Supporting Information

Toward a Neutral Single-Component Amidinate Iodide Aluminum Catalyst for the CO_2 Fixation into Cyclic Carbonates

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Figure S1. NMR spectra for N',N''-(naphthalen-1,8-diyl)bis(N-(2,6-dimetylphenyl)acetimidamide) (**1**) in [D_6]DMSO

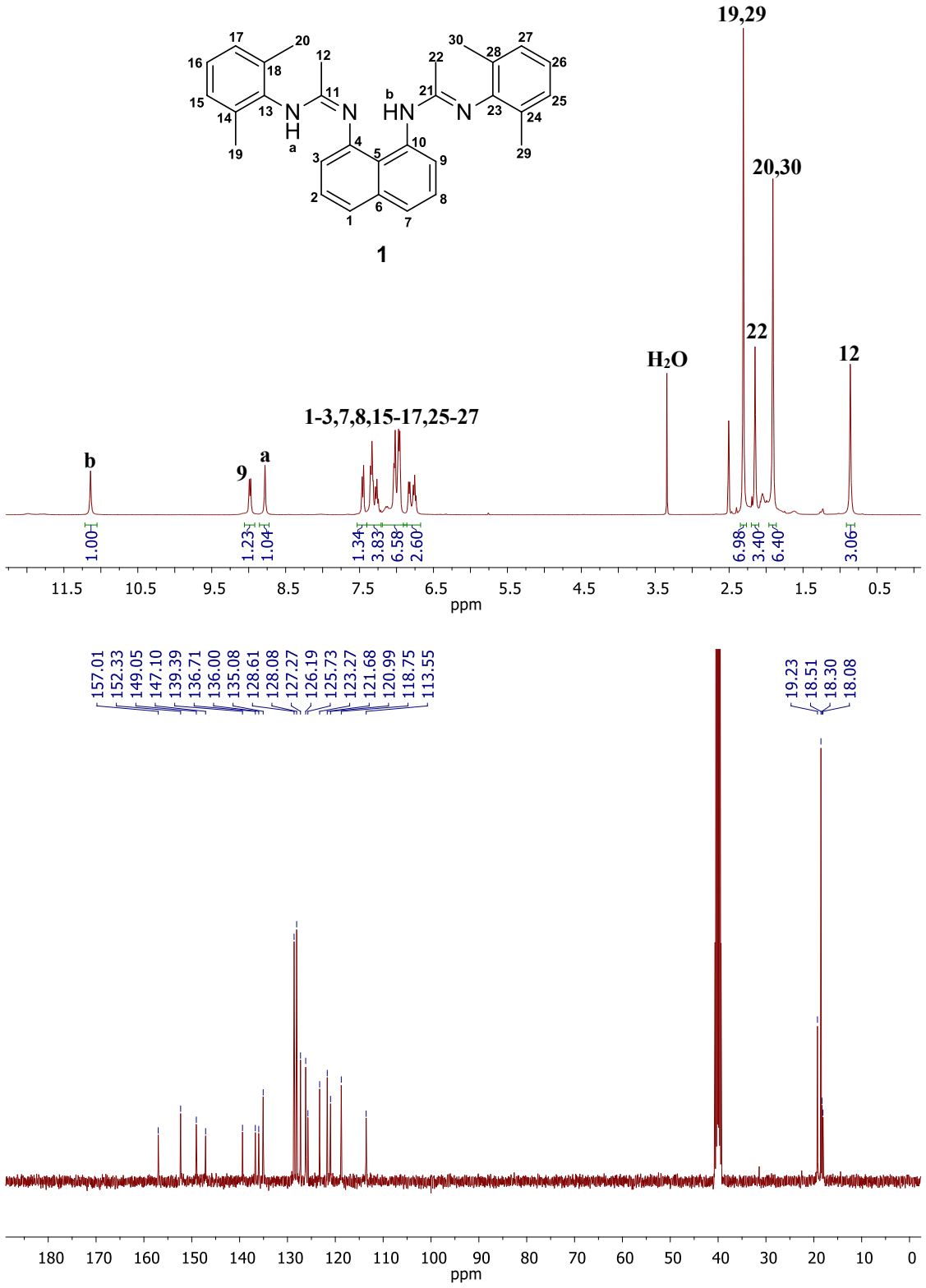


Figure S2. Crystal structure of compound **1**. Only one molecule (molecule "A") is shown. (Thermals ellipsoids are shown with 30% probability.)

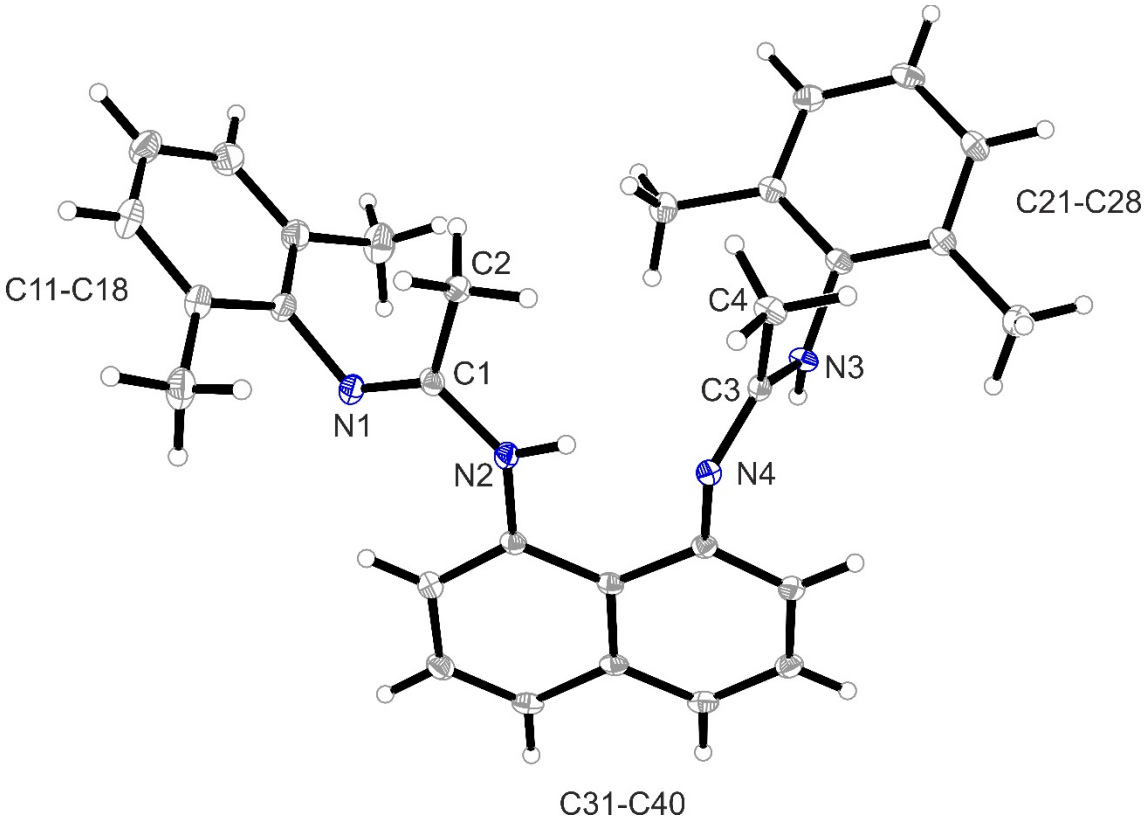


Figure S3. Non-covalent intermolecular and intramolecular interactions in compound **1** involving NH···N, CH···N and CH···π interactions: between two molecules "A"

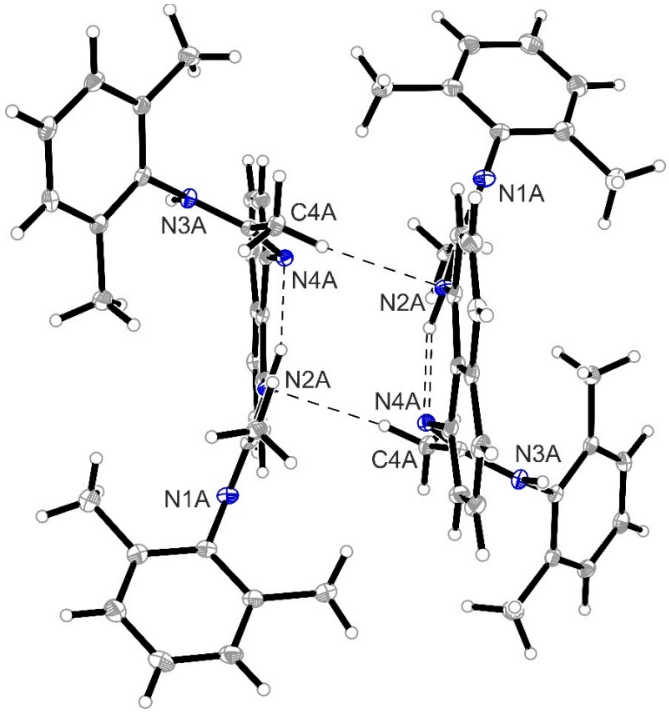


Figure S4. Non-covalent intermolecular and intramolecular interactions in compound **1** involving NH···N, CH···N and CH···π interactions: between two molecules "B"

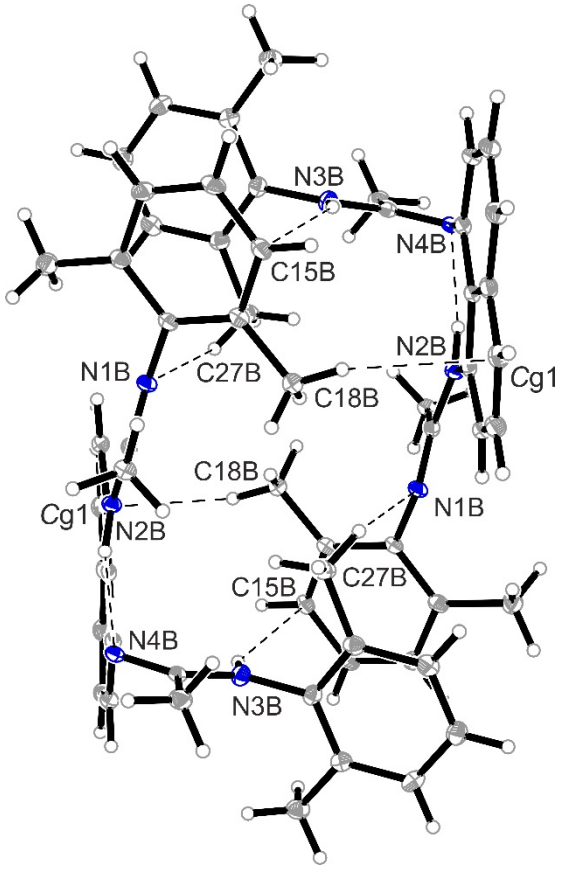


Figure S5. Non-covalent intermolecular and intramolecular interactions in compound **1** involving NH···N, CH···N and CH···π interactions: between the molecules "A" and "B".

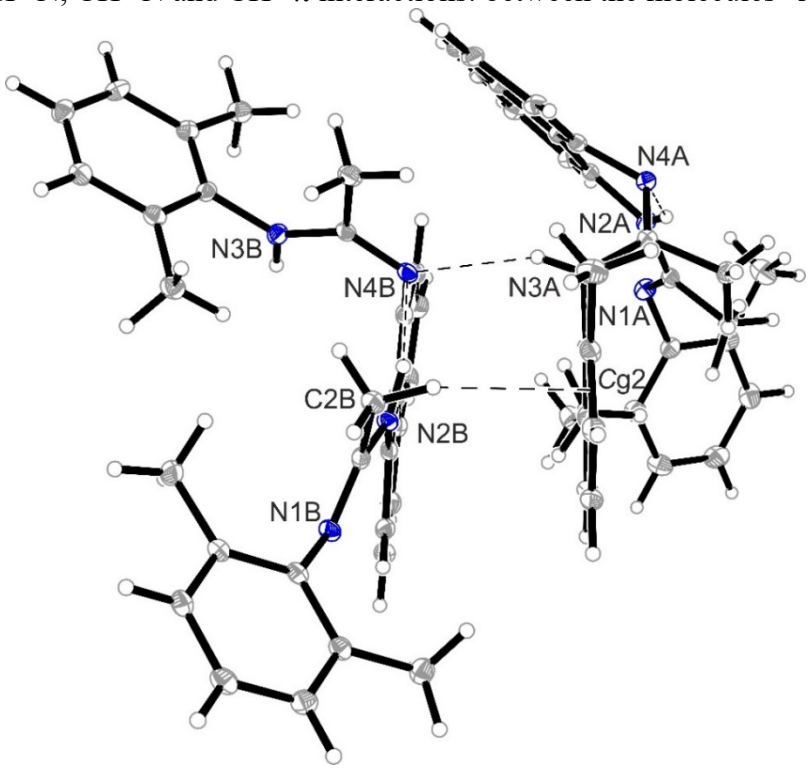


Table S1. Non-covalent intermolecular and intramolecular interactions in compound **1** (Å and deg)

D-H···*A*	*d*(*D*-H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
N2A-H2A···N4A	0.92(3)	1.88(3)	2.679(2)	144(2)
N3A-H3A···N4B	0.85(3)	2.23(3)	3.002(2)	150(2)
N2B-H2B···N4B	0.95(3)	1.94(3)	2.737(2)	140(2)
C4A-H401···N2A$^{\#1}$	0.98	2.59	3.554(3)	166.3
C18B-H18E···*Cg*1$^{\#2, a}$	0.98	2.51	3.393(3)	150.2
C27B-H27E···N1B$^{\#2}$	0.98	2.63	3.426(3)	138.8
C2B-H213···*Cg*2^{b}	0.98	2.69	3.596(2)	153.9
N3B-H3B···C15B$^{\#2}$	0.88(3)	2.75(3)	3.520(3)	146.1(3)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1.5, -y+0.5, -z; $^{\#2}$ -x+1.5, -y+0.5, -z+1. ^{a} *Cg*1 is the centroid of the aromatic ring C31B/C32B/C33B/C34B/C35B/C40B; ^{b} *Cg*2 is the centroid of the bond C25A/C26A.

Figure S6. NMR spectra for complex **2** in $CDCl_3$

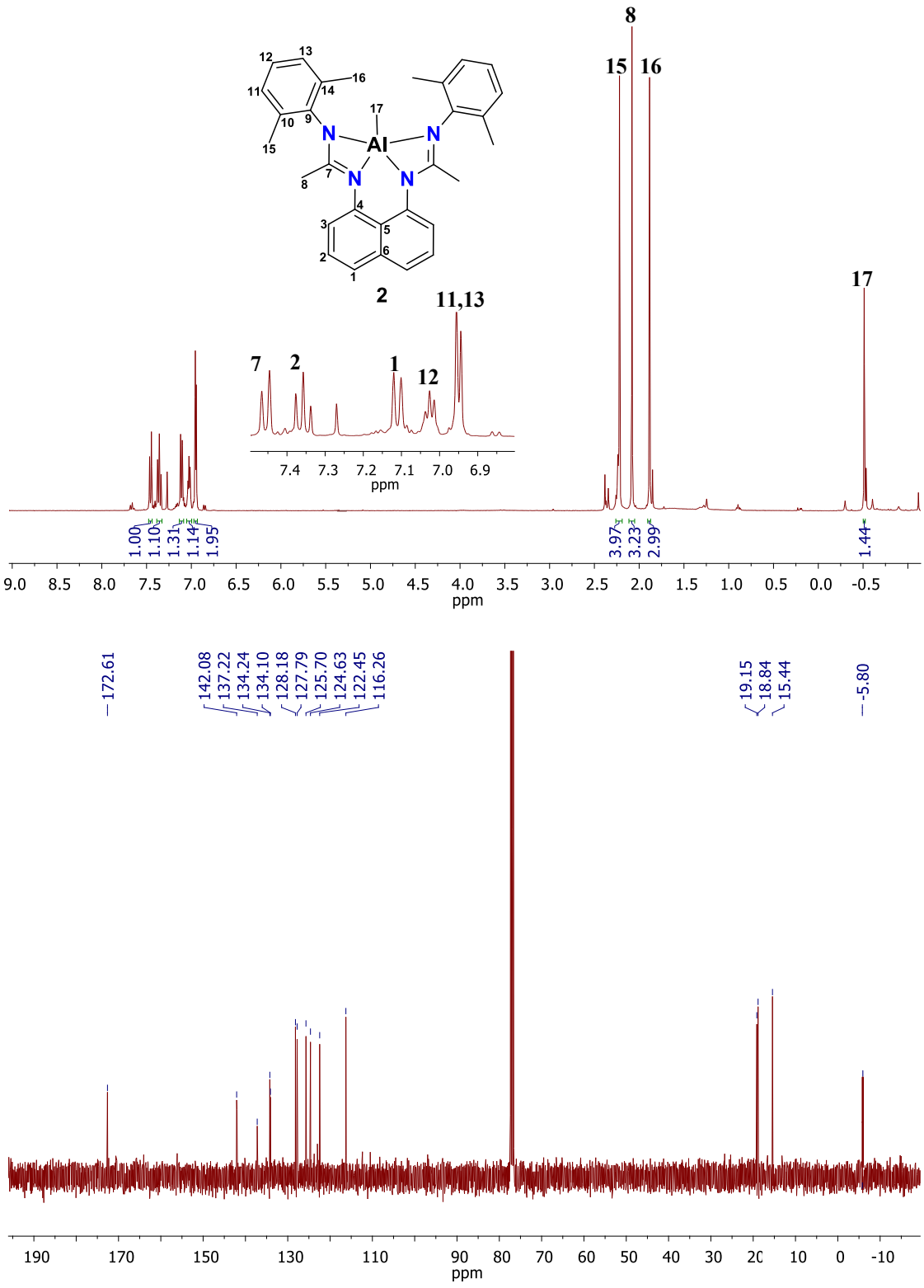


Figure S7. NMR spectra for complex **3** in $CDCl_3$

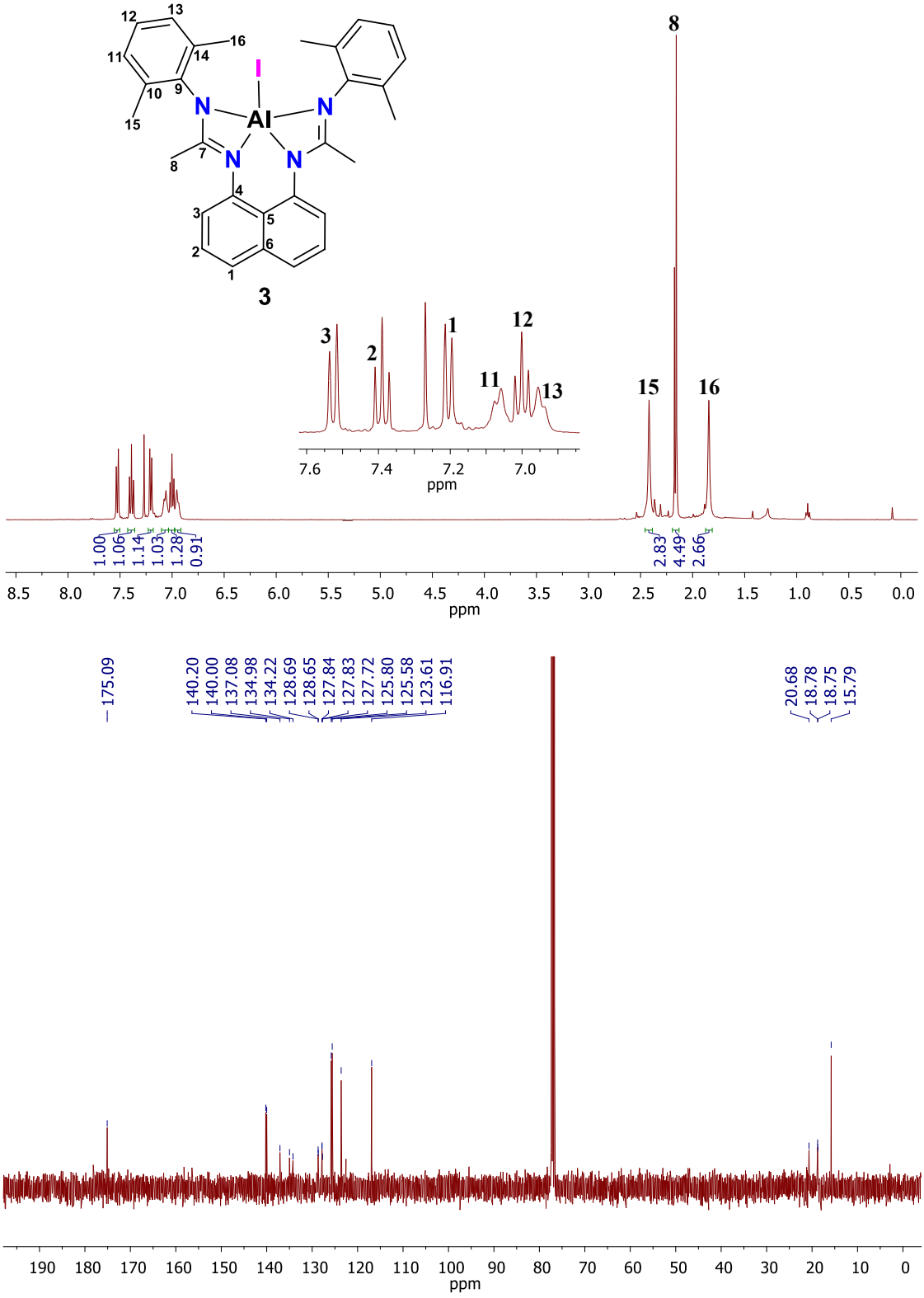


Table S2. Crystallographic data and structure refinement of ligand **1.**

	1
Empirical formula	$C_{30}H_{32}N_4$
Formula weight	448.59 g/mol
Temperature (K)	100(2)
Wavelength (Å)	1.54178
Crystal system	monoclinic
Space group	*C*2/*c*
a(Å)	22.8669(5)
b(Å)	20.2554(4)
c(Å)	22.9286(5)
α(°)	90
β(°)	110.6980(10)
γ(°)	90
Volume(Å^3)	9934.6(4)
Z	16
Density (calculated) (g/cm^3)	1.200
Absorption coefficient (mm^{-1})	0.549
F(000)	3840
Crystal size (mm^3)	0.087 x 0.101 x 0.231
Index ranges	$-27 \leq h \leq 27$ $-24 \leq k \leq 24$ $-27 \leq 1 \leq 27$
Reflections collected	62926
Independent reflections	8818 [R(int) = 0.1380]
Data/restraints/parameters	8818 / 0 / 641
Goodness-of-fit on F^2	1.108
Final R indices [I>2σ(I)]	R1 = 0.0541, wR2 = 0.1078
R indices (all data)	R1 = 0.0773 wR2 = 0.1183
Largest diff. peak / hole, e.Å^{-3}	0.190 and –0.233

Table S3. Bond lengths (Å) and angles (°) for ligand **1**

1 (Bond lengths, Å)		**1 (Bond angles, º)**	
N1A–C1A	1.286(3)	C1A–N1A–C11A	117.40(19)
N2A–C1A	1.373(3)	N1A–C1A–N2A	122.80(19)
N3A–C21A	1.433(3)	N2A–C1A–C2A	113.05(18)
N4A–C3A	1.298(3)	C3A–N3A–C21A	122.83(17)
N1B–C1B	1.277(3)	C1A–N2A–C31A	130.22(18)
N2B–C1B	1.382(3)	C31A–N2A–H2A	111.5(17)
N3B–C21B	1.436(3)	C3A–N3A–H3A	120.6(17)
N4B–C3B	1.299(3)	C3A–N4A–C39A	121.66(17)
C1A–C2A	1.509(3)	C1B–N2B–C31B	129.94(18)
C3A–C4A	1.501(3)	C31B–N2B–H2B	114.6(16)
C11A–C16A	1.401(3)	C3B–N3B–H3B	117.3(17)
C12A–C13A	1.395(3)	C3B–N4B–C39B	117.86(17)
C13A–C14A	1.384(4)	N1A–C1A–C2A	124.2(2)
C14A–C15A	1.382(3)	N4A–C3A–N3A	125.94(19)
C15A–C16A	1.395(3)	N3A–C3A–C4A	116.24(18)
C16A–C18A	1.503(3)	C16A–C11A–C12A	120.9(2)
N1A–C11A	1.422(3)	C12A–C11A–N1A	119.4(2)
N2A–C31A	1.405(3)	C13A–C12A–C17A	121.4(2)
N3A–C3A	1.356(3)	C14A–C13A–C12A	121.2(2)
N3A–H3A	0.85(3)	C16A–C11A–N1A	119.65(19)
N4A–C39A	1.416(3)	C13A–C12A–C11A	118.4(2)
N1B–C11B	1.413(3)	C11A–C12A–C17A	120.1(2)
N2B–C31B	1.405(3)	C14A–C13A–H13A	119.4
N3B–C3B	1.355(3)	C22A–C21A–C26A	121.77(19)
N3B–H3B	0.88(3)	C26A–C21A–N3A	118.60(19)
N4B–C39B	1.439(3)	C23A–C22A–C27A	119.7(2)
		C24A–C23A–C22A	121.4(2)
		C22A–C23A–H23A	119.3

Table S4. Crystallographic data and structure refinement for complexes **2** and **3.**

	2	**3**
Empirical formula	$C_{31}H_{33}AlN_4$	$C_{30}H_{30}AlIN_4$
Formula weight	488.59 g/mol	600.46 g/mol
Temperature (K)	100(2)	100(2)
Wavelength (Å)	1.54178	1.54178
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a(Å)	13.9815(5)	10.2822(2)
b(Å)	14.5523(5)	19.5288(4)
c(Å)	14.5393(5)	13.4122(3)
α(°)	90	90
β(°)	116.9610(10)	91.2100(10)
γ(°)	90	90
Volume(Å^3)	2636.70(16)	2692.56(10)
Z	4	4
Density (calculated) (g/cm^3)	1.231	1.481
Absorption coefficient (mm^{-1})	0.868	9.854
F(000)	1040	1216
Crystal size (mm^3)	0.141 x 0.190 x 0.210	0.040 x 0.120 x 0.140
Index ranges	$-17 \le h \le 17$ $-17 \le k \le 17$ $-17 \le l \le 17$	$-11 \le h \le 12$ $-23 \le k \le 23$ $-15 \le l \le 15$
Reflections collected	37564	48354
Independent reflections	4998 [R(int) = 0.0323]	4751 [R(int) = 0.0502]
Data/restraints/parameters	4998 / 0 / 332	4751 / 0 / 331
Goodness-of-fit on F^2	1.028	1.053
Final R indices [I>2σ(I)]	R1 = 0.0346, wR2 = 0.0880	R1 = 0.0253 wR2 = 0.0625
R indices (all data)	R1 = 0.0379 wR2 = 0.0906	R1 = 0.0279 wR2 = 0.0638
Largest diff. peak / hole, e.Å^{-3}	0.268 and –0.298	0.422 and –0.565

Table S5. Bond lengths (Å) and angles (°) for complexes **2** and **3**

2 (Bond lengths, Å)		**3 (Bond lengths, Å)**	
Al1–N2	1.939(11)	Al1–N4	1.911(2)
Al1–C5	1.964(14)	Al1–N3	1.962(2)
Al1–N3	1.999(11)	Al1–C3	2.392(3)
Al1–C3	2.430(13)	Al1–I1	2.553(7)
Al1–N4	1.942(11)	Al1–N2	1.918(2)
Al1–N1	1.992(11)	Al1–N1	1.973(2)
Al1–C1	2.424(13)	Al1–C1	2.397(3)
C1–N1	1.335(16)	N1–C1	1.345(3)
C1–C2	1.495(17)	N2–C1	1.337(3)
C11–C16	1.404(18)	N3–C3	1.337(3)
C11–N1	1.427(16)	N4–C3	1.341(3)
C12–C17	1.505(18)	C1–C2	1.493(3)
C3–N4	1.338(16)	N1–C11	1.437(3)
C3–C4	1.495(17)	N2–C31	1.407(3)
2 (Bond angles, °)		**3 (Bond angles, °)**	
N2–Al1–N4	85.25(5)	N4–Al1–N2	87.03(9)
N4–Al1–C5	112.21(6)	N2–Al1–N3	144.43(9)
N4–Al1–N1	134.59(5)	N2–Al1–N1	67.96(9)
N2–Al1–N3	131.88(5)	N2–Al1–I1	107.92(7)
C5–Al1–N3	113.23(5)	N1–Al1–I1	110.71(7)
N2–Al1–C1	33.47(4)	C1–Al1–I1	113.64(6)
C5–Al1–C1	116.88(5)	N4–Al1–N3	68.02(9)
N2–Al1–C5	113.39(5)	N4–Al1–N1	136.05(9)
N2–Al1–N1	66.87(4)	N3–Al1–N1	112.81(9)
C5–Al1–N1	111.60(5)	N2–Al1–C3	117.11(9)
N4–Al1–N3	66.72(4)	N1–Al1–C1	34.13(8)
N1–Al1–N3	105.67(4)	N4–Al1–I1	111.19(7)
N4–Al1–C1	112.06(4)	N3–Al1–I1	104.68(7)
N1–Al1–C1	33.41(4)	C3–Al1–I1	112.32(6)

NMR data for cyclic carbonates **5a–h**

Styrene carbonate (5a): Obtained as a white solid. (222.6 mg, 93 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 7.38–7.42 (m, 3H, ArH), 7.32–7.35 (m, 2H, ArH), 5.65 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, PhCHO), 4.77 (t, $^{3}J_{HH}$ =8.5 Hz, 1H, OCH_2), 4.29 ppm (t, $^{3}J_{HH}$ = 7.5 Hz, 1H, OCH_2); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 155.0, 135.9, 129.7, 129.2, 126.0, 78.1, 71.1 ppm.

1,2-hexylene carbonate (5b): Obtained as a colourless liquid (213.0 mg, 89 %); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 4.67–4.74 (m, 1H, OCH), 4.53 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH_2), 4.07 (dd, $^{3}J_{HH}$ = 8.5, 7.0 Hz, 1H, OCH_2), 1.76–1.86 (m, 1H, CH_2), 1.62–1.73 (m, 1H, CH_2), 1.31–1.52 (m, 4H, $2OCH_2$), 0.93 ppm (t, $^{3}J_{HH}$ = 7.0 Hz, 3H, CH_3); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 155.1, 77.1, 69.4, 33.6, 26.5, 22.3, 13.8 ppm.

3-chloropropylene carbonate (5c): Obtained as a colourless liquid. (194.9 mg, 86 %); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 4.96–5.01 (m, 1H, OCH), 4.58 (t, $^{3}J_{HH}$ = 8.5 Hz, 1H, CH_2Cl), 4.39 (dd, $^{3}J_{HH}$ = 8.5, 5.5 Hz, 1H, CH_2Cl), 3.79 (dd, $^{3}J_{HH}$ = 12.0, 5.5 Hz, 1H, CH_2O), 3.71 ppm (dd, $^{3}J_{HH}$ = 12.5, 3.5 Hz, CH_2O); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 154.4, 74.5, 67.0, 43.9 ppm.

3-phenoxyproplylene carbonate (5d): Obtained as a white solid. (297.4 mg, 92 %); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 7.27–7.33 (m, 2H, 2OArH), 7.03 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H, ArH), 6.90–6.95 (m, 2H, 2OArH), 5.00–5.07 (m, 1H, OCH), 4.62 (t, $^{3}J_{HH}$ = 8.5 Hz, 1H, OCH_2), 4.55 (dd, $^{3}J_{HH}$ = 9.0, 6.0 Hz, 1H, OCH_2), 4.25 (dd, $^{3}J_{HH}$ = 10.5, 4.5 Hz, 1H, CH_2OPh), 4.16 ppm (dd, $^{3}J_{HH}$ = 10.5, 3.5 Hz, 1H, CH_2OPh); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 157.8, 154.6, 129.7, 122.0, 114.6, 74.1, 66.9, 66.3 ppm.

4-chlorostyrene carbonate (5e): Obtained as a white solid. (214.3 mg, 65 %); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 7.39–7.41 (m, 2H, ArH), 7.29–7.31 (m, 2H, ArH), 5.67 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH), 4.81 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH), 4.30 ppm (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH_2); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 154.6, 135.7, 134.4, 129.5, 127.3, 77.3, 71.0 ppm.

4-bromostyrene carbonate (5f): Obtained as a white solid. (267.3 mg, 66 %) ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 7.44–7.39 (m, 2H, ArH), 7.33–7.28 (m, 2H, ArH), 5.67 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH), 4.80 (t, $^{3}J_{HH}$ = 8.0 Hz, 1H, OCH_2), 4.30 ppm (dd, $^{3}J_{HH}$ = 8.8, 7.6 Hz, 1H, OCH_2); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 154.4, 134.8, 132.5, 127.5, 127.2, 77.2, 70.9 ppm.

4-((2,2,3,3-tetrafluoropropoxy)methyl)-1,3-dioxolan-2-one (5g). Obtained as a colourless liquid (312.1 mg, 81 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 5.83 (tt, $^{3}J_{HH}$ = 52.8, 4.8 Hz, 1H, $CHCF_2$), 4.76–4.81 (m, 1H, OCH), 4.45 (t, $^{3}J_{HH}$ = 7.6 Hz, 1H, OCH_2), 4.29 (dd, $^{3}J_{HH}$ = 7.6, 6.0 Hz, 1H, OCH_2), 3.87 (dt, $^{3}J_{HH}$ = 12.8, 2.0 Hz, 2H OCH_2CF_2), 3.80 (dd, $^{3}J_{HH}$ = 11.2, 3,2 Hz, 1H, OCH_2CH), 3.70 ppm (dd, $^{3}J_{HH}$ = 11.2, 4.0 Hz, 1H, OCH_2CH); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 159.9 (C=O), 113.9 (tt, $^{3}J_{CF}$ = 994.0, 107.6 Hz, $CHCF_2$), 108.2 (tt, $^{3}J_{CF}$ = 991.6, 138.8 Hz, CF_2), 77.4 (CH), 70,4 (CH_2), 67.4 (t, $^{3}J_{CF}$ = 112.4 Hz, CF_2CH_2), 64.9 ppm (CH_2). ^{19}F NMR (400 MHz, $CDCl_3$, 298 K): δ = (−139.3)–(−139.4) (m, 2F), (−125.1)–(−125.0) ppm (m, 2F).

4-(((2,2,3,3,4,4,5,5-octafluoropentyl)oxy)methyl)-1,3-dioxolan- 2-one (5h). Obtained as a colourless liquid. (485.3 mg, 88 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 6.01 (tt, $^{3}J_{HH}$ = 52.0, 5.6 Hz, 1H, CHF_2), 4.75–4.83 (m, 1H, OCH), 4.46 (t, $^{3}J_{HH}$ = 8.8 Hz, 1H, OCH_2), 4.31 (dd, $^{3}J_{HH}$ = 8.4, 6.0 Hz, 1H, OCH_2), 3.90–4.10 (m, 2H, OCH_2CF_2), 3.83 (dd, $^{3}J_{HH}$ = 11.2, 3,2 Hz, 1H, O*CH*$_2$CH), 3.75 ppm (dd, $^{3}J_{HH}$ = 11.2, 3.6 Hz, 1H, O*CH*$_2$CH); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ = 153.8 (C=O), 103.9–117.2 (m, 3 x CF_2), 106.7 (tt, $^{3}J_{CF}$ = 1009.2, 123.2 Hz, $CHCF_2$), 73.8 (CH), 70,6 (CH_2), 67.3 (t, $^{3}J_{CF}$ = 102.8 Hz, CH_2), 64.8 ppm (CH_2).^{19}F NMR (400 MHz, $CDCl_3$, 298 K): δ = (−137.6)–(−136.7) (m, 2F), (−130.4)–(−129.5) (m, 2F), (−125.6)–(−125.7) (m, 2F), (−120.0)– (−120.1) ppm (m, 2F).

Figure S8. NMR spectra of styrene carbonate (**5a**) in $CDCl_3$

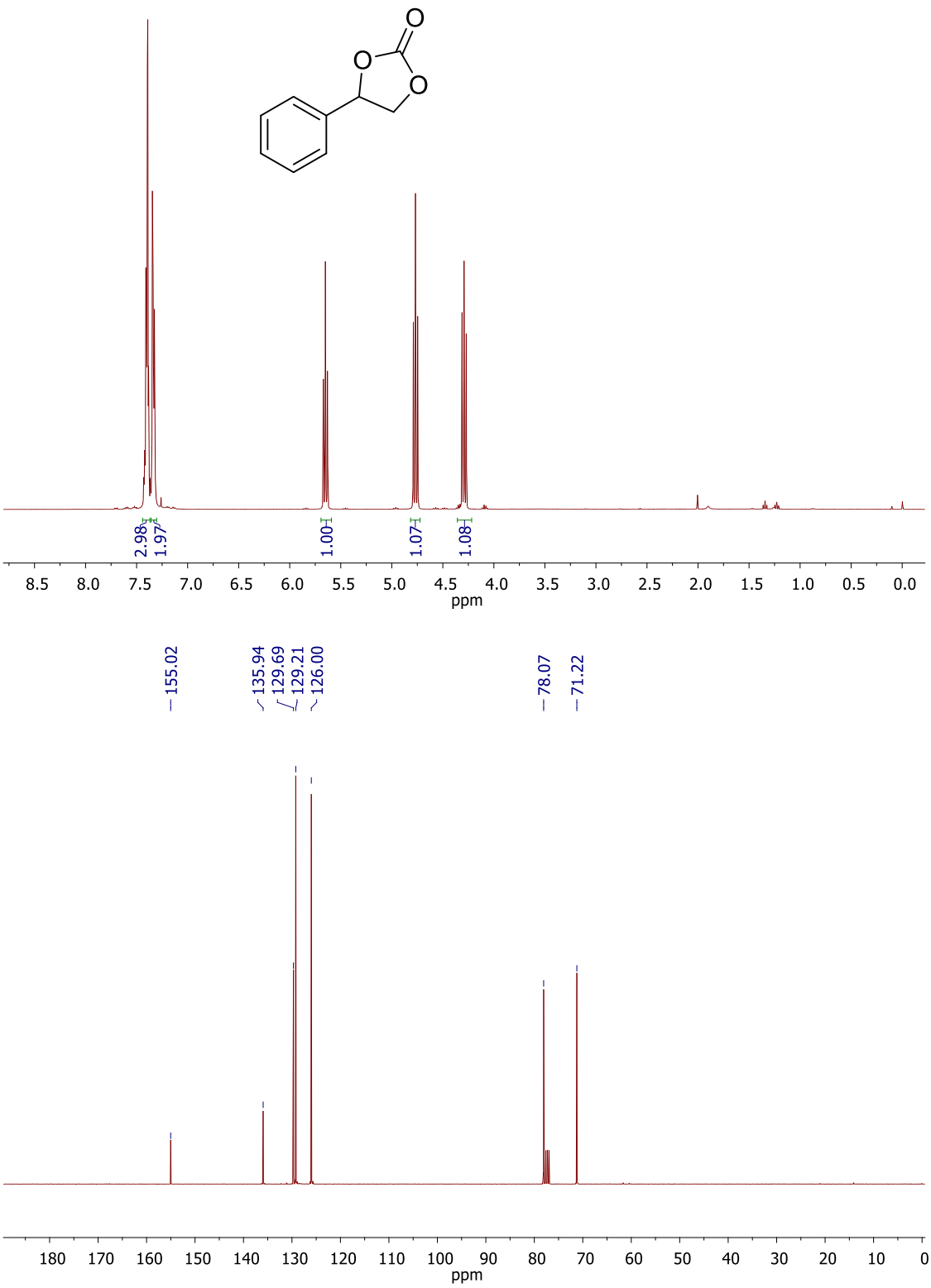


Figure S9. NMR spectra of 1,2-hexylene carbonate (**5b**) in $CDCl_3$

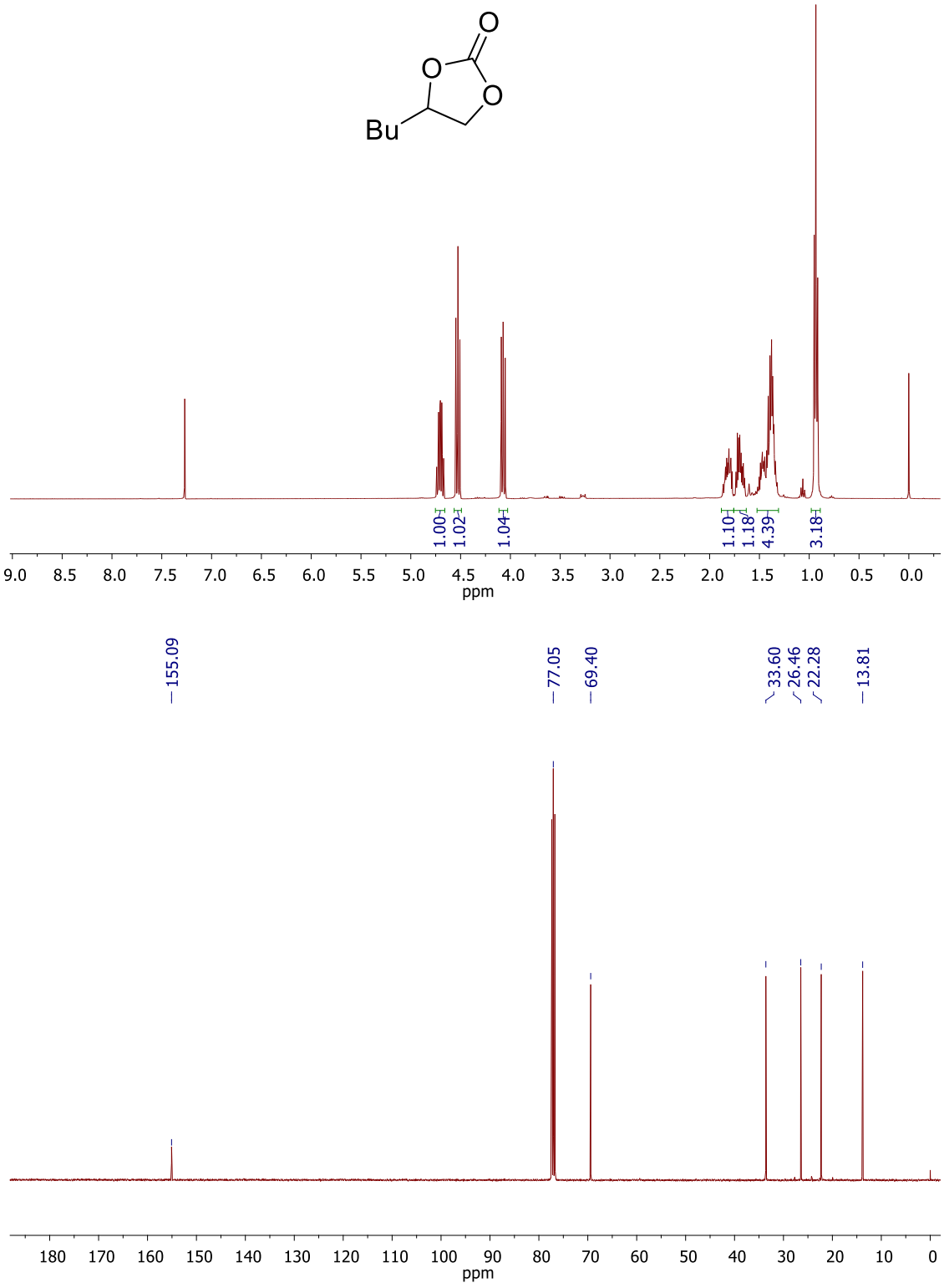


Figure S10. NMR spectra 3-chloropropylene carbonate (**5c**) in $CDCl_3$

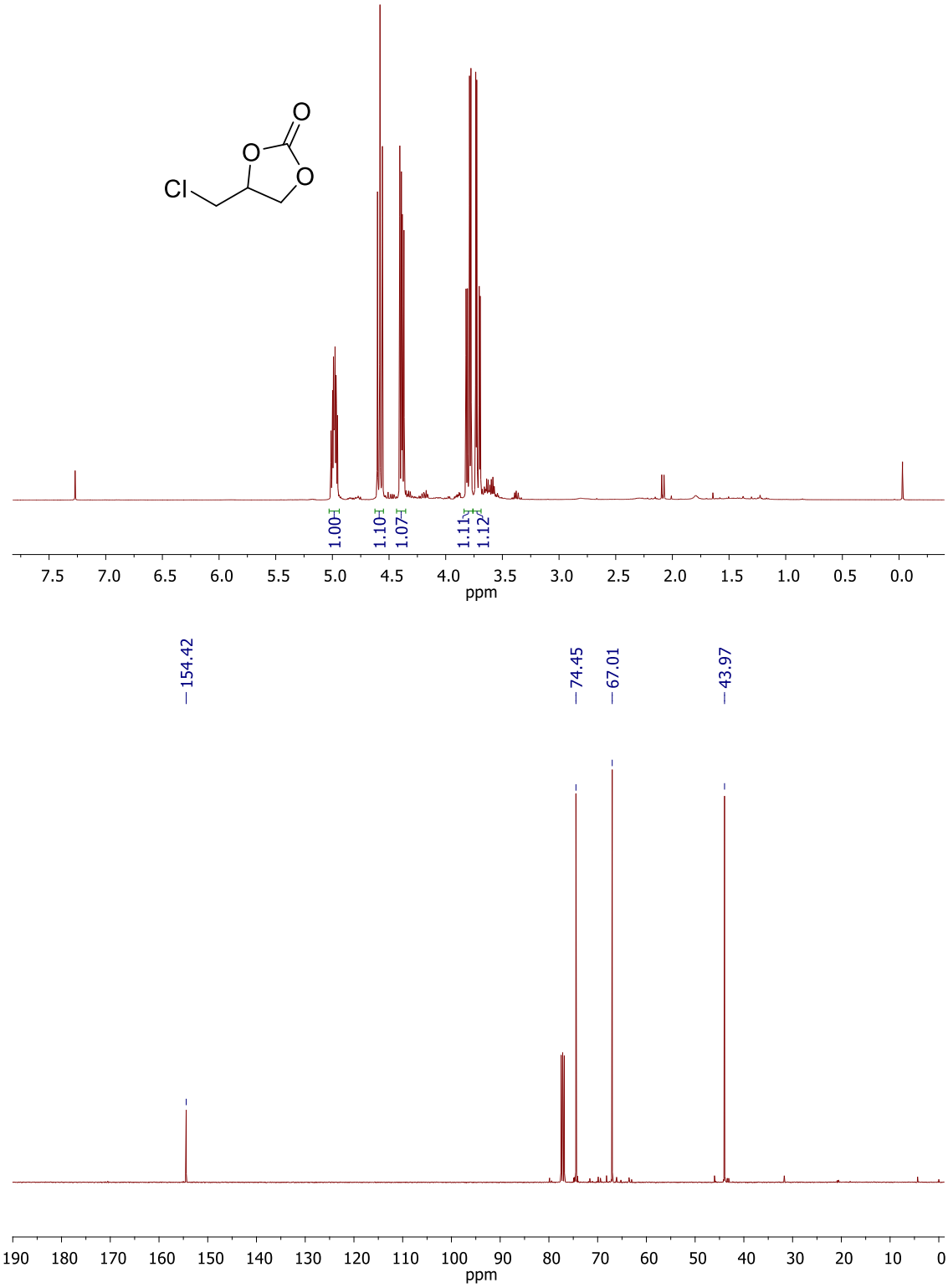


Figure S11. NMR spectra 3-phenoxyproplylene carbonate (**5d**) in $CDCl_3$

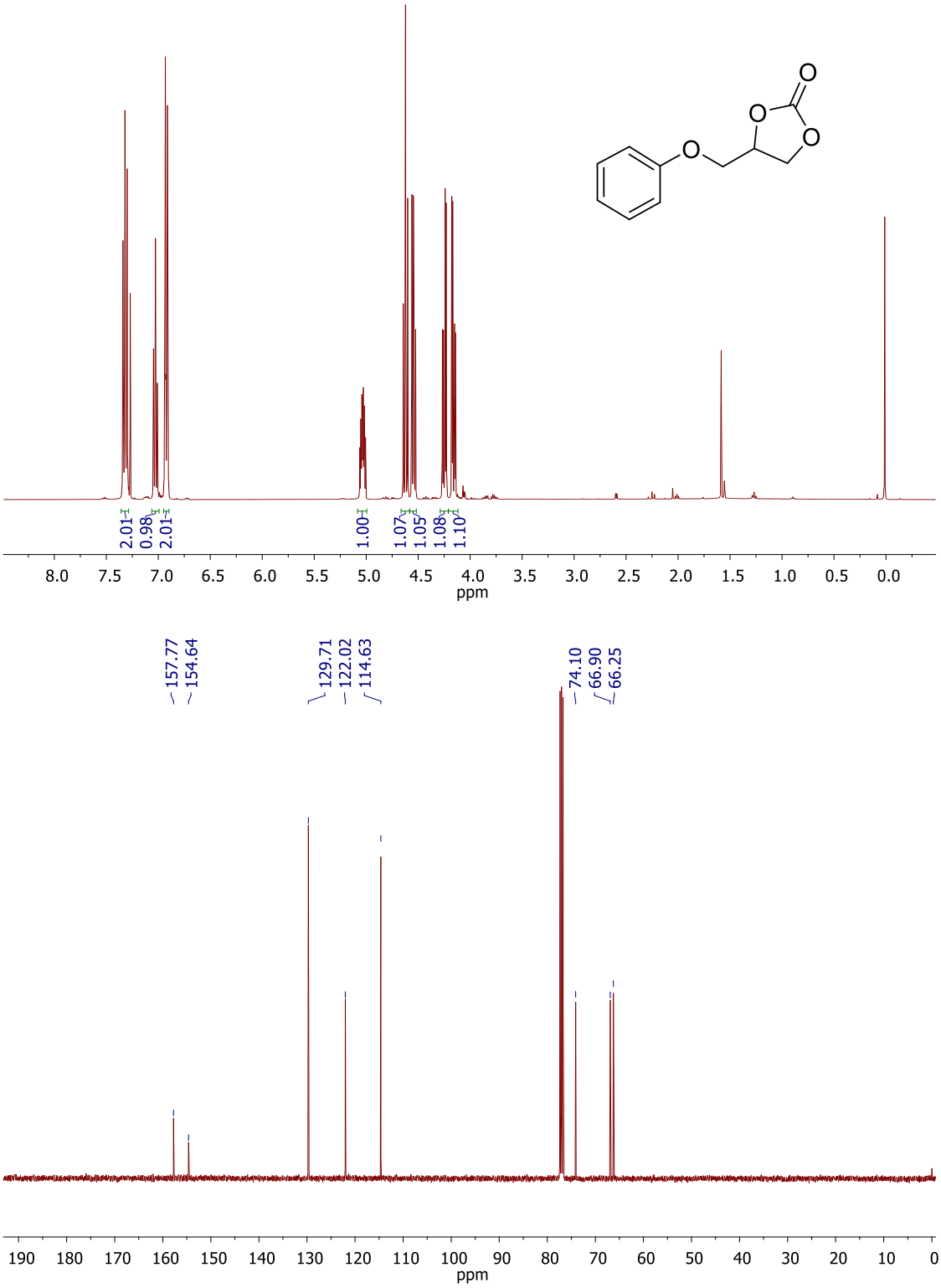


Figure S12. NMR spectra 4-chlorostyrene carbonate (**5e**) in $CDCl_3$

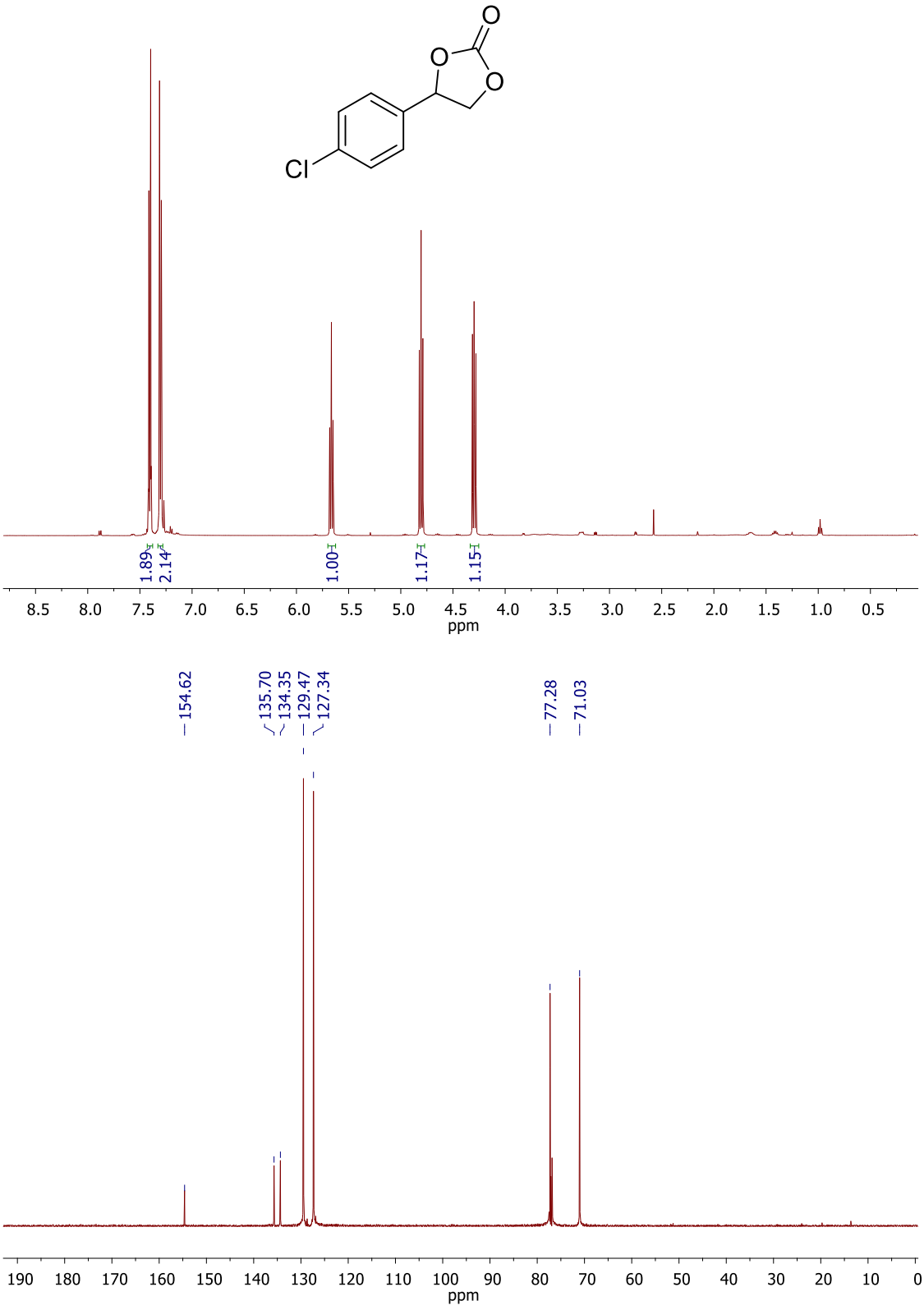


Figure S13. NMR spectra 4-bromostyrene carbonate (**5f**) in $CDCl_3$

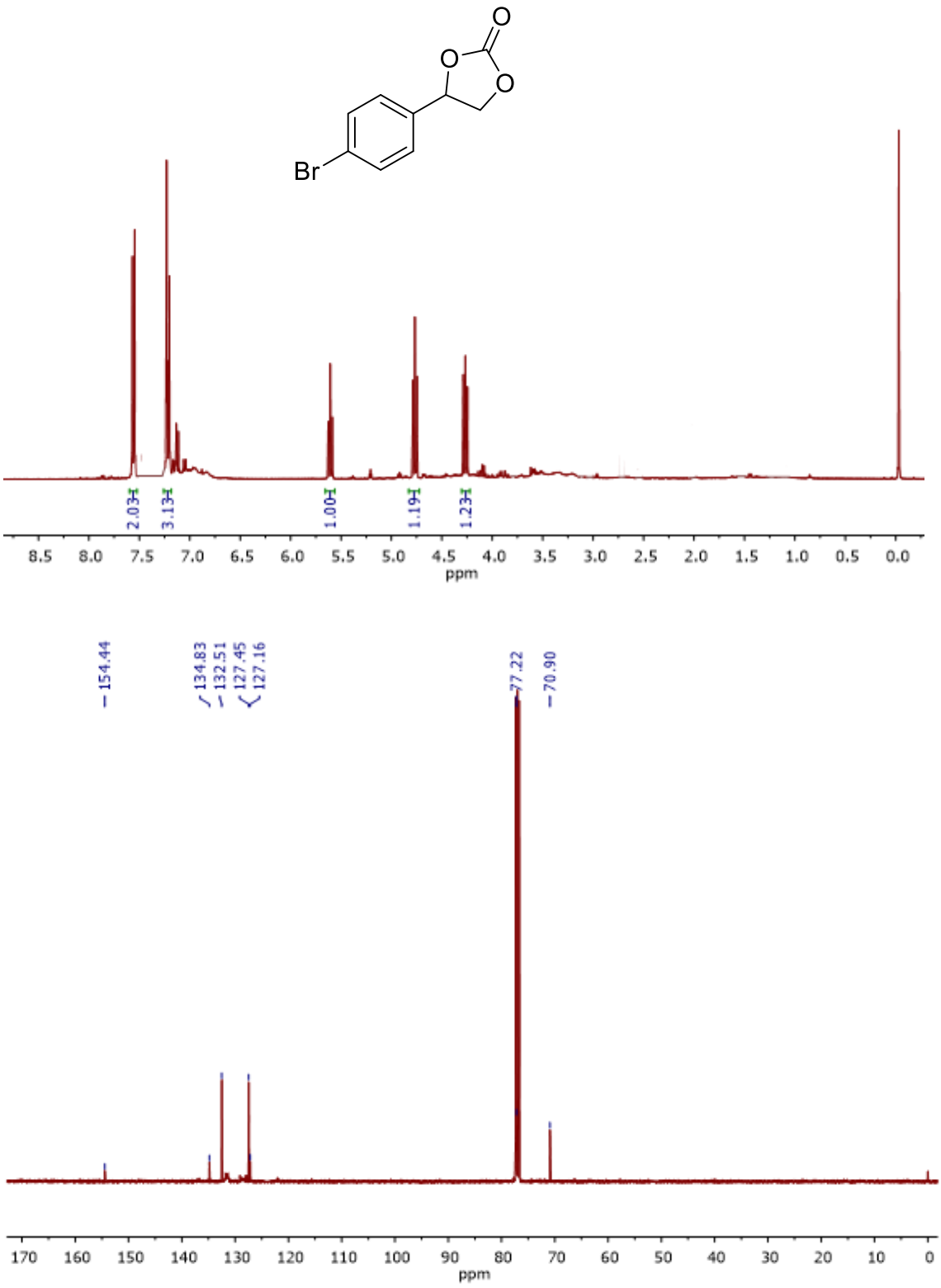


Figure S14. NMR spectra of 4-((2,2,3,3-tetrafluoropropoxy)methyl)-1,3-dioxolan-2-one (**5g**) in $CDCl_3$

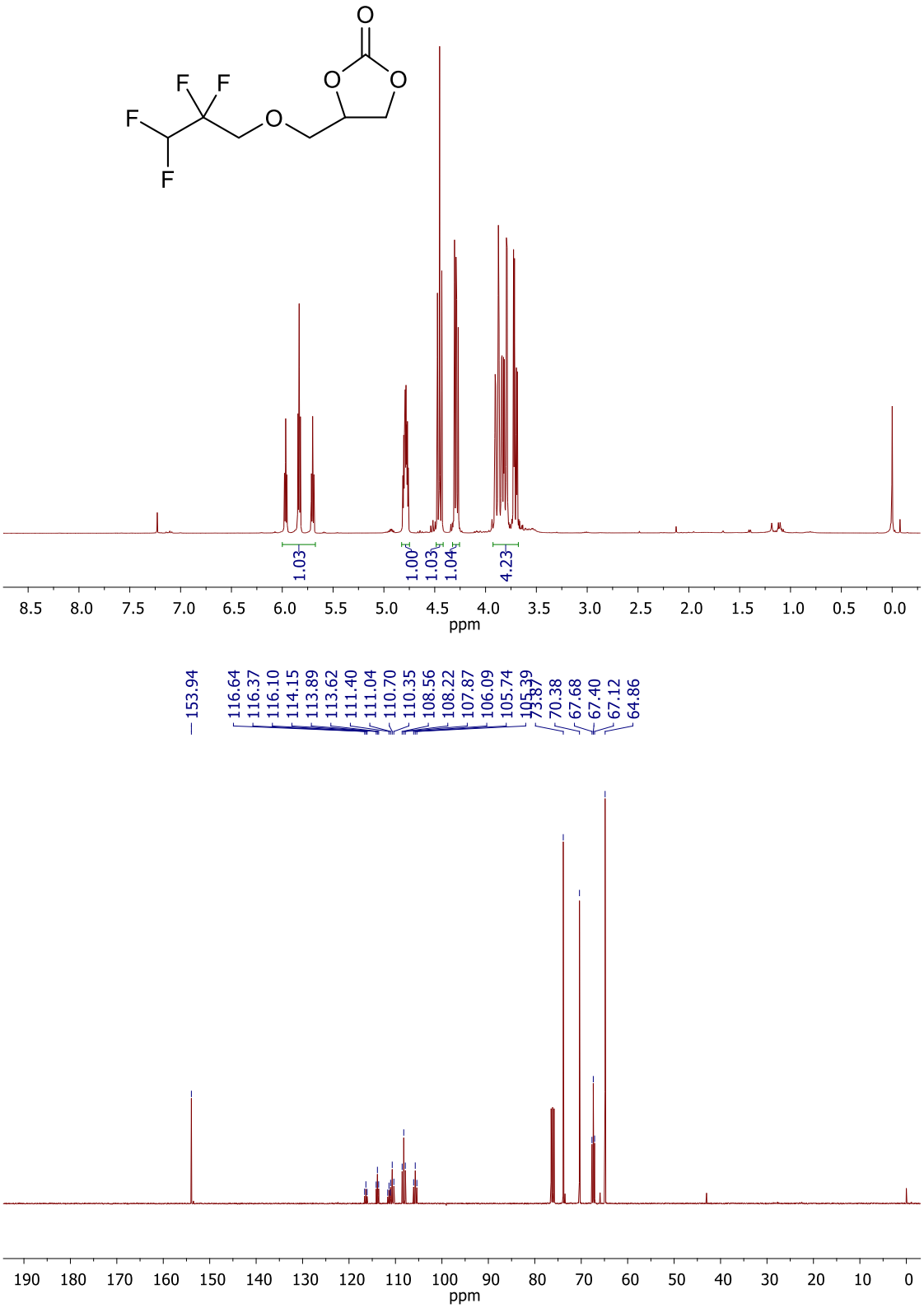


Figure S15. ^{19}F-NMR spectrum of 4-((2,2,3,3-tetrafluoropropoxy)methyl)-1,3-dioxolan-2-one (**5g**) in $CDCl_3$

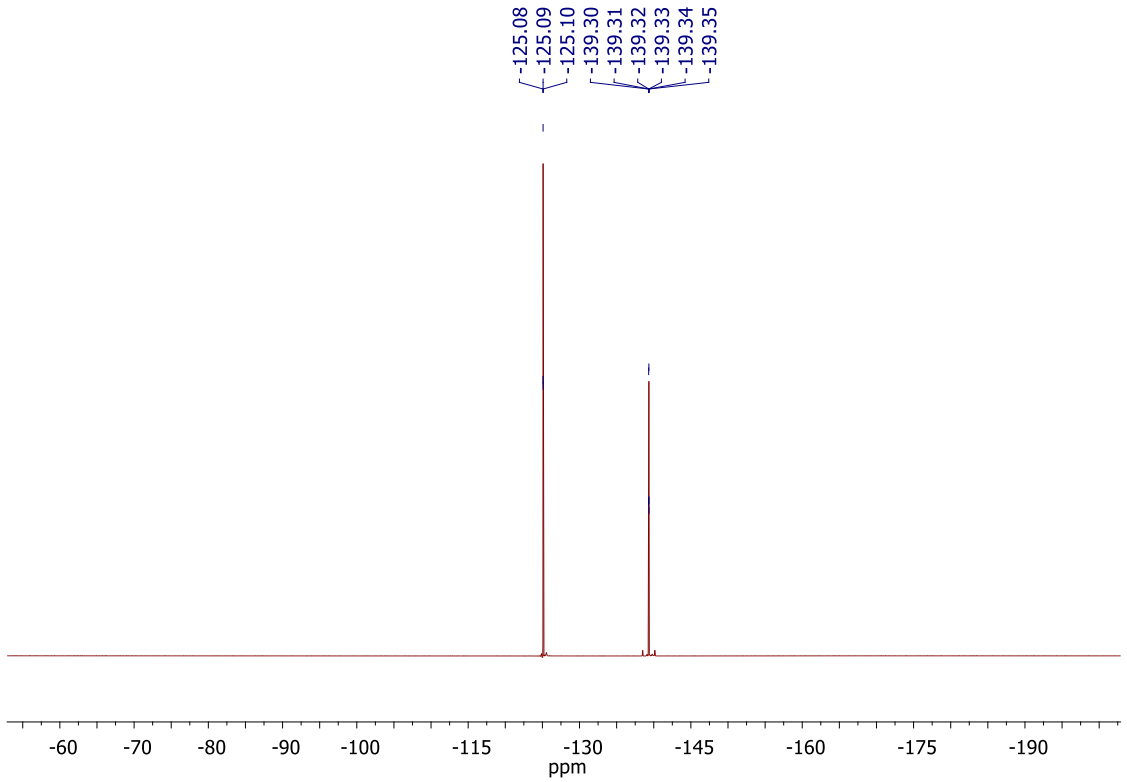
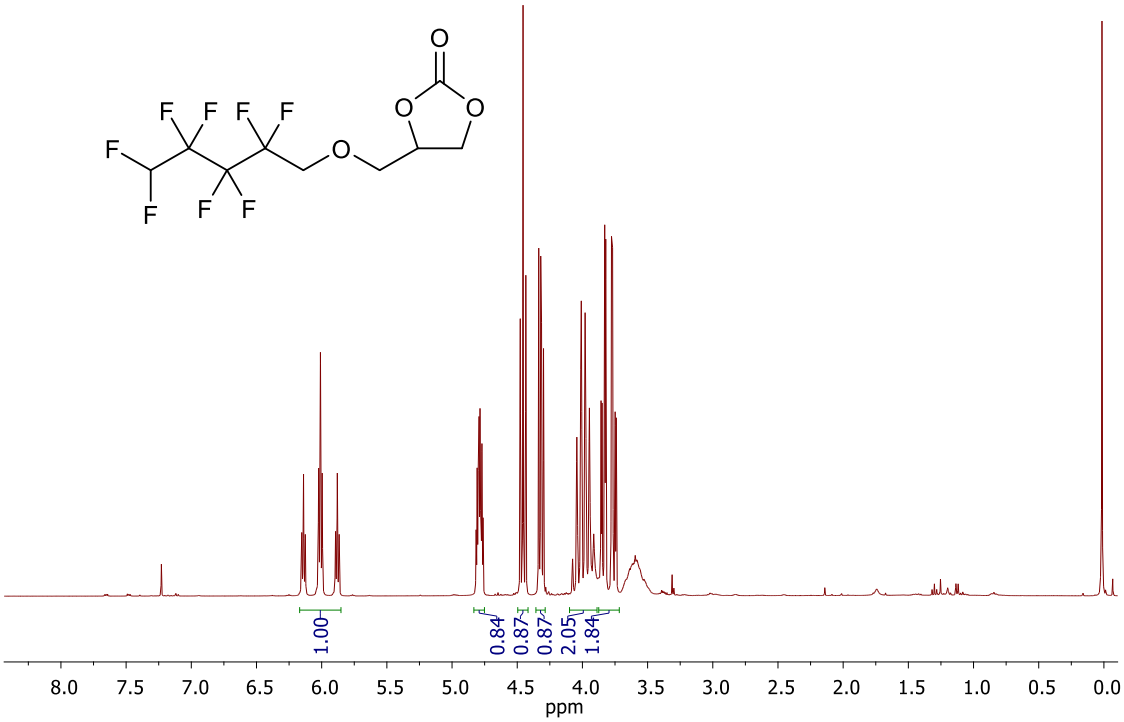


Figure S16. NMR spectra of 4-(((2,2,3,3,4,4,5,5-octafluoropentyl)oxy)methyl)-1,3-dioxolan- 2-one (**5h**) in $CDCl_3$



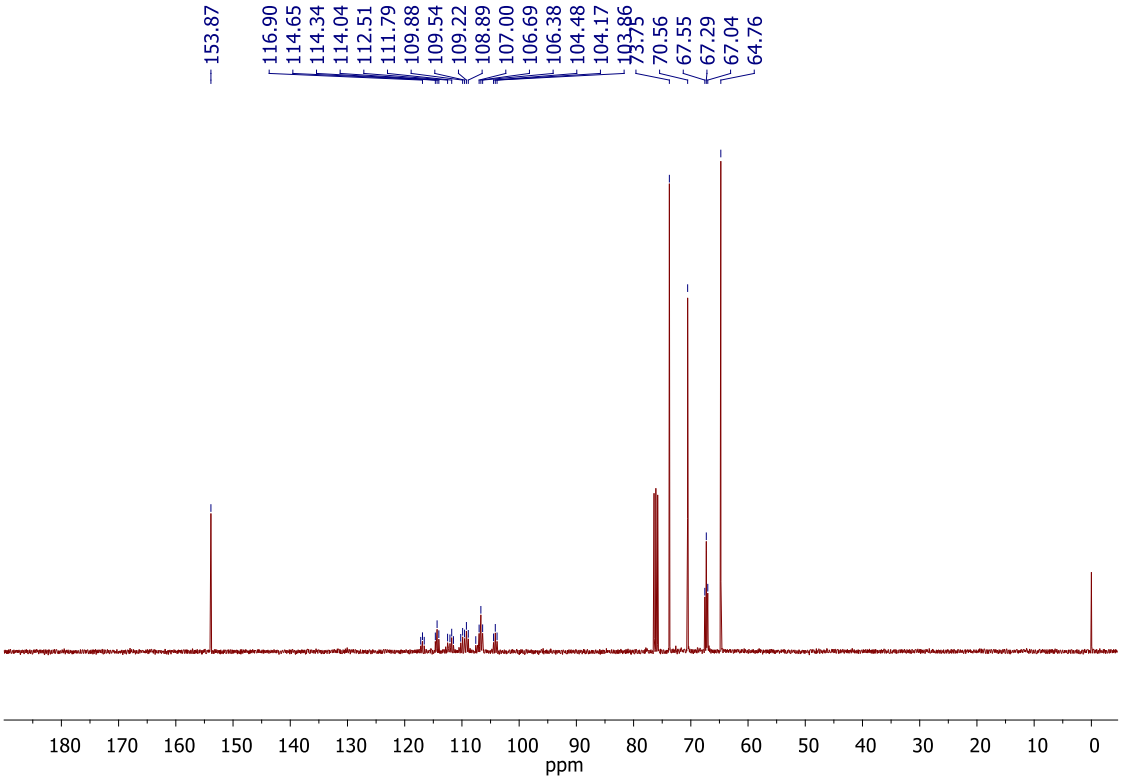


Figure S17. ^{19}F-NMR spectrum of 4-(((2,2,3,3,4,4,5,5-Octafluoropentyl)oxy)methyl)-1,3-dioxolan- 2-one (**5h**) in $CDCl_3$

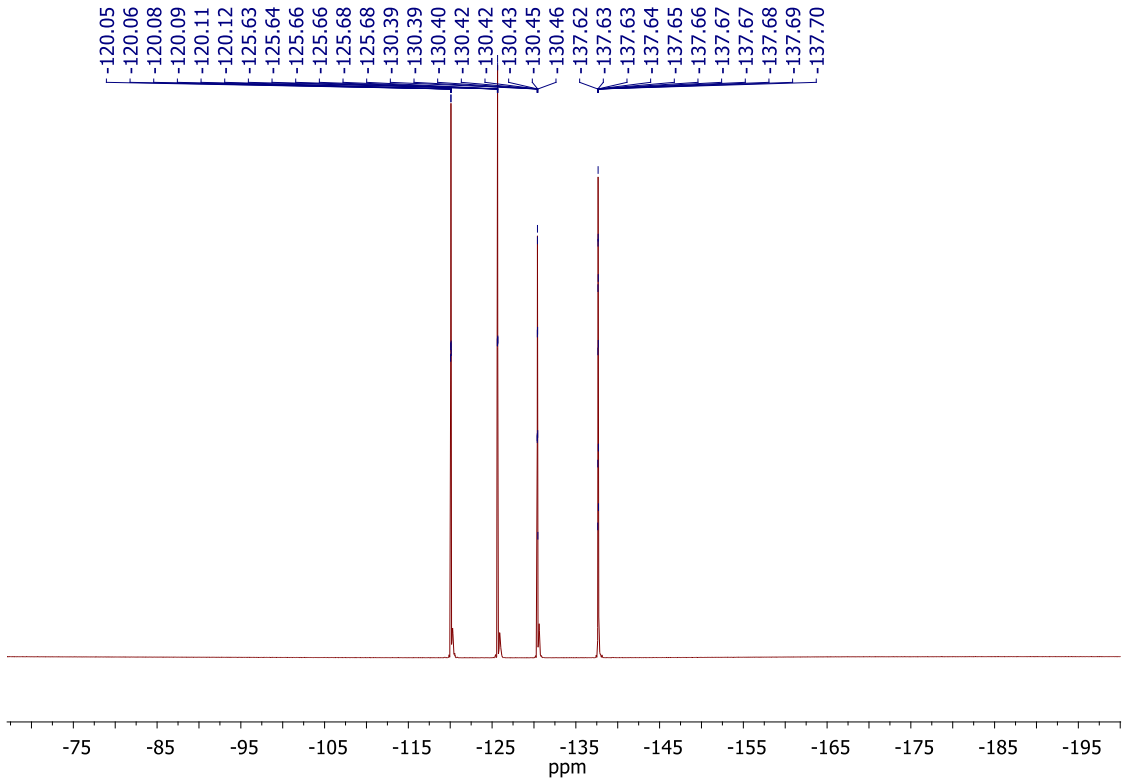


Figure S18. ^{1}H-NMR spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0) in $CDCl_3$

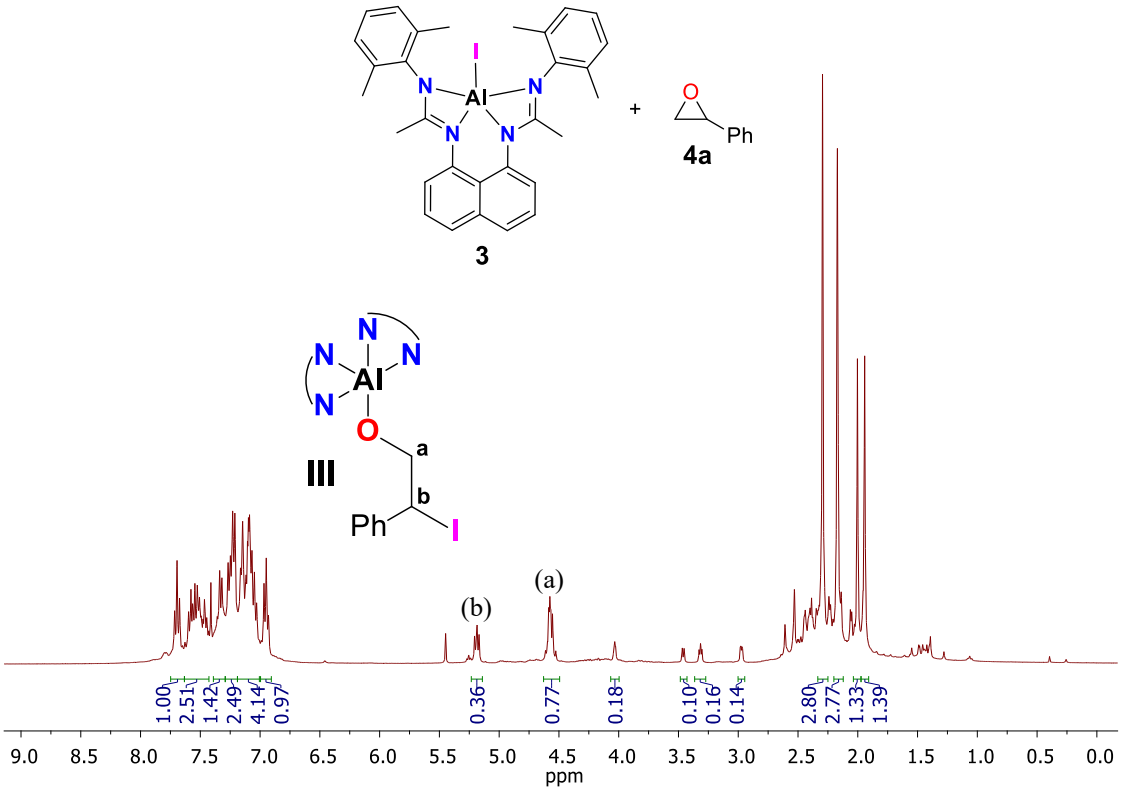


Figure S19. ^{13}C{^{1}H}-NMR spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0) in $CDCl_3$

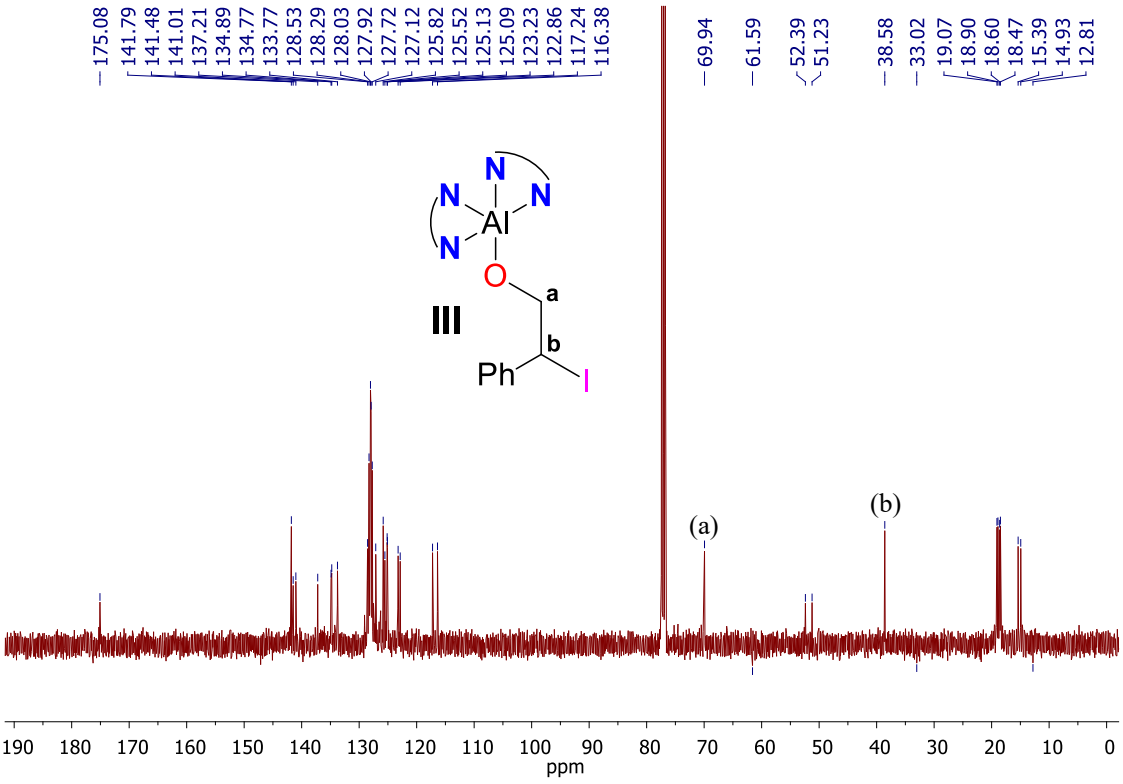


Figure S20. DEPT-135 spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0) in $CDCl_3$

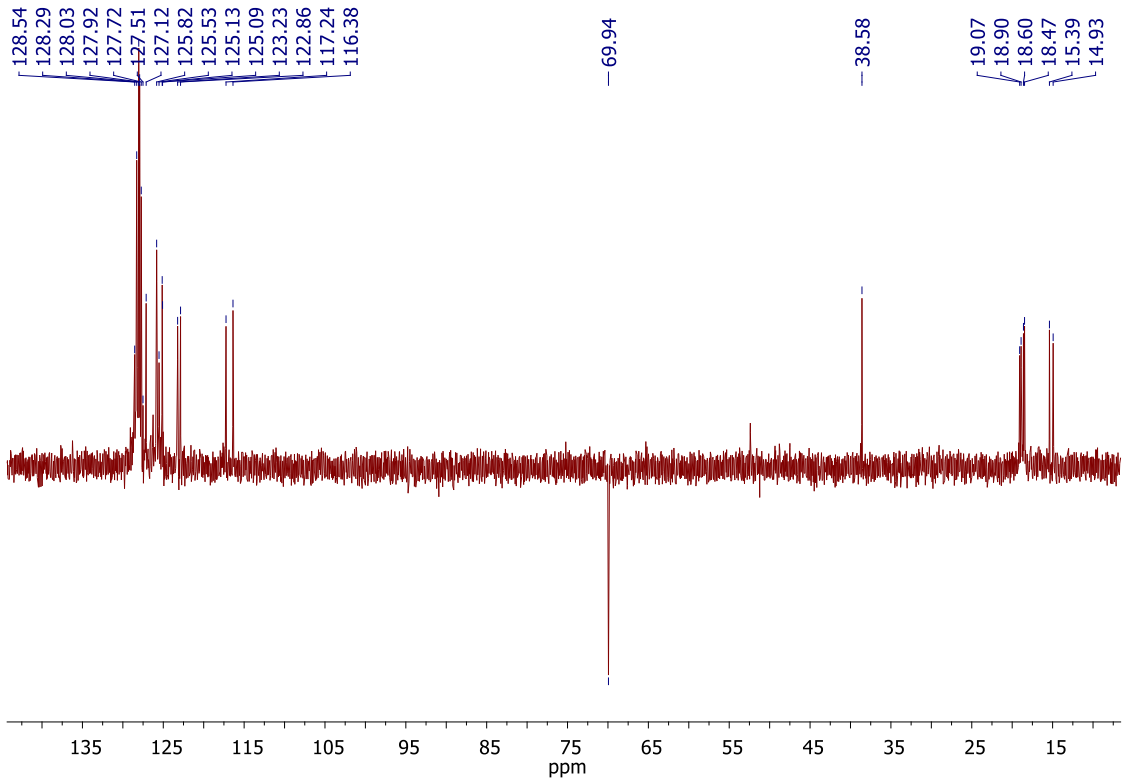


Figure S21. DEPT-135 spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0 in $CDCl_3$ (range 74.0–36.0 ppm)

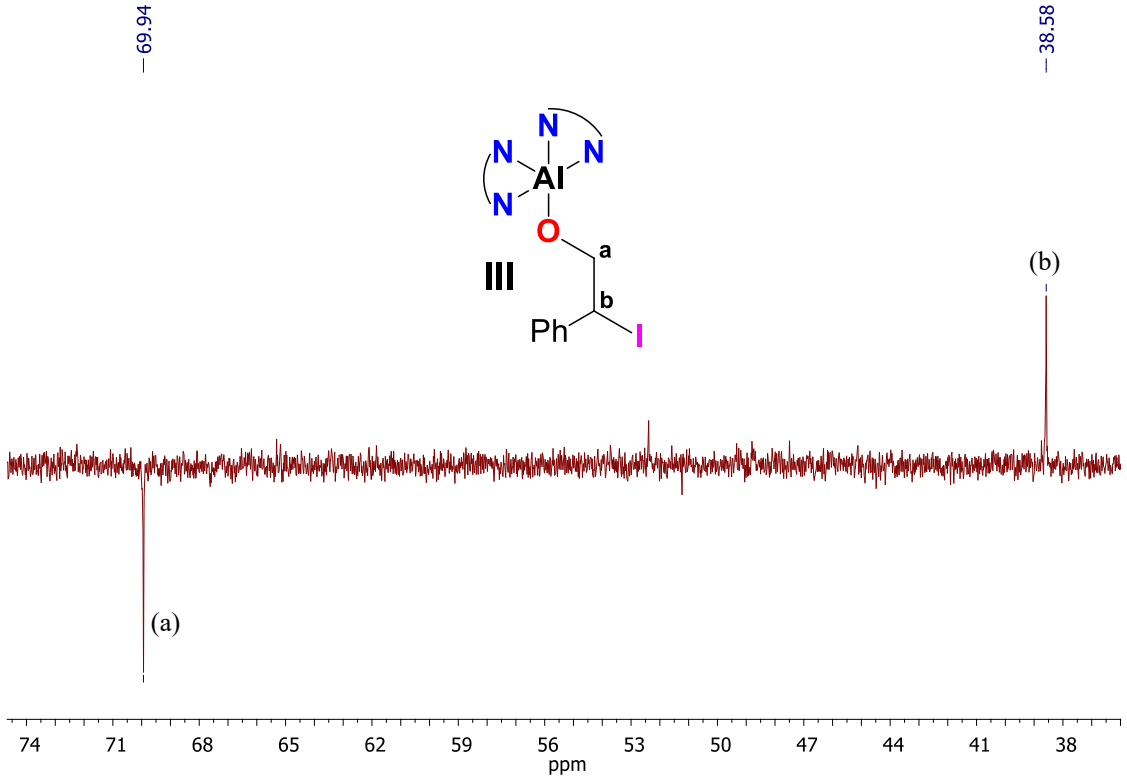


Figure S22. g-HSQC spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0) in $CDCl_3$

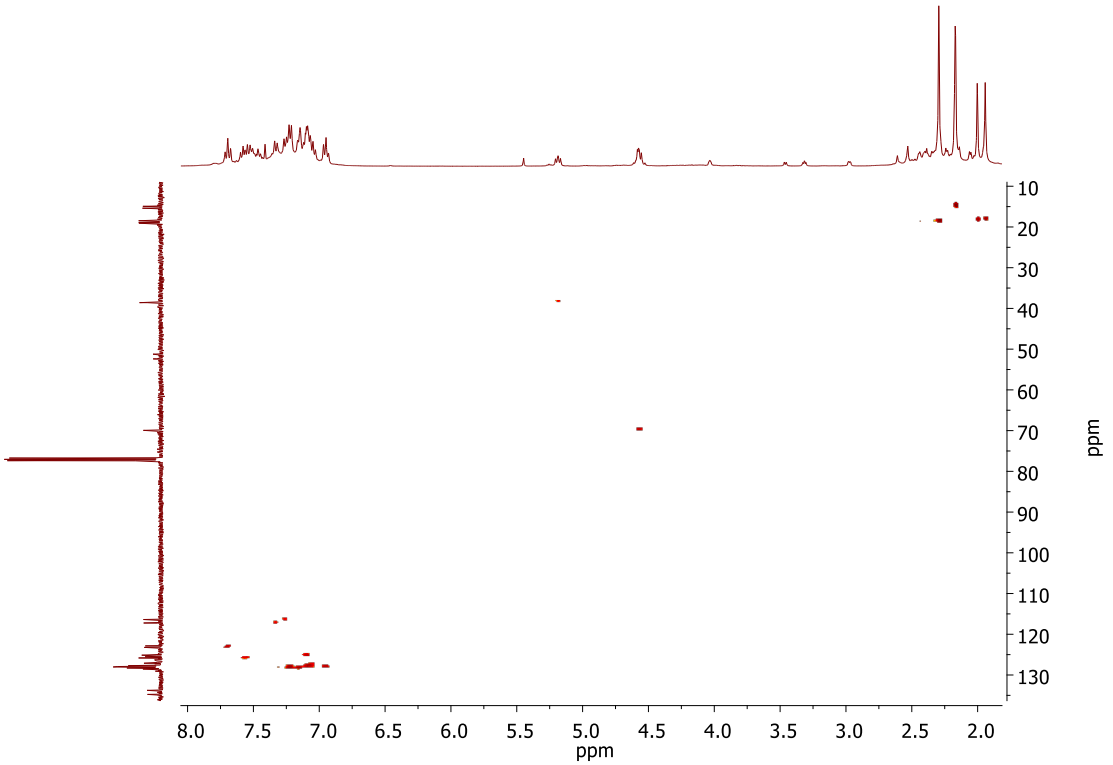
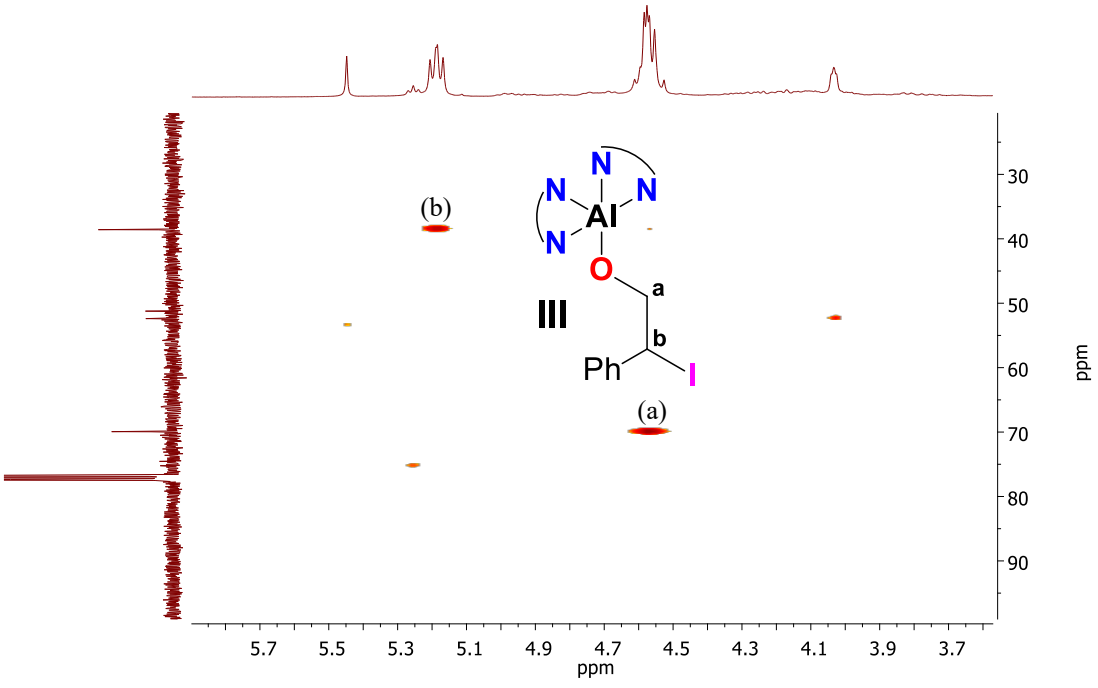


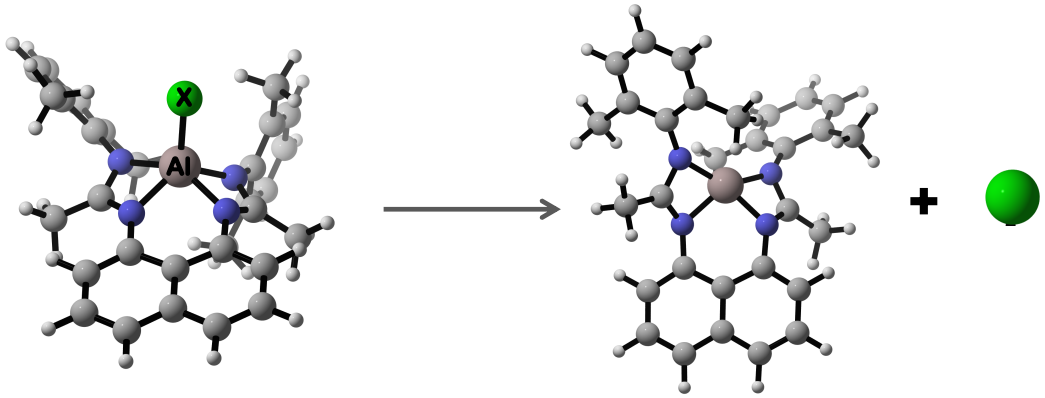
Figure S23. g-HSQC spectrum of complex **3** and styrene oxide **4a** in a molar ratio 1:1 at room temperature (t = 0) in $CDCl_3$ (range 5.9–3.6 ppm in ^{1}H-NMR and 100.0–20.0 ppm in ^{13}C-NMR)



Computational Section

Al–X Bond lengths and energies

Figure S24. Bond distances and dissociation energies for the chloride, bromide, and iodide catalyst computed at the B3LYP-D3/6-31G**.



bond distances
Al–Cl: 2.17 Å
Al–Br: 2.34 Å
Al–I: 2.55 Å

Al–X bond dissociation energies
Al–Cl: 135.3 kcal mol^{-1}
Al–Br: 118.0 kcal mol^{-1}
Al–I: 104.0 kcal mol^{-1}

XYZ coordinates for relevant structures

M06-2X/def2-TZVP

2

E = -1662.69011646 au

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4a

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C	1.268170	-1.517149	1.888097
C	1.737701	-2.792201	1.502152
C	2.948046	-3.251120	2.036219
C	3.697017	-2.465924	2.907432
C	3.230806	-1.202628	3.265711
C	2.015818	-0.717049	2.773651
H	3.310891	-4.231730	1.740951
H	3.806810	-0.582703	3.947326
C	0.022995	3.045094	0.561754
C	-0.013079	3.476995	1.899856
C	0.832495	4.523311	2.290122
C	1.673453	5.141703	1.369475
C	1.665226	4.730630	0.035333
C	0.840727	3.685484	-0.389071
H	0.820450	4.854308	3.324976
H	2.326142	5.950030	1.685510
H	2.303018	5.228198	-0.690245
Al	-0.820753	-0.007665	-0.137169
H	4.641668	-2.831448	3.298167
C	-0.978435	2.861421	2.881846
H	-0.649120	3.025633	3.911051
H	-1.977379	3.304481	2.782433
H	-1.088723	1.788590	2.716140
C	0.793221	3.263475	-1.833197
H	0.945648	2.187700	-1.938979
H	-0.183531	3.485012	-2.279626
H	1.550045	3.790678	-2.420261
C	1.499923	0.627713	3.197828
H	2.226417	1.146911	3.828383
H	1.285441	1.255831	2.332632
H	0.568655	0.531282	3.765531
C	0.992423	-3.646689	0.507806
H	0.137967	-4.164812	0.959351
H	0.614903	-3.050653	-0.325247
H	1.653243	-4.415207	0.099766

O	2.286096	0.962409	0.058540
C	3.441462	1.602652	0.608484
C	3.409584	1.185777	−0.807755
H	4.001982	0.994791	1.317137
H	3.304774	2.651090	0.867310
C	4.133562	−0.015301	−1.301165
C	4.852943	0.041981	−2.497657
C	4.104832	−1.207634	−0.570994
C	5.549143	−1.077835	−2.954429
C	4.794951	−2.325399	−1.028980
C	5.522262	−2.264258	−2.220599
H	4.862625	0.962214	−3.076342
H	3.519241	−1.257749	0.336320
H	6.103532	−1.025711	−3.886827
H	4.757286	−3.246385	−0.454893
H	6.057662	−3.138303	−2.579609
I	0.221044	−0.821130	−2.315572
H	3.244156	1.965622	−1.550279

TS1

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H	−2.190925	−3.843008	0.404115
H	−1.308465	−3.943093	1.945588
C	1.309866	−1.888987	1.769740
C	1.504086	−3.175205	2.257546
C	2.735986	−3.596589	2.787583
C	3.797799	−2.731890	2.854301
C	3.654453	−1.395189	2.405475
C	2.404149	−0.941194	1.857528
H	0.699667	−3.890606	2.226095
H	2.834568	−4.619508	3.137625
H	4.755553	−3.048212	3.255671
C	2.340134	0.440918	1.463794
C	3.438823	1.273229	1.590146
C	4.653495	0.804680	2.123004
C	4.755461	−0.505007	2.520495
H	3.362423	2.288158	1.218919
H	5.501144	1.478070	2.205297
H	5.683389	−0.889035	2.933707
N	1.157514	0.946809	0.899248
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C	0.418641	1.946737	1.368251
C	0.852437	2.949335	2.392364
H	1.418880	2.435628	3.174003
H	−0.013469	3.455271	2.820693
H	1.516215	3.697707	1.953150
C	−1.762956	2.918686	0.867335
C	−1.434894	4.174616	0.306881
C	−2.413032	5.177563	0.281653
C	−3.686814	4.960657	0.792111
C	−3.998788	3.720383	1.346319
C	−3.054850	2.694412	1.394137
H	−2.160226	6.140709	−0.154197
H	−4.988222	3.541753	1.757634
C	−3.167601	−1.600248	−0.117488
C	−4.068697	−1.898640	0.933268
C	−5.406289	−2.165386	0.621034
C	−5.856121	−2.149156	−0.694468
C	−4.957884	−1.869467	−1.720552
C	−3.612634	−1.595626	−1.456927
H	−6.097547	−2.387290	1.429686
H	−6.897304	−2.359146	−0.919807
H	−5.295565	−1.873885	−2.753182
Al	−0.395140	0.068531	0.147522
H	−4.431524	5.749914	0.760368
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H	−4.453854	−1.615411	3.030308

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H    -2.765449   -1.341330   2.583316
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H    -1.675809   -1.738016   -2.428246
H    -3.071868   -1.728545   -3.528682
H    -2.555095   -0.239580   -2.743199
C    -3.403760   1.368089   2.006613
H    -4.343569   1.428635   2.561009
H    -3.522158   0.596092   1.242353
H    -2.619146   1.027707   2.688321
C    -0.077074   4.492162   -0.272470
H    0.522307   5.095421   0.419765
H    0.508879   3.604546   -0.509464
H    -0.180998   5.082661   -1.188580
O    -0.292591   0.577112   -1.679016
C    -0.598841   1.638395   -2.611796
C    0.694042   0.939562   -2.735026
H    -0.642095   2.624422   -2.161303
H    -1.413132   1.386877   -3.284375
C    1.975917   1.574128   -2.332351
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C    2.160684   2.954728   -2.483354
C    4.250379   1.368898   -1.541033
C    3.382483   3.540819   -2.153591
C    4.427751   2.747189   -1.678244
H    2.880919   -0.292819   -1.762831
H    1.358957   3.571395   -2.876842
H    5.056958   0.748958   -1.164359
H    3.519086   4.610806   -2.277142
H    5.379825   3.201959   -1.420589
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II

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C    -0.520032   2.818072   2.011404
H    -1.019957   3.459275   1.270906
H    0.334012   3.352018   2.425823
H    -1.241310   2.567428   2.793232
C    -2.129436   0.171970   1.353648
C    -3.161313   1.087742   1.491550
C    -4.425318   0.687625   1.960280
C    -4.659053   -0.629544   2.271926
C    -3.647296   -1.609885   2.095670
C    -2.346128   -1.233616   1.614669
H    -2.994860   2.105855   1.159784
H    -5.213546   1.427465   2.060119
H    -5.629180   -0.951738   2.638597
C    -1.376207   -2.294561   1.408023
C    -1.729813   -3.609098   1.685703
C    -3.002726   -3.945769   2.181160
C    -3.943622   -2.968253   2.381659
H    -1.031166   -4.407025   1.480784
H    -3.234086   -4.986736   2.385649
H    -4.934694   -3.215598   2.750014
N    -0.140634   -1.973972   0.833090
N    1.902915   -1.795457   0.090702
C    1.021523   -2.617365   0.701434
C    1.384135   -3.980819   1.200526
H    1.031997   -4.098443   2.228834
H    2.464698   -4.121754   1.157989
H    0.907582   -4.758004   0.596056
C    3.131206   -2.218098   -0.476214
C    3.152303   -3.170300   -1.519179
C    4.383413   -3.524440   -2.083477
C    5.569502   -2.952404   -1.636935
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H    4.401279   -4.253819   -2.888903
H    6.458247   -1.557284   -0.258849
C    2.269279   2.198674   1.081829
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C    3.976917   3.079678   2.542293
C    4.511181   3.802250   1.477749
C    3.930946   3.710643   0.214495
C    2.805230   2.910147   -0.007969
H    4.437038   3.136426   3.524887
H    5.383535   4.430470   1.630986
H    4.349197   4.270257   -0.617210
Al    0.586151   -0.339292   0.110498
H    6.515814   -3.236771   -2.086520
C    2.313610   1.441536   3.503944
H    3.014021   1.436034   4.342712
H    1.356618   1.824175   3.875569
H    2.137582   0.405920   3.194993
C    2.180952   2.804353   -1.373393
H    1.116468   3.067569   -1.358895
H    2.690374   3.461768   -2.082155
H    2.246142   1.779151   -1.757458
C    4.310115   -0.595523   1.072881
H    5.311737   -0.437975   1.479679
H    3.952340   0.370946   0.706916
H    3.646419   -0.889411   1.890345
C    1.894545   -3.811813   -2.053558
H    1.726733   -4.804004   -1.617509
H    1.007407   -3.214049   -1.838349
H    1.963321   -3.951180   -3.136514
O    0.289358   -0.027266   -1.697456
C    0.280022   -0.472769   -3.067670
C    -0.996907   0.027771   -2.534560
H    0.443287   -1.538520   -3.194996
H    0.870519   0.170581   -3.714599
C    -2.104529   -0.833700   -2.077654
C    -3.295649   -0.200590   -1.694419
C    -2.000930   -2.230394   -1.992517
C    -4.370068   -0.961299   -1.238286
C    -3.070499   -2.982146   -1.518019
C    -4.256486   -2.347358   -1.140568
H    -3.350880   0.884784   -1.731576
H    -1.088568   -2.736652   -2.290473
H    -5.282198   -0.465177   -0.926468
H    -2.979134   -4.059819   -1.432687
H    -5.083572   -2.935602   -0.756759
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TS2

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Energy -2019.38548091 au
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C    4.120419   1.605751   -1.416541
H    4.106672   1.825370   -2.488755
H    4.965019   0.948785   -1.211851
H    4.236727   2.556913   -0.891189
C    1.491521   2.937808   -0.524133
C    1.896123   3.924902   -1.406469
C    1.738869   5.290769   -1.103321
C    1.158217   5.658742   0.084450
C    0.704090   4.681836   1.010409
C    0.860411   3.281336   0.725410
H    2.315718   3.624453   -2.360126
H    2.069558   6.041421   -1.814399
H    1.024003   6.706530   0.335627
C    0.347040   2.331384   1.694229
C    -0.280027   2.808759   2.839537
C    -0.403977   4.184140   3.103097
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H    -0.726287   2.114119   3.534644
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C    0.187800   -0.135120   2.139742
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H    0.640487   0.467828   4.131770
H    0.146223   -1.244000   3.954016
H    -1.059792   0.045428   3.882676
C    -0.182623   -2.503131   1.691510
C    -1.532732   -2.704678   2.060630
C    -1.962849   -4.012780   2.322001
C    -1.097755   -5.094586   2.224368
C    0.229056   -4.882489   1.853289
C    0.701142   -3.599099   1.579547
H    -3.003896   -4.170898   2.588194
H    0.913625   -5.722078   1.772714
C    3.707750   -1.308714   -0.928965
C    4.676992   -1.478622   0.076851
C    5.640733   -2.477731   -0.091613
C    5.638271   -3.288189   -1.225116
C    4.668572   -3.107388   -2.209579
C    3.689796   -2.117313   -2.079041
H    6.390912   -2.624620   0.680206
H    6.388795   -4.064380   -1.338631
H    4.664414   -3.741443   -3.091503
Al    0.844971   -0.049842   -0.175487
H    -1.455131   -6.099235   2.427720
C    4.655717   -0.621317   1.317407
H    5.329712   -1.022244   2.078081
H    4.966356   0.409755   1.111957
H    3.648650   -0.564769   1.742395
C    2.633424   -1.913601   -3.134547
H    2.708156   -0.917980   -3.587083
H    2.731391   -2.653894   -3.931887
H    1.624676   -1.984087   -2.715946
C    2.130619   -3.388791   1.166893
H    2.721133   -4.295693   1.315926
H    2.210895   -3.120941   0.109276
H    2.597690   -2.579450   1.732547
C    -2.564015   -1.604210   2.148873
H    -2.949053   -1.511310   3.170986
H    -2.180519   -0.627524   1.855458
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C    -1.712706   0.046629   -1.973434
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H    -1.765560   -2.136894   -1.866899
C    -1.983170   1.340641   -1.338213
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H    -1.301244   4.641512   -1.827975
H    -3.455641   2.755378   1.379352
H    -2.542887   4.802504   0.314525
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III

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C    3.913444   1.411442   -1.808468
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C	1.485539	5.134892	-1.717384
C	1.298816	5.592751	-0.436048
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C	1.147350	3.271298	0.413307
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C	0.886931	2.384900	1.532019
C	0.679053	2.945628	2.789140
C	0.709806	4.335461	3.002222
C	0.918863	5.197548	1.954835
H	0.427576	2.310703	3.624618
H	0.538478	4.718032	4.004097
H	0.919336	6.272842	2.104550
N	0.718143	1.023511	1.289922
N	0.350655	-1.120714	1.414138
C	0.634969	-0.025109	2.126455
C	0.986928	-0.051794	3.584453
H	1.889629	0.543851	3.745384
H	1.158960	-1.082327	3.898832
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C	-0.133192	-2.338663	1.931212
C	-1.189248	-2.384958	2.873991
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C	0.381268	-3.543727	1.392845
H	-2.448189	-3.664584	4.046754
H	0.306926	-5.680906	1.452214
C	3.505019	-1.434796	-1.100298
C	4.431775	-1.670721	-0.069108
C	5.390713	-2.671772	-0.250197
C	5.420163	-3.425262	-1.422852
C	4.486184	-3.185812	-2.429346
C	3.515280	-2.189163	-2.285807
H	6.111368	-2.865160	0.539581
H	6.166298	-4.204092	-1.548644
H	4.502779	-3.780491	-3.338569
Al	0.664840	-0.117192	-0.311306
H	-1.463961	-5.775554	3.196467
C	4.349642	-0.881205	1.213118
H	5.125228	-1.194902	1.916154
H	4.460078	0.194836	1.041258
H	3.373568	-1.021560	1.690486
C	2.488272	-1.923851	-3.357081
H	2.666748	-0.961427	-3.852581
H	2.516324	-2.701008	-4.125002
H	1.478244	-1.871908	-2.938352
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H	1.699522	-4.522986	0.003839
H	1.069918	-2.972144	-0.565596
H	2.338941	-3.010869	0.649062
C	-1.915762	-1.158319	3.372410
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H	-1.773296	-0.296608	2.719923
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C	-1.750978	-1.324167	-1.225115
C	-2.715204	-0.199253	-1.621029
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H	-1.937302	-2.199650	-1.858586
C	-2.604293	1.025505	-0.768776
C	-2.110964	2.211858	-1.325209
C	-2.903017	0.996632	0.600946
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C	-2.708518	2.125260	1.391994
C	-2.215609	3.304453	0.827144
H	-1.856815	2.238876	-2.380346
H	-3.312463	0.090183	1.033808
H	-1.509433	4.247624	-0.974994

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H    -2.942503   2.087295   2.451965
H    -2.039955   4.176605   1.447919
I    -4.801376   -1.046741   -1.598300
H    -2.573723   0.044607   -2.672722
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III+CO_2

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Energy -2208.03831565 au
C    -0.895031   -3.100713   -1.417444
O    -1.645462   -2.940529   -0.534193
O    -0.165221   -3.333615   -2.301537
N    -1.237336   0.235223   1.714906
N    0.440415   1.493413   1.106252
C    -0.340384   1.141222   2.127065
C    -0.249449   1.668562   3.524335
H    0.552271   1.133940   4.044767
H    -1.179408   1.503151   4.068162
H    0.008402   2.729887   3.515420
C    1.141954   2.693903   0.960596
C    2.157267   3.023666   1.845841
C    2.878833   4.225959   1.723500
C    2.582141   5.093389   0.702878
C    1.560081   4.795284   -0.238419
C    0.811608   3.570719   -0.139448
H    2.397803   2.322581   2.636733
H    3.668085   4.454387   2.433124
H    3.126355   6.026290   0.590981
C    -0.222341   3.319226   -1.132635
C    -0.439880   4.272026   -2.124129
C    0.299421   5.466282   -2.190531
C    1.282781   5.727416   -1.271035
H    -1.177261   4.090497   -2.890111
H    0.088082   6.172826   -2.987614
H    1.865439   6.642186   -1.317700
N    -0.909130   2.104711   -1.096336
N    -2.236014   0.386161   -1.340512
C    -1.973971   1.627537   -1.764425
C    -2.815363   2.324183   -2.791379
H    -3.132127   3.299878   -2.412578
H    -3.691929   1.718539   -3.023372
H    -2.252662   2.490235   -3.714501
C    -2.997671   -0.550309   -2.088049
C    -2.500093   -1.023116   -3.322578
C    -3.228731   -2.003239   -4.005382
C    -4.417177   -2.508968   -3.484833
C    -4.887691   -2.041470   -2.260230
C    -4.187212   -1.067835   -1.542716
H    -2.845114   -2.378353   -4.950005
H    -5.808001   -2.440285   -1.842788
C    -2.273936   -0.284171   2.528985
C    -3.416394   0.504801   2.768385
C    -4.457794   -0.041428   3.524940
C    -4.371823   -1.340144   4.022831
C    -3.235690   -2.107708   3.773280
C    -2.169676   -1.593990   3.027802
H    -5.346512   0.555383   3.710500
H    -5.191682   -1.754985   4.601585
H    -3.167502   -3.120191   4.161266
Al    -0.645714   0.429354   -0.134559
H    -4.968808   -3.271288   -4.026730
C    -3.524044   1.892397   2.187722
H    -4.537263   2.284374   2.305945
H    -2.838875   2.598850   2.670576
H    -3.274640   1.891509   1.122411
C    -0.925674   -2.397918   2.767529
H    -0.039252   -1.901836   3.171745
H    -0.996991   -3.389119   3.222617
H    -0.750001   -2.521264   1.696368
C    -4.672261   -0.609488   -0.196080
H    -5.673649   -0.994047   0.012720
H    -4.006968   -0.961470   0.597261
H    -4.699246   0.481292   -0.125064
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C    -1.186243   -0.531384   -3.879196
H    -1.265707   0.475204   -4.306386
H    -0.423980   -0.503659   -3.097739
H    -0.838471   -1.194284   -4.674556
O    0.374843   -0.803302   -0.844998
C    2.508054   -1.804982   -0.522719
C    1.730727   -0.663425   -1.174954
H    2.159625   -2.757361   -0.918736
H    2.143773   0.302972   -0.855020
H    1.862735   -0.728682   -2.262285
I    4.612320   -1.711949   -1.361268
C    2.560225   -1.825590   0.968702
C    2.772462   -0.657934   1.715138
C    2.416566   -3.042318   1.647679
C    2.834449   -0.711193   3.105305
C    2.484465   -3.098362   3.039033
C    2.693290   -1.930665   3.773769
H    2.904747   0.290455   1.208561
H    2.258824   -3.952407   1.075578
H    3.015780   0.198614   3.670979
H    2.371301   -4.050647   3.547877
H    2.750565   -1.969822   4.857360
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TS3

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Energy -2208.02075929 au
C    0.431990   0.609923   -2.469343
O    1.365070   0.927482   -1.752338
O    -0.090743   0.623989   -3.532595
N    1.612085   1.191203   1.157360
N    -0.355630   0.379048   1.625233
C    0.623094   1.171626   2.056524
C    0.645017   1.915248   3.356099
H    0.047540   2.827332   3.253587
H    1.661628   2.201177   3.626275
H    0.192873   1.312417   4.146546
C    -1.267414   -0.286667   2.456287
C    -2.208507   0.437619   3.173215
C    -3.146704   -0.194864   4.010087
C    -3.140887   -1.562245   4.120959
C    -2.196757   -2.350017   3.409515
C    -1.227704   -1.726043   2.547372
H    -2.213831   1.515917   3.067163
H    -3.871384   0.402702   4.554535
H    -3.857820   -2.071279   4.758051
C    -0.273416   -2.578760   1.855148
C    -0.344353   -3.954957   2.061980
C    -1.300597   -4.538638   2.911370
C    -2.213900   -3.758573   3.573071
H    0.334979   -4.612584   1.544383
H    -1.309739   -5.618182   3.029132
H    -2.959249   -4.199094   4.227875
N    0.627339   -1.993262   0.967448
N    2.107789   -1.536549   -0.563308
C    1.620414   -2.503060   0.221978
C    2.195548   -3.887963   0.245106
H    2.418884   -4.180964   1.274481
H    3.108441   -3.916835   -0.350726
H    1.491006   -4.616370   -0.165781
C    2.894078   -1.771819   -1.720394
C    2.355410   -2.498461   -2.805032
C    3.141006   -2.672972   -3.950177
C    4.420631   -2.133868   -4.034444
C    4.927514   -1.393920   -2.968237
C    4.176822   -1.195423   -1.807354
H    2.728563   -3.227382   -4.788701
H    5.919417   -0.955466   -3.033048
C    2.815754   1.922049   1.322029
C    3.847810   1.357402   2.097211
C    5.055066   2.052491   2.212535
C    5.233728   3.278988   1.575450
C    4.199128   3.828286   0.821038
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C    2.975426   3.164195   0.682923
H    5.860196   1.621733   2.801299
H    6.178315   3.806652   1.667931
H    4.335708   4.787556   0.329556
Al    0.775294   -0.216602   0.085321
H    5.014580   -2.275754   -4.932290
C    3.652089   0.022014   2.769874
H    4.594738   -0.347502   3.181273
H    2.931265   0.079620   3.593961
H    3.263504   -0.720228   2.067033
C    1.849706   3.757592   -0.121486
H    2.103153   4.765179   -0.461475
H    1.623231   3.140540   -0.994823
H    0.925476   3.816128   0.460547
C    4.717525   -0.367220   -0.675919
H    5.747042   -0.058115   -0.872211
H    4.118432   0.535247   -0.529097
H    4.699290   -0.915843   0.269767
C    0.952374   -3.056149   -2.774108
H    0.907912   -4.038303   -2.287820
H    0.269345   -2.391892   -2.241353
H    0.575529   -3.186827   -3.791502
O    -0.494688   -0.303121   -1.244114
C    -2.641825   0.632147   -1.832331
C    -1.890931   -0.556752   -1.228637
H    -2.457953   0.684315   -2.901512
H    -2.196095   -0.724963   -0.192230
H    -2.108135   -1.461120   -1.805810
I    -4.818836   0.086146   -1.753461
C    -2.372499   1.952213   -1.183816
C    -2.592238   2.160711   0.183662
C    -1.843727   2.996294   -1.953909
C    -2.291045   3.387779   0.766351
C    -1.536222   4.225062   -1.368591
C    -1.762114   4.425183   -0.007070
H    -3.016035   1.365171   0.785750
H    -1.660044   2.836796   -3.011661
H    -2.480906   3.543103   1.824672
H    -1.122394   5.023236   -1.976839
H    -1.531917   5.383355   0.448947
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IV

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Energy -2208.03949918 au
N    1.860142   1.395105   0.541915
N    0.637175   -0.194345   1.394247
C    1.107133   1.053557   1.590199
C    0.855403   1.971298   2.746279
H    -0.218323   2.148717   2.852486
H    1.361606   2.922842   2.583166
H    1.224592   1.525058   3.674056
C    -0.265900   -0.992937   2.089132
C    -0.786433   -0.642322   3.331749
C    -1.805807   -1.386852   3.952338
C    -2.318154   -2.506519   3.346964
C    -1.775368   -2.961714   2.116937
C    -0.714518   -2.233720   1.473412
H    -0.429051   0.243587   3.831694
H    -2.192469   -1.053684   4.910983
H    -3.121566   -3.074536   3.805191
C    -0.163653   -2.814284   0.271156
C    -0.681241   -3.987395   -0.249442
C    -1.743888   -4.663993   0.379821
C    -2.276657   -4.160071   1.539871
H    -0.261246   -4.365327   -1.175427
H    -2.134423   -5.577918   -0.056821
H    -3.088709   -4.672769   2.046474
N    0.878919   -2.155202   -0.394133
N    2.917830   -1.422737   -0.637495
C    2.159621   -2.513420   -0.445795
C    2.674641   -3.911484   -0.294234
H    2.222057   -4.378252   0.585227
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H    3.761132   -3.927337   -0.213913
H    2.377403   -4.504325   -1.164161
C    4.325856   -1.409261   -0.768091
C    4.883140   -1.119212   -2.027561
C    6.274313   -1.039787   -2.137270
C    7.092735   -1.239134   -1.026269
C    6.525211   -1.508516    0.216897
C    5.136779   -1.589009    0.369964
H    6.715789   -0.817954   -3.104758
H    7.161034   -1.641335    1.087855
C    2.381015   2.698578   0.323142
C    3.751403   2.933807   0.535634
C    4.256063   4.214316   0.287454
C    3.424100   5.236255   -0.163134
C    2.070548   4.984932   -0.376510
C    1.526808   3.717679   -0.143873
H    5.312914   4.404792   0.452216
H    3.829961   6.225760   -0.351123
H    1.420392   5.777285   -0.736671
Al    1.365775   -0.272574   -0.402921
H    8.171759   -1.172232   -1.127498
C    4.653437   1.825129   1.007951
H    5.653467   2.203757   1.233304
H    4.261176   1.338408   1.906608
H    4.754860   1.044691   0.248537
C    0.070558   3.442798   -0.416516
H    -0.461391   3.059611   0.458478
H    -0.441839   4.353295   -0.734821
H    -0.037334   2.696348   -1.207824
C    4.521306   -1.810852   1.729253
H    5.253233   -1.623329   2.518809
H    3.664247   -1.148982   1.884717
H    4.155950   -2.836100   1.859176
C    3.985283   -0.902248   -3.218238
H    4.570977   -0.668431   -4.110535
H    3.382364   -1.792243   -3.429587
H    3.274358   -0.087079   -3.048725
O    -1.201573   -0.239409   -1.108216
C    -3.460131   0.598650   -1.228357
C    -2.570222   -0.635010   -1.256991
H    -3.352613   1.148647   -2.160393
H    -2.767764   -1.310012   -0.424711
H    -2.699446   -1.166772   -2.200280
I    -5.576200   -0.177181   -1.388055
C    -3.317461   1.495631   -0.044781
C    -3.417908   2.881854   -0.226416
C    -3.077930   0.997236   1.243271
C    -3.285062   3.755011   0.851240
C    -2.947553   1.869596   2.321532
C    -3.050045   3.250248   2.131262
H    -3.602134   3.272908   -1.222961
H    -2.998737   -0.070303   1.413901
H    -3.361901   4.826077   0.691730
H    -2.771648   1.463414   3.312045
H    -2.951593   3.926591   2.975138
C    -0.546586   0.202861   -2.243253
O    -1.111198   0.391696   -3.296861
O    0.720638   0.381627   -1.960027
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TS4

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Energy -2207.99752773 au
N    1.551187   -1.129914   -1.215064
N    0.265424   0.616754   -1.426528
C    0.680982   -0.501788   -2.024703
C    0.281397   -0.999665   -3.374876
H    -0.691798   -1.493012   -3.294839
H    1.000497   -1.726945   -3.749667
H    0.180087   -0.163927   -4.071072
C    -0.290567   1.771344   -1.990250
C    -1.384706   1.682296   -2.838169
C    -1.972438   2.826577   -3.408403
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C	−1.464121	4.066492	−3.116838
C	−0.356343	4.214268	−2.240089
C	0.263028	3.061298	−1.642515
H	−1.806748	0.706571	−3.043401
H	−2.830688	2.718221	−4.063657
H	−1.906090	4.961988	−3.542368
C	1.388741	3.289472	−0.752043
C	1.806457	4.591939	−0.505117
C	1.188275	5.699875	−1.111813
C	0.129310	5.518514	−1.963684
H	2.608943	4.773467	0.193897
H	1.552113	6.697644	−0.887009
H	−0.362133	6.365161	−2.432493
N	1.975043	2.191375	−0.116810
N	3.191933	0.718390	0.936448
C	3.106631	2.011233	0.581434
C	4.168304	3.016052	0.901769
H	4.433707	3.575379	0.000723
H	5.049746	2.512715	1.300073
H	3.811742	3.733824	1.646654
C	4.090179	0.227848	1.923919
C	3.874360	0.551108	3.279596
C	4.755353	0.036167	4.235560
C	5.817642	−0.784744	3.864429
C	6.008414	−1.106223	2.523064
C	5.150916	−0.610491	1.536014
H	4.595405	0.277791	5.282463
H	6.832566	−1.750004	2.229356
C	2.075816	−2.425596	−1.467765
C	3.197061	−2.571725	−2.306337
C	3.720421	−3.855782	−2.498582
C	3.140855	−4.961866	−1.883179
C	2.021625	−4.799524	−1.067739
C	1.469744	−3.534724	−0.846313
H	4.590183	−3.981327	−3.137365
H	3.559525	−5.951375	−2.039527
H	1.564476	−5.663781	−0.594575
Al	1.487593	0.340601	0.051202
H	6.490948	−1.178021	4.619865
C	3.811070	−1.381344	−3.001237
H	4.846101	−1.588508	−3.284330
H	3.267507	−1.124620	−3.918760
H	3.797374	−0.493922	−2.364906
C	0.247955	−3.355698	0.018055
H	−0.573359	−2.883942	−0.531316
H	−0.112537	−4.319073	0.385144
H	0.451906	−2.719588	0.884089
C	5.349265	−0.972452	0.089464
H	6.292681	−1.504704	−0.054710
H	4.543558	−1.620943	−0.268318
H	5.354457	−0.085186	−0.550890
C	2.707088	1.408825	3.701177
H	2.598734	1.400580	4.788156
H	2.827185	2.455008	3.396367
H	1.773961	1.049461	3.259509
O	−1.472926	0.973213	1.192216
C	−3.112994	−0.740515	1.550233
C	−2.931703	0.763223	1.413202
H	−3.611460	−1.087506	2.441933
H	−3.433770	1.194377	0.555218
H	−3.208803	1.297146	2.319276
I	−6.090136	0.097228	1.550689
C	−3.278158	−1.581246	0.341431
C	−3.614306	−2.933195	0.494937
C	−2.998286	−1.086908	−0.939975
C	−3.685254	−3.773391	−0.611286
C	−3.094381	−1.925415	−2.048786
C	−3.430006	−3.271379	−1.889852
H	−3.838128	−3.313947	1.486235
H	−2.736514	−0.044628	−1.080398
H	−3.955671	−4.816266	−0.479921
H	−2.933623	−1.522297	−3.044687
H	−3.505348	−3.920933	−2.756281

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C    -0.814608   -0.100676   1.564750
O    -1.495164   -1.085339   1.996934
O    0.455412   -0.124762   1.481618
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V

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Energy -2208.00284267 au
N    2.065087   1.552261   0.297120
N    0.217627   0.727803   1.101616
C    0.998196   1.804374   1.087342
C    0.754922   3.081198   1.820650
H    -0.067132   3.615652   1.335221
H    1.640908   3.714951   1.818161
H    0.438718   2.864292   2.844867
C    -0.766716   0.333141   2.017854
C    -1.813403   1.185107   2.325601
C    -2.832875   0.797827   3.215031
C    -2.794295   -0.445942   3.792467
C    -1.749356   -1.361259   3.492061
C    -0.705319   -1.001033   2.570894
H    -1.868966   2.146949   1.833126
H    -3.649176   1.482387   3.419672
H    -3.573097   -0.763777   4.478523
C    0.304088   -2.004352   2.272420
C    0.239948   -3.239789   2.904322
C    -0.777505   -3.554647   3.823452
C    -1.757611   -2.639294   4.108330
H    0.969432   -4.000741   2.672043
H    -0.785699   -4.535709   4.287775
H    -2.559863   -2.876728   4.799662
N    1.273679   -1.712431   1.305316
N    2.907379   -1.587364   -0.137292
C    2.362878   -2.339454   0.839238
C    2.957743   -3.634189   1.293976
H    3.084716   -3.625099   2.379861
H    3.922314   -3.794259   0.811598
H    2.295830   -4.468479   1.042529
C    3.952258   -2.023411   -0.997451
C    3.663820   -2.942276   -2.026343
C    4.700920   -3.333263   -2.878802
C    5.987839   -2.823218   -2.722169
C    6.253402   -1.908342   -1.706241
C    5.244371   -1.493134   -0.831477
H    4.489489   -4.039929   -3.676112
H    7.255371   -1.507383   -1.583150
C    3.106925   2.471389   0.014397
C    4.094204   2.730067   0.985793
C    5.137420   3.602949   0.656513
C    5.204738   4.194762   -0.602183
C    4.225292   3.919035   -1.554948
C    3.165146   3.056249   -1.264267
H    5.906694   3.807937   1.395568
H    6.023280   4.865813   -0.843476
H    4.279084   4.377651   -2.538057
Al    1.492689   -0.275176   0.059051
H    6.781479   -3.135666   -3.393841
C    4.045270   2.067146   2.339990
H    5.009633   2.152903   2.846236
H    3.290991   2.518331   2.994681
H    3.796195   1.005687   2.253650
C    2.095201   2.761905   -2.283949
H    1.107533   3.064224   -1.918841
H    2.287944   3.295455   -3.217330
H    2.027739   1.692892   -2.510278
C    5.527952   -0.494550   0.258563
H    6.599520   -0.295988   0.336947
H    5.027361   0.458699   0.062417
H    5.173479   -0.847829   1.232077
C    2.266904   -3.477452   -2.219233
H    2.203768   -4.068842   -3.135337
H    1.952972   -4.124186   -1.391759
H    1.537553   -2.665060   -2.284088
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O    -1.395769   -1.112371   -0.595558
C    -2.838969   0.384566   -1.693297
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H    -3.548778   0.286469   -2.515102
H    -3.294133   -0.726268   0.176216
H    -3.279787   -1.742618   -1.300928
I    -6.088871   -0.935751   -1.638624
C    -2.961053   1.702334   -0.957515
C    -1.980215   2.694298   -1.061028
C    -4.098053   1.932721   -0.170520
C    -2.125960   3.901591   -0.373090
C    -4.234595   3.138224   0.515846
C    -3.249440   4.124344   0.424341
H    -1.112487   2.536460   -1.690116
H    -4.878150   1.174880   -0.131544
H    -1.368822   4.673598   -0.479579
H    -5.122070   3.307817   1.117691
H    -3.363993   5.064272   0.955967
C    -0.734990   -0.414553   -1.469802
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VI

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86
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C    -0.046495   1.702225   1.559480
C    0.239198   2.597499   2.723412
H    -0.051132   2.119581   3.659674
H    -0.271469   3.554145   2.601368
H    1.316266   2.792648   2.766980
C    -0.935588   3.333688   -0.001183
C    -0.168604   4.485476   0.029318
C    -0.732924   5.748781   -0.233045
C    -2.072020   5.845473   -0.517768
C    -2.896834   4.689641   -0.572984
C    -2.335451   3.384744   -0.346990
H    0.886723   4.388598   0.262780
H    -0.108560   6.636346   -0.198990
H    -2.531368   6.811826   -0.703432
C    -3.217711   2.231702   -0.454934
C    -4.575439   2.451261   -0.666801
C    -5.103600   3.741835   -0.853502
C    -4.283526   4.840799   -0.831875
H    -5.256040   1.615692   -0.705997
H    -6.169573   3.852958   -1.028115
H    -4.678289   5.838680   -0.995770
N    -2.658658   0.955619   -0.379547
N    -2.160195   -1.171111   -0.428812
C    -3.150196   -0.287416   -0.581462
C    -4.558469   -0.684257   -0.896893
H    -5.214040   -0.405793   -0.066020
H    -4.613145   -1.761887   -1.049124
H    -4.914611   -0.171108   -1.793764
C    -2.245585   -2.540212   -0.816920
C    -2.371290   -2.867103   -2.181632
C    -2.438611   -4.217319   -2.536715
C    -2.361648   -5.217362   -1.571956
C    -2.199787   -4.874650   -0.233140
C    -2.129834   -3.537963   0.164995
H    -2.529084   -4.479939   -3.586985
H    -2.104104   -5.650933   0.520128
C    0.118375   -0.349863   2.844270
C    -0.999670   -0.565072   3.673763
C    -0.827026   -1.295532   4.852130
C    0.428271   -1.788250   5.204109
C    1.526965   -1.541686   4.385461
C    1.395413   -0.816885   3.195275
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H    2.506831   -1.918851   4.663588
Al    -0.876031   0.275183   -0.125393
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H    -2.650935   -0.326786   2.297598
H    -3.114754   -0.337265   4.006433
H    -2.352746   1.088845   3.292651
C    2.583580   -0.570145   2.306983
H    3.513373   -0.796211   2.835950
H    2.517100   -1.218414   1.424305
H    2.626929   0.464681   1.954777
C    -1.888748   -3.176836   1.602970
H    -1.856317   -4.071542   2.228904
H    -0.927001   -2.665570   1.707352
H    -2.665829   -2.514546   1.995630
C    -2.371420   -1.803828   -3.252126
H    -1.525010   -1.123875   -3.125242
H    -2.291555   -2.263590   -4.240086
H    -3.284340   -1.196485   -3.252838
O    1.909061   -0.314656   -2.941260
C    3.506554   -0.013661   -1.213581
C    3.332334   -0.461768   -2.687349
H    3.729272   -0.882829   -0.591298
H    3.861622   0.166639   -3.403886
H    3.568371   -1.519596   -2.808830
I    1.606395   -3.007586   -0.633120
C    4.432256   1.136126   -0.957870
C    4.219516   2.376806   -1.572877
C    5.514379   0.973041   -0.089857
C    5.083866   3.439273   -1.323378
C    6.386447   2.035525   0.153547
C    6.171510   3.268257   -0.461855
H    3.368816   2.512767   -2.235219
H    5.669534   0.014330   0.396514
H    4.911593   4.399865   -1.798943
H    7.226987   1.900984   0.827061
H    6.846807   4.096512   -0.270275
C    1.320610   -0.007785   -1.809122
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TS5

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Energy -2208.00908498 au
N    0.111309   0.134493   1.659056
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C    0.905574   1.212752   1.620604
C    1.646780   1.756409   2.801949
H    1.116973   1.528922   3.728034
H    1.792731   2.832521   2.694781
H    2.633876   1.284989   2.857613
C    1.116570   3.093709   0.115027
C    2.412077   3.580668   0.088484
C    2.674470   4.947546   -0.128903
C    1.628110   5.819350   -0.302497
C    0.282183   5.363040   -0.292023
C    -0.006094   3.964715   -0.124230
H    3.223014   2.877179   0.248877
H    3.699646   5.305178   -0.141678
H    1.808422   6.880889   -0.444185
C    -1.395634   3.536505   -0.171869
C    -2.385591   4.513206   -0.238073
C    -2.078044   5.880787   -0.363787
C    -0.773720   6.301836   -0.421304
H    -3.425457   4.229037   -0.203081
H    -2.891176   6.597702   -0.428292
H    -0.527831   7.352143   -0.543648
N    -1.672322   2.169675   -0.180112
N    -2.499797   0.164455   -0.428424
C    -2.788443   1.468697   -0.464575
C    -4.156792   1.994309   -0.771616
H    -4.574793   2.479076   0.116094
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H    -4.811720   1.175018   -1.066365
H    -4.113085   2.737432   -1.571679
C    -3.382579   -0.856741   -0.886460
C    -3.656288   -0.969098   -2.263917
C    -4.513049   -1.987814   -2.691065
C    -5.068906   -2.885002   -1.783757
C    -4.764478   -2.775319   -0.430256
C    -3.917319   -1.768575   0.039143
H    -4.725895   -2.084260   -3.752074
H    -5.175090   -3.487323   0.279704
C    -0.053702   -0.658205   2.826250
C    -1.128759   -0.359002   3.684089
C    -1.323572   -1.156440   4.815371
C    -0.456497   -2.209598   5.098709
C    0.627181   -2.463584   4.261102
C    0.852063   -1.693550   3.115165
H    -2.156907   -0.941472   5.478478
H    -0.619553   -2.826159   5.977652
H    1.311617   -3.275280   4.490707
Al    -0.603899   0.544050   -0.091502
H    -5.724212   -3.677328   -2.133034
C    -2.017015   0.827701   3.406389
H    -2.397781   0.816656   2.383245
H    -2.868715   0.844303   4.091085
H    -1.472120   1.771929   3.528028
C    2.023668   -1.973635   2.212191
H    2.688326   -2.715787   2.662194
H    1.660619   -2.360476   1.253982
H    2.610869   -1.073327   2.003424
C    -3.563059   -1.684011   1.496962
H    -4.035436   -2.493894   2.057901
H    -2.481325   -1.769960   1.634074
H    -3.884285   -0.735208   1.938219
C    -3.008566   -0.054144   -3.272827
H    -1.921727   -0.058420   -3.160773
H    -3.249726   -0.378447   -4.288067
H    -3.340296   0.986509   -3.178181
O    1.382788   -0.985705   -3.189681
C    2.917285   -1.682805   -1.535501
C    2.625557   -1.727604   -3.052171
H    2.531853   -2.584929   -1.051688
H    3.385330   -1.224669   -3.653841
H    2.444804   -2.739979   -3.411544
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C    4.321750   -1.362585   -1.128399
C    4.887486   -0.116028   -1.426112
C    5.074320   -2.317662   -0.440892
C    6.196174   0.166169   -1.043154
C    6.389841   -2.038123   -0.067607
C    6.950961   -0.797213   -0.367797
H    4.294633   0.637943   -1.936098
H    4.626312   -3.275683   -0.193656
H    6.628204   1.136110   -1.269251
H    6.970060   -2.785114   0.464763
H    7.971945   -0.576624   -0.071914
C    1.085468   -0.455688   -2.022675
O    2.021287   -0.608475   -1.107004
O    0.069341   0.236177   -1.845648
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N    1.843638   1.847212   -0.481040
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C    0.577683   4.025729   -0.447447
H    -0.102481   4.305982   0.361680
H    0.141979   4.399620   -1.377936
H    1.551756   4.490195   -0.297168
C    -1.610364   1.985667   -0.043580
C    -2.485106   2.775688   -0.765925
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C    -4.100759   2.712081   1.007424
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H    -2.176420   3.110261   -1.750806
H    -4.414968   3.753714   -0.834591
H    -5.062617   2.983637   1.430640
C    -1.172562   0.532723   2.030991
C    -1.637305   0.156757   3.286254
C    -2.870601   0.605185   3.793697
C    -3.670834   1.436527   3.052403
H    -1.062319   -0.523549   3.892013
H    -3.186632   0.267308   4.776189
H    -4.635723   1.767685   3.424002
N    -0.000970   0.019535   1.470931
N    1.765550   -1.124083   0.897497
C    0.850605   -0.951523   1.858315
C    0.839194   -1.744989   3.125372
H    0.934927   -1.081601   3.989609
H    1.667234   -2.453774   3.129073
H    -0.108097   -2.285221   3.197431
C    2.781517   -2.119605   0.906419
C    2.461347   -3.470028   0.653538
C    3.500309   -4.407399   0.637340
C    4.820940   -4.027275   0.858028
C    5.121525   -2.689669   1.099868
C    4.114513   -1.720503   1.125794
H    3.260526   -5.448558   0.440933
H    6.149614   -2.384122   1.273455
C    3.128088   2.436043   -0.379792
C    3.552075   2.958026   0.858726
C    4.848226   3.474205   0.955212
C    5.704836   3.465287   -0.143327
C    5.272773   2.935840   -1.357879
C    3.983192   2.413039   -1.496502
H    5.188481   3.872347   1.907107
H    6.710852   3.863362   -0.051025
H    5.941377   2.923075   -2.213994
Al    0.853570   0.183625   -0.265124
H    5.612780   -4.770209   0.839013
C    2.645894   2.922523   2.064088
H    3.216561   3.092070   2.980471
H    1.866084   3.691495   2.017901
H    2.131265   1.960941   2.146823
C    3.512401   1.827547   -2.801804
H    4.273916   1.941859   -3.577133
H    3.278676   0.762871   -2.704030
H    2.592101   2.308415   -3.148875
C    4.454844   -0.276470   1.374822
H    5.488980   -0.170469   1.711625
H    4.341618   0.322988   0.467463
H    3.801305   0.170366   2.128991
C    1.045364   -3.912520   0.396017
H    0.583480   -3.306810   -0.387425
H    1.026247   -4.955685   0.071243
H    0.408847   -3.831512   1.280933
O    -2.824382   -3.366776   -0.464745
C    -2.958333   -1.155697   -1.229114
C    -3.062917   -2.629257   -1.679135
H    -2.364133   -0.571122   -1.933036
H    -4.050107   -2.894520   -2.057270
H    -2.285254   -2.886607   -2.402946
I    0.649232   -1.140883   -2.481150
C    -4.282440   -0.489570   -0.948262
C    -4.900131   -0.585949   0.301151
C    -4.922857   0.203171   -1.980539
C    -6.152807   -0.009223   0.507415
C    -6.176290   0.776496   -1.774523
C    -6.796137   0.667759   -0.528472
H    -4.390644   -1.072132   1.125348
H    -4.432916   0.300664   -2.946069
H    -6.618643   -0.079505   1.485555
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C    -2.238527   -2.554528   0.441172
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V+4a

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C    2.258208   -2.557903   0.362442
H    3.935557   -2.983874   1.735415
H    4.350771   -1.814983   0.370176
H    2.078958   -2.203987   -0.649443
C    1.396484   -3.691199   0.791083
C    0.841339   -4.530396   -0.177009
C    1.112403   -3.915724   2.139481
C    0.014862   -5.583859   0.203029
C    0.280042   -4.964549   2.516834
C    -0.272125   -5.802412   1.548949
H    1.020608   -4.326295   -1.225867
H    1.528539   -3.247963   2.883458
H    -0.414150   -6.227756   -0.556665
H    0.059426   -5.127914   3.566075
H    -0.921125   -6.619803   1.842958
N    0.092045   1.585827   2.068460
N    2.165187   1.565737   1.417995
C    1.361714   1.739178   2.475467
C    1.743997   2.055543   3.883273
H    2.511066   1.362294   4.233016
H    0.872376   2.003452   4.532934
H    2.156002   3.066535   3.932603
C    3.549393   1.517834   1.248462
C    4.430340   2.010459   2.199091
C    5.822133   1.862989   2.070680
C    6.350952   1.216294   0.987020
C    5.505243   0.731145   -0.042760
C    4.083681   0.906921   0.041696
H    4.047125   2.519170   3.069180
H    6.468548   2.256133   2.846771
H    7.420840   1.073382   0.890344
C    3.308453   0.453043   -1.088661
C    3.903813   -0.210000   -2.142859
C    5.296159   -0.406332   -2.180045
C    6.078738   0.069847   -1.161081
H    3.262286   -0.596941   -2.925379
H    5.740244   -0.930508   -3.018026
H    7.155331   -0.054626   -1.185115
N    1.929234   0.683042   -1.099046
N    0.132551   1.910417   -1.247166
C    1.256681   1.525307   -1.878453
C    1.668386   1.986257   -3.229940
H    1.325290   1.229872   -3.943915
H    2.754571   2.049268   -3.299793
H    1.207672   2.941981   -3.476818
C    -0.713567   2.965956   -1.684481
C    -1.813721   2.738395   -2.523341
C    -2.641870   3.823337   -2.837909
C    -2.385189   5.095183   -2.349791
C    -1.273434   5.312342   -1.539948
C    -0.425979   4.260966   -1.201656
H    -3.498194   3.653596   -3.482116
H    -1.058002   6.307774   -1.167412
C    -1.044917   1.340603   2.873310
C    -2.164887   2.177894   2.697501
C    -3.330615   1.901577   3.409687
C    -3.403306   0.807482   4.265999
C    -2.305261   -0.031075   4.404740
C    -1.113592   0.209200   3.712736
H    -4.190193   2.549717   3.281053
H    -4.316035   0.602774   4.813886
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H    -2.366946   -0.900729   5.049804
Al    0.707049   0.958028   0.323749
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C    -2.109887   3.333665   1.736835
H    -2.017108   2.990233   0.703462
H    -3.015714   3.937553   1.803485
H    -1.249827   3.977381   1.931625
C    0.033258   -0.758821   3.862532
H    0.620468   -0.861606   2.951506
H    0.714404   -0.456563   4.665020
H    -0.347023   -1.748710   4.118810
C    0.780565   4.501648   -0.331865
H    0.860530   5.557819   -0.070075
H    0.728437   3.925321   0.594933
H    1.707410   4.206798   -0.831812
C    -2.118305   1.385743   -3.107378
H    -2.109197   1.433230   -4.200273
H    -1.405306   0.622635   -2.807183
H    -3.119455   1.060979   -2.807925
O    -1.465589   -2.441942   0.285679
C    -3.123269   -1.393076   -1.028682
C    -2.631881   -2.770128   -0.514173
H    -3.088312   -1.366260   -2.116543
H    -3.342360   -3.273302   0.136256
H    -2.284289   -3.402764   -1.328750
I    0.001450   -1.993217   -3.045785
C    -4.435198   -0.915759   -0.479394
C    -4.539391   -0.467431   0.840927
C    -5.569526   -0.942265   -1.290092
C    -5.770212   -0.058357   1.340261
C    -6.803995   -0.541719   -0.784119
C    -6.905302   -0.099257   0.531673
H    -3.664568   -0.412738   1.477858
H    -5.485157   -1.271646   -2.320042
H    -5.836935   0.297576   2.360824
H    -7.680632   -0.564826   -1.420481
H    -7.863347   0.220736   0.924246
C    -1.144665   -1.198557   0.057413
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O    -0.122708   -0.689853   0.525203
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TS5’

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C    2.468622   0.255085   2.402581
C    1.929818   -1.053916   2.019529
H    2.450491   0.557137   3.446714
H    3.229046   0.714411   1.779282
H    2.297345   -1.462168   1.076193
C    1.357851   -2.031442   2.976593
C    1.553001   -3.393236   2.706276
C    0.679231   -1.642686   4.141218
C    1.079441   -4.353037   3.602887
C    0.199192   -2.606106   5.024348
C    0.401766   -3.964088   4.758242
H    2.094855   -3.688341   1.808695
H    0.510549   -0.590644   4.350160
H    1.242717   -5.405670   3.391964
H    -0.331515   -2.299646   5.921304
H    0.031585   -4.713563   5.452316
N    -0.742851   2.319655   0.721321
N    1.264325   2.865815   0.057668
C    0.133062   3.330597   0.604741
C    -0.162000   4.725549   1.080171
H    0.690497   5.127177   1.633230
H    -1.049401   4.731625   1.713252
H    -0.347966   5.389070   0.229008
C    2.480895   3.498625   -0.243563
C    2.622111   4.883580   -0.287204
C    3.876756   5.500820   -0.460914
C    5.010763   4.741523   -0.600527
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C	4.922128	3.324844	-0.645901
C	3.645361	2.673645	-0.515695
H	1.755502	5.519800	-0.188027
H	3.933526	6.585599	-0.469400
H	5.986423	5.207048	-0.706201
C	3.618953	1.243389	-0.706589
C	4.791957	0.527137	-0.889521
C	6.037053	1.185005	-0.951375
C	6.098307	2.553645	-0.850202
H	4.733812	-0.556992	-0.969052
H	6.939357	0.597970	-1.094350
H	7.048060	3.075596	-0.929791
N	2.373476	0.580793	-0.708091
N	0.462650	-0.048070	-1.555053
C	1.798530	0.007170	-1.761296
C	2.499505	-0.487772	-2.982213
H	2.956968	-1.457593	-2.733427
H	3.309826	0.192967	-3.254851
H	1.810045	-0.614357	-3.817739
C	-0.442993	-0.681164	-2.456426
C	-0.705638	-2.066372	-2.353609
C	-1.627322	-2.633856	-3.247143
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C	-1.989818	-0.502716	-4.312873
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H	-1.819573	-3.702477	-3.188752
H	-2.473059	0.098811	-5.078395
C	-2.031206	2.473843	1.318760
C	-3.150743	2.728970	0.498830
C	-4.406562	2.881843	1.099215
C	-4.562715	2.778327	2.479616
C	-3.451540	2.523004	3.279932
C	-2.177176	2.372250	2.720336
H	-5.268020	3.084237	0.468654
H	-5.543050	2.904354	2.930863
H	-3.564787	2.446418	4.358171
Al	0.613831	0.983368	0.097776
H	-2.976668	-2.326011	-4.900182
C	-3.015126	2.830124	-0.999234
H	-2.730720	1.864996	-1.429061
H	-3.962198	3.133539	-1.453362
H	-2.252422	3.557439	-1.295979
C	-0.986894	2.120947	3.612412
H	-0.273681	2.954180	3.585842
H	-1.303320	1.994789	4.651302
H	-0.445683	1.226200	3.297162
C	-0.709191	1.559397	-3.631141
H	-1.403060	2.049088	-4.319943
H	-0.718843	2.107154	-2.685993
H	0.300236	1.668575	-4.046201
C	0.005536	-2.939790	-1.351080
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H	-0.034655	-2.526624	-0.340610
H	-0.437125	-3.939477	-1.328547
O	-2.558826	-2.279409	0.961991
C	-4.111354	-1.598261	-0.648090
C	-3.894175	-2.582941	0.514802
H	-3.768928	-2.031639	-1.592267
H	-4.590151	-2.411545	1.341632
H	-3.929862	-3.628910	0.208656
I	3.928462	-3.371610	-0.568093
C	-5.506440	-1.055924	-0.788583
C	-6.075291	-0.248057	0.205792
C	-6.264022	-1.396005	-1.914512
C	-7.386551	0.205351	0.072436
C	-7.580881	-0.950333	-2.041402
C	-8.143799	-0.149450	-1.047529
H	-5.485916	0.049597	1.067740
H	-5.820422	-2.007929	-2.695584
H	-7.818693	0.836479	0.843437
H	-8.161081	-1.222521	-2.917946
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C	-2.211185	-1.065130	0.503543

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O    -3.149361   -0.551925   -0.309166
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II+5a

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C    2.740638   0.636697   2.044516
C    2.236740   -0.728664   1.843872
H    2.872002   1.013892   3.054495
H    3.336601   1.097175   1.264486
H    2.490856   -1.179099   0.883085
C    1.880079   -1.659171   2.938014
C    2.302177   -2.990142   2.834101
C    1.140557   -1.240646   4.050929
C    1.993549   -3.891807   3.852912
C    0.829677   -2.149000   5.059220
C    1.258543   -3.475730   4.963424
H    2.875098   -3.299516   1.962531
H    0.791240   -0.214974   4.110355
H    2.326385   -4.922041   3.772805
H    0.249275   -1.824699   5.917942
H    1.015942   -4.182116   5.751963
N    -1.119854   2.173285   0.317248
N    0.940686   2.856815   0.155028
C    -0.315662   3.257574   0.253844
C    -0.841995   4.661278   0.249395
H    -0.774825   5.099568   1.250836
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H    -0.249124   5.281578   -0.426423
C    2.110533   3.578133   -0.097766
C    2.280342   4.874611   0.374988
C    3.470478   5.592154   0.150870
C    4.513206   5.001864   -0.517811
C    4.415927   3.660055   -0.971970
C    3.200437   2.916169   -0.778020
H    1.497365   5.331886   0.965028
H    3.558960   6.606675   0.527673
H    5.441438   5.539046   -0.687817
C    3.170074   1.549575   -1.246342
C    4.314866   0.977094   -1.786892
C    5.487543   1.730641   -1.974758
C    5.534662   3.049708   -1.595530
H    4.328247   -0.086402   -1.990747
H    6.359502   1.245746   -2.402338
H    6.436818   3.638796   -1.731137
N    2.003152   0.803185   -1.064338
N    0.261792   -0.459573   -1.325435
C    1.466997   -0.132920   -1.839160
C    2.043818   -0.733770   -3.073628
H    2.735023   -1.532293   -2.765121
H    2.614460   0.013134   -3.629601
H    1.263835   -1.167000   -3.699561
C    -0.571971   -1.439787   -1.923847
C    -0.572724   -2.763805   -1.433074
C    -1.411075   -3.701025   -2.055397
C    -2.217191   -3.349059   -3.137102
C    -2.207130   -2.036129   -3.608156
C    -1.388134   -1.069379   -3.012877
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H    -2.825180   -1.755626   -4.456971
C    -2.425995   2.286983   0.875615
C    -3.555125   2.408475   0.045164
C    -4.812051   2.568791   0.636926
C    -4.959118   2.577950   2.021417
C    -3.837477   2.433248   2.835168
C    -2.560275   2.299150   2.280128
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H    -5.943077   2.700321   2.465020
H    -3.944408   2.442102   3.916446
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H    -2.848122   -4.094510   -3.612297
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C    -3.432121   2.331352   -1.451634
H    -3.285431   1.292134   -1.759812
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H    -2.577507   2.900941   -1.825370
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H    -0.635351   2.991098   3.005770
H    -1.643047   2.203292   4.224673
H    -0.813216   1.243760   2.984491
C    -1.334867   0.333158   -3.561189
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H    -1.258687   1.068926   -2.759466
H    -0.457325   0.471468   -4.204151
C    0.343474   -3.187173   -0.317982
H    1.394420   -3.165083   -0.636124
H    0.269679   -2.531728   0.550884
H    0.113963   -4.205226   0.005898
O    -2.337106   -2.200719   1.457870
C    -3.738648   -1.673589   -0.346092
C    -3.603816   -2.588383   0.881813
H    -3.330345   -2.156374   -1.231781
H    -4.386562   -2.426689   1.626548
H    -3.547912   -3.643188   0.614221
I    4.261332   -2.722838   -0.635116
C    -5.101873   -1.122727   -0.626091
C    -5.843071   -0.475221   0.368354
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H    -7.319241   -0.869866   -3.197092
H    -8.639720   0.258992   -1.420752
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O    -0.917602   -0.481648   1.236745
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5a

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Energy -573.501971642 au
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C    -2.602123   0.786624   0.556034
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H    -2.889225   0.474559   -0.448284
H    -3.086416   1.735757   0.807762
C    -3.005860   -1.694282   1.046896
C    -1.934940   -2.589510   1.007222
C    -4.238502   -2.069238   0.500920
C    -2.095774   -3.844115   0.417695
C    -4.396632   -3.320842   -0.089834
C    -3.322521   -4.211648   -0.133722
H    -0.985018   -2.314057   1.450958
H    -5.079314   -1.380476   0.540728
H    -1.259340   -4.535507   0.393242
H    -5.357549   -3.603209   -0.508537
H    -3.444473   -5.188894   -0.590090
C    -0.696595   0.451739   1.762651
O    -1.687238   -0.191449   2.446330
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