# Supplementary Materials: Synthesis and Characterization of a Sulfonyl- and Iminophosphoryl-Functionalized Methanide and Methandiide

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1. NMR Spectra of the Isolated Compounds
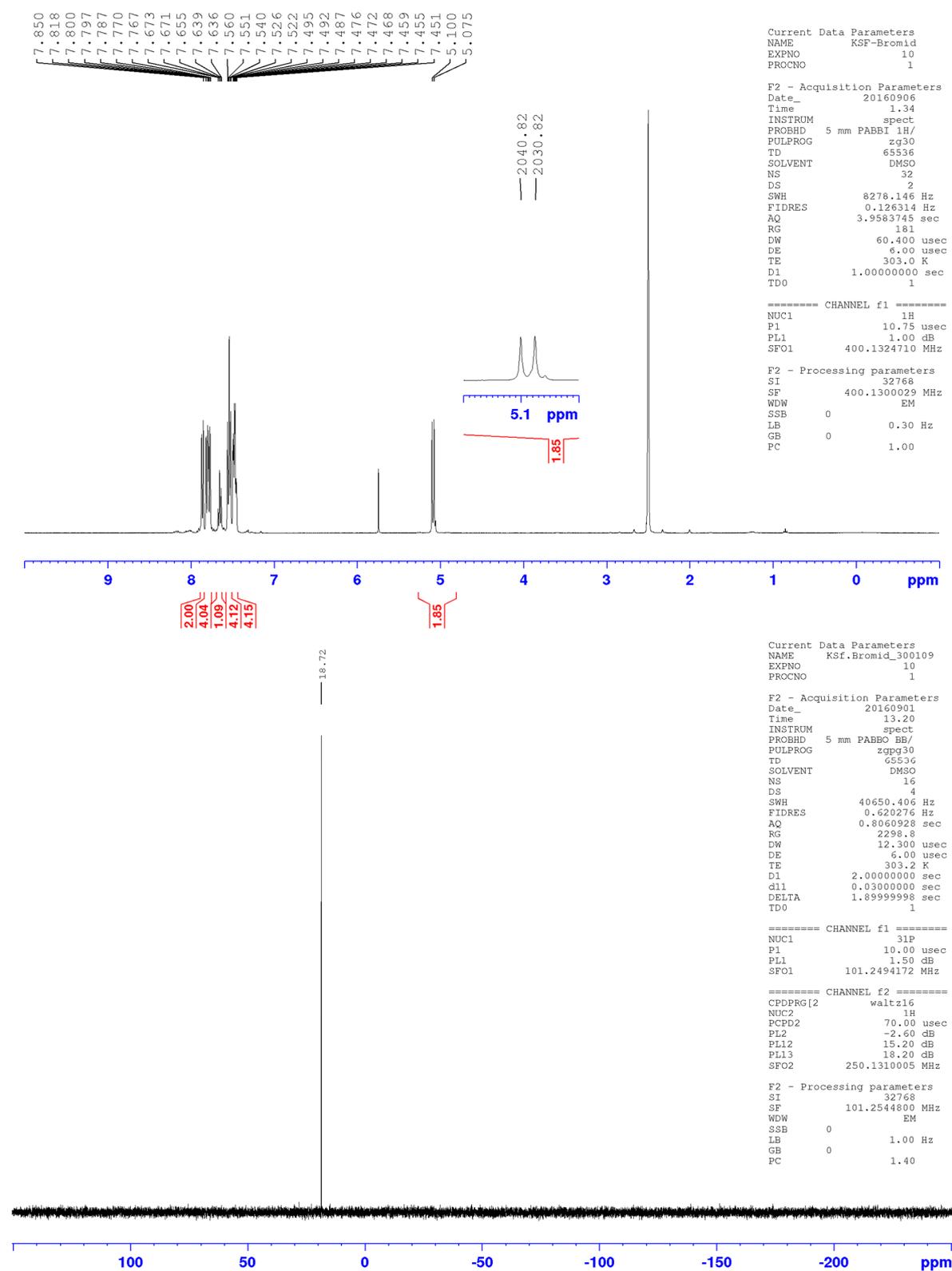
Figure S1. ^{1}H NMR and ^{31}P{^{1}H} NMR spectrum of bromide **3** in d$_6$-DMSO.
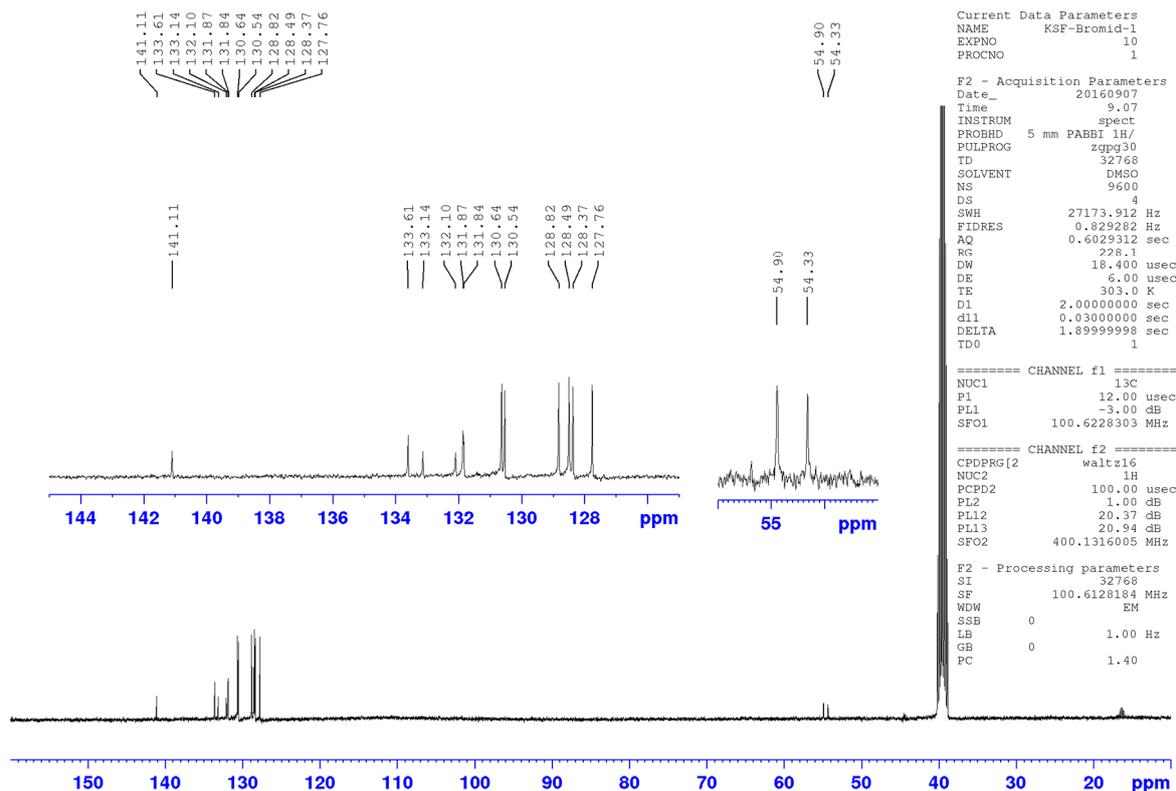
Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of bromide **3** d_6-DMSO.
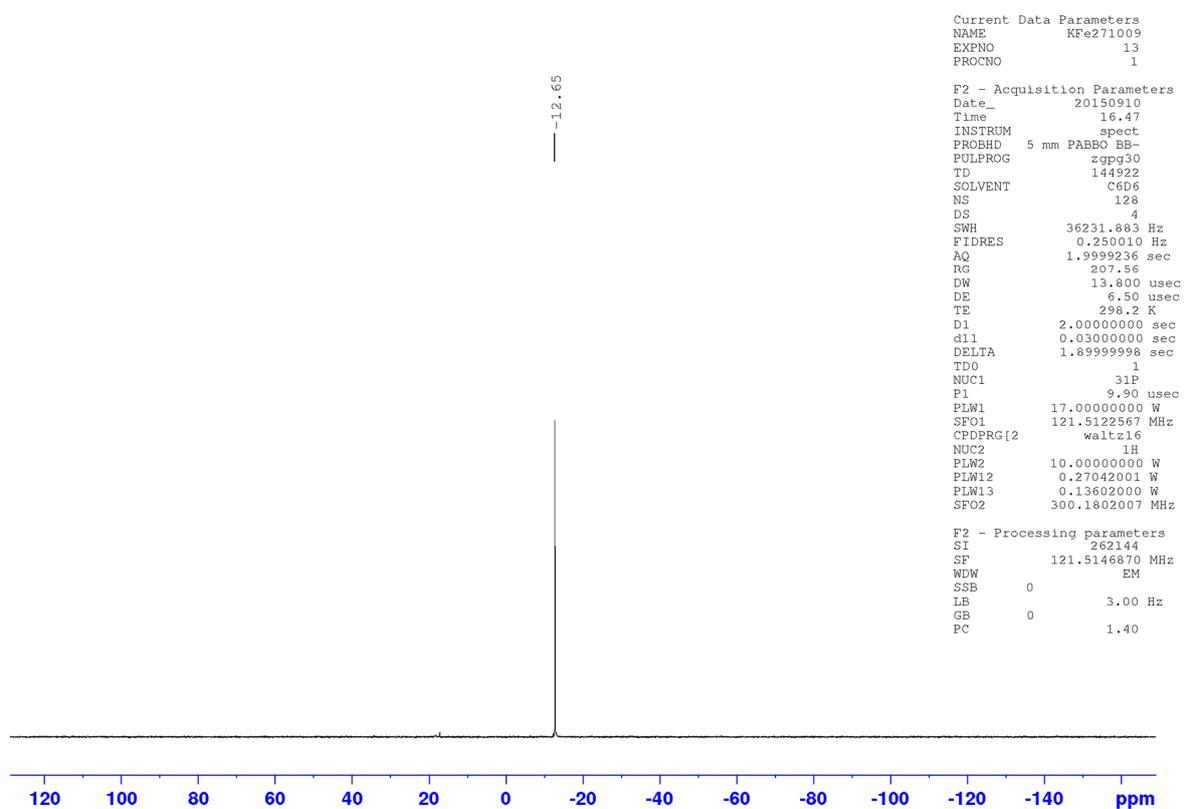
Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **1** in C_6D_6.

Figure S4. ^{1}H NMR and ^{13}C{^{1}H} NMR spectrum of ligand **1** in C$_6$D$_6$.
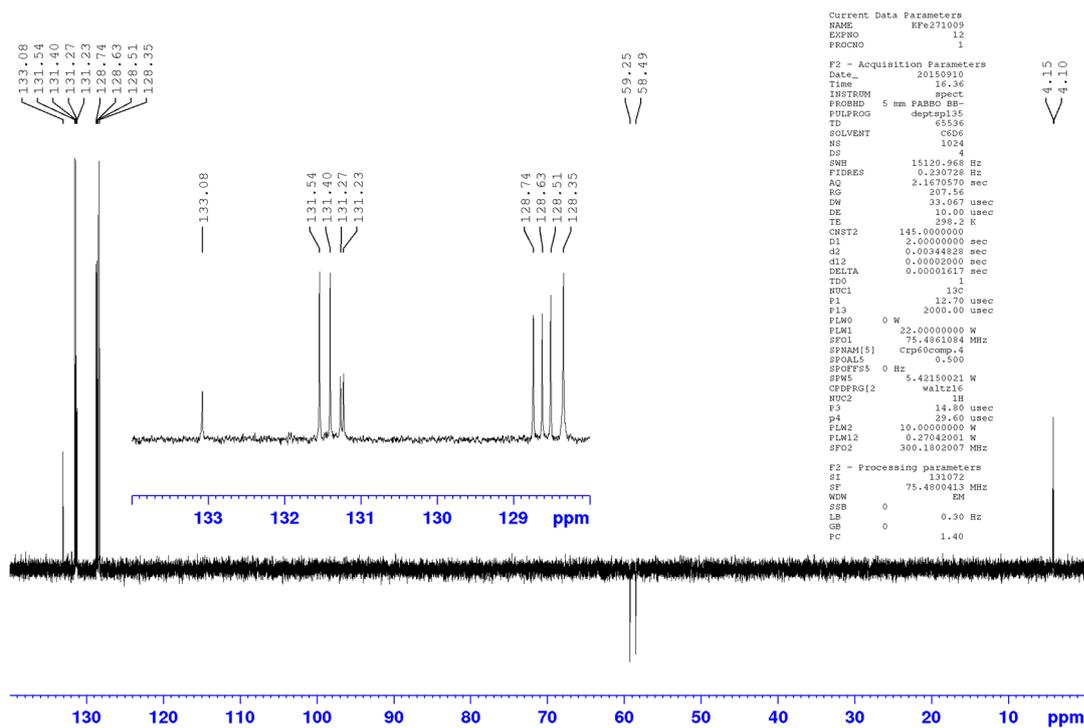
Figure S5. DEPT-135 NMR spectrum of ligand **1** in C$_6$D$_6$.
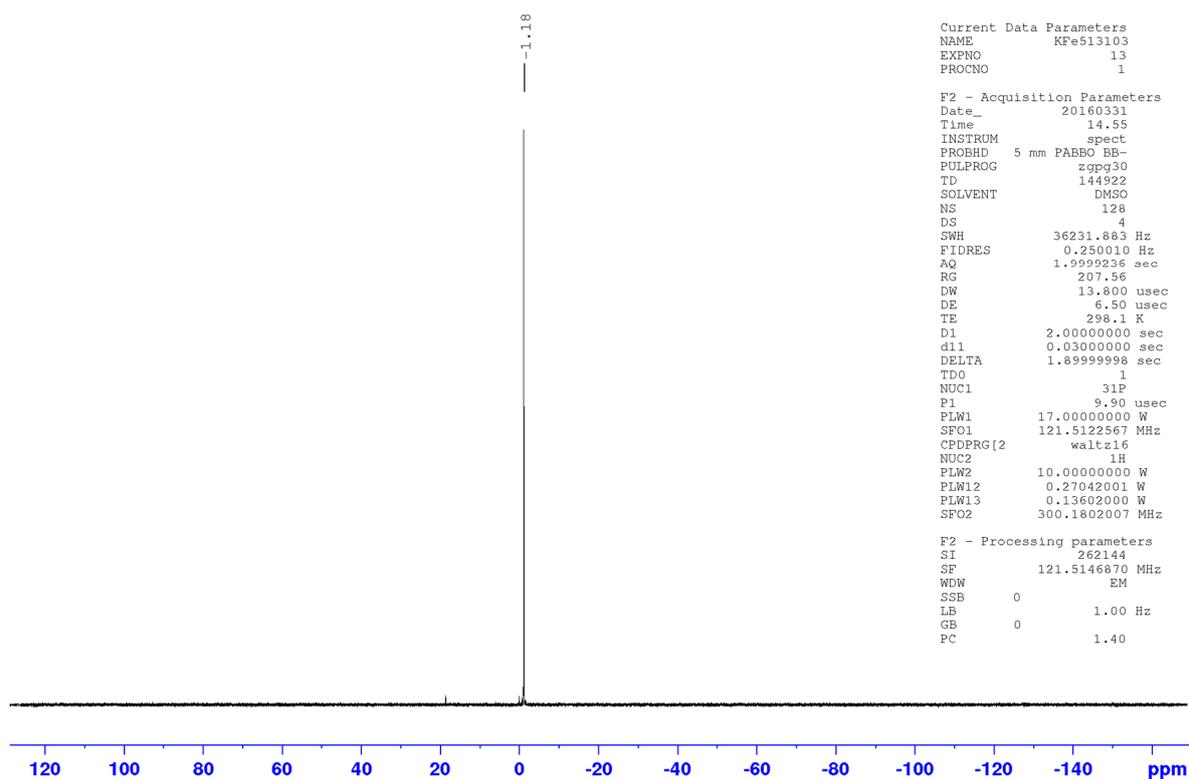
Figure S6. ^{31}P{^{1}H} NMR spectrum of monoanion **1-K** in d$_6$-DMSO.
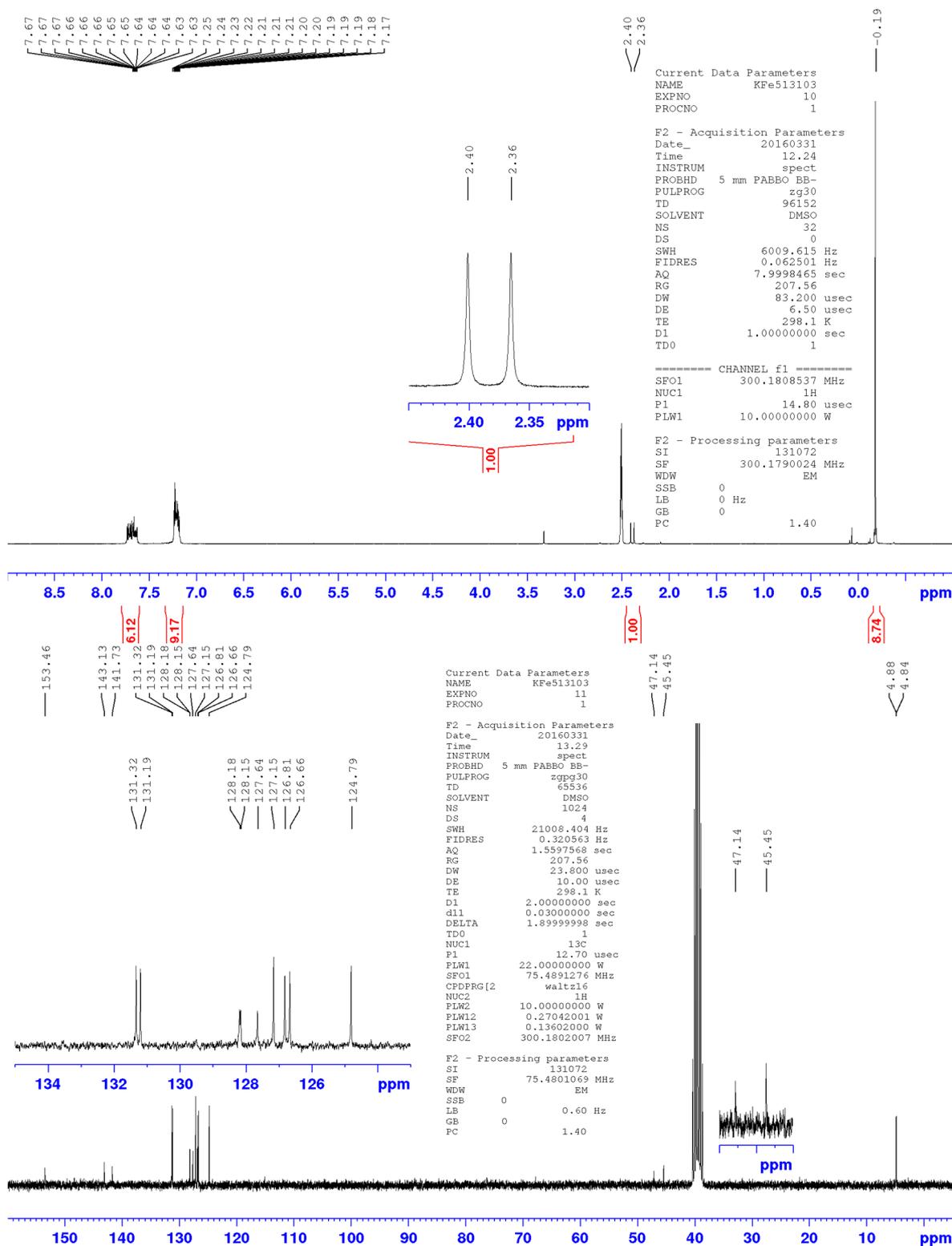
Figure S7. ¹H NMR and ¹³C{¹H} NMR spectrum of monoanion **1-K** in d₆-DMSO.

7.63

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PROCNO   1

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D11   0.03000000 sec
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PL12W   0.15631463 W
PL13W   0.09862786 W
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F2 - Processing parameters
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PL12   21.49 dB
PL13   23.49 dB
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PC   2.00

1.67   0.19

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Figure S8. $^{31}P\{^1H\}$ NMR and $^7Li\{^1H\}$ NMR spectrum of dianion **1-Li$_2$** in C$_6$D$_6$.
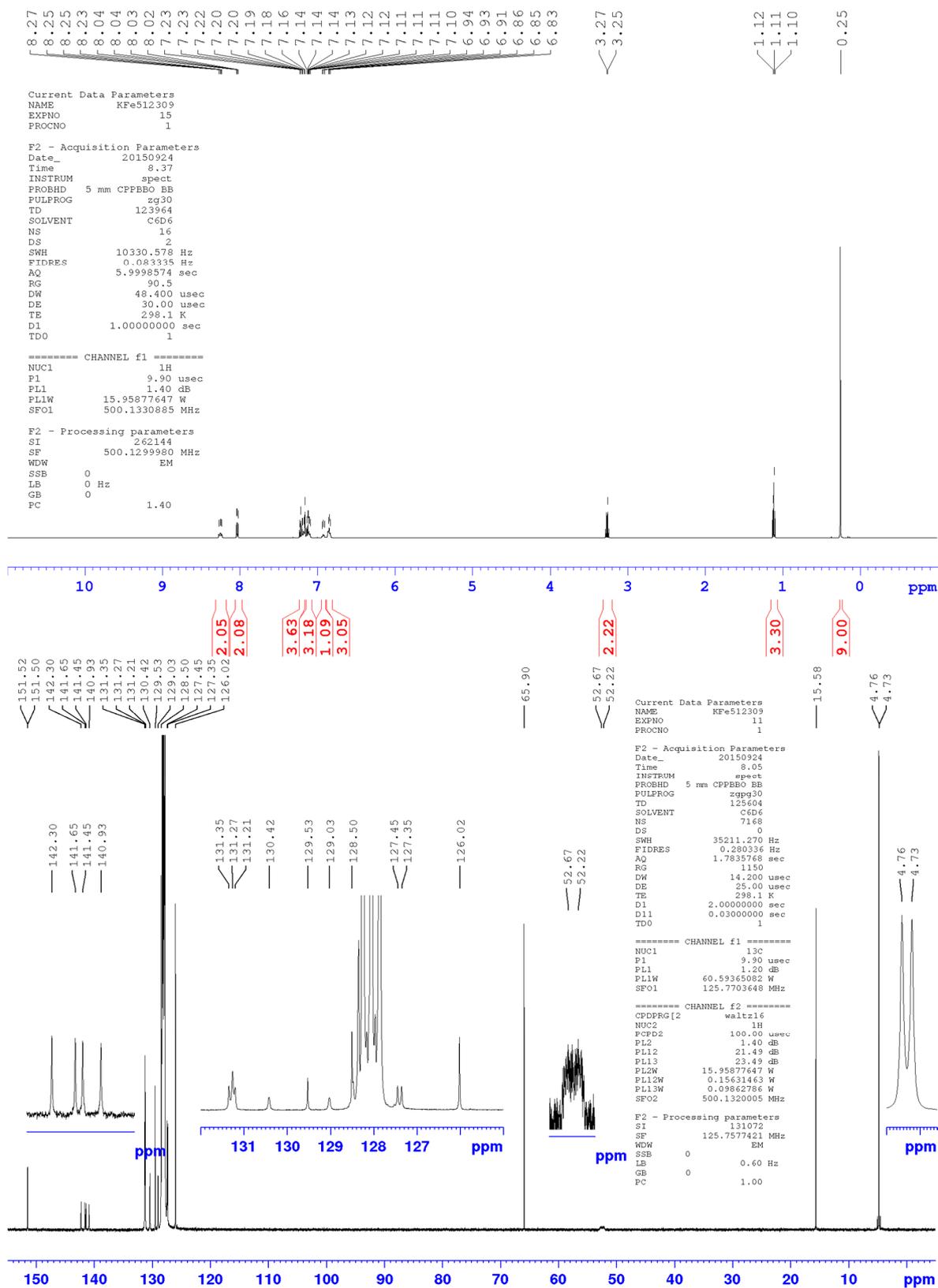
Figure S9. ^{1}H NMR and ^{13}C{^{1}H} NMR spectrum of dianion **1-Li$_2$** in C$_6$D$_6$.
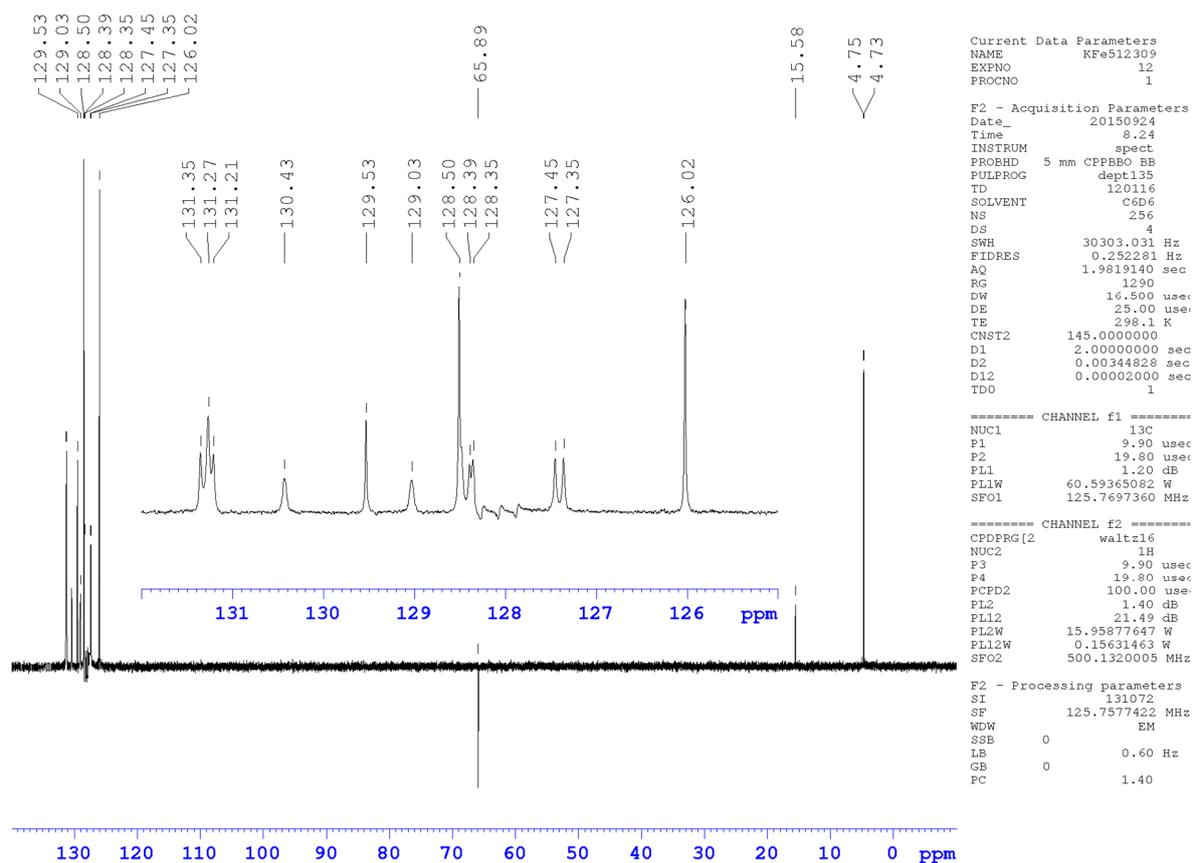
Figure S10. DEPT-135 NMR spectrum of dianion **1-Li₂** in C₆D₆.

2. Crystal Structure Determination

Data collection of all compounds was conducted with a Bruker APEX2-CCD (D8 three-circle goniometer). The structures were solved using direct methods, refined with the Shelx software package [50] and expanded using Fourier techniques. The crystals of all compounds were mounted in an inert oil (perfluoropolyalkylether). Crystal structure determinations were effected at 100 K. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1514516–1514518. Copies of the data can be obtained free of charge on application to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table S1. Data collection and structure refinement details for compounds **1**, **1-K** and **1-Li2**.

| Compound	1	1-K	1-Li$_2$
CCDC No.	1514516	1514518	1514517
Formula	$C_{22}H_{26}NO_2PSSi$	$C_{48}H_{58}K_2N_2O_5P_2S_2Si_2$	$C_{98}H_{121}Li_8N_4O_{10.50}P_4S_4Si_4$
Formula weight (g·mol^{-1})	427.56	1003.40	1942.98
Temperature (K)	100(2)	100(2)	100(2)
Wave length (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P*-1	*P*-1	*P*2$_1$/c
a (Å)	9.2087(4)	11.2841(10)	25.265(3)
b (Å)	10.5543(4)	15.3705(14)	18.972(2)
c (Å)	12.6990(5)	16.8163(15)	24.452(3)
α (°)	71.7520(10)	112.315(3)	90
β (°)	70.2450(10)	90.340(3)	116.547(3)
γ (°)	73.1050(10)	110.779(3)	90
Volume (Å^3)	1079.35(8)	2489.2(4)	10,485(2)
Z	2	2	4
Calc. density (Mg·m^{-3})	1.316	1.339	1.231
μ (Mo$_{K\alpha}$) (mm^{-1})	0.298	0.433	0.254
F(000)	452	1056	4100
Crystal dimensions (mm)	0.40 × 0.30 × 0.29	0.15 × 0.05 × 0.04	0.150 × 0.060 × 0.060
Theta range (°)	1.75–25.00	1.956–24.998	1.442–24.997
Index ranges	$-10 \le h \le 10$ $-12 \le k \le 12$ $-15 \le l \le 15$	$-13 \le h \le 13$ $-18 \le k \le 18$ $-19 \le l \le 19$	$-30 \le h \le 30$ $-22 \le k \le 22$ $-29 \le l \le 29$
Reflections collected	13,159	37,279	107,435
Independent reflections	3796 (*R*(int) = 0.0192)	8770 (*R*(int) = 0.0755)	18,468 (*R*(int) = 0.1048)
Data/Restraints/Parameter	3796/0/264	8770/0/605	18,468/0/1254
Goodness-of-fit on F^2	1.049	1.001	1.012
Final R indices (*I* > 2sigma(*I*))	*R*1 = 0.0290, *wR*2 = 0.1137	*R*1 = 0.0408, *wR*2 = 0.0917	*R*1 = 0.0494, *wR*2 = 0.0947
Largest diff. peak and hole hole (e·Å^{-3})	0.317 and −0.385 e·Å^{-3}	0.487 and −0.378 e·Å^{-3}	0.530 and −0.377 e·Å^{-3}

2.1. Crystal Structure Determination of 1
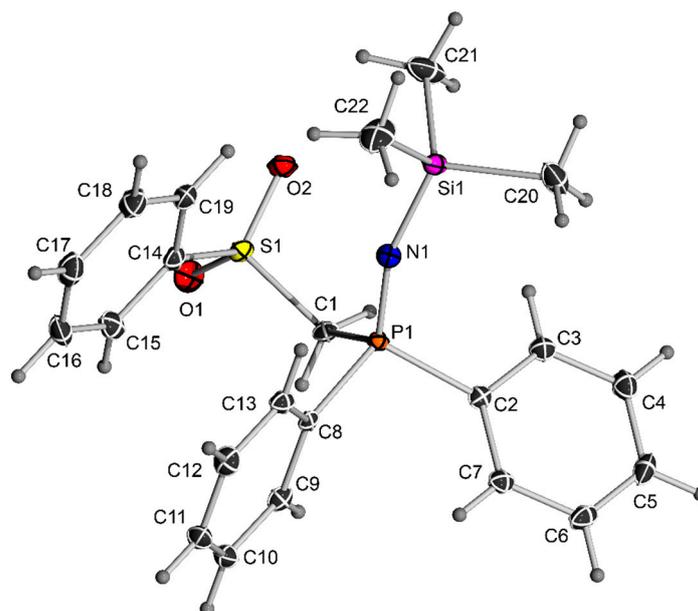
Figure S11. ORTEP Plot of **1**. Ellipsoids are drawn at the 50% probability level.

Table S2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	**U(eq)**
S(1)	5367(1)	7144(1)	4370(1)	12(1)
O(1)	4793(1)	7441(1)	5494(1)	20(1)
C(2)	9817(2)	4169(2)	3253(1)	11(1)
O(2)	4379(1)	6607(1)	4022(1)	16(1)
C(4)	10,049(2)	1722(2)	3791(1)	18(1)
C(3)	9135(2)	3031(2)	3581(1)	14(1)
C(5)	11,640(2)	1545(2)	3681(1)	19(1)
C(6)	12,326(2)	2664(2)	3362(1)	17(1)
C(7)	11,417(2)	3973(2)	3146(1)	13(1)
C(8)	9713(2)	7097(2)	2593(1)	10(1)
C(9)	10,353(2)	7224(2)	3400(1)	13(1)
C(10)	11,203(2)	8217(2)	3131(1)	15(1)
C(11)	11,435(2)	9105(2)	2044(1)	16(1)
C(12)	10,808(2)	8991(2)	1241(1)	16(1)
C(13)	9949(2)	7989(2)	1504(1)	13(1)
C(14)	5794(2)	8644(2)	3331(1)	13(1)
C(15)	6415(2)	9535(2)	3589(1)	18(1)
C(16)	6754(2)	10,697(2)	2759(2)	21(1)
C(17)	6456(2)	10,981(2)	1699(2)	22(1)
C(18)	5828(2)	10,090(2)	1457(2)	20(1)
C(19)	5481(2)	8912(2)	2279(1)	16(1)
C(20)	8235(2)	4085(2)	577(2)	23(1)
C(21)	4974(2)	5406(2)	1752(2)	29(1)
C(22)	7078(2)	7103(2)	−231(2)	29(1)
C(1)	7196(2)	5953(2)	4331(1)	12(1)
N(1)	7764(2)	6028(1)	1966(1)	13(1)
Si(1)	7045(1)	5660(1)	1069(1)	14(1)
P(1)	8554(1)	5831(1)	2900(1)	9(1)

Table S3. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + \ldots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

|	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	8(1)	15(1)	13(1)	−4(1)	0(1)	−3(1)
O(1)	15(1)	26(1)	15(1)	−10(1)	3(1)	−4(1)
C(2)	11(1)	13(1)	8(1)	−3(1)	−2(1)	−2(1)
O(2)	11(1)	18(1)	19(1)	−3(1)	−4(1)	−6(1)
C(4)	22(1)	13(1)	19(1)	−3(1)	−7(1)	−4(1)
C(3)	13(1)	15(1)	16(1)	−4(1)	−4(1)	−3(1)
C(5)	22(1)	14(1)	17(1)	−5(1)	−8(1)	5(1)
C(6)	12(1)	23(1)	17(1)	−10(1)	−4(1)	2(1)
C(7)	13(1)	17(1)	12(1)	−6(1)	−3(1)	−3(1)
C(8)	6(1)	10(1)	14(1)	−5(1)	0(1)	−1(1)
C(9)	12(1)	14(1)	12(1)	−2(1)	−2(1)	−1(1)
C(10)	13(1)	17(1)	18(1)	−7(1)	−6(1)	−2(1)
C(11)	13(1)	14(1)	23(1)	−4(1)	−5(1)	−5(1)
C(12)	16(1)	14(1)	14(1)	1(1)	−2(1)	−5(1)
C(13)	11(1)	15(1)	12(1)	−5(1)	−3(1)	−1(1)
C(14)	9(1)	12(1)	16(1)	−6(1)	−1(1)	0(1)
C(15)	16(1)	21(1)	19(1)	−11(1)	−1(1)	−4(1)
C(16)	18(1)	18(1)	28(1)	−13(1)	−1(1)	−6(1)
C(17)	21(1)	14(1)	28(1)	−3(1)	−4(1)	−3(1)
C(18)	22(1)	15(1)	21(1)	−2(1)	−9(1)	0(1)
C(19)	13(1)	14(1)	23(1)	−6(1)	−6(1)	0(1)
C(20)	23(1)	22(1)	27(1)	−12(1)	−1(1)	−10(1)
C(21)	16(1)	48(1)	34(1)	−24(1)	−2(1)	−11(1)
C(22)	36(1)	30(1)	19(1)	−6(1)	−16(1)	4(1)
C(1)	10(1)	13(1)	11(1)	−1(1)	−2(1)	−3(1)
N(1)	12(1)	13(1)	14(1)	−4(1)	−4(1)	−3(1)
Si(1)	11(1)	18(1)	14(1)	−7(1)	−4(1)	−3(1)
P(1)	8(1)	10(1)	10(1)	−2(1)	−2(1)	−2(1)

2.2. Crystal Structure Determination of **1-K**
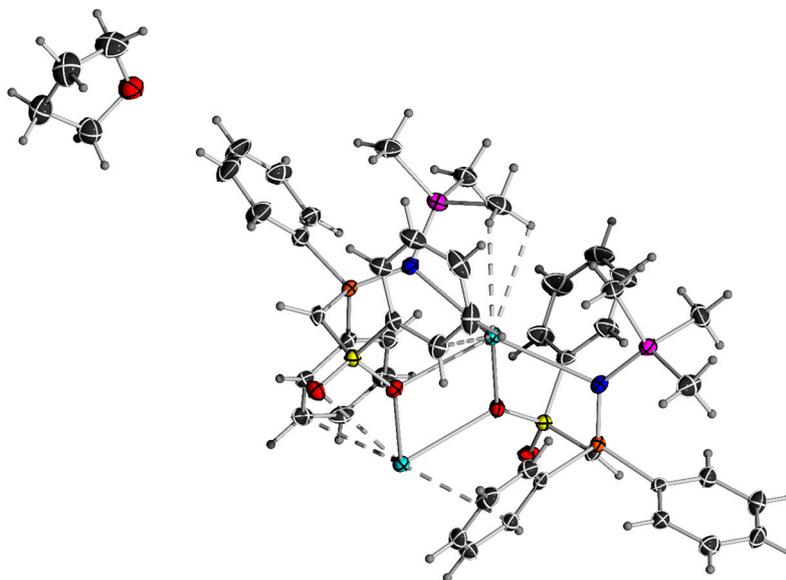
Figure S12. ORTEP Plot of **1-K**. Ellipsoids are drawn at the 50% probability level.

Table S4. Atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å² × 10³) **1-K**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
K(1)	3016(1)	5758(1)	2821(1)	22(1)
O(1)	−1072(2)	4638(2)	875(1)	23(1)
Si(1)	2400(1)	8035(1)	4597(1)	20(1)
N(1)	2103(2)	7356(2)	3505(2)	20(1)
P(1)	1440(1)	7413(1)	2714(1)	16(1)
S(1)	−144(1)	5233(1)	1669(1)	16(1)
C(1)	25(3)	6430(2)	2099(2)	18(1)
K(2)	2284(1)	4871(1)	179(1)	20(1)
O(2)	1124(2)	5187(1)	1596(1)	19(1)
Si(2)	3154(1)	3727(1)	3375(1)	20(1)
N(2)	3154(2)	3846(2)	2420(2)	19(1)
P(2)	3626(1)	3350(1)	1554(1)	15(1)
S(2)	5423(1)	5251(1)	1540(1)	16(1)
C(2)	1024(3)	8526(2)	3019(2)	16(1)
C(38)	6579(3)	7665(2)	3860(2)	32(1)
C(13)	2285(3)	7226(2)	1108(2)	20(1)
C(17)	−1651(3)	3645(3)	3464(2)	37(1)
C(11)	4475(3)	7986(2)	962(2)	27(1)
C(15)	−1382(3)	3568(2)	2032(2)	33(1)
C(14)	−754(3)	4610(2)	2372(2)	18(1)
C(44)	3483(4)	5001(3)	4276(2)	34(1)
C(16)	−1818(4)	3082(3)	2579(2)	41(1)
C(40)	7162(3)	6392(3)	4030(2)	33(1)
C(39)	7121(3)	7348(3)	4377(2)	35(1)
C(3)	−82(3)	8516(2)	3383(2)	23(1)
O(3)	4257(2)	5433(2)	1433(1)	20(1)
C(4)	−344(3)	9382(2)	3708(2)	28(1)
O(4)	6423(2)	5606(2)	1073(1)	24(1)
C(5)	491(3)	10,274(2)	3677(2)	27(1)
C(6)	1580(3)	10,290(2)	3313(2)	27(1)
C(7)	1849(3)	9423(2)	2986(2)	21(1)
C(8)	2627(3)	7598(2)	2001(2)	17(1)
C(9)	3908(3)	8162(2)	2365(2)	24(1)
C(10)	4825(3)	8363(2)	1850(2)	29(1)
C(12)	3210(3)	7407(2)	584(2)	25(1)
C(21)	2958(3)	9445(2)	4964(2)	34(1)
C(20)	958(3)	7649(3)	5114(2)	32(1)
C(19)	−553(3)	5168(2)	3254(2)	31(1)
C(18)	−1008(4)	4678(3)	3797(2)	38(1)
C(22)	3695(3)	7813(3)	5082(2)	30(1)
C(32)	1725(3)	2413(2)	−883(2)	24(1)
C(31)	2685(3)	2787(2)	−184(2)	19(1)
C(30)	2386(3)	2947(2)	647(2)	18(1)
C(29)	2613(3)	1361(2)	1361(2)	26(1)
C(28)	2626(3)	461(2)	1346(2)	34(1)
C(27)	3774(4)	349(3)	1397(3)	43(1)
C(26)	4890(4)	1118(3)	1456(3)	47(1)
C(25)	4881(3)	2017(3)	1456(2)	36(1)
C(24)	3737(3)	2153(2)	1415(2)	22(1)

C(23)	5073(3)	4054(2)	1354(2)	18(1)
C(33)	461(3)	2194(2)	−759(2)	26(1)
C(34)	160(3)	2368(2)	66(2)	26(1)
C(35)	1116(3)	2745(2)	768(2)	21(1)
C(36)	6097(3)	6067(2)	2659(2)	18(1)
C(37)	6084(3)	7038(2)	3006(2)	26(1)
C(41)	6650(3)	5750(2)	3170(2)	24(1)
C(42)	4355(3)	3242(3)	3612(2)	33(1)
C(43)	1553(3)	2882(2)	3456(2)	28(1)
O11	7169(2)	314(2)	1652(2)	40(1)
C21	8737(3)	69(3)	754(2)	39(1)
C31	9329(4)	556(3)	1681(3)	53(1)
C41	8214(4)	323(3)	2141(3)	48(1)
C11	7464(4)	207(3)	799(2)	42(1)

Table S5. Anisotropic displacement parameters ($\mathring{A}^2 \times 10^3$) for **1-K**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + \ldots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
K(1)	25(1)	28(1)	21(1)	10(1)	5(1)	18(1)
O(1)	26(1)	23(1)	18(1)	9(1)	−2(1)	8(1)
Si(1)	21(1)	21(1)	20(1)	8(1)	3(1)	11(1)
N(1)	23(1)	20(1)	22(1)	10(1)	6(1)	13(1)
P(1)	16(1)	17(1)	18(1)	9(1)	5(1)	10(1)
S(1)	16(1)	19(1)	16(1)	9(1)	4(1)	8(1)
C(1)	14(2)	23(2)	23(2)	12(1)	6(1)	10(1)
K(2)	22(1)	29(1)	18(1)	12(1)	6(1)	16(1)
O(2)	19(1)	21(1)	22(1)	9(1)	8(1)	12(1)
Si(2)	21(1)	22(1)	18(1)	10(1)	2(1)	6(1)
N(2)	18(1)	22(1)	22(1)	12(1)	5(1)	11(1)
P(2)	16(1)	17(1)	17(1)	8(1)	3(1)	9(1)
S(2)	15(1)	20(1)	17(1)	9(1)	5(1)	8(1)
C(2)	19(2)	17(1)	15(1)	7(1)	2(1)	10(1)
C(38)	20(2)	23(2)	38(2)	−1(2)	6(2)	4(1)
C(13)	20(2)	18(2)	25(2)	10(1)	6(1)	9(1)
C(17)	36(2)	41(2)	44(2)	32(2)	11(2)	9(2)
C(11)	25(2)	30(2)	40(2)	22(2)	20(2)	16(2)
C(15)	40(2)	26(2)	30(2)	14(2)	2(2)	5(2)
C(14)	12(1)	26(2)	21(2)	15(1)	3(1)	9(1)
C(44)	47(2)	31(2)	20(2)	11(2)	4(2)	9(2)
C(16)	46(2)	29(2)	46(2)	22(2)	9(2)	4(2)
C(40)	33(2)	37(2)	24(2)	15(2)	1(1)	6(2)
C(39)	26(2)	37(2)	21(2)	1(2)	2(1)	−1(2)
C(3)	22(2)	20(2)	27(2)	10(1)	6(1)	9(1)
O(3)	19(1)	25(1)	21(1)	11(1)	4(1)	12(1)
C(4)	23(2)	30(2)	34(2)	11(2)	7(1)	15(2)
O(4)	22(1)	28(1)	25(1)	14(1)	11(1)	10(1)
C(5)	33(2)	23(2)	28(2)	6(1)	4(1)	18(2)
C(6)	33(2)	20(2)	28(2)	11(1)	5(1)	10(2)
C(7)	22(2)	22(2)	22(2)	11(1)	5(1)	12(1)
C(8)	16(2)	14(1)	26(2)	10(1)	7(1)	9(1)
C(9)	22(2)	24(2)	28(2)	14(1)	4(1)	9(1)
C(10)	17(2)	34(2)	45(2)	23(2)	8(1)	11(2)

|						
C(12)	29(2)	27(2)	24(2)	13(1)	11(1)	13(2)
C(21)	44(2)	26(2)	27(2)	5(2)	−6(2)	14(2)
C(20)	33(2)	44(2)	23(2)	12(2)	10(2)	20(2)
C(19)	41(2)	26(2)	26(2)	14(1)	6(2)	8(2)
C(18)	53(2)	37(2)	23(2)	18(2)	9(2)	12(2)
C(22)	31(2)	39(2)	28(2)	16(2)	2(1)	19(2)
C(32)	31(2)	20(2)	20(2)	8(1)	1(1)	9(1)
C(31)	21(2)	18(2)	22(2)	10(1)	3(1)	9(1)
C(30)	19(2)	16(1)	19(1)	7(1)	1(1)	8(1)
C(29)	30(2)	23(2)	26(2)	11(1)	2(1)	12(2)
C(28)	43(2)	21(2)	36(2)	14(2)	2(2)	10(2)
C(27)	59(3)	32(2)	52(2)	23(2)	9(2)	28(2)
C(26)	47(2)	51(2)	67(3)	33(2)	17(2)	37(2)
C(25)	29(2)	37(2)	55(2)	27(2)	9(2)	18(2)
C(24)	25(2)	21(2)	23(2)	9(1)	4(1)	12(1)
C(23)	14(2)	23(2)	19(2)	6(1)	4(1)	11(1)
C(33)	26(2)	22(2)	26(2)	10(1)	−6(1)	6(1)
C(34)	17(2)	31(2)	29(2)	15(2)	0(1)	7(1)
C(35)	21(2)	22(2)	21(2)	11(1)	4(1)	8(1)
C(36)	11(1)	20(2)	20(2)	7(1)	4(1)	3(1)
C(37)	20(2)	26(2)	31(2)	10(2)	4(1)	8(1)
C(41)	24(2)	25(2)	22(2)	11(1)	2(1)	6(1)
C(42)	32(2)	40(2)	31(2)	20(2)	−1(2)	13(2)
C(43)	25(2)	32(2)	27(2)	16(2)	6(1)	8(2)
O11	34(1)	58(2)	42(1)	29(1)	10(1)	25(1)
C21	29(2)	34(2)	52(2)	16(2)	9(2)	10(2)
C31	33(2)	59(3)	54(3)	13(2)	−1(2)	17(2)
C41	35(2)	62(3)	49(2)	27(2)	−5(2)	15(2)
C11	37(2)	52(2)	41(2)	22(2)	11(2)	21(2)

2.3. Crystal Structure Determination of **1-Li₂**
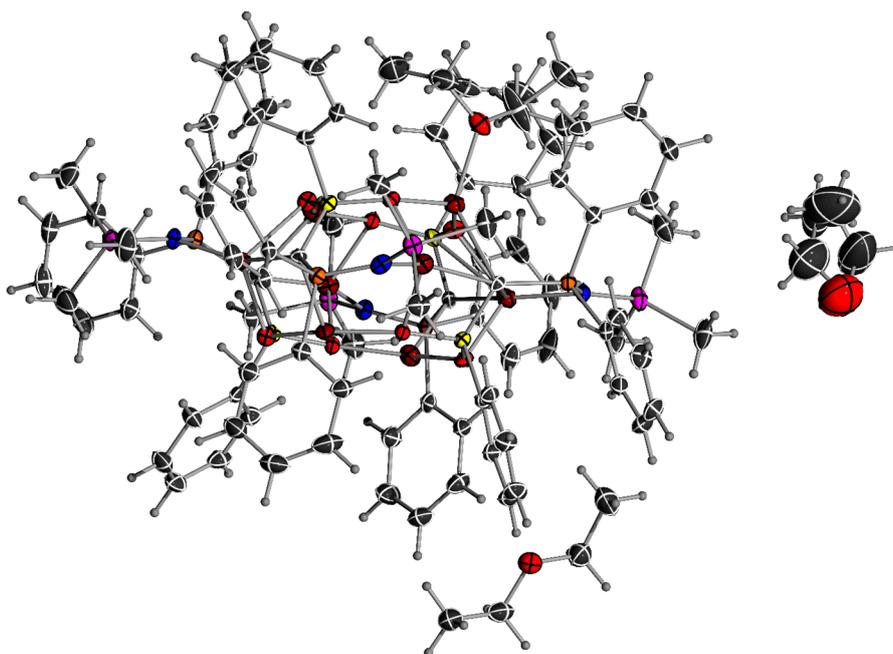
Figure S13. ORTEP Plot of **1-Li₂**. Ellipsoids are drawn at the 50% probability level.

Table S6. Atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å² × 10³) of **1-Li₂**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	**U(eq)**
S(1)	2909(1)	3838(1)	2835(1)	15(1)
P(1)	2270(1)	2808(1)	1893(1)	16(1)
Si(1)	3131(1)	2199(1)	1446(1)	20(1)
O(1)	2773(1)	4472(1)	3110(1)	18(1)
N(1)	2754(1)	2806(1)	1648(1)	16(1)
Li(1)	1891(2)	4266(3)	2817(3)	22(1)
C(1)	2296(1)	3498(2)	2357(1)	15(1)
C(52)	2925(1)	8458(2)	2142(2)	16(1)
P(2)	3941(1)	5097(1)	1417(1)	16(1)
Si(2)	4145(1)	6551(1)	1018(1)	21(1)
O(2)	3353(1)	4036(1)	2611(1)	18(1)
N(2)	3926(1)	5929(1)	1373(1)	17(1)
Li(2)	1845(2)	4342(3)	1694(3)	21(1)
C(2)	1536(1)	2898(2)	1246(2)	18(1)
S(2)	2670(1)	4968(1)	1069(1)	14(1)
C(53)	2588(2)	9069(2)	1922(2)	20(1)
S(3)	3359(1)	6472(1)	2734(1)	14(1)
P(3)	2556(1)	7630(1)	2141(1)	15(1)
Si(3)	2240(1)	8281(1)	3088(1)	19(1)
O(3)	2310(1)	4564(1)	1304(1)	17(1)
N(3)	2331(1)	7638(1)	2653(1)	18(1)
Li(3)	3015(2)	3802(3)	1732(3)	22(1)
C(3)	1072(1)	3259(2)	1286(2)	22(1)
C(54)	2857(2)	9715(2)	1988(2)	23(1)
Li(4)	3600(2)	4893(3)	2409(3)	21(1)
S(4)	1519(1)	5596(1)	2297(1)	14(1)
P(4)	1550(1)	5286(1)	3453(1)	16(1)
Si(4)	1271(1)	3727(1)	3604(1)	24(1)
O(4)	2557(1)	5741(1)	1084(1)	16(1)
N(4)	1502(1)	4452(1)	3369(1)	19(1)
C(4)	546(2)	3389(2)	772(2)	29(1)
C(57)	3536(2)	8514(2)	2406(2)	20(1)
C(56)	3805(2)	9166(2)	2472(2)	26(1)
C(5)	466(2)	3142(2)	207(2)	34(1)
Li(5)	3319(2)	6236(3)	1643(3)	20(1)
O(5)	3590(1)	5837(1)	2552(1)	16(1)
C(55)	3467(2)	9766(2)	2266(2)	28(1)
C(6)	912(2)	2761(2)	162(2)	34(1)
O(6)	3104(1)	6265(1)	3155(1)	16(1)
Li(6)	2221(2)	6219(3)	1553(3)	22(1)
C(58)	4018(1)	6939(2)	3226(2)	15(1)
C(7)	1445(2)	2652(2)	676(2)	26(1)
O(7)	1840(1)	6017(1)	2023(1)	16(1)
Li(7)	2277(2)	6610(3)	2821(3)	20(1)
C(59)	4026(1)	7355(2)	3690(2)	20(1)
C(8)	2250(2)	1961(2)	2238(2)	18(1)
Li(8)	2863(2)	5400(3)	3429(3)	22(1)
O(8)	1443(1)	4856(1)	2056(1)	16(1)
C(60)	4502(2)	7801(2)	3999(2)	25(1)

C(9)	1745(2)	1550(2)	2042(2)	29(1)
O(9)	3503(1)	5280(1)	4295(1)	29(1)
O(10)	−710(1)	4246(1)	613(1)	30(1)
C(10)	1762(2)	907(2)	2319(2)	38(1)
C(61)	4962(2)	7828(2)	3839(2)	25(1)
C(11)	2273(2)	674(2)	2789(2)	37(1)
C(62)	4953(2)	7406(2)	3381(2)	25(1)
C(12)	2781(2)	1072(2)	2994(2)	32(1)
C(45)	2953(1)	6904(2)	2122(1)	14(1)
C(13)	2768(2)	1717(2)	2718(2)	26(1)
C(46)	1929(1)	7663(2)	1377(2)	18(1)
C(14)	3345(2)	3315(2)	3491(2)	18(1)
C(51)	2015(2)	7658(2)	852(2)	25(1)
C(15)	3056(2)	2952(2)	3767(2)	26(1)
C(50)	1547(2)	7765(2)	280(2)	38(1)
C(16)	3381(2)	2593(2)	4310(2)	36(1)
C(49)	985(2)	7880(2)	225(2)	41(1)
C(17)	3990(2)	2604(2)	4568(2)	42(1)
C(48)	891(2)	7875(2)	737(2)	40(1)
C(18)	4278(2)	2954(2)	4284(2)	34(1)
C(47)	1357(2)	7764(2)	1311(2)	26(1)
C(19)	3957(2)	3310(2)	3739(2)	26(1)
C(20)	3315(2)	2602(2)	855(2)	27(1)
C(21)	2716(2)	1362(2)	1127(2)	30(1)
C(22)	3843(2)	1954(2)	2114(2)	32(1)
C(23)	3340(1)	4695(2)	1426(1)	15(1)
C(24)	4156(2)	4706(2)	866(2)	19(1)
C(25)	3738(2)	4432(2)	322(2)	27(1)
C(26)	3896(2)	4194(2)	−122(2)	33(1)
C(27)	4480(2)	4225(2)	−15(2)	34(1)
C(28)	4902(2)	4487(2)	528(2)	30(1)
C(29)	4747(2)	4724(2)	972(2)	24(1)
C(30)	4528(1)	4806(2)	2151(2)	18(1)
C(31)	4563(2)	4107(2)	2344(2)	26(1)
C(32)	4977(2)	3899(2)	2923(2)	32(1)
C(33)	5362(2)	4384(2)	3320(2)	33(1)
C(34)	5344(2)	5077(2)	3140(2)	30(1)
C(35)	4930(1)	5287(2)	2560(2)	23(1)
C(36)	2322(1)	4760(2)	275(2)	16(1)
C(38)	1947(2)	3867(2)	−501(2)	26(1)
C(37)	2161(1)	4061(2)	105(2)	22(1)
C(39)	1884(2)	4362(2)	−937(2)	31(1)
C(40)	2039(2)	5053(2)	−768(2)	32(1)
C(41)	2260(2)	5259(2)	−162(2)	23(1)
C(70)	−228(2)	5692(2)	2722(2)	30(1)
C(69)	315(2)	5367(2)	2883(2)	23(1)
C(68)	839(1)	5673(2)	3307(2)	19(1)
C(67)	1846(1)	5705(2)	3030(2)	14(1)
C(44)	3888(2)	7416(2)	1163(2)	42(1)
C(43)	4969(2)	6616(2)	1326(2)	42(1)
C(42)	3843(2)	6422(2)	180(2)	54(1)
C(74)	2011(1)	5561(2)	4244(2)	18(1)
C(73)	804(2)	6319(2)	3568(2)	25(1)

C(72)	263(2)	6644(2)	3404(2)	30(1)
C(71)	−251(2)	6336(2)	2982(2)	30(1)
C(78)	2246(2)	5458(2)	5313(2)	27(1)
C(77)	2693(2)	5954(2)	5464(2)	27(1)
C(76)	2788(2)	6257(2)	5004(2)	24(1)
C(75)	2449(1)	6066(2)	4398(2)	19(1)
C(79)	1908(2)	5262(2)	4710(2)	25(1)
C(80)	786(1)	5949(2)	1921(2)	16(1)
C(81)	317(1)	5567(2)	1492(2)	22(1)
C(82)	−243(2)	5866(2)	1225(2)	28(1)
C(83)	−327(2)	6539(2)	1386(2)	29(1)
C(85)	700(2)	6623(2)	2086(2)	22(1)
C(84)	140(2)	6922(2)	1814(2)	26(1)
C(86)	584(2)	3842(2)	3709(2)	37(1)
C(87)	1116(2)	3026(2)	3013(2)	31(1)
C(65)	1565(2)	8833(2)	2652(2)	27(1)
C(66)	2897(2)	8874(2)	3472(2)	24(1)
C(64)	2130(2)	7836(2)	3712(2)	33(1)
C(63)	4483(1)	6958(2)	3071(2)	22(1)
C(91)	3547(3)	4610(2)	4590(2)	65(2)
C(90)	4044(2)	5661(2)	4490(2)	46(1)
C(89)	4443(2)	5368(3)	4237(2)	70(2)
C(88)	1855(2)	3370(2)	4343(2)	36(1)
C(93)	−902(2)	4741(2)	−350(2)	42(1)
C(96)	−478(2)	3865(2)	1615(2)	49(1)
C(95)	−810(2)	3697(2)	948(2)	37(1)
C(94)	−996(2)	4118(2)	−29(2)	35(1)
C(92A)	3631(3)	4596(3)	5203(3)	39(2)
O1A1	0(60)	5320(40)	5090(70)	130(30)
C1A1	999(8)	4493(10)	5567(10)	123(8)
C2A1	546(9)	5038(10)	5187(9)	106(5)
O1B1	−30(30)	5150(20)	5090(30)	58(12)
C2B1	407(9)	4668(14)	5508(12)	182(12)
C1B1	923(11)	5006(11)	5799(11)	154(9)
C(92B)	3186(6)	4412(7)	4746(6)	29(4)

Table S7. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **1-Li₂**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	18(1)	13(1)	15(1)	2(1)	8(1)	2(1)
P(1)	18(1)	13(1)	18(1)	1(1)	10(1)	−1(1)
Si(1)	25(1)	15(1)	24(1)	2(1)	15(1)	4(1)
O(1)	18(1)	12(1)	22(1)	−1(1)	6(1)	1(1)
N(1)	18(2)	12(1)	21(2)	0(1)	10(1)	0(1)
Li(1)	25(3)	20(3)	20(3)	1(3)	11(3)	−1(3)
C(1)	16(2)	17(2)	14(2)	1(2)	9(2)	0(1)
C(52)	20(2)	15(2)	16(2)	0(2)	11(2)	−1(2)
P(2)	16(1)	15(1)	18(1)	0(1)	10(1)	0(1)
Si(2)	25(1)	20(1)	21(1)	1(1)	11(1)	−6(1)
O(2)	16(1)	19(1)	20(1)	3(1)	10(1)	−1(1)
N(2)	19(2)	14(1)	21(2)	0(1)	12(1)	−2(1)
Li(2)	28(3)	14(3)	21(3)	0(3)	10(3)	−1(3)

C(2)	20(2)	15(2)	20(2)	2(2)	10(2)	−3(2)
S(2)	15(1)	13(1)	14(1)	0(1)	7(1)	−1(1)
C(53)	26(2)	15(2)	21(2)	3(2)	14(2)	2(2)
S(3)	15(1)	12(1)	17(1)	−2(1)	7(1)	−1(1)
P(3)	17(1)	12(1)	16(1)	0(1)	7(1)	−1(1)
Si(3)	25(1)	15(1)	21(1)	0(1)	13(1)	2(1)
O(3)	15(1)	21(1)	18(1)	3(1)	10(1)	0(1)
N(3)	16(2)	13(1)	24(2)	−3(1)	9(1)	0(1)
Li(3)	21(3)	19(3)	23(3)	−1(3)	9(3)	1(3)
C(3)	19(2)	29(2)	20(2)	−5(2)	9(2)	−5(2)
C(54)	36(2)	14(2)	27(2)	2(2)	20(2)	4(2)
Li(4)	21(3)	22(3)	17(3)	−1(3)	6(3)	9(3)
S(4)	13(1)	15(1)	16(1)	0(1)	7(1)	0(1)
P(4)	17(1)	17(1)	16(1)	−1(1)	9(1)	−2(1)
Si(4)	31(1)	21(1)	26(1)	−1(1)	18(1)	−5(1)
O(4)	18(1)	12(1)	19(1)	−1(1)	9(1)	1(1)
N(4)	21(2)	22(2)	18(2)	−2(1)	14(1)	−5(1)
C(4)	19(2)	32(2)	35(2)	−5(2)	12(2)	0(2)
C(57)	26(2)	16(2)	22(2)	2(2)	13(2)	1(2)
C(56)	21(2)	23(2)	33(2)	−1(2)	12(2)	−8(2)
C(5)	19(2)	47(3)	30(2)	0(2)	5(2)	1(2)
Li(5)	15(3)	23(3)	19(3)	2(3)	6(3)	1(2)
O(5)	18(1)	12(1)	20(1)	−1(1)	10(1)	1(1)
C(55)	39(2)	15(2)	38(2)	−3(2)	23(2)	−9(2)
C(6)	31(2)	47(3)	23(2)	−9(2)	9(2)	−1(2)
O(6)	17(1)	14(1)	15(1)	−1(1)	6(1)	−2(1)
Li(6)	21(3)	25(3)	19(3)	−5(3)	9(3)	−9(3)
C(58)	15(2)	11(2)	15(2)	2(2)	3(2)	0(1)
C(7)	23(2)	33(2)	25(2)	−2(2)	13(2)	4(2)
O(7)	16(1)	17(1)	18(1)	0(1)	10(1)	−2(1)
Li(7)	21(3)	17(3)	23(3)	−1(3)	10(3)	0(2)
C(59)	18(2)	23(2)	20(2)	1(2)	11(2)	−3(2)
C(8)	29(2)	12(2)	20(2)	−2(2)	18(2)	1(2)
Li(8)	25(3)	21(3)	21(3)	−3(3)	10(3)	−1(3)
O(8)	14(1)	15(1)	17(1)	−3(1)	6(1)	−2(1)
C(60)	26(2)	24(2)	21(2)	−6(2)	6(2)	−5(2)
C(9)	32(2)	21(2)	42(3)	6(2)	23(2)	2(2)
O(9)	38(2)	24(1)	24(2)	5(1)	14(1)	4(1)
O(10)	27(1)	35(2)	25(2)	0(1)	10(1)	−2(1)
C(10)	43(3)	21(2)	68(3)	6(2)	40(3)	0(2)
C(61)	16(2)	25(2)	31(2)	0(2)	7(2)	−4(2)
C(11)	63(3)	18(2)	49(3)	9(2)	44(3)	8(2)
C(62)	16(2)	25(2)	33(2)	1(2)	12(2)	1(2)
C(12)	52(3)	26(2)	23(2)	3(2)	21(2)	9(2)
C(45)	15(2)	14(2)	12(2)	−3(1)	5(2)	−2(1)
C(13)	41(2)	20(2)	20(2)	−1(2)	18(2)	2(2)
C(46)	22(2)	9(2)	19(2)	1(2)	7(2)	−1(1)
C(14)	26(2)	13(2)	13(2)	0(2)	8(2)	5(2)
C(51)	26(2)	23(2)	24(2)	2(2)	9(2)	−4(2)
C(15)	36(2)	19(2)	22(2)	3(2)	14(2)	4(2)
C(50)	39(3)	46(3)	22(2)	5(2)	9(2)	−6(2)
C(16)	57(3)	26(2)	25(2)	8(2)	19(2)	5(2)
C(49)	33(2)	49(3)	26(2)	1(2)	0(2)	0(2)

C(17)	56(3)	32(2)	24(2)	7(2)	7(2)	15(2)
C(48)	22(2)	48(3)	40(3)	−7(2)	4(2)	3(2)
C(18)	33(2)	34(2)	23(2)	3(2)	2(2)	15(2)
C(47)	21(2)	30(2)	24(2)	−4(2)	6(2)	−2(2)
C(19)	28(2)	24(2)	22(2)	1(2)	7(2)	9(2)
C(20)	33(2)	24(2)	35(2)	2(2)	24(2)	6(2)
C(21)	43(2)	17(2)	37(2)	−3(2)	25(2)	2(2)
C(22)	33(2)	36(2)	35(2)	4(2)	21(2)	6(2)
C(23)	16(2)	14(2)	13(2)	3(2)	6(2)	3(1)
C(24)	26(2)	13(2)	26(2)	4(2)	18(2)	1(2)
C(25)	27(2)	26(2)	31(2)	−2(2)	17(2)	0(2)
C(26)	51(3)	27(2)	26(2)	−4(2)	23(2)	−1(2)
C(27)	55(3)	20(2)	46(3)	3(2)	41(2)	5(2)
C(28)	39(2)	19(2)	48(3)	6(2)	34(2)	5(2)
C(29)	28(2)	18(2)	34(2)	2(2)	19(2)	2(2)
C(30)	12(2)	21(2)	25(2)	2(2)	11(2)	4(2)
C(31)	16(2)	26(2)	34(2)	5(2)	10(2)	3(2)
C(32)	24(2)	30(2)	42(3)	17(2)	15(2)	8(2)
C(33)	25(2)	43(3)	26(2)	10(2)	8(2)	11(2)
C(34)	21(2)	36(2)	23(2)	−7(2)	2(2)	5(2)
C(35)	19(2)	24(2)	28(2)	−1(2)	11(2)	4(2)
C(36)	11(2)	20(2)	18(2)	−1(2)	7(2)	−1(1)
C(38)	21(2)	28(2)	25(2)	−9(2)	7(2)	−3(2)
C(37)	21(2)	21(2)	22(2)	0(2)	8(2)	1(2)
C(39)	27(2)	47(3)	18(2)	−8(2)	9(2)	−2(2)
C(40)	37(2)	36(2)	21(2)	6(2)	11(2)	−1(2)
C(41)	32(2)	21(2)	17(2)	2(2)	11(2)	−1(2)
C(70)	17(2)	40(2)	31(2)	−2(2)	9(2)	−4(2)
C(69)	25(2)	25(2)	22(2)	−1(2)	13(2)	−5(2)
C(68)	19(2)	25(2)	17(2)	1(2)	12(2)	−2(2)
C(67)	14(2)	14(2)	16(2)	−3(2)	7(2)	−2(1)
C(44)	52(3)	27(2)	57(3)	14(2)	34(2)	4(2)
C(43)	34(2)	41(3)	53(3)	7(2)	22(2)	−11(2)
C(42)	71(3)	58(3)	32(3)	2(2)	22(2)	−27(3)
C(74)	19(2)	18(2)	19(2)	0(2)	10(2)	4(2)
C(73)	24(2)	26(2)	23(2)	−6(2)	10(2)	−3(2)
C(72)	34(2)	30(2)	32(2)	−5(2)	20(2)	3(2)
C(71)	19(2)	40(2)	35(2)	1(2)	16(2)	5(2)
C(78)	36(2)	29(2)	21(2)	1(2)	17(2)	2(2)
C(77)	28(2)	31(2)	17(2)	−6(2)	5(2)	4(2)
C(76)	22(2)	23(2)	22(2)	−7(2)	6(2)	−3(2)
C(75)	21(2)	16(2)	20(2)	−1(2)	10(2)	3(2)
C(79)	26(2)	26(2)	22(2)	1(2)	12(2)	−2(2)
C(80)	14(2)	21(2)	12(2)	4(2)	5(2)	5(2)
C(81)	19(2)	29(2)	19(2)	−3(2)	9(2)	0(2)
C(82)	17(2)	42(2)	21(2)	−6(2)	5(2)	−2(2)
C(83)	20(2)	39(2)	27(2)	4(2)	8(2)	11(2)
C(85)	18(2)	23(2)	24(2)	2(2)	10(2)	2(2)
C(84)	24(2)	27(2)	27(2)	−1(2)	11(2)	6(2)
C(86)	45(3)	30(2)	51(3)	−1(2)	33(2)	−13(2)
C(87)	39(2)	26(2)	35(2)	−7(2)	24(2)	−13(2)
C(65)	28(2)	25(2)	29(2)	−5(2)	13(2)	3(2)
C(66)	30(2)	18(2)	22(2)	−2(2)	9(2)	3(2)

C(64)	53(3)	20(2)	39(3)	−1(2)	32(2)	1(2)
C(63)	18(2)	19(2)	29(2)	−6(2)	11(2)	−2(2)
C(91)	139(5)	31(3)	52(3)	22(2)	65(4)	31(3)
C(90)	40(3)	55(3)	28(3)	4(2)	3(2)	−1(2)
C(89)	35(3)	114(5)	58(3)	25(3)	17(3)	19(3)
C(88)	53(3)	30(2)	29(2)	7(2)	23(2)	−1(2)
C(93)	27(2)	64(3)	31(3)	1(2)	11(2)	−4(2)
C(96)	55(3)	61(3)	35(3)	6(2)	25(2)	2(2)
C(95)	30(2)	41(2)	39(3)	7(2)	16(2)	1(2)
C(94)	22(2)	45(3)	30(2)	−5(2)	6(2)	3(2)
C(92A)	60(5)	28(3)	28(4)	4(3)	20(4)	8(3)
O1A1	90(30)	160(70)	140(40)	40(60)	40(30)	10(60)
C1A1	74(11)	180(20)	133(17)	82(17)	64(11)	25(14)
C2A1	83(14)	125(15)	113(14)	0(12)	46(13)	5(12)
O1B1	50(20)	30(30)	80(30)	20(20)	26(18)	0(20)
C2B1	68(13)	310(30)	160(20)	120(20)	51(16)	30(18)
C1B1	109(17)	160(20)	140(20)	56(18)	12(15)	25(17)
C(92B)	33(8)	30(7)	28(9)	4(6)	19(7)	4(6)