

Table S2.9 - Hydrogen Bonds (Angstrom, Deg)
for: Complex3

C2	--	H2	..	N1	1.01(3)	2.42(3)	2.836(3)	104.3(17)	.	yes
C19	--	H19	..	N1	0.980(4)	2.438(4)	2.859(4)	105.4(3)	.	yes
C33	--	H33	..	N2	0.980(4)	2.445(3)	2.898(3)	107.7(2)	.	yes
C36	--	H36	..	N2	0.980(4)	2.448(3)	2.931(3)	110.0(2)	.	yes

Translation of Symmetry Code to Equiv.Pos

```
a =[ 1655.00 ] = 1+x,y,z
b =[ 1565.00 ] = x,1+y,z
c =[ 2765.00 ] = 2-x,1-y,-z
d =[ 1545.00 ] = x,-1+y,z
e =[ 2766.00 ] = 2-x,1-y,1-z
f =[ 2776.00 ] = 2-x,2-y,1-z
g =[ 1465.00 ] = -1+x,1+y,z
h =[ 1645.00 ] = 1+x,-1+y,z
i =[ 1455.00 ] = -1+x,y,z
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Table S3.1 - Crystal Data and Details of the Structure Determination
for: Complex4*0.5Et2O

Crystal Data			
Empirical Formula	2(C ₄₆ H ₇₂ Li ₂ N ₂ O), C ₄ O		
Formula Weight	1429.91		
Crystal System	Monoclinic		
Space group	P2 ₁ /c	(No. 14)	
a, b, c [Angstrom]	12.9790(10)	15.7030(10)	22.942(2)
alpha, beta, gamma [deg]	90	94.610(10)	90
V [Ang**3]	4660.7(6)		
Z	2		
D(obs), D(calc) [g/cm**3]	0.000, 1.019		
F(000)	1568		
Mu(MoKa) [/mm]	0.1		
Crystal Size [mm]	0.20 x 0.20 x 0.30		

Data Collection

Temperature (K)	183		
Radiation [Angstrom]	MoKa	0.71073	
Theta Min-Max [Deg]	2.0, 24.0		
Dataset	-14: 14 ;	0: 17 ;	0: 26
Tot., Uniq. Data, R(int)	7239,	7239,	0.000
Observed data [I > 2.0 sigma(I)]	2514		

Refinement

Nref, Npar	7236, 517		
R, wR, S	0.0429, 0.0719, 0.64		
w =			
Max. and Av. Shift/Error	0.00, 0.00		
Min. and Max. resd. dens. [e/Ang^3]	-0.30, 0.39		

Table S3.2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: Complex4*0.5Et2O

Atom	x	y	z	U(eq) [Ang ²]
O1	0.2847 (2)	0.56403 (14)	0.14232 (10)	0.0460 (11)
N1	0.5249 (2)	0.3476 (2)	0.20238 (10)	0.0267 (9)
N2	0.2447 (2)	0.3334 (2)	0.17518 (10)	0.0264 (10)
C1	0.4492 (2)	0.3752 (2)	0.10460 (12)	0.0254 (12)
C2	0.3907 (2)	0.2910 (2)	0.09772 (13)	0.0236 (12)
C3	0.2787 (2)	0.3125 (2)	0.07406 (12)	0.0260 (12)
C4	0.2792 (2)	0.3422 (2)	0.00996 (13)	0.0335 (12)
C5	0.3495 (2)	0.4205 (2)	0.01317 (13)	0.0348 (12)
C6	0.4259 (2)	0.4334 (2)	0.05650 (13)	0.0309 (12)
C7	0.4493 (2)	0.2196 (2)	0.06376 (13)	0.0333 (12)
C8	0.5275 (2)	0.1786 (2)	0.11033 (13)	0.0451 (12)
C9	0.3743 (2)	0.1487 (2)	0.04108 (13)	0.0458 (12)
C10	0.5132 (2)	0.2529 (2)	0.01456 (14)	0.0497 (14)
C11	0.1833 (2)	0.3515 (2)	-0.03494 (13)	0.0395 (12)
C12	0.1153 (3)	0.4298 (2)	-0.02592 (14)	0.0520 (14)
C13	0.1215 (2)	0.2671 (2)	-0.03798 (14)	0.0526 (14)
C14	0.2255 (2)	0.3615 (2)	-0.09608 (12)	0.0570 (14)
C15	0.5177 (2)	0.3960 (2)	0.15316 (13)	0.0243 (12)
C16	0.5800 (2)	0.4774 (2)	0.15056 (12)	0.0335 (12)
C17	0.6099 (2)	0.3539 (2)	0.24481 (13)	0.0313 (12)
C18	0.7143 (2)	0.3446 (2)	0.23254 (13)	0.0315 (12)
C19	0.7924 (2)	0.3474 (2)	0.2785 (2)	0.0434 (14)
C20	0.7691 (3)	0.3576 (2)	0.3353 (2)	0.0495 (16)
C21	0.6680 (3)	0.3655 (2)	0.34822 (14)	0.0402 (12)
C22	0.5873 (2)	0.3637 (2)	0.30454 (13)	0.0312 (12)
C23	0.7478 (2)	0.3259 (2)	0.17151 (14)	0.0408 (12)

Table S3.2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: Complex4*0.5Et2O

Atom	x	y	z	U(eq) [Ang ²]
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C24	0.7903 (2)	0.2348 (2)	0.1677 (2)	0.0559 (16)
C25	0.8304 (2)	0.3900 (2)	0.1532 (2)	0.0602 (16)
C26	0.4776 (2)	0.3735 (2)	0.31927 (14)	0.0388 (12)
C27	0.4643 (3)	0.4259 (3)	0.37518 (15)	0.0682 (16)
C28	0.4251 (3)	0.2867 (2)	0.32449 (15)	0.0523 (14)
C29	0.2087 (2)	0.3246 (2)	0.11454 (12)	0.0274 (12)
C30	0.0928 (2)	0.3345 (2)	0.10256 (12)	0.0418 (14)
C31	0.1780 (2)	0.3008 (2)	0.21654 (12)	0.0249 (12)
C32	0.1417 (2)	0.3537 (2)	0.26016 (13)	0.0299 (12)
C33	0.0744 (2)	0.3210 (2)	0.29851 (13)	0.0373 (14)
C34	0.0431 (2)	0.2372 (2)	0.29571 (14)	0.0400 (14)
C35	0.0822 (2)	0.1834 (2)	0.25525 (13)	0.0369 (12)
C36	0.1504 (2)	0.2132 (2)	0.21642 (13)	0.0276 (12)
C37	0.1720 (2)	0.4476 (2)	0.2640 (2)	0.0458 (14)
C38	0.0970 (3)	0.5016 (2)	0.2266 (2)	0.0676 (16)
C39	0.1800 (3)	0.4818 (2)	0.3275 (2)	0.0735 (17)
C40	0.1990 (2)	0.1489 (2)	0.17723 (13)	0.0365 (12)
C41	0.1207 (3)	0.0903 (2)	0.1444 (2)	0.0689 (17)
C42	0.2786 (3)	0.0943 (2)	0.2126 (2)	0.0604 (16)
C43	0.3911 (3)	0.5957 (2)	0.2307 (2)	0.0597 (17)
C44	0.3348 (3)	0.6303 (2)	0.1762 (2)	0.0714 (16)
C45	0.2061 (3)	0.5959 (3)	0.0994 (2)	0.0708 (17)
C46	0.2500 (4)	0.6469 (3)	0.0512 (2)	0.0940 (19)
Li1	0.3838 (4)	0.3163 (4)	0.2138 (2)	0.0362 (19)
Li2	0.3048 (4)	0.4415 (4)	0.1379 (2)	0.0404 (19)

Table S3.2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: Complex4*0.5Et2O

Atom	x	y	z	U(eq) [Ang ²]
*O2	-0.0140(11)	-0.0261(8)	0.0109(6)	0.200(4)
*C47	0.1230(10)	-0.1091(7)	-0.0089(5)	0.115(3)
*C48	0.0892(11)	-0.0173(9)	-0.0110(11)	0.210(4)
*C49	-0.0747(9)	0.0562(12)	0.0042(12)	0.210(4)
*C50	-0.1919(7)	0.0639(8)	0.0125(5)	0.115(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3.3 - Hydrogen Atom Positions and Isotropic Displacement
Parameters
for: Complex4*0.5Et2O

Atom	x	y	z	U(iso) [Ang ²]
H2	0.3824 (16)	0.2625 (14)	0.1373 (10)	0.010 (6)
H4	0.3181 (18)	0.2980 (17)	-0.0088 (11)	0.025 (8)
H5	0.340 (2)	0.4616 (19)	-0.0195 (12)	0.047 (10)
H6	0.4683 (19)	0.4865 (17)	0.0529 (10)	0.027 (8)
H8A	0.5681 (11)	0.1368 (9)	0.0920 (2)	0.0670
H8B	0.4905 (2)	0.1518 (11)	0.1400 (5)	0.0670
H8C	0.5721 (10)	0.2220 (3)	0.1278 (6)	0.0670
H9A	0.3334 (11)	0.1308 (9)	0.0719 (3)	0.0690
H9B	0.4130 (2)	0.1011 (5)	0.0283 (8)	0.0690
H9C	0.3297 (10)	0.1699 (4)	0.0089 (6)	0.0690
H10A	0.4676 (3)	0.2773 (12)	-0.0160 (5)	0.0740
H10B	0.5508 (12)	0.2066 (3)	-0.0010 (6)	0.0740
H10C	0.5609 (12)	0.2955 (10)	0.0301 (3)	0.0740
H12A	0.0847 (13)	0.4247 (7)	0.0106 (5)	0.0780
H12B	0.0619 (10)	0.4333 (8)	-0.0573 (5)	0.0780
H12C	0.1570 (4)	0.4803 (3)	-0.0255 (9)	0.0780
H13A	0.1106 (15)	0.2485 (8)	0.00091 (15)	0.0790
H13B	0.1596 (8)	0.2245 (4)	-0.0572 (8)	0.0790
H13C	0.0559 (7)	0.2760 (4)	-0.0596 (8)	0.0790
H14A	0.1687 (2)	0.3660 (15)	-0.1254 (2)	0.0850
H14B	0.2667 (15)	0.3127 (7)	-0.1040 (4)	0.0850
H14C	0.2672 (15)	0.4119 (8)	-0.0966 (3)	0.0850
H16A	0.5340 (2)	0.5247 (2)	0.1432 (7)	0.0500
H16B	0.6255 (9)	0.4732 (5)	0.1197 (5)	0.0500
H16C	0.6200 (10)	0.4857 (6)	0.1872 (3)	0.0500
H19	0.870 (2)	0.3414 (3)	0.2692 (3)	0.0520

Table S3.3 - Hydrogen Atom Positions and Isotropic Displacement
Parameters (continued)
for: Complex4*0.5Et2O

Atom	x	y	z	U(iso) [Ang ²]
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H20	0.8211 (17)	0.3591 (2)	0.3647 (9)	0.0590
H21	0.6530 (5)	0.3723 (3)	0.3876 (12)	0.0490
H23	0.6869 (2)	0.3308 (2)	0.14358 (14)	0.0490
H24A	0.7385 (6)	0.1948 (2)	0.1775 (9)	0.0840
H24B	0.8505 (10)	0.2286 (5)	0.1946 (7)	0.0840
H24C	0.8086 (16)	0.2240 (5)	0.1286 (3)	0.0840
H25A	0.8440 (13)	0.3798 (10)	0.1133 (4)	0.0900
H25B	0.8930 (6)	0.3828 (10)	0.1780 (7)	0.0900
H25C	0.8052 (7)	0.4471 (2)	0.1571 (9)	0.0900
H26	0.4404 (2)	0.4038 (2)	0.28664 (14)	0.0460
H27A	0.4919 (18)	0.3945 (7)	0.4088 (2)	0.1020
H27B	0.3922 (3)	0.4367 (14)	0.3784 (6)	0.1020
H27C	0.5004 (16)	0.4790 (7)	0.3731 (5)	0.1020
H28A	0.4333 (3)	0.2545 (2)	0.28959 (15)	0.0800
H28B	0.4572 (3)	0.2568 (2)	0.35765 (15)	0.0800
H28C	0.3529 (3)	0.2940 (2)	0.32931 (15)	0.0800
H30A	0.0719 (3)	0.3889 (6)	0.1167 (8)	0.0630
H30B	0.0584 (2)	0.2901 (8)	0.1222 (8)	0.0630
H30C	0.0747 (3)	0.3308 (13)	0.06124 (15)	0.0630
H33	0.0492 (8)	0.3575 (11)	0.3276 (9)	0.0440
H34	-0.0024 (15)	0.2177 (7)	0.3200 (8)	0.0480
H35	0.0605 (6)	0.1202 (18)	0.25393 (14)	0.0450
H37	0.2401 (2)	0.4534 (2)	0.2489 (2)	0.0550
H38A	0.1164 (12)	0.5605 (3)	0.2308 (9)	0.1010
H38B	0.0286 (4)	0.4939 (12)	0.2388 (8)	0.1010
H38C	0.0982 (15)	0.4850 (11)	0.1864 (2)	0.1010

Table S3.3 - Hydrogen Atom Positions and Isotropic Displacement
Parameters (continued)
for: Complex4*0.5Et2O

Atom	x	y	z	U(iso) [Ang ²]
H39A	0.2156 (18)	0.5354 (8)	0.3290 (3)	0.1100
H39B	0.2174 (18)	0.4418 (8)	0.3528 (2)	0.1100
H39C	0.1118 (3)	0.4894 (16)	0.3401 (4)	0.1100
H40	0.2351 (2)	0.1807 (2)	0.14822 (13)	0.0440
H41A	0.1553 (4)	0.0548 (12)	0.1181 (8)	0.1040
H41B	0.0692 (11)	0.1239 (2)	0.1227 (9)	0.1040
H41C	0.0882 (15)	0.0552 (12)	0.1719 (2)	0.1040
H42A	0.3105 (14)	0.0559 (11)	0.1869 (2)	0.0900
H42B	0.2449 (4)	0.0622 (12)	0.2412 (7)	0.0900
H42C	0.3304 (10)	0.1303 (2)	0.2320 (8)	0.0900
H43A	0.4273 (15)	0.6411 (3)	0.2516 (5)	0.0890
H43B	0.4396 (14)	0.5532 (11)	0.2205 (2)	0.0890
H43C	0.3424 (3)	0.5707 (14)	0.2550 (5)	0.0890
H44A	0.2838 (3)	0.6715 (2)	0.1867 (2)	0.0860
H44B	0.3834 (3)	0.6592 (2)	0.1531 (2)	0.0860
H45A	0.1584 (3)	0.6315 (3)	0.1190 (2)	0.0850
H45B	0.1672 (3)	0.5481 (3)	0.0822 (2)	0.0850
H46A	0.281 (2)	0.6981 (10)	0.0673 (3)	0.1410
H46B	0.1955 (5)	0.6613 (17)	0.0221 (7)	0.1410
H46C	0.3012 (17)	0.6136 (8)	0.0336 (9)	0.1410

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The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\text{Pi} ** 2) * U * (\text{Sin}(\text{Theta}) / \text{Lambda}) ** 2$ for Isotropic Atoms.

Table S3.4 - (An)isotropic Displacement Parameters
for: Complex4*0.5Et2O

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.057(2)	0.0284(14)	0.052(2)	-0.0024(13)	0.0014(12)	-0.0006(12)
N1	0.0250(14)	0.028(2)	0.0264(14)	0.0024(13)	-0.0020(11)	-0.0023(12)
N2	0.0250(14)	0.026(2)	0.0290(15)	0.0037(13)	0.0070(11)	-0.0017(13)
C1	0.024(2)	0.025(2)	0.028(2)	0.0017(15)	0.0065(14)	-0.0037(15)
C2	0.023(2)	0.024(2)	0.024(2)	0.005(2)	0.0035(14)	-0.0019(14)
C3	0.025(2)	0.025(2)	0.028(2)	0.000(2)	0.0027(14)	-0.0063(14)
C4	0.030(2)	0.039(2)	0.031(2)	0.006(2)	0.0000(15)	-0.008(2)
C5	0.041(2)	0.036(2)	0.027(2)	0.009(2)	0.000(2)	-0.012(2)
C6	0.028(2)	0.032(2)	0.033(2)	0.003(2)	0.005(2)	-0.010(2)
C7	0.033(2)	0.033(2)	0.034(2)	-0.012(2)	0.004(2)	-0.003(2)
C8	0.042(2)	0.033(2)	0.061(2)	-0.008(2)	0.009(2)	0.013(2)
C9	0.053(2)	0.040(2)	0.045(2)	-0.013(2)	0.007(2)	-0.005(2)
C10	0.047(2)	0.056(3)	0.049(2)	-0.009(2)	0.022(2)	0.000(2)
C11	0.039(2)	0.049(2)	0.029(2)	0.008(2)	-0.006(2)	-0.016(2)
C12	0.046(2)	0.060(3)	0.048(2)	0.015(2)	-0.008(2)	0.002(2)
C13	0.053(2)	0.066(3)	0.037(2)	0.008(2)	-0.007(2)	-0.022(2)
C14	0.062(2)	0.078(3)	0.029(2)	0.009(2)	-0.009(2)	-0.024(2)
C15	0.018(2)	0.026(2)	0.029(2)	0.000(2)	0.0030(14)	-0.0005(14)
C16	0.040(2)	0.031(2)	0.028(2)	0.006(2)	-0.006(2)	-0.007(2)
C17	0.032(2)	0.021(2)	0.040(2)	0.006(2)	-0.003(2)	0.000(2)
C18	0.027(2)	0.025(2)	0.042(2)	0.007(2)	-0.001(2)	-0.002(2)
C19	0.032(2)	0.037(2)	0.059(3)	0.010(2)	-0.010(2)	-0.004(2)
C20	0.053(3)	0.043(2)	0.048(3)	0.004(2)	-0.024(2)	-0.008(2)
C21	0.049(2)	0.036(2)	0.034(2)	0.007(2)	-0.007(2)	-0.003(2)
C22	0.040(2)	0.023(2)	0.030(2)	0.002(2)	0.000(2)	-0.004(2)
C23	0.027(2)	0.043(2)	0.052(2)	0.005(2)	0.001(2)	0.001(2)

Table S3.4 - (An)isotropic Displacement Parameters (continued)
for: Complex4*0.5Et2O

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C24	0.045(2)	0.054(3)	0.068(3)	0.000(2)	0.001(2)	0.018(2)
C25	0.036(2)	0.075(3)	0.071(3)	0.014(2)	0.013(2)	-0.007(2)
C26	0.050(2)	0.039(2)	0.028(2)	0.004(2)	0.007(2)	0.005(2)
C27	0.079(3)	0.083(3)	0.044(2)	-0.017(2)	0.014(2)	0.015(3)
C28	0.046(2)	0.060(3)	0.051(2)	0.013(2)	0.005(2)	-0.006(2)
C29	0.024(2)	0.024(2)	0.034(2)	0.005(2)	0.0013(15)	-0.0048(14)
C30	0.025(2)	0.060(3)	0.040(2)	0.015(2)	0.0009(14)	0.005(2)
C31	0.018(2)	0.028(2)	0.028(2)	0.002(2)	-0.0023(14)	0.0010(14)
C32	0.020(2)	0.034(2)	0.036(2)	0.002(2)	0.0036(14)	0.003(2)
C33	0.026(2)	0.055(3)	0.031(2)	0.002(2)	0.0032(15)	0.008(2)
C34	0.030(2)	0.053(3)	0.038(2)	0.017(2)	0.008(2)	-0.001(2)
C35	0.033(2)	0.039(2)	0.038(2)	0.012(2)	-0.001(2)	-0.006(2)
C36	0.023(2)	0.030(2)	0.029(2)	0.006(2)	-0.0035(14)	-0.0018(15)
C37	0.039(2)	0.036(2)	0.065(3)	-0.010(2)	0.020(2)	0.000(2)
C38	0.079(3)	0.031(2)	0.095(3)	0.002(2)	0.020(3)	0.014(2)
C39	0.087(3)	0.066(3)	0.071(3)	-0.035(3)	0.028(2)	-0.008(3)
C40	0.042(2)	0.027(2)	0.041(2)	0.002(2)	0.006(2)	-0.006(2)
C41	0.070(3)	0.066(3)	0.067(3)	-0.027(2)	-0.017(2)	-0.006(2)
C42	0.061(3)	0.045(2)	0.073(3)	-0.009(2)	-0.008(2)	0.015(2)
C43	0.062(3)	0.055(3)	0.061(3)	-0.006(2)	-0.001(2)	-0.008(2)
C44	0.097(3)	0.030(2)	0.084(3)	-0.004(2)	-0.012(3)	-0.012(2)
C45	0.092(3)	0.054(3)	0.064(3)	-0.001(2)	-0.009(3)	-0.005(2)
C46	0.146(4)	0.063(3)	0.073(3)	0.014(3)	0.008(3)	-0.003(3)
Li1	0.029(3)	0.042(4)	0.039(3)	0.003(3)	0.011(2)	0.002(3)
Li2	0.036(3)	0.030(3)	0.056(4)	0.001(3)	0.008(3)	-0.003(3)

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 \cdot (\text{Pi}^2) \cdot U \cdot (\text{Sin}(\text{Theta})/\text{Lambda})^2$ for Isotropic Atoms
 $T = 2 \cdot (\text{Pi}^2) \cdot \text{Sum}_{ij} (h(i) \cdot h(j) \cdot U(i,j) \cdot \text{Astar}(i) \cdot \text{Astar}(j))$, for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S3.5 - Bond Distances (Angstrom)
for: Complex4*0.5Et2O

O1	-C44	1.424(4)	C11	-C14	1.554(4)
O1	-C45	1.449(5)	C15	-C16	1.516(4)
O1	-Li2	1.945(7)	C17	-C18	1.413(4)
O2	-C48	1.47(2)	C17	-C22	1.433(4)
O2	-C49	1.51(2)	C18	-C23	1.528(4)
N1	-Li1	1.934(6)	C18	-C19	1.403(5)
N1	-C17	1.415(4)	C19	-C20	1.371(6)
N1	-C15	1.358(4)	C20	-C21	1.374(6)
N2	-Li1	1.965(6)	C21	-C22	1.390(5)
N2	-Li2	2.081(7)	C22	-C26	1.497(4)
N2	-C31	1.430(4)	C23	-C25	1.553(4)
N2	-C29	1.438(4)	C23	-C24	1.538(4)
C1	-C2	1.527(4)	C26	-C27	1.545(5)
C1	-Li2	2.326(6)	C26	-C28	1.533(5)
C1	-C6	1.446(4)	C29	-Li2	2.259(7)
C1	-C15	1.407(4)	C29	-C30	1.515(4)
C2	-C7	1.593(4)	C31	-C32	1.410(4)
C2	-C3	1.548(4)	C31	-C36	1.421(4)
C3	-C29	1.364(4)	C32	-C33	1.387(4)
C3	-C4	1.543(4)	C32	-C37	1.527(4)
C4	-C5	1.529(4)	C33	-C34	1.377(4)
C4	-C11	1.557(4)	C34	-C35	1.382(4)
C5	-C6	1.362(4)	C35	-C36	1.387(4)
C7	-C10	1.545(4)	C36	-C40	1.522(4)
C7	-C9	1.542(4)	C37	-C39	1.548(6)
C7	-C8	1.553(4)	C37	-C38	1.506(5)
C11	-C13	1.548(4)	C40	-C42	1.525(5)
C11	-C12	1.537(5)	C40	-C41	1.524(5)

Table S3.5 - Bond Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

C43	-C44	1.499(6)	C20	-H20	0.92(2)
C45	-C46	1.513(7)	C21	-H21	0.95(3)
C2	-H2	1.03(2)	C23	-H23	0.980(4)
C4	-H4	0.98(3)	C24	-H24C	0.961(10)
C5	-H5	0.99(3)	C24	-H24B	0.961(15)
C6	-H6	1.01(3)	C24	-H24A	0.960(8)
C8	-H8C	0.961(10)	C25	-H25A	0.960(11)
C8	-H8A	0.960(13)	C25	-H25B	0.960(12)
C8	-H8B	0.961(12)	C25	-H25C	0.961(6)
C9	-H9A	0.960(11)	C26	-H26	0.981(4)
C9	-H9B	0.959(9)	C27	-H27C	0.960(15)
C9	-H9C	0.960(13)	C27	-H27A	0.960(11)
C10	-H10A	0.960(12)	C27	-H27B	0.960(7)
C10	-H10C	0.960(15)	C28	-H28A	0.960(5)
C10	-H10B	0.960(11)	C28	-H28B	0.960(5)
C12	-H12C	0.960(6)	C28	-H28C	0.959(6)
C12	-H12A	0.959(13)	C30	-H30A	0.961(11)
C12	-H12B	0.960(13)	C30	-H30C	0.960(5)
C13	-H13B	0.960(11)	C30	-H30B	0.960(13)
C13	-H13A	0.960(7)	C33	-H33	0.957(18)
C13	-H13C	0.961(13)	C34	-H34	0.898(18)
C14	-H14B	0.960(15)	C35	-H35	1.03(3)
C14	-H14A	0.960(5)	C37	-H37	0.979(4)
C14	-H14C	0.959(15)	C38	-H38C	0.960(8)
C16	-H16B	0.960(12)	C38	-H38A	0.961(7)
C16	-H16C	0.961(9)	C38	-H38B	0.960(9)
C16	-H16A	0.959(5)	C39	-H39C	0.960(7)
C19	-H19	1.05(3)	C39	-H39A	0.959(16)

Table S3.5 - Bond Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

C39	-H39B	0.960(14)	C44	-H44B	0.969(6)
C40	-H40	0.981(4)	C44	-H44A	0.970(5)
C41	-H41C	0.960(15)	C45	-H45B	0.971(6)
C41	-H41A	0.959(17)	C45	-H45A	0.971(6)
C41	-H41B	0.959(15)	C46	-H46B	0.960(14)
C42	-H42C	0.960(13)	C46	-H46A	0.960(17)
C42	-H42B	0.960(16)	C46	-H46C	0.96(2)
C42	-H42A	0.960(15)	C47	-C48	1.506(18)
C43	-H43B	0.959(18)	C49	-C50	1.553(15)
C43	-H43A	0.961(12)	Li1	-H2	1.95(2)
C43	-H43C	0.960(12)	Li1	-H28A	2.049(6)

Table S3.6 - Bond Angles (Degrees)
for: Complex4*0.5Et2O

C44	-O1	-C45	112.6 (3)	C4	-C5	-C6	123.5 (3)
C44	-O1	-Li2	133.9 (3)	C1	-C6	-C5	124.0 (3)
C45	-O1	-Li2	113.3 (3)	C2	-C7	-C8	105.5 (2)
C48	-O2	-C49	111.4 (12)	C2	-C7	-C9	111.1 (2)
C15	-N1	-Li1	104.6 (2)	C8	-C7	-C9	107.0 (2)
C17	-N1	-Li1	128.2 (2)	C8	-C7	-C10	106.5 (2)
C15	-N1	-C17	122.0 (3)	C9	-C7	-C10	111.1 (2)
C29	-N2	-Li1	129.7 (2)	C2	-C7	-C10	115.1 (2)
C29	-N2	-Li2	77.5 (2)	C4	-C11	-C12	115.0 (3)
C29	-N2	-C31	116.1 (2)	C4	-C11	-C13	109.5 (2)
C31	-N2	-Li2	146.3 (3)	C12	-C11	-C13	112.9 (2)
Li1	-N2	-Li2	86.3 (2)	C12	-C11	-C14	106.8 (2)
C31	-N2	-Li1	103.6 (2)	C4	-C11	-C14	106.6 (2)
C2	-C1	-C6	113.4 (2)	C13	-C11	-C14	105.4 (2)
C2	-C1	-Li2	90.8 (2)	N1	-C15	-C16	120.2 (3)
C6	-C1	-C15	122.5 (3)	C1	-C15	-C16	118.0 (3)
C2	-C1	-C15	124.1 (3)	N1	-C15	-C1	121.7 (3)
C15	-C1	-Li2	96.3 (2)	N1	-C17	-C22	117.2 (2)
C6	-C1	-Li2	81.0 (2)	C18	-C17	-C22	118.4 (3)
C1	-C2	-C7	114.0 (2)	N1	-C17	-C18	124.2 (3)
C3	-C2	-C7	117.0 (2)	C17	-C18	-C23	123.4 (3)
C1	-C2	-C3	107.0 (2)	C19	-C18	-C23	116.9 (3)
C2	-C3	-C29	116.7 (2)	C17	-C18	-C19	119.6 (3)
C4	-C3	-C29	131.4 (3)	C18	-C19	-C20	121.1 (3)
C2	-C3	-C4	108.9 (2)	C19	-C20	-C21	120.2 (4)
C3	-C4	-C11	126.5 (2)	C20	-C21	-C22	121.3 (3)
C5	-C4	-C11	113.5 (2)	C17	-C22	-C21	119.4 (3)
C3	-C4	-C5	104.2 (2)	C17	-C22	-C26	119.9 (2)

Table S3.6 - Bond Angles (Degrees) (continued)
for: Complex4*0.5Et2O

C21	-C22	-C26	120.7(3)	C36	-C40	-C41	113.6(2)
C18	-C23	-C25	112.1(3)	C41	-C40	-C42	108.6(3)
C24	-C23	-C25	109.2(2)	C36	-C40	-C42	110.7(3)
C18	-C23	-C24	111.1(3)	O1	-C44	-C43	111.2(3)
C22	-C26	-C28	111.3(3)	O1	-C45	-C46	113.2(3)
C27	-C26	-C28	109.2(3)	C3	-C2	-H2	104.1(12)
C22	-C26	-C27	114.4(3)	C7	-C2	-H2	102.4(12)
N2	-C29	-C30	114.0(2)	C1	-C2	-H2	111.9(13)
N2	-C29	-Li2	64.0(2)	C5	-C4	-H4	105.3(15)
C3	-C29	-C30	126.6(2)	C11	-C4	-H4	100.9(15)
C3	-C29	-Li2	83.7(2)	C3	-C4	-H4	104.3(15)
C30	-C29	-Li2	118.7(3)	C6	-C5	-H5	119.7(16)
N2	-C29	-C3	119.3(2)	C4	-C5	-H5	116.8(16)
N2	-C31	-C32	121.0(3)	C5	-C6	-H6	115.7(14)
C32	-C31	-C36	118.2(3)	C1	-C6	-H6	120.3(14)
N2	-C31	-C36	120.7(3)	C7	-C8	-H8A	109.5(5)
C31	-C32	-C33	119.7(3)	H8A	-C8	-H8B	109.5(12)
C33	-C32	-C37	119.6(3)	C7	-C8	-H8B	109.4(5)
C31	-C32	-C37	120.7(3)	C7	-C8	-H8C	109.4(7)
C32	-C33	-C34	121.5(3)	H8B	-C8	-H8C	109.5(11)
C33	-C34	-C35	119.5(3)	H8A	-C8	-H8C	109.5(11)
C34	-C35	-C36	120.9(3)	C7	-C9	-H9A	109.5(8)
C31	-C36	-C35	119.9(3)	C7	-C9	-H9B	109.5(5)
C31	-C36	-C40	121.8(2)	H9A	-C9	-H9B	109.3(12)
C35	-C36	-C40	118.2(3)	H9A	-C9	-H9C	109.5(11)
C32	-C37	-C39	112.8(3)	C7	-C9	-H9C	109.5(6)
C38	-C37	-C39	109.4(3)	H9B	-C9	-H9C	109.5(12)
C32	-C37	-C38	111.0(3)	H10A	-C10	-H10B	109.4(12)

Table S3.6 - Bond Angles (Degrees) (continued)
for: Complex4*0.5Et2O

H10A	-C10	-H10C	109.5(13)	C15	-C16	-H16C	109.4(6)
C7	-C10	-H10C	109.4(6)	C18	-C19	-H19	119.4(6)
C7	-C10	-H10A	109.5(5)	C20	-C19	-H19	119.5(6)
C7	-C10	-H10B	109.5(7)	C19	-C20	-H20	119.8(14)
H10B	-C10	-H10C	109.5(13)	C21	-C20	-H20	119.9(14)
C11	-C12	-H12A	109.5(8)	C20	-C21	-H21	119.3(7)
C11	-C12	-H12B	109.4(8)	C22	-C21	-H21	119.3(7)
H12A	-C12	-H12B	109.6(13)	C18	-C23	-H23	108.1(3)
H12A	-C12	-H12C	109.5(14)	C25	-C23	-H23	108.1(3)
H12B	-C12	-H12C	109.4(13)	C24	-C23	-H23	108.1(3)
C11	-C12	-H12C	109.4(5)	C23	-C24	-H24A	109.5(5)
C11	-C13	-H13B	109.5(6)	C23	-C24	-H24B	109.5(6)
C11	-C13	-H13C	109.5(5)	H24A	-C24	-H24B	109.4(13)
H13A	-C13	-H13B	109.6(13)	H24A	-C24	-H24C	109.5(15)
H13B	-C13	-H13C	109.4(12)	H24B	-C24	-H24C	109.4(15)
H13A	-C13	-H13C	109.5(15)	C23	-C24	-H24C	109.5(6)
C11	-C13	-H13A	109.5(9)	C23	-C25	-H25A	109.5(10)
C11	-C14	-H14B	109.4(7)	C23	-C25	-H25B	109.5(9)
C11	-C14	-H14A	109.5(3)	H25A	-C25	-H25C	109.5(16)
H14A	-C14	-H14C	109.4(15)	H25B	-C25	-H25C	109.4(13)
H14B	-C14	-H14C	109.4(15)	C23	-C25	-H25C	109.4(7)
H14A	-C14	-H14B	109.5(14)	H25A	-C25	-H25B	109.5(13)
C11	-C14	-H14C	109.6(6)	C27	-C26	-H26	107.1(3)
C15	-C16	-H16A	109.5(3)	C22	-C26	-H26	107.2(3)
C15	-C16	-H16B	109.4(6)	C28	-C26	-H26	107.2(3)
H16A	-C16	-H16B	109.5(10)	C26	-C27	-H27A	109.5(8)
H16A	-C16	-H16C	109.5(11)	C26	-C27	-H27C	109.5(8)
H16B	-C16	-H16C	109.5(10)	C26	-C27	-H27B	109.4(10)

Table S3.6 - Bond Angles (Degrees) (continued)
for: Complex4*0.5Et2O

H27A	-C27	-H27C	109.5 (14)	H38A	-C38	-H38B	109.4 (15)
H27B	-C27	-H27C	109.5 (18)	C37	-C38	-H38C	109.6 (11)
H27A	-C27	-H27B	109.4 (17)	C37	-C39	-H39A	109.5 (6)
C26	-C28	-H28A	108.9 (4)	C37	-C39	-H39B	109.5 (6)
C26	-C28	-H28B	109.2 (4)	H39A	-C39	-H39B	109.5 (15)
H28B	-C28	-H28C	109.4 (5)	H39A	-C39	-H39C	109.5 (19)
H28A	-C28	-H28C	109.5 (5)	H39B	-C39	-H39C	109.4 (16)
C26	-C28	-H28C	110.3 (3)	C37	-C39	-H39C	109.4 (8)
H28A	-C28	-H28B	109.5 (4)	C36	-C40	-H40	107.8 (3)
C29	-C30	-H30C	109.5 (4)	C41	-C40	-H40	107.9 (3)
H30A	-C30	-H30C	109.5 (15)	C42	-C40	-H40	107.9 (3)
H30B	-C30	-H30C	109.5 (14)	H41A	-C41	-H41C	109.4 (15)
H30A	-C30	-H30B	109.4 (11)	H41A	-C41	-H41B	109.6 (15)
C29	-C30	-H30A	109.5 (5)	C40	-C41	-H41C	109.4 (9)
C29	-C30	-H30B	109.4 (6)	C40	-C41	-H41A	109.5 (7)
C34	-C33	-H33	119.3 (10)	H41B	-C41	-H41C	109.4 (15)
C32	-C33	-H33	119.2 (10)	C40	-C41	-H41B	109.5 (6)
C35	-C34	-H34	120.3 (9)	C40	-C42	-H42C	109.6 (6)
C33	-C34	-H34	120.2 (9)	C40	-C42	-H42A	109.5 (8)
C36	-C35	-H35	119.5 (5)	C40	-C42	-H42B	109.4 (7)
C34	-C35	-H35	119.6 (5)	H42A	-C42	-H42C	109.5 (14)
C32	-C37	-H37	107.8 (3)	H42B	-C42	-H42C	109.4 (14)
C38	-C37	-H37	107.8 (4)	H42A	-C42	-H42B	109.4 (14)
C39	-C37	-H37	107.8 (4)	C44	-C43	-H43B	109.5 (5)
C37	-C38	-H38B	109.5 (11)	C44	-C43	-H43C	109.5 (7)
C37	-C38	-H38A	109.4 (11)	C44	-C43	-H43A	109.5 (7)
H38A	-C38	-H38C	109.5 (16)	H43B	-C43	-H43C	109.4 (15)
H38B	-C38	-H38C	109.4 (16)	H43A	-C43	-H43C	109.4 (14)

Table S3.6 - Bond Angles (Degrees) (continued)
for: Complex4*0.5Et2O

H43A	-C43	-H43B	109.5(15)	H46A	-C46	-H46B	109.5(19)
O1	-C44	-H44B	109.4(4)	O2	-C48	-C47	99.8(11)
O1	-C44	-H44A	109.4(4)	O2	-C49	-C50	124.1(14)
H44A	-C44	-H44B	108.1(4)	N1	-Li1	-N2	138.6(3)
C43	-C44	-H44A	109.4(5)	N2	-Li2	-C1	96.2(3)
C43	-C44	-H44B	109.3(4)	N2	-Li2	-C29	38.43(14)
O1	-C45	-H45B	108.9(5)	O1	-Li2	-C1	125.1(3)
C46	-C45	-H45A	109.0(5)	O1	-Li2	-C29	137.9(3)
C46	-C45	-H45B	109.0(5)	C1	-Li2	-C29	90.1(2)
H45A	-C45	-H45B	107.7(5)	O1	-Li2	-N2	136.8(3)
O1	-C45	-H45A	108.9(5)	N1	-Li1	-H28A	90.0(2)
C45	-C46	-H46A	109.4(8)	H2	-Li1	-H28A	122.6(7)
C45	-C46	-H46B	109.5(11)	N2	-Li1	-H2	73.2(6)
H46B	-C46	-H46C	109.4(17)	N2	-Li1	-H28A	131.4(3)
H46A	-C46	-H46C	109.6(19)	N1	-Li1	-H2	85.9(7)
C45	-C46	-H46C	109.5(11)				

Table S3.7 - Torsion Angles (Degrees)
for: Complex4*0.5Et2O

C45	-O1	-C44	-C43	162.9 (3)
Li2	-O1	-C44	-C43	-21.7 (5)
C44	-O1	-C45	-C46	67.8 (4)
Li2	-O1	-C45	-C46	-108.6 (4)
C44	-O1	-Li2	-N2	94.1 (5)
C44	-O1	-Li2	-C1	-66.3 (5)
C44	-O1	-Li2	-C29	152.3 (4)
C45	-O1	-Li2	-N2	-90.5 (4)
C45	-O1	-Li2	-C1	109.1 (3)
C45	-O1	-Li2	-C29	-32.4 (5)
C48	-O2	-C49	-C50	168.6 (19)
C49	-O2	-C48	-C47	-170.7 (15)
Li1	-N1	-C15	-C1	-40.2 (4)
Li1	-N1	-C15	-C16	136.5 (3)
C15	-N1	-C17	-C18	-54.9 (5)
Li1	-N1	-C17	-C18	154.4 (3)
Li1	-N1	-C17	-C22	-20.5 (5)
C15	-N1	-Li1	-N2	1.2 (6)
C17	-N1	-Li1	-N2	155.8 (4)
C17	-N1	-C15	-C16	-20.1 (4)
C17	-N1	-C15	-C1	163.2 (3)
C15	-N1	-C17	-C22	130.2 (3)
C31	-N2	-C29	-Li2	147.2 (3)
Li1	-N2	-C31	-C36	-88.0 (3)
Li2	-N2	-C31	-C32	-15.0 (6)
Li2	-N2	-C31	-C36	167.9 (4)
C31	-N2	-C29	-C3	-147.3 (3)
C31	-N2	-C29	-C30	35.6 (4)

Table S3.7 - Torsion Angles (Degrees) (continued)
for: Complex4*0.5Et2O

Li2	-N2	-Li1	-N1	-23.6(5)
C29	-N2	-Li2	-O1	113.7(4)
C29	-N2	-Li2	-C1	-82.3(2)
C31	-N2	-Li2	-O1	-5.1(7)
C31	-N2	-Li2	-C1	158.9(4)
C29	-N2	-Li1	-N1	46.9(7)
C31	-N2	-Li1	-N1	-170.9(5)
Li1	-N2	-Li2	-C1	49.7(2)
Li1	-N2	-Li2	-C29	132.0(2)
Li2	-N2	-C29	-C30	-111.6(3)
C29	-N2	-C31	-C32	-122.6(3)
C29	-N2	-C31	-C36	60.3(4)
Li1	-N2	-C31	-C32	89.1(3)
Li1	-N2	-C29	-C3	-8.9(5)
Li1	-N2	-C29	-C30	174.0(3)
Li1	-N2	-C29	-Li2	-74.4(4)
Li2	-N2	-C29	-C3	65.5(3)
Li1	-N2	-Li2	-O1	-114.3(4)
C31	-N2	-Li2	-C29	-118.8(4)
C15	-C1	-C2	-C3	137.0(3)
C15	-C1	-C2	-C7	-92.0(3)
C6	-C1	-C2	-C7	89.2(3)
Li2	-C1	-C6	-C5	-78.4(3)
C2	-C1	-C15	-N1	-10.6(4)
C2	-C1	-C15	-C16	172.7(2)
Li2	-C1	-C2	-C3	38.8(2)
Li2	-C1	-C2	-C7	169.8(2)
C2	-C1	-C6	-C5	8.6(4)

Table S3.7 - Torsion Angles (Degrees) (continued)
for: Complex4*0.5Et2O

C6	-C1	-C2	-C3	-41.8(3)
C15	-C1	-Li2	-N2	-95.0(2)
C2	-C1	-Li2	-C29	-8.6(2)
C6	-C1	-Li2	-C29	105.0(2)
C15	-C1	-Li2	-C29	-133.0(2)
C2	-C1	-Li2	-O1	-163.9(3)
C6	-C1	-C15	-N1	168.1(3)
C15	-C1	-C6	-C5	-170.2(3)
C6	-C1	-Li2	-N2	143.0(2)
Li2	-C1	-C15	-C16	-92.0(3)
C15	-C1	-Li2	-O1	71.7(3)
C2	-C1	-Li2	-N2	29.5(2)
C6	-C1	-C15	-C16	-8.6(4)
Li2	-C1	-C15	-N1	84.8(3)
C6	-C1	-Li2	-O1	-50.3(3)
C7	-C2	-C3	-C29	138.6(3)
C1	-C2	-C7	-C8	82.6(3)
C3	-C2	-C7	-C9	-35.8(3)
C3	-C2	-C7	-C10	91.5(3)
C7	-C2	-C3	-C4	-58.6(3)
C3	-C2	-C7	-C8	-151.4(2)
C1	-C2	-C7	-C9	-161.7(2)
C1	-C2	-C7	-C10	-34.4(3)
C1	-C2	-C3	-C29	-92.0(3)
C1	-C2	-C3	-C4	70.7(3)
C29	-C3	-C4	-C11	-34.7(5)
C4	-C3	-C29	-Li2	-90.7(4)
C2	-C3	-C29	-Li2	67.4(3)

Table S3.7 - Torsion Angles (Degrees) (continued)
for: Complex4*0.5Et2O

C4	-C3	-C29	-C30	30.6(5)
C2	-C3	-C29	-C30	-171.3(3)
C2	-C3	-C4	-C5	-59.8(3)
C2	-C3	-C4	-C11	165.9(3)
C29	-C3	-C4	-C5	99.5(4)
C2	-C3	-C29	-N2	12.0(4)
C4	-C3	-C29	-N2	-146.1(3)
C5	-C4	-C11	-C13	176.1(2)
C5	-C4	-C11	-C12	-55.5(3)
C3	-C4	-C11	-C12	75.3(4)
C3	-C4	-C11	-C13	-53.1(4)
C11	-C4	-C5	-C6	167.0(3)
C3	-C4	-C5	-C6	25.9(4)
C3	-C4	-C11	-C14	-166.5(3)
C5	-C4	-C11	-C14	62.7(3)
C4	-C5	-C6	-C1	-0.4(5)
N1	-C17	-C18	-C23	-0.4(5)
N1	-C17	-C22	-C26	-4.6(4)
C18	-C17	-C22	-C21	1.3(5)
N1	-C17	-C18	-C19	-176.5(3)
N1	-C17	-C22	-C21	176.5(3)
C22	-C17	-C18	-C23	174.4(3)
C22	-C17	-C18	-C19	-1.6(5)
C18	-C17	-C22	-C26	-179.8(3)
C23	-C18	-C19	-C20	-175.2(3)
C17	-C18	-C23	-C24	-109.7(3)
C17	-C18	-C19	-C20	1.1(5)
C19	-C18	-C23	-C25	-56.1(4)

Table S3.7 - Torsion Angles (Degrees) (continued)
for: Complex4*0.5Et2O

C17	-C18	-C23	-C25	127.7(3)
C19	-C18	-C23	-C24	66.4(3)
C18	-C19	-C20	-C21	-0.1(5)
C19	-C20	-C21	-C22	-0.2(5)
C20	-C21	-C22	-C26	-179.2(3)
C20	-C21	-C22	-C17	-0.4(5)
C21	-C22	-C26	-C27	27.9(4)
C17	-C22	-C26	-C28	84.7(4)
C21	-C22	-C26	-C28	-96.5(4)
C17	-C22	-C26	-C27	-151.0(3)
C3	-C29	-Li2	-C1	-27.2(2)
C3	-C29	-Li2	-O1	122.2(4)
C30	-C29	-Li2	-O1	-6.4(5)
C3	-C29	-Li2	-N2	-127.0(3)
C30	-C29	-Li2	-N2	104.4(3)
N2	-C29	-Li2	-C1	99.9(2)
C30	-C29	-Li2	-C1	-155.8(2)
N2	-C29	-Li2	-O1	-110.8(4)
N2	-C31	-C36	-C35	-177.3(3)
N2	-C31	-C32	-C33	177.9(3)
N2	-C31	-C32	-C37	0.6(4)
C36	-C31	-C32	-C33	-4.9(4)
C36	-C31	-C32	-C37	177.7(3)
N2	-C31	-C36	-C40	6.7(4)
C32	-C31	-C36	-C35	5.5(4)
C32	-C31	-C36	-C40	-170.5(3)
C31	-C32	-C37	-C39	-148.1(3)
C33	-C32	-C37	-C39	34.5(4)

Table S3.7 - Torsion Angles (Degrees) (continued)
for: Complex4*0.5Et2O

C31	-C32	-C33	-C34	1.1(4)
C37	-C32	-C33	-C34	178.5(3)
C31	-C32	-C37	-C38	88.7(3)
C33	-C32	-C37	-C38	-88.7(4)
C32	-C33	-C34	-C35	2.3(4)
C33	-C34	-C35	-C36	-1.7(4)
C34	-C35	-C36	-C31	-2.3(4)
C34	-C35	-C36	-C40	173.9(3)
C31	-C36	-C40	-C42	104.3(3)
C31	-C36	-C40	-C41	-133.1(3)
C35	-C36	-C40	-C41	50.8(4)
C35	-C36	-C40	-C42	-71.7(3)

Table S3.8 - Contact Distances (Angstrom)
for: Complex4*0.5Et2O

O1	.C38	3.375 (5)	C15	.C8	3.558 (4)
N1	.C8	3.393 (4)	C15	.C23	3.179 (4)
N1	.C28	3.320 (4)	C16	.C23	3.235 (4)
N1	.H2	2.64 (2)	C16	.C25	3.524 (4)
N1	.H8C	2.713 (10)	C16	.C18	3.225 (4)
N1	.H23	2.601 (4)	C18	.C16	3.225 (4)
N1	.H26	2.462 (4)	C23	.C16	3.235 (4)
N1	.H28A	2.817 (4)	C23	.C15	3.179 (4)
N2	.H2	2.33 (2)	C25	.C16	3.524 (4)
N2	.H37	2.536 (5)	C29	.C40	3.119 (4)
N2	.H40	2.477 (4)	C30	.C11	3.464 (4)
C1	.N2	3.285 (4)	C30	.C40	3.598 (4)
C4	.C9	3.335 (4)	C30	.C36	3.271 (4)
C4	.C10	3.339 (4)	C30	.C13	3.442 (4)
C5	.C7	3.569 (4)	C30	.C12	3.339 (4)
C5	.C10	3.381 (4)	C36	.C30	3.271 (4)
C6	.C10	3.228 (4)	C37	.Li2	3.486 (6)
C7	.C5	3.569 (4)	C37	.Li1	3.694 (6)
C8	.Li1	3.808 (6)	C38	.O1	3.375 (5)
C8	.C15	3.558 (4)	C38	.Li2	3.632 (7)
C8	.N1	3.393 (4)	C40	.Li1	3.612 (6)
C9	.C4	3.335 (4)	C40	.C30	3.598 (4)
C10	.C4	3.339 (4)	C40	.C29	3.119 (4)
C10	.C5	3.381 (4)	C42	.Li1	3.743 (7)
C10	.C6	3.228 (4)	C1	.H10C	2.643 (13)
C11	.C30	3.464 (4)	C1	.H8C	2.912 (9)
C12	.C30	3.339 (4)	C2	.H40	2.966 (4)
C13	.C30	3.442 (4)	C3	.H9C	2.801 (10)

Table S3.8 - Contact Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

C3	.H13A	2.828(15)	C16	.H23	2.699(4)
C3	.H40	2.766(4)	C17	.H16C	2.465(9)
C3	.H9A	2.942(14)	C18	.H16C	2.699(10)
C4	.H10A	2.758(9)	C19	.H24B	2.826(13)
C4	.H30C	2.994(5)	C19	.H44A_b	3.061(5)
C4	.H9C	2.784(8)	C19	.H25B	2.795(15)
C5	.H12C	2.749(9)	C20	.H44A_b	3.035(5)
C5	.H10A	2.832(16)	C21	.H27A	2.81(2)
C5	.H14C	2.659(10)	C21	.H27C	2.904(18)
C6	.H10C	2.880(16)	C23	.H16C	3.045(11)
C6	.H16B	2.933(12)	C23	.H16B	2.997(10)
C6	.H10A	3.035(17)	C23	.H8C	2.916(12)
C6	.H16A	2.744(12)	C24	.H8C	2.912(13)
C7	.H4	2.59(3)	C24	.H19	2.985(10)
C8	.H24A	3.043(13)	C25	.H16B	3.007(11)
C9	.H4	2.68(3)	C25	.H19	2.777(9)
C10	.H4	2.64(2)	C27	.H21	2.584(8)
C11	.H30C	2.732(5)	C29	.H40	2.404(4)
C12	.H5	2.95(3)	C29	.H13A	3.051(9)
C12	.H30C	2.620(13)	C30	.H13A	2.721(8)
C13	.H30C	2.603(9)	C30	.H38C	3.044(14)
C14	.H5	2.71(3)	C30	.H12A	2.536(12)
C15	.H8C	2.893(7)	C31	.H30B	2.566(16)
C15	.H23	2.449(4)	C31	.H30A	2.924(15)
C16	.H43B	2.790(15)	C33	.H38B	3.077(19)
C16	.H25C	2.953(10)	C33	.H39C	2.84(2)
C16	.H14C_a	2.980(16)	C33	.H19_c	2.70(3)
C16	.H6	2.57(2)	C33	.H39B	2.868(17)

Table S3.8 - Contact Distances(Angstrom) (continued)
for: Complex4*0.5Et2O

C34	.H14A_d	2.843 (14)	Li1	.H42C	3.038 (8)
C34	.H19_c	2.81 (2)	Li1	.H37	3.001 (7)
C35	.H14A_d	2.977 (8)	Li1	.H40	3.171 (6)
C35	.H42B	2.880 (14)	Li2	.H16A	3.242 (6)
C35	.H41C	2.782 (14)	Li2	.H37	2.751 (6)
C36	.H30B	2.672 (16)	Li2	.H38C	3.062 (19)
C37	.H43C	2.957 (15)	Li2	.H43B	3.032 (15)
C38	.H30A	3.076 (16)	Li2	.H43C	3.371 (17)
C38	.H35_e	2.83 (2)	H2	.N1	2.64 (2)
C39	.H33	2.587 (15)	H2	.N2	2.33 (2)
C39	.H27B	2.989 (9)	H2	.H8B	2.23 (3)
C40	.H30B	3.077 (12)	H2	.H8C	2.57 (2)
C41	.H35	2.731 (8)	H2	.H40	2.33 (2)
C42	.H35	3.084 (9)	H4	.C7	2.59 (3)
C42	.H16C_b	3.072 (10)	H4	.C9	2.68 (3)
C43	.H16A	3.051 (12)	H4	.C10	2.64 (2)
C43	.H37	3.023 (5)	H4	.H9C	2.06 (3)
C44	.H46A	2.754 (11)	H4	.H10A	1.99 (2)
C45	.H38C	3.070 (15)	H4	.H13B	2.54 (3)
C46	.H44B	2.802 (6)	H4	.H14B	2.24 (3)
Li1	.C8	3.808 (6)	H5	.C12	2.95 (3)
Li1	.C37	3.694 (6)	H5	.C14	2.71 (3)
Li1	.C40	3.612 (6)	H5	.H12C	2.39 (3)
Li1	.C42	3.743 (7)	H5	.H14C	2.09 (3)
Li2	.C38	3.632 (7)	H5	.H16B_a	2.59 (3)
Li2	.C37	3.486 (6)	H6	.C16	2.57 (2)
Li1	.H26	2.241 (6)	H6	.H16A	2.26 (3)
Li1	.H8B	3.440 (15)	H6	.H16B	2.46 (3)

Table S3.8 - Contact Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

H8A	.H9B	2.455 (16)	H10B	.H8A	2.393 (15)
H8A	.H10B	2.393 (15)	H10B	.H9B	2.567 (14)
H8B	.Li1	3.440 (15)	H10C	.C1	2.643 (13)
H8B	.H2	2.23 (3)	H10C	.C6	2.880 (16)
H8B	.H9A	2.489 (14)	H10C	.H8C	2.515 (16)
H8C	.N1	2.713 (10)	H12A	.C30	2.536 (12)
H8C	.C1	2.912 (9)	H12A	.H30A	2.52 (2)
H8C	.C15	2.893 (7)	H12A	.H30C	1.89 (2)
H8C	.C23	2.916 (12)	H12B	.H13C	2.472 (14)
H8C	.C24	2.912 (13)	H12B	.H14A	2.414 (16)
H8C	.H2	2.57 (2)	H12C	.C5	2.749 (9)
H8C	.H10C	2.515 (16)	H12C	.H5	2.39 (3)
H8C	.H23	2.277 (10)	H12C	.H14C	2.50 (2)
H8C	.H24A	2.398 (18)	H13A	.C3	2.828 (15)
H9A	.C3	2.942 (14)	H13A	.C29	3.051 (9)
H9A	.H8B	2.489 (14)	H13A	.C30	2.721 (8)
H9A	.H40	2.380 (11)	H13A	.H30C	1.977 (17)
H9B	.H8A	2.455 (16)	H13B	.H4	2.54 (3)
H9B	.H10B	2.567 (14)	H13B	.H14B	2.290 (19)
H9C	.C3	2.801 (10)	H13C	.H12B	2.472 (14)
H9C	.C4	2.784 (8)	H14A	.H12B	2.414 (16)
H9C	.H4	2.06 (3)	H14A	.C34_f	2.843 (14)
H9C	.H10A	2.557 (17)	H14A	.C35_f	2.977 (8)
H10A	.C4	2.758 (9)	H14B	.H4	2.24 (3)
H10A	.C5	2.832 (16)	H14B	.H13B	2.290 (19)
H10A	.C6	3.035 (17)	H14B	.H28C_f	2.584 (13)
H10A	.H4	1.99 (2)	H14C	.C5	2.659 (10)
H10A	.H9C	2.557 (17)	H14C	.H5	2.09 (3)

Table S3.8 - Contact Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

H14C	.H12C	2.50 (2)	H21	.H27A	2.21 (2)
H14C	.C16_a	2.980 (16)	H21	.H27C	2.595 (19)
H14C	.H16B_a	2.365 (18)	H23	.N1	2.601 (4)
H16A	.C6	2.744 (12)	H23	.C15	2.449 (4)
H16A	.C43	3.051 (12)	H23	.C16	2.699 (4)
H16A	.Li2	3.242 (6)	H23	.H8C	2.277 (10)
H16A	.H6	2.26 (3)	H23	.H16B	2.422 (9)
H16A	.H43B	2.279 (17)	H24A	.C8	3.043 (13)
H16B	.C6	2.933 (12)	H24A	.H8C	2.398 (18)
H16B	.C23	2.997 (10)	H24A	.H39A_b	2.580 (14)
H16B	.C25	3.007 (11)	H24B	.C19	2.826 (13)
H16B	.H6	2.46 (3)	H24B	.H19	2.462 (14)
H16B	.H23	2.422 (9)	H24B	.H25B	2.519 (18)
H16B	.H25C	2.454 (16)	H24C	.H25A	2.519 (18)
H16B	.H5_a	2.59 (3)	H25A	.H24C	2.519 (18)
H16B	.H14C_a	2.365 (18)	H25B	.C19	2.795 (15)
H16C	.C17	2.465 (9)	H25B	.H19	2.234 (18)
H16C	.C18	2.699 (10)	H25B	.H24B	2.519 (18)
H16C	.C23	3.045 (11)	H25C	.C16	2.953 (10)
H16C	.C42_g	3.072 (10)	H25C	.H16B	2.454 (16)
H16C	.H42B_g	2.599 (17)	H26	.N1	2.462 (4)
H19	.C24	2.985 (10)	H26	.Li1	2.241 (6)
H19	.C25	2.777 (9)	H27A	.C21	2.81 (2)
H19	.C33_h	2.70 (3)	H27A	.H21	2.21 (2)
H19	.C34_h	2.81 (2)	H27A	.H28B	2.484 (11)
H19	.H24B	2.462 (14)	H27B	.C39	2.989 (9)
H19	.H25B	2.234 (18)	H27B	.H28C	2.54 (2)
H21	.C27	2.584 (8)	H27B	.H39B	2.30 (2)

Table S3.8 - Contact Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

H27C	.C21	2.904 (18)	H35	.H38A_i	2.530 (19)
H27C	.H21	2.595 (19)	H35	.H38B_i	2.31 (3)
H28A	.N1	2.817 (4)	H37	.N2	2.536 (5)
H28A	.C17	3.021 (5)	H37	.C43	3.023 (5)
H28B	.H27A	2.484 (11)	H37	.Li1	3.001 (7)
H28C	.H27B	2.54 (2)	H37	.Li2	2.751 (6)
H28C	.H14B_d	2.584 (13)	H37	.H43C	2.268 (18)
H30A	.C31	2.924 (15)	H38A	.H39A	2.53 (2)
H30A	.C38	3.076 (16)	H38A	.H35_e	2.53 (2)
H30A	.H12A	2.52 (2)	H38B	.C33	3.077 (19)
H30A	.H38C	2.205 (19)	H38B	.H39C	2.484 (19)
H30B	.C31	2.566 (16)	H38B	.H35_e	2.31 (3)
H30B	.C36	2.672 (16)	H38C	.C30	3.044 (14)
H30B	.C40	3.077 (12)	H38C	.C45	3.070 (15)
H30C	.C4	2.994 (5)	H38C	.Li2	3.062 (19)
H30C	.C11	2.732 (5)	H38C	.H30A	2.205 (19)
H30C	.C12	2.620 (13)	H39A	.H38A	2.53 (2)
H30C	.C13	2.603 (9)	H39A	.H43C	2.52 (2)
H30C	.H12A	1.89 (2)	H39A	.H24A_g	2.580 (14)
H30C	.H13A	1.977 (17)	H39B	.C33	2.868 (17)
H33	.C39	2.587 (15)	H39B	.H27B	2.30 (2)
H33	.H39B	2.58 (2)	H39B	.H33	2.58 (2)
H33	.H39C	2.23 (3)	H39C	.C33	2.84 (2)
H35	.C41	2.731 (8)	H39C	.H33	2.23 (3)
H35	.C42	3.084 (9)	H39C	.H38B	2.484 (19)
H35	.H41C	2.196 (17)	H40	.N2	2.477 (4)
H35	.H42B	2.599 (15)	H40	.C2	2.966 (4)
H35	.C38_i	2.83 (2)	H40	.C3	2.766 (4)

Table S3.8 - Contact Distances (Angstrom) (continued)
for: Complex4*0.5Et2O

H40	.C29	2.404(4)	H43B	.Li2	3.032(15)
H40	.Li1	3.171(6)	H43B	.H16A	2.279(17)
H40	.H2	2.33(2)	H43C	.C37	2.957(15)
H40	.H9A	2.380(11)	H43C	.Li2	3.371(17)
H41A	.H42A	2.457(19)	H43C	.H37	2.268(18)
H41C	.C35	2.782(14)	H43C	.H39A	2.52(2)
H41C	.H35	2.196(17)	H44A	.H45A	2.247(6)
H41C	.H42B	2.481(19)	H44A	.C19_g	3.061(5)
H42A	.H41A	2.457(19)	H44A	.C20_g	3.035(5)
H42B	.C35	2.880(14)	H44B	.C46	2.802(6)
H42B	.H35	2.599(15)	H44B	.H46A	2.365(15)
H42B	.H41C	2.481(19)	H45A	.H44A	2.247(6)
H42B	.H16C_b	2.599(17)	H46A	.C44	2.754(11)
H42C	.Li1	3.038(8)	H46A	.H44B	2.365(15)
H43B	.C16	2.790(15)			

Table S3.9 - Hydrogen Bonds (Angstrom, Deg)
for: Complex4*0.5Et2O

C2	--	H2	..	N2	1.03(2)	2.33(2)	2.781(4)	105.1(14)	.	yes
C23	--	H23	..	N1	0.980(4)	2.601(4)	3.052(4)	108.2(3)	.	yes
C26	--	H26	..	N1	0.981(4)	2.462(4)	2.828(4)	101.7(3)	.	yes
C37	--	H37	..	N2	0.979(4)	2.536(5)	2.927(5)	103.7(3)	.	yes
C40	--	H40	..	N2	0.981(4)	2.477(4)	2.958(4)	109.9(3)	.	yes

Translation of Symmetry Code to Equiv.Pos

a	= [3665.00]	= 1-x, 1-y, -z
b	= [2645.00]	= 1-x, -1/2+y, 1/2-z
c	= [1455.00]	= -1+x, y, z
d	= [4555.00]	= x, 1/2-y, 1/2+z
e	= [2555.00]	= -x, 1/2+y, 1/2-z
f	= [4554.00]	= x, 1/2-y, -1/2+z
g	= [2655.00]	= 1-x, 1/2+y, 1/2-z
h	= [1655.00]	= 1+x, y, z
i	= [2545.00]	= -x, -1/2+y, 1/2-z

Table S4.1 - Crystal Data and Details of the Structure Determination
for: Complex5

Crystal Data			
Empirical Formula	C42 H62 Li2 N2 O4		
Formula Weight	672.82		
Crystal System	Monoclinic		
Space group	I2/a	(No. 15)	
a, b, c [Angstrom]	14.3560(10)	14.8880(10)	19.760(2)
alpha, beta, gamma [deg]	90	99.000(10)	90
V [Ang**3]	4171.4(6)		
Z	4		
D(obs), D(calc) [g/cm**3]	0.000, 1.071		
F(000)	1464		
Mu(MoKa) [/mm]	0.1		
Crystal Size [mm]	0.10 x 0.20 x 0.30		
Data Collection			
Temperature (K)	193		
Radiation [Angstrom]	MoKa	0.71073	
Theta Min-Max [Deg]	3.0, 25.9		
Dataset	-17: 0 ; -18: 18 ; -21: 22		
Tot., Uniq. Data, R(int)	7383,	3771,	0.023
Observed data [I > 2.0 sigma(I)]	2528		
Refinement			
Nref, Npar	3770, 331		
R, wR, S	0.0631, 0.1657, 1.07		
w =			
Max. and Av. Shift/Error	0.81, 0.03		
Min. and Max. resd. dens. [e/Ang^3]	-0.16, 0.20		

Table S4.2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: Complex5

Atom	x	y	z	U(eq) [Ang ²]
----	---	---	---	-----
*O1	0.5470 (7)	0.3312 (8)	0.5716 (5)	0.054 (2)
*O2	0.5381 (14)	0.1569 (10)	0.5912 (10)	0.060 (3)
N1	0.58312 (14)	0.24114 (13)	0.42115 (10)	0.0436 (7)
C1	0.6910 (2)	0.11948 (14)	0.44786 (13)	0.0369 (7)
C2	3/4	0.1645 (2)	1/2	0.0340 (12)
C3	0.6924 (2)	0.0262 (2)	0.4487 (2)	0.0551 (11)
C4	3/4	-0.0190 (3)	1/2	0.0708 (18)
C5	0.6288 (2)	0.1726 (2)	0.39407 (13)	0.0397 (9)
C6	0.6263 (2)	0.1489 (2)	0.3277 (2)	0.0598 (12)
C7	0.5346 (2)	0.3037 (2)	0.37387 (12)	0.0402 (8)
C8	0.5834 (2)	0.3752 (2)	0.34838 (13)	0.0449 (11)
C9	0.5332 (2)	0.4386 (2)	0.30536 (13)	0.0482 (11)
C10	0.4367 (2)	0.4334 (2)	0.28737 (14)	0.0529 (12)
C11	0.3890 (2)	0.3641 (2)	0.3121 (2)	0.0582 (12)
C12	0.4358 (2)	0.2981 (2)	0.35481 (14)	0.0493 (11)
C13	0.6894 (2)	0.3862 (2)	0.3684 (2)	0.0601 (12)
*C14	0.7161 (5)	0.4860 (9)	0.3991 (7)	0.082 (3)
C15	0.7398 (2)	0.3841 (3)	0.3071 (2)	0.0860 (16)
C16	0.3802 (2)	0.2215 (2)	0.3802 (2)	0.0728 (14)
*C17	0.3666 (9)	0.1482 (10)	0.3264 (10)	0.110 (5)
*C18	0.2762 (8)	0.2541 (7)	0.3916 (9)	0.104 (5)
*C19	0.5137 (9)	0.4114 (10)	0.5434 (6)	0.069 (3)
*C20	0.5009 (8)	0.3012 (9)	0.6266 (5)	0.063 (3)
*C21	0.5433 (7)	0.2132 (8)	0.6515 (6)	0.062 (3)
*C22	0.5708 (7)	0.0660 (10)	0.6076 (5)	0.065 (3)
Li1	0.5737 (3)	0.2267 (4)	0.5156 (2)	0.0618 (17)

Table S4.2

Parameters of the non-Hydrogen atoms (continued)
for: Complex5

Atom	x	y	z	U(eq) [Ang ²]
----	---	---	---	-----
*C20A	0.479 (3)	0.266 (3)	0.6195 (18)	0.096 (11)
*O1A	0.527 (2)	0.3015 (16)	0.5692 (13)	0.068 (6)
*O2A	0.537 (3)	0.130 (3)	0.583 (3)	0.067 (9)
*C14A	0.7135 (9)	0.434 (3)	0.4256 (15)	0.088 (8)
*C17A	0.3241 (14)	0.1659 (13)	0.3243 (9)	0.097 (6)
*C18A	0.3319 (17)	0.2508 (10)	0.4355 (10)	0.116 (7)
*C19A	0.484 (4)	0.394 (3)	0.543 (2)	0.143 (17)
*C21A	0.531 (2)	0.181 (3)	0.6380 (18)	0.098 (11)
*C22A	0.572 (3)	0.042 (3)	0.602 (2)	0.160 (18)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S4.3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: Complex5

Atom	x	y	z	U(iso) [Ang ²]
*H2	0.754 (4)	0.233 (2)	0.505 (6)	0.038 (9)
*H14B	0.7828 (7)	0.4895 (13)	0.415 (2)	0.1230
*H14C	0.683 (2)	0.4974 (14)	0.4368 (15)	0.1230
H15A	0.7229 (14)	0.4362 (9)	0.2793 (7)	0.1300
H15B	0.7219 (14)	0.3310 (9)	0.2807 (8)	0.1300
H15C	0.8067 (2)	0.3837 (18)	0.3221 (2)	0.1300
H16	0.4288 (2)	0.1802 (2)	0.4023 (2)	0.0880
*H17A	0.4258 (12)	0.119 (3)	0.325 (3)	0.1660
*H17B	0.343 (5)	0.1741 (11)	0.2825 (11)	0.1660
*H17C	0.322 (4)	0.105 (2)	0.338 (2)	0.1660
*H18A	0.2436 (19)	0.2049 (13)	0.409 (3)	0.1550
*H18B	0.2414 (17)	0.274 (4)	0.3488 (11)	0.1550
*H18C	0.2820 (8)	0.303 (3)	0.424 (3)	0.1550
*H19A	0.545 (2)	0.4255 (18)	0.5052 (14)	0.1040
*H19B	0.526 (3)	0.4581 (10)	0.5772 (9)	0.1040
*H19C	0.4471 (10)	0.4068 (12)	0.528 (2)	0.1040
*H20A	0.4339 (8)	0.2941 (9)	0.6108 (5)	0.0750
*H20B	0.5094 (8)	0.3448 (9)	0.6635 (5)	0.0750
*H21A	0.6084 (7)	0.2210 (8)	0.6729 (6)	0.0740
*H21B	0.5082 (7)	0.1865 (8)	0.6845 (6)	0.0740
*H22A	0.572 (2)	0.0329 (12)	0.5660 (5)	0.0970
*H22B	0.5291 (15)	0.0370 (12)	0.6343 (16)	0.0970
*H22C	0.6333 (11)	0.0678 (10)	0.6334 (15)	0.0970
H3	0.6544 (2)	-0.0058 (2)	0.4146 (2)	0.0660
H4	3/4	-0.0814 (3)	1/2	0.0850
H6	0.583 (2)	0.1824 (19)	0.2899 (16)	0.064 (8)

Table S4.3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: Complex5

Atom	x	y	z	U(iso) [Ang ²]
H6A	0.6687(19)	0.0982(19)	0.3160(14)	0.055(8)
H9	0.5655(2)	0.4855(2)	0.28841(13)	0.0580
H10	0.4043(2)	0.4764(2)	0.25873(14)	0.0630
H11	0.3238(2)	0.3610(2)	0.3002(2)	0.0700
H13	0.7147(2)	0.3400(2)	0.4017(2)	0.0730
*H14A	0.698(3)	0.5300(10)	0.3639(9)	0.1230
*H14D	0.7802(14)	0.429(7)	0.441(3)	0.1340
*H14E	0.680(6)	0.412(5)	0.461(2)	0.1340
*H14F	0.697(7)	0.496(3)	0.4165(19)	0.1340
*H17D	0.362(2)	0.155(5)	0.289(2)	0.1450
*H17E	0.268(3)	0.198(3)	0.305(3)	0.1450
*H17F	0.307(5)	0.110(2)	0.3430(12)	0.1450
*H18D	0.298(5)	0.305(3)	0.422(2)	0.1740
*H18E	0.3772(18)	0.262(6)	0.4758(16)	0.1740
*H18F	0.288(5)	0.205(3)	0.445(3)	0.1740
*H19D	0.518(9)	0.417(7)	0.508(7)	0.2120
*H19E	0.489(11)	0.436(4)	0.580(3)	0.2120
*H19F	0.418(5)	0.387(4)	0.523(8)	0.2120
*H20C	0.413(3)	0.254(3)	0.6014(18)	0.1140
*H20D	0.482(3)	0.305(3)	0.6587(18)	0.1140
*H21C	0.594(2)	0.195(3)	0.6607(18)	0.1190
*H21D	0.500(2)	0.148(3)	0.6699(18)	0.1190
*H22D	0.551(8)	0.0003(19)	0.566(4)	0.2430
*H22E	0.549(7)	0.023(5)	0.643(4)	0.2430
*H22F	0.640(3)	0.0431(19)	0.610(6)	0.2430

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\text{Pi} ** 2) * U * (\text{Sin}(\text{Theta}) / \text{Lambda}) ** 2$ for Isotropic Atoms

Table S4.4 - (An)isotropic Displacement Parameters
for: Complex5

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.068(3)	0.058(5)	0.042(2)	0.004(3)	0.026(2)	0.005(3)
O2	0.073(3)	0.071(7)	0.038(4)	0.008(5)	0.016(2)	0.007(4)
N1	0.0492(12)	0.0505(12)	0.0321(13)	0.0078(9)	0.0096(9)	0.0143(9)
C1	0.0362(11)	0.0337(12)	0.0416(15)	-0.0036(10)	0.0085(10)	-0.0002(10)
C2	0.036(2)	0.031(2)	0.036(2)	0	0.0084(13)	0
C3	0.060(2)	0.0348(14)	0.066(2)	-0.0081(12)	-0.0044(13)	-0.0062(12)
C4	0.086(3)	0.033(2)	0.085(4)	0	-0.013(3)	0
C5	0.0380(12)	0.0439(13)	0.037(2)	-0.0035(10)	0.0057(10)	-0.0015(10)
C6	0.067(2)	0.067(2)	0.043(2)	-0.0139(14)	0.0008(13)	0.010(2)
C7	0.0487(14)	0.0459(14)	0.0268(14)	0.0034(10)	0.0082(10)	0.0096(11)
C8	0.0495(14)	0.055(2)	0.032(2)	0.0026(11)	0.0123(11)	0.0063(12)
C9	0.065(2)	0.0444(14)	0.038(2)	0.0071(11)	0.0168(12)	0.0011(12)
C10	0.065(2)	0.050(2)	0.043(2)	0.0122(12)	0.0061(12)	0.0176(13)
C11	0.050(2)	0.063(2)	0.058(2)	0.0135(14)	-0.0028(13)	0.0061(13)
C12	0.0518(15)	0.050(2)	0.044(2)	0.0102(12)	0.0010(11)	-0.0007(12)
C13	0.051(2)	0.083(2)	0.048(2)	0.014(2)	0.0132(13)	-0.0019(15)
C14	0.074(4)	0.092(7)	0.081(6)	-0.026(4)	0.015(4)	-0.015(4)
C15	0.062(2)	0.116(3)	0.086(3)	-0.016(2)	0.030(2)	-0.011(2)
C16	0.059(2)	0.070(2)	0.084(3)	0.035(2)	-0.006(2)	-0.005(2)
C17	0.068(7)	0.061(6)	0.205(12)	0.020(6)	0.030(8)	-0.016(5)
C18	0.076(6)	0.119(7)	0.126(11)	0.046(7)	0.048(6)	0.002(5)
C19	0.083(5)	0.072(4)	0.056(5)	0.002(3)	0.020(3)	0.019(4)
C20	0.071(5)	0.079(6)	0.044(4)	0.001(4)	0.027(3)	0.006(4)
C21	0.081(4)	0.074(6)	0.035(4)	-0.001(4)	0.023(3)	-0.002(4)
C22	0.067(4)	0.070(6)	0.060(5)	0.023(4)	0.020(3)	-0.007(4)
Li1	0.065(3)	0.086(3)	0.037(3)	0.014(2)	0.016(2)	0.017(3)