Synthesis and Stability of Li/Cl Carbenoids based on Bis(iminophosphorano)methanes

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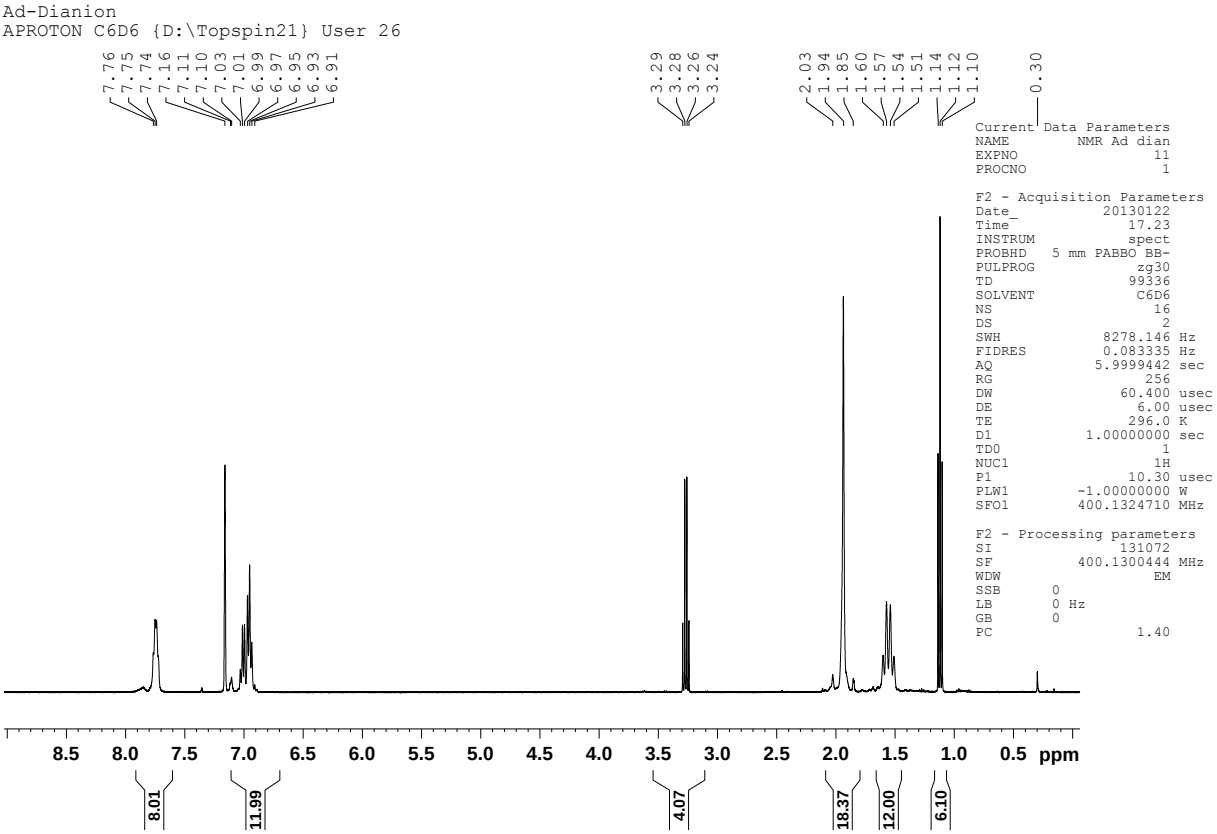
1. NMR spectra



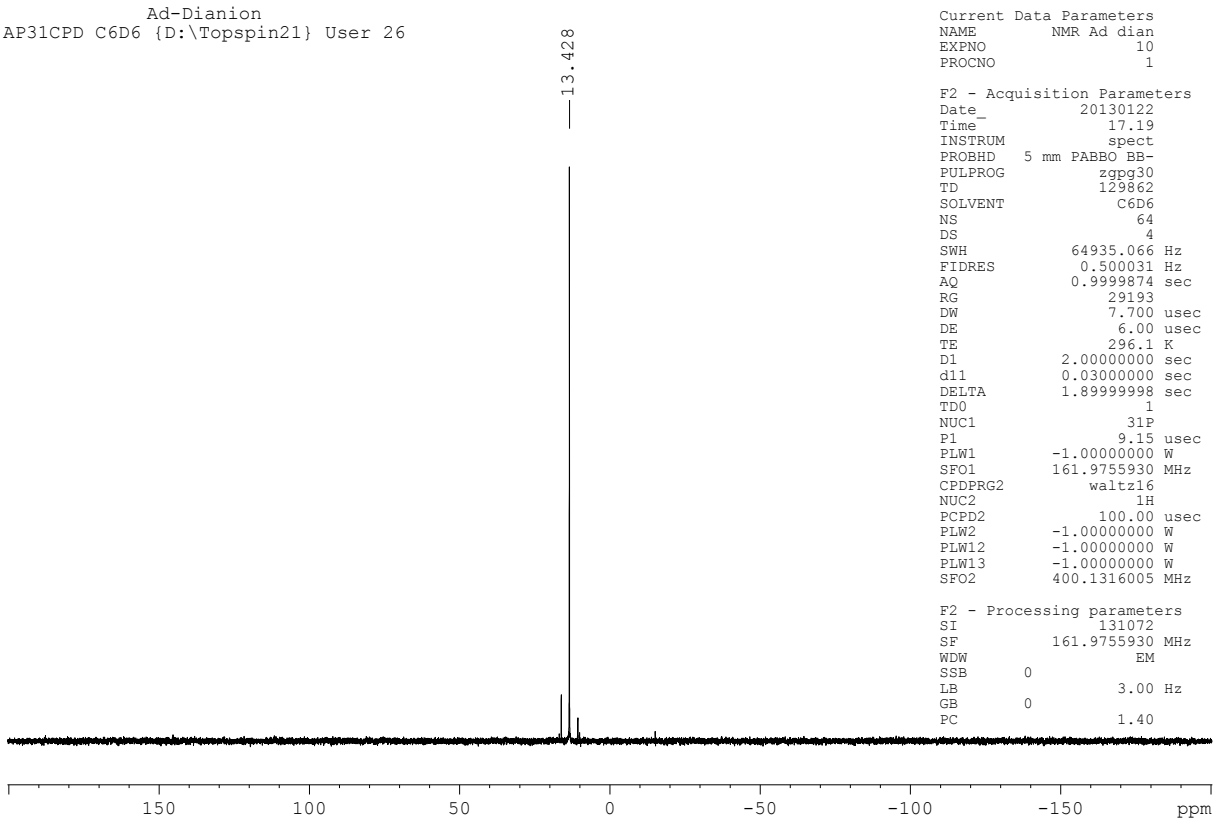
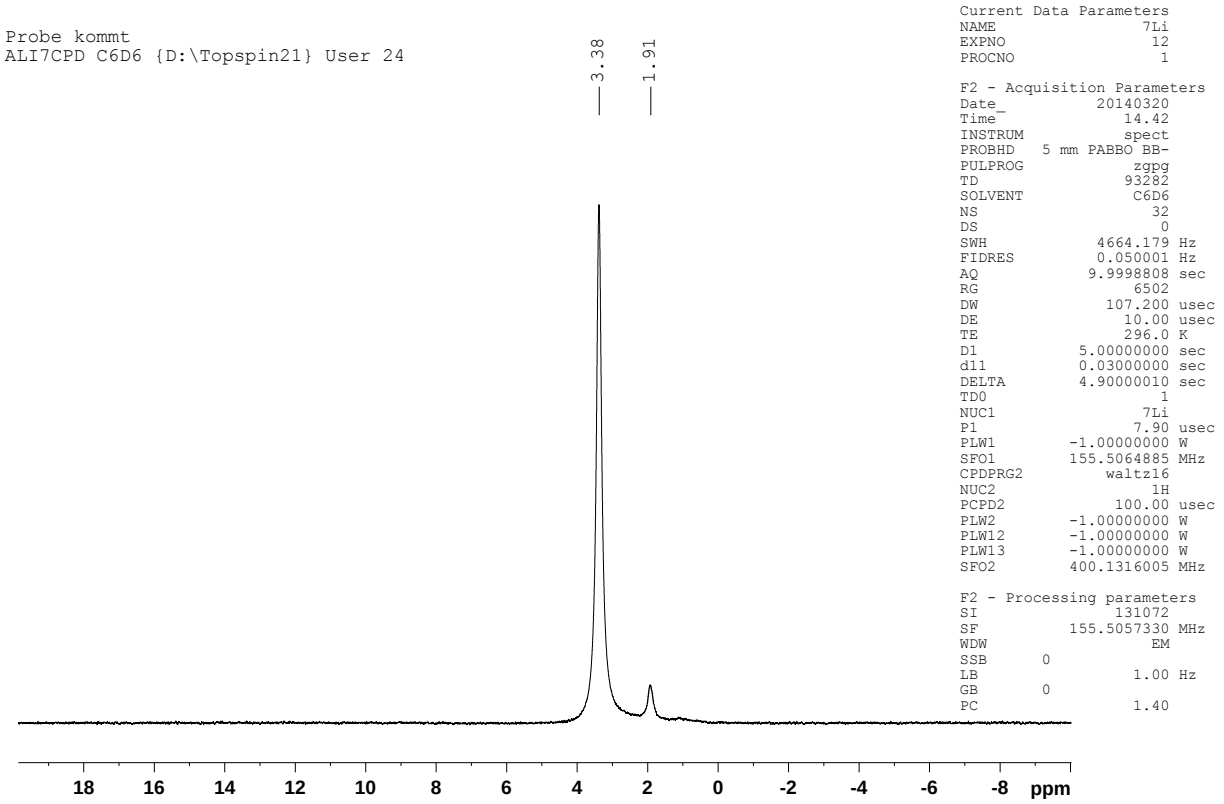


Figure S1a. $^{31}P\{^{1}H\}$ and ^{1}H NMR spectra of $BIPM^{Ad}$ in C_6D_6.



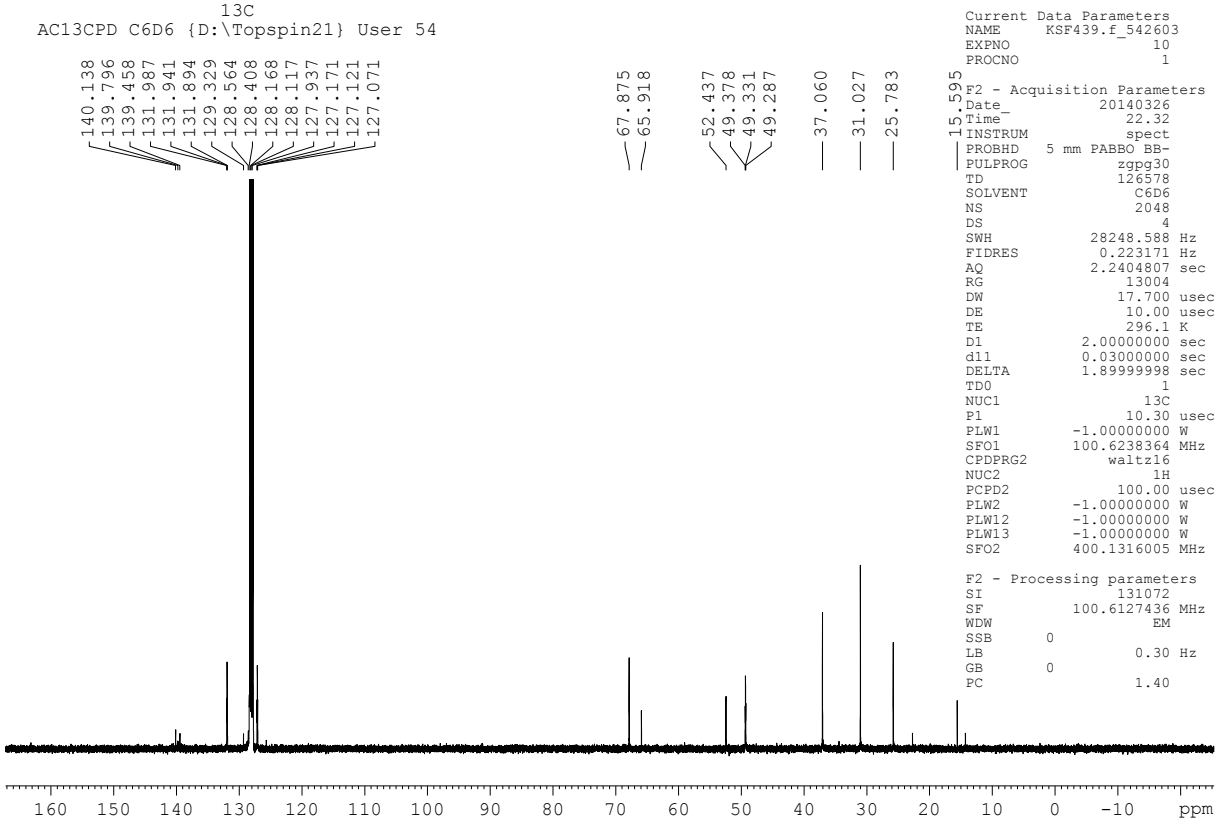


Figure S1b. ^{7}Li and $^{13}C\{^{1}H\}$ NMR spectra of $BIPM^{Ad}$ in C_6D_6.

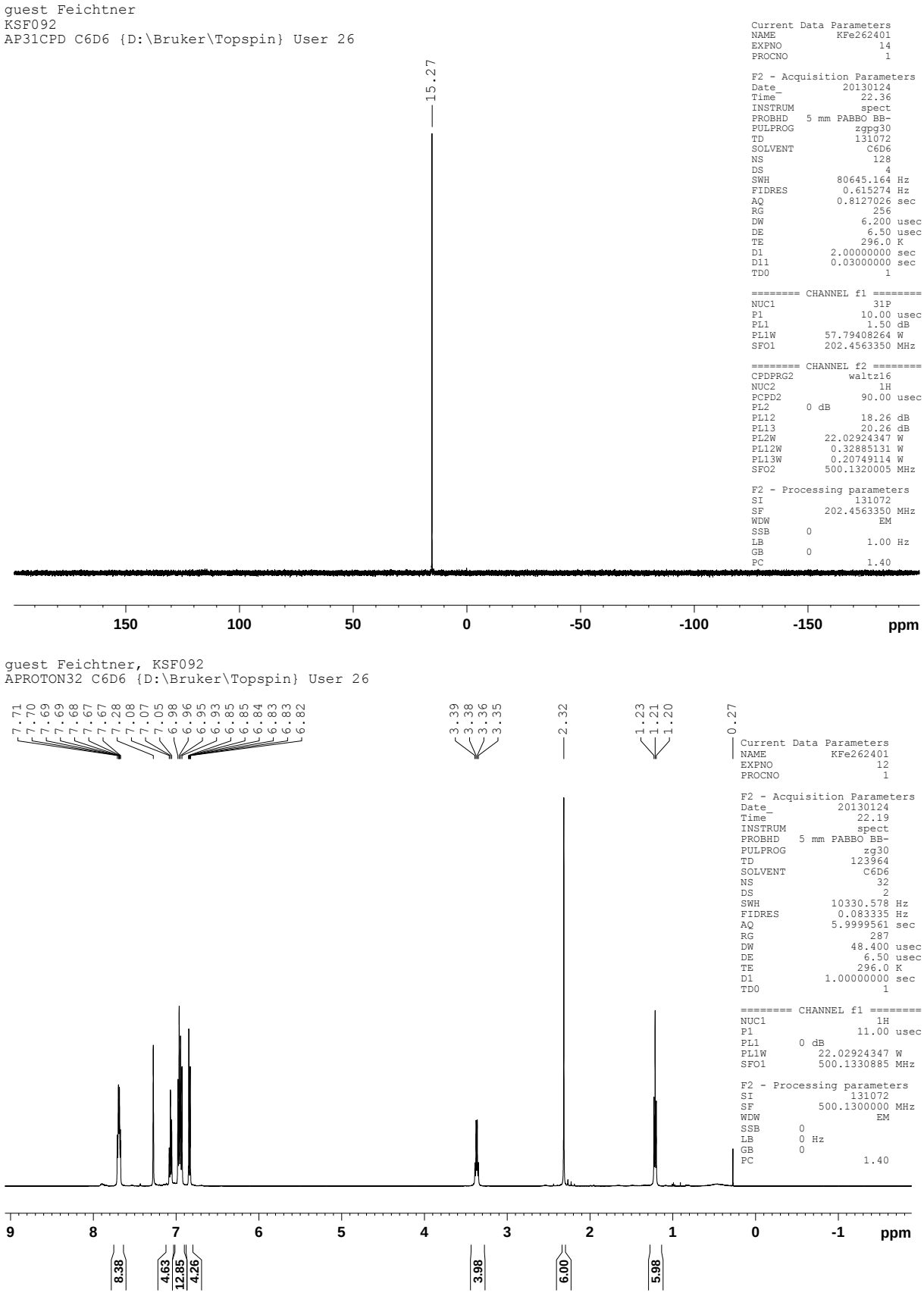
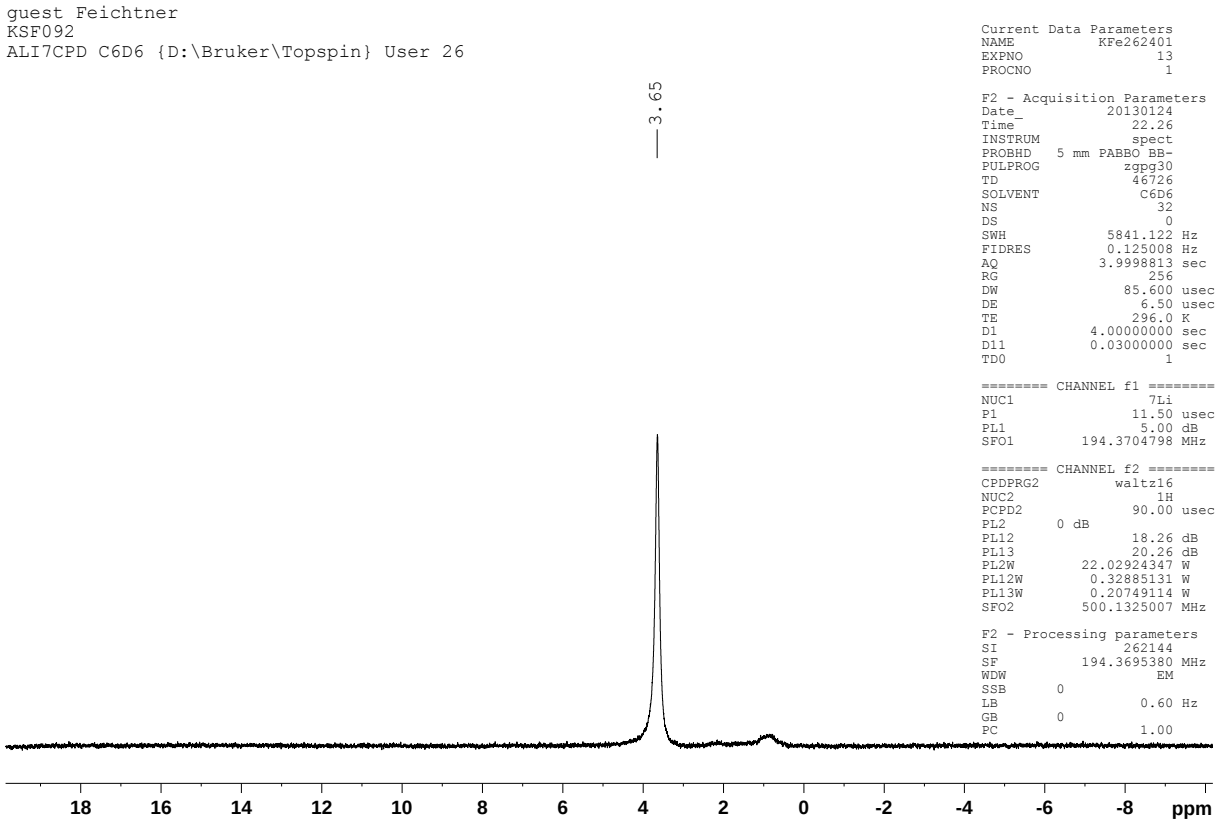


Figure S2a. $^{31}P\{^{1}H\}$ and ^{1}H NMR spectra of $BIPM^{Tol}$ in C_6D_6.



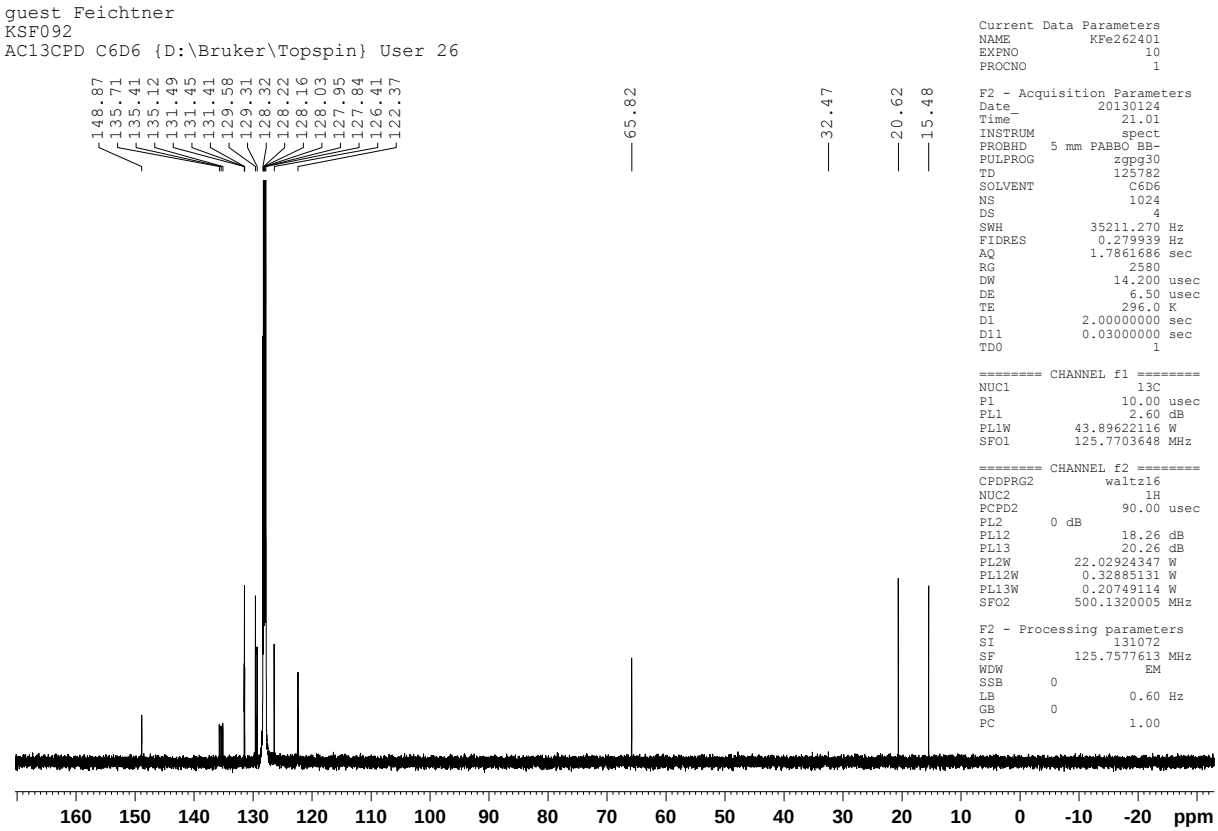
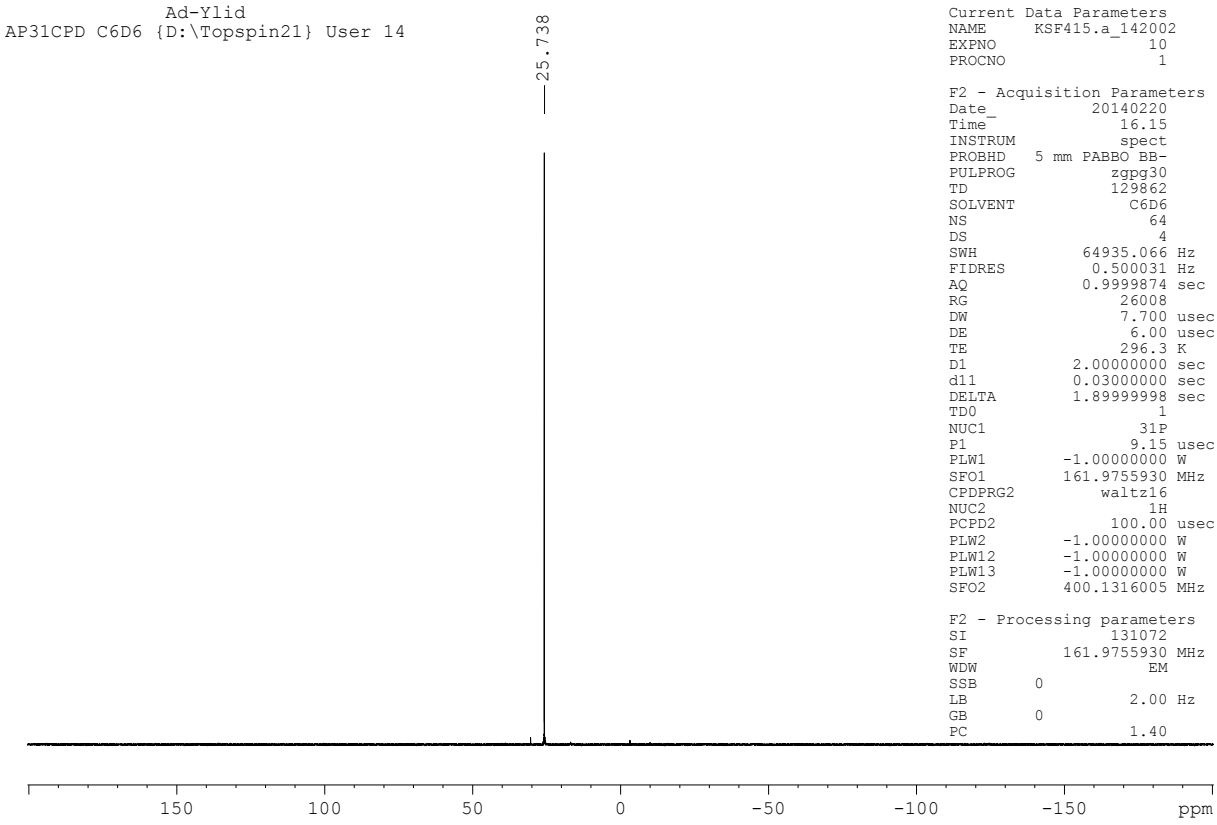


Figure S2b. ^{7}Li and $^{13}C\{^{1}H\}$ NMR spectra of BIPM^{Tol} in C_6D_6.



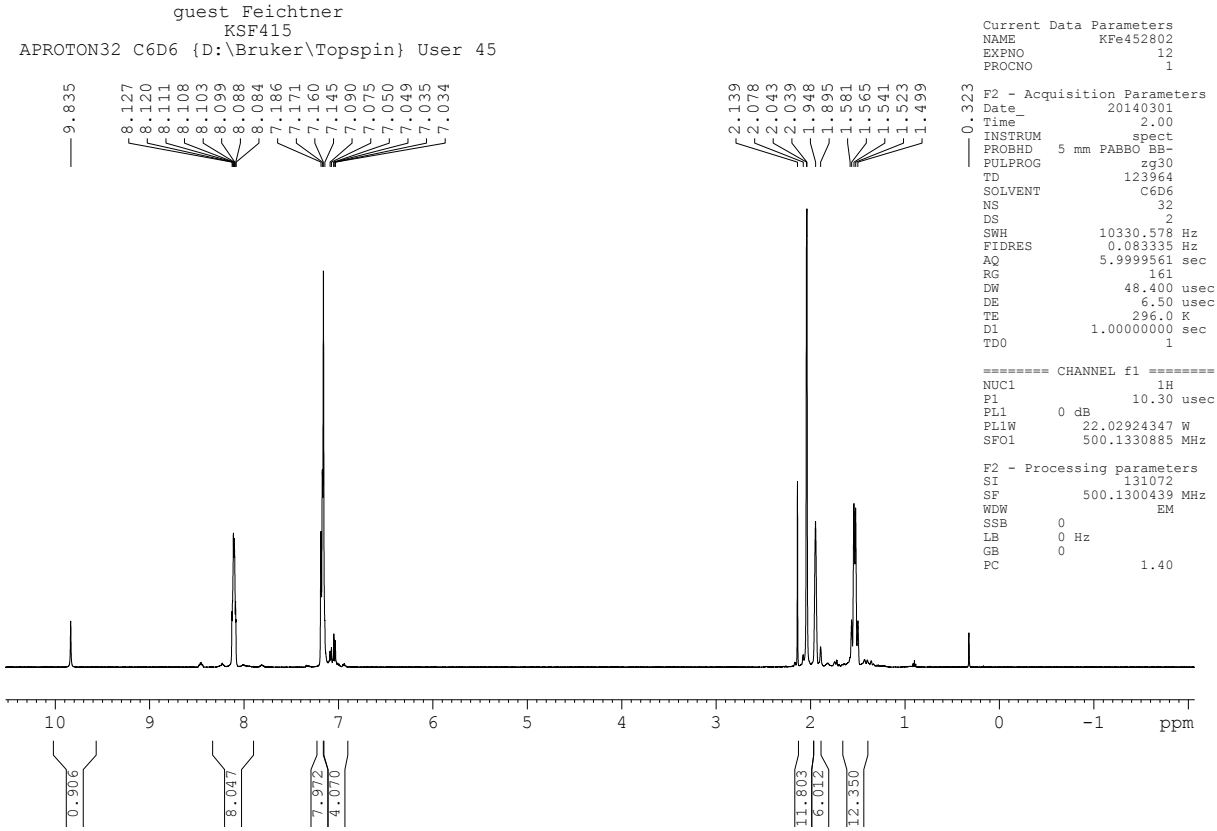
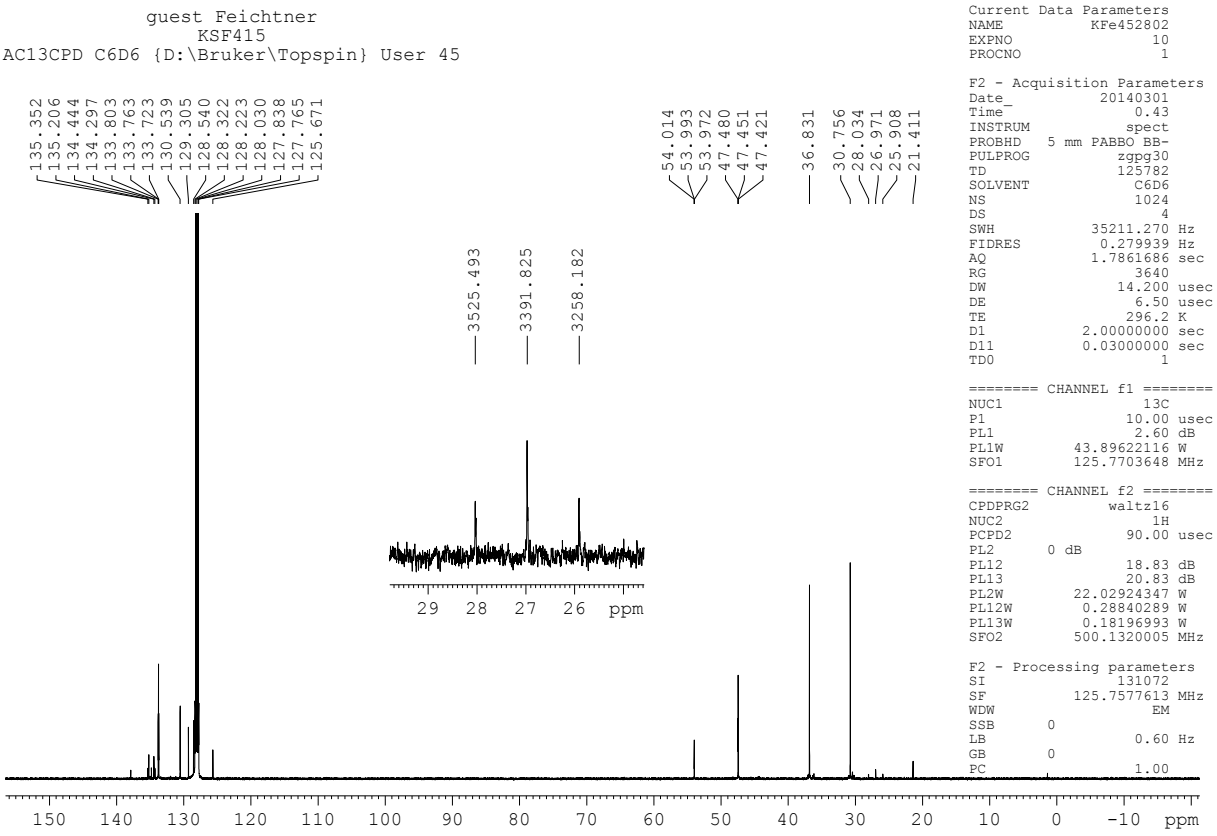


Figure S3a. $^{31}P\{^{1}H\}$ and ^{1}H NMR spectra of **5a** in C_6D_6.



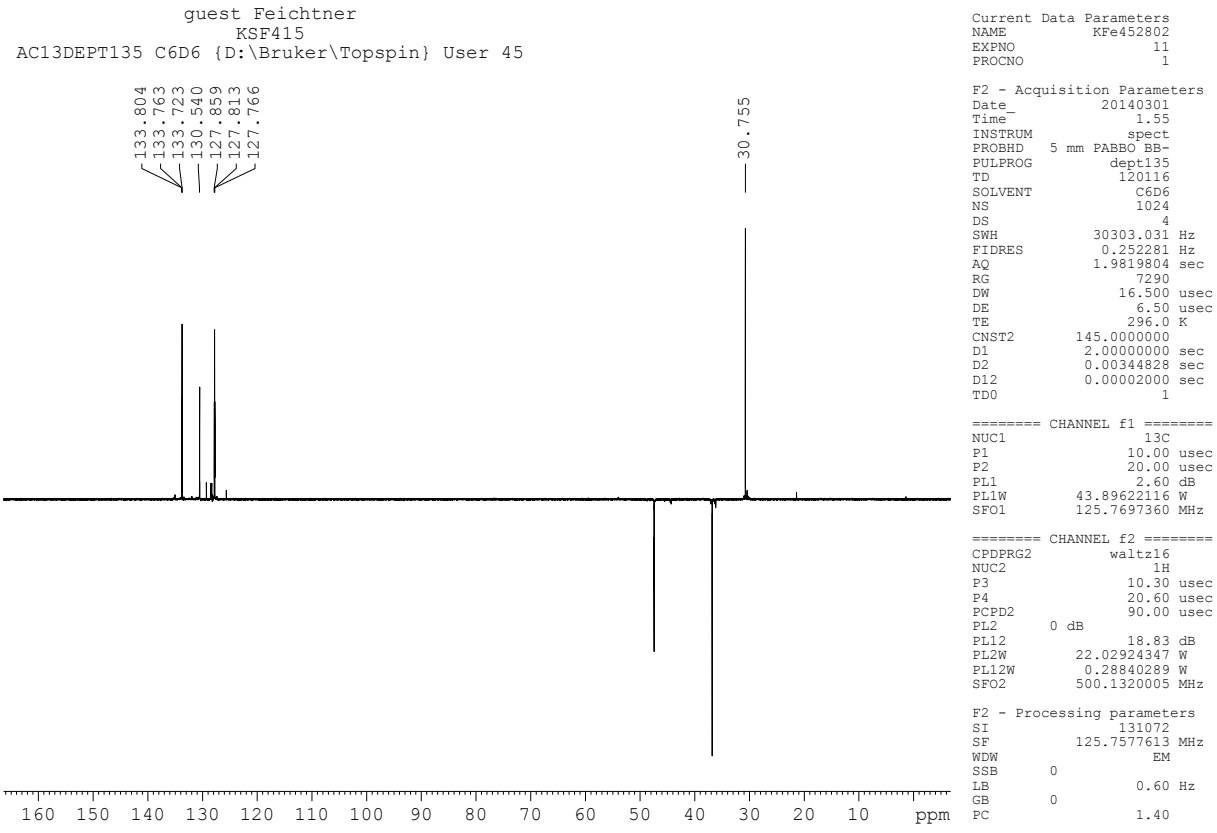
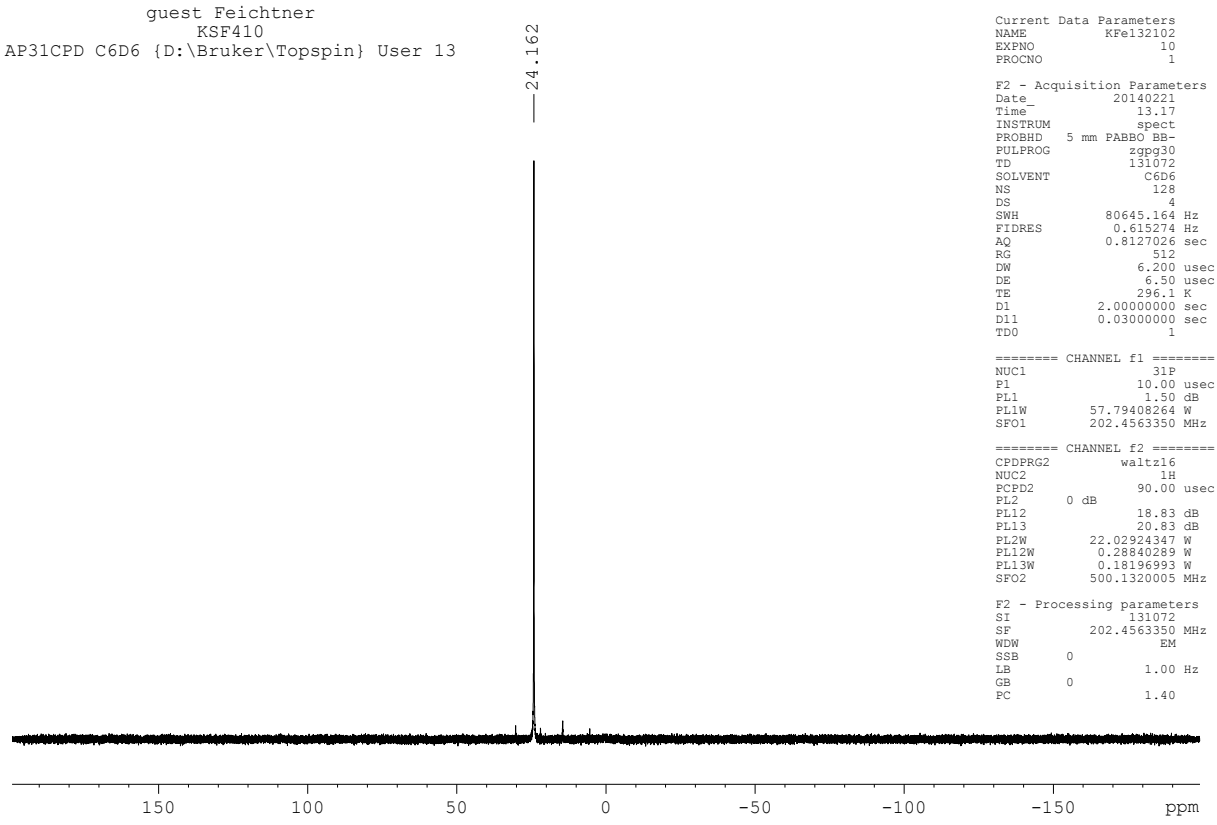


Figure S3b. $^{13}C\{^{1}H\}$ and ^{13}C-DEPT135 NMR spectra of **5a** in C_6D_6.



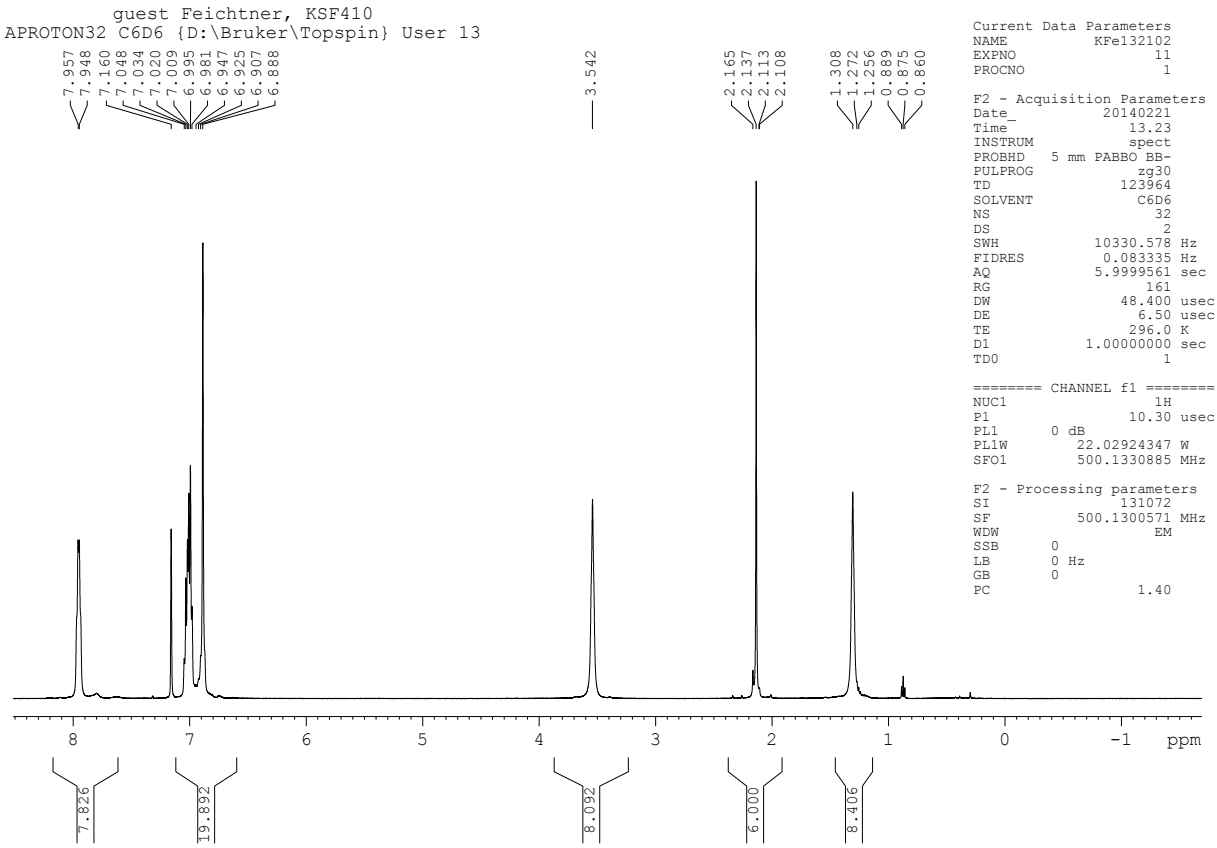
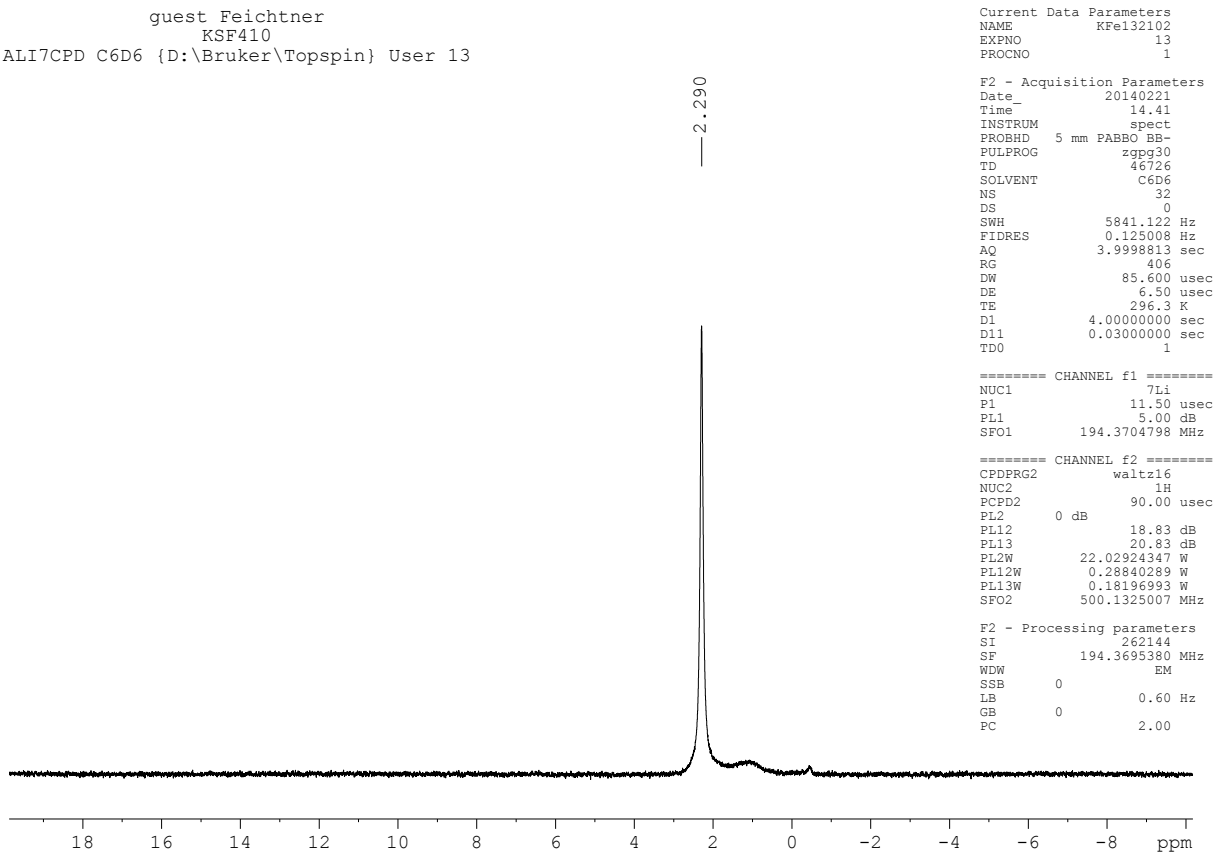


Figure S4a. $^{31}P\{^{1}H\}$ and ^{1}H NMR spectra of **4a** in C_6D_6.



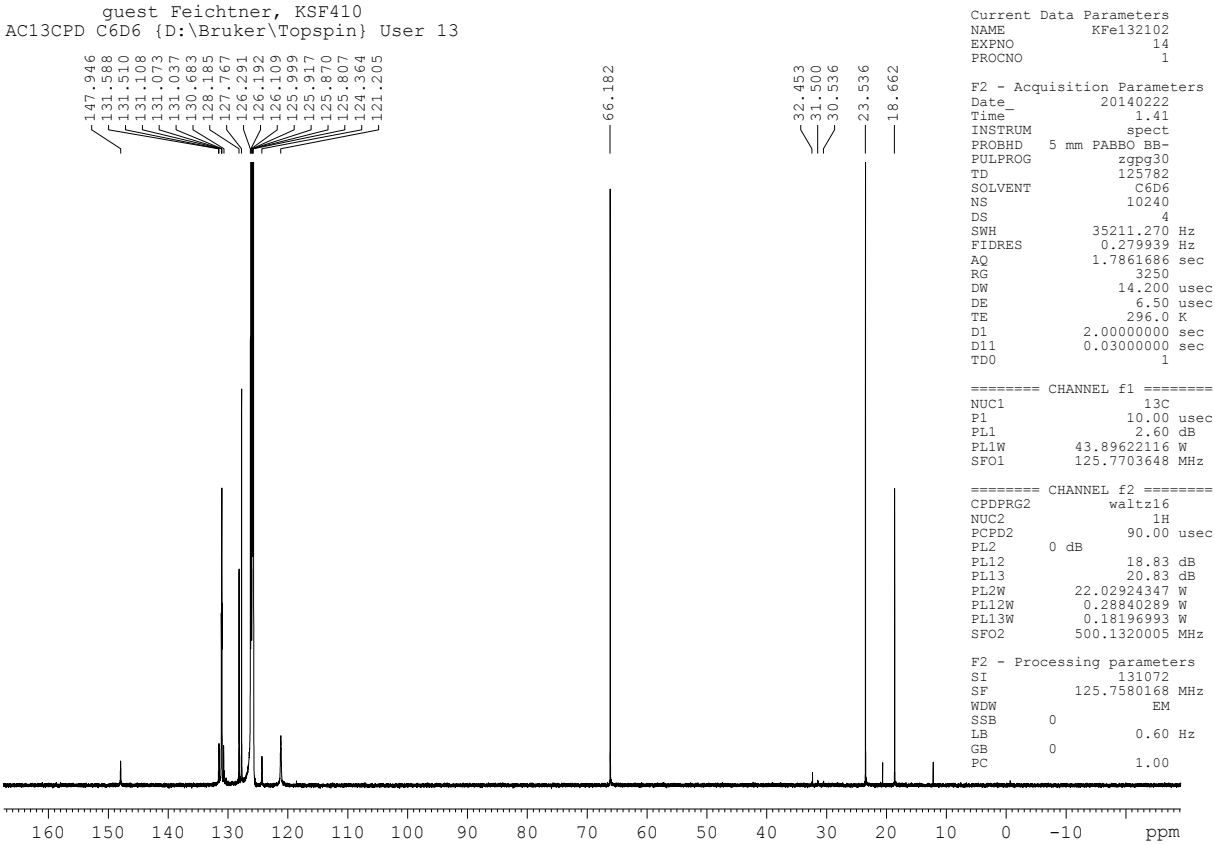
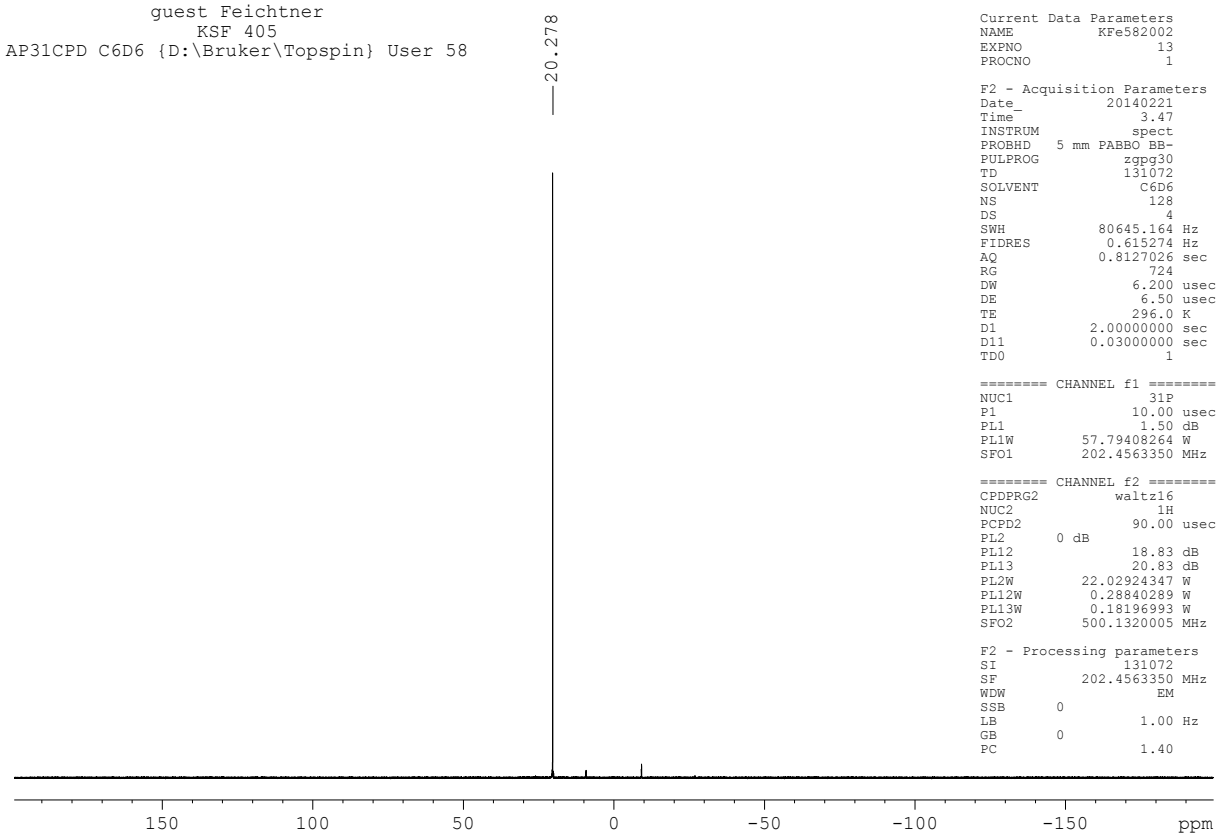


Figure S4b. ^{7}Li and $^{13}C\{^{1}H\}$ NMR spectra of **4a** in C_6D_6.



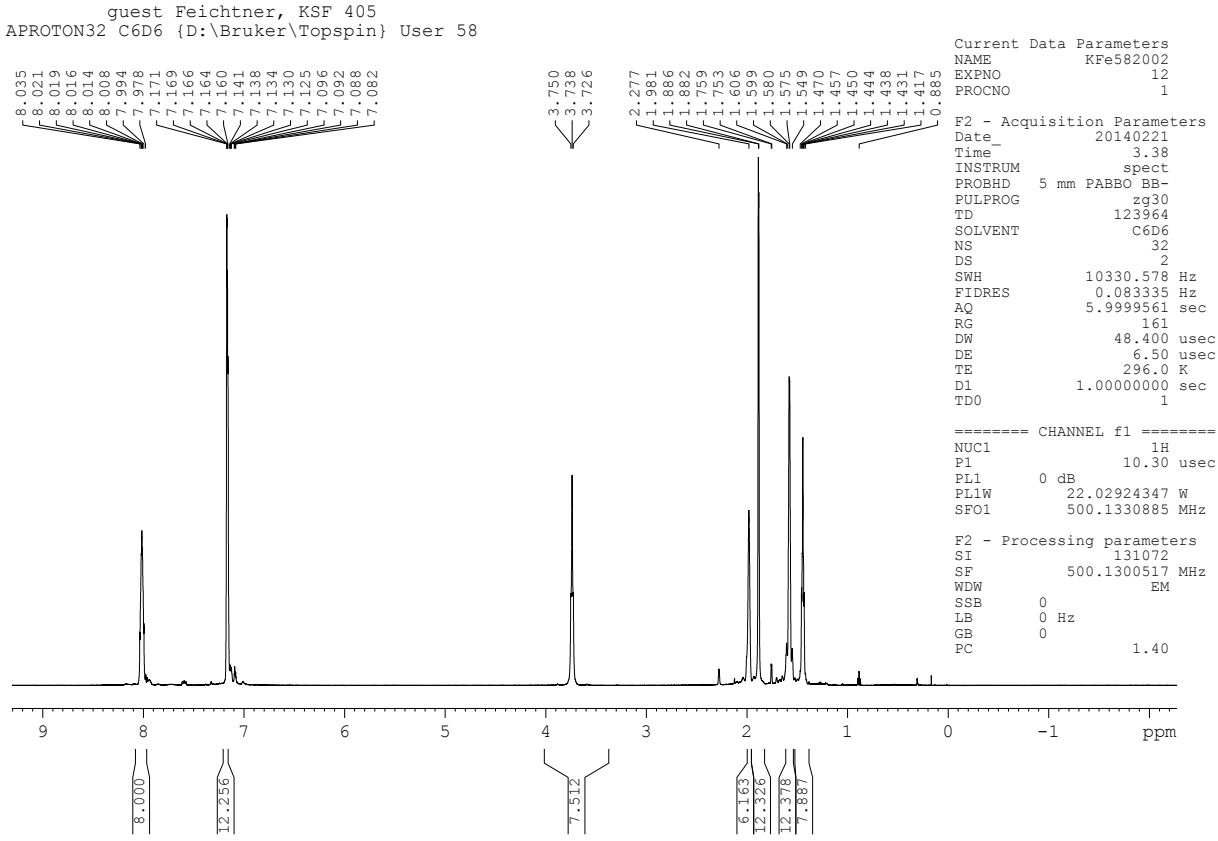


Figure S5a. $^{31}P\{^{1}H\}$ and ^{1}H NMR spectra of **4b** in C_6D_6.

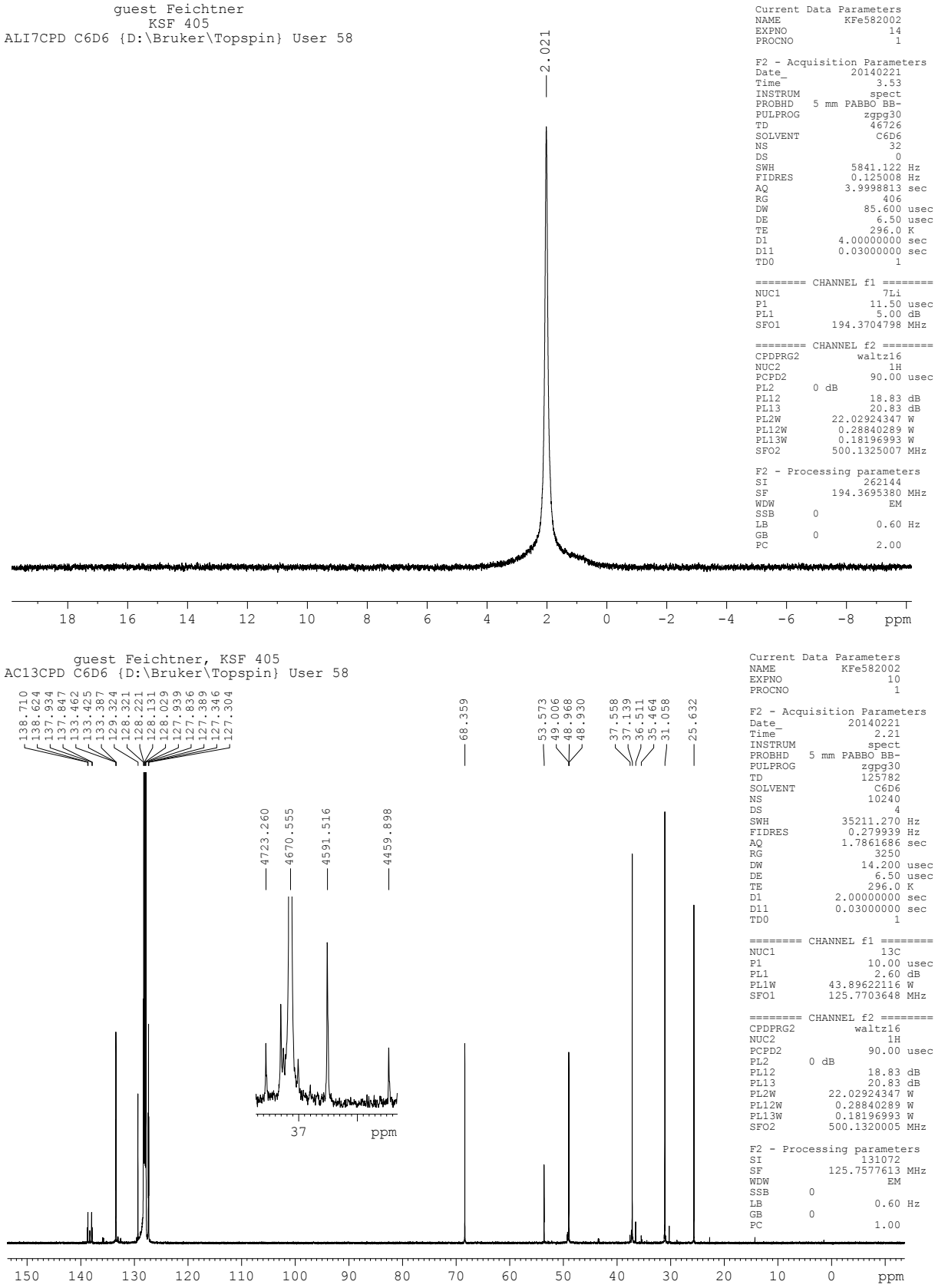


Figure S5b. ^{7}Li and $^{13}C\{^{1}H\}$ NMR spectra of **4b** in C_6D_6.

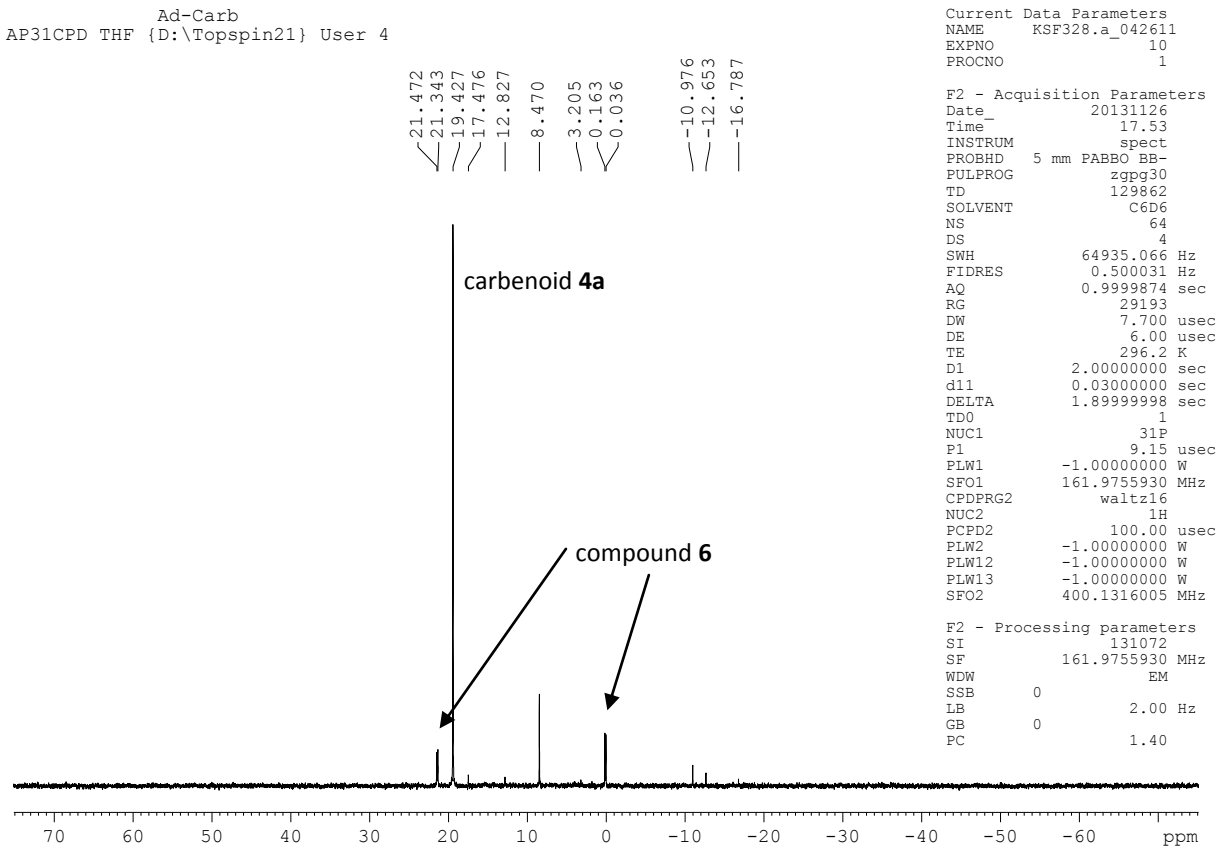


Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of the decomposition of **4a** in C_6D_6 (formation of **6**).

2. Crystal Structure Determination

Data collection of all compounds was conducted with a Bruker APEX-CCD (D8 three-circle goniometer) (Bruker AXS), cell determination and refinement with Smart version 5.622 (Bruker AXS, 2001), integration with SaintPlus version 6.02 (Bruker AXS, 1999); empirical absorption correction with Sadabs version 2.01 (Bruker AXS, 1999). The crystals of all two compounds were mounted in an inert oil (perfluoropolyalkylether). Crystal structure determinations were effected at –100 °C (type of radiation: Mo-K_α, α = 0.71073 Å). The structures were solved applying direct and fourier methods, using SHELXS-90 (G. M. Sheldrick, University of Göttingen 1990) and SHELXL-97 (G. M. Sheldrick, SHELXL97, University of Göttingen 1997). Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-990196 (compound **2a**), CCDC-990197 (compound **3a**), CCDC-990198 (compound **3a(THF)**), CCDC-990199 (compound **3b**), CCDC-990400 (compound **4b**), CCDC-990200 (compound **5a**), and CCDC-990201 (**6a**). 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 S1a Data collection and structure refinement details for compounds **2, 3a** and **3a(THF)**.

Compound	**2a**	**3a**	**3a (THF)**	**3b**
CCDC No.	CCDC 990196	CCDC 990197	CCDC 990198	CCDC 990199
Formula	$C_{46}H_{54}Cl_2N_2P_2$	$C_{98}H_{120}Li_4N_4O_2P_4$	$C_{110}H_{140}Li_4N_4O_5P_4$	$C_{96}H_{104}Li_4N_4O_{4.50}P_4$
Formula weight [g·mol^{-1}]	767.75	1537.62	1749.90	1537.47
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Wave length [Å]	0.71073	0.71073	0.71073	0.71073
Crystal system	trilcinic	trilcinic	triclinic	monoclinic
Space group	*P*-1 (2)	*P*-1 (2)	*P*-1 (2)	*P*2(1)/n (14)
a [Å]	10.1916(4)	15.2691(6)	12.9112(5)	23.2710(12)
b [Å]	11.1132(5)	15.6945(6)	15.4801(6)	16.1806(8)
c [Å]	18.1884(7)	17.5037(7)	23.1811(9)	45.312(2)
α [°]	90.3220(10)	86.1380(10)	90.009(2)	90
β [°]	106.2020(10)	89.8310(10)	92.105(2)	101.3850(10)
γ [°]	91.2680(10)	86.2670(10)	90.346(2)	90
Volume [Å^3]	1977.59(14)	4176.2(3)	4629.9(3)	16726.1(14)
Z	2	2	2	8
Calc. density [Mg·m^{-3}]	1.289	1.223	1.255	1.221
μ ($Mo_{K\alpha}$) [mm^{-1}]	0.281	0.143	0.140	0.146
F(000)	816	1648	1880	6528
Crystal dimensions [mm]	0.32 x 0.31 x 0.28	0.32 x 0.30 x 0.21	0.32 x 0.22 x 0.08	0.25 x 0.22 x 0.21
Theta range [°]	1.83 to 25.00	1.17 to 25.00	1.32 to 25.00	1.34 to 25.00
Index ranges	$-12 \le h \le 12$	$-18 \le h \le 18$	$-15 \le k \le 15$	$-27 \le k \le 27$
	$-13 \le k \le 13$	$-18 \le k \le 18$	$-18 \le k \le 18$	$-19 \le k \le 19$
	$-21 \le l \le 20$	$-20 \le l \le 20$	$-27 \le k \le 27$	$-53 \le k \le 53$
Reflections collected	17442	55213	62666	203987
Independent reflections	6927 [R_{int} = 0.0205]	14710 [R_{int}= 0.0357]	16268 [R_{int}= 0.0653]	29458 [R_{int}= 0.0704]
Data/Restraints/Parameter	6927 / 0 / 469	14710 / 0 / 1024	16268 / 24 / 1168	29458 / 0 / 2097

Goodness-of-fit on F^2	1.023	1.034	1.052	1.065
Final R indices [I>2sigma(I)]	*R*1 = 0.0378 w*R*2 = 0.0955	*R*1 = 0.0385 w*R*2 = 0.0906	*R*1 = 0.0732 w*R*2 = 0.2015	*R*1 = 0.0531 w*R*2 = 0.1163
R indices (all data)	*R*1 = 0.0474 w*R*2 = 0.1018	*R*1 = 0.0553 w*R*2 = 0.0993	*R*1 = 0.1297 w*R*2 = 0.2395	*R*1 = 0.0867 w*R*2 = 0.1339
Largest diff. peak and hole	0.560 and –0.658	0.341 and –0.360	0.977 and –0.844	0.678 and –0.520

Table S1b Data collection and structure refinement details for compounds **4b, 5a,** and **6a**.

Compound	**4b**	**5a**	**6a**
CCDC No.	CCDC 990400	CCDC 990200	CCDC 990201
Formula	$C_{43}H_{44}ClLiN_2OP_2$	$C_{49}H_{59}ClN_2OP_2$	$C_{53}H_{66}N_2O_2P_2$
Formula weight [g·mol^{-1}]	709.13	789.37	825.02
Temperature [K]	100(2)	100(2)	100(2)
Wave length [Å]	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P*-1 (2)	*P*2(1)/n (14)	*P*2(1)/c (14)
a [Å]	9.1841(13)	10.5406(4)	19.5729(9)
b [Å]	13.989(2)	18.6971(7)	22.0037(11)
c [Å]	15.738(2)	21.1513(9)	21.0614(10)
α [°]	95.644(5)	90	90
β [°]	105.321(5)	102.9820(10)	102.206(2)
γ [°]	101.501(5)	90	90
Volume [Å^3]	1886.5(5)	4061.9(3)	8865.6(7)
Z	2	4	8
Calc. density [Mg·m^{-3}]	1.248	1.291	1.236
μ ($Mo_{K\alpha}$) [mm^{-1}]	0.222	0.214	0.142
F(000)	748	1688	3552
Crystal dimensions [mm]	0.14 x 0.13 x 0.07	0.29 x 0.25 x 0.21	0.48 x 0.35 x 0.21
Theta range [°]	2.72 to 25.00	1.47 to 25.00	1.41 to 25.00
Index ranges	–10 ≤ k ≤ 10 –16 ≤ k ≤ 16 –18 ≤ k ≤ 18	–12 ≤ k ≤ 12 –22 ≤ k ≤ 22 –25 ≤ k ≤ 25	–23 ≤ k ≤ 23 –26 ≤ k ≤ 26 –25 ≤ k ≤ 25
Reflections collected	22801	39344	104908
Independent reflections	6617 [R_{int}= 0.0487]	7169 [R_{int}= 0.0231]	15601 [R_{int}= 0.0667]
Data/Restraints/Parameter	6617 / 0 / 455	7169 / 26 / 537	15601 / 0 / 1111
Goodness-of-fit on F^2	1.015	1.045	1.071
Final R indices [I>2sigma(I)]	*R*1 = 0.0402 w*R*2 = 0.0848	*R*1 = 0.0342 w*R*2 = 0.0918	*R*1 = 0.0486 w*R*2 = 0.1145
R indices (all data)	*R*1 = 0.0617 w*R*2 = 0.0943	*R*1 = 0.0391 w*R*2 = 0.0958	*R*1 = 0.0808 w*R*2 = 0.1319
Largest diff. peak and hole	0.318 and –0.315	0.476 and –0.403	0.678 and –0.520

2.1 Crystal Structure Determination of **2a**

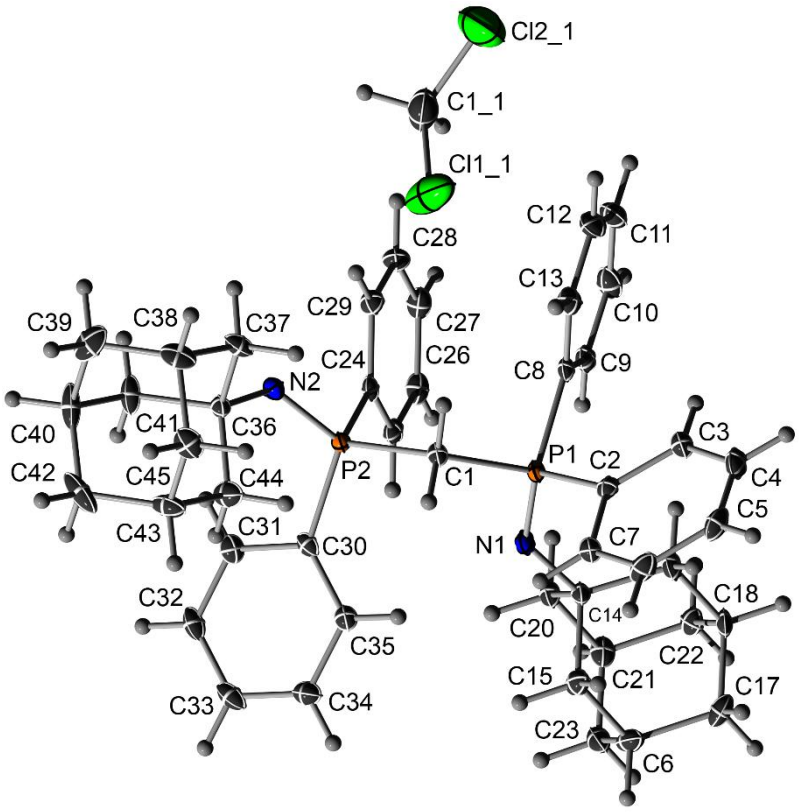


Figure S7. ORTEP Plot of compound **2a**. Ellipsoids are drawn at the 50% probability level.

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

	x	y	z	U(eq)
P(1)	7065(1)	1598(1)	2031(1)	10(1)
P(2)	8227(1)	-848(1)	2861(1)	10(1)
N(1)	5629(2)	984(1)	1798(1)	14(1)
N(2)	9619(2)	-1403(1)	3277(1)	15(1)
C(1)	8323(2)	417(2)	2219(1)	12(1)
C(2)	7550(2)	2528(2)	1316(1)	12(1)
C(3)	7736(2)	3778(2)	1390(1)	16(1)
C(4)	8027(2)	4446(2)	809(1)	20(1)
C(5)	8148(2)	3880(2)	151(1)	21(1)
C(6)	7945(2)	2646(2)	67(1)	21(1)
C(7)	7640(2)	1979(2)	641(1)	16(1)
C(8)	7556(2)	2558(2)	2891(1)	13(1)
C(9)	6598(2)	2811(2)	3280(1)	16(1)
C(10)	6942(2)	3556(2)	3928(1)	22(1)
C(11)	8256(2)	4038(2)	4193(1)	25(1)
C(12)	9223(2)	3779(2)	3815(1)	23(1)
C(13)	8882(2)	3047(2)	3169(1)	17(1)
C(14)	4248(2)	1393(2)	1459(1)	13(1)
C(15)	3700(2)	860(2)	642(1)	19(1)

C(16)	2201(2)	1185(2)	285(1)	23(1)
C(17)	2089(2)	2563(2)	245(1)	22(1)
C(18)	2600(2)	3098(2)	1054(1)	18(1)
C(19)	4101(2)	2771(2)	1402(1)	18(1)
C(20)	3335(2)	902(2)	1939(1)	15(1)
C(21)	1838(2)	1226(2)	1585(1)	18(1)
C(22)	1729(2)	2598(2)	1552(1)	18(1)
C(23)	1323(2)	692(2)	777(1)	23(1)
C(24)	7563(2)	-219(2)	3597(1)	12(1)
C(25)	6164(2)	-222(2)	3517(1)	14(1)
C(26)	5675(2)	287(2)	4085(1)	17(1)
C(27)	6578(2)	805(2)	4729(1)	18(1)
C(28)	7977(2)	811(2)	4815(1)	19(1)
C(29)	8469(2)	299(2)	4250(1)	16(1)
C(30)	6937(2)	-1915(2)	2307(1)	13(1)
C(31)	6789(2)	-2987(2)	2681(1)	17(1)
C(32)	6005(2)	-3940(2)	2280(1)	19(1)
C(33)	5366(2)	-3839(2)	1504(1)	20(1)
C(34)	5488(2)	-2775(2)	1132(1)	19(1)
C(35)	6262(2)	-1812(2)	1532(1)	15(1)
C(36)	10516(2)	-2164(2)	2983(1)	12(1)
C(37)	11897(2)	-1505(2)	3089(1)	17(1)
C(38)	12923(2)	-2319(2)	2862(1)	21(1)
C(39)	13135(2)	-3442(2)	3350(1)	28(1)
C(40)	11768(2)	-4128(2)	3221(1)	28(1)
C(41)	10751(2)	-3317(2)	3459(1)	22(1)
C(42)	11219(2)	-4472(2)	2379(1)	31(1)
C(43)	10992(2)	-3343(2)	1892(1)	23(1)
C(44)	9971(2)	-2537(2)	2132(1)	22(1)
C(45)	12357(2)	-2660(2)	2015(1)	21(1)
C11	12467(3)	2259(2)	4738(1)	41(1)
Cl11	12313(1)	1916(1)	3781(1)	63(1)
Cl21	13471(1)	3555(1)	5047(1)	71(1)

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2**. 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}
P(1)	11(1)	8(1)	13(1)	1(1)	4(1)	0(1)
P(2)	11(1)	9(1)	12(1)	0(1)	3(1)	0(1)
N(1)	13(1)	10(1)	18(1)	3(1)	4(1)	-1(1)
N(2)	17(1)	13(1)	14(1)	-1(1)	3(1)	3(1)
C(1)	11(1)	10(1)	16(1)	1(1)	4(1)	1(1)
C(2)	9(1)	13(1)	14(1)	2(1)	2(1)	1(1)
C(3)	18(1)	12(1)	19(1)	1(1)	5(1)	1(1)
C(4)	22(1)	12(1)	26(1)	7(1)	6(1)	-1(1)
C(5)	21(1)	24(1)	20(1)	12(1)	7(1)	3(1)
C(6)	25(1)	26(1)	14(1)	4(1)	7(1)	7(1)

C(7)	19(1)	12(1)	17(1)	1(1)	2(1)	1(1)
C(8)	18(1)	8(1)	14(1)	3(1)	4(1)	1(1)
C(9)	19(1)	11(1)	16(1)	3(1)	6(1)	0(1)
C(10)	33(1)	17(1)	21(1)	0(1)	12(1)	3(1)
C(11)	40(1)	16(1)	18(1)	-4(1)	5(1)	-3(1)
C(12)	26(1)	17(1)	21(1)	2(1)	2(1)	-7(1)
C(13)	20(1)	16(1)	17(1)	2(1)	6(1)	-2(1)
C(14)	11(1)	9(1)	16(1)	1(1)	2(1)	1(1)
C(15)	18(1)	19(1)	17(1)	-1(1)	3(1)	6(1)
C(16)	22(1)	25(1)	17(1)	-7(1)	-3(1)	7(1)
C(17)	20(1)	26(1)	21(1)	9(1)	4(1)	10(1)
C(18)	18(1)	8(1)	26(1)	4(1)	4(1)	4(1)
C(19)	17(1)	10(1)	26(1)	3(1)	5(1)	-1(1)
C(20)	14(1)	11(1)	20(1)	2(1)	5(1)	0(1)
C(21)	13(1)	16(1)	27(1)	5(1)	7(1)	0(1)
C(22)	15(1)	16(1)	23(1)	0(1)	4(1)	5(1)
C(23)	13(1)	14(1)	37(1)	-3(1)	-3(1)	2(1)
C(24)	16(1)	8(1)	13(1)	3(1)	5(1)	1(1)
C(25)	14(1)	12(1)	15(1)	4(1)	3(1)	-1(1)
C(26)	16(1)	17(1)	22(1)	5(1)	9(1)	3(1)
C(27)	23(1)	18(1)	17(1)	3(1)	11(1)	6(1)
C(28)	22(1)	19(1)	14(1)	-1(1)	3(1)	1(1)
C(29)	14(1)	16(1)	18(1)	1(1)	4(1)	1(1)
C(30)	11(1)	11(1)	18(1)	-3(1)	6(1)	0(1)
C(31)	17(1)	16(1)	19(1)	1(1)	8(1)	0(1)
C(32)	19(1)	12(1)	31(1)	2(1)	12(1)	-1(1)
C(33)	14(1)	16(1)	31(1)	-8(1)	9(1)	-3(1)
C(34)	16(1)	21(1)	18(1)	-5(1)	3(1)	-1(1)
C(35)	14(1)	13(1)	18(1)	1(1)	5(1)	1(1)
C(36)	12(1)	10(1)	15(1)	0(1)	3(1)	1(1)
C(37)	20(1)	15(1)	17(1)	-4(1)	7(1)	-6(1)
C(38)	14(1)	25(1)	25(1)	-6(1)	9(1)	-7(1)
C(39)	18(1)	40(1)	26(1)	4(1)	7(1)	14(1)
C(40)	31(1)	16(1)	45(1)	14(1)	23(1)	12(1)
C(41)	22(1)	15(1)	33(1)	10(1)	16(1)	5(1)
C(42)	26(1)	14(1)	61(2)	-12(1)	24(1)	-2(1)
C(43)	17(1)	25(1)	24(1)	-12(1)	4(1)	1(1)
C(44)	17(1)	25(1)	22(1)	-8(1)	2(1)	6(1)
C(45)	24(1)	21(1)	22(1)	-2(1)	13(1)	0(1)
C11	52(2)	31(1)	39(1)	9(1)	12(1)	12(1)
Cl11	56(1)	84(1)	41(1)	-21(1)	-4(1)	41(1)
Cl21	64(1)	51(1)	86(1)	-26(1)	-1(1)	2(1)

2.2 Crystal Structure Determination of **3a**

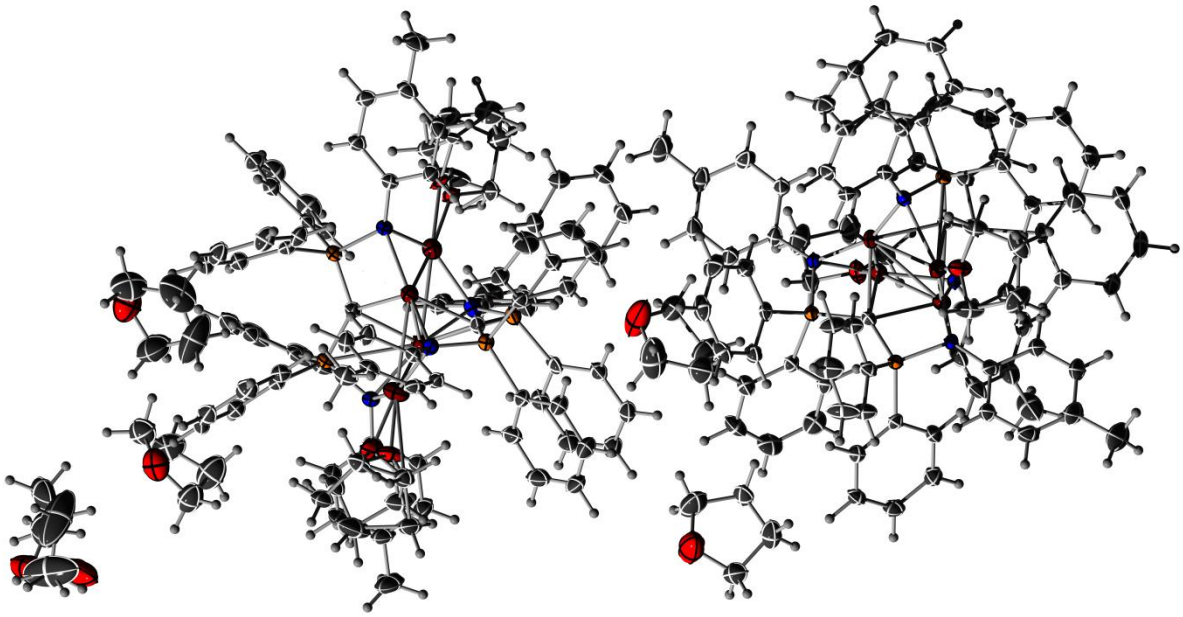


Figure S8. ORTEP Plot of compound **3a**. Ellipsoids are drawn at the 50% probability level (for the solvent molecules at the 30 % probability level).

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **3a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	2331(1)	6091(1)	1522(1)	11(1)
P(2)	4149(1)	6501(1)	2109(1)	13(1)
N(1)	1390(1)	6561(1)	1747(1)	12(1)
N(2)	4341(1)	7210(1)	2713(1)	15(1)
C(1)	2374(1)	4917(1)	1694(1)	13(1)
C(2)	2184(1)	4358(1)	1140(1)	16(1)
C(3)	2244(1)	3478(1)	1305(1)	20(1)
C(4)	2492(1)	3141(1)	2031(1)	23(1)
C(5)	2676(1)	3687(1)	2590(1)	21(1)
C(6)	2617(1)	4566(1)	2425(1)	16(1)
C(7)	2580(1)	6224(1)	499(1)	14(1)
C(8)	2215(1)	6942(1)	67(1)	18(1)
C(9)	2480(1)	7130(1)	-681(1)	25(1)
C(10)	3113(1)	6601(1)	-1015(1)	28(1)
C(11)	3479(1)	5888(1)	-597(1)	24(1)
C(12)	3222(1)	5705(1)	152(1)	18(1)
C(13)	3039(1)	6595(1)	2056(1)	13(1)
C(14)	4580(1)	5420(1)	2444(1)	16(1)
C(15)	4689(1)	4753(1)	1952(1)	20(1)
C(16)	4956(1)	3930(1)	2227(1)	27(1)
C(17)	5104(1)	3746(1)	3002(1)	31(1)
C(18)	4976(1)	4390(1)	3502(1)	27(1)
C(19)	4721(1)	5222(1)	3224(1)	20(1)
C(20)	4738(1)	6690(1)	1199(1)	15(1)
C(21)	5551(1)	6290(1)	1031(1)	19(1)
C(22)	5971(1)	6492(1)	343(1)	24(1)
C(23)	5585(1)	7095(1)	-183(1)	27(1)
C(24)	4782(1)	7506(1)	-22(1)	25(1)

C(25)	4362(1)	7303(1)	663(1)	19(1)
C(26)	496(1)	6342(1)	1545(1)	13(1)
C(27)	172(1)	5650(1)	2123(1)	19(1)
C(28)	-791(1)	5480(1)	1962(1)	25(1)
C(29)	-871(1)	5174(1)	1154(1)	25(1)
C(30)	-568(1)	5867(1)	571(1)	19(1)
C(31)	393(1)	6039(1)	734(1)	15(1)
C(32)	-1150(1)	6692(1)	636(1)	22(1)
C(33)	-1070(1)	6997(1)	1445(1)	23(1)
C(34)	-1365(1)	6309(2)	2029(1)	28(1)
C(35)	-105(1)	7159(1)	1594(1)	18(1)
C(36)	5186(1)	7575(1)	2868(1)	14(1)
C(37)	5093(1)	7968(1)	3646(1)	16(1)
C(38)	5903(1)	8444(1)	3841(1)	18(1)
C(39)	6702(1)	7801(1)	3884(1)	23(1)
C(40)	6823(1)	7399(1)	3117(1)	22(1)
C(41)	5995(1)	6938(1)	2924(1)	19(1)
C(42)	5360(1)	8297(1)	2254(1)	17(1)
C(43)	6185(1)	8750(1)	2442(1)	19(1)
C(44)	6054(1)	9146(1)	3211(1)	19(1)
C(45)	6976(1)	8095(1)	2486(1)	23(1)
Li(1)	1828(2)	7737(2)	1826(2)	22(1)
Li(2)	1848(2)	6682(2)	2874(2)	19(1)
Li(3)	3232(2)	8009(2)	2290(2)	22(1)
Li(4)	3254(2)	6969(2)	3332(2)	22(1)
P11	1876(1)	9089(1)	2688(1)	12(1)
P21	1885(1)	7722(1)	4040(1)	11(1)
N11	2232(1)	8937(1)	1826(1)	15(1)
N21	2201(1)	6714(1)	4013(1)	13(1)
C11	2402(1)	9971(1)	3115(1)	13(1)
C21	3252(1)	9789(1)	3401(1)	19(1)
C31	3704(1)	10399(1)	3739(1)	24(1)
C41	3311(1)	11210(1)	3808(1)	24(1)
C51	2473(1)	11410(1)	3524(1)	20(1)
C61	2022(1)	10800(1)	3177(1)	16(1)
C71	705(1)	9438(1)	2734(1)	14(1)
C81	328(1)	9761(1)	3392(1)	17(1)
C91	-573(1)	9917(1)	3456(1)	23(1)
C101	-1117(1)	9743(1)	2863(1)	27(1)
C111	-759(1)	9417(1)	2208(1)	28(1)
C121	143(1)	9270(1)	2144(1)	21(1)
C131	2080(1)	8102(1)	3131(1)	14(1)
C141	748(1)	7883(1)	4373(1)	13(1)
C151	90(1)	7673(1)	3876(1)	16(1)
C161	-787(1)	7759(1)	4080(1)	21(1)
C171	-1027(1)	8067(1)	4779(1)	21(1)
C181	-386(1)	8276(1)	5279(1)	20(1)
C191	496(1)	8176(1)	5077(1)	16(1)
C201	2526(1)	8265(1)	4726(1)	15(1)
C211	2294(1)	9093(1)	4936(1)	18(1)
C221	2854(1)	9524(1)	5375(1)	23(1)
C231	3665(1)	9140(1)	5602(1)	25(1)
C241	3907(1)	8325(1)	5394(1)	24(1)
C251	3345(1)	7893(1)	4964(1)	18(1)
C261	2391(1)	9585(1)	1196(1)	16(1)
C271	2242(1)	9175(1)	438(1)	23(1)
C281	2452(2)	9782(1)	-258(1)	30(1)
C291	1857(2)	10600(1)	-243(1)	34(1)
C301	2009(2)	11028(1)	500(1)	31(1)
C311	1797(1)	10414(1)	1190(1)	23(1)
C321	3352(1)	9821(1)	1211(1)	22(1)
C331	3562(1)	10434(1)	523(1)	30(1)

C341	3412(2)	9997(2)	-216(1)	33(1)
C351	2962(2)	11248(1)	539(1)	35(1)
C361	2107(1)	6004(1)	4605(1)	14(1)
C371	1866(1)	6275(1)	5408(1)	19(1)
C381	1812(1)	5489(1)	5980(1)	21(1)
C391	1104(1)	4924(1)	5712(1)	23(1)
C401	1337(1)	4634(1)	4918(1)	21(1)
C411	1396(1)	5424(1)	4353(1)	17(1)
C421	2698(1)	4975(1)	6022(1)	25(1)
C431	2933(1)	4674(1)	5227(1)	23(1)
C441	2222(1)	4118(1)	4954(1)	24(1)
C451	2984(1)	5461(1)	4657(1)	18(1)
O12	6390(1)	1918(1)	2491(1)	35(1)
C12	7667(2)	2457(3)	2994(2)	84(1)
C22	7301(2)	1731(2)	2643(1)	48(1)
C32	6026(2)	1272(2)	2102(2)	50(1)
C42	5047(2)	1416(2)	2088(2)	63(1)
C13	385(2)	3429(2)	3260(1)	46(1)
C23	94(2)	3261(2)	2477(2)	48(1)
O1A3	222(3)	2259(3)	2577(3)	40(1)
C3A3	-225(4)	1856(4)	2016(3)	50(1)
C4A3	-52(5)	2133(5)	1212(5)	64(1)
O1B3	19(3)	2496(2)	2243(2)	40(1)
C3B3	-232(4)	2465(4)	1466(3)	50(1)
C4B3	-428(4)	1557(3)	1321(4)	64(1)

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3a**. 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}
P(1)	11(1)	11(1)	12(1)	-2(1)	1(1)	-1(1)
P(2)	11(1)	13(1)	16(1)	-2(1)	2(1)	-1(1)
N(1)	11(1)	13(1)	14(1)	-4(1)	-1(1)	-1(1)
N(2)	10(1)	17(1)	18(1)	-5(1)	1(1)	-2(1)
C(1)	9(1)	13(1)	18(1)	-1(1)	4(1)	0(1)
C(2)	14(1)	17(1)	17(1)	-2(1)	1(1)	-2(1)
C(3)	23(1)	15(1)	23(1)	-5(1)	3(1)	-5(1)
C(4)	28(1)	12(1)	28(1)	1(1)	4(1)	-1(1)
C(5)	22(1)	21(1)	18(1)	4(1)	1(1)	-1(1)
C(6)	15(1)	18(1)	16(1)	-4(1)	2(1)	-2(1)
C(7)	15(1)	14(1)	14(1)	-4(1)	1(1)	-5(1)
C(8)	20(1)	16(1)	17(1)	-3(1)	2(1)	-3(1)
C(9)	33(1)	22(1)	20(1)	4(1)	0(1)	-4(1)
C(10)	39(1)	30(1)	16(1)	1(1)	8(1)	-7(1)
C(11)	28(1)	24(1)	22(1)	-7(1)	10(1)	-3(1)
C(12)	20(1)	16(1)	20(1)	-3(1)	2(1)	-4(1)
C(13)	13(1)	13(1)	15(1)	-3(1)	1(1)	-1(1)
C(14)	7(1)	16(1)	24(1)	0(1)	4(1)	0(1)
C(15)	16(1)	19(1)	26(1)	-2(1)	5(1)	-1(1)
C(16)	23(1)	17(1)	39(1)	-5(1)	9(1)	1(1)
C(17)	22(1)	19(1)	48(1)	9(1)	4(1)	4(1)
C(18)	20(1)	27(1)	31(1)	10(1)	-1(1)	-1(1)
C(19)	13(1)	23(1)	25(1)	0(1)	1(1)	-3(1)
C(20)	15(1)	13(1)	19(1)	-5(1)	3(1)	-5(1)
C(21)	17(1)	18(1)	23(1)	-5(1)	3(1)	-4(1)
C(22)	20(1)	25(1)	27(1)	-10(1)	9(1)	-6(1)
C(23)	28(1)	32(1)	23(1)	-6(1)	11(1)	-14(1)
C(24)	28(1)	26(1)	22(1)	3(1)	1(1)	-10(1)
C(25)	16(1)	18(1)	22(1)	-3(1)	2(1)	-4(1)

C(26)	10(1)	15(1)	15(1)	-3(1)	-1(1)	-1(1)
C(27)	15(1)	25(1)	17(1)	2(1)	-1(1)	-6(1)
C(28)	19(1)	36(1)	22(1)	5(1)	1(1)	-12(1)
C(29)	17(1)	26(1)	32(1)	-4(1)	-5(1)	-7(1)
C(30)	16(1)	25(1)	17(1)	-7(1)	-2(1)	-4(1)
C(31)	14(1)	18(1)	14(1)	-5(1)	1(1)	-1(1)
C(32)	15(1)	29(1)	21(1)	-3(1)	-5(1)	-1(1)
C(33)	13(1)	31(1)	26(1)	-10(1)	-2(1)	5(1)
C(34)	13(1)	52(1)	21(1)	-10(1)	2(1)	-4(1)
C(35)	17(1)	19(1)	18(1)	-7(1)	-2(1)	1(1)
C(36)	9(1)	15(1)	18(1)	-3(1)	-1(1)	-1(1)
C(37)	11(1)	19(1)	18(1)	-2(1)	-1(1)	0(1)
C(38)	16(1)	20(1)	18(1)	-5(1)	-3(1)	-1(1)
C(39)	14(1)	23(1)	31(1)	1(1)	-9(1)	-2(1)
C(40)	8(1)	19(1)	38(1)	-6(1)	-2(1)	1(1)
C(41)	13(1)	16(1)	29(1)	-4(1)	-1(1)	-2(1)
C(42)	18(1)	17(1)	17(1)	-3(1)	0(1)	-3(1)
C(43)	20(1)	16(1)	21(1)	-2(1)	1(1)	-6(1)
C(44)	16(1)	16(1)	26(1)	-7(1)	-4(1)	-2(1)
C(45)	14(1)	25(1)	32(1)	-12(1)	6(1)	-8(1)
Li(1)	31(2)	14(2)	22(2)	-2(1)	0(1)	-5(1)
Li(2)	19(2)	21(2)	17(2)	-2(1)	-1(1)	-3(1)
Li(3)	22(2)	24(2)	21(2)	1(1)	0(1)	-1(1)
Li(4)	19(2)	27(2)	21(2)	-4(1)	2(1)	-2(1)
P11	14(1)	10(1)	12(1)	-2(1)	1(1)	-1(1)
P21	11(1)	13(1)	11(1)	-2(1)	1(1)	-1(1)
N11	21(1)	11(1)	13(1)	-1(1)	3(1)	-1(1)
N21	14(1)	13(1)	13(1)	1(1)	2(1)	-2(1)
C11	16(1)	13(1)	12(1)	-1(1)	2(1)	-2(1)
C21	16(1)	19(1)	21(1)	-2(1)	2(1)	-1(1)
C31	16(1)	31(1)	24(1)	-3(1)	0(1)	-5(1)
C41	28(1)	24(1)	22(1)	-6(1)	2(1)	-13(1)
C51	27(1)	15(1)	20(1)	-5(1)	7(1)	-5(1)
C61	18(1)	15(1)	16(1)	-1(1)	2(1)	-2(1)
C71	15(1)	9(1)	19(1)	2(1)	0(1)	-1(1)
C81	17(1)	14(1)	20(1)	0(1)	0(1)	-1(1)
C91	21(1)	19(1)	30(1)	-2(1)	6(1)	1(1)
C101	14(1)	23(1)	44(1)	-1(1)	-1(1)	-2(1)
C111	23(1)	28(1)	35(1)	-2(1)	-10(1)	-7(1)
C121	22(1)	20(1)	22(1)	-2(1)	-2(1)	-3(1)
C131	15(1)	12(1)	14(1)	-2(1)	1(1)	0(1)
C141	13(1)	12(1)	13(1)	2(1)	1(1)	-1(1)
C151	17(1)	18(1)	14(1)	-3(1)	1(1)	-2(1)
C161	15(1)	26(1)	22(1)	-2(1)	-4(1)	-4(1)
C171	12(1)	26(1)	24(1)	-1(1)	4(1)	0(1)
C181	21(1)	24(1)	16(1)	-5(1)	6(1)	-1(1)
C191	16(1)	17(1)	15(1)	-2(1)	0(1)	-2(1)
C201	16(1)	20(1)	10(1)	-1(1)	3(1)	-6(1)
C211	18(1)	22(1)	15(1)	-2(1)	1(1)	-3(1)
C221	26(1)	23(1)	20(1)	-8(1)	2(1)	-6(1)
C231	22(1)	36(1)	20(1)	-11(1)	0(1)	-12(1)
C241	16(1)	36(1)	22(1)	-5(1)	-1(1)	-4(1)
C251	15(1)	23(1)	17(1)	-4(1)	3(1)	-3(1)
C261	23(1)	12(1)	13(1)	0(1)	2(1)	-3(1)
C271	37(1)	17(1)	16(1)	-1(1)	0(1)	-5(1)
C281	53(1)	24(1)	13(1)	-1(1)	-1(1)	-10(1)
C291	49(1)	30(1)	23(1)	11(1)	-10(1)	-7(1)
C301	51(1)	16(1)	23(1)	5(1)	-3(1)	3(1)
C311	31(1)	17(1)	21(1)	2(1)	0(1)	3(1)
C321	25(1)	23(1)	19(1)	3(1)	1(1)	-5(1)
C331	34(1)	35(1)	23(1)	5(1)	3(1)	-16(1)
C341	48(1)	32(1)	20(1)	4(1)	11(1)	-7(1)

C351	65(2)	20(1)	21(1)	5(1)	-2(1)	-18(1)
C361	13(1)	14(1)	15(1)	2(1)	0(1)	-1(1)
C371	22(1)	19(1)	16(1)	2(1)	2(1)	-2(1)
C381	23(1)	24(1)	16(1)	5(1)	2(1)	-3(1)
C391	15(1)	24(1)	28(1)	12(1)	1(1)	-1(1)
C401	17(1)	18(1)	27(1)	6(1)	-4(1)	-6(1)
C411	15(1)	17(1)	20(1)	2(1)	-2(1)	-2(1)
C421	20(1)	28(1)	24(1)	11(1)	-6(1)	-5(1)
C431	14(1)	22(1)	31(1)	10(1)	-1(1)	3(1)
C441	26(1)	16(1)	30(1)	7(1)	1(1)	0(1)
C451	13(1)	20(1)	20(1)	3(1)	1(1)	-1(1)
O12	47(1)	29(1)	28(1)	-6(1)	-5(1)	1(1)
C12	59(2)	146(4)	52(2)	-25(2)	-20(2)	-21(2)
C22	48(2)	64(2)	27(1)	19(1)	9(1)	17(1)
C32	89(2)	24(1)	39(2)	-3(1)	3(1)	-17(1)
C42	79(2)	66(2)	47(2)	7(1)	-4(2)	-44(2)
C13	42(1)	53(2)	40(1)	10(1)	10(1)	1(1)
C23	37(1)	51(2)	56(2)	-13(1)	4(1)	11(1)
O1A3	41(2)	20(2)	57(3)	7(2)	4(2)	3(1)
C3A3	48(2)	41(2)	60(3)	-5(2)	5(2)	-3(2)
C4A3	46(3)	46(3)	101(4)	-17(3)	5(3)	4(2)
O1B3	41(2)	20(2)	57(3)	7(2)	4(2)	3(1)
C3B3	48(2)	41(2)	60(3)	-5(2)	5(2)	-3(2)
C4B3	46(3)	46(3)	101(4)	-17(3)	5(3)	4(2)

2.3 Crystal Structure Determination of **3a (THF)**

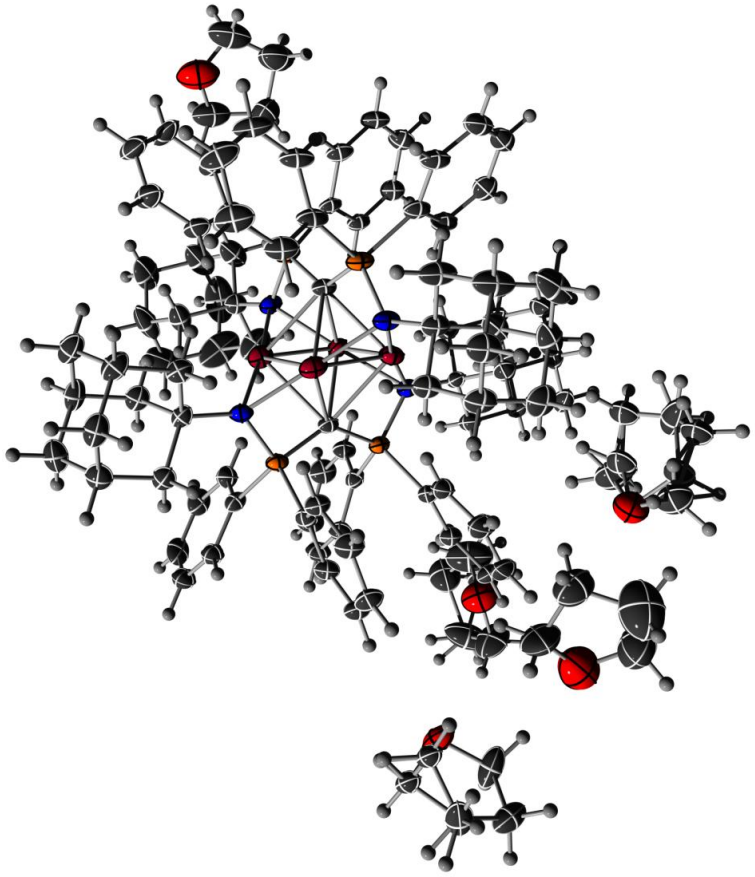


Figure S9. ORTEP Plot of compound **3a x 4 THF**. Ellipsoids are drawn at the 50% probability level.

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **3a (THF)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	8980(1)	3930(1)	1993(1)	22(1)
P(2)	11102(1)	3369(1)	1568(1)	25(1)
N(1)	8361(2)	3504(2)	2524(1)	24(1)
N(2)	11830(2)	2606(2)	1837(1)	25(1)
C(1)	10084(3)	3336(3)	2004(2)	24(1)
C(2)	9175(3)	5103(3)	2073(2)	27(1)
C(3)	8517(4)	5727(3)	1819(2)	39(1)
C(4)	8730(4)	6601(3)	1891(2)	52(1)
C(5)	9585(4)	6870(3)	2226(2)	54(2)
C(6)	10218(4)	6260(3)	2487(2)	43(1)
C(7)	10025(3)	5392(3)	2409(2)	33(1)
C(8)	8268(3)	3848(2)	1294(2)	22(1)
C(9)	7519(3)	3199(3)	1200(2)	25(1)
C(10)	7063(3)	3058(3)	662(2)	28(1)
C(11)	7336(3)	3560(3)	194(2)	34(1)
C(12)	8081(3)	4212(3)	278(2)	34(1)
C(13)	8537(3)	4348(3)	814(2)	30(1)
C(14)	7407(3)	3805(3)	2794(2)	24(1)
C(15)	6845(4)	3005(3)	3012(3)	53(1)
C(16)	5880(4)	3266(4)	3363(4)	80(2)
C(17)	6212(5)	3868(5)	3864(3)	77(2)
C(18)	6714(4)	4634(4)	3633(2)	62(2)
C(19)	7689(3)	4384(3)	3309(2)	41(1)
C(20)	6647(3)	4311(4)	2398(2)	46(1)
C(21)	5678(4)	4553(4)	2724(2)	56(2)
C(22)	5976(4)	5120(4)	3238(2)	63(2)
C(23)	5135(4)	3754(5)	2934(3)	82(2)
C(24)	11756(3)	4427(3)	1583(2)	31(1)
C(25)	12550(3)	4583(3)	1996(2)	35(1)
C(26)	12966(3)	5399(3)	2081(2)	42(1)
C(27)	12610(3)	6089(3)	1741(2)	47(1)
C(28)	11827(3)	5939(3)	1323(2)	42(1)
C(29)	11399(3)	5130(3)	1250(2)	34(1)
C(30)	10768(3)	3191(3)	798(2)	29(1)
C(31)	11263(3)	3583(3)	338(2)	34(1)
C(32)	10963(4)	3400(3)	-228(2)	41(1)
C(33)	10166(4)	2827(3)	-347(2)	42(1)
C(34)	9676(3)	2416(3)	103(2)	37(1)
C(35)	9974(3)	2599(3)	666(2)	31(1)
C(36)	12754(3)	2218(3)	1571(2)	29(1)
C(37)	13399(3)	2844(3)	1212(2)	43(1)
C(38)	14343(3)	2380(4)	966(2)	49(1)
C(39)	15041(3)	2054(3)	1468(2)	40(1)
C(40)	14420(3)	1416(3)	1830(2)	35(1)
C(41)	13468(3)	1881(3)	2061(2)	29(1)
C(42)	12432(3)	1455(3)	1189(2)	38(1)
C(43)	13373(3)	989(4)	949(2)	45(1)
C(44)	13983(4)	1622(4)	593(2)	60(2)
C(45)	14061(3)	659(3)	1450(2)	45(1)
Li(1)	9782(5)	3294(4)	2985(3)	28(2)
Li(2)	11446(5)	2877(5)	2666(3)	30(2)
Li(3)	10511(5)	1901(5)	2061(3)	29(2)
Li(4)	8862(5)	2290(4)	2386(3)	28(2)
P32	9694(1)	869(1)	2868(1)	21(1)
P42	10844(1)	2180(1)	3662(1)	21(1)
N32	9239(2)	1047(2)	2213(1)	23(1)
N42	11133(2)	3168(2)	3501(1)	23(1)
C502	10229(3)	1844(2)	3047(2)	22(1)

C512	8681(3)	536(2)	3360(2)	24(1)
C522	7649(3)	758(3)	3235(2)	29(1)
C532	6882(3)	598(3)	3621(2)	39(1)
C542	7125(3)	218(3)	4152(2)	40(1)
C552	8137(3)	5(3)	4291(2)	36(1)
C562	8910(3)	170(3)	3902(2)	28(1)
C572	10609(3)	-36(3)	2903(2)	25(1)
C582	10380(3)	-874(3)	3090(2)	31(1)
C592	11142(4)	-1515(3)	3105(2)	39(1)
C602	12134(4)	-1323(3)	2932(2)	46(1)
C612	12366(4)	-500(3)	2742(2)	42(1)
C622	11621(3)	134(3)	2729(2)	30(1)
C632	8805(3)	421(2)	1787(2)	23(1)
C642	7953(3)	889(3)	1428(2)	29(1)
C652	7491(4)	308(3)	945(2)	38(1)
C662	8354(4)	50(3)	545(2)	43(1)
C672	9182(4)	-446(3)	893(2)	38(1)
C682	9644(3)	138(3)	1374(2)	32(1)
C692	8312(3)	-389(3)	2038(2)	29(1)
C702	7849(3)	-984(3)	1556(2)	34(1)
C712	8708(4)	-1244(3)	1156(2)	40(1)
C722	7009(4)	-493(3)	1214(2)	38(1)
C732	10081(3)	2089(3)	4313(2)	25(1)
C742	9013(3)	2243(3)	4244(2)	30(1)
C752	8368(3)	2187(3)	4709(2)	36(1)
C762	8762(4)	1966(3)	5249(2)	39(1)
C772	9817(3)	1812(3)	5325(2)	34(1)
C782	10462(3)	1874(3)	4861(2)	29(1)
C792	11993(3)	1523(3)	3835(2)	24(1)
C802	12948(3)	1768(3)	3610(2)	27(1)
C812	13806(3)	1236(3)	3661(2)	34(1)
C822	13740(3)	448(3)	3939(2)	37(1)
C832	12805(3)	195(3)	4165(2)	33(1)
C842	11946(3)	721(3)	4108(2)	27(1)
C852	11548(3)	3872(2)	3887(2)	24(1)
C862	12202(3)	3571(3)	4417(2)	29(1)
C872	12626(3)	4357(3)	4764(2)	33(1)
C882	13306(3)	4922(3)	4380(2)	34(1)
C892	12663(3)	5233(3)	3858(2)	35(1)
C902	12241(3)	4451(3)	3520(2)	27(1)
C912	10657(3)	4429(3)	4095(2)	29(1)
C922	11071(3)	5211(3)	4442(2)	34(1)
C932	11717(3)	4901(3)	4967(2)	37(1)
C942	11743(3)	5771(3)	4059(2)	39(1)
O13	13999(3)	-1703(3)	4532(2)	75(1)
C13	14087(5)	-2587(4)	4412(4)	84(2)
C23	15139(5)	-2878(4)	4582(3)	80(2)
C33	15672(6)	-2079(6)	4823(3)	105(3)
C4A3	14789(7)	-1503(5)	4951(5)	53(3)
C4B3	15100(18)	-1351(16)	4581(18)	45(10)
O14	13198(5)	-1752(4)	1607(2)	112(2)
C24	12820(8)	-1432(6)	640(4)	127(4)
C1A4	13686(12)	-1763(10)	1066(6)	84(4)
C3A4	12026(10)	-1060(9)	929(5)	80(3)
C4A4	11963(15)	-1654(16)	1484(10)	117(6)
C1B4	12370(20)	-1487(18)	1357(10)	84(4)
C3B4	13786(14)	-1491(12)	666(8)	80(3)
C4B4	14206(18)	-1780(17)	1294(10)	117(6)
O1B5	6325(5)	6700(5)	1159(4)	132(2)
C1A5	6139(8)	6736(9)	595(5)	138(4)
C4A5	5619(7)	6060(6)	1380(4)	112(3)
C2B5	5745(9)	5878(8)	399(4)	136(4)

C3B5	5532(8)	5369(6)	942(4)	113(3)
O16	9064(5)	-2418(4)	3443(3)	120(2)
C16	7997(8)	-2136(8)	3215(5)	154(5)
C2A6	7218(15)	-2849(14)	3328(9)	130(5)
C2B6	7200(20)	-2300(20)	3608(13)	130(5)
C36	7846(7)	-3167(8)	3957(4)	144(4)
C46	8878(8)	-3201(6)	3743(5)	131(4)
O17	14765(5)	-2243(6)	3086(3)	147(3)
C17	15117(12)	-1367(6)	3105(5)	171(6)
C27	15307(7)	-1131(6)	2535(5)	116(3)
C37	15606(12)	-1978(10)	2276(7)	205(6)
C47	15007(10)	-2578(7)	2577(5)	144(4)

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3a (THF)**. 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}
P(1)	16(1)	20(1)	31(1)	7(1)	1(1)	3(1)
P(2)	16(1)	29(1)	30(1)	13(1)	4(1)	4(1)
N(1)	17(2)	26(2)	29(2)	5(2)	4(1)	7(1)
N(2)	16(2)	31(2)	28(2)	12(2)	7(1)	7(1)
C(1)	20(2)	24(2)	27(2)	10(2)	3(2)	3(2)
C(2)	25(2)	20(2)	35(2)	6(2)	2(2)	2(2)
C(3)	39(3)	31(3)	45(3)	5(2)	-16(2)	6(2)
C(4)	71(4)	18(3)	64(4)	1(2)	-26(3)	10(2)
C(5)	81(4)	21(3)	58(3)	6(2)	-21(3)	-5(2)
C(6)	49(3)	30(3)	47(3)	6(2)	-16(2)	-3(2)
C(7)	33(2)	27(3)	38(3)	9(2)	-6(2)	2(2)
C(8)	19(2)	20(2)	28(2)	8(2)	2(2)	7(2)
C(9)	21(2)	24(2)	31(2)	8(2)	5(2)	5(2)
C(10)	19(2)	33(2)	32(2)	6(2)	3(2)	1(2)
C(11)	28(2)	41(3)	31(2)	6(2)	-5(2)	4(2)
C(12)	32(2)	36(3)	34(3)	18(2)	2(2)	3(2)
C(13)	24(2)	28(2)	37(3)	12(2)	-2(2)	3(2)
C(14)	16(2)	28(2)	28(2)	3(2)	3(2)	3(2)
C(15)	29(3)	43(3)	89(4)	3(3)	28(3)	-3(2)
C(16)	29(3)	67(4)	146(7)	22(4)	47(4)	6(3)
C(17)	49(4)	137(7)	46(4)	17(4)	22(3)	49(4)
C(18)	50(3)	102(5)	35(3)	-23(3)	-6(2)	38(3)
C(19)	31(2)	56(3)	37(3)	-14(2)	-6(2)	14(2)
C(20)	30(3)	74(4)	34(3)	-1(2)	2(2)	29(2)
C(21)	28(3)	102(5)	39(3)	-7(3)	-4(2)	36(3)
C(22)	51(3)	84(4)	55(4)	-18(3)	2(3)	41(3)
C(23)	17(3)	125(6)	104(5)	-48(5)	11(3)	5(3)
C(24)	23(2)	35(3)	35(2)	15(2)	7(2)	3(2)
C(25)	22(2)	41(3)	42(3)	16(2)	2(2)	2(2)
C(26)	22(2)	46(3)	58(3)	17(2)	-6(2)	-4(2)
C(27)	30(3)	37(3)	72(4)	17(3)	-1(2)	-9(2)
C(28)	29(2)	40(3)	56(3)	28(2)	-2(2)	-3(2)
C(29)	23(2)	40(3)	40(3)	19(2)	2(2)	2(2)
C(30)	23(2)	32(3)	33(2)	13(2)	5(2)	12(2)
C(31)	28(2)	36(3)	38(3)	17(2)	5(2)	9(2)
C(32)	40(3)	50(3)	34(3)	17(2)	11(2)	17(2)
C(33)	44(3)	54(3)	28(3)	5(2)	2(2)	26(2)
C(34)	30(2)	39(3)	41(3)	2(2)	-1(2)	10(2)
C(35)	25(2)	34(3)	34(3)	12(2)	6(2)	7(2)
C(36)	19(2)	36(3)	32(2)	11(2)	6(2)	7(2)
C(37)	24(2)	56(3)	50(3)	29(2)	17(2)	17(2)
C(38)	24(2)	72(4)	52(3)	33(3)	17(2)	18(2)

C(39)	22(2)	54(3)	46(3)	14(2)	10(2)	12(2)
C(40)	17(2)	48(3)	40(3)	12(2)	3(2)	14(2)
C(41)	17(2)	39(3)	32(2)	9(2)	5(2)	7(2)
C(42)	23(2)	58(3)	33(3)	0(2)	3(2)	14(2)
C(43)	29(3)	65(4)	42(3)	-11(3)	0(2)	15(2)
C(44)	34(3)	108(5)	37(3)	9(3)	12(2)	37(3)
C(45)	28(2)	52(3)	54(3)	2(3)	8(2)	19(2)
Li(1)	19(3)	30(4)	35(4)	3(3)	3(3)	2(3)
Li(2)	22(3)	32(4)	37(4)	8(3)	2(3)	2(3)
Li(3)	26(4)	32(4)	29(4)	8(3)	1(3)	4(3)
Li(4)	29(4)	22(4)	32(4)	1(3)	-1(3)	6(3)
P32	21(1)	20(1)	23(1)	5(1)	1(1)	2(1)
P42	18(1)	22(1)	23(1)	4(1)	1(1)	2(1)
N32	22(2)	21(2)	26(2)	5(1)	2(1)	2(1)
N42	19(2)	25(2)	25(2)	4(1)	-2(1)	2(1)
C502	21(2)	20(2)	25(2)	4(2)	2(2)	5(2)
C512	25(2)	19(2)	27(2)	1(2)	4(2)	-1(2)
C522	26(2)	30(3)	30(2)	5(2)	4(2)	-3(2)
C532	24(2)	45(3)	48(3)	6(2)	7(2)	0(2)
C542	34(3)	46(3)	40(3)	12(2)	16(2)	-4(2)
C552	42(3)	35(3)	30(2)	9(2)	4(2)	-4(2)
C562	28(2)	27(2)	28(2)	4(2)	2(2)	-2(2)
C572	30(2)	23(2)	21(2)	2(2)	-1(2)	7(2)
C582	41(3)	26(2)	25(2)	4(2)	-1(2)	4(2)
C592	63(3)	22(3)	31(3)	3(2)	-5(2)	16(2)
C602	55(3)	49(3)	36(3)	7(2)	5(2)	32(3)
C612	41(3)	47(3)	38(3)	8(2)	10(2)	19(2)
C622	31(2)	33(3)	25(2)	6(2)	5(2)	8(2)
C632	25(2)	18(2)	25(2)	4(2)	-1(2)	4(2)
C642	29(2)	25(2)	33(2)	5(2)	-6(2)	4(2)
C652	45(3)	30(3)	39(3)	1(2)	-17(2)	5(2)
C662	61(3)	39(3)	27(3)	2(2)	-7(2)	-6(2)
C672	43(3)	41(3)	30(3)	-9(2)	-1(2)	9(2)
C682	31(2)	35(3)	30(2)	0(2)	-1(2)	7(2)
C692	33(2)	26(2)	28(2)	5(2)	-3(2)	1(2)
C702	44(3)	23(2)	35(3)	3(2)	-9(2)	-1(2)
C712	47(3)	30(3)	41(3)	-9(2)	-12(2)	10(2)
C722	41(3)	29(3)	42(3)	-3(2)	-10(2)	-2(2)
C732	24(2)	20(2)	30(2)	1(2)	6(2)	2(2)
C742	28(2)	32(3)	29(2)	1(2)	4(2)	3(2)
C752	27(2)	39(3)	44(3)	-1(2)	14(2)	5(2)
C762	44(3)	37(3)	38(3)	-1(2)	21(2)	0(2)
C772	40(3)	35(3)	26(2)	5(2)	5(2)	4(2)
C782	31(2)	28(2)	27(2)	3(2)	4(2)	3(2)
C792	22(2)	28(2)	22(2)	0(2)	-3(2)	4(2)
C802	26(2)	25(2)	29(2)	7(2)	1(2)	2(2)
C812	20(2)	42(3)	39(3)	6(2)	3(2)	5(2)
C822	33(3)	37(3)	39(3)	4(2)	-6(2)	13(2)
C832	37(3)	28(3)	33(3)	6(2)	-5(2)	8(2)
C842	27(2)	29(2)	25(2)	6(2)	0(2)	1(2)
C852	18(2)	20(2)	32(2)	-1(2)	-2(2)	-1(2)
C862	26(2)	26(2)	34(2)	-1(2)	-3(2)	0(2)
C872	24(2)	37(3)	37(3)	-2(2)	-5(2)	2(2)
C882	21(2)	33(3)	50(3)	-10(2)	2(2)	0(2)
C892	28(2)	26(3)	52(3)	0(2)	3(2)	-6(2)
C902	20(2)	26(2)	35(2)	4(2)	2(2)	-2(2)
C912	17(2)	32(3)	37(3)	-2(2)	1(2)	3(2)
C922	21(2)	33(3)	48(3)	-14(2)	0(2)	6(2)
C932	25(2)	45(3)	39(3)	-12(2)	2(2)	-2(2)
C942	33(3)	28(3)	55(3)	-6(2)	-9(2)	1(2)
O13	57(3)	55(3)	110(4)	4(2)	-20(2)	7(2)
C13	52(4)	55(4)	145(7)	-31(4)	19(4)	-3(3)

C23	71(4)	59(4)	110(6)	21(4)	20(4)	17(3)
C33	78(5)	136(7)	98(6)	-53(5)	-46(4)	61(5)
C4A3	50(5)	42(4)	66(6)	0(4)	-16(4)	6(3)
C4B3	36(14)	26(14)	70(20)	11(13)	29(14)	-2(10)
O14	139(5)	108(4)	91(4)	12(3)	21(4)	4(4)
C24	148(9)	116(7)	112(7)	-38(6)	-61(6)	60(7)
C1A4	93(10)	109(9)	50(7)	-7(6)	-24(6)	31(7)
C3A4	89(7)	92(8)	59(6)	3(5)	-11(5)	15(6)
C4A4	97(13)	150(14)	103(11)	27(9)	-11(8)	45(10)
C1B4	93(10)	109(9)	50(7)	-7(6)	-24(6)	31(7)
C3B4	89(7)	92(8)	59(6)	3(5)	-11(5)	15(6)
C4B4	97(13)	150(14)	103(11)	27(9)	-11(8)	45(10)
O1B5	97(4)	140(6)	159(7)	51(5)	-5(4)	6(4)
C1A5	118(8)	174(12)	122(9)	65(9)	9(7)	22(8)
C4A5	88(6)	121(8)	127(8)	55(7)	24(5)	22(5)
C2B5	159(10)	139(10)	110(8)	42(7)	19(7)	43(8)
C3B5	138(8)	86(6)	114(7)	-5(6)	-1(6)	21(5)
O16	99(4)	114(5)	148(6)	20(4)	-1(4)	-14(4)
C16	100(8)	176(11)	184(11)	69(9)	-22(7)	-35(7)
C2A6	141(7)	123(8)	127(7)	-4(6)	26(6)	-29(6)
C2B6	141(7)	123(8)	127(7)	-4(6)	26(6)	-29(6)
C36	88(7)	233(13)	110(7)	66(8)	1(5)	-19(7)
C46	144(9)	72(6)	179(10)	20(6)	43(8)	-27(6)
O17	113(5)	189(9)	139(6)	-3(6)	10(4)	19(5)
C17	321(18)	62(6)	130(10)	29(6)	-9(10)	31(8)
C27	109(7)	101(7)	141(9)	23(6)	33(6)	13(5)
C37	212(9)	194(9)	211(9)	-33(8)	56(8)	-36(8)
C47	177(8)	106(6)	152(8)	-5(6)	21(7)	6(6)

2.4 Crystal Structure Determination of **3b**

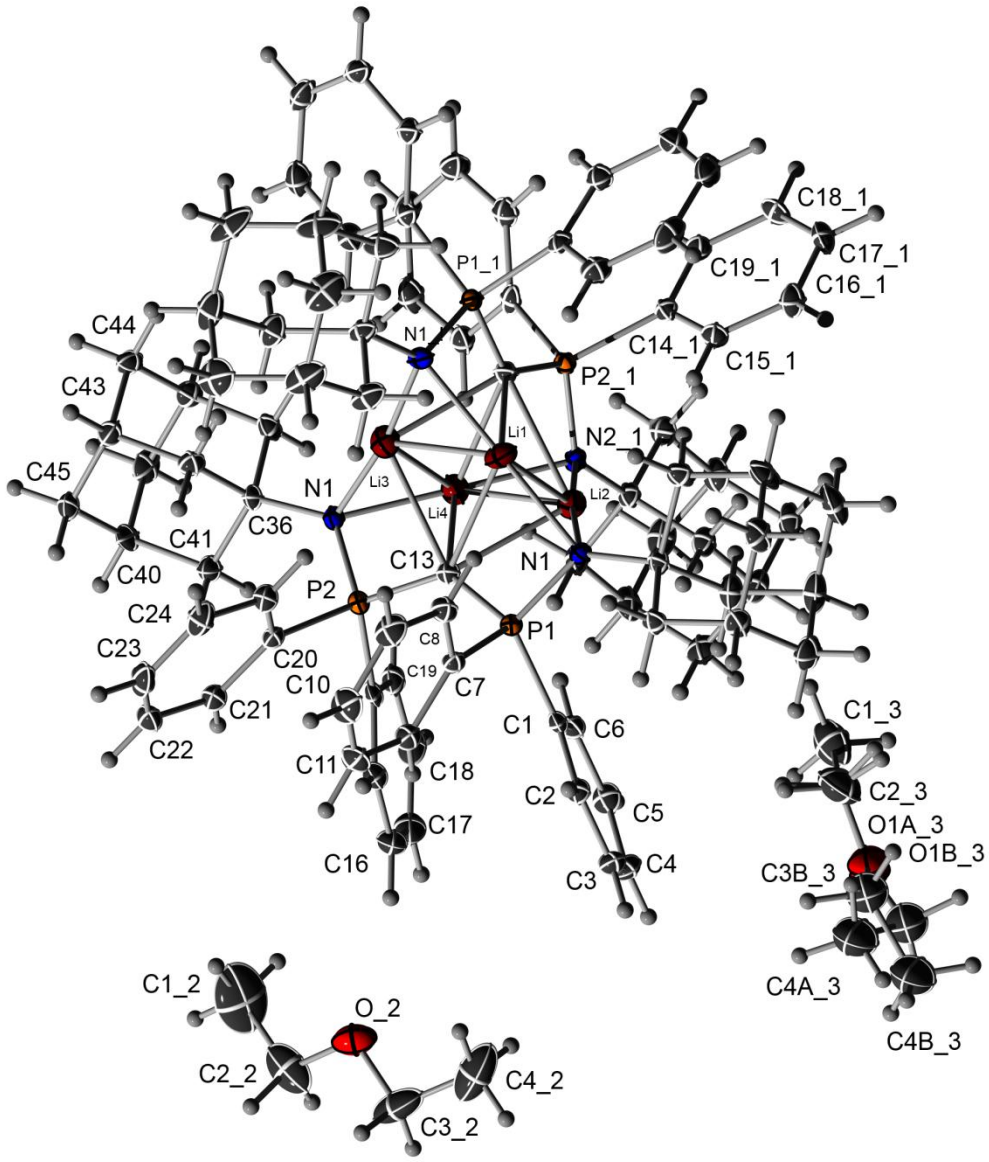


Figure S10. ORTEP Plot of compound **3b**. Ellipsoids are drawn at the 50% probability level.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **3b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	8031(1)	9385(2)	1704(1)	19(1)
C(2)	8002(1)	10681(2)	2155(1)	21(1)
C(3)	8316(1)	11307(2)	2329(1)	25(1)
C(4)	8246(1)	11437(2)	2624(1)	34(1)
C(5)	7853(1)	10966(2)	2744(1)	34(1)
C(6)	7533(1)	10356(2)	2573(1)	31(1)
C(7)	7613(1)	10211(2)	2284(1)	26(1)
C(8)	8701(1)	10935(2)	1692(1)	20(1)
C(9)	8682(1)	11269(2)	1406(1)	26(1)
C(10)	9179(1)	11617(2)	1330(1)	32(1)
C(11)	9697(1)	11635(2)	1535(1)	37(1)
C(12)	9729(1)	11293(2)	1817(1)	34(1)
C(13)	9235(1)	10940(2)	1896(1)	26(1)

C(14)	7333(1)	11541(2)	1436(1)	20(1)
C(15)	6918(1)	11663(2)	1171(1)	29(1)
C(16)	6763(1)	12443(2)	1063(1)	40(1)
C(17)	7005(1)	13149(2)	1207(1)	35(1)
C(18)	7406(1)	13036(2)	1471(1)	29(1)
C(19)	7571(1)	12258(2)	1586(1)	25(1)
C(20)	6848(2)	14004(2)	1080(1)	57(1)
C(21)	8431(1)	8507(2)	2277(1)	21(1)
C(22)	8794(1)	8969(2)	2499(1)	25(1)
C(23)	8719(1)	8952(2)	2795(1)	31(1)
C(24)	8274(1)	8484(2)	2873(1)	31(1)
C(25)	7910(1)	8026(2)	2655(1)	28(1)
C(26)	7988(1)	8032(2)	2359(1)	23(1)
C(27)	9221(1)	8692(2)	1855(1)	21(1)
C(28)	9336(1)	9059(2)	1593(1)	24(1)
C(29)	9899(1)	9091(2)	1537(1)	31(1)
C(30)	10359(1)	8775(2)	1743(1)	37(1)
C(31)	10260(1)	8432(2)	2007(1)	36(1)
C(32)	9695(1)	8387(2)	2063(1)	27(1)
C(33)	8266(1)	6975(2)	1760(1)	19(1)
C(34)	8741(1)	6685(2)	1975(1)	24(1)
C(35)	8851(1)	5848(2)	2017(1)	24(1)
C(36)	8500(1)	5253(2)	1853(1)	24(1)
C(37)	8016(1)	5533(2)	1646(1)	25(1)
C(38)	7900(1)	6369(2)	1602(1)	23(1)
C(39)	8635(1)	4345(2)	1900(1)	34(1)
C(40)	6888(1)	8794(2)	1135(1)	19(1)
C(41)	5621(1)	9093(2)	1046(1)	20(1)
C(42)	5066(1)	8755(2)	940(1)	26(1)
C(43)	4620(1)	9224(2)	774(1)	35(1)
C(44)	4711(1)	10046(2)	716(1)	37(1)
C(45)	5249(1)	10401(2)	827(1)	35(1)
C(46)	5699(1)	9928(2)	986(1)	25(1)
C(47)	6050(1)	7444(2)	1171(1)	20(1)
C(48)	6154(1)	6859(2)	1401(1)	27(1)
C(49)	6036(1)	6028(2)	1340(1)	37(1)
C(50)	5814(1)	5771(2)	1049(1)	35(1)
C(51)	5713(1)	6342(2)	818(1)	31(1)
C(52)	5828(1)	7166(2)	878(1)	25(1)
C(53)	6077(1)	8536(2)	1815(1)	21(1)
C(54)	6349(1)	8527(2)	2120(1)	23(1)
C(55)	6036(1)	8376(2)	2344(1)	29(1)
C(56)	5437(1)	8241(2)	2281(1)	31(1)
C(57)	5161(1)	8267(2)	1979(1)	32(1)
C(58)	5470(1)	8398(2)	1752(1)	28(1)
C(59)	5103(2)	8059(2)	2528(1)	50(1)
C(60)	6638(1)	9411(2)	515(1)	19(1)
C(61)	6103(1)	9157(2)	344(1)	20(1)
C(62)	5749(1)	9703(2)	154(1)	24(1)
C(63)	5917(1)	10517(2)	137(1)	29(1)
C(64)	6442(1)	10785(2)	309(1)	31(1)
C(65)	6800(1)	10237(2)	494(1)	24(1)
C(66)	7064(1)	7719(2)	640(1)	20(1)
C(67)	7230(1)	7090(2)	850(1)	25(1)
C(68)	7259(1)	6274(2)	766(1)	33(1)
C(69)	7111(2)	6068(2)	465(1)	44(1)
C(70)	6940(2)	6677(2)	250(1)	43(1)
C(71)	6922(1)	7494(2)	338(1)	30(1)
C(72)	8099(1)	9309(2)	663(1)	24(1)
C(73)	7950(1)	9144(2)	354(1)	28(1)
C(74)	8328(1)	9340(2)	164(1)	38(1)
C(75)	8864(1)	9698(2)	267(1)	46(1)

C(76)	9011(1)	9883(2)	572(1)	43(1)
C(77)	8637(1)	9698(2)	764(1)	30(1)
C(78)	9279(2)	9893(3)	58(1)	80(2)
C(80)	3298(1)	4494(2)	1182(1)	24(1)
C(81)	4157(1)	5495(2)	1599(1)	24(1)
C(82)	4520(1)	6189(2)	1657(1)	28(1)
C(83)	5012(1)	6175(2)	1887(1)	33(1)
C(84)	5140(1)	5487(2)	2064(1)	35(1)
C(85)	4790(1)	4791(2)	2008(1)	35(1)
C(86)	4308(1)	4799(2)	1775(1)	29(1)
C(87)	3541(1)	6238(2)	1046(1)	24(1)
C(88)	3057(1)	6722(2)	923(1)	31(1)
C(89)	3084(1)	7282(2)	692(1)	39(1)
C(90)	3597(1)	7364(2)	584(1)	38(1)
C(91)	4081(1)	6892(2)	707(1)	32(1)
C(92)	4054(1)	6336(2)	934(1)	28(1)
C(93)	2758(1)	6379(2)	1600(1)	26(1)
C(94)	3089(1)	7109(2)	1638(1)	34(1)
C(95)	2892(1)	7808(2)	1764(1)	35(1)
C(96)	2355(1)	7820(2)	1855(1)	31(1)
C(97)	2019(1)	7104(2)	1812(1)	31(1)
C(98)	2212(1)	6406(2)	1687(1)	27(1)
C(99)	2148(2)	8579(2)	1996(1)	45(1)
C(100)	3640(1)	4358(2)	596(1)	26(1)
C(101)	3194(1)	4890(2)	462(1)	34(1)
C(102)	3229(2)	5325(2)	204(1)	49(1)
C(103)	3713(2)	5233(3)	76(1)	62(1)
C(104)	4161(2)	4707(3)	203(1)	54(1)
C(105)	4126(1)	4270(2)	463(1)	37(1)
C(106)	4297(1)	3461(2)	1096(1)	24(1)
C(107)	4405(1)	2627(2)	1152(1)	39(1)
C(108)	4965(2)	2346(2)	1275(1)	56(1)
C(109)	5422(2)	2897(2)	1352(1)	50(1)
C(110)	5321(1)	3724(2)	1305(1)	36(1)
C(111)	4769(1)	4006(2)	1174(1)	30(1)
C(112)	3101(1)	2330(2)	771(1)	21(1)
C(113)	2811(1)	1674(2)	880(1)	26(1)
C(114)	2774(1)	896(2)	754(1)	28(1)
C(115)	3033(1)	724(2)	509(1)	26(1)
C(116)	3333(1)	1361(2)	402(1)	25(1)
C(117)	3365(1)	2151(2)	527(1)	22(1)
C(118)	2999(1)	-134(2)	374(1)	35(1)
C(120)	2029(1)	3672(2)	1390(1)	24(1)
C(121)	997(1)	3024(2)	967(1)	25(1)
C(122)	386(1)	2989(2)	870(1)	30(1)
C(123)	123(1)	2293(2)	725(1)	35(1)
C(124)	458(2)	1625(2)	671(1)	39(1)
C(125)	1060(2)	1651(2)	762(1)	37(1)
C(126)	1323(1)	2339(2)	909(1)	29(1)
C(127)	867(1)	4436(2)	1335(1)	26(1)
C(128)	857(1)	5296(2)	1352(1)	33(1)
C(129)	501(1)	5687(2)	1521(1)	44(1)
C(130)	144(1)	5224(3)	1669(1)	49(1)
C(131)	153(1)	4374(3)	1657(1)	44(1)
C(132)	516(1)	3981(2)	1492(1)	34(1)
C(133)	1301(1)	5061(2)	705(1)	23(1)
C(134)	703(1)	5005(2)	591(1)	42(1)
C(135)	419(1)	5579(2)	385(1)	51(1)
C(136)	705(1)	6221(2)	279(1)	37(1)
C(137)	1300(1)	6274(2)	388(1)	37(1)
C(138)	1592(1)	5710(2)	597(1)	31(1)
C(139)	389(2)	6852(3)	57(1)	55(1)

C(140)	1854(1)	3435(2)	2014(1)	21(1)
C(141)	1703(1)	2898(2)	2228(1)	25(1)
C(142)	1476(1)	3193(2)	2468(1)	33(1)
C(143)	1395(1)	4029(2)	2498(1)	39(1)
C(144)	1537(1)	4570(2)	2288(1)	38(1)
C(145)	1763(1)	4276(2)	2047(1)	29(1)
C(146)	1979(1)	2010(2)	1655(1)	21(1)
C(147)	2383(1)	1413(2)	1610(1)	26(1)
C(148)	2208(1)	609(2)	1532(1)	34(1)
C(149)	1624(1)	393(2)	1497(1)	34(1)
C(150)	1218(1)	971(2)	1546(1)	31(1)
C(151)	1393(1)	1771(2)	1625(1)	26(1)
C(152)	3303(1)	2738(2)	2000(1)	20(1)
C(153)	3888(1)	2693(2)	1969(1)	27(1)
C(154)	4308(1)	2281(2)	2173(1)	35(1)
C(155)	4170(1)	1876(2)	2419(1)	30(1)
C(156)	3593(1)	1923(2)	2455(1)	27(1)
C(157)	3168(1)	2341(2)	2252(1)	24(1)
C(158)	4623(1)	1400(2)	2640(1)	44(1)
Li(1)	7574(2)	9716(3)	1250(1)	22(1)
Li(2)	8141(2)	8275(3)	1243(1)	27(1)
Li(3)	7328(2)	8457(3)	1596(1)	22(1)
Li(4)	6793(2)	9930(3)	1599(1)	29(1)
Li(5)	2383(2)	4816(3)	1221(1)	27(1)
Li(6)	2272(2)	3700(3)	779(1)	38(1)
Li(7)	2921(2)	3376(3)	1334(1)	25(1)
Li(8)	2981(2)	4536(3)	1768(1)	33(1)
N(1)	7473(1)	10724(1)	1524(1)	19(1)
N(2)	8129(1)	7808(1)	1691(1)	19(1)
N(3)	6429(1)	8710(1)	1604(1)	20(1)
N(4)	7759(1)	9110(1)	877(1)	19(1)
N(5)	2913(1)	5630(1)	1483(1)	25(1)
N(6)	3085(1)	3103(1)	910(1)	22(1)
N(7)	1638(1)	4521(1)	914(1)	23(1)
N(8)	2910(1)	3187(1)	1784(1)	21(1)
P(1)	8049(1)	10409(1)	1767(1)	18(1)
P(2)	8442(1)	8614(1)	1878(1)	18(1)
P(3)	6265(1)	8523(1)	1242(1)	17(1)
P(4)	7084(1)	8762(1)	800(1)	17(1)
P(5)	3466(1)	5440(1)	1320(1)	23(1)
P(6)	3562(1)	3860(1)	950(1)	21(1)
P(7)	1404(1)	3915(1)	1156(1)	22(1)
P(8)	2194(1)	3097(1)	1703(1)	20(1)
O11	8677(1)	7557(1)	1089(1)	30(1)
C11	9179(1)	7118(2)	1254(1)	32(1)
C21	9648(1)	7196(2)	1064(1)	41(1)
C31	9324(2)	7497(2)	761(1)	48(1)
C41	8687(1)	7394(2)	777(1)	40(1)
O12	6279(1)	10664(1)	1761(1)	32(1)
C12	5675(1)	10528(2)	1772(1)	37(1)
C22	5641(2)	10712(2)	2092(1)	47(1)
C32	6075(2)	11420(2)	2177(1)	47(1)
C42	6442(1)	11407(2)	1934(1)	29(1)
O1A3	3261(4)	5023(4)	2155(2)	28(1)
O1B3	3256(13)	4760(15)	2219(5)	25(5)
C1B3	3726(8)	4358(9)	2413(3)	26(4)
C2B3	4062(8)	5023(9)	2613(4)	44(5)
C4B3	3147(10)	5523(13)	2350(4)	63(7)
C33	3838(2)	5754(2)	2545(1)	40(1)
C1A3	3308(3)	4528(3)	2426(1)	38(1)
C2A3	3494(2)	5127(3)	2686(1)	38(1)
C4A3	3504(1)	5841(1)	2237(1)	29(1)

O1A4	2056(1)	3443(1)	346(1)	34(1)
O1B4	1846(1)	3388(1)	403(1)	40(3)
C34	1201(1)	3741(1)	-9(1)	75(2)
C1A4	1888(2)	2639(3)	224(1)	32(1)
C2A4	1248(2)	2745(3)	78(1)	41(1)
C4A4	1790(2)	4022(3)	117(1)	43(1)
C1B4	1234(5)	3412(9)	247(3)	35(4)
C2B4	2158(6)	3392(8)	159(3)	32(3)
C4B4	1835(6)	4041(10)	-64(4)	41(4)
O15	4467(2)	6705(2)	-327(1)	88(1)
C15	4558(2)	6980(3)	-8(1)	79(2)
C25	5034(1)	7570(2)	46(1)	40(1)
C35	5193(2)	7717(2)	-240(1)	47(1)
C45	4696(2)	7403(2)	-472(1)	43(1)
O16	3661(2)	9538(2)	1714(1)	101(1)
C16	3744(2)	9434(3)	1407(1)	87(2)
C26	4092(2)	10181(3)	1348(1)	68(1)
C36	3984(2)	10813(3)	1565(1)	60(1)
C46	3892(2)	10287(2)	1826(1)	53(1)
O1A7	-2232(7)	2894(8)	108(3)	140(3)
O1B7	-2737(3)	2639(4)	181(2)	140(3)
C17	-2460(3)	2858(4)	441(2)	102(2)
C27	-2130(2)	2168(3)	572(1)	90(2)
C37	-1906(3)	1759(4)	318(2)	152(3)
C47	-2296(1)	2092(1)	39(1)	149(4)
O48	-1049(1)	3562(1)	759(1)	56(1)
C18	-1186(1)	3818(1)	1040(1)	55(1)
C28	-1228(2)	4732(2)	1031(1)	63(1)
C38	-846(2)	4960(3)	818(1)	74(1)
C48	-973(2)	4274(3)	588(1)	61(1)
O19	859(1)	-1340(2)	1070(1)	72(1)
C19	911(2)	-969(3)	794(1)	90(2)
C29	1523(3)	-1119(4)	748(2)	131(3)
C39	1723(2)	-1845(4)	961(1)	96(2)
C49	1192(2)	-2060(3)	1070(1)	74(1)

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3b**. 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}
C(1)	17(1)	24(2)	15(1)	1(1)	1(1)	-4(1)
C(2)	19(1)	25(2)	20(1)	-1(1)	3(1)	3(1)
C(3)	28(2)	28(2)	20(2)	-2(1)	5(1)	0(1)
C(4)	43(2)	29(2)	27(2)	-7(1)	2(1)	4(2)
C(5)	48(2)	38(2)	19(2)	0(1)	13(1)	12(2)
C(6)	32(2)	37(2)	30(2)	6(1)	16(1)	6(1)
C(7)	24(2)	32(2)	24(2)	2(1)	7(1)	1(1)
C(8)	20(1)	17(1)	25(2)	-6(1)	7(1)	-4(1)
C(9)	22(2)	27(2)	29(2)	1(1)	7(1)	-3(1)
C(10)	27(2)	33(2)	41(2)	6(2)	15(2)	-4(1)
C(11)	23(2)	32(2)	58(2)	4(2)	16(2)	-8(1)
C(12)	19(2)	35(2)	46(2)	-4(2)	1(1)	-5(1)
C(13)	23(2)	27(2)	29(2)	-4(1)	5(1)	-4(1)
C(14)	17(1)	22(2)	24(2)	-1(1)	10(1)	-2(1)
C(15)	22(2)	20(2)	40(2)	-1(1)	-4(1)	-3(1)
C(16)	26(2)	29(2)	55(2)	4(2)	-14(2)	0(1)
C(17)	24(2)	23(2)	55(2)	3(2)	2(2)	2(1)
C(18)	30(2)	21(2)	40(2)	-6(1)	14(1)	-4(1)
C(19)	24(2)	26(2)	25(2)	-4(1)	7(1)	-3(1)

C(20)	48(2)	26(2)	88(3)	8(2)	-10(2)	3(2)
C(21)	19(1)	25(2)	18(1)	3(1)	4(1)	1(1)
C(22)	22(2)	35(2)	19(2)	0(1)	2(1)	-6(1)
C(23)	28(2)	45(2)	19(2)	-4(1)	0(1)	-4(1)
C(24)	36(2)	40(2)	17(2)	3(1)	8(1)	5(2)
C(25)	26(2)	33(2)	26(2)	7(1)	8(1)	-2(1)
C(26)	21(1)	27(2)	20(1)	3(1)	1(1)	-1(1)
C(27)	20(1)	24(2)	19(1)	-2(1)	3(1)	-3(1)
C(28)	24(2)	24(2)	23(2)	-2(1)	4(1)	-1(1)
C(29)	28(2)	36(2)	30(2)	0(1)	11(1)	-5(1)
C(30)	21(2)	52(2)	40(2)	0(2)	9(1)	-5(2)
C(31)	18(2)	51(2)	36(2)	3(2)	-3(1)	-2(1)
C(32)	22(2)	38(2)	21(2)	3(1)	1(1)	-4(1)
C(33)	18(1)	24(2)	16(1)	2(1)	2(1)	-2(1)
C(34)	23(2)	24(2)	22(2)	-1(1)	1(1)	-2(1)
C(35)	20(2)	29(2)	20(2)	2(1)	1(1)	3(1)
C(36)	28(2)	26(2)	19(1)	3(1)	7(1)	1(1)
C(37)	31(2)	23(2)	20(2)	1(1)	-1(1)	-7(1)
C(38)	23(2)	28(2)	16(1)	5(1)	1(1)	-2(1)
C(39)	40(2)	26(2)	32(2)	5(1)	1(2)	1(1)
C(40)	16(1)	23(2)	17(1)	-1(1)	1(1)	-4(1)
C(41)	18(1)	24(2)	18(1)	-1(1)	6(1)	0(1)
C(42)	22(2)	26(2)	30(2)	-2(1)	3(1)	-1(1)
C(43)	21(2)	44(2)	36(2)	-6(2)	-2(1)	3(1)
C(44)	30(2)	41(2)	40(2)	3(2)	7(2)	15(2)
C(45)	38(2)	28(2)	42(2)	4(2)	17(2)	8(2)
C(46)	24(2)	24(2)	30(2)	-3(1)	11(1)	-1(1)
C(47)	14(1)	22(2)	25(2)	0(1)	5(1)	-2(1)
C(48)	27(2)	26(2)	28(2)	3(1)	6(1)	0(1)
C(49)	43(2)	23(2)	45(2)	10(2)	12(2)	1(2)
C(50)	31(2)	21(2)	53(2)	-3(2)	8(2)	-4(1)
C(51)	28(2)	28(2)	37(2)	-9(1)	2(1)	-3(1)
C(52)	23(2)	22(2)	29(2)	0(1)	3(1)	-3(1)
C(53)	20(1)	21(2)	23(2)	-1(1)	9(1)	-3(1)
C(54)	20(1)	26(2)	23(2)	-2(1)	6(1)	-4(1)
C(55)	35(2)	33(2)	20(2)	-4(1)	11(1)	-6(1)
C(56)	33(2)	34(2)	31(2)	-5(1)	19(1)	-7(1)
C(57)	24(2)	40(2)	36(2)	-6(2)	14(1)	-10(1)
C(58)	24(2)	36(2)	24(2)	-1(1)	8(1)	-9(1)
C(59)	51(2)	65(3)	41(2)	-7(2)	28(2)	-14(2)
C(60)	18(1)	23(2)	16(1)	0(1)	6(1)	0(1)
C(61)	20(1)	21(2)	20(1)	-1(1)	5(1)	2(1)
C(62)	18(1)	33(2)	21(2)	-2(1)	2(1)	2(1)
C(63)	26(2)	31(2)	29(2)	9(1)	3(1)	7(1)
C(64)	28(2)	27(2)	36(2)	8(1)	5(1)	-2(1)
C(65)	17(1)	30(2)	24(2)	4(1)	2(1)	-1(1)
C(66)	16(1)	25(2)	19(1)	0(1)	2(1)	2(1)
C(67)	30(2)	26(2)	19(1)	1(1)	3(1)	3(1)
C(68)	43(2)	30(2)	25(2)	7(1)	4(1)	12(2)
C(69)	66(2)	26(2)	35(2)	-7(2)	-2(2)	13(2)
C(70)	67(2)	36(2)	21(2)	-8(2)	-5(2)	17(2)
C(71)	40(2)	29(2)	19(2)	0(1)	0(1)	9(1)
C(72)	16(1)	34(2)	21(2)	6(1)	5(1)	4(1)
C(73)	19(2)	44(2)	22(2)	3(1)	5(1)	-1(1)
C(74)	26(2)	68(2)	20(2)	8(2)	8(1)	6(2)
C(75)	28(2)	78(3)	36(2)	13(2)	16(2)	-2(2)
C(76)	23(2)	70(3)	36(2)	11(2)	9(2)	-11(2)
C(77)	22(2)	44(2)	24(2)	6(1)	4(1)	-4(1)
C(78)	48(2)	148(5)	53(3)	17(3)	31(2)	-19(3)
C(80)	19(1)	25(2)	28(2)	0(1)	4(1)	-5(1)
C(81)	20(2)	27(2)	24(2)	-2(1)	3(1)	-1(1)
C(82)	23(2)	25(2)	36(2)	0(1)	4(1)	-1(1)

C(83)	26(2)	33(2)	37(2)	-4(2)	1(1)	-8(1)
C(84)	24(2)	46(2)	31(2)	2(2)	-4(1)	-3(2)
C(85)	31(2)	37(2)	33(2)	10(2)	0(1)	1(2)
C(86)	25(2)	30(2)	30(2)	1(1)	3(1)	-5(1)
C(87)	22(2)	21(2)	28(2)	-4(1)	-2(1)	-7(1)
C(88)	25(2)	27(2)	41(2)	1(1)	4(1)	-2(1)
C(89)	32(2)	29(2)	52(2)	12(2)	1(2)	3(1)
C(90)	35(2)	33(2)	46(2)	12(2)	6(2)	-7(2)
C(91)	27(2)	30(2)	39(2)	3(2)	5(1)	-8(1)
C(92)	21(2)	28(2)	32(2)	1(1)	-2(1)	-2(1)
C(93)	23(2)	28(2)	25(2)	0(1)	1(1)	2(1)
C(94)	23(2)	35(2)	44(2)	-10(2)	6(1)	-4(1)
C(95)	34(2)	28(2)	42(2)	-6(2)	3(2)	-2(1)
C(96)	36(2)	30(2)	25(2)	3(1)	0(1)	13(1)
C(97)	30(2)	38(2)	27(2)	10(1)	8(1)	9(1)
C(98)	25(2)	28(2)	27(2)	6(1)	3(1)	3(1)
C(99)	48(2)	38(2)	49(2)	3(2)	14(2)	18(2)
C(100)	27(2)	24(2)	25(2)	6(1)	1(1)	-7(1)
C(101)	36(2)	33(2)	29(2)	4(1)	-6(1)	-6(2)
C(102)	56(2)	41(2)	40(2)	16(2)	-16(2)	-14(2)
C(103)	70(3)	69(3)	37(2)	27(2)	-10(2)	-42(2)
C(104)	49(2)	78(3)	35(2)	14(2)	11(2)	-27(2)
C(105)	34(2)	45(2)	31(2)	10(2)	7(2)	-12(2)
C(106)	23(2)	29(2)	21(2)	5(1)	6(1)	0(1)
C(107)	33(2)	34(2)	44(2)	16(2)	-5(2)	-7(2)
C(108)	44(2)	40(2)	73(3)	30(2)	-13(2)	3(2)
C(109)	30(2)	58(3)	55(2)	25(2)	-10(2)	5(2)
C(110)	22(2)	46(2)	40(2)	5(2)	0(1)	-4(2)
C(111)	24(2)	29(2)	37(2)	3(1)	4(1)	-1(1)
C(112)	19(1)	23(2)	19(1)	1(1)	1(1)	-2(1)
C(113)	26(2)	28(2)	27(2)	-1(1)	13(1)	-3(1)
C(114)	26(2)	28(2)	32(2)	-1(1)	11(1)	-6(1)
C(115)	22(2)	27(2)	24(2)	-2(1)	-3(1)	2(1)
C(116)	27(2)	33(2)	16(1)	2(1)	5(1)	6(1)
C(117)	21(2)	25(2)	21(2)	5(1)	7(1)	1(1)
C(118)	37(2)	32(2)	34(2)	-6(2)	1(2)	3(2)
C(120)	19(1)	29(2)	23(2)	7(1)	1(1)	-2(1)
C(121)	24(2)	31(2)	19(1)	6(1)	2(1)	-7(1)
C(122)	29(2)	36(2)	26(2)	8(1)	4(1)	-6(1)
C(123)	30(2)	48(2)	28(2)	4(2)	4(1)	-18(2)
C(124)	51(2)	41(2)	25(2)	-6(2)	8(2)	-22(2)
C(125)	49(2)	34(2)	30(2)	-4(2)	10(2)	-6(2)
C(126)	30(2)	34(2)	22(2)	4(1)	3(1)	-2(1)
C(127)	16(1)	37(2)	24(2)	1(1)	-3(1)	0(1)
C(128)	24(2)	39(2)	32(2)	0(2)	-4(1)	5(1)
C(129)	31(2)	50(2)	42(2)	-14(2)	-10(2)	10(2)
C(130)	26(2)	82(3)	37(2)	-25(2)	0(2)	8(2)
C(131)	25(2)	77(3)	31(2)	-10(2)	6(2)	-5(2)
C(132)	21(2)	47(2)	30(2)	0(2)	1(1)	-3(1)
C(133)	22(2)	28(2)	18(1)	4(1)	0(1)	0(1)
C(134)	25(2)	54(2)	41(2)	25(2)	-5(2)	-9(2)
C(135)	22(2)	77(3)	49(2)	31(2)	-7(2)	-3(2)
C(136)	32(2)	47(2)	30(2)	16(2)	5(1)	11(2)
C(137)	35(2)	35(2)	41(2)	16(2)	7(2)	0(2)
C(138)	23(2)	33(2)	34(2)	9(1)	0(1)	-1(1)
C(139)	47(2)	71(3)	47(2)	33(2)	8(2)	18(2)
C(140)	14(1)	27(2)	20(1)	-1(1)	-1(1)	-1(1)
C(141)	20(2)	28(2)	27(2)	-2(1)	4(1)	-1(1)
C(142)	29(2)	44(2)	26(2)	-4(2)	9(1)	-3(2)
C(143)	35(2)	48(2)	36(2)	-13(2)	13(2)	3(2)
C(144)	37(2)	29(2)	47(2)	-10(2)	3(2)	8(2)
C(145)	28(2)	28(2)	30(2)	-1(1)	2(1)	-1(1)

C(146)	23(2)	26(2)	13(1)	3(1)	3(1)	-3(1)
C(147)	28(2)	27(2)	26(2)	2(1)	13(1)	-2(1)
C(148)	41(2)	30(2)	37(2)	-3(1)	21(2)	2(2)
C(149)	44(2)	27(2)	33(2)	-2(1)	14(2)	-9(2)
C(150)	27(2)	34(2)	31(2)	1(1)	4(1)	-9(1)
C(151)	24(2)	31(2)	23(2)	3(1)	4(1)	-2(1)
C(152)	19(1)	22(2)	18(1)	2(1)	1(1)	-1(1)
C(153)	21(2)	30(2)	31(2)	11(1)	6(1)	1(1)
C(154)	19(2)	37(2)	47(2)	11(2)	4(1)	3(1)
C(155)	25(2)	26(2)	33(2)	5(1)	-6(1)	2(1)
C(156)	34(2)	26(2)	21(2)	5(1)	2(1)	1(1)
C(157)	20(2)	28(2)	23(2)	3(1)	3(1)	2(1)
C(158)	34(2)	42(2)	49(2)	14(2)	-11(2)	8(2)
Li(1)	22(2)	25(3)	19(2)	0(2)	2(2)	-2(2)
Li(2)	23(2)	34(3)	23(3)	3(2)	6(2)	0(2)
Li(3)	17(2)	27(3)	23(2)	2(2)	5(2)	-2(2)
Li(4)	28(3)	33(3)	27(3)	-4(2)	8(2)	-9(2)
Li(5)	25(3)	27(3)	28(3)	-1(2)	1(2)	-2(2)
Li(6)	37(3)	41(3)	31(3)	0(2)	-5(2)	5(3)
Li(7)	22(2)	28(3)	23(2)	1(2)	3(2)	0(2)
Li(8)	31(3)	35(3)	31(3)	0(2)	4(2)	-7(2)
N(1)	17(1)	18(1)	21(1)	-1(1)	4(1)	-4(1)
N(2)	19(1)	19(1)	17(1)	0(1)	0(1)	-2(1)
N(3)	16(1)	28(1)	18(1)	-2(1)	5(1)	-6(1)
N(4)	14(1)	28(1)	16(1)	3(1)	4(1)	-1(1)
N(5)	20(1)	26(1)	28(1)	-4(1)	3(1)	-2(1)
N(6)	24(1)	21(1)	22(1)	0(1)	7(1)	-4(1)
N(7)	20(1)	28(1)	20(1)	6(1)	-1(1)	-2(1)
N(8)	17(1)	24(1)	20(1)	5(1)	1(1)	-1(1)
P(1)	16(1)	22(1)	17(1)	-2(1)	4(1)	-5(1)
P(2)	16(1)	24(1)	15(1)	0(1)	1(1)	-4(1)
P(3)	16(1)	21(1)	16(1)	0(1)	3(1)	-4(1)
P(4)	15(1)	23(1)	14(1)	1(1)	2(1)	-1(1)
P(5)	18(1)	23(1)	27(1)	-1(1)	2(1)	-2(1)
P(6)	19(1)	22(1)	20(1)	3(1)	3(1)	-3(1)
P(7)	17(1)	26(1)	21(1)	5(1)	-1(1)	-1(1)
P(8)	16(1)	24(1)	19(1)	3(1)	2(1)	0(1)
O11	28(1)	41(1)	21(1)	1(1)	4(1)	11(1)
C11	33(2)	32(2)	27(2)	2(1)	-1(1)	9(1)
C21	27(2)	47(2)	47(2)	-11(2)	7(2)	3(2)
C31	54(2)	49(2)	48(2)	5(2)	29(2)	10(2)
C41	45(2)	51(2)	22(2)	1(2)	3(2)	23(2)
O12	24(1)	38(1)	35(1)	-9(1)	11(1)	-9(1)
C12	22(2)	33(2)	53(2)	6(2)	2(2)	-2(1)
C22	41(2)	42(2)	64(2)	3(2)	28(2)	3(2)
C32	39(2)	58(2)	49(2)	-10(2)	25(2)	-5(2)
C42	25(2)	32(2)	30(2)	-3(1)	4(1)	0(1)
O1A3	39(2)	23(3)	19(3)	6(2)	1(2)	-10(2)
O1B3	44(8)	22(13)	9(12)	4(8)	6(8)	-9(10)
C1B3	31(10)	29(9)	14(7)	5(6)	-10(7)	-9(7)
C2B3	58(12)	22(9)	49(11)	-1(8)	-1(9)	8(8)
C4B3	83(16)	55(13)	39(11)	-13(10)	-18(11)	24(12)
C33	48(2)	31(2)	38(2)	-7(2)	5(2)	-4(2)
C1A3	55(4)	31(3)	23(3)	7(2)	-3(2)	-10(2)
C2A3	49(3)	40(3)	22(2)	0(2)	1(2)	-6(2)
C4A3	33(2)	23(2)	30(2)	0(2)	3(2)	-6(2)
O1A4	35(2)	47(2)	17(2)	-3(2)	-1(2)	13(2)
O1B4	31(6)	66(8)	26(6)	0(5)	15(5)	7(5)
C34	40(2)	140(5)	38(2)	3(3)	-6(2)	20(3)
C1A4	28(2)	40(3)	26(2)	-5(2)	3(2)	5(2)
C2A4	28(2)	59(3)	31(3)	11(2)	-2(2)	2(2)
C4A4	44(3)	50(3)	32(3)	6(3)	3(3)	14(2)

C1B4	18(6)	48(9)	36(8)	6(7)	1(5)	4(6)
C2B4	28(7)	38(8)	29(8)	4(6)	6(6)	4(6)
C4B4	36(8)	61(10)	26(8)	12(8)	5(7)	6(7)
O15	102(3)	102(3)	61(2)	-8(2)	19(2)	-56(2)
C15	96(4)	106(4)	38(2)	7(2)	21(2)	-38(3)
C25	36(2)	60(2)	24(2)	-10(2)	4(1)	-18(2)
C35	46(2)	44(2)	53(2)	-11(2)	18(2)	-14(2)
C45	48(2)	44(2)	35(2)	4(2)	6(2)	1(2)
O16	147(3)	106(3)	61(2)	-26(2)	49(2)	-78(3)
C16	79(3)	107(4)	89(4)	-44(3)	50(3)	-32(3)
C26	61(3)	84(3)	56(3)	0(2)	9(2)	8(2)
C36	54(2)	73(3)	58(3)	18(2)	25(2)	17(2)
C46	57(2)	55(3)	49(2)	12(2)	11(2)	-11(2)
O1A7	169(7)	88(4)	119(5)	34(3)	-79(5)	-53(4)
O1B7	169(7)	88(4)	119(5)	34(3)	-79(5)	-53(4)
C17	83(4)	95(4)	124(5)	20(4)	12(4)	-13(3)
C27	72(3)	69(3)	114(4)	28(3)	-21(3)	-35(3)
C37	139(6)	79(4)	268(10)	81(6)	115(7)	41(4)
C47	295(11)	49(3)	75(4)	-11(3)	-32(5)	-21(5)
O48	56(2)	45(2)	68(2)	-16(1)	17(1)	-4(1)
C18	63(3)	51(2)	50(2)	-5(2)	8(2)	-4(2)
C28	89(3)	48(3)	53(3)	0(2)	17(2)	13(2)
C38	100(4)	49(3)	81(3)	-3(2)	36(3)	-6(2)
C48	74(3)	62(3)	53(2)	-6(2)	26(2)	-12(2)
O19	74(2)	69(2)	82(2)	-4(2)	35(2)	4(2)
C19	100(4)	93(4)	78(3)	39(3)	16(3)	5(3)
C29	149(6)	117(5)	158(6)	14(5)	106(5)	-22(5)
C39	64(3)	115(5)	109(4)	-14(4)	22(3)	31(3)
C49	77(3)	74(3)	73(3)	6(3)	15(3)	25(3)

2.5 Crystal Structure Determination of **4b**

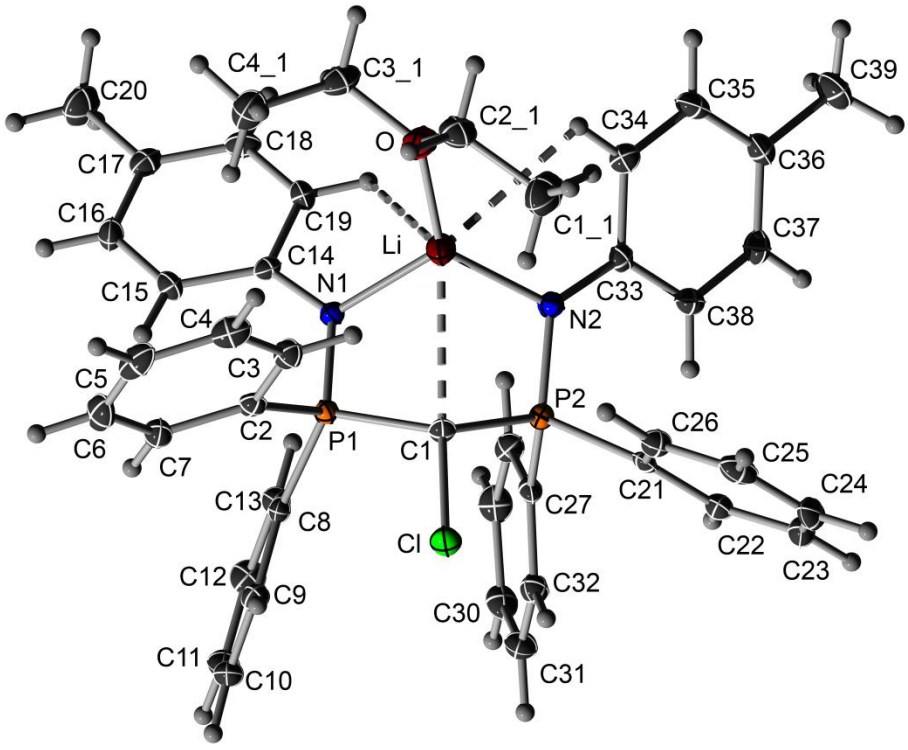


Figure S11. ORTEP Plot of compound **4b**. Ellipsoids are drawn at the 50% probability level.

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	5670(1)	3781(1)	3993(1)	19(1)
P(1)	3353(1)	3547(1)	2294(1)	12(1)
N(1)	2018(2)	2714(1)	1590(1)	13(1)
C(1)	4152(2)	2912(2)	3136(1)	13(1)
Li(1)	2729(5)	1494(3)	1793(3)	23(1)
P(2)	2968(1)	2077(1)	3587(1)	11(1)
N(2)	2126(2)	1136(1)	2823(1)	14(1)
C(2)	4937(2)	4061(2)	1853(1)	14(1)
C(3)	5950(3)	3466(2)	1739(2)	18(1)
C(4)	7016(3)	3735(2)	1275(2)	23(1)
C(5)	7105(3)	4610(2)	932(2)	26(1)
C(6)	6130(3)	5214(2)	1052(2)	25(1)
C(7)	5042(3)	4939(2)	1503(2)	19(1)
C(8)	2681(2)	4591(2)	2695(1)	14(1)
C(9)	3718(3)	5462(2)	3210(2)	17(1)
C(10)	3162(3)	6207(2)	3574(2)	20(1)
C(11)	1583(3)	6108(2)	3422(2)	22(1)
C(12)	547(3)	5251(2)	2921(2)	21(1)
C(13)	1090(3)	4496(2)	2562(2)	17(1)
C(14)	847(2)	2781(2)	846(1)	13(1)
C(15)	806(3)	3591(2)	391(2)	17(1)
C(16)	-415(3)	3562(2)	-362(2)	19(1)
C(17)	-1648(3)	2736(2)	-704(2)	19(1)
C(18)	-1607(3)	1929(2)	-256(2)	19(1)
C(19)	-402(3)	1944(2)	497(2)	16(1)
C(20)	-2949(3)	2709(2)	-1528(2)	30(1)
C(21)	4220(2)	1749(2)	4563(1)	13(1)
C(22)	3712(3)	1558(2)	5302(2)	16(1)
C(23)	4613(3)	1207(2)	5997(2)	22(1)
C(24)	6044(3)	1048(2)	5969(2)	25(1)
C(25)	6567(3)	1239(2)	5241(2)	23(1)
C(26)	5656(3)	1580(2)	4536(2)	18(1)
C(27)	1641(2)	2664(2)	4001(1)	13(1)
C(28)	68(2)	2436(2)	3531(2)	17(1)
C(29)	-934(3)	2928(2)	3818(2)	21(1)
C(30)	-369(3)	3645(2)	4571(2)	21(1)
C(31)	1200(3)	3890(2)	5038(2)	21(1)
C(32)	2204(3)	3410(2)	4750(2)	17(1)
C(33)	1128(2)	259(2)	2873(1)	13(1)
C(34)	762(3)	-532(2)	2174(2)	17(1)
C(35)	-190(3)	-1439(2)	2173(2)	20(1)
C(36)	-839(3)	-1602(2)	2864(2)	19(1)
C(37)	-497(3)	-821(2)	3551(2)	20(1)
C(38)	468(3)	92(2)	3569(2)	18(1)
C(39)	-1908(3)	-2589(2)	2851(2)	29(1)
O11	3497(2)	864(1)	935(1)	24(1)
C11	5420(3)	453(2)	2093(2)	37(1)
C21	4940(3)	568(2)	1130(2)	24(1)
C31	2844(3)	918(2)	-1(2)	25(1)
C41	3688(3)	1801(2)	-298(2)	31(1)

Table S11. Anisotropic displacement parameters ($Å^2$x 10^3) for compound **4b**. 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}
Cl(1)	15(1)	18(1)	18(1)	2(1)	0(1)	0(1)
P(1)	12(1)	11(1)	12(1)	2(1)	3(1)	2(1)

N(1)	14(1)	12(1)	12(1)	1(1)	1(1)	3(1)
C(1)	10(1)	13(1)	12(1)	1(1)	-1(1)	-1(1)
Li(1)	32(2)	20(2)	20(2)	6(2)	10(2)	11(2)
P(2)	11(1)	12(1)	11(1)	2(1)	3(1)	3(1)
N(2)	15(1)	14(1)	14(1)	1(1)	5(1)	2(1)
C(2)	13(1)	14(1)	12(1)	0(1)	1(1)	-1(1)
C(3)	17(1)	19(1)	17(1)	3(1)	5(1)	2(1)
C(4)	15(1)	30(2)	21(1)	-2(1)	6(1)	3(1)
C(5)	19(1)	36(2)	18(1)	4(1)	8(1)	-5(1)
C(6)	26(1)	23(1)	23(2)	9(1)	6(1)	-5(1)
C(7)	20(1)	18(1)	16(1)	4(1)	4(1)	2(1)
C(8)	18(1)	13(1)	10(1)	4(1)	3(1)	5(1)
C(9)	17(1)	17(1)	15(1)	3(1)	2(1)	3(1)
C(10)	27(1)	15(1)	15(1)	1(1)	3(1)	3(1)
C(11)	32(2)	18(1)	19(1)	2(1)	11(1)	11(1)
C(12)	17(1)	26(1)	23(1)	4(1)	8(1)	9(1)
C(13)	18(1)	15(1)	16(1)	2(1)	4(1)	4(1)
C(14)	14(1)	15(1)	10(1)	0(1)	3(1)	4(1)
C(15)	19(1)	13(1)	18(1)	3(1)	6(1)	1(1)
C(16)	24(1)	19(1)	17(1)	8(1)	6(1)	7(1)
C(17)	18(1)	24(1)	14(1)	2(1)	3(1)	8(1)
C(18)	14(1)	19(1)	18(1)	-2(1)	3(1)	1(1)
C(19)	20(1)	12(1)	17(1)	5(1)	6(1)	3(1)
C(20)	27(1)	37(2)	23(2)	7(1)	-2(1)	8(1)
C(21)	15(1)	7(1)	14(1)	0(1)	1(1)	1(1)
C(22)	19(1)	13(1)	16(1)	1(1)	4(1)	2(1)
C(23)	31(1)	17(1)	16(1)	5(1)	4(1)	2(1)
C(24)	32(2)	16(1)	21(1)	4(1)	-5(1)	9(1)
C(25)	19(1)	18(1)	27(2)	-2(1)	0(1)	7(1)
C(26)	18(1)	16(1)	19(1)	1(1)	4(1)	5(1)
C(27)	16(1)	12(1)	14(1)	5(1)	7(1)	5(1)
C(28)	15(1)	19(1)	16(1)	2(1)	4(1)	2(1)
C(29)	13(1)	24(1)	25(1)	6(1)	6(1)	4(1)
C(30)	24(1)	22(1)	25(1)	7(1)	13(1)	11(1)
C(31)	27(1)	19(1)	20(1)	1(1)	8(1)	9(1)
C(32)	17(1)	16(1)	18(1)	3(1)	4(1)	5(1)
C(33)	12(1)	14(1)	14(1)	4(1)	1(1)	4(1)
C(34)	15(1)	19(1)	16(1)	2(1)	5(1)	4(1)
C(35)	21(1)	15(1)	22(1)	-3(1)	2(1)	3(1)
C(36)	17(1)	14(1)	24(1)	5(1)	3(1)	3(1)
C(37)	21(1)	21(1)	21(1)	8(1)	10(1)	3(1)
C(38)	20(1)	16(1)	16(1)	0(1)	4(1)	2(1)
C(39)	31(2)	17(1)	35(2)	4(1)	10(1)	-2(1)
O11	29(1)	28(1)	20(1)	3(1)	12(1)	13(1)
C11	46(2)	43(2)	29(2)	11(1)	12(1)	25(1)
C21	26(1)	23(1)	26(1)	2(1)	12(1)	9(1)
C31	25(1)	33(2)	19(1)	-2(1)	7(1)	11(1)
C41	33(2)	36(2)	24(2)	8(1)	6(1)	8(1)

2.6 Crystal Structure Determination of **5a**

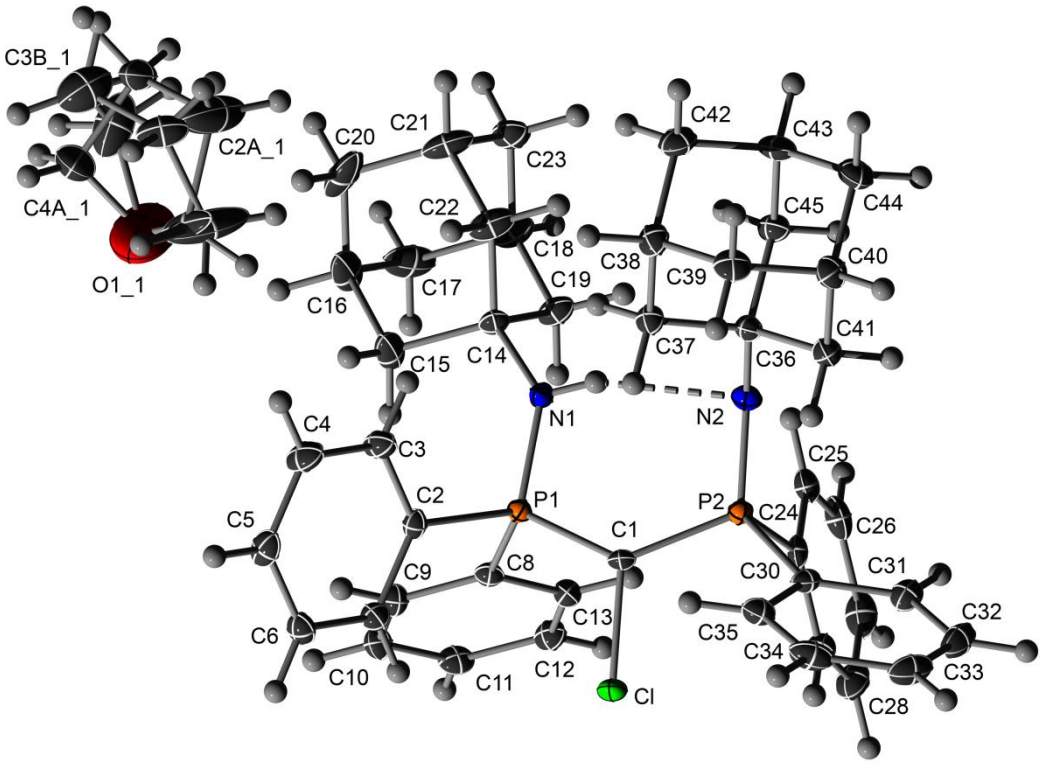


Figure S12. ORTEP Plot of compound **5a**. Ellipsoids are drawn at the 50% probability level.

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **5a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	41(1)	6444(1)	1143(1)	17(1)
P(1)	2669(1)	5981(1)	1629(1)	11(1)
P(2)	2083(1)	7592(1)	1343(1)	12(1)
N(1)	4156(1)	6277(1)	1856(1)	14(1)
N(2)	3563(1)	7785(1)	1433(1)	14(1)
C(1)	1720(2)	6677(1)	1249(1)	13(1)
C(2)	2609(2)	5248(1)	1063(1)	14(1)
C(3)	3651(2)	5122(1)	775(1)	20(1)
C(4)	3566(2)	4599(1)	303(1)	24(1)
C(5)	2432(2)	4207(1)	103(1)	20(1)
C(6)	1380(2)	4339(1)	375(1)	18(1)
C(7)	1468(2)	4851(1)	857(1)	16(1)
C(8)	2063(2)	5629(1)	2306(1)	13(1)
C(9)	1977(2)	4903(1)	2443(1)	17(1)
C(10)	1585(2)	4687(1)	2999(1)	19(1)
C(11)	1274(2)	5195(1)	3418(1)	19(1)
C(12)	1349(2)	5917(1)	3282(1)	18(1)
C(13)	1733(2)	6135(1)	2727(1)	15(1)
C(14)	5307(2)	6000(1)	2336(1)	16(1)
C(15)	5211(2)	5198(1)	2470(1)	33(1)
C(16)	6444(2)	4959(1)	2967(1)	40(1)
C(17)	6558(2)	5378(1)	3594(1)	37(1)
C(18)	6679(2)	6174(1)	3464(1)	24(1)
C(19)	5446(2)	6413(1)	2972(1)	20(1)
C(20)	7635(2)	5087(1)	2691(1)	41(1)

C(21)	7747(2)	5883(1)	2555(1)	29(1)
C(22)	6518(2)	6129(1)	2066(1)	26(1)
C(23)	7872(2)	6307(1)	3184(1)	24(1)
C(24)	1603(2)	7899(1)	2072(1)	14(1)
C(25)	294(2)	7933(1)	2099(1)	19(1)
C(26)	-59(2)	8082(1)	2681(1)	25(1)
C(27)	889(2)	8191(1)	3240(1)	26(1)
C(28)	2193(2)	8154(1)	3220(1)	23(1)
C(29)	2554(2)	8013(1)	2640(1)	17(1)
C(30)	907(2)	8021(1)	687(1)	14(1)
C(31)	506(2)	8721(1)	756(1)	19(1)
C(32)	-306(2)	9070(1)	237(1)	24(1)
C(33)	-703(2)	8728(1)	-352(1)	26(1)
C(34)	-307(2)	8033(1)	-426(1)	24(1)
C(35)	490(2)	7678(1)	91(1)	18(1)
C(36)	4351(2)	7925(1)	953(1)	14(1)
C(37)	4602(2)	7250(1)	581(1)	16(1)
C(38)	5525(2)	7414(1)	133(1)	19(1)
C(39)	4911(2)	7983(1)	-362(1)	21(1)
C(40)	4677(2)	8665(1)	-3(1)	20(1)
C(41)	3753(2)	8494(1)	445(1)	17(1)
C(42)	6826(2)	7691(1)	536(1)	23(1)
C(43)	6593(2)	8377(1)	891(1)	23(1)
C(44)	5974(2)	8945(1)	394(1)	24(1)
C(45)	5668(2)	8214(1)	1338(1)	18(1)
O4A1	7076(2)	3647(1)	1502(2)	99(1)
C1A1	6958(9)	4013(4)	926(4)	34(2)
C2A1	8136(5)	3250(3)	1499(3)	40(2)
C3A1	9114(4)	3823(3)	1445(3)	33(1)
C4A1	8334(6)	4338(5)	983(5)	79(3)
C1B1	6921(12)	4151(8)	1009(6)	72(3)
C2B1	8597(8)	3558(4)	1797(3)	55(2)
C3B1	8993(6)	3433(5)	1199(3)	52(2)
C4B1	8170(5)	3973(4)	725(2)	33(1)

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **5a**. 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}
Cl(1)	10(1)	17(1)	21(1)	0(1)	0(1)	-2(1)
P(1)	11(1)	11(1)	11(1)	-1(1)	2(1)	0(1)
P(2)	11(1)	12(1)	11(1)	0(1)	2(1)	0(1)
N(1)	12(1)	11(1)	18(1)	3(1)	0(1)	0(1)
N(2)	14(1)	17(1)	13(1)	-1(1)	2(1)	-1(1)
C(1)	8(1)	15(1)	16(1)	0(1)	1(1)	-1(1)
C(2)	16(1)	12(1)	12(1)	0(1)	1(1)	2(1)
C(3)	15(1)	23(1)	21(1)	-6(1)	2(1)	-1(1)
C(4)	18(1)	30(1)	24(1)	-9(1)	7(1)	3(1)
C(5)	22(1)	20(1)	16(1)	-6(1)	0(1)	4(1)
C(6)	19(1)	16(1)	17(1)	-2(1)	1(1)	-2(1)
C(7)	17(1)	17(1)	16(1)	-1(1)	5(1)	0(1)
C(8)	12(1)	15(1)	13(1)	0(1)	1(1)	-1(1)
C(9)	19(1)	15(1)	17(1)	-1(1)	4(1)	1(1)
C(10)	21(1)	15(1)	21(1)	4(1)	5(1)	0(1)
C(11)	18(1)	24(1)	16(1)	4(1)	6(1)	0(1)
C(12)	18(1)	21(1)	17(1)	-4(1)	5(1)	1(1)
C(13)	14(1)	14(1)	18(1)	0(1)	3(1)	0(1)
C(14)	11(1)	17(1)	17(1)	0(1)	-2(1)	1(1)
C(15)	24(1)	17(1)	48(1)	4(1)	-14(1)	1(1)
C(16)	27(1)	19(1)	61(2)	10(1)	-19(1)	2(1)
C(17)	19(1)	50(1)	36(1)	26(1)	-6(1)	0(1)

C(18)	18(1)	36(1)	16(1)	-1(1)	-2(1)	5(1)
C(19)	16(1)	27(1)	16(1)	-2(1)	2(1)	4(1)
C(20)	29(1)	40(1)	42(1)	-15(1)	-16(1)	21(1)
C(21)	13(1)	52(1)	22(1)	0(1)	2(1)	7(1)
C(22)	16(1)	44(1)	18(1)	1(1)	3(1)	6(1)
C(23)	15(1)	29(1)	25(1)	2(1)	-4(1)	-1(1)
C(24)	20(1)	8(1)	15(1)	1(1)	6(1)	1(1)
C(25)	21(1)	18(1)	20(1)	2(1)	7(1)	3(1)
C(26)	27(1)	23(1)	29(1)	2(1)	15(1)	4(1)
C(27)	42(1)	20(1)	21(1)	-1(1)	18(1)	2(1)
C(28)	36(1)	15(1)	16(1)	-1(1)	4(1)	-3(1)
C(29)	22(1)	12(1)	18(1)	1(1)	4(1)	-1(1)
C(30)	10(1)	18(1)	16(1)	4(1)	3(1)	0(1)
C(31)	20(1)	20(1)	19(1)	3(1)	7(1)	3(1)
C(32)	22(1)	24(1)	29(1)	11(1)	10(1)	8(1)
C(33)	16(1)	37(1)	23(1)	16(1)	1(1)	4(1)
C(34)	20(1)	33(1)	18(1)	5(1)	-1(1)	-7(1)
C(35)	16(1)	20(1)	19(1)	2(1)	3(1)	-4(1)
C(36)	13(1)	15(1)	15(1)	-1(1)	4(1)	-2(1)
C(37)	17(1)	16(1)	16(1)	0(1)	4(1)	0(1)
C(38)	22(1)	19(1)	20(1)	-2(1)	9(1)	1(1)
C(39)	23(1)	26(1)	18(1)	2(1)	9(1)	-1(1)
C(40)	21(1)	19(1)	22(1)	5(1)	7(1)	0(1)
C(41)	16(1)	15(1)	19(1)	0(1)	5(1)	0(1)
C(42)	17(1)	28(1)	26(1)	3(1)	10(1)	2(1)
C(43)	14(1)	29(1)	26(1)	-2(1)	5(1)	-6(1)
C(44)	23(1)	22(1)	33(1)	0(1)	13(1)	-6(1)
C(45)	15(1)	21(1)	19(1)	-3(1)	4(1)	-2(1)
O4A1	83(2)	87(2)	155(3)	39(2)	85(2)	13(1)
C1A1	13(3)	53(3)	33(3)	-36(3)	4(2)	3(2)
C2A1	31(3)	28(3)	65(4)	4(2)	18(2)	-6(2)
C3A1	18(2)	27(3)	53(3)	11(2)	4(2)	-2(2)
C4A1	28(3)	84(5)	122(6)	65(4)	14(4)	8(3)
C1B1	23(4)	137(8)	61(6)	51(5)	20(4)	15(5)
C2B1	73(5)	44(4)	48(4)	7(3)	17(4)	25(4)
C3B1	39(3)	65(5)	52(4)	9(3)	11(3)	14(3)
C4B1	20(2)	52(4)	26(2)	2(2)	3(2)	1(2)

2.7 Crystal Structure Determination of **6**

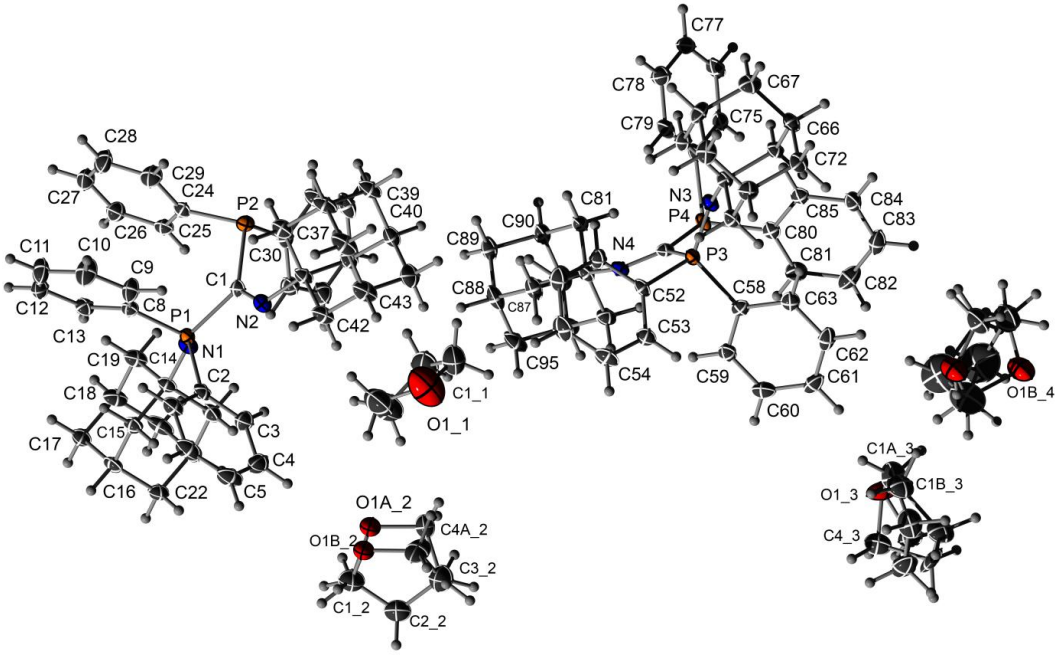


Figure S13. ORTEP Plot of compound **6**. Ellipsoids are drawn at the 50% probability level.

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	5221(1)	7978(1)	7361(1)	16(1)
C(1)	4400(1)	7527(1)	7306(1)	17(1)
P(2)	4382(1)	6705(1)	7569(1)	18(1)
C(2)	4909(1)	8710(1)	6997(1)	20(1)
P(3)	41(1)	5426(1)	3045(1)	14(1)
C(3)	4685(1)	8722(1)	6328(1)	27(1)
P(4)	841(1)	4208(1)	2683(1)	16(1)
C(4)	4436(2)	9258(1)	6011(2)	36(1)
N(1)	5739(1)	7622(1)	7040(1)	20(1)
N(2)	3863(1)	7861(1)	7134(1)	19(1)
N(3)	-458(1)	5019(1)	3336(1)	17(1)
N(4)	1397(1)	5271(1)	3358(1)	17(1)
C(14)	6372(1)	7785(1)	6808(1)	18(1)
C(19)	6967(1)	7355(1)	7120(1)	25(1)
C(18)	7635(1)	7476(1)	6860(1)	27(1)
C(17)	7868(1)	8133(1)	7015(1)	25(1)
C(16)	7287(1)	8565(1)	6690(1)	22(1)
C(5)	4410(1)	9784(1)	6372(2)	35(1)
C(15)	6620(1)	8441(1)	6949(1)	20(1)
C(95)	3556(1)	5511(1)	3394(2)	31(1)
C(94)	3332(1)	4410(1)	3179(1)	26(1)
C(93)	3162(1)	5049(1)	2910(1)	27(1)
C(92)	2371(1)	5151(1)	2800(1)	22(1)
C(91)	2315(1)	4446(1)	3730(1)	19(1)
C(6)	4636(1)	9778(1)	7029(2)	33(1)
C(20)	6237(1)	7687(1)	6068(1)	24(1)
C(7)	4892(1)	9246(1)	7348(1)	25(1)
C(8)	5467(1)	8142(1)	8229(1)	18(1)
C(21)	6896(1)	7814(1)	5802(1)	26(1)
C(9)	4975(1)	8347(1)	8568(1)	28(1)
C(22)	7130(1)	8471(1)	5955(1)	24(1)
C(10)	5173(2)	8501(1)	9214(1)	36(1)
C(11)	5865(1)	8444(1)	9538(1)	34(1)
C(12)	6354(1)	8229(1)	9209(1)	27(1)
C(13)	6156(1)	8075(1)	8557(1)	22(1)
C(36)	3120(1)	7693(1)	7065(1)	19(1)
C(24)	5209(1)	6600(1)	8154(1)	19(1)
C(23)	7481(1)	7383(1)	6126(1)	30(1)
C(37)	2937(1)	7567(1)	7728(1)	23(1)
C(25)	5849(1)	6464(1)	7998(1)	21(1)
C(38)	2142(1)	7458(1)	7632(1)	25(1)
C(26)	6434(1)	6363(1)	8490(1)	27(1)
C(39)	1932(1)	6919(1)	7175(1)	26(1)
C(27)	6388(2)	6398(1)	9134(1)	30(1)
C(40)	2102(1)	7056(1)	6514(1)	25(1)
C(28)	5756(2)	6529(1)	9296(1)	34(1)
C(41)	2897(1)	7152(1)	6605(1)	22(1)
C(29)	5168(2)	6623(1)	8806(1)	29(1)
C(42)	2714(1)	8260(1)	6769(1)	26(1)
C(30)	4500(1)	6286(1)	6845(1)	19(1)
C(44)	1746(1)	8024(1)	7339(2)	31(1)
C(31)	4240(1)	5693(1)	6774(1)	25(1)
C(43)	1924(1)	8161(1)	6686(2)	31(1)
C(32)	4297(1)	5347(1)	6239(1)	30(1)
C(45)	1709(1)	7623(1)	6220(2)	33(1)
C(33)	4596(1)	5586(1)	5762(1)	30(1)
C(35)	4804(1)	6521(1)	6359(1)	26(1)
C(34)	4850(1)	6172(1)	5826(1)	32(1)

C(64)	-1092(1)	5132(1)	3577(1)	16(1)
C(51)	852(1)	4982(1)	3077(1)	15(1)
C(65)	-1636(1)	4651(1)	3281(1)	18(1)
C(52)	329(1)	6138(1)	3463(1)	16(1)
C(53)	276(1)	6704(1)	3158(1)	22(1)
C(66)	-2313(1)	4717(1)	3537(1)	21(1)
C(54)	495(1)	7230(1)	3512(1)	30(1)
C(67)	-2147(1)	4641(1)	4276(1)	25(1)
C(55)	766(2)	7193(1)	4174(1)	32(1)
C(56)	814(1)	6635(1)	4486(1)	30(1)
C(63)	-863(1)	5535(1)	1827(1)	20(1)
C(57)	597(1)	6110(1)	4134(1)	21(1)
C(62)	-1034(1)	5678(1)	1172(1)	25(1)
C(58)	-187(1)	5635(1)	2186(1)	18(1)
C(61)	-535(2)	5917(1)	863(1)	27(1)
C(59)	315(1)	5870(1)	1871(1)	21(1)
C(60)	142(2)	6012(1)	1216(1)	28(1)
C(86)	2136(1)	5088(1)	3451(1)	16(1)
C(69)	-938(1)	5053(1)	4322(1)	21(1)
C(68)	-1612(1)	5120(1)	4587(1)	24(1)
C(87)	2541(1)	5553(1)	3932(1)	23(1)
C(70)	-1414(1)	5766(1)	3418(1)	19(1)
C(88)	3328(1)	5446(1)	4045(1)	26(1)
C(71)	-2089(1)	5836(1)	3676(1)	22(1)
C(72)	-1924(1)	5755(1)	4414(1)	25(1)
C(73)	-2620(1)	5353(1)	3360(1)	23(1)
C(74)	625(1)	3694(1)	3298(1)	17(1)
C(75)	582(1)	3077(1)	3137(1)	22(1)
C(89)	3498(1)	4807(1)	4317(1)	25(1)
C(76)	433(1)	2647(1)	3571(1)	30(1)
C(90)	3105(1)	4341(1)	3830(1)	22(1)
C(77)	335(1)	2827(1)	4178(1)	29(1)
C(78)	385(1)	3434(1)	4344(1)	27(1)
C(79)	526(1)	3868(1)	3909(1)	23(1)
C(80)	42(1)	4174(1)	2048(1)	17(1)
C(81)	118(1)	4277(1)	1414(1)	25(1)
C(82)	-439(2)	4191(1)	892(1)	33(1)
C(83)	-1076(1)	3988(1)	997(1)	30(1)
C(85)	-607(1)	3984(1)	2149(1)	19(1)
C(84)	-1159(1)	3890(1)	1623(1)	24(1)
O11	2696(2)	7842(1)	4867(2)	88(1)
C11	2665(2)	7234(2)	4634(2)	62(1)
C21	3395(2)	7024(2)	4658(2)	58(1)
C31	3811(2)	7591(2)	4772(2)	64(1)
C41	3414(2)	7981(2)	5115(2)	65(1)
O12	3722(1)	9244(1)	4387(1)	42(1)
O1B2	3476(7)	9805(7)	4471(6)	42(1)
C12	4074(2)	9784(2)	4185(2)	53(1)
C22	3813(2)	9807(2)	3476(2)	47(1)
C32	3089(2)	9527(2)	3379(2)	50(1)
C4A2	3180(2)	9049(2)	3864(2)	35(1)
C4B2	2883(10)	9671(11)	3981(9)	44(6)
O13	-1017(1)	6732(1)	-492(1)	47(1)
C13	-1597(4)	6930(3)	-281(4)	40(1)
C23	-1855(2)	7500(2)	-650(3)	40(1)
C33	-1321(3)	7594(2)	-1078(2)	45(1)
C4A3	-1062(3)	6964(2)	-1144(3)	38(1)
C1B3	-1707(10)	7064(12)	-383(13)	42(4)
C2B3	-1952(7)	7304(7)	-1099(8)	42(4)
C3B3	-1360(9)	7233(8)	-1423(7)	48(5)
C4B3	-747(9)	7170(7)	-859(9)	37(4)
O14	-2221(1)	5514(1)	-260(1)	41(1)

C14	-2593(2)	4995(2)	-143(2)	41(1)
C24	-2486(2)	4513(2)	-608(2)	54(1)
C3A4	-1791(4)	4745(3)	-824(3)	89(2)
O1B4	-2405(7)	4856(6)	-1139(7)	41(1)
C44	-1874(2)	5381(2)	-783(2)	66(1)
C1B4	-1444(19)	5052(14)	-472(16)	89(2)
C3B4	-1805(10)	4294(9)	-547(11)	41(1)

Table S15. Anisotropic displacement parameters ($Å^2x\ 10^3$) for compound **6**. 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}
P(1)	15(1)	14(1)	19(1)	0(1)	3(1)	-1(1)
C(1)	19(1)	15(1)	15(1)	-3(1)	4(1)	-1(1)
P(2)	17(1)	16(1)	20(1)	1(1)	5(1)	1(1)
C(2)	14(1)	20(1)	27(2)	4(1)	3(1)	-1(1)
P(3)	12(1)	13(1)	18(1)	0(1)	2(1)	1(1)
C(3)	23(2)	28(2)	29(2)	5(1)	2(1)	0(1)
P(4)	13(1)	15(1)	21(1)	-2(1)	4(1)	0(1)
C(4)	27(2)	45(2)	33(2)	15(1)	1(1)	-1(1)
N(1)	19(1)	17(1)	24(1)	-1(1)	7(1)	-2(1)
N(2)	17(1)	18(1)	22(1)	-2(1)	5(1)	-1(1)
N(3)	13(1)	16(1)	22(1)	0(1)	4(1)	0(1)
N(4)	15(1)	15(1)	22(1)	1(1)	6(1)	0(1)
C(14)	17(1)	16(1)	22(1)	-1(1)	8(1)	-1(1)
C(19)	23(1)	20(1)	36(2)	6(1)	12(1)	2(1)
C(18)	20(1)	24(2)	38(2)	9(1)	12(1)	4(1)
C(17)	20(1)	31(2)	27(2)	2(1)	7(1)	-5(1)
C(16)	25(1)	15(1)	26(2)	-3(1)	7(1)	-7(1)
C(5)	24(2)	24(2)	57(2)	15(1)	8(1)	3(1)
C(15)	23(1)	17(1)	21(1)	-2(1)	6(1)	-2(1)
C(95)	16(1)	25(2)	53(2)	4(1)	8(1)	-3(1)
C(94)	18(1)	26(2)	35(2)	-7(1)	5(1)	4(1)
C(93)	19(1)	34(2)	30(2)	5(1)	12(1)	2(1)
C(92)	19(1)	23(1)	26(2)	3(1)	7(1)	0(1)
C(91)	15(1)	15(1)	25(1)	2(1)	2(1)	-1(1)
C(6)	25(2)	22(2)	52(2)	3(1)	9(1)	1(1)
C(20)	25(1)	24(1)	25(2)	-7(1)	9(1)	-9(1)
C(7)	20(1)	19(1)	37(2)	1(1)	7(1)	-1(1)
C(8)	19(1)	16(1)	19(1)	0(1)	4(1)	-1(1)
C(21)	30(2)	31(2)	22(2)	-6(1)	11(1)	-11(1)
C(9)	20(1)	38(2)	24(2)	-4(1)	2(1)	3(1)
C(22)	24(1)	26(1)	24(2)	3(1)	9(1)	-5(1)
C(10)	29(2)	54(2)	25(2)	-10(1)	9(1)	5(2)
C(11)	28(2)	51(2)	20(2)	-8(1)	2(1)	-4(1)
C(12)	19(1)	36(2)	25(2)	4(1)	0(1)	-3(1)
C(13)	19(1)	24(1)	23(2)	2(1)	6(1)	1(1)
C(36)	14(1)	16(1)	27(2)	1(1)	6(1)	-1(1)
C(24)	23(1)	14(1)	19(1)	0(1)	2(1)	-1(1)
C(23)	31(2)	19(1)	47(2)	-7(1)	25(1)	-7(1)
C(37)	23(1)	20(1)	27(2)	-2(1)	9(1)	-1(1)
C(25)	23(1)	16(1)	23(1)	1(1)	6(1)	-2(1)
C(38)	23(1)	22(1)	35(2)	-2(1)	17(1)	-2(1)
C(26)	22(1)	26(2)	31(2)	4(1)	4(1)	2(1)
C(39)	20(1)	21(1)	39(2)	1(1)	11(1)	-2(1)
C(27)	27(2)	31(2)	29(2)	3(1)	-5(1)	-2(1)
C(40)	17(1)	24(2)	33(2)	-4(1)	2(1)	-4(1)
C(28)	37(2)	45(2)	19(2)	-3(1)	1(1)	-2(2)
C(41)	19(1)	22(1)	24(2)	0(1)	5(1)	0(1)
C(29)	28(2)	36(2)	25(2)	-2(1)	10(1)	2(1)
C(42)	22(1)	19(1)	37(2)	5(1)	10(1)	0(1)
C(30)	14(1)	19(1)	22(1)	-1(1)	2(1)	4(1)
C(44)	22(2)	24(2)	51(2)	-2(1)	16(1)	1(1)

C(31)	24(1)	19(1)	32(2)	0(1)	9(1)	0(1)
C(43)	16(1)	23(2)	55(2)	9(1)	9(1)	6(1)
C(32)	23(2)	23(2)	42(2)	-9(1)	5(1)	-1(1)
C(45)	16(1)	40(2)	40(2)	6(1)	1(1)	0(1)
C(33)	19(1)	39(2)	29(2)	-17(1)	-1(1)	0(1)
C(35)	29(2)	23(1)	25(2)	-3(1)	7(1)	-5(1)
C(34)	30(2)	42(2)	24(2)	-7(1)	9(1)	-9(1)
C(64)	14(1)	18(1)	17(1)	1(1)	5(1)	2(1)
C(51)	16(1)	14(1)	16(1)	3(1)	6(1)	0(1)
C(65)	15(1)	20(1)	21(1)	0(1)	5(1)	-1(1)
C(52)	12(1)	16(1)	22(1)	-2(1)	5(1)	-1(1)
C(53)	23(1)	18(1)	24(2)	-1(1)	6(1)	1(1)
C(66)	16(1)	24(1)	26(2)	-1(1)	7(1)	-4(1)
C(54)	35(2)	14(1)	42(2)	-1(1)	11(1)	-2(1)
C(67)	21(1)	29(2)	28(2)	4(1)	11(1)	4(1)
C(55)	36(2)	20(2)	39(2)	-12(1)	4(1)	-3(1)
C(56)	30(2)	28(2)	28(2)	-7(1)	1(1)	0(1)
C(63)	20(1)	15(1)	24(2)	-1(1)	3(1)	4(1)
C(57)	20(1)	20(1)	21(1)	-1(1)	2(1)	2(1)
C(62)	25(2)	21(1)	26(2)	-3(1)	-4(1)	7(1)
C(58)	20(1)	13(1)	20(1)	1(1)	4(1)	4(1)
C(61)	39(2)	21(1)	19(2)	3(1)	2(1)	7(1)
C(59)	22(1)	17(1)	25(2)	1(1)	4(1)	-1(1)
C(60)	36(2)	20(1)	30(2)	4(1)	13(1)	-1(1)
C(86)	12(1)	13(1)	23(1)	-1(1)	3(1)	0(1)
C(69)	17(1)	22(1)	22(1)	1(1)	1(1)	3(1)
C(68)	23(1)	34(2)	16(1)	2(1)	5(1)	6(1)
C(87)	17(1)	18(1)	34(2)	-8(1)	3(1)	1(1)
C(70)	16(1)	17(1)	24(1)	0(1)	4(1)	1(1)
C(88)	15(1)	19(1)	43(2)	-8(1)	0(1)	-1(1)
C(71)	19(1)	21(1)	27(2)	1(1)	7(1)	6(1)
C(72)	20(1)	31(2)	25(2)	-7(1)	8(1)	6(1)
C(73)	13(1)	30(2)	25(2)	2(1)	6(1)	2(1)
C(74)	10(1)	17(1)	24(1)	2(1)	1(1)	0(1)
C(75)	19(1)	18(1)	26(2)	-2(1)	0(1)	-1(1)
C(89)	14(1)	27(2)	32(2)	-5(1)	0(1)	2(1)
C(76)	27(2)	14(1)	42(2)	4(1)	-4(1)	-2(1)
C(90)	16(1)	16(1)	31(2)	0(1)	0(1)	2(1)
C(77)	21(1)	31(2)	34(2)	14(1)	0(1)	-4(1)
C(78)	26(2)	29(2)	27(2)	4(1)	6(1)	0(1)
C(79)	21(1)	19(1)	29(2)	0(1)	6(1)	-1(1)
C(80)	19(1)	11(1)	21(1)	-2(1)	5(1)	3(1)
C(81)	23(1)	26(2)	26(2)	0(1)	9(1)	3(1)
C(82)	39(2)	38(2)	20(2)	2(1)	7(1)	11(1)
C(83)	28(2)	29(2)	27(2)	-3(1)	-6(1)	6(1)
C(85)	18(1)	13(1)	23(1)	0(1)	2(1)	2(1)
C(84)	19(1)	19(1)	31(2)	2(1)	0(1)	0(1)
O11	60(2)	69(2)	135(3)	-8(2)	22(2)	9(2)
C11	60(3)	71(3)	49(2)	-4(2)	-2(2)	-21(2)
C21	64(3)	38(2)	66(3)	-3(2)	-2(2)	2(2)
C31	53(2)	62(3)	82(3)	2(2)	22(2)	-8(2)
C41	69(3)	55(2)	74(3)	-6(2)	18(2)	-23(2)
O12	36(2)	55(2)	31(1)	13(1)	0(1)	-19(1)
O1B2	36(2)	55(2)	31(1)	13(1)	0(1)	-19(1)
C12	55(2)	63(2)	41(2)	7(2)	11(2)	-22(2)
C22	52(2)	43(2)	46(2)	11(2)	6(2)	-9(2)
C32	40(2)	58(2)	49(2)	10(2)	1(2)	-2(2)
C4A2	31(2)	38(2)	32(2)	-1(2)	0(2)	-7(2)
C4B2	26(11)	77(16)	32(12)	9(11)	14(9)	-1(11)
O13	39(1)	55(2)	51(2)	31(1)	18(1)	15(1)
C13	32(2)	37(2)	50(3)	-7(2)	9(2)	8(2)
C23	32(2)	37(2)	50(3)	-7(2)	9(2)	8(2)
C33	65(3)	27(2)	39(3)	8(2)	1(2)	8(2)
C4A3	56(3)	31(3)	28(3)	5(2)	12(3)	-1(3)
C1B3	30(7)	50(8)	49(9)	6(6)	17(6)	0(5)
C2B3	30(7)	50(8)	49(9)	6(6)	17(6)	0(5)
C3B3	79(12)	44(11)	14(8)	7(7)	-8(7)	4(9)
C4B3	40(9)	31(9)	44(10)	4(7)	15(8)	0(7)
O14	44(2)	40(2)	44(2)	-11(1)	23(1)	-8(1)

C14	38(2)	33(2)	50(2)	-4(2)	8(2)	-7(2)
C24	57(2)	46(2)	56(2)	-7(2)	5(2)	-7(2)
C3A4	125(6)	65(4)	82(4)	-25(3)	34(4)	19(4)
O1B4	44(2)	40(2)	44(2)	-11(1)	23(1)	-8(1)
C44	69(3)	62(3)	78(3)	-12(2)	39(2)	1(2)
C1B4	125(6)	65(4)	82(4)	-25(3)	34(4)	19(4)
C3B4	38(2)	33(2)	50(2)	-4(2)	8(2)	-7(2)

3. Computational details

All calculations were performed without symmetry restrictions. Starting coordinates were obtained with Chem3DUltra 10.0 or directly from the crystal structure analysis. All calculations were done with the Gaussian 09 (Revision B.01) program package.[1] Geometry optimizations were performed using Density-Functional Theory (DFT) with the B3LYP (Becke 3-parameter-Lee-Yang-Parr) functional[2] and the 6-311++G(d) basis. Harmonic vibrational frequency analyses were performed on the same levels of theory. The vibrational frequency analyses showed no imaginary frequencies for the ground states and a single negative frequency for the transition states.

3.1 Electronic structure of a bis(iminophosphoryl)methandiide

For computational cost a model system analogous to the dimeric structure of BIPM^{Tol} was chosen, in which the substituents at the phosphorus and nitrogen atoms were replaced by methyl groups. Natural bond orbital analysis studies were performed on the energy-optimized system with the NBO 3.1[3] program implemented in the Gaussian program package. The natural atomic charges and Wiberg bond indices are given in Figure S14, the results of the NBO analysis and second-order perturbation theory analysis are given in Figure S15 and S16. The Cartesian coordinates are given in Table S16.

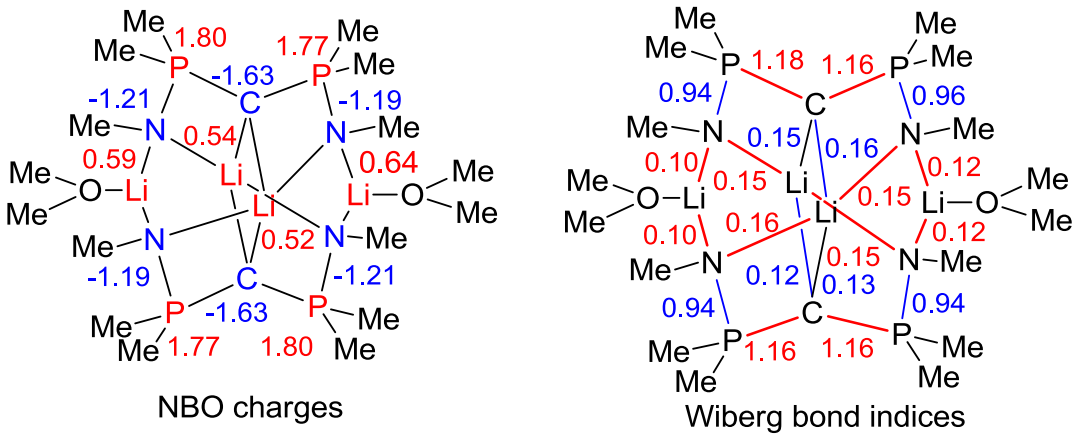


Figure S14. NBO charges and Wiberg bond indices in a bis(iminophosphoryl) substituted methandiide.

```
   (Occupancy)   Bond orbital/ Coefficients/ Hybrids
-------------------------------------------------------------------------------
 1. (1.93776) BD ( 1) C   1 - P  11
           ( 59.99%)   0.7745* C   1 s( 39.23%)p 1.55( 60.72%)d 0.00(  0.05%)
                                    -0.0011  0.6262  0.0158 -0.0010 -0.0001
                                    -0.3487 -0.0102 -0.0054 -0.0017 -0.1301
                                    -0.0081 -0.0078  0.0015  0.6840  0.0237
                                     0.0018  0.0034  0.0044 -0.0124 -0.0112
                                    -0.0010  0.0140
           ( 40.01%)   0.6326* P  11 s( 32.15%)p 2.09( 67.11%)d 0.02(  0.73%)
                                     0.0000 -0.0023  0.5663  0.0279 -0.0049
                                    -0.0003  0.0001 -0.0001  0.3512  0.0005
                                    -0.0031  0.0029 -0.0002 -0.0005  0.0042
                                     0.0032 -0.0073  0.0047  0.0003  0.0000
                                    -0.7397 -0.0224  0.0023 -0.0068  0.0004
                                     0.0020 -0.0565 -0.0041  0.0173  0.0617
 2. (1.94183) BD ( 1) C   1 - P  12
           ( 59.94%)   0.7742* C   1 s( 40.49%)p 1.47( 59.46%)d 0.00(  0.05%)
                                    -0.0010  0.6361  0.0181  0.0021 -0.0001
                                     0.3748  0.0121 -0.0025  0.0025 -0.4712
                                    -0.0251 -0.0051 -0.0004 -0.4806 -0.0170
                                    -0.0012 -0.0032 -0.0134 -0.0096  0.0127
                                    -0.0078 -0.0041
           ( 40.06%)   0.6329* P  12 s( 32.85%)p 2.02( 66.40%)d 0.02(  0.75%)
                                     0.0000 -0.0015  0.5723  0.0313 -0.0040
                                    -0.0004  0.0001 -0.0002 -0.4431 -0.0145
                                    -0.0025 -0.0012  0.0003 -0.0004  0.4328
                                     0.0110 -0.0069  0.0051 -0.0004  0.0000
                                     0.5290  0.0082 -0.0015  0.0053 -0.0003
                                    -0.0452 -0.0501  0.0523  0.0029  0.0128
 3. (1.94363) BD ( 1) C   2 - P  13
           ( 59.85%)   0.7737* C   2 s( 40.48%)p 1.47( 59.47%)d 0.00(  0.05%)
                                    -0.0010  0.6360  0.0172 -0.0001 -0.0001
                                     0.5523  0.0192  0.0048  0.0031  0.1888
                                     0.0111  0.0055 -0.0013  0.5032  0.0154
                                    -0.0019  0.0031  0.0102  0.0164  0.0095
                                     0.0027  0.0040
           ( 40.15%)   0.6336* P  13 s( 32.77%)p 2.03( 66.51%)d 0.02(  0.72%)
                                     0.0000 -0.0020  0.5717  0.0282  0.0062
                                    -0.0009  0.0001  0.0002 -0.5690 -0.0028
                                     0.0015 -0.0040  0.0004  0.0004 -0.0837
                                    -0.0081  0.0058 -0.0068 -0.0003 -0.0001
                                    -0.5775 -0.0231 -0.0012 -0.0045  0.0003
                                     0.0116  0.0704  0.0141  0.0375  0.0219
 4. (1.94380) BD ( 1) C   2 - P  14
           ( 60.09%)   0.7752* C   2 s( 40.20%)p 1.49( 59.75%)d 0.00(  0.05%)
                                    -0.0010  0.6338  0.0179 -0.0018 -0.0001
                                    -0.5260 -0.0132  0.0029 -0.0039  0.4184
                                     0.0210  0.0058  0.0000 -0.3807 -0.0124
                                    -0.0021 -0.0023 -0.0159  0.0104 -0.0088
                                    -0.0029 -0.0075
           ( 39.91%)   0.6318* P  14 s( 32.64%)p 2.04( 66.62%)d 0.02(  0.74%)
                                     0.0000 -0.0016  0.5706  0.0284 -0.0051
                                    -0.0004  0.0001  0.0001  0.6038  0.0117
                                     0.0017  0.0035 -0.0006  0.0004 -0.3573
                                    -0.0054  0.0067 -0.0037  0.0005  0.0000
                                     0.4167  0.0072 -0.0031  0.0036 -0.0004
                                    -0.0496  0.0544 -0.0335  0.0280 -0.0075
 5. (1.95469) BD ( 1) N   7 - P  11
```

```
121. (1.65162) LP ( 1) C   1           s( 18.38%)p 4.44( 81.59%)d 0.00(  0.03%)
                                        -0.0007  0.4281 -0.0235  0.0011  0.0001
                                        -0.3000  0.0013  0.0003  0.0022  0.7502
                                        -0.0237 -0.0234  0.0002 -0.4024  0.0068
                                        -0.0049  0.0004  0.0049 -0.0060  0.0096
                                         0.0089  0.0042
122. (1.61026) LP ( 2) C   1           s(  1.87%)p52.34( 98.10%)d 0.02(  0.03%)
                                        -0.0007  0.1350 -0.0222 -0.0058 -0.0003
                                         0.8042 -0.0060  0.0094 -0.0041  0.4427
                                        -0.0122  0.0027  0.0000  0.3712 -0.0043
                                         0.0083 -0.0009 -0.0099  0.0070 -0.0009
                                         0.0093  0.0080
123. (1.63717) LP ( 1) C   2           s( 19.30%)p 4.18( 80.67%)d 0.00(  0.03%)
                                        -0.0007  0.4381 -0.0327  0.0025  0.0000
                                        -0.0612  0.0032  0.0051  0.0009 -0.8819
                                         0.0247  0.0167  0.0003 -0.1557  0.0050
                                        -0.0052  0.0007  0.0016  0.0026 -0.0071
                                         0.0128  0.0076
124. (1.61696) LP ( 2) C   2           s(  0.06%)p99.99( 99.91%)d 0.44(  0.03%)
                                         0.0007  0.0135  0.0176  0.0103  0.0005
                                         0.6426  0.0019  0.0048 -0.0036  0.0958
                                        -0.0022  0.0036 -0.0001 -0.7595  0.0103
                                        -0.0108  0.0026  0.0091  0.0047 -0.0090
                                        -0.0042 -0.0078
```

Figure S15. Extracts of the output of the NBO analysis of the C-P bonds and the lone pairs at the metallated carbon atoms C1 and C2.

120.	CR	(1)	C	77	/803.	RY*(1)	H	78			0.54	11.03	0.069
120.	CR	(1)	C	77	/805.	RY*(1)	H	79			0.82	11.76	0.088
121.	LP	(1)	C	1	/156.	RY*(4)	C	1			0.52	1.50	0.028
121.	LP	(1)	C	1	/324.	RY*(2)	P	11			3.56	1.12	0.062
121.	LP	(1)	C	1	/325.	RY*(3)	P	11			1.33	1.01	0.036
121.	LP	(1)	C	1	/332.	RY*(10)	P	11			0.66	0.90	0.024
121.	LP	(1)	C	1	/344.	RY*(1)	P	12			0.97	1.03	0.031
121.	LP	(1)	C	1	/345.	RY*(2)	P	12			1.09	1.05	0.033
121.	LP	(1)	C	1	/346.	RY*(3)	P	12			2.41	1.08	0.050
121.	LP	(1)	C	1	/353.	RY*(10)	P	12			0.58	1.25	0.026
121.	LP	(1)	C	1	/809.	BD*(1)	C	1	- P	11	0.55	0.54	0.017
121.	LP	(1)	C	1	/810.	BD*(1)	C	1	- P	12	0.70	0.55	0.019
121.	LP	(1)	C	1	/813.	BD*(1)	N	7	- P	11	4.78	0.48	0.046
121.	LP	(1)	C	1	/815.	BD*(1)	N	8	- P	12	2.18	0.47	0.031
121.	LP	(1)	C	1	/821.	BD*(1)	P	11	- C	73	0.54	0.39	0.014
121.	LP	(1)	C	1	/822.	BD*(1)	P	11	- C	77	15.18	0.39	0.072
121.	LP	(1)	C	1	/824.	BD*(1)	P	12	- C	53	17.73	0.38	0.078
121.	LP	(1)	C	1	/860.	BD*(1)	C	53	- H	54	0.52	0.56	0.017
121.	LP	(1)	C	1	/878.	BD*(1)	C	77	- H	78	0.53	0.57	0.017
122.	LP	(2)	C	1	/323.	RY*(1)	P	11			2.58	0.98	0.050
122.	LP	(2)	C	1	/324.	RY*(2)	P	11			0.97	1.07	0.032
122.	LP	(2)	C	1	/325.	RY*(3)	P	11			2.15	0.96	0.045
122.	LP	(2)	C	1	/344.	RY*(1)	P	12			1.14	0.98	0.033
122.	LP	(2)	C	1	/345.	RY*(2)	P	12			3.45	1.00	0.058
122.	LP	(2)	C	1	/346.	RY*(3)	P	12			0.82	1.03	0.029
122.	LP	(2)	C	1	/813.	BD*(1)	N	7	- P	11	2.09	0.43	0.029
122.	LP	(2)	C	1	/815.	BD*(1)	N	8	- P	12	6.04	0.42	0.049
122.	LP	(2)	C	1	/821.	BD*(1)	P	11	- C	73	22.12	0.34	0.082
122.	LP	(2)	C	1	/822.	BD*(1)	P	11	- C	77	5.84	0.33	0.042
122.	LP	(2)	C	1	/823.	BD*(1)	P	12	- C	49	18.82	0.34	0.076
122.	LP	(2)	C	1	/824.	BD*(1)	P	12	- C	53	0.74	0.33	0.015
122.	LP	(2)	C	1	/857.	BD*(1)	C	49	- H	50	0.64	0.51	0.018
141.	LP	(1)	N	7	/257.	RY*(3)	N	7			0.75	1.36	0.030
141.	LP	(1)	N	7	/324.	RY*(2)	P	11			2.87	1.29	0.057
141.	LP	(1)	N	7	/326.	RY*(4)	P	11			1.46	1.55	0.044
141.	LP	(1)	N	7	/327.	RY*(5)	P	11			0.68	1.70	0.032

Figure S16. Extract of the output of the second order perturbation theory analysis. Donor-acceptor interaction of the two lone pairs at the metallated carbon atom with the antibonding orbitals σ^*(P-X).

Table S16. Cartesian coordinates of the $[(MeNPMe_2)_2CLi_2{\cdot}OMe_2]_2$.

Atomic symbol	x	y	z
C	6.5300478012	7.2557669343	5.6688341505
C	3.2365730251	5.7334453263	5.988679526
Li	4.2651667415	7.6470349064	5.5869402381
Li	4.5040401387	5.8776922615	3.5399036284
Li	5.361637114	5.297839519	5.9653935405
Li	5.6526890331	7.0474904048	7.7690741554
N	5.1120370065	8.9883341523	6.9359390984
N	6.342530505	5.0917893764	4.1430888548
N	2.995670933	7.2515531624	3.8966356578
N	4.8556454875	5.1294814051	7.9797023636
P	6.486576506	8.9073660775	6.0251031573
P	7.3806129079	6.3124631629	4.5629920894
P	2.0740577018	6.423091528	4.9957970926
P	3.2646693276	5.0627671108	7.5306135987
O	6.7470840295	7.4683150711	9.4685161025
C	7.9343372209	6.8128773016	9.8883836139
C	6.1097419369	8.1913533933	10.5125582886
O	4.3105327196	5.3727528729	1.5447509691
C	3.0631506226	5.2921417004	0.8671344065
C	5.4149898082	5.19744852	0.666912844
H	8.6658844623	7.5395687317	10.2631353887
H	8.3473410962	6.3031740354	9.0189569474
H	7.7231693541	6.0795807885	10.6754253464
H	6.7857191368	8.9474908637	10.9298740307
H	5.7859202183	7.5168554083	11.3144130114
H	5.2431137183	8.6875857053	10.0789764259
H	2.9976363923	6.0546574906	0.0820425025
H	2.9319315911	4.3007596119	0.4163770487
H	2.2827137857	5.4672717211	1.602359443
H	5.4059417072	5.9603981836	-0.1211604903
H	5.3906080008	4.2039120777	0.2032327533

H	6.3178142293	5.2974072909	1.2626803524
C	4.6732187053	10.2553201353	7.5045026396
H	4.4628475588	11.0366696767	6.7550661513
H	5.3861301016	10.6962031797	8.2229702959
H	3.7366589982	10.1029122763	8.0530370056
C	6.8803755057	3.8544014475	3.5790816712
H	7.4723560627	3.2647924686	4.2961128257
H	7.5233273322	3.9941485241	2.6925380424
H	6.0538500414	3.2108866601	3.2588306623
C	2.3611217058	8.1546358856	2.9434541262
H	1.898145391	9.0385320384	3.4108590151
H	1.5764367571	7.6868962363	2.3229691265
H	3.114097367	8.5359638553	2.2447154432
C	5.3042713307	4.3281198686	9.1133865068
H	5.114952303	3.248897836	9.0004955109
H	4.8598527147	4.6247467084	10.0802512749
H	6.3879222761	4.4324489045	9.2293214891
C	8.9516815239	5.5728035604	5.218189173
H	9.4482023547	4.9246808786	4.4896848913
H	8.7217284472	4.9849715872	6.1097415531
H	9.6418070359	6.370932056	5.5026277289
C	8.0456727559	7.1642394236	3.0498302482
H	8.4911980023	6.4416418077	2.3588914549
H	8.8159965893	7.8932614085	3.316848552
H	7.2352901861	7.6865047582	2.5377769044
C	2.6522320635	3.315466575	7.6513880313
H	2.7236782494	2.9114721336	8.6655869198
H	3.2393866499	2.6870017096	6.9783161903
H	1.6070376228	3.2716297121	7.334744016
C	2.1956142522	5.8678162463	8.8207535419
H	2.4015271844	5.4521410044	9.8122234642
H	1.1332914159	5.7233558013	8.6050559772
H	2.405398749	6.9390361253	8.8384686556
C	0.8994916168	5.2545101706	4.1504489784
H	0.3016133013	5.7546454573	3.3810376327
H	0.2141580795	4.8157222598	4.8811352986
H	1.469809709	4.4431069987	3.6940909775
C	0.841941555	7.5706132493	5.7830537656
H	0.1821013352	8.0234314044	5.0368137378
H	1.3730519066	8.3677481976	6.3076877204
H	0.2226051395	7.0334860126	6.5055215514
C	7.9398422397	9.6344436911	6.925089469
H	7.7667071634	10.6824277497	7.1896627998
H	8.8379776371	9.5812308186	6.3034980261
H	8.1089500348	9.0636458746	7.8385785482
C	6.4006672594	10.0828767059	4.587298582
H	6.2324967948	11.1088126623	4.9290000549
H	5.5744273951	9.7941208633	3.9341488884
H	7.3276595203	10.0647600792	4.0085043345

3.2 Calculations on carbenoid 4b

For computational cost a model system **4b'** was chosen, in which the tolyl subsitutent was replaced by a phenyl group and diethyl ether by dimethyl ether. The energy-optimized structure (B3LYP functional) well reproduces the experimental data showing a boat conformation of the $C(PN)_2Li$ ring with stabilizing contacts to the *ortho*-hydrogen atoms. This geometry of **4b'** (Figure S17) turned out to be the thermodynamically most stable structure. An alternative coordination **4b-Alt** mode with only one iminophosphoryl moiety, but two dimethyl ether binding to the lithium turned out to be higher in energy (ΔE =46 kJ/mol; ΔG = 90 kJ/mol). The coordination of a second dimethyl ether to the structure of **4b** observed in the molecular structure, was found to be no minimum on the potential energy surface. Optimization always resulted in the elimination of one of the ether molecules under formation of **4b'**. The calculations also showed that **4b'** is preferred over conformer **4b'-chair** (ΔE =10 kJ/mol; ΔG = 16 kJ/mol) with a flattened chair conformation of the $C(PN)_2Li$ ring and over **4b'-NoH** (ΔE =6 kJ/mol; ΔG = 13 kJ/mol), which does not feature the stabilizing Li-H contacts found in the molecular structure of **4b**. The latter could only be calculated by freezing the $CNC_{ipso}C_{ortho}$ dihedral angle. Otherwise, optimization always resulted in structure **4b'** with stabilizing Li–H interactions. The calculations were also performed using the M062X functional to also account for dispersion effects. These studies revealed the same tendencies as observed with the B3LYP functional (Table 17). Figure S17 shows the calculated structures, Table S17 contains the corresponding energies, Table S18-S22 the Cartesian coordinates of the calculated compounds.

The interactions between the lithium and the central carbon atom as well as the ortho-hydrogen of the tolyl substituents were also confirmed by NBO analyses. Second-order perturbation theory analysis showed donor-acceptor interactions for these contacts. For the Li–H interactions the B3LYP and the M062X functional delivered similar energies of the corresponding donor-acceptor interactions (approx. 7 kcal/mol). In the case of the C–Li contact the dispersion-corrected functional showed a higher energetic contribution (13 kcal/mol) than the B3LYP calculations (8 kcal/mol).

Table S17. Energies [in kJ/mol] of the calculated structures

Compound	Method	SCF	ZPE	Free Energy	ΔZPE	ΔG
4b'	B3LYP/6-311+g(d)	-7077863.121	-7075998.107	-7076210.569	0	0
4b'-Alt		-7484954.344	-7482878.367	-7483112.816	45.7	90.3
Me2O		-407135.345	-406925.975	-406992.676	-	-
4b'	B3LYP/6-311+g(d,p)	-7465701.102	-7464003.285	-7464225.509	0	0
4b'-NoH		-7465692.751	-7463994.038	-7464211.642	6.1	12.9
4b'-chair		-7465691.108	-7463993.290	-7464209.999	10.0	15.5
4b'	M062x/6-311+g(d)	-7463522.476	-7461801,522	-7462016,831	0	0
4b'-NoH		-7463510.027	-7461788.316	-7461999.385	13.2	17.4
4b'-chair		-7463515.476	-7461792.677	-7461998.642	8.8	18.2

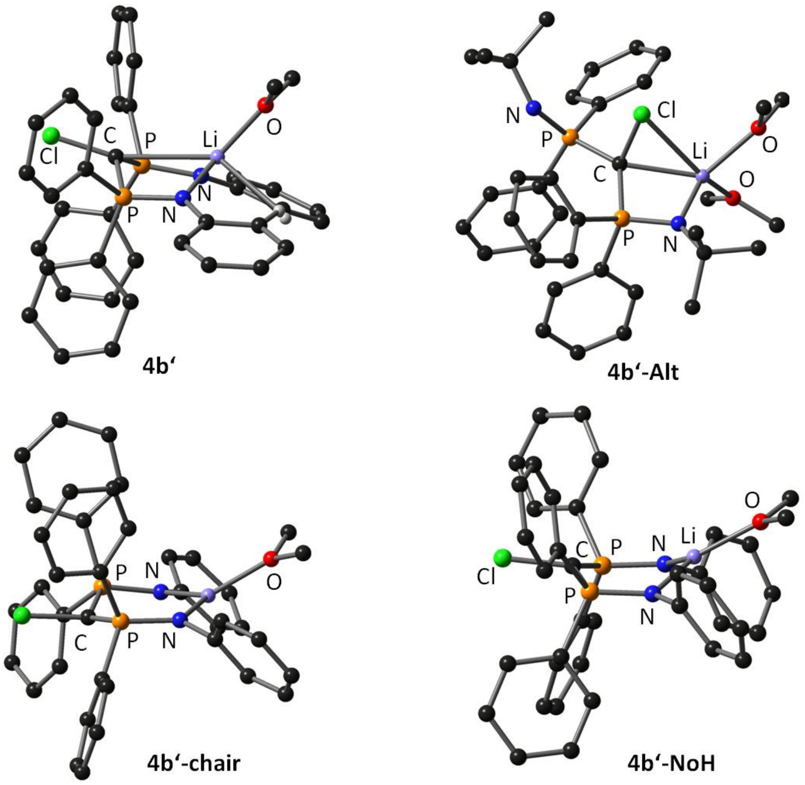


Figure S17. Geometries of the energy-optimized structures.

52. BD (	1) C	24	– H	59	/168. LP*(	1) Li	5		0.10	0.64	0.007
52. BD (	1) C	24	– H	59	/169. LP*(	2) Li	5		0.11	0.63	0.008
52. BD (	1) C	24	– H	59	/171. LP*(	4) Li	5		0.12	0.66	0.008
53. BD (	1) C	25	– H	60	/168. LP*(	1) Li	5		1.28	0.64	0.026
53. BD (	1) C	25	– H	60	/169. LP*(	2) Li	5		3.53	0.62	0.042
53. BD (	1) C	25	– H	60	/170. LP*(	3) Li	5		0.21	0.66	0.011
53. BD (	1) C	25	– H	60	/171. LP*(	4) Li	5		1.96	0.65	0.032
54. BD (	1) C	26	– C	27	/168. LP*(	1) Li	5		0.12	0.85	0.009
54. BD (	1) C	26	– C	27	/171. LP*(	4) Li	5		0.12	0.87	0.009
56. BD (	1) C	26	– C	31	/168. LP*(	1) Li	5		0.16	0.85	0.011
56. BD (	1) C	26	– C	31	/171. LP*(	4) Li	5		0.07	0.86	0.007
64. BD (	1) C	30	– C	31	/168. LP*(	1) Li	5		0.08	0.85	0.008
64. BD (	1) C	30	– C	31	/171. LP*(	4) Li	5		0.08	0.86	0.007
67. BD (	1) C	31	– H	65	/168. LP*(	1) Li	5		0.51	0.66	0.017
85. BD (	1) C	39	– C	40	/169. LP*(	2) Li	5		0.27	0.81	0.013
85. BD (	1) C	39	– C	40	/170. LP*(	3) Li	5		0.40	0.85	0.017
85. BD (	1) C	39	– C	40	/171. LP*(	4) Li	5		0.50	0.84	0.019
86. BD (	2) C	39	– C	40	/169. LP*(	2) Li	5		0.13	0.36	0.006
86. BD (	2) C	39	– C	40	/170. LP*(	3) Li	5		0.15	0.40	0.007
87. BD (	1) C	39	– H	71	/168. LP*(	1) Li	5		1.64	0.64	0.029
87. BD (	1) C	39	– H	71	/169. LP*(	2) Li	5		1.77	0.62	0.030
87. BD (	1) C	39	– H	71	/170. LP*(	3) Li	5		3.83	0.66	0.045
87. BD (	1) C	39	– H	71	/171. LP*(	4) Li	5		0.33	0.65	0.013
87. BD (	1) C	39	– H	71	/260. RY*(	9) Li	5		0.08	1.83	0.011
88. BD (	1) C	40	– C	41	/168. LP*(	1) Li	5		0.10	0.82	0.008
88. BD (	1) C	40	– C	41	/169. LP*(	2) Li	5		0.06	0.80	0.006
88. BD (	1) C	40	– C	41	/170. LP*(	3) Li	5		0.16	0.84	0.010
166. LP (	2) N	3			/171. LP*(	4) Li	5		1.31	0.36	0.021
166. LP (	2) N	3			/253. RY*(	2) Li	5		0.07	1.16	0.009
166. LP (	2) N	3			/255. RY*(	4) Li	5		0.11	0.87	0.010
167. LP (	1) C	4			/168. LP*(	1) Li	5		2.89	0.34	0.029
167. LP (	1) C	4			/169. LP*(	2) Li	5		2.50	0.33	0.027
167. LP (	1) C	4			/170. LP*(	3) Li	5		1.92	0.36	0.025
167. LP (	1) C	4			/171. LP*(	4) Li	5		0.37	0.36	0.011
167. LP (	1) C	4			/254. RY*(	3) Li	5		0.05	0.79	0.006

Figure S18. Extract of the output of the second order perturbation theory analysis of **4b**. Donor-acceptor interactions between the lone pair at the metallated carbon atom or bonding orbitals of the C_{ortho}–H bonds with empty orbitals of the lithium atom.

Table S18. Cartesian coordinates of **4b'** (B3LYP/6-311+g(d)).

Atomic symbol	x	y	z
Cl	1.6698078332	-2.5019677441	0.7085295476
P	-1.0109939742	-1.3045301942	0.2985219744
P	1.7455484103	0.3495426389	-0.0308342001
N	-1.8364413482	-0.2502776479	-0.5873237276
N	0.8904475076	1.5446585286	-0.6715059532
C	0.7327782765	-1.0976244431	0.0269543826
C	-1.3831778745	-1.1981074502	2.1140799476
C	-1.8761599309	0.0125656951	2.6194144585
C	-2.0598570062	0.1946355467	3.9879407349
C	-1.7460602771	-0.83220326	4.8783718544
C	-1.2375132196	-2.0351116627	4.3906002531
C	-1.0529381023	-2.2172417022	3.0203051278
C	-1.3570444206	-3.0760427704	-0.1381333047
C	-2.3377042544	-3.8337050031	0.5116192472
C	-2.6800711717	-5.1049630281	0.0489081201
C	-2.0447709165	-5.6367742841	-1.0701501153
C	-1.0626305368	-4.8913839923	-1.7236597859
C	-0.7243044198	-3.623312297	-1.2622163041
C	-3.2769492035	-0.2421422285	-0.932987367
C	-4.2320699521	-0.6647742961	0.2012656644
C	-3.5438001348	-1.1441628077	-2.1587166853
C	-3.6247170341	1.2111916054	-1.3138857716
C	3.1979899583	-0.1133400383	-1.1064318959
C	4.2612928155	-0.9226247028	-0.6841389893
C	5.2892771975	-1.2599896428	-1.5633607731
C	5.2732544701	-0.7928353697	-2.8767410662
C	4.2220961085	0.015312361	-3.3068449567
C	3.1938778832	0.3497136485	-2.4269615038
C	2.5615806826	0.6939166129	1.6007236104
C	3.8311531106	1.281488994	1.6868124345
C	4.3876698254	1.595196292	2.9255283059
C	3.685961669	1.3181734625	4.0977905143
C	2.4290375142	0.720193263	4.0238717068
C	1.8733642862	0.4086213183	2.7849340178
C	0.9937269034	3.0064183255	-0.4939169909
C	0.5722814698	3.4458978708	0.9239372032
C	2.3946820794	3.5700099235	-0.8087816225
C	0.0024801801	3.6286406677	-1.4984683062
H	-2.1019321184	0.8175179999	1.9290482017
H	-2.4462395	1.1387478355	4.3596572469
H	-1.892536738	-0.6940868844	5.945118088
H	-0.980042824	-2.8355003873	5.0775222143
H	-0.642180266	-3.1532166776	2.6613431474
H	-2.840381441	-3.4417218519	1.3880205627
H	-3.4424850598	-5.678148296	0.5673460796
H	-2.3086397126	-6.6266858555	-1.4290436607
H	-0.5533675845	-5.3036172048	-2.5893895792
H	0.0511788547	-3.0529768068	-1.760529459
H	-4.1251073369	-0.0263844887	1.0793371305
H	-4.0642542665	-1.6972337818	0.5120130492
H	-3.337186775	-2.191820179	-1.9328270005
H	-2.9023553835	-0.8494153371	-2.9933328461
H	-3.0177825095	1.5526117418	-2.1592166995
H	-3.4427764018	1.8862917322	-0.4738032113
H	4.2930411739	-1.291507036	0.3335361224
H	6.105070973	-1.8886016034	-1.2196416061
H	6.076910761	-1.0535711963	-3.5585651497
H	4.2068209096	0.39142303	-4.3256998171
H	2.3784365333	0.9851598872	-2.7552749558

H	4.3987954794	1.489269756	0.7870353935
H	5.3715134422	2.0518194495	2.9736580428
H	4.120395405	1.5594766935	5.0629894479
H	1.8797791679	0.4883107272	4.9307675672
H	0.9013839213	-0.0653242159	2.7391673411
H	-0.4222880537	3.0582615862	1.1592354456
H	1.2643188312	3.0758201911	1.6815851677
H	3.1425346142	3.2063125186	-0.1024722314
H	2.7141129258	3.287515981	-1.8148277513
H	0.2693059707	3.3539657444	-2.5235092248
H	-1.0196475276	3.2896351497	-1.2978476325
H	2.3968315359	4.6636808127	-0.7490563189
H	0.0017100056	4.7207748507	-1.4336421116
H	0.5423097735	4.5381932946	1.0050353027
H	-4.6744138134	1.3064153119	-1.6090767947
H	-4.5862620738	-1.0697518994	-2.4880812509
H	-5.2713237673	-0.5952509034	-0.1359824069
C	-1.1382307888	1.4073994762	-4.6828267398
H	-1.9939702665	0.8920403624	-5.1341175132
H	-0.4168833885	1.6621468911	-5.4677795696
H	-1.4810555755	2.3228246333	-4.2023919969
C	-0.0095033395	-0.6250434202	-4.2044464974
H	-0.8148373981	-1.2404103536	-4.6202909253
H	0.464474197	-1.151770838	-3.378154345
H	0.7359856043	-0.4251295574	-4.9817842139
Li	-0.5760967553	0.7575490777	-1.6779689918
O	-0.5282238179	0.5988388508	-3.6854648362

Table S19. Cartesian coordinates of **Me_2O** (B3LYP/6-311+g(d)).

Atomic symbol	x	y	z
C	1.1753020387	0.1946251137	0.0000244826
O	0.0000015684	-0.5859678502	-0.0000841761
C	-1.1752997935	0.1946279971	0.0000244978
H	2.0210436128	-0.4930366655	-0.0000979087
H	1.2341854493	0.8343896737	0.8923496513
H	1.2341595211	0.8346757671	-0.8920969067
H	-1.234162674	0.8346687273	-0.8921041834
H	-1.2341741392	0.8344047268	0.8923408697
H	-2.0210397218	-0.49303449	-0.0000853264

Table S20. Cartesian coordinates of **4b'-Alt** (B3LYP/6-311+g(d)).

Atomic symbol	x	y	z
Cl	0.8204271474	-0.8625375865	-1.1762423279
P	0.7962378798	-2.1602835989	1.4507904229
P	-1.7804582576	-0.5898429917	0.1822063099
N	0.9889377766	-3.5086274843	0.6814465453
N	-1.7953424743	0.8634882616	-0.5211914655
C	-0.0325691585	-0.8598458337	0.4910257135
C	-0.1755801158	-2.4272672098	3.0094883163
C	-0.6979395078	-3.7069331344	3.2159932021
C	-1.3327516112	-4.030694593	4.4148002982
C	-1.4473764636	-3.0764402618	5.423116495
C	-0.9347311475	-1.7942396526	5.2237032456
C	-0.3041456231	-1.4726936275	4.0248010756
C	2.3492384531	-1.3711266867	2.1342786599
C	2.902443429	-1.8641609429	3.3251354268

C	4.1108812947	-1.3722929738	3.8162412464
C	4.7979740802	-0.3792236858	3.1205603717
C	4.2630707339	0.1172938325	1.932768636
C	3.0516648346	-0.3723382443	1.4463171885
C	2.0516220958	-4.4624933394	0.391645802
C	2.4541020994	-5.2785537329	1.6400459836
C	3.3099686362	-3.790573093	-0.197913875
C	1.487288821	-5.4377516183	-0.6623321861
C	-2.6953648654	-0.5458892024	1.7949240262
C	-3.4148575283	-1.630666366	2.3075026954
C	-4.1798058814	-1.4893007447	3.4640415191
C	-4.2311756391	-0.2648012218	4.1266522495
C	-3.5072490061	0.8191660609	3.6316182282
C	-2.7495585081	0.6786339541	2.471832585
C	-2.5916427897	-2.0132812327	-0.7035710747
C	-3.9773871218	-2.0598898924	-0.9215765825
C	-4.5618807365	-3.129483387	-1.5938254588
C	-3.7688922099	-4.1789930705	-2.0584536403
C	-2.3966614418	-4.1557818776	-1.8266762086
C	-1.8087966602	-3.0850220591	-1.1507523807
C	-2.8224845216	1.5478423907	-1.3271952998
C	-2.977480915	0.9029370793	-2.7213406906
C	-4.202471711	1.6459005279	-0.6408667271
C	-2.3287623725	2.9956521287	-1.5259007584
H	-0.5801977732	-4.4437060061	2.4291087749
H	-1.728231778	-5.0310696101	4.5633954903
H	-1.9318885856	-3.3284821274	6.3615800402
H	-1.0240755799	-1.0454976967	6.0047058763
H	0.1024968719	-0.4772854556	3.8899583639
H	2.3832109665	-2.6345164141	3.884392808
H	4.515154644	-1.7679225079	4.74305415
H	5.7420699595	0.0009754738	3.4982161775
H	4.7941767342	0.885936739	1.3785502888
H	2.6594754892	0.0150325283	0.5145497616
H	1.5832675209	-5.782343898	2.0681736244
H	2.883255163	-4.6322931133	2.4101286559
H	3.7917583641	-3.1347096647	0.5305564103
H	3.0438563297	-3.1895173435	-1.0706325178
H	1.2247445601	-4.8982211567	-1.5761836169
H	0.5832529098	-5.9239698132	-0.2854467144
H	-3.386126674	-2.5889057762	1.80357298
H	-4.7350292188	-2.3394149257	3.8471118462
H	-4.8332724798	-0.1550743242	5.0234043003
H	-3.5463692962	1.7774301583	4.1415311306
H	-2.2147543472	1.5280007472	2.0618994972
H	-4.6182025005	-1.269368814	-0.5512131962
H	-5.6364112897	-3.1452782443	-1.7490307058
H	-4.2221926506	-5.0136561252	-2.5845236321
H	-1.7724646742	-4.9787354596	-2.1605461345
H	-0.7471309072	-3.1144485416	-0.9365193539
H	-2.0103479728	0.8629326521	-3.229478515
H	-3.3541275394	-0.1183760229	-2.6565113036
H	-4.6563693854	0.6688376878	-0.4737980876
H	-4.1203091166	2.1385749258	0.3306310395
H	-2.2554386601	3.5104267779	-0.5636992828
H	-1.345254913	3.0168762114	-2.0000765853
H	-4.9001204392	2.2254924463	-1.2547243634
H	-3.0185898036	3.5642321318	-2.1572051613
H	-3.6695063118	1.4759133849	-3.3486234191
H	2.2152085339	-6.2147492574	-0.9195358905
H	4.0464550118	-4.5404667767	-0.5078015873
H	3.1995694787	-6.0436479625	1.3948968854
C	1.3267746357	2.1798980867	-2.6630057899
H	2.1604035067	1.5278939513	-2.9439282093
H	1.3868392291	3.1154038621	-3.2316553646
H	0.3913660927	1.6716076175	-2.8816312077
C	2.5693323141	3.0582124344	-0.8567704936
H	2.7048465072	4.0259053455	-1.3550073833
H	3.4234604735	2.4135304166	-1.0958464283

H	2.5161361979	3.205156754	0.2196844998
C	-0.0405943846	4.0800016303	1.5404391004
H	0.7396936576	4.7600516255	1.9030468845
H	-0.9388097015	4.2099427411	2.1555795823
H	-0.2746241826	4.3179082066	0.5046396975
C	0.8095469235	2.3242284513	2.8861811117
H	1.6048005813	2.9770952794	3.2643135476
H	1.185384987	1.3075338579	2.8050638895
H	-0.0401698192	2.3535533236	3.5774457654
Li	0.0578019301	1.41425408	0.0076758259
O	1.350291978	2.4500214428	-1.2624036348
O	0.4110269292	2.7318691457	1.5791968365

Table S21. Cartesian coordinates of **4b'-chair** (B3LYP/6-311+g(d,p)).

Atomic symbol	x	y	z
Cl	0.111681369	-2.1183576744	2.1621533818
P	-1.4982806478	-0.2853081972	0.5821656275
N	-1.4991733601	1.1202926269	-0.2204938195
C	0.0984229023	-0.5679936007	1.2538055282
Li	0.1031970912	1.9818588555	-0.844183957
P	1.5407561589	-0.3613358242	0.2709380614
N	1.6983778487	1.1931253397	-0.1362176754
C	-2.6595097152	-0.2936028818	1.9861497122
C	-2.2261714879	0.274784727	3.186293337
C	-3.0980895757	0.3772525369	4.2625099994
C	-4.4072875922	-0.0825442824	4.146030963
C	-4.8434767291	-0.6471680349	2.9527013698
C	-3.9715248881	-0.7545522032	1.8734210367
C	-2.005580577	-1.6852744826	-0.4902555836
C	-2.3483458543	-2.9396116459	0.0235602594
C	-2.5967645124	-4.0034181726	-0.8393803399
C	-2.5049247802	-3.8244721377	-2.2161792481
C	-2.161406662	-2.5783764215	-2.732950038
C	-1.9099807561	-1.5160062365	-1.8739684934
C	-2.6621299823	1.7841455491	-0.6180007822
C	-2.6120693038	3.1889383566	-0.7124281856
C	-3.6877230587	3.9269961566	-1.182760829
C	-4.8689589167	3.2930460424	-1.5624242576
C	-4.9454428549	1.9089274866	-1.4604023155
C	-3.8639237437	1.1621112277	-1.0031104275
C	2.9397731137	-0.9517865507	1.2719179069
C	3.8850741009	-1.861071818	0.8032330834
C	4.9686446064	-2.2112283652	1.604339049
C	5.1078607984	-1.6526255787	2.8693730508
C	4.165470957	-0.7398228039	3.3378166442
C	3.0839777258	-0.3880960975	2.5418757248
C	1.4762461688	-1.4305058332	-1.2204495694
C	1.4900829356	-0.832309507	-2.4805830993
C	1.326785278	-1.6035457291	-3.629357004
C	1.1386525008	-2.9765420608	-3.5220661892
C	1.1051080231	-3.578277476	-2.2652874375
C	1.2714278149	-2.8124598437	-1.1184233366
C	2.8878886569	1.792982107	-0.5406129086
C	3.0122623786	3.1824820915	-0.3400660749
C	4.1224567229	3.8845121379	-0.7859063764
C	5.1637472651	3.2240920754	-1.4357355958
C	5.0716470748	1.8482378078	-1.6179758714
C	3.9567846858	1.1395407443	-1.1818197372
O	0.1602723236	2.4423427479	-2.7250572798
C	1.3153939786	2.811743152	-3.4641313652
C	-0.8670431299	1.9468040357	-3.5703213595
H	-1.2000726196	0.6190466842	3.2660330454
H	-2.755700942	0.8119965623	5.1947999615
H	-5.086939792	-0.0023062615	4.9872868118

H	-5.862174313	-1.0063388307	2.8601594386
H	-4.3161721024	-1.2071128877	0.9504351141
H	-2.4257058793	-3.0851430379	1.0951995189
H	-2.865280275	-4.972599911	-0.4337008197
H	-2.7017512637	-4.6549577341	-2.8855381512
H	-2.0819191173	-2.4350298244	-3.805064269
H	-1.6381375717	-0.542904222	-2.2706871465
H	-1.7086966585	3.6998140046	-0.3897854452
H	-3.6075155771	5.0074431845	-1.2404331208
H	-5.8560554746	1.39452933	-1.7496274937
H	-3.9466196469	0.0824252692	-0.9717594531
H	3.7816623913	-2.2976171099	-0.1844028034
H	5.703226042	-2.9193449912	1.237812809
H	5.9521611116	-1.926652907	3.4922648165
H	4.274207703	-0.3043821048	4.3246016468
H	2.3392088218	0.31623153	2.8988822083
H	1.6339312227	0.2412564516	-2.5531934565
H	1.351743533	-1.1318709661	-4.6064995045
H	1.0094582332	-3.579061438	-4.4146888462
H	0.9376235369	-4.6460906024	-2.1788121125
H	1.2316339266	-3.2852638802	-0.1425137125
H	2.2134106924	3.6953882034	0.187631254
H	4.1799815561	4.9546349685	-0.6155865384
H	5.8758319265	1.3133277615	-2.1125670515
H	3.9090551579	0.0704595046	-1.3580648962
H	1.070372829	3.6244603071	-4.155049134
H	1.6910851813	1.9565679426	-4.0375003156
H	-1.7498056787	1.7680423142	-2.9597953703
H	-0.5426493247	1.0130556804	-4.0451085319
H	6.0337922734	3.7696558318	-1.781510173
H	-5.7132547608	3.8681868545	-1.9236956706
H	-1.1061280196	2.6842529177	-4.3427515672
H	2.0799843167	3.1371604308	-2.7620087398

Table S22. Cartesian coordinates of **4b'-NoH** (B3LYP/6-311+g(d,p)).

Atomic symbol	x	y	z
Cl	-0.1144748451	-2.9017833837	0.7646297729
P	1.5692259836	-0.6448415842	-0.0978612015
P	-1.6099346969	-0.4154887816	0.2900376695
N	1.6591307103	0.9656369069	-0.2398327204
N	-1.5093615564	1.1983231727	0.241178333
C	-0.0207240203	-1.1190389836	0.4651049799
C	1.9981800255	-1.4825238408	-1.6916286454
C	1.8751119788	-0.7583193979	-2.8840685095
C	2.0948479549	-1.3725214187	-4.115019393
C	2.4310263035	-2.7241250991	-4.1719845907
C	2.5445188472	-3.4578946128	-2.9919677094
C	2.3309379593	-2.8436302809	-1.7593901537
C	2.7772692432	-1.3468669983	1.1111511247
C	4.086101903	-1.6731649543	0.7374407025
C	5.0169989709	-2.0679986186	1.6974895242
C	4.6499904967	-2.1395008347	3.039654108
C	3.3482584647	-1.8122574812	3.4202966607
C	2.4181981639	-1.417009401	2.4628247632
C	-2.585759575	-1.0184141792	1.746160822
C	-3.4290623633	-2.1327994089	1.7086663504
C	-4.1057261423	-2.5456278222	2.8565413259
C	-3.9433732515	-1.8520444636	4.0532806021
C	-3.0968654348	-0.7439089861	4.1020785076
C	-2.4228979739	-0.3323167666	2.9558192773
C	-2.5375801287	-1.0709031126	-1.16473545
C	-3.9107286846	-0.8301291151	-1.3176554888
C	-4.5783061675	-1.2597624085	-2.462002807
C	-3.8845691954	-1.9375219546	-3.464200891

C	-2.52041421	-2.181186351	-3.3193440857
C	-1.8498770033	-1.7490154114	-2.1759997815
H	1.6031911686	0.2879571322	-2.8416077273
H	2.0046142648	-0.7949090406	-5.0284555559
H	2.6033016209	-3.2032129294	-5.1295151053
H	2.8001725128	-4.5111796003	-3.0289329252
H	2.4218648526	-3.4271176689	-0.8521974047
H	4.3879015949	-1.6137395522	-0.3011026341
H	6.0279223236	-2.3178222124	1.394940725
H	5.37319773	-2.4506257115	3.7855117888
H	3.0550344461	-1.8731310449	4.4626079301
H	1.4025017225	-1.1730134084	2.7520882787
H	-3.5557998766	-2.686692249	0.7869550732
H	-4.7563514919	-3.4121846872	2.8141264936
H	-4.4702683835	-2.1737862187	4.9448562739
H	-2.9631096676	-0.2022823017	5.0322602974
H	-1.7658565585	0.5296907839	2.9928006416
H	-4.4632694097	-0.304553506	-0.5478611249
H	-5.6391040383	-1.0630332973	-2.5711972022
H	-4.406532782	-2.2747852549	-4.3530678628
H	-1.9754713438	-2.7114905597	-4.0923431429
H	-0.790529185	-1.9434230206	-2.064922651
C	-0.7071094589	4.5582281868	1.8018669567
H	-0.7755170432	5.5070615515	1.2581308315
H	-0.6137927805	4.7619578139	2.8750292369
H	-1.6028029938	3.9705795846	1.612459433
C	1.6474712209	4.5097852816	1.5075387897
H	1.6209363809	5.4523271084	0.9496678978
H	2.4467211215	3.8809824632	1.1218190943
H	1.822006562	4.7213996942	2.5687912269
Li	0.2161054702	2.0287317538	0.5277001854
O	0.4153070017	3.8025649219	1.3415364398
C	2.8472347989	1.6873088532	-0.4865718278
C	3.9212125607	1.7418958135	0.4247436488
C	2.9485936385	2.4779186199	-1.6479418825
C	5.0394980373	2.5350678851	0.1754284736
H	3.8660893524	1.165792796	1.3396034117
C	4.0620979981	3.279163172	-1.8876340363
H	2.1264756547	2.4672713479	-2.3546216348
C	5.1211106745	3.3101621942	-0.9809179455
H	5.8491944237	2.552280001	0.8978016037
H	4.1030142725	3.8789734779	-2.7909683292
H	5.9909775681	3.928651648	-1.1700067545
C	-2.5904307585	2.0181904169	-0.1570163557
C	-3.5911560033	2.4230406944	0.7462428288
C	-2.6671126504	2.5048269321	-1.4745452415
C	-4.6123370224	3.2857402213	0.3505529806
H	-3.5616020993	2.0485157582	1.7629772178
C	-3.684705823	3.3715620912	-1.8654983788
H	-1.9120425774	2.1885238531	-2.1853103146
C	-4.6650443012	3.7690377123	-0.9563244642
H	-5.3708127342	3.5800938918	1.0687806944
H	-3.7157109373	3.7325472516	-2.8882986069
H	-5.4582468099	4.4418019273	-1.2620164414

3.3 Calculation on the tautomerism of 5a

Calculations were performed on the b3lyp/6-311+g(d,p) level of theory. For computational costs a model system was chosen, in which the adamantyl substituents were replaced by *tert*-butyl groups. The transition state was located by using the qst3 method. For the evaluation of solvent effects on the tautomerization process and on the stabilities of both tautomers, calculations including solvent effects (polarizable continuum model with thf and toluene as solvent) were performed. These calculations showed no distinct influence of the solvent on the tautomerization process. Table 23 gives the energies of all calculated structures, Table 24-26 the coordinates of the optimized compounds without inclusion of solvent effects. Figure S19 gives the NBO charges as well as the Wiberg bond indices in **5a**.

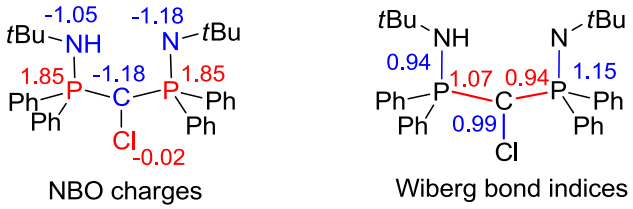


Figure S19. NBO charges and WBIs of **5a**.

Table 23. Energies [in kJ/mol] of the calculated structures.

	Solvent	SCF	ZPE	Free Energy	ΔZPE	ΔG
*N*H tautomer	None	-6652316.641	-6650645.939	-6.650838.638	0	0
*C*H tautomer	None	-6652302.102	-6650626.805	-6.650820.719	19.1	17.9
N-H-N TS	None	-6652297.198	-6650630.948	-6.650819.333	15.0	19.3
*N*H tautomer	THF	-6652348.622	-6650671.990	-6650865.208	0	0
*C*H tautomer	THF	-6652327.962	-6650651.839	-6650840.027	20.2	25.2
N-H-N TS	THF	-6652319.784	-6650654.759	-6650843.041	17.2	22.2
*N*H tautomer	Toluene	-6652336.687	-6650659.293	-6650851.311	0	0
*C*H tautomer	Toluene	-6652315.186	-6650639.990	-6650832.387	19.3	18.9
N-H-N TS	Toluene	-6652308.897	-6650643.395	-6650832.106	15.9	19.2

Table 24. Cartesian coordinates of the *N*H tautomer.

Atomic symbol	x	y	z
Cl	-0.6840838513	12.0920306654	2.8330028631
P	1.9436261294	11.0115279299	3.4918818189
P	1.5467380109	14.1085465507	2.8571257097
N	3.556818769	11.4111379079	3.5209743922
N	3.1033772019	14.2249060559	3.1629319468
C	1.0689991112	12.4237905144	3.0429157435
C	1.6956036209	9.6646510178	2.2656639805
C	2.626189067	9.5304251464	1.2267214543
C	2.4191967586	8.6043953465	0.2081791649
C	1.2726722559	7.8096397485	0.2073536687
C	0.3323868124	7.9506653164	1.2255593329
C	0.5392678725	8.8740091125	2.2494873046
C	1.3073020188	10.3444484849	5.0938814009
C	1.2852632581	8.9840243953	5.4262344368

C	0.8258651209	8.5700705483	6.6753956907
C	0.3820214108	9.5099481768	7.6040994309
C	0.390182208	10.8654070728	7.2769976834
C	0.8436058196	11.2797478883	6.0276183614
C	4.7084883709	10.7923870011	4.2398023325
C	4.6375287531	9.259708608	4.2410061379
C	4.7841847872	11.3158154991	5.686394311
C	5.9694053141	11.2154330522	3.4657665823
C	0.482495239	15.089937721	4.0248130717
C	-0.8690489342	15.382610924	3.7995127246
C	-1.6201347605	16.0505802198	4.7663978944
C	-1.0340801539	16.4312811848	5.9722477193
C	0.3080862337	16.136310574	6.2107918827
C	1.0577654168	15.4687436098	5.2445867805
C	0.9598258155	14.6199863439	1.1715079455
C	0.5119232557	15.9135126637	0.8753327363
C	0.1807369349	16.2693691887	-0.4315467741
C	0.2929240909	15.3364557031	-1.4607844654
C	0.7336872446	14.044289018	-1.1762134632
C	1.0611677909	13.6893823452	0.1298736483
C	4.0691428814	15.2823402404	2.813044566
C	4.7264327536	14.9610503945	1.4536691299
C	3.4775379491	16.7062302334	2.7517558173
C	5.1539327699	15.2805803224	3.9084147407
H	3.5091595778	10.1593501474	1.2217207274
H	3.1519095774	8.5046194175	-0.5863839512
H	1.1102662539	7.0887505285	-0.5876087917
H	-0.5680657005	7.3448501941	1.2233882091
H	-0.2074805013	8.9806023591	3.0270943206
H	1.6184749474	8.2391149894	4.7130812014
H	0.8118602052	7.5127685741	6.9203219199
H	0.0222035325	9.1861007964	8.575560613
H	0.0317219847	11.6009958004	7.9897006177
H	0.8250205799	12.331080033	5.7604608723
H	4.5498575337	8.8575151537	3.2300927299
H	3.8066831746	8.8844199681	4.8381230383
H	3.9082038717	11.0099481464	6.2623263722
H	4.8324618038	12.4071493212	5.7010902091
H	6.0570013221	12.3017225479	3.407695667
H	5.9487751556	10.8253819592	2.4453032534
H	-1.3427539669	15.0895570838	2.8701995999
H	-2.6659039123	16.2718791222	4.576103909
H	-1.619919435	16.9539474693	6.7220753385
H	0.7722889987	16.4299808917	7.1475082353
H	2.1016134041	15.2346826426	5.4256611117
H	0.4133982144	16.6510163104	1.6638554885
H	-0.1674530764	17.2755856687	-0.6436972883
H	0.032846282	15.6130144462	-2.4778053512
H	0.8134558774	13.308863677	-1.9708128793
H	1.3839983077	12.6782740179	0.3548813891
H	5.1822251666	13.9675215121	1.4737979133
H	3.9829302876	14.9695602402	0.652722769
H	2.7644133495	16.8119734209	1.9327706517
H	2.9727489822	16.96910422	3.6842787064
H	4.7205756249	15.5312210709	4.8805491077
H	5.6214514756	14.2978264979	3.9969954847
H	3.6374519344	12.4440452114	3.4093681001
H	4.2707380338	17.4422365237	2.5840809073
H	5.94183651	16.0083316073	3.688383789
H	5.5056447233	15.6888589915	1.2001922517
H	6.8673067419	10.8344053929	3.9603832333
H	5.6736040869	10.9296186519	6.1943862006
H	5.5538041237	8.8580405974	4.681815171

Table 25. Cartesian coordinates of the *C*H tautomer.

Atomic symbol	x	y	z
Cl	-0.4290857663	11.9814095949	2.1886195204
P	2.1852307847	11.0224733756	3.4237594446
P	1.6219219151	14.2676199586	2.6929565663
N	3.5692927246	11.5355470203	3.8884830445

N	3.0798067557	14.7975915636	2.7742651708
C	2.2608523848	9.672570023	2.1402405321
C	3.5377297466	9.3440908464	1.6722440719
C	3.7086713822	8.3739979894	0.6854168826
C	2.6007167092	7.7199342206	0.15184819
C	1.3222923916	8.0408513606	0.6084180354
C	1.1505306649	9.0101405954	1.5946546431
C	0.9817324592	10.4194171639	4.6891258737
C	0.7108201802	9.0539693436	4.8463220548
C	-0.0731913334	8.6042153425	5.9076921276
C	-0.595875573	9.511413189	6.8263772458
C	-0.3223716476	10.8713698203	6.6847516921
C	0.46657353	11.3210939755	5.6297309551
C	4.5271130499	11.2516273233	4.9593618291
C	4.3209704914	9.8764756886	5.6256984898
C	4.419733233	12.3535696481	6.0318367789
C	5.9413676119	11.2922162136	4.3477600817
C	0.8091769739	14.681091645	4.2798827366
C	-0.5801134841	14.6326742664	4.4549402768
C	-1.1431136926	14.9788477918	5.6820847096
C	-0.3269638653	15.3745788279	6.7411504878
C	1.0559671589	15.4297410088	6.5689135669
C	1.6228714044	15.0888037034	5.3428087397
C	0.5448598079	15.010723401	1.3742300548
C	0.0132913364	16.2869941677	1.6043443382
C	-0.6411658825	16.9803852433	0.588783786
C	-0.7647447261	16.4141477781	-0.6786295317
C	-0.228581303	15.1513288159	-0.923685696
C	0.4212912152	14.4565945728	0.0938500397
C	4.1780827344	14.983023753	1.8277694909
C	4.450295958	13.7196089545	0.9884009448
C	3.9005834809	16.1772262909	0.8911660063
C	5.427231909	15.3022043176	2.6709915868
H	4.3946555505	9.8634050929	2.0862330253
H	4.7069481903	8.1314599956	0.3348542242
H	2.7304513355	6.9637033367	-0.6159735024
H	0.4547390356	7.5340151371	0.1973433192
H	0.1500432328	9.2437734037	1.9361683575
H	1.1185925054	8.3313686152	4.1500832348
H	-0.271863251	7.5425647366	6.0156492578
H	-1.2075232759	9.1608481412	7.651676212
H	-0.7198870152	11.5860786437	7.3979434103
H	0.679222731	12.3791291259	5.5443995598
H	4.3775523276	9.070519968	4.8877406725
H	3.3513618877	9.8144251813	6.1245568821
H	3.4336070028	12.3373940449	6.5033752302
H	4.5598898016	13.3358269151	5.5763584844
H	6.1150401687	12.2447552898	3.8438294676
H	6.0729240151	10.4935212052	3.6121343771
H	-1.2256323431	14.3324091622	3.6392151023
H	-2.2205008934	14.9422060837	5.8076557517
H	-0.7681907626	15.6465624161	7.6950534348
H	1.6950538313	15.7439363117	7.387937517
H	2.6925389316	15.1411022227	5.1822027833
H	0.1131832071	16.7475898839	2.5811449805
H	-1.0509065249	17.9655087238	0.7883536205
H	-1.2723599736	16.9544278031	-1.4712491486
H	-0.3181902104	14.7025613968	-1.9078731426
H	0.8237748047	13.4745306801	-0.1273135911
H	4.5755100238	12.8526307137	1.639736849
H	3.6216721227	13.5209621082	0.2991052261
H	3.0316605156	15.9944559577	0.2545064976

H	3.7049000786	17.0804703516	1.4748594307
H	5.2547700803	16.1936268118	3.2797642141
H	5.6555045608	14.4740578096	3.3446463389
H	4.7592006388	16.3713511502	0.2393177551
H	6.3001331182	15.4840084883	2.0356243628
H	5.353448149	13.8352275789	0.3800332669
H	6.7083917536	11.1665955886	5.1188625086
H	5.1737553761	12.2223828428	6.8156179383
H	5.0928361427	9.6911639383	6.3799001774
C	1.3479611128	12.3840244124	2.3878871774
H	1.7785803779	12.2221075258	1.3983610893

Table 26. Cartesian coordinates of the transition state for the proton shift between both imino groups.

Atomic symbol	x	y	z
Cl	0.0008620549	0.38578245	-2.5520179439
P	-1.5734313383	-0.1090409389	-0.0678510247
P	1.5465764909	0.1672620605	-0.0108167245
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