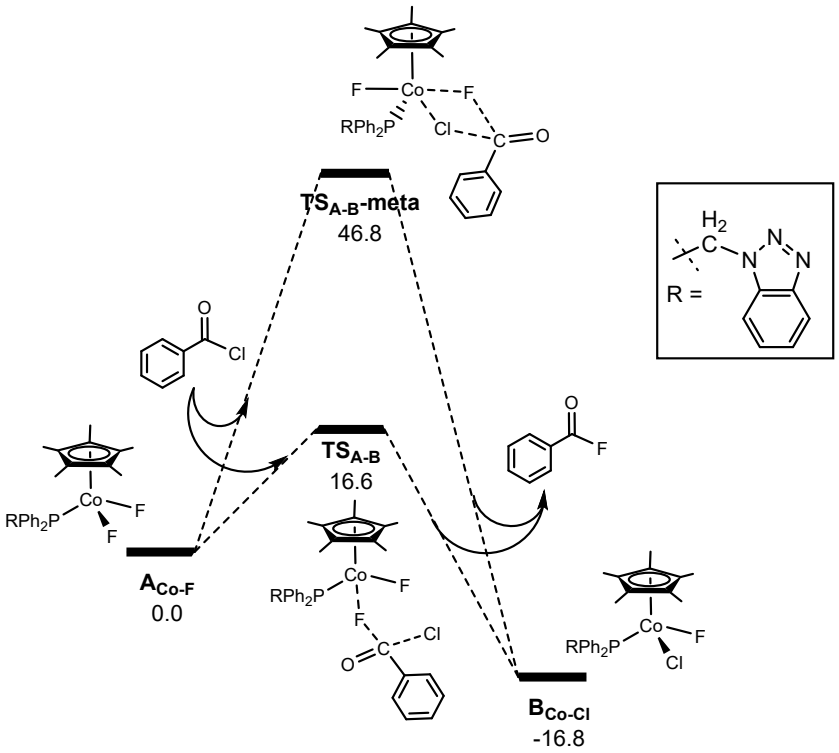


Figure S62. Comparison between the two possible alternatives for the fluorination of benzoyl chloride.

Table S6. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the M06-L (SMD =

dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^3\mathbf{A}_{\mathbf{Co\text{-}F}}$	-3210.3682	0.4679	-3212.2674	-3211.7996
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$	-4015.1355	0.5596	-4017.5436	-4016.9841
$^3\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	-3570.7012	0.4666	-3572.6256	-3572.1589

Table S7. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the M06 (SMD = dichloromethane)/def2-TZVP//M06-L/def2-SVP level of theory in the singlet electronic state. Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A}_{\mathbf{Co\text{-}F}}$ and benzoyl chloride) in kcal·mol^{-1}.

	Corr. G(1M)	E (TZ)	G (TZ) 1M	**ΔG 1M (TZ)**
$\mathbf{A}_{\mathbf{Co\text{-}F}}$	0.4727	-3211.3787	-3210.9060	**0.0**
$\mathbf{TS}_{\mathbf{A\text{-}B}}$	0.5643	-4016.4387	-4015.8743	**23.7**
$\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	0.4714	-3571.7429	-3571.2715	**-18.5**
Benzoyl chloride	0.0707	-805.0768	-805.0060	
Benzoyl fluoride	0.0739	-444.7439	-444.6700	

Note that, for M06 results, optimization was performed by means of M06-L functional, M06 single point calculations with def2-TZVP being performed afterwards. This way, Corr. G(1M) corresponds to the M06-L computed one.

Table S8. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the M06 (SMD = dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^3\mathbf{A}_{\mathbf{Co\text{-}F}}$	0.4679	-3211.3721	-3210.9042
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$	0.5596	-4016.4334	-4015.8739
$^3\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	0.4666	-3571.7339	-3571.2673

Note that, for M06 results, optimization was performed by means of M06-L functional, M06 single point calculations with def2-TZVP being performed afterwards. This way, Corr. G(1M) corresponds to the M06-L computed one.

Table S9. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the B3LYP-D3BJ (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the singlet electronic state. Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A_{Co\text{-}F}}$ and benzoyl chloride) in kcal·mol^{-1}.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)	**ΔG (1M, TZ)**
$\mathbf{A_{Co\text{-}F}}$	-3210.7670	0.4757	-3212.7085	-3212.2329	**0.0**
$\mathbf{TS_{A\text{-}B}}$	-4015.6169	0.5674	-4018.0863	-4017.5190	**15.3**
$\mathbf{B_{Co\text{-}Cl}}$	-3571.1029	0.4742	-3573.0770	-3572.6028	**-19.4**
Benzoyl chloride	-804.8404	0.0710	-805.3815	-805.3105	
Benzoyl fluoride	-444.5407	0.0740	-445.0454	-444.9714	

Table S10. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the B3LYP-D3BJ (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^{3}\mathbf{A_{Co\text{-}F}}$	-3210.7578	0.4676	-3212.7004	-3212.2328
$^{3}\mathbf{TS_{A\text{-}B}}$	-4015.6069	0.5591	-4018.0778	-4017.5187
$^{3}\mathbf{B_{Co\text{-}Cl}}$	-3571.0928	0.4678	-3573.0670	-3572.5993

Table S11. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the TPSSh (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the singlet electronic state. Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A_{Co\text{-}F}}$ and benzoyl chloride) in kcal·mol^{-1}.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)	**ΔG (1M, TZ)**
$\mathbf{A_{Co\text{-}F}}$	-3210.7196	0.4693	-3212.6110	-3212.1417	**0.0**
$\mathbf{TS_{A\text{-}B}}$	-4015.5472	0.5626	-4017.9542	-4017.3916	**30.7**
$\mathbf{B_{Co\text{-}Cl}}$	-3571.0572	0.4697	-3572.9786	-3572.5088	**-15.9**
Benzoyl chloride	-804.8412	0.0707	-805.3695	-805.2988	
Benzoyl fluoride	-444.5376	0.0736	-445.0307	-444.9571	

Table S12. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the TPSSh (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^3\mathbf{A}_{\mathbf{Co\text{-}F}}$	-3210.7038	0.46494	-3212.5945	-3212.1296
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$	-4015.5343	0.55438	-4017.9431	-4017.38878
$^3\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	-3571.0407	0.46414	-3572.9616	-3572.4975

Table S13. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the TPSS (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the singlet electronic state. Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A}_{\mathbf{Co\text{-}F}}$ and benzoyl chloride) in kcal·mol^{-1}.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)	**ΔG (1M, TZ)**
$\mathbf{A}_{\mathbf{Co\text{-}F}}$	-3210.9274	0.4621	-3212.8228	-3212.3607	**0.0**
$\mathbf{TS}_{\mathbf{A\text{-}B}}$	-4015.8032	0.5533	-4018.2148	-4017.6615	**29.1**
$\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	-3571.2596	0.4621	-3573.1853	-3572.7231	**-15.2**
Benzoyl chloride	-804.8876	0.0693	-805.4164	-805.3471	
Benzoyl fluoride	-444.5877	0.0722	-445.0812	-445.0090	

Table S14. Energy data for the DFT-computed intermediates and transition states for the nucleophilic fluorination reaction computed at the TPSS (PCM = dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^3\mathbf{A}_{\mathbf{Co\text{-}F}}$	-3210.9042	0.4580	-3212.7986	-3212.3405
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$	-4015.7812	0.5450	-4018.1947	-4017.6497
$^3\mathbf{B}_{\mathbf{Co\text{-}Cl}}$	-3571.2353	0.4566	-3573.1603	-3572.7038

Table S15. Energy data for the DFT-computed intermediates and transition states for the Co–F assisted S_N2 fluorination reaction of benzyl bromide and 1-iodooctane computed at the M06-L (SMD = dichloromethane)/def2-TZVP//def2-SVP level of theory in the singlet electronic state. Absolute energies are in a.u. and relative Gibbs energies (with respect to $\mathbf{A_{Co\text{-}F}}$ and acyl chloride) in kcal·mol^{-1}.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)	**ΔG (1M, TZ)**
$A_{Co\text{-}F}$	-3210.3869	0.4727	-3212.2876	-3211.8149	**0.0**
$TS_{A\text{-}B'}$-S_N2 (BnBr)	-6054.8653	0.5807	-6057.3628	-6056.7822	**22.8**
$TS_{A\text{-}B'}$- S_N2 (1-I)	-3823.0855	0.6870	-3825.3266	-3824.6395	**19.6**
$B'_{Co\text{-}Br}$	-5684.4085	0.4708	-5686.5003	-5686.0294	**-4.2**
$B'_{Co\text{-}I}$	-3408.5254	0.4705	-3410.3143	-3409.8437	**-7.8**
Benzyl Bromide (BnBr)	-2844.4941	0.0886	-2845.0921	-2845.0035	
Benzyl Fluoride (BnF)	-370.4834	0.0924	-370.8880	-370.7956	
1-iodooctane (1-I)	-612.7064	0.1968	-613.0527	-612.8559	
1-fluorooctane (1-F)	-414.5836	0.2005	-415.0400	-414.8396	

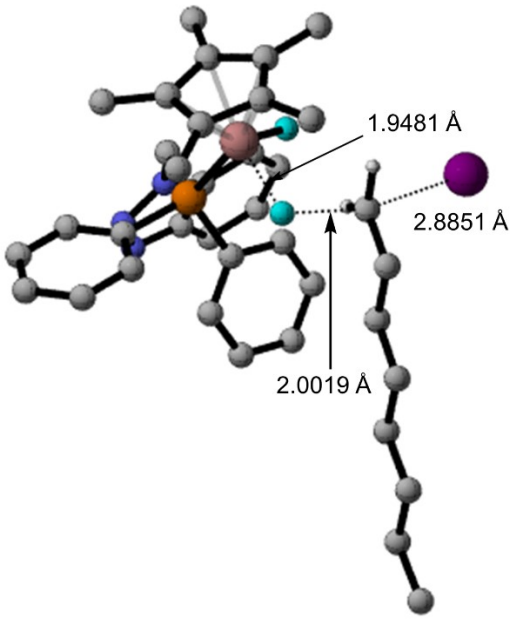


Figure S63. DFT-optimized geometrical structure of $TS_{A\text{-}B'}$-S_N2 for 1-iodooctane substrate. Note that non-relevant hydrogen atoms have been omitted for clarity.

Table S16. Energy data for the DFT-computed intermediates and transition states for the Co–F assisted S_N2 fluorination reaction of benzyl bromide and 1-iodooctane computed at the M06-L (SMD = dichloromethane)/def2-TZVP//def2-SVP level of theory in the triplet electronic state. Energies are in a.u.

	E (DZ)	Corr. G(1M)	E (TZ)	G (1M, TZ)
$^3\mathbf{A}_{\mathbf{Co\text{-}F}}$	-3210.3682	0.4679	-3212.2674	-3211.7996
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$**- S_N2 (BnBr)**	-6054.8489	0.5762	-6057.3447	-6056.7684
$^3\mathbf{TS}_{\mathbf{A\text{-}B}}$**- S_N2 (1-I)**	-3823.0630	0.6792	-3825.3002	-3824.6210
$^3\mathbf{B'}_{\mathbf{Co\text{-}Br}}$	-5684.3888	0.4667	-5686.4792	-5686.0124
$^3\mathbf{B'}_{\mathbf{Co\text{-}I}}$	-3408.5099	0.4647	-3410.2968	-3409.8322

Table S17. Cartesian coordinates.

Structures optimized at the M06-L (SMD = dichloromethane)/def2-SVP level of theory

model-3 N3-coordinated

71

C	-3.06186800	0.72711500	0.43734200
P	-1.28060300	0.84219900	0.84771500
C	-1.27379700	1.24968400	2.62401300
C	-4.02746900	1.34849100	1.24373000
C	-3.48148300	0.00648300	-0.68820000
C	-0.76884800	2.42782400	0.08399000
C	-5.38173400	1.24201300	0.92981000
H	-3.73491400	1.92062300	2.12672400
C	-4.83576300	-0.09209600	-1.00359900
H	-2.73901100	-0.48550200	-1.32208900
C	0.13724400	3.27746300	0.73600600
C	-1.28017000	2.81299900	-1.16412900
H	-6.12232300	1.72757300	1.56969400
C	-5.78988400	0.52121700	-0.19251800
H	-5.14435100	-0.65903500	-1.88532300
H	0.52289400	3.01891800	1.72377300
C	0.54274300	4.47101200	0.13934600
H	-2.00447300	2.17703700	-1.67934700
C	-0.87912200	4.01012200	-1.75335600
H	-6.85215300	0.43858800	-0.43434500
H	1.24786700	5.12283600	0.66138400
C	0.04060100	4.83752200	-1.10875400
H	-1.29022300	4.29732000	-2.72383500
H	0.35707300	5.77398100	-1.57402400
Co	0.00163000	-0.99618500	0.28521400
C	-0.99488300	-2.81007800	0.01390500
C	0.43543300	-3.02063000	-0.07637400
C	-1.28557600	-2.29200400	1.31015500
C	1.00792800	-2.61615800	1.15876800
C	-0.03741900	-2.10514200	2.00630900
C	-1.98370900	-3.26511600	-0.99262200
H	-2.96036200	-2.78015600	-0.87229500
H	-1.63756300	-3.10013100	-2.02162500
H	-2.14842400	-4.34930800	-0.87844700
C	-2.63678000	-2.14011600	1.90078000
H	-2.87602500	-3.06037400	2.45871800
H	-2.70781100	-1.31633000	2.62230400
H	-3.42198900	-2.01127300	1.14646900
C	1.12782500	-3.70355100	-1.19532600
H	2.21377100	-3.54844900	-1.17251100
H	0.95655300	-4.79041200	-1.12851600
H	0.75203200	-3.38122500	-2.17577400
C	2.43109100	-2.71444900	1.55757600
H	2.73818700	-1.88640900	2.21117000
H	2.58028300	-3.64041100	2.13618200
H	3.11469600	-2.75878800	0.70062300
C	0.14851900	-1.69828300	3.42156300
H	0.44640800	-2.56812900	4.02904600
H	0.94460600	-0.94859000	3.53845500
H	-0.77031300	-1.29648100	3.86444600
I	-0.07235700	-0.37461200	-2.32905300
H	-1.67528300	2.25781600	2.79387300
H	-0.24998200	1.21118900	3.01267200
H	-1.88588800	0.53143000	3.18257400
N	1.67804000	0.03852900	0.54168000
N	1.77258500	0.80463300	1.59172300
C	2.87691200	0.03832600	-0.13473100
N	2.98988700	1.33394400	1.62908800
C	3.73631600	0.90173800	0.57185100
C	3.33987000	-0.65654600	-1.26464200
C	3.35615700	2.26613300	2.66695900
C	5.05849400	1.14779600	0.18012100
H	2.69701700	-1.35001600	-1.80621000
C	4.64832200	-0.42224500	-1.65006800
H	2.57341100	2.26008600	3.43098800
H	4.30723300	1.96274600	3.11968500
H	3.46055500	3.27771200	2.25317100
C	5.49110100	0.47118900	-0.94692600
H	5.70471500	1.82816300	0.73620100
H	5.04650200	-0.94223400	-2.52368700
H	6.51331800	0.62167600	-1.30010400

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C	3.85883200	0.00632000	-0.08875900
C	-2.78630100	1.28793700	0.71945400
N	1.70500800	-0.35551300	0.23668700
N	2.77022800	-0.67152100	-0.54314500
P	-0.97395300	1.04488900	0.85936000
C	3.38665600	0.73661300	1.01934700

C	5.19340500	0.06108700	-0.51305200
C	-0.62633400	1.47528100	2.59411100
C	-3.49208600	2.00000100	1.70149100
C	-3.49625000	0.74471400	-0.35988600
N	2.06105600	0.46777400	1.17133800
C	-0.27810700	2.47670500	-0.04957100
C	4.24610500	1.57277300	1.75342800
C	6.02684500	0.88634300	0.22349800
H	5.55123700	-0.50500800	-1.37402800
C	-4.87411300	2.15660700	1.60406600
H	-2.97373400	2.43770900	2.55661800
C	-4.87691000	0.90938500	-0.45846900
H	-2.96342900	0.18206600	-1.13122000
C	0.82275800	3.17973800	0.46212900
C	-0.84671100	2.89738100	-1.26108200
H	3.88310300	2.14262500	2.61038900
C	5.56318600	1.63101900	1.33629700
H	7.07725400	0.97019900	-0.06315400
H	-5.40814200	2.70992600	2.38012100
C	-5.57122400	1.61095500	0.52648800
H	-5.41147100	0.47808400	-1.30828800
H	1.26820600	2.88992500	1.41498900
C	1.35704100	4.26244800	-0.23530700
H	-1.71775500	2.37809200	-1.66841300
C	-0.31474700	3.98459000	-1.95122500
H	6.27030300	2.26627200	1.87350600
H	-6.65449000	1.73352100	0.45521600
H	2.21626600	4.79676300	0.17787400
C	0.79342000	4.66470400	-1.44544000
H	-0.77269900	4.30270300	-2.89059200
H	1.21136700	5.51501600	-1.98945300
Co	-0.17959600	-1.05191900	0.21929500
C	-1.56337700	-2.61438300	0.19830400
C	-0.24361800	-3.15250300	-0.04385100
C	-1.56341200	-1.99443800	1.48308700
C	0.56514300	-2.82264900	1.07697100
C	-0.22357300	-2.05706300	2.00801200
C	-2.75340900	-2.86890100	-0.64708500
H	-3.50449900	-2.07186800	-0.57199900
H	-2.48983400	-2.99642300	-1.70447500
H	-3.24266100	-3.80014200	-0.31633900
C	-2.77202200	-1.54691700	2.21404100
H	-3.12775300	-2.38678700	2.83332600
H	-2.58723200	-0.71232600	2.90124100
H	-3.59688700	-1.27328500	1.54494200
C	0.11224000	-4.03226300	-1.18409100
H	1.18113100	-4.27809200	-1.20654000
H	-0.43671900	-4.98371400	-1.10078400
H	-0.16433700	-3.59275100	-2.15340900
C	1.97525400	-3.21335400	1.30937800
H	2.54089700	-2.43667900	1.84215600
H	2.00044600	-4.10914400	1.95060400
H	2.50797600	-3.47194100	0.38595500
C	0.23632400	-1.64571100	3.35780900
H	0.45946900	-2.53610500	3.96720000
H	1.16185300	-1.05288800	3.31949000
H	-0.52033200	-1.06476700	3.89715300
I	-0.53065000	-0.52807400	-2.39401700
H	-0.80728800	2.54426800	2.76994700
H	0.42052100	1.25098000	2.82497000
C	2.73557400	-1.60546300	-1.63918700
H	1.81297900	-2.18669700	-1.58269100
H	2.76793400	-1.07682000	-2.60075000
H	3.60122800	-2.27551500	-1.56265100
H	-1.26765700	0.89828700	3.27105800

$A_{Co\text{-}F}$

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C	-4.25137400	-1.27074000	-0.99614500
C	-0.80919800	-0.38352500	-1.55098500
H	-0.77988300	0.42998800	-2.28855500
H	-0.17731000	-1.20781600	-1.90823400
C	-0.31422700	1.90220100	0.32162800
N	-2.32248900	-2.22453800	-1.20005900
N	-3.56685900	-2.45869400	-0.95527100
P	-0.00879500	0.13020400	0.05942600
C	-3.33572700	-0.24029800	-1.29683600
C	-5.60668900	-0.98280600	-0.77146900
C	-0.05222600	2.39257200	1.61289200
C	-0.66148400	2.80719600	-0.68941100
N	-2.14570700	-0.89595600	-1.42749500
C	-1.06921900	-0.68789300	1.30014800
C	-3.72609300	1.10115300	-1.39154800
C	-5.99414400	0.34467400	-0.85261500
H	-6.31525700	-1.77900400	-0.53625600
C	-0.16774700	3.75136400	1.88959900
H	0.25554700	1.69972900	2.40328400
C	-0.77144400	4.17062400	-0.40967000
H	-0.84731800	2.45918200	-1.70867600
C	-2.24092800	-0.06669700	1.75939400
C	-0.76665100	-1.99056100	1.72071500
H	-3.01818400	1.89696900	-1.62628500
C	-5.06752000	1.36788400	-1.15987100
H	-7.03833600	0.61402800	-0.67893100
H	0.03262000	4.11619700	2.89977400
C	-0.53051800	4.64450900	0.87891800
H	-1.04999000	4.86388600	-1.20684800
H	-2.49407700	0.94760100	1.43791200
C	-3.10075700	-0.74158100	2.62520800
H	0.14357800	-2.45885400	1.34728500
C	-1.63127100	-2.65721600	2.58638900
H	-5.42025000	2.40026200	-1.21660900
H	-0.62021000	5.71134100	1.09656100
H	-4.01382300	-0.25060900	2.97141800
C	-2.79805700	-2.03897600	3.03784600
H	-1.39087500	-3.67316900	2.90935800
H	-3.47315300	-2.56908700	3.71448800
Co	2.12486200	-0.57395900	0.03911800
C	3.25185200	1.11355200	-0.24788400
C	4.02171000	0.12352500	0.43649900
C	2.85053800	0.55144600	-1.52377900
C	4.06025300	-1.06181300	-0.36560400
C	3.36317400	-0.77390300	-1.59687900
C	3.05033500	2.51567600	0.19472700
H	2.18232700	2.98573800	-0.28654400
H	2.91914700	2.59193700	1.28272500
H	3.92993900	3.12901000	-0.06293100
C	2.12561100	1.28511400	-2.59184500
H	2.83217300	1.87016700	-3.20292600
H	1.59135600	0.61266400	-3.27543500
H	1.40284900	2.00388800	-2.18039200
C	4.57555000	0.27435900	1.80040700
H	4.73852600	-0.69369400	2.28811800
H	5.54488800	0.79667300	1.76389900
H	3.90934300	0.86542900	2.44121100
C	4.66600600	-2.36596200	-0.00366500
H	5.71626300	-2.43793300	-0.32949900
H	4.64825300	-2.53021700	1.08203900
H	4.12300200	-3.19822900	-0.47086300
C	3.14045300	-1.76006300	-2.67955000
H	4.09863200	-2.11265300	-3.09012000
H	2.60401400	-2.63622100	-2.28746700
H	2.55385600	-1.34538000	-3.50862000
F	1.94110900	-0.93222600	1.87173400
F	1.29857400	-2.22850200	-0.41177300

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C	4.60437100	0.11301800	-1.73752400
C	1.51314800	-1.67961300	-1.27801700
H	1.75178000	-2.72500900	-1.04145900
H	0.87117500	-1.65520700	-2.16676300
C	0.87207000	-1.77133300	1.62561200
N	2.73473600	-0.22734800	-2.76799000
N	3.85465100	0.40577200	-2.84880200
P	0.46197200	-0.91044900	0.07320600
C	3.86834800	-0.77798300	-0.92853500
C	5.87253100	0.56391400	-1.33775700
C	0.39931300	-1.21596600	2.82728800
C	1.54207500	-3.00187100	1.67048100
N	2.70867200	-0.96219400	-1.62354800
C	1.20622000	0.75034500	0.20905100
C	4.35835400	-1.25628000	0.29296900
C	6.35729500	0.09803800	-0.12672800
H	6.44109900	1.25689400	-1.96053500
C	0.61551000	-1.86494000	4.04057700
H	-0.14596700	-0.26954200	2.80779800
C	1.75186000	-3.65126300	2.88707900
H	1.90688500	-3.47808600	0.75744100
C	2.05897400	1.11985700	1.25951000
C	1.02639800	1.62263400	-0.87543600
H	3.78349600	-1.93904900	0.92066800
C	5.61126600	-0.79876900	0.67302600
H	7.33787700	0.42705300	0.22431300
H	0.24679500	-1.41443800	4.96503500
C	1.29127400	-3.08546600	4.07468700
H	2.27856800	-4.60823500	2.90184600
H	2.22867100	0.44758400	2.10381300
C	2.72723500	2.34291400	1.21914900
H	0.35784700	1.32677700	-1.68737700
C	1.71671800	2.83177000	-0.91825900
H	6.03481800	-1.13942700	1.62070700
H	1.45669900	-3.59650400	5.02599900
H	3.39122700	2.62054300	2.04162800
C	2.56622300	3.19504100	0.12619700
H	1.58423100	3.49648700	-1.77557000
H	3.10022600	4.14822600	0.09210600
Co	-1.67074300	-0.93128500	-0.77499900
C	-3.28783100	-1.68251000	0.26822400
C	-3.69601000	-1.27454000	-1.06463900
C	-2.30390600	-2.69743300	0.13210400
C	-2.93485400	-2.01591500	-2.00220700
C	-2.00817000	-2.84886900	-1.27241900
C	-3.89554500	-1.22587800	1.53898500
H	-3.22190000	-1.37332800	2.39267400
H	-4.17433000	-0.16446500	1.50545900
H	-4.81276400	-1.80335300	1.74316100
C	-1.77561900	-3.53769200	1.22940300
H	-2.50982600	-4.33328600	1.43848300
H	-0.83456700	-4.03702100	0.97182600
H	-1.63580100	-2.98516400	2.16704500
C	-4.71536700	-0.24502600	-1.36263500
H	-4.61723700	0.14802100	-2.38228400
H	-5.72704400	-0.67253900	-1.27100600
H	-4.65008500	0.59641500	-0.65940900
C	-2.98597800	-1.89044900	-3.47421500
H	-3.69469000	-2.62432100	-3.89011800
H	-3.32064900	-0.89564700	-3.79194400
H	-2.00869300	-2.08179000	-3.93207400
C	-1.06418000	-3.82330100	-1.87084400
H	-1.58468300	-4.75946300	-2.13108400
H	-0.61279800	-3.44343500	-2.79711600
H	-0.25337500	-4.08975800	-1.17947700
F	-0.79586100	-0.32642100	-2.33254700
F	-2.02901300	0.99765200	-0.40185400
Cl	-4.06848500	2.35927200	1.15557800
C	-1.96122500	1.87396900	1.10115700
O	-1.63665200	1.13785600	1.97177900
C	-1.39437300	3.17508300	0.68553200
C	-0.55383900	3.81507100	1.60146900
C	-1.69532500	3.78650700	-0.53761300
C	-0.02419200	5.06972600	1.29899300
H	-0.32367700	3.32799100	2.55204700
C	-1.15226000	5.02957300	-0.83789800
H	-2.35930000	3.27991900	-1.23896300
C	-0.31929400	5.67729000	0.08088000
H	0.62966600	5.56815900	2.01899700
H	-1.38270900	5.50414300	-1.79471000
H	0.09716100	6.65918200	-0.15721200

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C	1.03382300	0.67011200	-1.05968500
H	0.20451400	0.43981900	-1.74220200
H	1.09558500	1.76910800	-1.01554300
C	1.62188900	-1.28885700	1.06937700
P	0.48456400	0.06024000	0.61723600
C	2.14847200	-1.38625200	2.36451200
C	1.92878400	-2.28686300	0.13239300
C	0.86059100	1.42532000	1.77497600
C	2.98825200	-2.44552200	2.70413500
H	1.91046900	-0.62795000	3.11470200
C	2.78471700	-3.33237500	0.46946700
H	1.50141300	-2.25069100	-0.87339300
C	0.20848800	1.41989000	3.01941100
C	1.72725100	2.48474000	1.46947700
H	3.39247000	-2.50854900	3.71716000
C	3.31795700	-3.41413500	1.75613400
H	3.02819500	-4.09169300	-0.27781100
H	-0.48486700	0.60608000	3.24482500
C	0.43515300	2.44171200	3.93860100
H	2.23918600	2.53708400	0.50566600
C	1.94723400	3.50780400	2.39212800
H	3.98569600	-4.23707200	2.02168300
H	-0.07972400	2.42275600	4.90212600
C	1.30261300	3.48959900	3.62792400
H	2.62349900	4.32704300	2.13565000
H	1.47309100	4.29416600	4.34728900
Co	-1.67673500	-0.61221700	0.65391800
C	-3.17605100	-2.12107300	0.65881800
C	-3.94691200	-1.67071600	-0.44466600
C	-1.91757200	-2.60167100	0.12785300
C	-3.25245500	-1.93809800	-1.66717200
C	-2.02174100	-2.48646000	-1.33429500
C	-3.75316600	-2.40572100	2.00523100
H	-2.97674900	-2.65034600	2.73724800
H	-4.31557700	-1.54696700	2.40377300
H	-4.45966700	-3.25291900	1.96368900
C	-1.08115600	-3.63905800	0.80448300
H	-1.63785800	-4.58728000	0.90657100
H	-0.16897900	-3.87113300	0.23940100
H	-0.78200300	-3.32383700	1.81254500
C	-5.27420000	-1.02999600	-0.32749300
H	-5.64183600	-0.62876300	-1.27963400
H	-6.02271900	-1.74963600	0.04607900
H	-5.25603900	-0.21034800	0.40707100
C	-3.69977800	-1.48292800	-3.00941100
H	-3.02994500	-1.83238700	-3.80643900
H	-4.71278100	-1.83573200	-3.25832000
H	-3.72964700	-0.38257100	-3.07337300
C	-0.91729100	-2.76859400	-2.27919800
H	-1.29143200	-3.08022900	-3.26429700

H	-0.29896300	-1.87009000	-2.46221800
H	-0.23835300	-3.55253400	-1.91397400
F	-1.25808400	-1.14230600	2.38256500
F	-1.92893900	0.26604000	-1.08057300
C	-2.81670700	1.91506900	-0.88292700
C	-1.69022900	2.79639200	-1.20594500
C	-1.34817700	2.83614700	-2.56943900
C	-1.01224200	3.59573100	-0.28299500
C	-0.32300300	3.67058800	-2.99713200
H	-1.87990600	2.20015700	-3.28073200
C	-0.00039100	4.44510300	-0.73055000
H	-1.27978800	3.55804500	0.77388900
C	0.35089100	4.47969400	-2.07878900
H	-0.05137500	3.69163700	-4.05464700
H	0.52017000	5.08093600	-0.01106000
H	1.15125700	5.14094500	-2.41849500
O	-3.90727900	1.78428200	-1.27647400
Cl	-2.70389500	1.45998700	1.34104900
N	2.21567900	0.11315000	-1.66367600
N	2.08338300	-0.50407200	-2.87025800
C	3.51453400	0.03370100	-1.24609200
N	3.22437200	-0.96677200	-3.24865800
C	4.15583000	-0.67057500	-2.28789800
C	4.20078500	0.42559300	-0.08854300
C	5.52049700	-0.99251100	-2.21069900
H	3.70363200	0.93736700	0.73628400
C	5.54528700	0.09368300	-0.02579500
C	6.19940200	-0.60072400	-1.07014000
H	6.01057200	-1.53878600	-3.01852400
H	6.11654500	0.37047900	0.86330400
H	7.26064900	-0.83612700	-0.96477300

$B_{Co\text{-}Cl}$

67

C	-0.88002000	-0.43924600	-1.57360100
H	-0.88615700	0.30439500	-2.38323300
H	-0.23465200	-1.27452600	-1.87163400
C	-0.18402000	2.05850700	-0.06727900
P	-0.06474900	0.24443800	-0.03442100
C	0.37532800	2.72109500	1.03885200
C	-0.70437200	2.81512100	-1.12369100
C	-1.23146400	-0.25625300	1.28262800
C	0.39151500	4.11218700	1.09236100
H	0.80350100	2.13162600	1.85777300
C	-0.68239100	4.20951200	-1.06835300
H	-1.12191000	2.32799200	-2.00799300
C	-2.16022900	0.64651200	1.81733400
C	-1.25003900	-1.59518400	1.70163700
H	0.82471000	4.61524500	1.96014400
C	-0.13734000	4.85979600	0.03789800
H	-1.09237400	4.78910100	-1.89881300
H	-2.16722900	1.69275500	1.50108700
C	-3.10110200	0.21414200	2.75312200
H	-0.51274600	-2.28346400	1.28403300
C	-2.19691500	-2.02001700	2.62988700
H	-0.12140900	5.95151200	0.07797300
H	-3.82267000	0.92697800	3.16003300
C	-3.12452100	-1.11927500	3.15719900
H	-2.20792800	-3.06599500	2.94633200
H	-3.86490600	-1.45811300	3.88618000
Co	2.00781900	-0.61600300	0.07608800
C	3.60536500	0.66431700	-0.06415800
C	4.09409700	-0.67760000	0.19378700
C	2.90188600	0.63898700	-1.30764100
C	3.63764900	-1.51937400	-0.84702700
C	2.85288700	-0.72133900	-1.76248800
C	3.91038500	1.84940500	0.77403600
H	3.30818700	2.72310500	0.49332800
H	3.72485000	1.63724900	1.83660500
H	4.96959200	2.13772300	0.67688400
C	2.37393000	1.81091800	-2.04526200
H	3.11654700	2.12944900	-2.79487300
H	1.45070300	1.58316600	-2.59580800
H	2.18516000	2.67392200	-1.39475500
C	4.93876400	-1.06816300	1.34607400
H	4.79221800	-2.11808700	1.62921700
H	6.00433800	-0.93988100	1.09486200
H	4.72798000	-0.45195500	2.22818900
C	3.80389500	-2.98557900	-0.95989300
H	4.32513100	-3.25296500	-1.89170300
H	4.37300100	-3.40604400	-0.12219800
H	2.81793700	-3.47281600	-0.98305500
C	2.24368400	-1.23059300	-3.01511100
H	3.01384200	-1.39390900	-3.78667700
H	1.74742700	-2.19836300	-2.85490700
H	1.51045300	-0.53205000	-3.43839900
F	1.01522100	-2.23215000	-0.10946300
Cl	1.88374600	-0.49891300	2.38912500
N	-2.19193500	-0.99865500	-1.39235400
C	-3.39769500	-0.39830000	-1.17207300
N	-2.32657800	-2.34974300	-1.30770900
C	-4.27545500	-1.48231600	-0.96007900
C	-3.83108800	0.93271000	-1.11966500
N	-3.55635100	-2.64600100	-1.06035100
C	-5.63396700	-1.26334800	-0.68242400
C	-5.17529700	1.13040700	-0.84209500
H	-3.14973100	1.77114500	-1.27078200
H	-6.31162400	-2.10239500	-0.51505300
C	-6.06441600	0.05183000	-0.62620000
H	-5.56026000	2.15114600	-0.78514500
H	-7.11279300	0.26803900	-0.40939800

Benzoyl chloride

14

C	0.12281800	0.19921300	0.00011500
C	0.56474500	-1.13195800	0.00017100
C	1.92781600	-1.40999700	0.00011300
C	2.85684700	-0.36875000	-0.00006300
C	2.42358600	0.95904700	-0.00016800
C	1.06459200	1.24502300	-0.00009600
H	-0.15831200	-1.94818500	0.00030800
H	2.26708300	-2.44783000	0.00020300
H	3.92610200	-0.59317000	-0.00012300
H	3.15065500	1.77387500	-0.00029900
H	0.71160300	2.27813600	-0.00017000
C	-1.29293200	0.60034000	0.00018500
O	-1.72074300	1.71180800	0.00018300
Cl	-2.47859000	-0.78322400	-0.00017200

Benzoyl fluoride

14

C	-0.23791500	0.04039500	0.00000000
C	0.42869300	-1.19407800	0.00000100
C	1.81982200	-1.22765100	0.00000100
C	2.54817100	-0.03685000	0.00000000
C	1.88758100	1.19420300	-0.00000100
C	0.49854300	1.23546900	-0.00000100
H	-0.14524300	-2.12177600	0.00000200
H	2.33979200	-2.18790800	0.00000200
H	3.64037100	-0.06774200	0.00000000
H	2.46060600	2.12376500	-0.00000200
H	-0.03438200	2.18865200	-0.00000100
C	-1.70249700	0.13417300	0.00000000
O	-2.37800800	1.11697000	0.00000200
F	-2.29905200	-1.08274600	-0.00000200

$^3A_{Co\text{-}F}$

67

C	-4.26198500	-1.42579700	-0.99634100
C	-0.83751300	-0.48066300	-1.57371000
H	-0.80247300	0.25972800	-2.38499300
H	-0.19055600	-1.32526000	-1.84553700
C	-0.22647200	2.00445400	0.00413900
N	-2.33670500	-2.35540800	-1.31950900
N	-3.57609900	-2.61158600	-1.07458400
P	-0.08139200	0.19971900	-0.00785700
C	-3.35190700	-0.37158600	-1.22021500
C	-5.61279000	-1.15965100	-0.72280600
C	0.14772900	2.63740300	1.20280900
C	-0.56731400	2.78790600	-1.10638600
N	-2.16434200	-1.01054600	-1.42716200
C	-1.20571600	-0.38766600	1.30018400
C	-3.73927700	0.97374200	-1.18157300
C	-5.99933100	0.16988800	-0.67863400
H	-6.31856500	-1.97347600	-0.54738500
C	0.14140100	4.02568900	1.29569300
H	0.45996400	2.02492200	2.05469600
C	-0.56040600	4.18034500	-1.01038500
H	-0.84527900	2.32440300	-2.05633700
C	-2.20643500	0.43089700	1.84213600
C	-1.10276500	-1.72393000	1.71443200
H	-3.02947800	1.78693100	-1.34408200
C	-5.07619600	1.21753000	-0.90425100
H	-7.04007900	0.42218700	-0.46386400
H	0.42562100	4.50640600	2.23466300
C	-0.21344400	4.80051300	0.18921300
H	-0.83226500	4.78180400	-1.88092100
H	-2.30528700	1.47230000	1.52491600
C	-3.09742600	-0.08348600	2.78356000
H	-0.32027200	-2.35176900	1.28091100
C	-2.00098900	-2.23099800	2.65050000
H	-5.42832400	2.25055000	-0.85682200
H	-0.21387300	5.89062800	0.26115500
H	-3.87703800	0.56128700	3.19675500
C	-2.99851200	-1.41490500	3.18626300
H	-1.91895800	-3.27412800	2.96518400
H	-3.70024800	-1.81736700	3.92098600
Co	1.99673800	-0.62350200	0.24164400
C	3.38696400	0.89591500	-0.33232800
C	4.09982800	-0.00008100	0.50051000
C	2.98503900	0.16910000	-1.53900600
C	4.04294800	-1.29260600	-0.11933900
C	3.45664700	-1.15468100	-1.42839700
C	3.23661300	2.35473400	-0.10573000
H	2.41394600	2.79005900	-0.68897800
H	3.06182900	2.58500600	0.95518000
H	4.15352600	2.89378500	-0.39945700
C	2.33305900	0.79858500	-2.71542600
H	3.06854600	1.36300200	-3.31230400
H	1.87348900	0.06019800	-3.38518100
H	1.55932800	1.52336700	-2.42181400
C	4.66342600	0.33117600	1.83228500
H	5.16193500	-0.53024000	2.29435300
H	5.40340200	1.14349400	1.76501600
H	3.86836600	0.66027700	2.51703500
C	4.56434800	-2.56607100	0.43188800
H	5.56174900	-2.80150600	0.02574000
H	4.65441400	-2.53729200	1.52517300
H	3.90884100	-3.40843400	0.16986300
C	3.23623000	-2.27696400	-2.37134800
H	4.18484800	-2.75518700	-2.66133300
H	2.60802800	-3.05329600	-1.90916800
H	2.73719000	-1.95019000	-3.29279300
F	1.72546200	-0.25327300	2.10638700
F	1.18033000	-2.31266000	-0.15803500

$^3TS_{A\text{-}B}$

81

C	4.68696100	0.08263200	-1.69518200
C	1.57041700	-1.66730900	-1.25216200
H	1.78049100	-2.71369000	-0.99401300
H	0.94275800	-1.65103300	-2.15118100
C	0.95727200	-1.67170700	1.64982900
N	2.81697300	-0.23294100	-2.73202800
N	3.94226100	0.39029800	-2.80581100
P	0.52775300	-0.85350000	0.08003400
C	3.94194800	-0.80808600	-0.89382300
C	5.95693400	0.52247900	-1.29016200
C	0.55598400	-1.06679900	2.85381400
C	1.57057300	-2.93294200	1.70308700
N	2.78281800	-0.97857100	-1.59412000
C	1.23556300	0.82268000	0.12246800
C	4.42644800	-1.29734400	0.32562300
C	6.43530000	0.04728800	-0.08017600
H	6.53149300	1.21488500	-1.90801200
C	0.78545300	-1.69899000	4.07405000
H	0.05568700	-0.09696000	2.83081900
C	1.79548800	-3.56234200	2.92649500
H	1.87840500	-3.44950000	0.79162500
C	2.13791300	1.25263100	1.10522500
C	0.95779400	1.64948300	-0.97708300
H	3.84864100	-1.98288700	0.94733500
C	5.68125200	-0.84940300	0.71173000
H	7.41698200	0.36795100	0.27541500
H	0.47270300	-1.20943800	4.99926100
C	1.40604400	-2.94784800	4.11552300
H	2.27821500	-4.54216100	2.94564600
H	2.37684800	0.61465400	1.95998900
C	2.76142300	2.49361200	0.98170500
H	0.25210600	1.30756100	-1.73883800
C	1.60343600	2.87719200	-1.10403600
H	6.10016200	-1.19930300	1.65809700
H	1.58260400	-3.44370200	5.07285900
H	3.46562200	2.82213800	1.75016300
C	2.50454600	3.30062000	-0.12751900
H	1.39430600	3.50810700	-1.97147500
H	3.00413000	4.26773400	-0.22712200
Co	-1.62902900	-0.95477000	-0.83569200
C	-3.18495600	-1.83054400	0.39438000
C	-3.77719000	-1.32071400	-0.78484100
C	-2.25504600	-2.88433600	0.00652500
C	-3.16569100	-1.99924800	-1.90190300
C	-2.28200700	-3.01532900	-1.40469900
C	-3.48289800	-1.43973700	1.79305000
H	-2.58918600	-1.49347600	2.43014800
H	-3.87323400	-0.41544800	1.85764700
H	-4.23123400	-2.11647700	2.23850100
C	-1.56272000	-3.77877500	0.95996500
H	-2.23186600	-4.61629600	1.21991300
H	-0.65003200	-4.22204300	0.54040500
H	-1.31083100	-3.27745900	1.90337700
C	-4.80910900	-0.26593000	-0.90399300
H	-4.55329200	0.46602200	-1.68311600
H	-5.77991400	-0.70333800	-1.18858800
H	-4.93871200	0.28813000	0.03185200
C	-3.46615600	-1.74182800	-3.32608200
H	-4.35460300	-2.31535000	-3.63813100
H	-3.68945600	-0.68325600	-3.51187700
H	-2.63849000	-2.03890800	-3.98158100
C	-1.47712400	-3.93973700	-2.24112800
H	-2.10872800	-4.71834200	-2.69830300

H	-0.98391300	-3.41530100	-3.07305600
H	-0.70274900	-4.45609600	-1.65915000
F	-0.82753000	-0.47391600	-2.45692300
F	-2.12374800	0.97737900	-0.23738700
Cl	-3.98162600	2.25931000	1.51734600
C	-1.93293800	1.92726100	1.20972400
O	-1.43411700	1.25817100	2.05754100
C	-1.47534300	3.22913100	0.66512000
C	-0.57109800	3.95847400	1.44278100
C	-1.92842200	3.74855100	-0.55317800
C	-0.12699100	5.20722800	1.00663900
H	-0.22173100	3.54337200	2.39137800
C	-1.47152400	4.98690200	-0.98882300
H	-2.63871500	3.17080900	-1.14606300
C	-0.57237400	5.72175500	-0.20895400
H	0.57880600	5.77457900	1.61875500
H	-1.82116100	5.38749400	-1.94349000
H	-0.22185500	6.69816100	-0.55267000

$^3B_{Co\text{-}Cl}$

67

C	-0.93555200	-0.42065100	-1.59883400
H	-0.92899100	0.33879100	-2.39302300
H	-0.30052400	-1.25985800	-1.90810800
C	-0.22260800	2.03745800	-0.04150800
P	-0.12812000	0.22210100	-0.04090200
C	0.31748500	2.68491500	1.08371500
C	-0.69624200	2.81089300	-1.10878000
C	-1.27895500	-0.32301800	1.26437600
C	0.35711400	4.07507900	1.14547200
H	0.71524000	2.08662200	1.91048500
C	-0.65096100	4.20425100	-1.04403600
H	-1.09630700	2.33900600	-2.00910400
C	-2.19880200	0.55185700	1.85706900
C	-1.27582400	-1.67880000	1.62525900
H	0.77464800	4.56483400	2.02834800
C	-0.12752600	4.83866900	0.08143400
H	-1.02538500	4.79525900	-1.88313400
H	-2.21653500	1.61000600	1.58282900
C	-3.11345200	0.07236900	2.79503300
H	-0.54697300	-2.34585900	1.15765600
C	-2.19679400	-2.14969700	2.55756700
H	-0.09257400	5.92962600	0.12842300
H	-3.83056200	0.76057200	3.24929600
C	-3.11659700	-1.27767100	3.14326400
H	-2.19390700	-3.20768700	2.83072000
H	-3.83664500	-1.65175600	3.87526800
Co	1.96691000	-0.64601600	0.15620800
C	3.82698400	0.62377500	-0.04832200
C	4.14120300	-0.76545100	0.15710700
C	3.02738400	0.70507600	-1.21237800
C	3.65490200	-1.51898300	-0.96819700
C	2.92669900	-0.63042900	-1.79012100
C	4.20517900	1.73259300	0.86296800
H	3.72101600	2.67768500	0.58394000
H	3.92916200	1.50889800	1.90439300
H	5.29296300	1.90825500	0.85036400
C	2.52926500	1.93911000	-1.86536000
H	3.26605800	2.29598000	-2.60433300
H	1.59357100	1.77023200	-2.41615800
H	2.36529300	2.75954000	-1.15432500
C	4.95754500	-1.29466000	1.27430800
H	4.67898000	-2.32301100	1.53946300
H	6.02561600	-1.30909400	1.00048300
H	4.85777200	-0.67656000	2.17538900
C	3.78716200	-2.98024800	-1.18593400
H	4.17413500	-3.20208900	-2.19176200
H	4.46384400	-3.44761200	-0.45962900
H	2.80391500	-3.46741500	-1.09994000
C	2.26112800	-0.98591400	-3.06692600
H	2.98815500	-1.01759800	-3.89573300
H	1.79633600	-1.98041300	-3.01439400
H	1.48849700	-0.26111900	-3.35531000
F	0.98864400	-2.27457200	-0.30386100
Cl	1.89349100	-0.37372000	2.44908200
N	-2.25552600	-0.96085600	-1.42513300
C	-3.44781400	-0.34015300	-1.18946700
N	-2.41239800	-2.30976900	-1.34327100
C	-4.34336200	-1.40922500	-0.97686600
C	-3.85361300	0.99848300	-1.12182000
N	-3.64539100	-2.58516800	-1.08815500
C	-5.69479600	-1.16622800	-0.68543400
C	-5.19104300	1.21987900	-0.82916900
H	-3.15751800	1.82432100	-1.27533600
H	-6.38762300	-1.99292200	-0.51876700
C	-6.09877600	0.15678500	-0.61431900
H	-5.55558500	2.24736400	-0.76017000
H	-7.14078100	0.39148400	-0.38625100

$TS_{A\text{-}B'}$-S_N2 (BnBr)

82

P	-1.29356100	-0.83470800	-0.17075400
Co	0.78975200	-1.23831300	0.61761100
C	1.18528500	-3.19759700	0.17272300
C	2.42945900	-2.53763900	0.44812200
C	0.37680400	-3.11029400	1.36533800
C	2.36649600	-1.96316400	1.75239800
C	1.08779100	-2.32145000	2.31889100
C	0.88239200	-3.99897700	-1.03907900
H	-0.18763600	-4.22769100	-1.12801000
H	1.20168200	-3.49143900	-1.96017300
H	1.41761400	-4.96225800	-1.00736100
C	-0.89594600	-3.83370500	1.59406100
H	-0.67148600	-4.89674500	1.77778300
H	-1.43862400	-3.46777800	2.47418700
H	-1.56713900	-3.81122700	0.72498700
C	3.55775400	-2.45773200	-0.50460800
H	4.30799600	-1.69949400	-0.23430400
H	4.07183100	-3.43254700	-0.53010100
H	3.20951500	-2.26586500	-1.52884400
C	3.40368800	-1.16805900	2.45348800
H	3.84842700	-1.75224500	3.27503400
H	4.22590000	-0.85092400	1.79372400
H	2.96986100	-0.26616600	2.91017500
C	0.62255300	-1.91178700	3.66216100
H	1.15149900	-2.48222200	4.44192300
H	0.82764000	-0.84833800	3.84148400
H	-0.45188300	-2.08277200	3.80256500
F	0.48246100	0.33213400	1.63266000
F	1.44617200	-0.11842600	-0.88275600
C	3.03368700	0.66475800	-0.64263800
H	3.50688900	0.13471600	-1.46312400
H	3.17185500	0.25963300	0.35392100
Br	5.85271000	0.75882800	-0.05458600
C	2.79473900	2.08918200	-0.78540300
C	2.80849100	2.68793900	-2.05599000
C	2.53125800	2.88607800	0.34240500
C	2.58790300	4.05493800	-2.19401500
H	3.01011800	2.07009700	-2.93526600
C	2.31688600	4.25245400	0.20362100
H	2.51129200	2.41891500	1.33053900
C	2.34919400	4.84063600	-1.06442500
H	2.60897200	4.51384900	-3.18523800
H	2.12596700	4.86659600	1.08691700
H	2.18475100	5.91577700	-1.17165600
C	-2.40897100	-0.77783500	1.31411500

H	-2.67531800	-1.79533700	1.62903700
H	-1.78676500	-0.32986900	2.10202900
C	-2.00427200	-1.98607800	-1.38204200
C	-1.36837100	-2.03390700	-2.63450300
C	-3.09227700	-2.83170800	-1.13222200
C	-1.81823900	-2.90844100	-3.61856900
H	-0.51123000	-1.38229200	-2.83559500
C	-3.53474900	-3.71232200	-2.12087200
H	-3.61556700	-2.79571700	-0.17428400
C	-2.90109500	-3.75251000	-3.36177600
H	-1.31880700	-2.93492800	-4.58978200
H	-4.38801300	-4.36357600	-1.91803500
H	-3.25342900	-4.44069400	-4.13371200
C	-1.56878500	0.79790500	-0.93995700
C	-2.68153800	0.99064200	-1.77506100
C	-0.74450300	1.88500500	-0.62361200
C	-2.96335000	2.25748600	-2.28254300
H	-3.34285400	0.15501400	-2.02157600
C	-1.03227900	3.14788400	-1.13874200
H	0.10664700	1.72437000	0.03848400
C	-2.13979700	3.33812600	-1.96479200
H	-3.83551300	2.39903200	-2.92533900
H	-0.38410200	3.99080700	-0.88556700
H	-2.36308000	4.33105900	-2.36295000
N	-4.74188400	-0.52102000	0.65396500
C	-5.11360000	1.57370300	1.05157400
N	-3.60551000	0.00439900	1.17554300
N	-5.64565400	0.39950300	0.58260500
C	-3.77980000	1.33197300	1.43809800
C	-5.66756600	2.85915400	1.17018300
H	-6.69885500	3.05521200	0.87158800
C	-2.94490700	2.33273200	1.94983700
H	-1.90715300	2.13241400	2.22565600
C	-4.84704100	3.85459400	1.67415000
H	-5.23559900	4.86990200	1.77952000
C	-3.50955300	3.59447400	2.05784800
H	-2.90296900	4.41653800	2.44476400

$TS_{A\text{-}B'}$- S_N2 (1-I)

93

P	1.51063200	0.80691200	0.53194900
Co	1.65025700	-1.46982300	0.39130800
C	2.63268100	-2.16988300	2.13653400
C	1.90765400	-3.28284700	1.61971400
C	3.66633000	-1.80475600	1.16383200
C	2.37850700	-3.52101200	0.29778400
C	3.52471300	-2.65748600	0.05923700
C	2.49405900	-1.61535000	3.49858000
H	2.94011400	-0.61459900	3.59468900
H	1.44429800	-1.55325300	3.81062600
H	3.00749100	-2.26257500	4.23326700
C	4.72468800	-0.79099100	1.39787800
H	5.63415900	-1.27842900	1.86912300
H	5.05542300	-0.31141300	0.43595000
H	4.37506100	0.00283600	2.12188600
C	0.80765800	-3.98935200	2.32275200
H	0.07520500	-4.45906600	1.60260400
H	1.23441000	-4.82325700	2.97071800
H	0.24330500	-3.27762100	2.99423000
C	1.86544700	-4.49546500	-0.68850500
H	0.96364200	-5.01645700	-0.33408000
H	1.63056200	-4.00847800	-1.64127200
H	2.62446500	-5.27147200	-0.90779100
C	4.30358800	-2.64655200	-1.20031200
H	4.85662700	-3.59004300	-1.33021900
H	3.63354100	-2.54240800	-2.07616300
H	5.03724300	-1.82357400	-1.23602600
F	1.53171500	-1.25633800	-1.47731000
F	-0.16365500	-1.38119200	1.36586200
C	-1.36390900	-2.21899100	-0.01087200
H	-0.78566000	-3.13873100	0.04366100
H	-0.98120400	-1.43843800	-0.65955300
C	2.82528800	1.54923700	-0.55431900
H	3.77627900	1.62016200	-0.00621300
H	2.97179500	0.83185600	-1.37087900
C	-2.61843300	-2.06112400	0.75170700
H	-3.30214100	-2.89169100	0.51281300
H	-2.36079000	-2.22433500	1.81516900
C	-3.29430900	-0.71879900	0.56499800
H	-3.52530400	-0.58089300	-0.50846600
H	-2.57555400	0.08209900	0.81801600
C	-4.56661100	-0.55350300	1.38151600
H	-4.34124200	-0.72800400	2.44975800
H	-5.28493100	-1.34695200	1.10043000
C	-5.22129800	0.80430200	1.22134100
H	-5.42210500	0.99080100	0.15018600
H	-4.50851700	1.59461500	1.52146300
C	-6.51348700	0.95675900	2.00671600
H	-6.31244500	0.75955800	3.07602500
H	-7.22674800	0.16949300	1.70020600
C	-7.16958300	2.31697300	1.86303200
H	-7.36622900	2.51464800	0.79440900
H	-6.45778200	3.10201900	2.17452000
C	-8.45968300	2.45013500	2.65231300
H	-8.29127700	2.30170900	3.72962000
H	-8.91416000	3.44695800	2.53416100
H	-9.20791900	1.71144700	2.33707300
I	-2.27283800	-3.18795700	-2.49733700
C	-0.02176400	1.50383300	-0.17474700
C	-0.64077500	2.62534900	0.40205200
C	-0.54025500	0.96084400	-1.36106200
C	-1.76473600	3.18739100	-0.20197000
H	-0.23949800	3.07770600	1.31226600
C	-1.66475900	1.52834300	-1.95253300
H	-0.04572500	0.10014100	-1.81852700
C	-2.28002600	2.64004400	-1.37731300
H	-2.23633000	4.06344000	0.24976400
H	-2.06683900	1.09172100	-2.87254900
H	-3.16728900	3.08304500	-1.84592800
C	1.66301200	1.54711500	2.17803500
C	2.73462800	2.35742400	2.57293700
C	0.66813500	1.21283300	3.12036800
C	2.81146300	2.82738900	3.88438800
H	3.51225900	2.64896700	1.86017900
C	0.74511600	1.69586300	4.42323000
H	-0.15472000	0.55842500	2.82023900
C	1.82130900	2.50124400	4.81171800
H	3.65270400	3.45780300	4.18144300
H	-0.03146500	1.43434000	5.14214800
H	1.88345100	2.87089700	5.83612200
C	1.97374800	3.09804900	-2.35374600
C	1.67850500	4.47541200	-2.28996400
C	1.73479500	2.32655900	-3.49835700
C	1.12171800	5.13770500	-3.39670800
C	1.18376000	2.99780600	-4.57878600
H	1.95099700	1.25660900	-3.53149200
C	0.88097600	4.37973500	-4.53022500
H	0.88900600	6.20313600	-3.35290200
H	0.97044100	2.44333400	-5.49552000
H	0.44543600	4.85373200	-5.41257100
N	2.48124700	2.82294000	-1.11662500
N	2.47391400	3.94136900	-0.35000000
N	2.01062600	4.93080400	-1.03947900

$B'_{Co\text{-}Br}$

67

C	-1.05949000	-0.26194400	-1.68728600
H	-1.12159500	0.55630700	-2.41843400
H	-0.41285900	-1.04777600	-2.09569600
C	-0.34337100	2.09659400	0.01229500
P	-0.18521500	0.28783200	-0.12297500
C	0.23950800	2.68021900	1.15033500
C	-0.92334200	2.92660800	-0.95444500
C	-1.29602200	-0.35516700	1.18115800
C	0.22292400	4.06194900	1.32192200
H	0.71410200	2.03855300	1.90199100
C	-0.93565900	4.31130800	-0.78090500
H	-1.36266200	2.50660000	-1.86213900
C	-2.23625900	0.47032500	1.81168100
C	-1.25819600	-1.72275300	1.49173100
H	0.67606100	4.50219400	2.21339700
C	-0.36515400	4.88140400	0.35605600
H	-1.39272600	4.94633800	-1.54349300
H	-2.28632100	1.53719600	1.57928100
C	-3.13304800	-0.06651400	2.73664700
H	-0.50872200	-2.34876700	1.00291500
C	-2.16239900	-2.25212700	2.40879500
H	-0.37549600	5.96569300	0.48952300
H	-3.86441300	0.58631700	3.21977900
C	-3.10109800	-1.42791900	3.03283500
H	-2.13034900	-3.31934700	2.64189500
H	-3.80754900	-1.84803500	3.75322200
Co	1.90438100	-0.54159000	-0.21104000
C	3.46803300	0.78796900	-0.33881500
C	4.00174700	-0.55720000	-0.23407300
C	2.68560700	0.85190400	-1.53414100
C	3.48582200	-1.31852400	-1.30959600
C	2.63601100	-0.46227900	-2.10504700
C	3.81520400	1.91608300	0.56053300
H	3.13856400	2.77086300	0.43039800
H	3.77319900	1.61232700	1.61618700
H	4.83758800	2.27684600	0.36174500
C	2.09323900	2.07228000	-2.13187500
H	2.77514600	2.46507100	-2.90359900
H	1.13427200	1.87839700	-2.63198300
H	1.94541200	2.87511100	-1.39918600
C	4.96032900	-1.02619500	0.79450200
H	4.78992300	-2.07357400	1.07450700
H	5.98953100	-0.95378200	0.40588700
H	4.90620200	-0.42574500	1.71002400
C	3.68340200	-2.76271300	-1.56719900
H	4.22533900	-2.92275800	-2.51217500
H	4.25073200	-3.25487400	-0.76796400
H	2.71124200	-3.26800200	-1.65733600
C	1.96032100	-0.87508200	-3.35865800
H	2.68971200	-0.98861300	-4.17721900
H	1.46285800	-1.84881000	-3.24320600
H	1.21513100	-0.14211100	-3.69348800
F	0.92234400	-2.14882800	-0.50148000
N	-2.35087300	-0.86662500	-1.50414100
C	-3.55966000	-0.31306200	-1.19660200
N	-2.45232800	-2.22293700	-1.50905900
C	-4.40460700	-1.43015400	-1.02782100
C	-4.01970600	0.99985800	-1.03617000
N	-3.66443800	-2.56607500	-1.23642700
C	-5.75510700	-1.26419100	-0.68225200
C	-5.35567000	1.14528200	-0.69325900
H	-3.36397500	1.86356200	-1.15580500
H	-6.40713100	-2.12904300	-0.54758200
C	-6.21143600	0.03309500	-0.51736100
H	-5.76009700	2.15017300	-0.55173100
H	-7.25463700	0.20791800	-0.24510400
Br	1.95298000	-0.67909100	2.24545400

B'$_{\text{Co-I}}$

67

C	1.24102700	0.24006700	1.76919700
H	1.33414900	1.21931000	2.25991700
H	0.59854100	-0.40021000	2.38510900
C	0.53401100	2.09064300	-0.47522500
P	0.32530000	0.38944600	0.14044400
C	-0.08979400	2.38703000	-1.69892600
C	1.19933900	3.11433700	0.21079500
C	1.37125900	-0.62266000	-0.96870600
C	-0.03316100	3.67348700	-2.22889600
H	-0.62797700	1.59901100	-2.23816500
C	1.25098500	4.40350300	-0.32033100
H	1.67184100	2.92623400	1.17739100
C	2.23953300	-0.04098800	-1.90164200
C	1.35068100	-2.01817400	-0.82028400
H	-0.52114400	3.88691300	-3.18280000
C	0.63686400	4.68593900	-1.53956700
H	1.77242800	5.19176400	0.22766400
H	2.27824500	1.04387400	-2.02752100
C	3.07949200	-0.84513100	-2.67313600
H	0.65910100	-2.45988700	-0.09905800
C	2.19880400	-2.81268000	-1.58705000
H	0.67719100	5.69662500	-1.95236000
H	3.75423300	-0.38027200	-3.39621600
C	3.06378800	-2.22981100	-2.51519800
H	2.17952600	-3.89788300	-1.46086700
H	3.72605700	-2.85688200	-3.11723000
Co	-1.78688200	-0.29718900	0.55569300
C	-3.23071400	1.16533700	0.42486500
C	-3.88944200	-0.10143600	0.66563900
C	-2.37472100	1.42626200	1.54381300
C	-3.35903200	-0.65606300	1.85597200
C	-2.40112300	0.27893200	2.40101700
C	-3.54673700	2.09668300	-0.68693600
H	-2.76996700	2.86133000	-0.81784000
H	-3.65927500	1.56613200	-1.64333700
H	-4.49504300	2.62651700	-0.49859700
C	-1.66080900	2.69545900	1.82166100
H	-2.24793000	3.28747500	2.54238000
H	-0.67248300	2.54076300	2.27694100
H	-1.53604100	3.31495800	0.92524000
C	-4.99570700	-0.66551300	-0.14390900
H	-4.96986100	-1.76170200	-0.19055200
H	-5.95703400	-0.38349200	0.31723200
H	-5.00164700	-0.28110800	-1.17080700
C	-3.66458100	-1.97975600	2.44397700
H	-4.20192300	-1.87405900	3.39934900
H	-4.28217400	-2.59501600	1.77813100
H	-2.73582800	-2.53008400	2.65063500
C	-1.68085900	0.09281800	3.68320500
H	-2.37143500	0.20328800	4.53488100
H	-1.24972300	-0.91588800	3.75566200
H	-0.87644300	0.82575600	3.82534600
F	-0.85441200	-1.81695400	1.22420800
N	2.51519000	-0.42303400	1.71009200
C	3.71393300	-0.02104000	1.19452000
N	2.58996500	-1.72801200	2.08816600
C	4.52329300	-1.17225500	1.29923200
C	4.19203700	1.17689400	0.64741400
N	3.77525600	-2.17736300	1.85743400
C	5.85301500	-1.16075800	0.84948800
C	5.50674700	1.16941200	0.20602800
H	3.56447100	2.06440900	0.55576200
H	6.47645500	-2.05317900	0.92828600
C	6.32594900	0.02061400	0.30296300
H	5.92322100	2.07881900	-0.23326900
H	7.35371700	0.07313800	-0.06277700

I	-2.05706800	-1.32320200	-1.91936800

Benzyl bromide (BnBr)

15

C	0.76314900	0.00669700	1.11952600
H	0.97915900	-0.88165400	1.72378100
H	0.97825100	0.90235300	1.71322000
C	-0.61857300	0.00303300	0.57143500
C	-1.27670700	-1.20583300	0.30465900
C	-1.28041600	1.20856100	0.29893800
C	-2.56887300	-1.20933600	-0.21614500
H	-0.76502400	-2.15093500	0.50923700
C	-2.57263100	1.20568000	-0.22182700
H	-0.77160200	2.15612700	0.49914400
C	-3.21991200	-0.00343000	-0.48141100
H	-3.07240200	-2.15850300	-0.41544500
H	-3.07904700	2.15236800	-0.42554300
H	-4.23331300	-0.00596100	-0.88998600
Br	2.13165000	-0.00131500	-0.31329900

Benzyl fluoride (BnF)

15

C	-1.91057800	0.61548600	-0.02767900
H	-2.17574800	1.16461200	-0.94703500
H	-2.17067500	1.26770600	0.82264700
C	-0.45381200	0.27256500	-0.01174400
C	-0.01790300	-1.05511300	-0.01623000
C	0.49623800	1.30258400	0.00317300
C	1.34694800	-1.34879600	-0.00631000
H	-0.75371200	-1.86159800	-0.02580000
C	1.85725900	1.00796100	0.01184500
H	0.16162700	2.34447200	0.00870400
C	2.28797600	-0.32071100	0.00749200
H	1.67485800	-2.39148000	-0.00900200
H	2.58828700	1.82039100	0.02385800
H	3.35591100	-0.55187100	0.01569900
F	-2.70192400	-0.51512200	0.03862800

1-iodooctane (1-I)

26

C	-7.18804100	-0.56806500	0.00625700
H	-7.20945900	-1.18694700	0.91668000
H	-7.19120600	-1.25962200	-0.85049600
H	-8.13334300	-0.00743800	-0.02606000
C	-5.98169100	0.34647600	-0.01822300
H	-6.01945500	0.98981500	-0.91517000
H	-6.02565100	1.04397700	0.83705700
C	-4.65542600	-0.39397600	0.00811500
H	-4.60570300	-1.08611400	-0.85263500
H	-4.61636200	-1.04487800	0.90096800
C	-3.43992500	0.51542800	-0.00551500
H	-3.48313800	1.19872100	0.86238700
H	-3.48440000	1.17449400	-0.89189100
C	-2.11616700	-0.22778800	0.00312900
H	-2.06699200	-0.90148700	-0.87151900
H	-2.07413400	-0.89503600	0.88307900
C	-0.90141100	0.68355600	0.00522300
H	-0.94043200	1.34833800	0.88667100
H	-0.94292000	1.35688900	-0.86959500
C	0.41879900	-0.07469300	-0.00087100
H	0.46678000	-0.72647100	-0.88939100
H	0.46227400	-0.74971500	0.87040300
C	1.59857500	0.86343400	0.01510600
H	1.62533600	1.49086100	0.91605800
H	1.62552800	1.52217100	-0.86323100
I	3.51330200	-0.17233600	-0.00231400

1-fluorooctane (1-F)

26

C	-5.04908100	-0.33851700	-0.00335600
H	-5.11923600	-0.94990200	0.90964100
H	-5.09767500	-1.03211900	-0.85710700
H	-5.95165900	0.28807500	-0.04340100
C	-3.77936400	0.48546600	-0.02609700
H	-3.76374500	1.12165700	-0.92881400
H	-3.77774200	1.19179300	0.82306400
C	-2.51192700	-0.35100600	0.01595600
H	-2.50913900	-1.05344300	-0.83789300
H	-2.52685600	-0.99426900	0.91506500
C	-1.23193100	0.46471900	0.00134100
H	-1.22570900	1.15384800	0.86574700
H	-1.22539000	1.12099800	-0.88827000
C	0.03310300	-0.37411700	0.01548900
H	0.03365000	-1.05241400	-0.85706500
H	0.02427100	-1.04024100	0.89731100
C	1.31079500	0.44534300	0.01646900
H	1.32159500	1.10653600	0.90175100
H	1.30964000	1.12704600	-0.85318200
C	2.57434300	-0.39516300	-0.00376600
H	2.58973900	-1.03697800	-0.90095700
H	2.59265000	-1.07940800	0.86149700
C	3.82285600	0.44153700	0.01291700
H	3.88363100	1.05905900	0.92482700
H	3.86404400	1.12288600	-0.85348500
F	4.95168400	-0.36918900	-0.02805000

$^{3}TS_{A\text{-}B}$- S_N2 (BnBr)

82

P	1.33313000	-0.78115300	0.22797900
Co	-0.77981900	-1.13286600	-0.58719500
C	-1.21821200	-3.15665400	-0.15943800
C	-2.48583300	-2.54748000	-0.40127700
C	-0.45360800	-3.13448600	-1.40851500
C	-2.45341200	-2.01986000	-1.72412100
C	-1.22062900	-2.44870700	-2.36395800
C	-0.84467300	-3.90463700	1.06513200
H	0.23595600	-4.08430700	1.13807200
H	-1.17328300	-3.38758000	1.97799300
H	-1.33572900	-4.89235000	1.07028300
C	0.82261600	-3.86149400	-1.61777200
H	0.63006700	-4.94404100	-1.69497900
H	1.33398600	-3.55882000	-2.54025600
H	1.52161300	-3.74124200	-0.77731200
C	-3.59776900	-2.47554000	0.57749500
H	-4.37890800	-1.75623500	0.28935600
H	-4.08190000	-3.46114500	0.67487500
H	-3.23675700	-2.20536500	1.57984200
C	-3.51430600	-1.25251400	-2.41619100
H	-4.01161900	-1.88242300	-3.17207400
H	-4.29462400	-0.87527500	-1.73740300
H	-3.09072700	-0.39639400	-2.96271200
C	-0.84001300	-2.08626700	-3.74825500
H	-1.55489200	-2.49508900	-4.47906800
H	-0.84328800	-0.99383400	-3.88107800
H	0.15772800	-2.45534800	-4.01600200
F	-0.43929900	0.31541300	-1.73392400
F	-1.50581100	-0.11325700	1.05419700
C	-3.14301300	0.65403400	0.72226100
H	-3.60511000	0.16468200	1.57267100
H	-3.21978000	0.16949000	-0.24464600
Br	-5.87908900	0.77283600	0.07308200
C	-2.88831300	2.08026900	0.76813400
C	-2.93603400	2.77658500	1.98753200
C	-2.57205900	2.78366200	-0.40781400
C	-2.70323100	4.14784400	2.02547800

H	-3.17506600	2.23110900	2.90438200
C	-2.34306000	4.15410400	-0.36845200
H	-2.51980100	2.23975300	-1.35489500
C	-2.41519800	4.84076200	0.84736200
H	-2.75295800	4.68315400	2.97663700
H	-2.11125400	4.69506600	-1.28912100
H	-2.24133900	5.91935800	0.87624900
C	2.43102300	-0.82018000	-1.27135200
H	2.64464500	-1.85924200	-1.55407000
H	1.82319400	-0.37433400	-2.07181700
C	2.02624100	-1.90492400	1.47090300
C	1.42582600	-1.87446300	2.74165700
C	3.06035700	-2.81623600	1.22040400
C	1.85829900	-2.73814000	3.74306400
H	0.61061500	-1.17150900	2.94289400
C	3.48630000	-3.68257100	2.22841500
H	3.55572700	-2.84399200	0.24756600
C	2.88764300	-3.64674800	3.48685700
H	1.38672400	-2.70479000	4.72783400
H	4.29846100	-4.38468200	2.02663600
H	3.22599100	-4.32559100	4.27313500
C	1.62776700	0.87488000	0.92421700
C	2.79540700	1.12788200	1.66204800
C	0.73586200	1.91903800	0.65342800
C	3.06700700	2.41716400	2.11431100
H	3.50428600	0.32119200	1.87293600
C	1.01155800	3.20460700	1.11635200
H	-0.16439700	1.71229800	0.07411200
C	2.17530000	3.45610300	1.84281000
H	3.98210100	2.60996200	2.67950000
H	0.31044100	4.01499400	0.90245000
H	2.38966500	4.46638200	2.19991600
N	4.79019700	-0.66970700	-0.67444300
C	5.24219700	1.40775900	-1.08181000
N	3.66436600	-0.09385400	-1.16653400
N	5.73417900	0.21081300	-0.62606700
C	3.89025400	1.22418800	-1.43557100
C	5.84782300	2.66805300	-1.21565500
H	6.89385500	2.81947800	-0.94342300
C	3.08645400	2.25899700	-1.92788500
H	2.03558400	2.10161100	-2.18203200
C	5.05833900	3.69800500	-1.69985700
H	5.48781600	4.69542800	-1.81629300
C	3.70175400	3.49565200	-2.05031700
H	3.12205900	4.34274600	-2.42431600

$^{3}TS_{A\text{-}B}$- S_N2 (1-I)

93

P	1.50885400	0.80992600	0.53668700
Co	1.65316600	-1.46670700	0.39418700
C	2.63651200	-2.16239100	2.13064900
C	1.91890000	-3.28754000	1.62014600
C	3.66969700	-1.79647200	1.16273800
C	2.39062900	-3.51654300	0.29866200
C	3.53014400	-2.64599900	0.05425900
C	2.50136100	-1.60627700	3.49690600
H	2.93035600	-0.59946400	3.58676600
H	1.45135700	-1.56589200	3.81860200
H	3.03091500	-2.24648700	4.22260600
C	4.71591600	-0.77022500	1.39570400
H	5.49124500	-1.15515700	2.07787000
H	5.22095300	-0.47128200	0.46821100
H	4.30946200	0.13387700	1.87353100
C	0.83513500	-4.00533800	2.33384600
H	0.28360900	-4.68765900	1.67440600
H	1.24365500	-4.61223900	3.15777600
H	0.11412600	-3.30396900	2.77421000
C	1.87984200	-4.49838900	-0.68644500
H	0.99898300	-5.04075000	-0.32154600
H	1.60424700	-4.00313800	-1.62995400
H	2.65052900	-5.24318600	-0.93948300
C	4.29936100	-2.62518900	-1.21008900
H	4.93936200	-3.51773000	-1.29855500
H	3.62934900	-2.62860600	-2.08126500
H	4.95134500	-1.74575700	-1.28671600
F	1.53472400	-1.25600900	-1.47475400
F	-0.16119200	-1.37044800	1.37309100
C	-1.35934900	-2.22256200	0.00217100
H	-0.78424600	-3.14602500	0.06812700
H	-0.97305800	-1.44712500	-0.65245700
C	2.81730300	1.54845500	-0.55521700
H	3.77298900	1.61206800	-0.01693800
H	2.95050800	0.83026400	-1.37575800
C	-2.61940500	-2.06122000	0.75917200
H	-3.30134800	-2.89350600	0.52121500
H	-2.36672900	-2.21745200	1.82292100
C	-3.29796700	-0.72054600	0.56044300
H	-3.52394100	-0.58957900	-0.51326600
H	-2.58092000	0.08216200	0.81257400
C	-4.56583700	-0.55674300	1.37637400
H	-4.34041900	-0.72932900	2.44491700
H	-5.28245600	-1.35203300	1.10116500
C	-5.22824900	0.79950900	1.21416500
H	-5.42912800	0.98414000	0.14270000
H	-4.51716900	1.59168400	1.51341200
C	-6.51597100	0.95039700	2.00396400
H	-6.31483300	0.75506300	3.07359800
H	-7.22753600	0.16126000	1.69832400
C	-7.17980200	2.30907800	1.85824200
H	-7.37654400	2.50489600	0.78929400
H	-6.46969400	3.09599800	2.16886200
C	-8.46539700	2.44067300	2.64697500
H	-8.29700300	2.28905900	3.72453600
H	-8.92688000	3.43141100	2.52734200
H	-9.21203900	1.69503100	2.33253400
I	-2.26558500	-3.19677900	-2.49323000
C	-0.02475900	1.50275500	-0.17139200
C	-0.64622400	2.62378900	0.39870400
C	-0.54180100	0.95709500	-1.35711300
C	-1.77115700	3.18271300	-0.20640200
H	-0.24613200	3.07820200	1.30841500
C	-1.66729200	1.52149100	-1.95467600
H	-0.04538400	0.09678000	-1.81326600
C	-2.28499100	2.63271500	-1.38114500
H	-2.24466700	4.05841000	0.24400500
H	-2.06321500	1.08279600	-2.87421100
H	-3.16802300	3.07326500	-1.85061500
C	1.65925000	1.55267900	2.18180700
C	2.73409600	2.36071100	2.57590900
C	0.66478800	1.22264900	3.11931200
C	2.80959600	2.83261700	3.88674200
H	3.51133500	2.64287000	1.86297600
C	0.74040800	1.70760800	4.42153600
H	-0.16163800	0.57115500	2.81983400
C	1.81484400	2.51071300	4.80923300
H	3.64946300	3.46515100	4.18317700
H	-0.04083700	1.45047900	5.14058300
H	1.87593800	2.88688600	5.83315100
C	1.96811800	3.09807500	-2.35699300
C	1.67004700	4.47491800	-2.29517100
C	1.73106900	2.32454100	-3.50062100
C	1.11222600	5.13456500	-3.40297300
C	1.17897500	2.99319000	-4.58211800
H	1.94946500	1.25499100	-3.53223700
C	0.87335800	4.37456300	-4.53552600
H	0.87732700	6.19957700	-3.36068400
H	0.96705100	2.43703600	-5.49815700

H	0.43710200	4.84646800	-5.41863900
N	2.47582400	2.82568600	-1.11935400
N	2.46598800	3.94514100	-0.35425500
N	2.00087800	4.93268900	-1.04521200

^{3}B'$_{Co\text{-}Br}$

67

C	-1.09437800	-0.30660800	-1.68624300
H	-1.13040300	0.49831400	-2.43346600
H	-0.45320700	-1.11234600	-2.06389000
C	-0.37842300	2.07260200	-0.01744200
P	-0.24224700	0.26046000	-0.11976300
C	0.17167600	2.67730500	1.12648300
C	-0.90529700	2.88782200	-1.02737300
C	-1.34218500	-0.37540600	1.18861700
C	0.17544800	4.06311900	1.26005400
H	0.60384500	2.05041800	1.91423300
C	-0.89747700	4.27653200	-0.89105800
H	-1.32032000	2.45225100	-1.93908300
C	-2.28159300	0.44168900	1.83074400
C	-1.28103900	-1.74230500	1.49749500
H	0.60262200	4.51847000	2.15661600
C	-0.35861600	4.86691200	0.25077400
H	-1.31354200	4.89841300	-1.68712700
H	-2.34480500	1.50768000	1.59645800
C	-3.15823700	-0.10637000	2.76745100
H	-0.53675800	-2.36102900	0.98931300
C	-2.16547900	-2.28239900	2.42771200
H	-0.35180500	5.95447900	0.35415900
H	-3.89103400	0.53644200	3.26152100
C	-3.10432300	-1.46777400	3.06367100
H	-2.11862700	-3.34897500	2.66064400
H	-3.79512800	-1.89556900	3.79450700
Co	1.87239100	-0.58590700	-0.10286500
C	3.65141800	0.75716100	-0.43750400
C	4.04381800	-0.61617800	-0.27042800
C	2.76956000	0.80956900	-1.54468100
C	3.49547100	-1.38626700	-1.35673700
C	2.68915500	-0.52145400	-2.12810000
C	4.06150100	1.88103200	0.44187300
H	3.48256100	2.79230900	0.24249700
H	3.93428600	1.63094400	1.50592800
H	5.12423900	2.13522100	0.29749800
C	2.17306100	2.02692800	-2.14525600
H	2.80764200	2.39023700	-2.97062500
H	1.18095100	1.83663900	-2.57823600
H	2.07925200	2.85053100	-1.42554400
C	4.99621800	-1.11209600	0.75047700
H	4.78239600	-2.14636800	1.05039600
H	6.02437600	-1.09739100	0.35171100
H	4.98409000	-0.49161100	1.65554900
C	3.67444800	-2.83746800	-1.60078000
H	4.25819200	-3.02349900	-2.51626700
H	4.19591800	-3.33539800	-0.77361400
H	2.69882300	-3.32781300	-1.72678000
C	1.94893600	-0.89971400	-3.35606400
H	2.63222600	-0.98957700	-4.21691900
H	1.45620400	-1.87619400	-3.24326500
H	1.18809100	-0.15891500	-3.63428300
F	0.88554800	-2.20644700	-0.59134800
N	-2.39778200	-0.88317000	-1.50348300
C	-3.59440000	-0.29981900	-1.20368700
N	-2.52619200	-2.23747700	-1.48317600
C	-4.46144900	-1.39614300	-1.01348200
C	-4.02591500	1.02531300	-1.06719400
N	-3.74470000	-2.55049700	-1.20316300
C	-5.80748400	-1.19571900	-0.66899300
C	-5.35785000	1.20468400	-0.72431900
H	-3.35342100	1.87284800	-1.20649000
H	-6.47761300	-2.04387500	-0.51812100
C	-6.23600700	0.11382900	-0.52674800
H	-5.74133200	2.22013200	-0.60100100
H	-7.27475100	0.31549500	-0.25611800
Br	1.98439000	-0.48960800	2.32996900

^{3}B'$_{Co\text{-}I}$

67

C	1.24993500	0.28155800	1.76436400
H	1.33483800	1.28239500	2.20850500
H	0.59831200	-0.32916900	2.40247500
C	0.56696500	2.04455000	-0.55785300
P	0.37181600	0.36451800	0.11082900
C	0.08003500	2.26588100	-1.85831700
C	1.07863600	3.13055100	0.16670600
C	1.40861700	-0.70724200	-0.94072800
C	0.11768000	3.53821100	-2.42123200
H	-0.33448100	1.43004700	-2.43232000
C	1.10713500	4.40601400	-0.39907300
H	1.46380200	3.00002100	1.18076500
C	2.30155900	-0.18938600	-1.88790200
C	1.34337200	-2.09373300	-0.73261300
H	-0.25939300	3.69056000	-3.43508000
C	0.62821200	4.61323500	-1.69152200
H	1.51074200	5.24113800	0.17799200
H	2.37199400	0.88803700	-2.05659600
C	3.12302800	-1.05018800	-2.61593800
H	0.63877200	-2.48661100	0.00460500
C	2.17371300	-2.94462200	-1.45724100
H	0.65248900	5.61288900	-2.13137500
H	3.81808600	-0.63785300	-3.35137600
C	3.06303500	-2.42626500	-2.40010900
H	2.12188700	-4.02231200	-1.28555500
H	3.71071500	-3.09777700	-2.96907200
Co	-1.76034300	-0.36451200	0.52514600
C	-2.95130900	1.37958000	0.79293600
C	-3.85576000	0.30408900	0.58178200
C	-2.26249200	1.14556900	2.06419900
C	-3.61997300	-0.65350100	1.62006800
C	-2.71868300	-0.07640100	2.59014900
C	-2.87489300	2.62780600	-0.00677500
H	-1.93770800	3.17483900	0.16229800
H	-2.96526200	2.43209500	-1.08522500
H	-3.69713100	3.31285300	0.26030500
C	-1.38180000	2.13595000	2.73118700
H	-1.98858600	2.93244200	3.19296100
H	-0.77377200	1.69112600	3.52874800
H	-0.70970700	2.64382500	2.02538700
C	-4.90013500	0.22158900	-0.46813300
H	-5.10801700	-0.81181500	-0.77484600
H	-5.84700700	0.63965600	-0.08636600
H	-4.63516900	0.79277800	-1.36714500
C	-4.27077200	-1.97650300	1.75945700
H	-5.14631400	-1.91909900	2.42720300
H	-4.62126100	-2.36448200	0.79429200
H	-3.58571100	-2.71555900	2.19687200
C	-2.26567700	-0.76576500	3.81997300
H	-3.11963500	-1.08297700	4.43786000
H	-1.69778900	-1.67402100	3.56597000
H	-1.62337700	-0.12959200	4.44192200
F	-0.86921100	-1.82348200	1.36557400
N	2.53002200	-0.36795600	1.74310200
C	3.72142600	0.04429700	1.22076500
N	2.62994000	-1.65728700	2.16452400
C	4.55688100	-1.08234800	1.36975400
C	4.16766500	1.23536000	0.63441200
N	3.82800100	-2.08547800	1.95745500

C	5.88821400	-1.05072100	0.92536000
C	5.48428700	1.24724500	0.19878800
H	3.51382600	2.10095400	0.51096700
H	6.53577500	-1.92216900	1.03698100
C	6.33205000	0.12380900	0.34033200
H	5.87994700	2.15096400	-0.27044000
H	7.35996000	0.19055800	-0.02270000
I	-2.08202500	-1.22311300	-2.13833800

Structures optimized at the B3LYP-D3BJ (PCM = dichloromethane)/def2-SVP level of theory

A_{Co-F}

67

C	-4.21196100	-1.39481800	-0.90874000
C	-0.79939100	-0.47929500	-1.61842800
H	-0.76793200	0.27586800	-2.41458700
H	-0.17522000	-1.33054500	-1.91371600
C	-0.05847600	1.99561100	-0.05515000
N	-2.30665000	-2.33904100	-1.31961400
N	-3.53042700	-2.58800100	-1.01130600
P	-0.01185000	0.17586300	-0.03751600
C	-3.30908900	-0.34503600	-1.19374900
C	-5.54969600	-1.12220200	-0.57160200
C	0.47373000	2.60824500	1.09560000
C	-0.51659700	2.79040000	-1.11424400
N	-2.13222400	-0.99527100	-1.45145700
C	-1.22930200	-0.29990200	1.24132100
C	-3.69996000	1.00293100	-1.16271600
C	-5.93714000	0.20981100	-0.53167600
H	-6.24354200	-1.93374600	-0.34710300
C	0.50568300	3.99819500	1.19392500
H	0.88434000	1.97021600	1.88243800
C	-0.46747900	4.18525200	-1.01559400
H	-0.90992700	2.34086500	-2.02717300
C	-2.15869400	0.62826100	1.73558300
C	-1.29859100	-1.64190700	1.64990400
H	-3.00529700	1.81503100	-1.36943300
C	-5.02376400	1.25450500	-0.82590800
H	-6.96570600	0.46613400	-0.26942300
H	0.91493300	4.46774400	2.09125200
C	0.03381400	4.78982600	0.13985900
H	-0.82616700	4.79777700	-1.84559400
H	-2.11912600	1.67135900	1.42274600
C	-3.15586500	0.21645900	2.62232800
H	-0.55441200	-2.34011100	1.26606600
C	-2.30358900	-2.04571000	2.53007100
H	-5.37186300	2.28878300	-0.78110600
H	0.06493700	5.87897700	0.21662700
H	-3.87901800	0.94454200	2.99653000
C	-3.23476800	-1.12208800	3.01543800
H	-2.35933100	-3.09230500	2.83849800
H	-4.02139400	-1.44526200	3.70148900
Co	2.02629400	-0.61115400	0.25701700
C	3.46184500	0.77894900	-0.32943000
C	4.11717200	-0.25224400	0.43787800
C	2.90410300	0.16324900	-1.50509700
C	3.88873900	-1.49417900	-0.20315800
C	3.11539200	-1.24073700	-1.40482700
C	3.53634100	2.24098100	-0.03281300
H	2.77000000	2.80859000	-0.57504400
H	3.40003000	2.43314900	1.04003100
H	4.52284500	2.64288400	-0.32235900
C	2.27135900	0.89292600	-2.64565500
H	3.05793800	1.25900900	-3.32686700
H	1.60627200	0.24677400	-3.23373800
H	1.70368700	1.77035600	-2.30872500
C	4.74940800	-0.01741100	1.76800300
H	5.25371500	-0.91605400	2.14686600
H	5.48323100	0.80175400	1.71853600
H	3.95525100	0.26343900	2.47935200
C	4.23922300	-2.86172300	0.27974000
H	4.81924000	-3.41256500	-0.47790200
H	4.82301600	-2.83151200	1.20915300
H	3.30651000	-3.41749900	0.46854000
C	2.61929000	-2.31476800	-2.31627000
H	3.45414800	-2.90451800	-2.72746500
H	1.96827700	-2.99040100	-1.73949700
H	2.04652000	-1.90730100	-3.16050300
F	1.74598900	-0.14140600	2.04530000
F	1.21473700	-2.30787400	0.37853000

TS_{A-B}

81

C	4.58951700	-0.11674200	-1.69090900
C	1.38351000	-1.74690700	-1.36303500
H	1.49552700	-2.82279500	-1.17951600
H	0.75199700	-1.58238400	-2.24379600
C	0.75097300	-1.83156500	1.55856500
N	2.75993800	-0.40556900	-2.81045900
N	3.89998900	0.18744400	-2.84401700
P	0.39861900	-0.92226700	0.01527700
C	3.78620300	-0.97949700	-0.90990500
C	5.85339400	0.30209200	-1.23898700
C	0.26933200	-1.28827100	2.76411500
C	1.39493800	-3.07825900	1.58234200
N	2.65037600	-1.12996800	-1.66199800
C	1.25583600	0.68296800	0.15181500
C	4.21609300	-1.46222000	0.33687400
C	6.27488000	-0.16579800	-0.00260400
H	6.46556900	0.97264600	-1.84408800
C	0.45465900	-1.97205300	3.96680500
H	-0.26187100	-0.33662700	2.75224500
C	1.57264100	-3.76151300	2.78836300
H	1.75887500	-3.54146400	0.66529200
C	2.14135800	0.97167500	1.20049700
C	1.12549900	1.57797400	-0.92282600
H	3.60191000	-2.11839400	0.94907800
C	5.46598800	-1.03803100	0.76934800
H	7.24794800	0.13834600	0.38872700
H	0.07985400	-1.53659000	4.89572400
C	1.10660200	-3.20939600	3.98378400
H	2.07664500	-4.73031700	2.78865200
H	2.25805000	0.27975400	2.03392500
C	2.90225800	2.14094400	1.16555100
H	0.42648300	1.34134200	-1.72518100
C	1.90389600	2.73404300	-0.95712200
H	5.83581400	-1.38383500	1.73718400
H	1.24618400	-3.74435100	4.92574100
H	3.59269400	2.35949500	1.98312000
C	2.79266100	3.01691300	0.08238700
H	1.80318700	3.42497700	-1.79570700
H	3.39369300	3.92837100	0.05426500
Co	-1.72172700	-0.79252100	-0.77136100
C	-3.36754000	-1.51701100	0.32361400
C	-3.82198000	-1.04384100	-0.97481400
C	-2.45891600	-2.58500000	0.10671600
C	-3.15430800	-1.79324900	-1.97197800
C	-2.23587100	-2.69410200	-1.31481600
C	-3.88021800	-1.06259300	1.64911400

H	-3.13963500	-1.23551800	2.44087000
H	-4.12350800	0.00742100	1.64133700
H	-4.79343000	-1.62726000	1.90684100
C	-1.94186300	-3.50809300	1.15559800
H	-2.72471500	-4.25815700	1.36262700
H	-1.04330200	-4.04828400	0.83777900
H	-1.72261500	-2.99051800	2.09701300
C	-4.81430000	0.04804200	-1.18187700
H	-4.83990200	0.37789900	-2.22855500
H	-5.82250700	-0.30753000	-0.90895900
H	-4.58059400	0.91239700	-0.54468000
C	-3.23390800	-1.62205900	-3.44971900
H	-3.44596400	-2.58575400	-3.93864200
H	-4.01363400	-0.90569500	-3.73736800
H	-2.26508200	-1.24999200	-3.81837100
C	-1.39200500	-3.70465900	-2.02048200
H	-2.01484200	-4.55260500	-2.35274000
H	-0.92109900	-3.27327800	-2.91462000
H	-0.60386800	-4.11087200	-1.37312700
F	-0.86925800	-0.22437100	-2.33058500
F	-1.97199700	1.11880800	-0.32621500
Cl	-3.85196800	2.53332900	1.25687400
C	-1.80179400	1.94808700	1.12104000
O	-1.48099300	1.20604300	1.99594900
C	-1.14810800	3.22054500	0.70319200
C	-0.24009800	3.79209000	1.60032600
C	-1.43091700	3.85624900	-0.51322600
C	0.38173600	5.00280900	1.28443900
H	-0.02032700	3.27901400	2.53726800
C	-0.80164600	5.05802200	-0.82717000
H	-2.14295800	3.39839300	-1.19818100
C	0.10344100	5.63687400	0.07265300
H	1.09457500	5.44396700	1.98468600
H	-1.01612200	5.54997000	-1.77873700
H	0.59324300	6.58126600	-0.17644900

$B_{Co\text{-}Cl}$

67

C	-0.86791500	-0.45730400	-1.63491300
H	-0.77671900	0.27552600	-2.44795200
H	-0.26405100	-1.34283300	-1.86497300
C	-0.18496700	1.99305900	-0.00330800
P	-0.07810800	0.17587000	-0.05070500
C	0.34262800	2.60785500	1.14812800
C	-0.64866000	2.79062600	-1.05757200
C	-1.26925800	-0.40664000	1.20873700
C	0.37896500	3.99870500	1.24504000
H	0.73569600	1.98462400	1.95538600
C	-0.60728600	4.18478000	-0.95758000
H	-1.02964200	2.34039400	-1.97486700
C	-2.19163800	0.46622600	1.80157200
C	-1.31950100	-1.78059100	1.49661600
H	0.78732300	4.46755500	2.14304200
C	-0.09688600	4.79058400	0.19282000
H	-0.97096500	4.79612900	-1.78621800
H	-2.16671600	1.53299900	1.57965600
C	-3.16462900	-0.03165300	2.67246000
H	-0.58591800	-2.43870000	1.03049900
C	-2.30059300	-2.27015200	2.35827300
H	-0.06380300	5.87966000	0.26880000
H	-3.88326600	0.65405400	3.12687600
C	-3.22502000	-1.39973800	2.94692300
H	-2.34378300	-3.34055000	2.57242500
H	-3.99240100	-1.78919200	3.62019100
Co	1.98423500	-0.63954800	0.09114400
C	3.64825400	0.65045400	0.08679500
C	4.11809000	-0.72021400	0.20433500
C	2.97341300	0.77948900	-1.15864400
C	3.67231000	-1.43023200	-0.93370600
C	2.90324400	-0.52565500	-1.75728400
C	3.95332000	1.74013200	1.06089700
H	3.32128800	2.62164700	0.89091100
H	3.78185500	1.39205700	2.08881400
H	5.00731200	2.05370500	0.97180500
C	2.52315500	2.05949100	-1.77954600
H	3.35457700	2.47006400	-2.37804300
H	1.67100700	1.92584900	-2.45700600
H	2.25023100	2.81170300	-1.03027800
C	4.94031800	-1.23445000	1.33773300
H	5.09500600	-2.31910500	1.26781900
H	5.92839300	-0.74479000	1.34295400
H	4.44538200	-1.01878300	2.29576500
C	3.81309100	-2.88667900	-1.21841500
H	4.24968100	-3.05021900	-2.21626400
H	4.44289800	-3.39199900	-0.47496600
H	2.81078400	-3.34376700	-1.19688700
C	2.31368700	-0.88982300	-3.08099100
H	3.10453800	-0.98204600	-3.84482800
H	1.79843200	-1.85941900	-3.02344400
H	1.59823700	-0.13701300	-3.43733500
F	1.08325800	-2.26390800	-0.20096900
Cl	1.79201700	-0.59674700	2.36911600
N	-2.22282200	-0.92916300	-1.49877900
C	-3.38465400	-0.26931300	-1.19468000
N	-2.43978600	-2.27401500	-1.48310600
C	-4.31879400	-1.31339500	-1.00221600
C	-3.74457000	1.08025800	-1.05044200
N	-3.67126600	-2.51280200	-1.20185300
C	-5.65069700	-1.03617900	-0.64648500
C	-5.06311800	1.33714400	-0.69729300
H	-3.03095300	1.88976600	-1.18477800
H	-6.36510300	-1.84657800	-0.49357500
C	-6.00513500	0.29672300	-0.49444200
H	-5.38340200	2.37317300	-0.56672700
H	-7.02804700	0.55650500	-0.21405100

Benzoyl chloride

14

C	0.12633100	0.20278200	-0.00002900
C	0.56459400	-1.13149100	-0.00007000
C	1.93035500	-1.41394800	-0.00004100
C	2.86354400	-0.37212700	0.00001500
C	2.43174200	0.95982400	0.00005600
C	1.06980600	1.24895000	0.00004700
H	-0.16504500	-1.94043000	-0.00011800
H	2.26791100	-2.45227200	-0.00006800
H	3.93229100	-0.59828000	0.00002600
H	3.16054000	1.77296000	0.00009800
H	0.71651600	2.28095500	0.00008600
C	-1.30070200	0.59899600	-0.00001600
O	-1.72493100	1.71292200	-0.00009800
Cl	-2.48392900	-0.78377800	0.00005800

Benzoyl fluoride

14

C	-0.23557400	0.04265800	-0.00013500
C	0.42822200	-1.19549000	-0.00020000
C	1.82252500	-1.23184300	-0.00008000
C	2.55444200	-0.03949100	0.00008200
C	1.89448900	1.19565800	0.00013800
C	0.50223900	1.23931600	0.00003800
H	-0.14966100	-2.11979100	-0.00033400
H	2.34105900	-2.19277400	-0.00012000
H	3.64641900	-0.07221700	0.00016400
H	2.46929200	2.12401700	0.00026600
H	-0.03113000	2.19128200	0.00008300

C	-1.70852900	0.13438300	-0.00022600
O	-2.38316500	1.11777600	-0.00013300
F	-2.30639300	-1.08265300	0.00036700

$^{3}A_{Co\text{-}F}$

67

C	-4.28291500	-1.31936400	-0.98870900
C	-0.82326000	-0.51524800	-1.61376700
H	-0.71312400	0.20213100	-2.43787900
H	-0.21257100	-1.40381400	-1.81840700
C	-0.19020400	1.96297600	0.01415600
N	-2.40679000	-2.31882700	-1.40037300
N	-3.64266800	-2.53271100	-1.11757700
P	-0.08508400	0.15199200	-0.02316800
C	-3.33937200	-0.29439100	-1.22965300
C	-5.61369100	-1.01148800	-0.65541200
C	0.24135100	2.56449300	1.21213200
C	-0.55368600	2.76750800	-1.07510500
N	-2.18142500	-0.97843000	-1.49090100
C	-1.24514200	-0.45134400	1.24724900
C	-3.68419500	1.06452000	-1.15570300
C	-5.95475000	0.33121900	-0.57210900
H	-6.33741700	-1.80559500	-0.46552000
C	0.25745600	3.95350500	1.32714400
H	0.59742400	1.92220000	2.02119700
C	-0.51984600	4.16082800	-0.95722300
H	-0.86313500	2.32553800	-2.02339200
C	-2.23258800	0.38038300	1.79529300
C	-1.19290500	-1.80930800	1.60229300
H	-2.96100100	1.85869700	-1.32915400
C	-5.00178600	1.35145500	-0.82141200
H	-6.97630800	0.61475900	-0.31052100
H	0.58693400	4.41499400	2.26068400
C	-0.12532400	4.75449900	0.24462800
H	-0.80646300	4.78124800	-1.80902400
H	-2.28318200	1.43409900	1.52104000
C	-3.16929500	-0.14492100	2.68807100
H	-0.41626700	-2.43738600	1.16230100
C	-2.13609600	-2.32575500	2.49180400
H	-5.31297900	2.39556700	-0.74452000
H	-0.10570700	5.84279900	0.33510000
H	-3.94026300	0.50589200	3.10647600
C	-3.12536800	-1.49848100	3.03371900
H	-2.09884800	-3.38358000	2.76205300
H	-3.86321700	-1.90937100	3.72691600
Co	1.98466500	-0.64847900	0.29491100
C	3.40323500	0.90786500	-0.35845200
C	4.11638000	0.04569100	0.49909300
C	3.00215300	0.13826000	-1.54963300
C	4.06835100	-1.27021000	-0.08582200
C	3.48010000	-1.17563000	-1.40109400
C	3.24577600	2.38244500	-0.18283700
H	2.38677000	2.77772600	-0.73946200
H	3.11057400	2.64441200	0.87495900
H	4.14649600	2.90848200	-0.54615800
C	2.34025800	0.73142500	-2.75226900
H	3.09027100	1.21396600	-3.40283500
H	1.82205800	-0.02940600	-3.35170800
H	1.61611700	1.51052900	-2.47509100
C	4.65423700	0.41468800	1.84479000
H	5.33073200	-0.35645700	2.23844900
H	5.20945100	1.36433900	1.80404800
H	3.81181000	0.52977100	2.54593500
C	4.58161900	-2.54142400	0.50432000
H	5.45653900	-2.91208500	-0.05646100
H	4.87333500	-2.41792500	1.55547700
H	3.80263600	-3.31798200	0.45014900
C	3.25439700	-2.34253700	-2.30540000
H	4.18772400	-2.90238100	-2.47624500
H	2.52377500	-3.02333300	-1.83933900
H	2.86191000	-2.03056800	-3.28308700
F	1.67881800	-0.15522100	2.11397600
F	1.21596900	-2.35015700	-0.07060400

$^{3}TS_{A\text{-}B}$

81

C	4.62460500	-0.22916500	-1.67954400
C	1.40118400	-1.80889100	-1.31154400
H	1.49040600	-2.87887100	-1.08258800
H	0.76847400	-1.67261200	-2.19697100
C	0.77969700	-1.77332600	1.61603700
N	2.78790700	-0.51086700	-2.79021900
N	3.93380900	0.07000200	-2.83361100
P	0.44768900	-0.91132000	0.04482900
C	3.81542900	-1.07559900	-0.88710200
C	5.89241800	0.18404000	-1.23374100
C	0.33698500	-1.16387400	2.80511900
C	1.35624400	-3.05201000	1.67712900
N	2.67681000	-1.22513000	-1.63502300
C	1.30726400	0.69204000	0.10605500
C	4.24051700	-1.54635900	0.36565400
C	6.30984400	-0.27136100	0.00894400
H	6.51026500	0.84168800	-1.84715500
C	0.49638800	-1.81632800	4.02897000
H	-0.14298200	-0.18592800	2.76382700
C	1.50992600	-3.70084900	2.90479500
H	1.68399000	-3.56604800	0.77368400
C	2.22648300	1.02307300	1.11175000
C	1.11971000	1.55159000	-0.98887700
H	3.62070700	-2.19059500	0.98536900
C	5.49395400	-1.12638700	0.79271600
H	7.28549600	0.02966600	0.39620500
H	0.15265700	-1.33074300	4.94496600
C	1.08354300	-3.08457900	4.08382400
H	1.96244200	-4.69427000	2.93522000
H	2.38258600	0.35666000	1.95992000
C	2.96605200	2.20231800	1.01279000
H	0.39996100	1.28083800	-1.76231800
C	1.87582200	2.71863900	-1.08659800
H	5.86141700	-1.46239600	1.76487900
H	1.20344600	-3.59374700	5.04262300
H	3.68403600	2.45642400	1.79560900
C	2.79863500	3.04458500	-0.09002400
H	1.73106300	3.38427100	-1.93902100
H	3.38149300	3.96491800	-0.16684600
Co	-1.69904000	-0.75243300	-0.85695100
C	-3.38389300	-1.54355000	0.39081100
C	-3.90621600	-1.04996400	-0.81510900
C	-2.49262200	-2.66403400	0.06890900
C	-3.31253000	-1.82761900	-1.89862200
C	-2.47757400	-2.84318600	-1.33837000
C	-3.68855800	-1.08935200	1.77942700
H	-2.77825800	-1.06406600	2.39495600
H	-4.11280900	-0.07800400	1.78610500
H	-4.40107000	-1.78024200	2.26310400
C	-1.90459200	-3.57450100	1.08801500
H	-2.67796800	-4.30262500	1.39171600
H	-1.04997700	-4.14137300	0.69945100
H	-1.59068900	-3.03852800	1.99196000
C	-4.87173000	0.07510300	-0.99174500
H	-4.68228700	0.61691400	-1.92937200
H	-5.90705000	-0.30499500	-1.03271400
H	-4.79113400	0.79771600	-0.17045900
C	-3.52909300	-1.63073800	-3.35840400
H	-3.91566300	-2.55370900	-3.82006600
H	-4.23242900	-0.81456500	-3.56534600

H	-2.56537000	-1.39072000	-3.83656800
C	-1.69358100	-3.84783700	-2.12174000
H	-2.33440300	-4.67957300	-2.46063300
H	-1.25089700	-3.38944300	-3.01855400
H	-0.87880100	-4.28048500	-1.52399600
F	-0.87118900	-0.37961600	-2.48864600
F	-2.00275100	1.16179100	-0.22596400
Cl	-3.75959100	2.57802400	1.43267700
C	-1.77494400	2.07488200	1.21252900
O	-1.36165300	1.36692800	2.08107800
C	-1.13779600	3.31681500	0.68036400
C	-0.16852300	3.92880400	1.48140200
C	-1.49254700	3.88500600	-0.55048700
C	0.44111400	5.11245900	1.05704200
H	0.10791600	3.46740200	2.43022300
C	-0.87468200	5.05916000	-0.97437400
H	-2.24774600	3.39312900	-1.16189900
C	0.09085300	5.67878400	-0.16960300
H	1.20104200	5.58501400	1.68349700
H	-1.14517100	5.49699500	-1.93813900
H	0.57137900	6.60122200	-0.50447800

$^{3}B_{Co\text{-}Cl}$

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C	-0.93591600	-0.44002000	-1.65391400
H	-0.83435600	0.30055500	-2.45842800
H	-0.33947100	-1.33109100	-1.88530600
C	-0.22356500	1.98687500	-0.00185000
P	-0.14732700	0.16812700	-0.06201200
C	0.30885100	2.59384300	1.15186100
C	-0.65776900	2.79433000	-1.06276300
C	-1.31866400	-0.44030700	1.19784000
C	0.37243700	3.98400200	1.24723200
H	0.68876300	1.96761500	1.96261900
C	-0.58751600	4.18716500	-0.96438000
H	-1.04105500	2.35206500	-1.98301800
C	-2.22013100	0.41147600	1.84998300
C	-1.35511500	-1.82411800	1.43825000
H	0.78326900	4.44500600	2.14817700
C	-0.07722700	4.78449300	0.19052400
H	-0.92994700	4.80424400	-1.79783800
H	-2.20064300	1.48538100	1.66277300
C	-3.16322400	-0.11947400	2.73361700
H	-0.63863200	-2.46437300	0.91968600
C	-2.30704100	-2.34570400	2.31427200
H	-0.02223200	5.87275300	0.26538200
H	-3.86803300	0.54714300	3.23560900
C	-3.21209400	-1.49722200	2.96190400
H	-2.34271200	-3.42285800	2.49275900
H	-3.95631100	-1.91121900	3.64638100
Co	1.95312500	-0.72291000	0.17006600
C	3.88354400	0.62264000	0.08459500
C	4.17546400	-0.80532800	0.14228500
C	3.12157600	0.85158800	-1.06371300
C	3.68224500	-1.42497000	-1.05111200
C	2.95164400	-0.43943800	-1.75738700
C	4.29771700	1.61118600	1.12383700
H	3.89446900	2.61066500	0.91211300
H	3.93344700	1.29843600	2.11469100
H	5.39642300	1.69109200	1.17875200
C	2.67314700	2.17211300	-1.59555400
H	3.46777800	2.60746500	-2.22653100
H	1.77715300	2.08323200	-2.22137700
H	2.45230500	2.88712100	-0.79232700
C	4.98152400	-1.44015500	1.22325400
H	4.99129100	-2.53464600	1.13886700
H	6.02440800	-1.08142400	1.18087100
H	4.57500700	-1.17155900	2.20972700
C	3.77774300	-2.86491500	-1.44283000
H	4.22625600	-2.97453500	-2.44335300
H	4.38875100	-3.43874500	-0.73312900
H	2.76685200	-3.30035100	-1.45969900
C	2.29464200	-0.65016300	-3.08143000
H	3.04645700	-0.62878100	-3.88988900
H	1.80000900	-1.63092700	-3.11805800
H	1.55047900	0.12434600	-3.30905300
F	1.00682100	-2.32985700	-0.38961200
Cl	1.83099300	-0.50502500	2.43542100
N	-2.29760800	-0.89285200	-1.52106100
C	-3.44399300	-0.21968300	-1.18839800
N	-2.54133900	-2.23291000	-1.54503700
C	-4.39796300	-1.25008500	-1.02242200
C	-3.77425400	1.13172700	-0.99799900
N	-3.77588000	-2.45551500	-1.26309600
C	-5.72202000	-0.95694300	-0.65058300
C	-5.08535800	1.40430700	-0.62895500
H	-3.04425800	1.92997800	-1.11051000
H	-6.45238500	-1.75682100	-0.51914000
C	-6.04785300	0.37756600	-0.45453500
H	-5.38327700	2.44195700	-0.46308900
H	-7.06376100	0.64931200	-0.16034800

Structures optimized at the TPSSh (PCM = dichloromethane)/def2-SVP level of theory

$A_{Co\text{-}F}$

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C	-4.48182200	-1.16361800	-1.03584400
C	-0.94789200	-0.43560000	-1.39694100
H	-0.87222800	0.33785500	-2.17324900
H	-0.38311800	-1.32402900	-1.71245500
C	-0.30392500	1.82699600	0.54886000
N	-2.56744300	-2.17112100	-0.98638000
N	-3.83518500	-2.36645100	-0.86037800
P	-0.00158800	0.06526300	0.15583700
C	-3.51046600	-0.16579000	-1.28853500
C	-5.85488600	-0.85360600	-1.01352800
C	0.10272500	2.24535900	1.83335000
C	-0.79178400	2.78347900	-0.35666400
N	-2.32455900	-0.85669300	-1.24383600
C	-0.89434900	-0.83269400	1.48260300
C	-3.87297700	1.16930200	-1.54237400
C	-6.21258500	0.46663700	-1.25407000
H	-6.59766800	-1.62855700	-0.81794900
C	-0.01518000	3.58464600	2.20986400
H	0.52335500	1.51192700	2.52571200
C	-0.90321300	4.12703600	0.02320900
H	-1.08440600	2.49660000	-1.36810700
C	-2.05519600	-0.27543400	2.04963500
C	-0.45862200	-2.10479600	1.89254400
H	-3.13927500	1.94593100	-1.75125400
C	-5.23351000	1.45903300	-1.51727700
H	-7.26645800	0.75308900	-1.24681900
H	0.29589200	3.89389400	3.21042500
C	-0.52265400	4.52870700	1.30729200
H	-1.29162100	4.85828400	-0.68937900
H	-2.40386300	0.71282300	1.74112800
C	-2.76977700	-0.98217400	3.02299100

H	0.43430000	-2.51925700	1.42561300
C	-1.17695300	-2.80093500	2.86877700
H	-5.55901900	2.48408500	-1.70869000
H	-0.61547100	5.57610800	1.60346800
H	-3.67033200	-0.54227000	3.45818400
C	-2.32998200	-2.24456700	3.43566300
H	-0.83313800	-3.78784500	3.18861900
H	-2.88646000	-2.79453100	4.19880700
Co	2.14057200	-0.51108400	-0.07428300
C	3.40280900	1.09007700	-0.30166700
C	4.18261200	-0.06835600	0.07283700
C	2.76934900	0.79819700	-1.56758500
C	3.95911600	-1.08937700	-0.89213500
C	3.07019400	-0.55564400	-1.90954600
C	3.40671200	2.40025100	0.42418200
H	2.53852500	3.01670600	0.15393500
H	3.38715400	2.24452100	1.51222600
H	4.31794300	2.97489400	0.18203800
C	2.02202200	1.78213200	-2.41354100
H	2.74401400	2.35191600	-3.02350400
H	1.32621500	1.28847600	-3.10600900
H	1.46423500	2.50764900	-1.80615800
C	4.94718700	-0.18651500	1.35139200
H	5.53699000	-1.11224400	1.38841900
H	5.62872000	0.66885200	1.47918300
H	4.22761000	-0.19499800	2.18673600
C	4.43701000	-2.50637700	-0.86248600
H	5.00479800	-2.74989600	-1.77507800
H	5.07775400	-2.70217600	0.00778800
H	3.56222900	-3.17475500	-0.81091200
C	2.59130700	-1.33416100	-3.09417000
H	3.42338800	-1.53562800	-3.78957300
H	2.18094200	-2.29818500	-2.75821000
H	1.80916800	-0.79724700	-3.64845900
F	2.06308500	-0.65563100	1.78316100
F	1.39323600	-2.21715600	-0.36485800

TS_{A-B}

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C	4.84955300	0.66278900	-1.66931000
C	1.85055700	-1.32370100	-1.20594700
H	2.17567200	-2.35086900	-0.99380600
H	1.23268900	-1.30555100	-2.11316200
C	1.12409700	-1.47544500	1.70747200
N	2.97801400	0.22360800	-2.66160100
N	4.06634000	0.90231300	-2.77640200
P	0.62954300	-0.72637700	0.10835400
C	4.16315900	-0.23886100	-0.82168400
C	6.12316800	1.15670100	-1.32949800
C	0.48420700	-1.00562700	2.87321400
C	2.02897600	-2.54668100	1.81497700
N	2.99153100	-0.48238600	-1.49539500
C	1.07029400	1.04913700	0.23163000
C	4.72103700	-0.67968000	0.39203600
C	6.67438900	0.72154800	-0.13137700
H	6.64530700	1.85158600	-1.98909700
C	0.77345700	-1.57579900	4.11627500
H	-0.24863900	-0.19884700	2.80265900
C	2.31103100	-3.11724700	3.06174000
H	2.51832100	-2.96053800	0.93148300
C	1.87460700	1.54621200	1.27300100
C	0.69501400	1.89694400	-0.82673800
H	4.20087200	-1.36551100	1.05896900
C	5.98025400	-0.18268800	0.71301300
H	7.66061200	1.07843400	0.17330700
H	0.27503300	-1.19586700	5.01104400
C	1.68916100	-2.63041900	4.21542500
H	3.01899000	-3.94662900	3.12580400
H	2.18171300	0.89834400	2.09573200
C	2.29900800	2.87866400	1.25275000
H	0.06890600	1.49642600	-1.62552200
C	1.13941500	3.22150700	-0.84551600
H	6.44970400	-0.49824300	1.64761900
H	1.91158400	-3.07573300	5.18779800
H	2.92296300	3.25730100	2.06583500
C	1.93882700	3.71532900	0.19085600
H	0.84965600	3.87348900	-1.67229300
H	2.27935900	4.75343300	0.17322700
Co	-1.43921900	-1.17404400	-0.77210400
C	-2.91573800	-2.28041300	0.19617600
C	-3.36765000	-1.91216300	-1.13879500
C	-1.74280000	-3.07601300	0.05790200
C	-2.45380700	-2.45908500	-2.07822700
C	-1.39781000	-3.12445400	-1.34677500
C	-3.64505900	-2.00711700	1.47267600
H	-2.96738000	-2.03967300	2.33631100
H	-4.13590400	-1.02444400	1.45299000
H	-4.41960100	-2.78053400	1.62087200
C	-1.08093100	-3.84649000	1.15392000
H	-1.65432600	-4.77679700	1.31121600
H	-0.05196700	-4.13021600	0.90167500
H	-1.07052500	-3.29686500	2.10430500
C	-4.59151300	-1.11176500	-1.44024100
H	-4.58491500	-0.73895200	-2.47318700
H	-5.48639700	-1.74486900	-1.31055900
H	-4.67595100	-0.25725700	-0.75350700
C	-2.47141400	-2.29443000	-3.56236800
H	-2.42238700	-3.27771100	-4.05650700
H	-3.37798100	-1.77785700	-3.90272500
H	-1.59479300	-1.70274300	-3.86976800
C	-0.30574400	-3.93307700	-1.97601200
H	-0.71132000	-4.90575000	-2.30472000
H	0.10774900	-3.43296600	-2.86283800
H	0.51221000	-4.14037300	-1.27288500
F	-0.66198400	-0.36630100	-2.26243800
F	-2.20019400	0.59540900	-0.31752300
Cl	-4.55272000	1.44936300	1.09893900
C	-2.44342800	1.56209800	1.11914800
O	-1.95371100	1.01735900	2.05827900
C	-2.20927100	2.94245400	0.60611000
C	-1.60816500	3.84829700	1.49208400
C	-2.60772400	3.36530000	-0.67127900
C	-1.41100900	5.17751900	1.10245600
H	-1.30455300	3.50679100	2.48340100
C	-2.39764000	4.68899300	-1.05754400
H	-3.07814500	2.65092200	-1.34610500
C	-1.80327000	5.59954200	-0.17120600
H	-0.94773900	5.88225500	1.79715000
H	-2.70271800	5.01694000	-2.05419500
H	-1.64942600	6.63770000	-0.47584000

B_{Co-Cl}

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C	-0.96785200	-0.47443300	-1.45358900
H	-0.91611400	0.24226600	-2.28490900
H	-0.36809700	-1.36302100	-1.69042100
C	-0.26224200	2.00375200	0.15395500
P	-0.06817800	0.18457500	0.07020900
C	0.25643000	2.62636800	1.30879200
C	-0.78374000	2.80375400	-0.87593500
C	-1.11592100	-0.45182100	1.44034400
C	0.21826800	4.01672000	1.43854900
H	0.69818300	2.01091200	2.09775900
C	-0.81700600	4.19753300	-0.74303700
H	-1.15718700	2.35599700	-1.79881600
C	-2.09606500	0.35881800	2.03823500

C	-0.98071700	-1.79307800	1.84390600
H	0.61627300	4.48614800	2.34116100
C	-0.32237800	4.80580800	0.41455200
H	-1.22949700	4.80610300	-1.55099300
H	-2.21761400	1.39968100	1.73240500
C	-2.92571800	-0.16394800	3.03754200
H	-0.21316500	-2.40400900	1.36677100
C	-1.81810100	-2.30775100	2.83656800
H	-0.35123200	5.89301400	0.51713400
H	-3.68192200	0.47561800	3.49904900
C	-2.78843700	-1.49641300	3.43815200
H	-1.70792200	-3.34996500	3.14614500
H	-3.43712400	-1.90312200	4.21797900
Co	2.04786500	-0.57640600	-0.01801200
C	3.71601400	0.65769300	-0.11045500
C	4.14335600	-0.73402700	-0.08058500
C	2.92285100	0.85124800	-1.28115700
C	3.57352600	-1.38704500	-1.20552000
C	2.76934300	-0.42819100	-1.93177200
C	4.15849800	1.70763800	0.85969800
H	3.53900400	2.61181500	0.78667900
H	4.09460400	1.32751200	1.88902400
H	5.20474000	1.99391000	0.65610900
C	2.45616700	2.17088900	-1.80965500
H	3.26856500	2.61344900	-2.41212600
H	1.57938500	2.07364900	-2.46284800
H	2.21426500	2.87838200	-1.00576700
C	5.05338600	-1.32196900	0.94998600
H	5.13375400	-2.41210200	0.84424700
H	6.06360300	-0.89039600	0.84993400
H	4.67889800	-1.09790400	1.96007600
C	3.65403700	-2.83858900	-1.55058000
H	4.00380100	-2.97199300	-2.58662300
H	4.33426200	-3.38010900	-0.88024000
H	2.64778200	-3.27819100	-1.45876600
C	2.09807500	-0.70523300	-3.24230200
H	2.84727000	-0.72114500	-4.05300300
H	1.60061100	-1.68574700	-3.23612100
H	1.35471400	0.06230500	-3.49685200
F	1.11382900	-2.19843000	-0.18839200
Cl	2.07734400	-0.55796400	2.26803900
N	-2.32238300	-0.95678100	-1.28307900
C	-3.53294100	-0.31599000	-1.18548600
N	-2.50895700	-2.30425000	-1.20157800
C	-4.45723500	-1.37807500	-1.04103700
C	-3.95251500	1.02635600	-1.21511800
N	-3.76195900	-2.56633800	-1.05885200
C	-5.83764000	-1.13158800	-0.91766000
C	-5.31963200	1.25315800	-1.09216600
H	-3.25368000	1.85467900	-1.31902100
H	-6.54279900	-1.95679600	-0.80643300
C	-6.25152600	0.19376000	-0.94495300
H	-5.68776900	2.28156500	-1.10828700
H	-7.31319800	0.43261500	-0.85227100

Benzoyl chloride

14

C	-0.12650600	0.20526600	-0.00002900
C	-0.56159500	-1.13200800	0.00000700
C	-1.92817500	-1.41673800	0.00000800
C	-2.86377000	-0.37482100	-0.00002700
C	-2.43454600	0.95950900	-0.00006200
C	-1.07190500	1.25221800	-0.00006300
H	0.17236100	-1.93828600	0.00003300
H	-2.26458900	-2.45549700	0.00003600
H	-3.93218500	-0.60279300	-0.00002600
H	-3.16514900	1.77110700	-0.00009000
H	-0.71964800	2.28506100	-0.00009000
C	1.29810700	0.60366500	-0.00003300
O	1.72914700	1.71792500	-0.00000500
Cl	2.48272800	-0.78738500	0.00008100

Benzoyl fluoride

14

C	0.23592700	0.04300500	-0.00000200
C	-0.42808700	-1.19710100	0.00006100
C	-1.82386400	-1.23313600	0.00003200
C	-2.55626400	-0.03925700	-0.00006300
C	-1.89587500	1.19733300	-0.00012700
C	-0.50210900	1.24149100	-0.00009600
H	0.15077400	-2.12126200	0.00013200
H	-2.34269000	-2.19401800	0.00008400
H	-3.64831400	-0.07189200	-0.00008600
H	-2.47104000	2.12559300	-0.00020200
H	0.03164900	2.19367100	-0.00014300
C	1.70857500	0.13511000	0.00003200
O	2.38704500	1.12036100	0.00002400
F	2.30593900	-1.08662800	0.00011200

$^{3}A_{Co\text{-}F}$

67

C	-4.51226900	-1.23577300	-1.11654500
C	-0.98314000	-0.47385200	-1.46367900
H	-0.88552500	0.26772300	-2.26924900
H	-0.41204200	-1.37265900	-1.73552000
C	-0.34670400	1.87863900	0.34933400
N	-2.60276700	-2.24337200	-1.25814900
N	-3.86815200	-2.45256900	-1.13298200
P	-0.08549100	0.09072300	0.09430200
C	-3.54161200	-0.21344600	-1.24226300
C	-5.88223000	-0.92946300	-1.01015700
C	-0.01464200	2.39317200	1.61977400
C	-0.71544700	2.76917100	-0.67524800
N	-2.35893700	-0.90517200	-1.33003800
C	-1.01500000	-0.75194300	1.42814700
C	-3.90046600	1.14641600	-1.26954900
C	-6.23697700	0.41306200	-1.03461200
H	-6.62467600	-1.72322700	-0.91395300
C	-0.10144000	3.76511600	1.86714000
H	0.33665000	1.70581700	2.39215400
C	-0.79167900	4.14416000	-0.42281700
H	-0.94228500	2.40658000	-1.68003800
C	-2.10594400	-0.13323200	2.06238600
C	-0.65017800	-2.06222800	1.78700500
H	-3.16410100	1.94337400	-1.36079900
C	-5.25799800	1.43187800	-1.16303000
H	-7.28834400	0.69770200	-0.95457200
H	0.14900200	4.15121900	2.85805600
C	-0.49458900	4.64369700	0.84958000
H	-1.08651600	4.82372500	-1.22568500
H	-2.40226800	0.88207500	1.79038900
C	-2.81718000	-0.81471300	3.05675300
H	0.18433600	-2.53753900	1.26831500
C	-1.36703800	-2.73516200	2.77973900
H	-5.58106700	2.47532600	-1.17813600
H	-0.56023400	5.71641800	1.04547000
H	-3.66225100	-0.32557400	3.54709800
C	-2.44742200	-2.11412400	3.41873100
H	-1.07868700	-3.75212000	3.05684400
H	-3.00225200	-2.64381500	4.19706700
Co	2.08733500	-0.59937700	0.05917200
C	3.40903000	1.05595800	-0.32638900
C	4.18023000	0.05253500	0.32616100
C	2.99921000	0.54380800	-1.64497800
C	4.10931600	-1.12049600	-0.49112500
C	3.46151800	-0.77679000	-1.75223300

C	3.22294000	2.45470000	0.17066900
H	2.36982700	2.95369200	-0.30879400
H	3.05744600	2.45959700	1.25688000
H	4.12493100	3.05705400	-0.03873900
C	2.33049500	1.36118700	-2.70870800
H	3.08554400	1.93460800	-3.27455000
H	1.78351500	0.73282100	-3.42574800
H	1.62956400	2.09172000	-2.27981200
C	4.78994400	0.18211600	1.68868100
H	5.38057900	-0.70639300	1.95220700
H	5.45463600	1.05942800	1.74076600
H	3.98620900	0.30200900	2.43229500
C	4.66075200	-2.47802700	-0.18777100
H	5.48719200	-2.72645100	-0.87506900
H	5.03622200	-2.54566800	0.84202300
H	3.87474300	-3.23769300	-0.32235800
C	3.22764100	-1.75172700	-2.86226700
H	4.17771700	-2.18211000	-3.21935300
H	2.59640000	-2.57867000	-2.49761000
H	2.72367800	-1.28094300	-3.71756400
F	1.81134500	-0.16284300	1.93436300
F	1.38095100	-2.26890400	-0.40796000

$^{3}TS_{A-B}$

81

C	4.97061000	1.30051700	-1.57314800
C	2.15879600	-0.96064000	-1.20511100
H	2.56728500	-1.96133600	-1.00716600
H	1.56164000	-0.98665200	-2.12659400
C	1.42256100	-1.09582900	1.72667500
N	3.10825800	0.79108800	-2.54882500
N	4.13024700	1.56996100	-2.63028300
P	0.86758900	-0.48594800	0.09190300
C	4.39446400	0.26921500	-0.79362900
C	6.21024500	1.87043300	-1.22729800
C	0.75683900	-0.60146300	2.86830600
C	2.39354900	-2.10183700	1.88627700
N	3.22434000	-0.01468500	-1.45525200
C	1.02655700	1.33616100	0.13910700
C	5.03484300	-0.23152800	0.35441400
C	6.84159600	1.37764800	-0.09273100
H	6.64647400	2.66507700	-1.83455600
C	1.08683200	-1.08416800	4.13800000
H	-0.02096700	0.15915100	2.76097300
C	2.71662500	-2.58160400	3.16068600
H	2.90418100	-2.53185600	1.02285900
C	1.85448500	1.98348100	1.07277000
C	0.35854500	2.08686700	-0.84424500
H	4.60227400	-1.01925900	0.96875700
C	6.25920100	0.34235400	0.68255300
H	7.80512700	1.78997600	0.21445700
H	0.56844500	-0.68701100	5.01373000
C	2.06851900	-2.07082800	4.28956700
H	3.47741400	-3.35830700	3.26613900
H	2.38111300	1.41030600	1.83827200
C	2.00573500	3.37278300	1.02496600
H	-0.26941800	1.57169700	-1.57242500
C	0.52174400	3.47420200	-0.88796800
H	6.78933000	-0.01597900	1.56794700
H	2.32292500	-2.44500400	5.28384600
H	2.64877200	3.87070300	1.75448300
C	1.34110300	4.11926000	0.04537500
H	0.00090000	4.05359500	-1.65360700
H	1.46277400	5.20460800	0.00971600
Co	-1.17867500	-1.23877400	-0.85139200
C	-2.09377700	-2.85015900	0.25013700
C	-3.01030600	-2.42707100	-0.75470900
C	-0.92842200	-3.46192900	-0.41390300
C	-2.35055300	-2.60525300	-2.01694200
C	-1.08951900	-3.31023600	-1.79786300
C	-2.34458000	-2.85422700	1.72442500
H	-1.40501800	-2.82030900	2.29380600
H	-2.96328300	-1.99472900	2.02040200
H	-2.87439400	-3.78006100	2.01197800
C	0.12734800	-4.24494500	0.29740100
H	-0.26812500	-5.24924900	0.53047000
H	1.02890100	-4.37776900	-0.31613300
H	0.41422200	-3.78280500	1.25137600
C	-4.38788700	-1.88644700	-0.53327400
H	-4.72732500	-1.29126800	-1.39259200
H	-5.10036800	-2.71996800	-0.40552100
H	-4.42827000	-1.25417800	0.36478200
C	-2.86520500	-2.23692300	-3.36922400
H	-2.10582900	-1.65113300	-3.90975100
H	-3.07276000	-3.14671000	-3.95754100
H	-3.78781600	-1.64546100	-3.30904700
C	-0.16000200	-3.72761100	-2.89281300
H	-0.60822700	-4.53498900	-3.49642800
H	0.04241000	-2.88451200	-3.57135700
H	0.79706200	-4.09281000	-2.49626300
F	-0.54250300	-0.41327700	-2.37884500
F	-2.21090900	0.22703600	0.17385300
Cl	-4.11878500	0.42876500	2.26458500
C	-2.52134800	1.44248100	1.37721400
O	-1.58422800	1.55647300	2.10706500
C	-3.16582500	2.50702100	0.55049000
C	-2.79076100	3.83080500	0.82452800
C	-4.11149800	2.23967300	-0.45057500
C	-3.36420600	4.88407300	0.10353600
H	-2.05055900	4.02327100	1.60313900
C	-4.67351700	3.29286500	-1.17337300
H	-4.39667100	1.20745100	-0.64986700
C	-4.30403600	4.61736600	-0.89702700
H	-3.07271100	5.91383700	0.32411000
H	-5.40641400	3.08258700	-1.95605500
H	-4.75128700	5.43898800	-1.46189100

$^{3}B_{Co-Cl}$

67

C	-1.02582800	-0.46299100	-1.46851100
H	-0.94432900	0.26440200	-2.28828800
H	-0.43766600	-1.36078800	-1.70347600
C	-0.33383200	1.97396000	0.19586300
P	-0.14066600	0.15723300	0.07435100
C	0.12062200	2.58404300	1.38409000
C	-0.78401300	2.78904800	-0.85759700
C	-1.15084000	-0.54913200	1.43089800
C	0.08506000	3.97364800	1.52293000
H	0.51442300	1.96225900	2.19238700
C	-0.81517100	4.18138500	-0.71436200
H	-1.10582300	2.35346900	-1.80552000
C	-2.12132200	0.20969700	2.10679800
C	-0.97197100	-1.90704800	1.75499000
H	0.43264200	4.43160400	2.45188200
C	-0.38748400	4.77619900	0.47653700
H	-1.17364400	4.79954700	-1.54058800
H	-2.27338900	1.26254700	1.86104000
C	-2.90082800	-0.38426400	3.10615100
H	-0.21711600	-2.47695100	1.20805600
C	-1.76032800	-2.49191500	2.74902800
H	-0.41446800	5.86265000	0.58714500
H	-3.65180200	0.21212100	3.62976700
C	-2.72183900	-1.73347600	3.42859900
H	-1.61974100	-3.54678800	2.99708100
H	-3.33231300	-2.19451900	4.20896400
Co	2.03698500	-0.62299700	0.06757900

C	3.89891800	0.70647600	-0.17315800
C	4.20695900	-0.71723700	-0.10212000
C	3.04566900	0.90040600	-1.27063700
C	3.64313700	-1.36845300	-1.25028800
C	2.85400000	-0.40279000	-1.92964300
C	4.39864700	1.73155000	0.79583300
H	3.96493500	2.72077700	0.59553600
H	4.14074700	1.44320000	1.82706300
H	5.49647800	1.82205700	0.73390600
C	2.55171400	2.21077000	-1.79977700
H	3.30172400	2.63692300	-2.48929000
H	1.61729900	2.10007600	-2.36579900
H	2.38087600	2.94089600	-0.99676800
C	5.10946900	-1.32486000	0.92358300
H	5.09266300	-2.42219200	0.88298300
H	6.14801300	-0.99049300	0.75575900
H	4.81060200	-1.00870500	1.93419200
C	3.74229400	-2.81714400	-1.61942600
H	4.13407500	-2.93639000	-2.64267100
H	4.40747900	-3.36273500	-0.93616000
H	2.74098800	-3.27195100	-1.56773300
C	2.13320800	-0.63999300	-3.22012500
H	2.84616000	-0.59256200	-4.06239400
H	1.66946700	-1.63630800	-3.23428700
H	1.35560900	0.11266100	-3.40850700
F	1.06551300	-2.25157700	-0.39399400
Cl	2.09146200	-0.38078600	2.32570700
N	-2.39229300	-0.91678200	-1.32038800
C	-3.58566400	-0.25020500	-1.18754900
N	-2.61493800	-2.26159100	-1.31391600
C	-4.53830600	-1.29346900	-1.10420900
C	-3.96833800	1.10258100	-1.13878500
N	-3.87479700	-2.49721500	-1.18725400
C	-5.91191200	-1.01720400	-0.96859200
C	-5.32925800	1.35877500	-1.00464000
H	-3.24648400	1.91601100	-1.19222300
H	-6.63941600	-1.82795600	-0.90552800
C	-6.28984800	0.31832600	-0.92074500
H	-5.66936000	2.39602000	-0.96123600
H	-7.34498800	0.58011800	-0.81617800

Structures optimized at the TPSS (PCM = dichloromethane)/def2-SVP level of theory

$A_{Co\text{-}F}$

67

C	-4.50304800	-1.16426800	-1.03434600
C	-0.95464300	-0.44018200	-1.39801000
H	-0.87745700	0.33317400	-2.17809300
H	-0.38926300	-1.33411500	-1.70658600
C	-0.30318700	1.83008300	0.55643200
N	-2.58295700	-2.18270800	-0.97806000
N	-3.85920100	-2.37288300	-0.85248500
P	0.00563400	0.06530000	0.15662900
C	-3.52566900	-0.16496900	-1.29078300
C	-5.87847100	-0.85022900	-1.01563300
C	0.11132300	2.24937200	1.84289600
C	-0.80279400	2.78937900	-0.34637000
N	-2.33616600	-0.85843300	-1.24218100
C	-0.88292000	-0.83959300	1.49115100
C	-3.88698500	1.17213500	-1.55210000
C	-6.23480500	0.47390300	-1.26355500
H	-6.62479800	-1.62484700	-0.81743300
C	-0.01186400	3.59082500	2.22430800
H	0.54135500	1.51456200	2.53211300
C	-0.91958900	4.13495300	0.03885600
H	-1.10045300	2.50227600	-1.35914100
C	-2.03256300	-0.27610300	2.08385200
C	-0.45314200	-2.12466900	1.88069600
H	-3.14967400	1.94830500	-1.76404900
C	-5.25163900	1.46559200	-1.53052500
H	-7.29087500	0.76257700	-1.25913900
H	0.30481600	3.90007300	3.22608100
C	-0.53219000	4.53693600	1.32510800
H	-1.31761100	4.86750600	-0.67125000
H	-2.37716200	0.72107000	1.79102600
C	-2.74107600	-0.98943900	3.06277200
H	0.43090600	-2.54226500	1.39360100
C	-1.16547500	-2.82696500	2.86215700
H	-5.57551500	2.49289800	-1.72783000
H	-0.62945800	5.58558400	1.62529100
H	-3.63264400	-0.54438300	3.51769100
C	-2.30704000	-2.26426500	3.45541200
H	-0.82599000	-3.82351800	3.16574800
H	-2.85856300	-2.81875200	4.22273100
Co	2.14467400	-0.50102400	-0.09291400
C	3.43012600	1.08217200	-0.27250200
C	4.19284700	-0.10591800	0.06866000
C	2.77705300	0.83203700	-1.54283800
C	3.95036700	-1.09867300	-0.92813000
C	3.05769000	-0.52337400	-1.92722600
C	3.46130600	2.37389900	0.48999400
H	2.60584800	3.01842300	0.23410400
H	3.43698000	2.18890700	1.57620600
H	4.38840300	2.93582000	0.26426300
C	2.05148200	1.85625600	-2.36520900
H	2.78966300	2.42856800	-2.95882200
H	1.34565900	1.39611700	-3.07506200
H	1.50492200	2.57830800	-1.73858900
C	4.95784300	-0.27449900	1.34450000
H	5.53775600	-1.21052700	1.35281900
H	5.65009300	0.57081600	1.50254800
H	4.23317000	-0.30075100	2.17975400
C	4.40493200	-2.52631700	-0.93641000
H	4.95367600	-2.76144600	-1.86618000
H	5.05725900	-2.75326900	-0.07883600
H	3.51516500	-3.18031700	-0.88522400
C	2.56796100	-1.25730400	-3.13907000
H	3.39385400	-1.41989900	-3.85686000
H	2.17182400	-2.24267500	-2.84138400
H	1.77021100	-0.70412100	-3.65959100
F	2.06432500	-0.67287800	1.77743600
F	1.38239600	-2.21627900	-0.39700300

$TS_{A\text{-}B}$

81

C	4.87276000	0.73580200	-1.66777600
C	1.88644400	-1.29369300	-1.20265900
H	2.22528100	-2.31806400	-0.98437400
H	1.26772000	-1.28370200	-2.11302300
C	1.16015200	-1.43505000	1.72122800
N	2.99251200	0.28541100	-2.66098800
N	4.08048100	0.97878000	-2.77338000
P	0.64160500	-0.71104000	0.11108300
C	4.19763700	-0.18344900	-0.82010900
C	6.14603900	1.24061500	-1.32990600
C	0.52391700	-0.95973500	2.89182700
C	2.08349800	-2.49582900	1.83298800

N	3.02044900	-0.43573500	-1.49029800
C	1.04733300	1.08052300	0.21811200
C	4.76930300	-0.62905700	0.38897400
C	6.71077600	0.80000200	-0.13470300
H	6.65842600	1.94783000	-1.98842800
C	0.83486500	-1.51263600	4.14183500
H	-0.22277600	-0.16267700	2.81988100
C	2.38705200	-3.04905200	3.08680700
H	2.57018200	-2.91444100	0.94698400
C	1.84383100	1.60823300	1.25604400
C	0.64897500	1.91115700	-0.85073800
H	4.25911100	-1.32731800	1.05494900
C	6.02955900	-0.12019700	0.70797600
H	7.69748500	1.16562200	0.16766700
H	0.33901600	-1.12793300	5.03929000
C	1.76879100	-2.55593700	4.24448600
H	3.10888300	-3.86980800	3.15312000
H	2.16986500	0.97423300	2.08571300
C	2.23595600	2.95440900	1.22193700
H	0.03167000	1.48469400	-1.64645400
C	1.06077300	3.24992500	-0.88239300
H	6.50855700	-0.43968500	1.63952800
H	2.00796000	-2.98756200	5.22203800
H	2.85385700	3.35667200	2.03196800
C	1.85124000	3.77489200	0.15085400
H	0.75319000	3.88810300	-1.71709400
H	2.16608400	4.82365900	0.12346200
Co	-1.41158500	-1.21592600	-0.76719600
C	-2.86854800	-2.32913800	0.21055800
C	-3.33480000	-1.98363600	-1.13077400
C	-1.67151200	-3.10312300	0.07456200
C	-2.40658800	-2.51763800	-2.07172700
C	-1.33267900	-3.16341900	-1.33647800
C	-3.60441700	-2.06677400	1.48857800
H	-2.92443100	-2.08196400	2.35441200
H	-4.12062300	-1.09352500	1.46555400
H	-4.36292200	-2.85999900	1.63968900
C	-0.99571300	-3.85892800	1.17633000
H	-1.54978700	-4.80442100	1.33385300
H	0.04316200	-4.12023200	0.92830200
H	-1.00155900	-3.30632400	2.12825400
C	-4.58003900	-1.21451100	-1.43782200
H	-4.58704500	-0.85436500	-2.47828500
H	-5.46109200	-1.86953900	-1.29589700
H	-4.68507300	-0.35215500	-0.75825500
C	-2.43066500	-2.36111600	-3.55945900
H	-2.34663900	-3.34621900	-4.05155700
H	-3.35597000	-1.87489000	-3.90326900
H	-1.57116000	-1.73979200	-3.86878300
C	-0.22760600	-3.95969500	-1.96433700
H	-0.62008400	-4.94378800	-2.28565600
H	0.17567700	-3.45877700	-2.85881800
H	0.59744200	-4.14922400	-1.26027600
F	-0.64400000	-0.39879300	-2.27597600
F	-2.21323300	0.56069400	-0.35769500
Cl	-4.63059900	1.35509900	1.08163700
C	-2.48158300	1.51607800	1.10021300
O	-1.98481200	0.97053700	2.04002400
C	-2.29501000	2.90859800	0.60107300
C	-1.71096000	3.82678800	1.49364100
C	-2.71789200	3.33348600	-0.67253200
C	-1.55672000	5.16822400	1.11405400
H	-1.38803600	3.48461000	2.48148300
C	-2.54992900	4.67002800	-1.04835200
H	-3.17529900	2.61024900	-1.35081100
C	-1.97374500	5.59196400	-0.15563400
H	-1.10767400	5.88142700	1.81366000
H	-2.87441200	4.99915500	-2.04140700
H	-1.85354600	6.63978500	-0.45173700

$B_{Co\text{-}Cl}$

67

C	-0.96995900	-0.48249800	-1.45204900
H	-0.91754500	0.23343100	-2.28757200
H	-0.36874500	-1.37561100	-1.68135700
C	-0.26128300	2.00886400	0.15712700
P	-0.05895600	0.18458700	0.07404900
C	0.25521000	2.63635900	1.31548100
C	-0.78609600	2.80899300	-0.87685800
C	-1.10859200	-0.45187800	1.45200100
C	0.21055800	4.03044800	1.44488200
H	0.69995800	2.02142000	2.10677300
C	-0.82539900	4.20652200	-0.74405400
H	-1.15783700	2.35772900	-1.80184300
C	-2.08946000	0.36192700	2.05399800
C	-0.97331300	-1.79705000	1.85649400
H	0.60637100	4.50302900	2.35009800
C	-0.33363600	4.81920000	0.41718400
H	-1.24057500	4.81439700	-1.55481700
H	-2.21175200	1.40513400	1.74726900
C	-2.91904900	-0.16193000	3.05835700
H	-0.20571900	-2.40955500	1.37528000
C	-1.81067900	-2.31227800	2.85425400
H	-0.36744300	5.90896400	0.51960900
H	-3.67550700	0.48000200	3.52265900
C	-2.78145700	-1.49802400	3.46029700
H	-1.70019400	-3.35721400	3.16423800
H	-3.42988000	-1.90500100	4.24396700
Co	2.05538300	-0.56707600	-0.02870000
C	3.71423900	0.66516900	-0.11703800
C	4.15343500	-0.72748500	-0.07894400
C	2.91339300	0.84543700	-1.29475900
C	3.58137100	-1.39547800	-1.20118200
C	2.77426600	-0.44208900	-1.94322600
C	4.15341900	1.72836900	0.84451200
H	3.52493200	2.62935400	0.76687400
H	4.09776200	1.35514300	1.87992400
H	5.19938000	2.02236800	0.63350400
C	2.44794100	2.16250600	-1.83933100
H	3.26320400	2.59841600	-2.44838100
H	1.56876500	2.05926900	-2.49334900
H	2.20682100	2.88152500	-1.04168800
C	5.06848200	-1.30474400	0.95716300
H	5.17467100	-2.39476800	0.84346600
H	6.07216000	-0.84817200	0.87104600
H	4.67822400	-1.09562000	1.96812800
C	3.66511100	-2.85306600	-1.53144700
H	4.01157100	-2.99862900	-2.57003300
H	4.34909000	-3.38793600	-0.85493800
H	2.65602100	-3.29290600	-1.43164600
C	2.10758400	-0.73230900	-3.25617700
H	2.86201500	-0.75165800	-4.06628100
H	1.61295900	-1.71736200	-3.24481400
H	1.36053700	0.03268400	-3.51961900
F	1.11200400	-2.20312900	-0.19347800
Cl	2.08801600	-0.55675300	2.27085300
N	-2.32891900	-0.96328700	-1.27918900
C	-3.54387900	-0.32040200	-1.18867400
N	-2.51762300	-2.32163200	-1.18731300
C	-4.47331600	-1.38494900	-1.03825300
C	-3.96328500	1.02479200	-1.22929900
N	-3.77922800	-2.57937200	-1.04514300
C	-5.85672300	-1.13462500	-0.92047400
C	-5.33513100	1.25502000	-1.11165100
H	-3.26128600	1.85338000	-1.33763500
H	-6.56498600	-1.96008900	-0.80493900
C	-6.27048300	0.19535300	-0.95900000

H	-5.70267900	2.28630600	-1.13648600
H	-7.33484400	0.43629200	-0.87096700

Benzoyl chloride

14

C	-0.12766300	0.20925100	-0.00003100
C	-0.56037900	-1.13345000	0.00000200
C	-1.92947900	-1.42324800	0.00000600
C	-2.87130300	-0.38153900	-0.00002300
C	-2.44504800	0.95787600	-0.00005900
C	-1.08000700	1.25630700	-0.00006400
H	0.17937500	-1.93798500	0.00002600
H	-2.26330600	-2.46563600	0.00003400
H	-3.94156400	-0.61346100	-0.00002000
H	-3.18007400	1.76907700	-0.00008200
H	-0.73029400	2.29277900	-0.00008900
C	1.29665700	0.61262100	-0.00003600
O	1.73176500	1.73059300	0.00000300
Cl	2.49324000	-0.79273100	0.00007900

Benzoyl fluoride

14

C	0.23706000	0.04420100	0.00000600
C	-0.42880800	-1.19999300	0.00006300
C	-1.82816200	-1.23705400	0.00002800
C	-2.56381400	-0.04054100	-0.00006400
C	-1.90230600	1.19989200	-0.00012100
C	-0.50496500	1.24553600	-0.00008500
H	0.15278600	-2.12544400	0.00013300
H	-2.34750300	-2.20070900	0.00007100
H	-3.65848500	-0.07409000	-0.00009100
H	-2.47960900	2.12998300	-0.00019300
H	0.02950400	2.20032200	-0.00012800
C	1.71152600	0.13828400	0.00004000
O	2.39492700	1.12678600	-0.00000500
F	2.31341100	-1.09403300	0.00011600

$^{3}A_{Co\text{-}F}$

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C	-4.51805400	-1.24446200	-1.11503700
C	-0.97566900	-0.48014900	-1.46125800
H	-0.87743000	0.26103300	-2.27072900
H	-0.40194900	-1.38314900	-1.72461300
C	-0.33490600	1.88731800	0.34747800
N	-2.60092400	-2.26079400	-1.24995000
N	-3.87444800	-2.46683400	-1.12639200
P	-0.07106800	0.09349600	0.10069900
C	-3.54299800	-0.21835200	-1.24174500
C	-5.89107200	-0.93614500	-1.01267300
C	-0.00562200	2.41245100	1.61899700
C	-0.70606000	2.77329100	-0.68614300
N	-2.35546100	-0.91107800	-1.32562200
C	-1.00265700	-0.74639000	1.44298000
C	-3.90296500	1.14420800	-1.27327000
C	-6.24679400	0.41082300	-1.04171900
H	-6.63576100	-1.73139000	-0.91599200
C	-0.09773900	3.78937500	1.85838700
H	0.34654500	1.72925900	2.39815600
C	-0.78758400	4.15316000	-0.44117000
H	-0.93077500	2.40271000	-1.69131800
C	-2.08797900	-0.12040700	2.08841400
C	-0.64322600	-2.06409300	1.79629000
H	-3.16446400	1.94279900	-1.36492400
C	-5.26530900	1.43137800	-1.17058500
H	-7.30098000	0.69622300	-0.96488900
H	0.15011700	4.18317900	2.84989800
C	-0.49339200	4.66294200	0.83221200
H	-1.08436800	4.82844100	-1.25057000
H	-2.38099600	0.89949400	1.81975800
C	-2.79793500	-0.80216500	3.08910100
H	0.18534900	-2.54471900	1.26739900
C	-1.35867900	-2.73655600	2.79558000
H	-5.58858700	2.47750100	-1.18922600
H	-0.56330700	5.73920100	1.02197900
H	-3.63842100	-0.30762000	3.58790000
C	-2.43296200	-2.10833200	3.44643600
H	-1.07436700	-3.75875100	3.06826400
H	-2.98668300	-2.63758500	4.22959500
Co	2.07199900	-0.58647600	0.04471800
C	3.40693800	1.05363400	-0.33191800
C	4.17044200	0.04391200	0.33262800
C	2.99169100	0.53022500	-1.64533600
C	4.10122800	-1.13777600	-0.48315300
C	3.46387900	-0.79760300	-1.74930100
C	3.23527300	2.46212500	0.15368200
H	2.39380400	2.97144000	-0.34163800
H	3.05560200	2.47903000	1.24047500
H	4.15073400	3.05202900	-0.04861600
C	2.33122700	1.34230800	-2.72296800
H	3.09511200	1.90020500	-3.29837200
H	1.77535900	0.70925100	-3.43346300
H	1.63707500	2.08858100	-2.30320700
C	4.78014200	0.17861100	1.69738000
H	5.36789900	-0.71302900	1.96869500
H	5.44921100	1.05654400	1.74666800
H	3.97332300	0.30741100	2.44096800
C	4.64542000	-2.49883900	-0.16539200
H	5.47529100	-2.75978300	-0.84867200
H	5.01738600	-2.56047000	0.86915500
H	3.85389100	-3.25755200	-0.29727300
C	3.23083200	-1.77603600	-2.86066500
H	4.18273400	-2.21837800	-3.20728300
H	2.58676500	-2.59853500	-2.49920500
H	2.73875800	-1.30283900	-3.72520200
F	1.80914400	-0.14917200	1.93143700
F	1.36176700	-2.26170600	-0.43379800

$^{3}TS_{A\text{-}B}$

81

C	4.99539500	1.41145600	-1.49290000
C	2.18421400	-0.88533900	-1.22841400
H	2.60420300	-1.88681800	-1.04577000
H	1.59582100	-0.89722000	-2.15882100
C	1.43356400	-1.03970900	1.71055100
N	3.08653600	0.99733400	-2.44711300
N	4.11326600	1.78536800	-2.48857200
P	0.85983300	-0.45665400	0.06721100
C	4.44669600	0.30223000	-0.79432700
C	6.25362300	1.94474400	-1.14275500
C	0.77446000	-0.53466400	2.85634600
C	2.41747900	-2.03833300	1.87285500
N	3.24607900	0.08081300	-1.43477300
C	0.95678500	1.37481100	0.11539900
C	5.13722500	-0.31517200	0.26810300
C	6.93334300	1.33762100	-0.08873100
H	6.66818300	2.79853500	-1.68629700
C	1.12337000	-1.00012700	4.13159200
H	-0.01328200	0.21889100	2.74861600
C	2.75999400	-2.50002300	3.15290700
H	2.92222400	-2.47478200	1.00618700
C	1.82138100	2.04299000	1.00711100
C	0.21244300	2.11258800	-0.82755000
H	4.73139100	-1.16814800	0.81424100
C	6.38089600	0.22457100	0.60151200
H	7.91307200	1.71828900	0.21758500
H	0.60981000	-0.59523000	5.00997500

C	2.11794000	-1.97902400	4.28545300
H	3.53104200	-3.27012900	3.26003100
H	2.40628400	1.47972500	1.74088700
C	1.93332100	3.43981000	0.95665300
H	-0.44213500	1.58276100	-1.52416100
C	0.33529200	3.50774400	-0.87264200
H	6.94951600	-0.22504400	1.42229300
H	2.38722500	-2.33893300	5.28400300
H	2.60524000	3.95366700	1.65234800
C	1.19186000	4.17331800	0.01761000
H	-0.24541300	4.07696200	-1.60593200
H	1.28257800	5.26429500	-0.01977200
Co	-1.13062700	-1.27488100	-0.85249200
C	-2.03123200	-2.87848100	0.26226900
C	-2.95622500	-2.46942100	-0.75089800
C	-0.85668100	-3.47194500	-0.39803700
C	-2.29233700	-2.64721400	-2.01703900
C	-1.02350800	-3.33550300	-1.79334500
C	-2.28792400	-2.87819100	1.73926300
H	-1.34825600	-2.83797400	2.31349200
H	-2.91446200	-2.01895800	2.03094700
H	-2.81558400	-3.80806200	2.02952500
C	0.21375000	-4.24094300	0.31323700
H	-0.16677600	-5.25525200	0.54219200
H	1.12076600	-4.35750100	-0.30072700
H	0.49123800	-3.77688300	1.27215400
C	-4.34780300	-1.95813400	-0.53272000
H	-4.71004900	-1.39260500	-1.40636400
H	-5.03861500	-2.80993200	-0.38047000
H	-4.40160900	-1.30600100	0.35449000
C	-2.81536000	-2.29013800	-3.37329500
H	-3.01805300	-3.20612500	-3.95907400
H	-3.74507700	-1.70443400	-3.31293800
H	-2.06179200	-1.69821900	-3.92113000
C	-0.08479800	-3.75330500	-2.88442100
H	-0.51856000	-4.58326400	-3.47347700
H	0.09900200	-2.91825300	-3.58255900
H	0.88327500	-4.09230000	-2.48343700
F	-0.54143800	-0.42248600	-2.38534800
F	-2.19588200	0.16276600	0.21909900
Cl	-4.21117800	0.35140200	2.26690700
C	-2.57030100	1.40279400	1.39463500
O	-1.66349700	1.54574900	2.16283100
C	-3.22668500	2.44117800	0.54411700
C	-2.95702400	3.78476200	0.86807100
C	-4.08562900	2.13655900	-0.52783800
C	-3.55066200	4.81752900	0.12756000
H	-2.28276300	4.00784700	1.70035500
C	-4.66722600	3.17116900	-1.26927800
H	-4.28538300	1.09070600	-0.76810600
C	-4.40476000	4.51357000	-0.94264500
H	-3.34163600	5.86101200	0.38714500
H	-5.33135500	2.93167500	-2.10677000
H	-4.86717000	5.31967900	-1.52259800

$^3B_{Co\text{-}Cl}$

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C	-1.01438600	-0.47269700	-1.46603200
H	-0.93421900	0.25673400	-2.28758900
H	-0.42589300	-1.37390600	-1.69924400
C	-0.31653700	1.97422200	0.19878600
P	-0.11929400	0.15193100	0.08214100
C	0.12617200	2.59267600	1.39197300
C	-0.76687800	2.78547900	-0.86322100
C	-1.13697600	-0.54908800	1.44458200
C	0.07935800	3.98622800	1.52659600
H	0.51949700	1.97392600	2.20625200
C	-0.80957800	4.18171400	-0.72345000
H	-1.07973800	2.34377500	-1.81427000
C	-2.11489100	0.21619200	2.11093500
C	-0.95867100	-1.90813700	1.78127000
H	0.41782600	4.45040300	2.45898600
C	-0.39324200	4.78466100	0.47194900
H	-1.16799200	4.79627600	-1.55590200
H	-2.26747300	1.26921800	1.85514400
C	-2.90103000	-0.37241200	3.11380600
H	-0.20004900	-2.48372400	1.24089100
C	-1.75296300	-2.48697600	2.77934700
H	-0.42912300	5.87383400	0.57956400
H	-3.65728600	0.22905400	3.62960700
C	-2.72143700	-1.72215300	3.44989000
H	-1.61197400	-3.54223700	3.03725700
H	-3.33659300	-2.17846600	4.23309200
Co	2.02227600	-0.59803000	0.05858100
C	3.90093100	0.69454000	-0.18294200
C	4.20285100	-0.72273500	-0.09743100
C	3.02446000	0.87626700	-1.28249800
C	3.63007600	-1.38774400	-1.24543700
C	2.85119800	-0.42480000	-1.94727400
C	4.39994800	1.73728400	0.77293400
H	3.95283800	2.72263000	0.56717300
H	4.15652500	1.45751800	1.81308100
H	5.49902200	1.83991500	0.69809500
C	2.53954100	2.19010800	-1.82051100
H	3.30744300	2.61792900	-2.49397900
H	1.61555500	2.08005000	-2.40870700
H	2.35169900	2.92174700	-1.01887400
C	5.10026400	-1.33139600	0.93745800
H	5.07718900	-2.43178900	0.90339700
H	6.14482500	-1.00412400	0.77385200
H	4.79767800	-1.00730700	1.94784600
C	3.73031300	-2.84284100	-1.59764300
H	4.09807500	-2.97425900	-2.63135100
H	4.41509700	-3.37851100	-0.92132700
H	2.72907400	-3.30215900	-1.51847400
C	2.13732200	-0.67169400	-3.24435300
H	2.85691000	-0.64068100	-4.08571800
H	1.66173600	-1.66582000	-3.25225100
H	1.36584100	0.08778300	-3.44736900
F	1.07165000	-2.24883000	-0.38098200
Cl	2.08797500	-0.34479200	2.32613900
N	-2.38479000	-0.92470300	-1.31344200
C	-3.58321400	-0.25524700	-1.19527200
N	-2.60851000	-2.28103400	-1.28203800
C	-4.53992500	-1.30116400	-1.09449800
C	-3.96730000	1.10090300	-1.17337900
N	-3.87650900	-2.51171100	-1.15352000
C	-5.91673900	-1.02088300	-0.96756500
C	-5.33315400	1.36074900	-1.04725900
H	-3.24342900	1.91507200	-1.24089700
H	-6.64634800	-1.83214400	-0.89107700
C	-6.29596200	0.31978100	-0.94581300
H	-5.67381700	2.40127300	-1.02451200
H	-7.35400700	0.58387900	-0.84869000