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Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Compounds **3**, **4**, **6** and **9**.

	3	**4**	**6**	**9**
formula	$C_{40}H_{56}F_3N_4NbO_4S{\cdot}C_4H_8O$	$C_{37}H_{51}N_4Nb$	$C_{47}H_{69}N_6Nb$	$C_{50}H_{74}LiN_4NbO_4{\cdot}0.5C_4H_8O$
cryst habit	prism	prism	prism	prism
cryst colour	black	black	orange	yellow-green
fw	923.0	644.7	811.0	931.1
cryst syst	triclinic	monoclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2_1/n$	$P2_1/c$	$C2/c$
cell parameters at 295 K [a]				
a, Å	11.820(3)	12.275(9)	19.423(3)	43.080(7)
b, Å	19.171(4)	12.728(5)	11.091(2)	11.988(7)
c, Å	10.994(3)	21.465(4)	20.805(3)	20.474(7)
α, deg	105.27(3)	90	90	90
β, deg	109.36(3)	96.40(3)	90.29(2)	103.26(2)
γ, deg	87.88(2)	90	90	90
V, Å^3	2263.9(11)	3333(3)	4481.8(13)	10292(7)
Z	2	4	4	8
d_{calc}, Mg m^{-3}	1.354	1.285	1.203	1.202
cryst dimens, mm	0.39x050x0.68	0.20x0.32x0.48	0.27x0.34x0.35	0.26x0.32x0.54
linear abs coeff, cm^{-1}	3.56	3.74	2.92	2.67
diffractometer	Philips PW1100	Rigaku AFC6S	Siemens AED	Rigaku AFC6S
diffraction geometry	equatorial	equatorial	equatorial	equatorial
scan type	ω/2θ	ω/2θ	ω/2θ	ω/2θ
scan speed, deg/min	4-12	4	3-12	1-4
scan width, deg	b	b	b	b
radiation	c	c	c	d

Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Compounds **3**, **4**, **6** and **9**. (cont.)

	3	**4**	**6**	**9**
data collcn range of 2θ, deg	6-60	6-50	6-50	6-50
reflcns measd	±h,±k,l	h,k,±l	±h,k,l	h,k,±l
unique total data	13204	6212	7868	9073
criterion for obsn	$I > 3\sigma(I)$	$I > 2\sigma(I)$	$I > 2\sigma(I)$	$I > 2\sigma(I)$
unique obsd data (NO)	8428	3425	3593	4836
no. of params refined (NV)	530	372	481	553
overdetermn ratio (NO/NV)	15.9	9.2	7.5	8.8
transm factors	0.938-1.000	0.690-1.000	0.780-1.000	0.982-1.000
R	0.041	0.063	0.072	0.075
wR2	0.102	0.169	0.156	0.203
GOF	1.008	1.102	1.082	1.177
largest shift/esd, final cycle	0.3	0.02	0.001	0.1
largest peak, e/Å^3	0.50	0.76	0.48	0.68

[a] unit cell parameters were obtained by least-squares analysis of the setting angles of 25 carefully centered reflections chosen from diverse regions of reciprocal space

[b] $(\theta - 0.6) - [\theta + (0.6 + \Delta\theta)]$; $\Delta\theta = [(\lambda\alpha_2 - \lambda\alpha_1)/\theta]\tan\theta$

[c] graphite monochromated Mo Kα (λ = 0.71069 Å)

$R = \Sigma|\Delta F|/\Sigma|F_o|$

$wR2 = [\Sigma(w\Delta F^2)^2/\Sigma(wF_o^2)^2]^{1/2}$

$GOF = [\Sigma w|\Delta F|^2/(NO-NV)]^{1/2}$

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Table S2. Fractional atomic coordinates ($x10^4$) for complex **3**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Nb1	2216.7(2)	2559.3(1)	2348.7(2)	C19	2192(2)	1572(1)	3401(3)
S1	845.8(9)	1325.8(5)	-746.4(8)	C20	1177(2)	1525(2)	3912(3)
F1	188(2)	2125(1)	-2428(2)	C21	146(3)	4503(2)	3249(4)
F2	-1159(2)	1937(2)	-1634(3)	C22	-20(5)	5116(2)	2592(5)
F3	-732(2)	1082(1)	-3090(2)	C23	-1688(3)	3703(2)	1624(4)
O1	1249(2)	2000(1)	354(2)	C24	-2248(3)	2958(3)	786(4)
O2	181(4)	823(2)	-469(3)	C25	3255(3)	4244(2)	2(4)
O3	1766(3)	1076(2)	-1278(3)	C26	3174(4)	4906(2)	1069(5)
O4	2886(2)	3520(1)	4224(2)	C27	3017(3)	2879(2)	-1004(3)
N1	724(2)	2633(1)	3037(2)	C28	4148(4)	2815(3)	-1366(4)
N2	1520(2)	3418(1)	1500(2)	C29	5498(3)	2752(2)	5440(3)
N3	3835(2)	2918(1)	2155(2)	C30	6723(4)	3160(3)	6091(4)
N4	3180(2)	2045(1)	4168(2)	C31	6099(3)	1789(2)	3691(4)
C1	607(2)	2245(2)	3933(3)	C32	6278(4)	1220(3)	4470(5)
C2	-140(3)	2582(2)	4595(3)	C33	1683(3)	1413(2)	5341(3)
C3	-538(3)	3193(2)	4100(3)	C34	2325(4)	721(2)	5408(4)
C4	-36(2)	3210(2)	3156(3)	C35	252(3)	904(2)	2919(3)
C5	-307(2)	3730(2)	2295(3)	C36	-802(4)	776(2)	3343(4)
C6	288(2)	3567(2)	1233(3)	C37	-287(4)	1644(2)	-2039(3)
C7	-167(3)	3694(2)	2(3)	C41	3469(3)	4188(2)	4235(3)
C8	777(3)	3652(2)	-534(3)	C42	3554(5)	4717(2)	5546(4)
C9	1794(2)	3501(2)	378(3)	C43	3344(4)	4305(2)	6399(4)
C10	3024(2)	3502(2)	249(3)	C44	2666(3)	3613(2)	5505(3)
C11	3995(2)	3401(2)	1463(3)	C1S	5645(16)	996(8)	77(12)
C12	5190(3)	3618(2)	1889(3)	C2S	6765(15)	635(10)	-5(17)
C13	5822(2)	3260(2)	2887(3)	C3S	6839(14)	730(10)	-1260(23)
C14	4998(2)	2844(2)	3034(3)	C4SA	5764(23)	371(14)	-2159(17)
C15	5154(2)	2347(2)	3934(3)	C5SA	5043(20)	372(19)	-1234(26)
C16	3945(2)	1946(2)	3442(3)	C4SB	5788(20)	1048(12)	-1903(18)
C17	3422(3)	1450(2)	2184(3)	C5SB	4932(15)	888(16)	-1201(24)
C18	2325(3)	1187(2)	2179(3)				

The site occupation factor for the A and B positions of the disordered C4S and C5S carbon atoms is 0.5.

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Table S3. Fractional atomic coordinates ($x10^4$) for complex **4**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Nb1	1940.9(6)	1653.2(5)	2477.5(3)	C21A	-1365(19)	1846(17)	1075(11)
N1	1338(5)	1085(5)	1573(3)	C22A	-536(18)	2742(19)	1016(12)
N2	329(5)	1199(5)	2682(3)	C21B	-874(27)	2133(19)	1127(13)
N3	2361(5)	1047(6)	3403(3)	C22B	-1615(32)	3027(20)	1121(18)
N4	3656(5)	1045(5)	2273(3)	C23A	-1749(20)	625(18)	1408(12)
C1	2022(7)	663(7)	1155(4)	C24A	-1709(18)	-390(17)	1798(11)
C2	1464(8)	-60(8)	772(4)	C23B	-1675(17)	213(18)	1610(9)
C3	367(7)	-43(8)	921(4)	C24B	-1408(18)	-630(16)	2118(10)
C4	294(7)	648(8)	1396(4)	C25	594(12)	1659(14)	4450(7)
C5	-715(7)	1175(9)	1583(5)	C26A	1190(24)	2656(18)	4294(15)
C6	-530(6)	1567(7)	2235(4)	C26B	1556(20)	2424(21)	4605(15)
C7	-1239(8)	2143(9)	2544(6)	C27A	-275(22)	434(24)	4196(11)
C8	-870(8)	2117(8)	3181(5)	C28A	-470(22)	-473(21)	3717(11)
C9	52(7)	1513(8)	3261(4)	C27B	-134(16)	9(14)	3965(12)
C10	566(8)	1008(10)	3848(5)	C28B	-1336(18)	-131(23)	3964(13)
C11	1675(7)	587(8)	3800(4)	C29	4739(8)	2169(9)	3856(5)
C12	2263(8)	-96(8)	4193(4)	C30	5254(13)	1762(13)	4494(6)
C13	3369(8)	-38(8)	4077(4)	C31	5319(8)	482(9)	3282(5)
C14	3421(7)	677(6)	3616(3)	C32	6264(8)	1065(12)	3011(7)
C15	4365(7)	1241(7)	3378(4)	C33	3014(8)	2046(8)	618(4)
C16	3896(5)	1705(7)	2771(3)	C34	2871(9)	1653(9)	-54(4)
C17	3675(7)	2754(7)	2587(4)	C35	4015(7)	349(8)	1036(4)
C18	3320(7)	2719(6)	1951(4)	C36	5161(9)	831(10)	1019(6)
C19	3360(6)	1672(7)	1763(3)	C37	1375(8)	3248(7)	2570(5)
C20	3108(7)	1177(7)	1132(4)				

The site occupation factor for the A and B positions of the disordered C21, C22, C23, C24, C26 carbon atoms is 0.5.

Table S4. Fractional atomic coordinates ($x10^4$) for complex **6**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Nb1	2324.1(4)	1295.3(8)	1483.8(4)	C24	4541(9)	-1570(20)	1413(8)
N1	2394(4)	-455(7)	2050(4)	C25	4321(6)	3374(13)	312(6)
N2	3421(4)	1046(7)	1412(3)	C26	4278(8)	4596(16)	628(8)
N3	2464(4)	2427(7)	596(4)	C27	3899(6)	1307(13)	49(5)
N4	1177(4)	743(8)	1111(4)	C28	3753(9)	1325(19)	-654(8)
N5	2636(4)	2866(8)	2071(4)	C29	717(5)	3754(14)	461(7)
N6	2469(5)	-951(8)	353(4)	C30A	-24(9)	3746(32)	722(14)
C1	1804(6)	-1050(10)	2282(5)	C30B	-29(9)	3230(27)	493(14)
C2	2015(8)	-1906(12)	2722(7)	C31A	1006(11)	1599(15)	-104(7)
C3	2711(8)	-1864(12)	2755(7)	C32A	963(12)	2042(22)	-806(8)
C4	2956(6)	-975(9)	2353(5)	C31B	760(14)	1947(30)	-110(13)
C5	3683(6)	-684(11)	2191(5)	C32B	1257(18)	974(32)	-355(18)
C6	3797(5)	579(11)	1945(5)	C33	575(7)	-768(12)	2557(7)
C7	4368(5)	1281(14)	2045(5)	C34	-131(8)	-433(15)	2328(8)
C8	4410(6)	2114(13)	1549(6)	C35	907(6)	-1614(10)	1452(6)
C9	3835(5)	1952(11)	1160(5)	C36	819(8)	-2929(13)	1647(8)
C10	3754(6)	2429(11)	471(5)	C37	2663(6)	1682(10)	3125(5)
C11	3051(5)	2884(10)	324(5)	C38	2591(5)	1956(10)	2417(4)
C12	2877(6)	3713(12)	-138(4)	C39	2754(6)	4162(10)	2224(5)
C13	2159(6)	3774(11)	-172(5)	C40	2631(7)	4884(11)	1605(6)
C14	1916(5)	2980(9)	285(4)	C41	3495(7)	4291(13)	2466(7)
C15	1203(5)	2576(9)	403(5)	C42	2242(8)	4559(10)	2755(6)
C16	1206(5)	1955(11)	1057(5)	C43	2414(5)	-191(10)	719(5)
C17	1258(5)	2500(10)	1659(5)	C44	2556(8)	-1952(12)	-107(6)
C18	1254(5)	1553(9)	2109(5)	C45A	1933(16)	-2007(29)	-541(15)
C19	1180(5)	505(10)	1756(6)	C46A	3246(21)	-1704(38)	-511(20)
C20	1118(6)	-757(10)	2011(5)	C47A	2616(19)	-3089(33)	348(17)
C21	4151(6)	-998(13)	2782(5)	C46B	3273(17)	-2330(31)	-170(16)
C22	4036(7)	-276(14)	3395(6)	C45B	2305(19)	-1359(36)	-761(17)
C23	3862(8)	-1575(14)	1632(7)	C47B	2066(22)	-2973(38)	170(19)

The site occupation factor is 0.7 for C31B, C32B; 0.5 for C30A, C30B, C45A, C45B, C46A, C46B, C47A, C47B; 0.3 for C31A, C32A.

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Table S5. Fractional atomic coordinates ($x10^4$) for complex **9**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Nb1	3765.7(2)	2033.2(7)	5261.2(4)	C27	2799(4)	3206(18)	6116(12)
Li1	3425(4)	-760(15)	4996(10)	C28	3555(5)	5029(12)	6616(7)
O1	3626(2)	666(5)	5217(3)	C29	3891(6)	5051(17)	6545(10)
O2	3758(2)	-1796(6)	4922(5)	C30	3485(2)	2051(10)	4194(4)
O3	3142(2)	-866(7)	5606(5)	C31	3618(3)	1197(10)	3788(5)
O4	3119(2)	-1061(8)	4142(4)	C32	3275(3)	3447(11)	3223(6)
N1	4252(2)	1720(6)	5721(4)	C33	2946(3)	2949(14)	3093(6)
N2	3708(2)	2302(7)	6269(4)	C34	4331(3)	5737(10)	3355(7)
N3	3444(2)	3451(7)	5116(4)	C35	4786(2)	2042(11)	4490(6)
N4	4032(2)	3065(7)	4522(3)	C36	4580(3)	1321(13)	3958(6)
C1	4506(2)	1651(8)	5402(5)	C37	4852(3)	3314(10)	5492(6)
C2	4694(3)	758(10)	5650(6)	C38	4708(4)	3926(12)	5988(8)
C3	4564(3)	275(9)	6155(6)	C39A	3797(7)	-2912(26)	5288(16)
C4	4297(2)	867(8)	6198(5)	C39B	3780(7)	-2963(29)	4931(16)
C5	4109(3)	674(9)	6724(5)	C40	4126(5)	-3251(17)	5132(13)
C6	3858(3)	1557(10)	6769(5)	C41A	4302(8)	-2325(29)	5088(19)
C7	3746(3)	1759(12)	7334(5)	C41B	4255(10)	-2251(37)	4697(23)
C8	3542(3)	2645(13)	7209(6)	C42	4048(3)	-1368(13)	4733(9)
C9	3520(2)	2982(10)	6557(5)	C43	2962(5)	-1832(15)	5722(12)
C10	3346(3)	4032(9)	6248(6)	C44A	2812(15)	-1516(51)	6261(30)
C11	3312(2)	4166(9)	5512(6)	C45A	2840(10)	-385(37)	6384(22)
C12	3148(3)	5013(9)	5129(7)	C44B	2653(10)	-1331(36)	5895(22)
C13	3166(3)	4811(10)	4465(7)	C45B	2724(11)	-36(36)	6051(23)
C14	3348(2)	3877(9)	4465(5)	C46	3041(5)	154(13)	5889(10)
C15	3473(2)	3225(8)	3953(5)	C47	3164(4)	-1779(14)	3591(8)
C16	3819(2)	3612(8)	4035(5)	C48A	2877(7)	-1758(25)	3074(14)
C17	3908(2)	4446(9)	3652(5)	C49A	2691(7)	-751(26)	3273(15)
C18	4225(3)	4772(9)	3760(5)	C48B	2933(9)	-1227(33)	2933(18)
C19	4434(3)	4181(10)	4235(6)	C49B	2775(8)	-292(28)	3090(16)
C20	4347(2)	3302(8)	4587(5)	C50	2832(3)	-446(13)	3943(8)
C21	4607(2)	2573(9)	4990(5)	C61	4712(7)	2927(22)	2504(18)
C22	3952(4)	-524(11)	6600(7)	C62	4802(9)	2922(24)	1941(17)
C23	3807(4)	-1036(15)	7104(9)	C63	4919(8)	3685(28)	2993(16)
C24	4354(3)	633(12)	7422(6)	C64	4797(11)	4014(26)	2275(17)
C25	4546(4)	1680(13)	7590(7)	C65	5000(-)	2236(39)	2500(-)
C26	3023(5)	4117(15)	6422(8)				

The site occupation factor is 0.5 for C39A, C39B, C41A, C41B, C44A, C44B, C45A, C45B, C48A, C48B, C49A, C49B, C61, C62, C64, C64.

Table S6. Fractional atomic coordinates ($x10^4$) for hydrogen atoms for complex 3.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	-330	2448	5440	H291	5434	2366	6031
H3	-1132	3511	4439	H292	4820	2957	5428
H7	-981	3813	-361	H301	6847	3382	7023
H8	686	3677	-1400	H302	6774	3515	5652
H12	5464	3929	1429	H303	7336	2815	6029
H13	6689	3314	3434	H311	6816	2122	4034
H17	3735	1319	1424	H312	5798	1569	2833
H18	1638	826	1413	H321	6882	898	4248
H211	990	4481	3804	H322	5544	945	4207
H212	-218	4599	4040	H323	6555	1447	5401
H221	297	5564	3260	H331	991	1456	5605
H222	-847	5150	2124	H332	2259	1834	6017
H223	421	5029	1965	H341	2629	687	6322
H231	-1859	4135	1239	H342	3005	715	5095
H232	-2036	3842	2437	H343	1794	309	4865
H241	-3105	3002	389	H351	-27	1005	2040
H242	-2093	2637	1312	H352	679	469	2800
H243	-1919	2805	63	H361	-1324	385	2674
H251	4062	4213	25	H362	-1236	1206	3445
H252	2556	4297	-782	H363	-509	648	4177
H261	3498	5323	967	H411	2969	4297	3420
H262	3897	4913	2025	H412	4166	4009	4027
H263	2577	4954	963	H421	4348	4965	5958
H271	2744	2394	-781	H422	2962	5075	5412
H272	2415	2949	-1782	H431	2893	4577	6936
H281	4053	2420	-2139	H432	4111	4201	7000
H282	4809	2734	-625	H441	1751	3682	5214
H283	4320	3259	-1539	H442	2993	3202	5821

Table S7. Fractional atomic coordinates ($x10^4$) for hydrogen atoms for complex **4**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	1792	-396	511	H322	6537	1611	3295
H3	-119	-445	756	H323	5995	1369	2613
H7	-1869	2373	2343	H331	2275	2529	661
H8	-1101	2441	3515	H332	3589	2330	751
H12	3920	-444	4311	H341	2793	2187	-311
H13	1961	-502	4536	H342	2169	1036	-114
H17	3824	3223	2892	H343	3454	1164	-103
H18	3119	3169	1768	H351	4145	-153	1528
H291	5234	2564	3613	H352	3771	42	751
H292	4078	2326	3872	H361	5645	250	964
H301	5506	2281	4801	H362	5300	1251	1390
H302	5859	1283	4389	H363	5219	1294	629
H303	4659	1494	4727	H371	1811	3448	3026
H311	5450	188	3651	H372	675	3259	2611
H312	4989	-110	2937	H373	1513	3521	2276
H321	6840	578	2955				

Table S8. Fractional atomic coordinates ($x10^4$) for hydrogen atoms for complex 6.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	1612	-2230	2873	H281	3869	573	-851
H3	3112	-2383	2962	H282	4013	1964	-861
H7	4715	1141	2452	H283	3267	1486	-731
H8	4703	2697	1564	H331	739	-207	2910
H12	3171	4060	-416	H332	441	-1474	2671
H13	1765	4157	-435	H341	-473	-628	2704
H17	1382	3417	1740	H342	-419	-1036	2052
H18	1170	1601	2560	H343	-55	533	2086
H211	4541	-623	2611	H351	1256	-1603	1222
H212	4038	-2130	2925	H352	496	-1169	1272
H221	4338	-579	3729	H361	695	-3409	1278
H222	3561	-417	3541	H362	473	-3004	1969
H223	4104	546	3327	H363	1252	-3239	1819
H231	3583	-1531	1380	H371	2719	1098	3204
H232	3981	-2640	1702	H372	2270	1972	3346
H241	4592	-2169	1074	H373	3106	2154	3287
H242	4855	-1773	1755	H401	2526	5745	1566
H243	4661	-796	1241	H402	2046	4933	1501
H251	4924	2979	394	H403	2986	4776	1232
H252	4253	3605	-91	H411	3597	5088	2532
H261	4700	5299	486	H412	3821	3925	1956
H262	4318	4799	1145	H413	3544	3954	2905
H263	3869	4983	536	H421	2361	5359	2864
H271	3706	525	95	H422	2427	4170	3156
H272	4417	899	73	H423	1818	4301	2518

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Table S9. Fractional atomic coordinates ($x10^4$) for hydrogen atoms for complex **9**.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	4870	508	5508	H282	3556	4982	7085
H3	4652	-335	6419	H291	3968	5708	6792
H7	3798	1369	7738	H292	3869	5142	6084
H8	3439	2971	7513	H293	3975	4405	6730
H12	3039	5598	5279	H30	3268	1815	4196
H13	3066	5236	4087	H311	3616	473	3987
H17	3752	4792	3323	H312	3836	1393	3788
H19	4648	4385	4324	H313	3494	1190	3339
H221	3791	-500	6183	H321	3390	3111	2909
H222	4117	-1040	6523	H322	3264	4239	3139
H231	3729	-1761	6956	H331	2835	3110	2636
H232	3636	-573	7169	H332	2830	3299	3392
H233	3966	-1099	7518	H333	2956	2170	3166
H241	4241	484	7766	H351	4881	2623	4278
H242	4500	14	7415	H352	4957	1578	4744
H251	4690	1578	8021	H361	4709	1027	3668
H252	4404	2281	7612	H362	4412	1772	3691
H253	4662	1814	7256	H363	4490	723	4158
H261	3046	4074	6896	H371	5022	2825	5743
H262	2922	4814	6259	H372	4951	3836	5246
H271	2594	3284	6239	H381	4866	4361	6282
H272	2883	2481	6259	H382	4614	3404	6245
H273	2755	3230	5627	H383	4542	4413	5746
H281	3450	5715	6441				

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Table S10. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ (x10^4 Å^2) for complex **3**. $U_{(i,j)}$ are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2}+...+2U_{12}hka^*b^*+...)]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	228(1)	287(1)	220(1)	78(1)	82(1)	25(1)
S1	628(6)	462(5)	320(4)	8(4)	30(4)	-42(4)
F1	1131(21)	887(18)	474(13)	260(13)	140(14)	-108(15)
F2	584(15)	1374(26)	809(18)	138(17)	181(14)	229(16)
F3	1024(20)	925(19)	417(13)	-70(12)	-125(13)	-184(15)
O1	434(12)	404(12)	265(10)	69(9)	74(9)	-16(9)
O2	1401(30)	839(22)	557(18)	240(16)	-109(18)	-601(21)
O3	785(21)	928(23)	781(21)	-215(18)	208(17)	282(18)
O4	367(10)	335(10)	241(9)	68(8)	108(8)	-57(8)
N1	252(11)	308(12)	262(11)	62(9)	94(9)	3(9)
N2	249(11)	341(12)	258(11)	120(9)	80(9)	46(9)
N3	214(10)	396(13)	270(11)	112(10)	88(9)	20(9)
N4	301(12)	356(13)	289(12)	135(10)	86(10)	47(10)
C1	331(14)	362(15)	316(14)	105(12)	150(12)	-24(12)
C2	430(17)	488(18)	469(18)	166(15)	289(15)	48(14)
C3	421(17)	527(19)	502(19)	163(16)	302(15)	102(15)
C4	275(13)	373(15)	391(16)	108(12)	172(12)	58(12)
C5	298(14)	410(16)	381(15)	148(13)	148(12)	126(12)
C6	262(13)	369(16)	366(15)	162(12)	100(12)	87(12)
C7	323(15)	617(21)	425(18)	260(16)	83(13)	122(14)
C8	411(17)	613(21)	339(16)	259(15)	118(13)	95(15)
C9	313(14)	412(16)	312(14)	181(12)	110(12)	38(12)
C10	343(15)	480(18)	306(15)	171(13)	135(12)	11(13)
C11	290(14)	410(16)	287(14)	111(12)	131(11)	6(12)
C12	333(15)	580(20)	403(17)	157(15)	155(13)	-48(14)
C13	244(14)	606(21)	443(18)	162(16)	87(13)	-17(14)
C14	229(13)	516(18)	340(15)	139(13)	102(11)	39(12)
C15	247(14)	507(18)	408(16)	179(14)	98(12)	85(13)
C16	304(14)	376(16)	326(14)	181(12)	92(12)	100(12)
C17	391(16)	375(16)	393(16)	149(13)	184(13)	136(13)
C18	445(16)	307(15)	325(15)	108(12)	150(13)	66(12)
C19	347(14)	286(14)	311(14)	137(11)	112(12)	43(11)
C20	368(15)	318(14)	331(15)	102(12)	151(12)	-36(12)
C21	684(23)	408(18)	462(19)	140(15)	221(17)	109(16)
C22	1393(45)	445(23)	868(34)	261(23)	380(32)	121(26)
C23	323(16)	771(26)	540(21)	214(19)	194(15)	218(17)
C24	355(19)	1203(39)	611(25)	47(25)	170(18)	-40(22)
C25	489(19)	641(23)	552(21)	347(19)	168(17)	-34(17)
C26	759(28)	498(23)	868(31)	308(22)	139(24)	-18(20)
C27	384(17)	759(24)	318(16)	83(16)	163(14)	41(16)
C28	531(23)	1138(37)	502(22)	50(23)	264(19)	80(23)
C29	314(16)	728(24)	362(17)	160(16)	13(13)	-4(15)
C30	502(23)	1126(38)	564(25)	176(25)	13(19)	-151(24)
C31	357(17)	625(23)	725(25)	253(20)	157(17)	183(16)
C32	615(26)	879(33)	1146(40)	557(31)	239(26)	353(24)
C33	567(20)	507(19)	367(16)	225(15)	187(15)	55(16)
C34	916(31)	732(28)	664(26)	451(23)	281(24)	202(24)
C35	500(19)	433(18)	446(18)	71(15)	165(15)	-120(15)
C36	651(26)	694(27)	790(29)	26(22)	307(22)	-317(21)
C37	579(23)	774(27)	316(18)	55(18)	86(16)	-28(20)

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Table S10. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex 3. (cont.)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C41	494(18)	353(16)	365(16)	47(13)	154(14)	-121(14)
C42	1281(40)	557(24)	511(23)	-112(19)	393(25)	-454(25)
C43	1016(33)	638(25)	402(20)	-57(18)	338(21)	-283(23)
C44	455(17)	440(17)	237(13)	53(12)	145(12)	-39(14)
C1S	3064(149)	2653(133)	1299(83)	-235(86)	485(97)	233(117)
C2S	2601(159)	3435(171)	2616(162)	1568(144)	254(130)	970(133)
C3S	1923(122)	3126(154)	3893(194)	985(159)	1168(140)	186(116)

Atom	U_{iso}	Atom	U_{iso}
C4SA	2157(91)	C4SB	1778(70)
C5SA	3092(143)	C5SB	2184(96)

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Table S11. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex **4**. $U_{(i,j)}$ are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2}+...+2U_{12}hka^*b^*+...)]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	349(4)	302(3)	402(4)	-1(4)	121(3)	-9(4)
N1	444(38)	491(41)	214(32)	-30(30)	93(28)	33(32)
N2	396(37)	433(38)	470(40)	-7(33)	166(31)	-38(31)
N3	391(37)	481(42)	389(39)	-23(33)	131(30)	-52(32)
N4	342(34)	386(37)	389(38)	-40(32)	144(28)	-75(29)
C1	482(48)	397(48)	428(48)	-49(39)	118(39)	-27(39)
C2	662(60)	590(61)	539(56)	-120(49)	222(46)	-25(51)
C3	520(54)	677(64)	588(62)	-62(53)	74(44)	-200(50)
C4	419(49)	606(60)	431(51)	-26(45)	42(39)	-98(43)
C5	321(47)	922(78)	640(64)	79(58)	22(43)	25(48)
C6	361(41)	576(54)	512(49)	81(48)	131(36)	64(45)
C7	452(54)	730(68)	935(84)	117(63)	293(55)	155(49)
C8	589(59)	626(61)	772(74)	-16(55)	371(54)	98(50)
C9	480(48)	617(60)	549(52)	-10(49)	269(41)	5(47)
C10	502(57)	1154(94)	606(64)	-46(65)	286(50)	-24(60)
C11	540(55)	551(59)	463(53)	-21(46)	140(43)	-121(46)
C12	744(65)	553(60)	410(52)	27(46)	165(46)	-73(51)
C13	655(60)	512(55)	469(54)	55(44)	57(44)	61(48)
C14	524(50)	423(48)	219(39)	-35(35)	82(35)	-17(39)
C15	395(48)	547(55)	589(58)	-58(46)	85(42)	-42(40)
C16	334(37)	434(43)	290(36)	15(39)	120(29)	-53(38)
C17	472(49)	408(50)	526(55)	-73(41)	110(39)	-178(41)
C18	510(49)	365(47)	532(54)	51(39)	211(41)	-69(39)
C19	313(36)	491(46)	390(41)	-1(44)	132(31)	-63(40)
C20	390(43)	459(46)	392(47)	24(38)	127(36)	4(37)
C25	1282(124)	2070(190)	1002(107)	-308(120)	393(94)	873(133)
C29	697(66)	685(67)	595(65)	-47(54)	-38(50)	-271(56)
C30	1261(114)	1498(140)	679(80)	-55(93)	-366(76)	-319(108)
C31	400(52)	831(77)	914(82)	205(66)	108(53)	108(51)
C32	396(58)	1388(121)	1309(116)	-70(99)	251(65)	-75(68)
C33	659(59)	670(61)	343(48)	133(42)	115(42)	-39(47)
C34	897(73)	828(74)	490(54)	119(60)	157(50)	100(68)
C35	508(54)	638(66)	582(59)	-87(50)	136(44)	22(46)
C36	534(64)	1023(97)	1203(105)	-131(81)	362(66)	53(64)
C37	632(56)	330(46)	811(65)	-67(48)	224(49)	55(45)

Atom	U(iso)	Atom	U(iso)
C21A	1076(102)	C21B	983(81)
C22A	803(66)	C22B	1506(132)
C23A	757(68)	C23B	572(48)
C24A	696(58)	C24B	669(56)
C26A	970(85)	C26B	998(88)
C27A	1390(132)	C27B	634(52)
C28A	870(72)	C28B	1038(84)

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Table S12. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex **6**. $U_{(i,j)}$ are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2}+...+2U_{12}hka^*b^*+...)]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	430(4)	435(4)	382(4)	5(5)	11(3)	27(6)
N1	610(55)	500(53)	434(48)	87(41)	-8(42)	58(45)
N2	484(46)	547(58)	404(44)	45(39)	-44(36)	-30(41)
N3	428(47)	510(50)	429(46)	53(39)	-13(38)	-66(41)
N4	369(49)	370(50)	745(66)	45(47)	-12(44)	12(40)
N5	638(60)	491(57)	426(51)	-57(44)	48(42)	22(45)
N6	855(66)	514(59)	425(48)	-84(44)	-110(45)	99(47)
C1	743(76)	624(82)	625(66)	188(60)	-4(57)	0(63)
C2	1197(123)	669(84)	939(102)	421(79)	-28(88)	-204(85)
C3	964(107)	770(91)	941(100)	224(80)	-226(84)	246(84)
C4	701(76)	474(71)	644(69)	77(55)	-59(58)	169(55)
C5	657(73)	813(83)	472(61)	-2(59)	-101(53)	292(64)
C6	562(72)	785(84)	534(65)	-60(61)	-67(55)	190(64)
C7	553(67)	1137(99)	748(77)	97(89)	-270(57)	-34(84)
C8	645(82)	1121(112)	753(86)	57(83)	-45(67)	-184(78)
C9	543(69)	820(81)	559(67)	-78(63)	16(56)	5(64)
C10	627(72)	876(86)	495(66)	25(61)	100(54)	-230(66)
C11	539(66)	637(71)	440(58)	-10(54)	151(49)	-64(57)
C12	917(85)	738(74)	418(56)	69(68)	33(54)	-276(82)
C13	842(80)	599(68)	568(62)	172(65)	-97(55)	17(76)
C14	694(73)	466(60)	426(56)	127(51)	-35(50)	23(55)
C15	580(69)	693(74)	559(66)	60(57)	-109(54)	16(60)
C16	376(60)	688(81)	502(66)	106(61)	6(49)	93(57)
C17	391(58)	640(72)	634(70)	-131(61)	-20(51)	108(54)
C18	488(58)	537(75)	576(62)	77(55)	142(48)	136(49)
C19	389(61)	511(72)	774(86)	37(62)	88(56)	15(51)
C20	743(80)	559(69)	753(79)	198(62)	82(64)	-47(61)
C21	804(82)	1179(119)	649(74)	114(77)	-146(62)	142(81)
C22	1103(108)	1431(131)	619(78)	-76(86)	-466(75)	433(98)
C23	989(104)	1253(136)	948(100)	-119(91)	-79(81)	638(99)
C24	1378(149)	2154(220)	1036(120)	-219(130)	-87(104)	773(152)
C25	698(81)	1133(124)	813(89)	135(80)	112(65)	-324(78)
C26	978(114)	1295(145)	1386(144)	124(115)	200(100)	-619(107)
C27	985(89)	1052(96)	520(64)	-116(82)	199(60)	-134(91)
C28	1510(150)	1903(185)	1063(121)	-175(142)	377(104)	-67(150)
C29	724(81)	1237(115)	1285(111)	678(102)	121(76)	481(91)
C33	918(100)	800(92)	1166(110)	187(81)	420(86)	-216(79)
C34	780(102)	1163(128)	1804(162)	-11(115)	556(104)	-329(97)
C35	731(79)	492(77)	1090(99)	52(64)	-80(70)	-197(59)
C36	1123(121)	767(101)	1569(146)	36(98)	64(102)	-353(90)
C37	1058(94)	776(88)	403(59)	49(55)	-145(58)	138(69)
C38	550(65)	662(72)	388(57)	-19(55)	31(47)	105(56)
C39	784(80)	584(69)	529(65)	-181(56)	85(58)	-222(60)
C40	1300(119)	575(77)	695(85)	94(64)	88(76)	-82(74)
C41	907(98)	1008(104)	1070(106)	-121(87)	-165(81)	-341(84)
C42	1480(130)	514(75)	734(84)	-243(68)	98(84)	-133(80)
C43	605(69)	549(68)	351(56)	0(53)	-53(49)	89(55)
C44	1343(131)	772(91)	634(82)	-161(75)	-123(82)	-146(93)

Table S12. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex **6**. (cont.)

Atom	U(iso)	Atom	U(iso)
C30A	1031(97)	C30B	904(92)
C31A	748(53)	C31B	567(107)
C32A	1249(77)	C32B	741(111)
C45A	1036(90)	C46B	1073(99)
C46A	1485(145)	C45B	1382(117)
C47A	1267(113)	C47B	1483(136)

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Table S13. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex **9**. $U_{(i,j)}$ are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2}+...+2U_{12}hka^*b^*+...)]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	347(4)	348(4)	340(4)	26(5)	33(3)	7(5)
LI1	523(113)	426(101)	752(130)	-37(90)	127(94)	6(84)
O1	606(46)	397(38)	410(39)	6(31)	46(34)	-36(33)
O2	397(41)	431(49)	1300(72)	-195(44)	187(44)	108(34)
O3	879(68)	627(56)	1107(74)	-117(52)	549(58)	-167(49)
O4	554(54)	1068(72)	742(59)	230(53)	48(44)	-150(50)
N1	327(43)	441(50)	377(42)	-20(34)	26(34)	44(34)
N2	490(50)	475(55)	404(45)	5(37)	188(38)	53(39)
N3	386(47)	426(45)	421(47)	115(38)	92(38)	7(37)
N4	341(41)	403(44)	359(39)	12(38)	15(31)	6(38)
C1	375(56)	509(61)	472(59)	-19(47)	-10(46)	110(46)
C2	554(74)	569(72)	704(81)	80(62)	104(60)	183(58)
C3	712(82)	515(69)	572(70)	132(57)	84(60)	267(61)
C4	577(67)	374(56)	392(55)	28(45)	55(48)	70(49)
C5	629(72)	446(60)	364(56)	53(46)	11(49)	104(53)
C6	781(86)	692(77)	342(59)	54(53)	101(57)	-125(66)
C7	827(93)	1146(120)	400(63)	246(69)	224(62)	255(84)
C8	605(79)	1145(115)	525(69)	-8(70)	273(59)	249(77)
C9	543(62)	584(63)	511(60)	-27(62)	228(48)	15(62)
C10	658(80)	496(66)	650(75)	-18(56)	292(61)	161(57)
C11	450(64)	499(64)	628(71)	-19(56)	117(53)	74(52)
C12	673(82)	429(65)	845(91)	30(63)	170(69)	243(59)
C13	535(74)	614(79)	761(89)	236(67)	-8(64)	33(60)
C14	384(60)	476(63)	563(66)	103(52)	2(49)	26(50)
C15	220(46)	599(76)	514(59)	125(50)	56(41)	10(43)
C16	517(65)	410(58)	453(58)	63(48)	94(49)	-8(49)
C17	455(63)	647(72)	435(60)	189(53)	50(48)	-101(53)
C18	610(74)	521(66)	535(67)	145(54)	148(57)	-148(57)
C19	428(66)	689(78)	618(73)	74(62)	84(55)	-185(57)
C20	528(66)	460(62)	373(52)	-40(44)	74(46)	-80(47)
C21	342(54)	548(60)	457(57)	-28(48)	74(44)	-39(46)
C22	1043(114)	676(87)	740(91)	318(72)	127(80)	-121(79)
C23	1200(146)	1247(140)	1038(125)	384(112)	375(108)	-217(116)
C24	572(78)	948(99)	521(71)	-6(67)	0(57)	285(72)
C25	944(110)	1089(122)	578(78)	-222(77)	-71(72)	12(90)
C26	1173(143)	961(119)	1017(120)	294(98)	556(108)	594(108)
C27	721(112)	1449(180)	1898(207)	551(157)	606(125)	269(116)
C28	1427(160)	631(90)	668(93)	-114(73)	55(99)	-81(98)
C29	1967(248)	1215(159)	1097(153)	33(122)	-255(153)	-881(165)
C30	342(50)	574(59)	418(51)	43(58)	113(39)	-44(54)
C31	647(79)	627(74)	483(65)	-85(57)	89(57)	-69(62)
C32	581(76)	859(87)	499(67)	225(62)	46(55)	-46(65)
C33	494(72)	1305(122)	722(83)	240(93)	-295(60)	-85(88)
C34	685(85)	668(81)	880(94)	332(72)	157(70)	-157(67)
C35	481(63)	726(74)	676(71)	53(72)	228(53)	33(66)
C36	789(97)	989(106)	631(81)	-141(76)	219(71)	77(81)
C37	419(64)	789(87)	619(71)	-159(62)	0(54)	-138(57)
C38	824(105)	819(100)	944(109)	-278(86)	-5(83)	-99(81)

Table S13. Anisotropic and isotropic thermal parameters $U_{(i,j)}$ ($x10^4$ Å^2) for complex **9**. (cont.)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C40	1308(178)	1082(158)	2521(280)	344(160)	823(183)	637(134)
C42	633(93)	815(100)	1362(138)	-279(97)	430(92)	-105(77)
C43	1320(164)	1000(138)	2054(218)	-73(137)	994(162)	-368(118)
C46	1428(161)	757(105)	1520(159)	-157(104)	969(138)	75(104)
C47	873(107)	1247(139)	920(106)	597(101)	-31(83)	-294(95)
C50	536(85)	1094(119)	1074(119)	331(96)	-8(78)	-169(81)

Atom	U(iso)	Atom	U(iso)
C39A	797(77)	C39B	812(80)
C41A	890(97)	C41B	1235(142)
C44A	1681(203)	C44B	1205(131)
C45A	1155(129)	C45B	1210(135)
C48A	718(79)	C48B	985(108)
C49A	765(81)	C49B	870(92)
C61	1136(109)	C64	1981(228)
C62	1479(151)	C65	2668(237)
C63	1231(123)		

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Table S14. Bond distances (Å) and angles (°) for complex **3**.

Nb1	- O1	2.111(2)	C8	- C9	1.365(4)
Nb1	- O4	2.301(2)	C9	- C10	1.507(4)
Nb1	- N1	2.125(3)	C10	- C11	1.497(4)
Nb1	- N2	2.111(2)	C10	- C25	1.566(6)
Nb1	- N3	2.150(3)	C10	- C27	1.565(5)
Nb1	- N4	2.391(2)	C11	- C12	1.375(4)
Nb1	- C16	2.437(3)	C12	- C13	1.431(5)
Nb1	- C17	2.516(4)	C13	- C14	1.357(5)
Nb1	- C18	2.589(4)	C14	- C15	1.511(6)
Nb1	- C19	2.470(3)	C15	- C16	1.508(4)
S1	- O1	1.484(2)	C15	- C29	1.552(4)
S1	- O2	1.417(5)	C15	- C31	1.556(5)
S1	- O3	1.410(4)	C16	- C17	1.408(4)
S1	- C37	1.822(4)	C17	- C18	1.406(6)
F1	- C37	1.324(5)	C18	- C19	1.408(5)
F2	- C37	1.306(6)	C19	- C20	1.498(4)
F3	- C37	1.325(3)	C20	- C33	1.555(5)
O4	- C41	1.472(5)	C20	- C35	1.557(4)
O4	- C44	1.480(5)	C21	- C22	1.509(7)
N1	- C1	1.424(5)	C23	- C24	1.516(6)
N1	- C4	1.406(4)	C25	- C26	1.509(6)
N2	- C6	1.421(3)	C27	- C28	1.508(7)
N2	- C9	1.423(5)	C29	- C30	1.524(6)
N3	- C11	1.397(5)	C31	- C32	1.524(8)
N3	- C14	1.421(3)	C33	- C34	1.510(6)
N4	- C16	1.370(4)	C35	- C36	1.516(7)
N4	- C19	1.386(3)	C41	- C42	1.502(5)
C1	- C2	1.365(5)	C42	- C43	1.457(7)
C1	- C20	1.511(5)	C43	- C44	1.496(5)
C2	- C3	1.419(6)	C1S	- C2S	1.49(3)
C3	- C4	1.363(5)	C1S	- C5SA	1.58(3)
C4	- C5	1.505(6)	C1S	- C5SB	1.34(3)
C5	- C6	1.514(5)	C2S	- C3S	1.47(3)
C5	- C21	1.565(5)	C3S	- C4SA	1.39(3)
C5	- C23	1.549(4)	C3S	- C4SB	1.42(3)
C6	- C7	1.364(5)	C4SA	- C5SA	1.53(4)
C7	- C8	1.415(6)	C4SB	- C5SB	1.54(4)

C18	- Nb1 - C19	32.2(1)	C6	- C5 - C21	109.1(3)
C17	- Nb1 - C19	53.6(1)	N2	- C6 - C5	123.2(3)
C17	- Nb1 - C18	31.9(1)	C5	- C6 - C7	125.8(3)
C16	- Nb1 - C19	53.3(1)	N2	- C6 - C7	109.5(3)
C16	- Nb1 - C18	53.2(1)	C6	- C7 - C8	107.9(3)
C16	- Nb1 - C17	33.0(1)	C7	- C8 - C9	108.0(3)
N4	- Nb1 - C19	33.1(1)	N2	- C9 - C8	109.3(3)
N4	- Nb1 - C18	54.7(1)	C8	- C9 - C10	124.0(3)
N4	- Nb1 - C17	55.4(1)	N2	- C9 - C10	126.4(3)
N4	- Nb1 - C16	32.9(1)	C9	- C10 - C27	108.2(3)
N3	- Nb1 - C19	121.7(1)	C9	- C10 - C25	107.5(3)
N3	- Nb1 - C18	107.7(1)	C9	- C10 - C11	112.7(3)
N3	- Nb1 - C17	75.9(1)	C25	- C10 - C27	108.7(3)
N3	- Nb1 - C16	68.6(1)	C11	- C10 - C27	109.7(3)

Table S14. Bond distances (Å) and angles (°) for complex **3** (cont.)

N3	- Nb1 -	N4	96.4(1)	C11	- C10 -	C25	109.9(3)
N2	- Nb1 -	C19	156.3(1)	N3	- C11 -	C10	121.7(3)
N2	- Nb1 -	C18	150.3(1)	C10	- C11 -	C12	127.3(3)
N2	- Nb1 -	C17	146.0(1)	N3	- C11 -	C12	109.6(3)
N2	- Nb1 -	C16	149.4(1)	C11	- C12 -	C13	107.6(3)
N2	- Nb1 -	N4	154.1(1)	C12	- C13 -	C14	107.2(3)
N2	- Nb1 -	N3	81.8(1)	N3	- C14 -	C13	109.9(3)
N1	- Nb1 -	C19	69.9(1)	C13	- C14 -	C15	130.3(3)
N1	- Nb1 -	C18	91.8(1)	N3	- C14 -	C15	119.7(3)
N1	- Nb1 -	C17	122.1(1)	C14	- C15 -	C31	109.3(3)
N1	- Nb1 -	C16	117.5(1)	C14	- C15 -	C29	113.7(3)
N1	- Nb1 -	N4	85.0(1)	C14	- C15 -	C16	103.8(3)
N1	- Nb1 -	N3	157.1(1)	C29	- C15 -	C31	110.8(3)
N1	- Nb1 -	N2	87.0(1)	C16	- C15 -	C31	108.3(3)
O4	- Nb1 -	C19	100.1(1)	C16	- C15 -	C29	110.6(3)
O4	- Nb1 -	C18	128.6(1)	N4	- C16 -	C15	123.3(3)
O4	- Nb1 -	C17	119.1(1)	Nb1	- C16 -	C15	116.7(3)
O4	- Nb1 -	C16	86.1(1)	Nb1	- C16 -	N4	71.7(2)
O4	- Nb1 -	N4	74.0(1)	C15	- C16 -	C17	126.0(3)
O4	- Nb1 -	N3	78.7(1)	N4	- C16 -	C17	110.6(3)
O4	- Nb1 -	N2	80.3(1)	Nb1	- C16 -	C17	76.6(2)
O4	- Nb1 -	N1	79.7(1)	Nb1	- C17 -	C16	70.4(2)
O1	- Nb1 -	C19	98.2(1)	C16	- C17 -	C18	106.6(3)
O1	- Nb1 -	C18	72.5(1)	Nb1	- C17 -	C18	76.9(2)
O1	- Nb1 -	C17	81.7(1)	Nb1	- C18 -	C17	71.1(2)
O1	- Nb1 -	C16	114.6(1)	C17	- C18 -	C19	106.1(3)
O1	- Nb1 -	N4	127.2(1)	Nb1	- C18 -	C19	69.2(2)
O1	- Nb1 -	N3	101.6(1)	N4	- C19 -	C18	110.5(3)
O1	- Nb1 -	N2	78.1(1)	Nb1	- C19 -	C18	78.6(2)
O1	- Nb1 -	N1	95.5(1)	Nb1	- C19 -	N4	70.3(1)
O1	- Nb1 -	O4	158.1(1)	C18	- C19 -	C20	129.1(3)
O3	- S1 -	C37	105.9(2)	N4	- C19 -	C20	120.4(3)
O2	- S1 -	C37	103.1(2)	Nb1	- C19 -	C20	117.6(2)
O2	- S1 -	O3	119.0(3)	C1	- C20 -	C19	104.5(3)
O1	- S1 -	C37	102.2(2)	C19	- C20 -	C35	109.6(3)
O1	- S1 -	O3	111.2(2)	C19	- C20 -	C33	109.4(3)
O1	- S1 -	O2	113.4(2)	C1	- C20 -	C35	109.6(3)
Nb1	- O1 -	S1	152.0(2)	C1	- C20 -	C33	111.2(3)
Nb1	- O4 -	C44	126.8(2)	C33	- C20 -	C35	112.2(3)
Nb1	- O4 -	C41	122.9(2)	C5	- C21 -	C22	116.3(3)
C41	- O4 -	C44	109.8(2)	C5	- C23 -	C24	114.4(4)
Nb1	- N1 -	C4	128.0(2)	C10	- C25 -	C26	115.2(3)
Nb1	- N1 -	C1	123.2(2)	C10	- C27 -	C28	116.8(3)
C1	- N1 -	C4	104.8(2)	C15	- C29 -	C30	116.5(3)
Nb1	- N2 -	C9	119.9(2)	C15	- C31 -	C32	114.6(3)
Nb1	- N2 -	C6	120.3(2)	C20	- C33 -	C34	114.2(3)
C6	- N2 -	C9	105.1(3)	C20	- C35 -	C36	115.2(3)
Nb1	- N3 -	C14	122.7(2)	F2	- C37 -	F3	109.1(4)
Nb1	- N3 -	C11	129.6(2)	F1	- C37 -	F3	107.8(3)
C11	- N3 -	C14	105.7(2)	F1	- C37 -	F2	108.5(4)
Nb1	- N4 -	C19	76.6(2)	S1	- C37 -	F3	108.2(3)
Nb1	- N4 -	C16	75.4(2)	S1	- C37 -	F2	112.0(3)
C16	- N4 -	C19	106.0(3)	S1	- C37 -	F1	111.2(3)

Table S14. Bond distances (Å) and angles (°) for complex 3 (cont.).

N1	- C1	- C20	118.7(3)	O4	- C41 - C42	105.7(3)
N1	- C1	- C2	110.4(3)	C41	- C42 - C43	107.3(3)
C2	- C1	- C20	130.6(3)	C42	- C43 - C44	107.4(3)
C1	- C2	- C3	106.5(3)	O4	- C44 - C43	105.1(3)
C2	- C3	- C4	108.7(3)	C2S	- C1S - C5SB	104.6(16)
N1	- C4	- C3	109.6(3)	C2S	- C1S - C5SA	82.8(16)
C3	- C4	- C5	125.9(3)	C1S	- C2S - C3S	102.7(15)
N1	- C4	- C5	124.4(3)	C2S	- C3S - C4SB	109.1(18)
C4	- C5	- C23	107.5(3)	C2S	- C3S - C4SA	100.2(18)
C4	- C5	- C21	107.0(3)	C3S	- C4SA- C5SA	101.7(18)
C4	- C5	- C6	113.9(3)	C1S	- C5SA- C4SA	106.1(21)
C21	- C5	- C23	109.6(3)	C3S	- C4SB- C5SB	101.0(18)
C6	- C5	- C23	109.7(3)	C1S	- C5SB- C4SB	103.3(18)

Table S15. Bond distances (Å) and angles (°) for complex **4**.

Nb1	- N1	2.126(6)	C9	- C10	1.490(14)
Nb1	- N2	2.153(6)	C10	- C11	1.477(14)
Nb1	- N3	2.140(7)	C10	- C25	1.532(20)
Nb1	- N4	2.330(6)	C10	- C27A	1.53(3)
Nb1	- C16	2.413(6)	C10	- C27B	1.57(2)
Nb1	- C17	2.537(9)	C11	- C12	1.361(13)
Nb1	- C18	2.532(9)	C12	- C13	1.409(14)
Nb1	- C19	2.446(7)	C13	- C14	1.351(12)
Nb1	- C37	2.162(9)	C14	- C15	1.500(12)
N1	- C1	1.402(11)	C15	- C16	1.487(11)
N1	- C4	1.410(11)	C15	- C29	1.598(14)
N2	- C6	1.423(10)	C15	- C31	1.549(14)
N2	- C9	1.383(11)	C16	- C17	1.410(12)
N3	- C11	1.392(12)	C17	- C18	1.387(12)
N3	- C14	1.411(10)	C18	- C19	1.395(12)
N4	- C16	1.366(10)	C19	- C20	1.495(11)
N4	- C19	1.371(10)	C20	- C33	1.557(13)
C1	- C2	1.366(13)	C20	- C35	1.563(13)
C1	- C20	1.491(12)	C21A	- C22A	1.54(3)
C2	- C3	1.418(13)	C21B	- C22B	1.46(4)
C3	- C4	1.357(13)	C23A	- C24A	1.54(3)
C4	- C5	1.502(13)	C23B	- C24B	1.54(3)
C5	- C6	1.479(14)	C25	- C26A	1.52(3)
C5	- C21A	1.54(2)	C25	- C26B	1.54(3)
C5	- C21B	1.56(3)	C27A	- C28A	1.55(4)
C5	- C23A	1.46(3)	C27B	- C28B	1.49(3)
C5	- C23B	1.71(2)	C29	- C30	1.533(17)
C6	- C7	1.365(14)	C31	- C32	1.544(17)
C7	- C8	1.392(16)	C33	- C34	1.518(13)
C8	- C9	1.363(13)	C35	- C36	1.539(15)

C19	- Nb1 - C37	107.9(3)	C5	- C6 - C7	127.0(8)
C18	- Nb1 - C37	77.0(3)	N2	- C6 - C7	108.3(8)
C18	- Nb1 - C19	32.5(3)	C6	- C7 - C8	108.0(9)
C17	- Nb1 - C37	75.4(3)	C7	- C8 - C9	108.2(9)
C17	- Nb1 - C19	53.4(3)	N2	- C9 - C8	109.5(8)
C17	- Nb1 - C18	31.7(3)	C8	- C9 - C10	128.1(9)
C16	- Nb1 - C37	105.7(3)	N2	- C9 - C10	120.8(8)
C16	- Nb1 - C19	53.6(2)	C9	- C10 - C27B	107.3(11)
C16	- Nb1 - C18	53.6(3)	C9	- C10 - C27A	112.0(13)
C16	- Nb1 - C17	33.0(3)	C9	- C10 - C25	116.6(10)
N4	- Nb1 - C37	129.5(3)	C9	- C10 - C11	113.8(8)
N4	- Nb1 - C19	33.2(2)	C25	- C10 - C27B	105.3(12)
N4	- Nb1 - C18	55.3(3)	C25	- C10 - C27A	78.4(12)
N4	- Nb1 - C17	55.6(3)	C11	- C10 - C27B	104.0(10)
N4	- Nb1 - C16	33.4(2)	C11	- C10 - C27A	122.6(14)
N3	- Nb1 - C37	107.4(3)	C11	- C10 - C25	108.7(9)
N3	- Nb1 - C19	118.1(3)	N3	- C11 - C10	121.0(8)
N3	- Nb1 - C18	120.2(3)	C10	- C11 - C12	128.1(9)
N3	- Nb1 - C17	90.0(3)	N3	- C11 - C12	109.4(8)
N3	- Nb1 - C16	68.8(2)	C11	- C12 - C13	108.2(8)
N3	- Nb1 - N4	85.7(2)	C12	- C13 - C14	106.8(8)
N2	- Nb1 - C37	85.5(3)	N3	- C14 - C13	110.2(8)
N2	- Nb1 - C19	149.9(2)	C13	- C14 - C15	132.3(8)
N2	- Nb1 - C18	155.5(3)	N3	- C14 - C15	116.7(7)
N2	- Nb1 - C17	155.5(3)	C14	- C15 - C31	111.8(8)

Table S15. Bond distances (Å) and angles (°) for complex **4**.(cont.)

N2	- Nb1 -	C16	149.8(2)	C14	- C15 -	C29	108.2(7)
N2	- Nb1 -	N4	145.0(2)	C14	- C15 -	C16	104.5(6)
N2	- Nb1 -	N3	81.1(3)	C29	- C15 -	C31	112.3(7)
N1	- Nb1 -	C37	108.7(3)	C16	- C15 -	C31	110.8(7)
N1	- Nb1 -	C19	68.3(2)	C16	- C15 -	C29	108.9(7)
N1	- Nb1 -	C18	87.5(3)	N4	- C16 -	C15	118.0(7)
N1	- Nb1 -	C17	118.4(3)	Nb1	- C16 -	C15	119.6(5)
N1	- Nb1 -	C16	118.8(2)	Nb1	- C16 -	N4	70.0(4)
N1	- Nb1 -	N4	86.8(2)	C15	- C16 -	C17	131.7(7)
N1	- Nb1 -	N3	138.5(3)	N4	- C16 -	C17	110.2(6)
N1	- Nb1 -	N2	82.0(2)	Nb1	- C16 -	C17	78.3(4)
Nb1	- N1 -	C4	126.4(5)	Nb1	- C17 -	C16	68.7(4)
Nb1	- N1 -	C1	122.8(5)	C16	- C17 -	C18	105.9(7)
C1	- N1 -	C4	105.5(7)	Nb1	- C17 -	C18	73.9(5)
Nb1	- N2 -	C9	115.4(5)	Nb1	- C18 -	C17	74.3(5)
Nb1	- N2 -	C6	113.7(5)	C17	- C18 -	C19	107.3(7)
C6	- N2 -	C9	105.8(6)	Nb1	- C18 -	C19	70.4(5)
Nb1	- N3 -	C14	122.6(5)	N4	- C19 -	C18	109.9(6)
Nb1	- N3 -	C11	128.3(5)	Nb1	- C19 -	C18	77.1(5)
C11	- N3 -	C14	105.1(6)	Nb1	- C19 -	N4	68.7(4)
Nb1	- N4 -	C19	78.0(4)	C18	- C19 -	C20	130.9(8)
Nb1	- N4 -	C16	76.6(4)	N4	- C19 -	C20	119.2(7)
C16	- N4 -	C19	106.4(6)	Nb1	- C19 -	C20	118.3(5)
N1	- C1 -	C20	117.0(7)	C1	- C20 -	C19	104.5(7)
N1	- C1 -	C2	110.3(8)	C19	- C20 -	C35	109.0(7)
C2	- C1 -	C20	131.7(8)	C19	- C20 -	C33	109.5(7)
C1	- C2 -	C3	106.2(8)	C1	- C20 -	C35	111.2(8)
C2	- C3 -	C4	108.8(8)	C1	- C20 -	C33	109.8(7)
N1	- C4 -	C3	108.9(8)	C33	- C20 -	C35	112.5(7)
C3	- C4 -	C5	128.0(8)	C5	- C21A-	C22A	100.0(16)
N1	- C4 -	C5	120.2(8)	C5	- C21B-	C22B	131(3)
C4	- C5 -	C23B	106.4(10)	C5	- C23A-	C24A	106.8(18)
C4	- C5 -	C23A	115.8(12)	C5	- C23B-	C24B	115.6(15)
C4	- C5 -	C21B	103.3(13)	C10	- C25 -	C27A	50.7(10)
C4	- C5 -	C21A	115.9(11)	C10	- C25 -	C26B	118.0(14)
C4	- C5 -	C6	111.1(7)	C10	- C25 -	C26A	103.4(15)
C21B	- C5 -	C23B	122.9(15)	C10	- C27A-	C28A	95.4(18)
C21A	- C5 -	C23A	73.5(14)	C10	- C27B-	C28B	131.1(17)
C6	- C5 -	C23B	104.1(10)	C15	- C29 -	C30	112.6(10)
C6	- C5 -	C23A	116.2(12)	C15	- C31 -	C32	111.2(9)
C6	- C5 -	C21B	108.9(12)	C20	- C33 -	C34	115.5(8)
C6	- C5 -	C21A	119.8(11)	C20	- C35 -	C36	113.6(8)
N2	- C6 -	C5	123.4(7)				

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Table S16. Bond distances (Å) and angles (°) for complex 6.

Nb1 - N1	2.274(8)	C10 - C25	1.557(18)
Nb1 - N2	2.154(8)	C10 - C27	1.550(18)
Nb1 - N3	2.251(8)	C11 - C12	1.371(15)
Nb1 - N4	2.434(8)	C12 - C13	1.398(17)
Nb1 - N5	2.211(9)	C13 - C14	1.381(15)
Nb1 - C16	2.454(10)	C14 - C15	1.477(14)
Nb1 - C17	2.493(10)	C15 - C16	1.525(15)
Nb1 - C18	2.474(10)	C15 - C29	1.617(17)
Nb1 - C19	2.458(10)	C15 - C31A	1.559(19)
Nb1 - C38	2.137(9)	C15 - C31B	1.54(3)
Nb1 - C43	2.298(11)	C16 - C17	1.394(15)
N1 - C1	1.410(14)	C17 - C18	1.407(15)
N1 - C4	1.384(14)	C18 - C19	1.382(15)
N2 - C6	1.422(13)	C19 - C20	1.502(16)
N2 - C9	1.391(14)	C20 - C33	1.554(18)
N3 - C11	1.372(13)	C20 - C35	1.555(16)
N3 - C14	1.386(12)	C21 - C22	1.523(18)
N4 - C16	1.350(15)	C23 - C24	1.40(2)
N4 - C19	1.368(15)	C25 - C26	1.51(2)
N5 - C38	1.243(13)	C27 - C28	1.49(2)
N5 - C39	1.490(14)	C29 - C30A	1.54(2)
N6 - C43	1.141(14)	C29 - C30B	1.56(2)
N6 - C44	1.476(16)	C31A - C32A	1.54(2)
C1 - C2	1.380(18)	C31B - C32B	1.54(5)
C1 - C20	1.480(16)	C33 - C34	1.496(2)
C2 - C3	1.354(22)	C35 - C36	1.524(18)
C3 - C4	1.379(18)	C37 - C38	1.510(13)
C4 - C5	1.489(16)	C39 - C40	1.534(16)
C5 - C6	1.508(17)	C39 - C41	1.529(18)
C5 - C21	1.565(16)	C39 - C42	1.554(18)
C5 - C23	1.567(19)	C44 - C45A	1.51(3)
C6 - C7	1.370(16)	C44 - C46A	1.61(4)
C7 - C8	1.388(19)	C44 - C47A	1.58(4)
C8 - C9	1.388(16)	C44 - C46B	1.46(4)
C9 - C10	1.535(15)	C44 - C45B	1.59(4)
C10 - C11	1.486(15)	C44 - C47B	1.59(4)

C38 - Nb1 - C43	148.9(4)	C5 - C6 - C7	126.6(10)
C19 - Nb1 - C43	88.6(4)	N2 - C6 - C7	108.9(10)
C19 - Nb1 - C38	97.4(4)	C6 - C7 - C8	108.4(10)
C18 - Nb1 - C43	120.9(3)	C7 - C8 - C9	107.3(11)
C18 - Nb1 - C38	71.5(3)	N2 - C9 - C8	109.8(10)
C18 - Nb1 - C19	32.5(3)	C8 - C9 - C10	125.3(10)
C17 - Nb1 - C43	123.5(3)	N2 - C9 - C10	123.0(9)
C17 - Nb1 - C38	83.2(3)	C9 - C10 - C27	103.5(9)
C17 - Nb1 - C19	53.5(3)	C9 - C10 - C25	111.2(9)
C17 - Nb1 - C18	32.9(3)	C9 - C10 - C11	113.5(9)
C16 - Nb1 - C43	91.9(4)	C25 - C10 - C27	106.8(9)
C16 - Nb1 - C38	115.9(4)	C11 - C10 - C27	109.0(9)
C16 - Nb1 - C19	52.4(3)	C11 - C10 - C25	112.2(10)
C16 - Nb1 - C18	53.9(3)	N3 - C11 - C10	123.6(9)
C16 - Nb1 - C17	32.7(3)	C10 - C11 - C12	126.5(9)
N5 - Nb1 - C43	157.9(3)	N3 - C11 - C12	109.5(9)
N5 - Nb1 - C38	33.2(3)	C11 - C12 - C13	108.1(9)
N5 - Nb1 - C19	113.5(3)	C12 - C13 - C14	106.2(9)

Table S16. Bond distances (Å) and angles (°) for complex 6.(cont.)

N5	- Nb1 -	C18	81.2(3)	N3	- C14 -	C13	109.8(9)
N5	- Nb1 -	C17	73.9(3)	C13	- C14 -	C15	129.2(9)
N5	- Nb1 -	C16	101.8(3)	N3	- C14 -	C15	120.4(8)
N4	- Nb1 -	C43	70.8(3)	C14	- C15 -	C31B	123.0(13)
N4	- Nb1 -	C38	126.4(3)	C14	- C15 -	C31A	109.0(9)
N4	- Nb1 -	C19	32.5(3)	C14	- C15 -	C29	108.4(9)
N4	- Nb1 -	C18	55.0(3)	C14	- C15 -	C16	106.6(8)
N4	- Nb1 -	C17	54.7(3)	C29	- C15 -	C31B	95.4(12)
N4	- Nb1 -	C16	32.1(3)	C29	- C15 -	C31A	118.1(10)
N4	- Nb1 -	N5	128.5(3)	C16	- C15 -	C31B	114.5(14)
N3	- Nb1 -	C43	79.7(3)	C16	- C15 -	C31A	106.8(10)
N3	- Nb1 -	C38	121.6(4)	C16	- C15 -	C29	107.3(9)
N3	- Nb1 -	C19	120.1(3)	N4	- C16 -	C15	121.6(10)
N3	- Nb1 -	C18	118.2(3)	Nb1	- C16 -	C15	117.2(6)
N3	- Nb1 -	C17	85.7(3)	Nb1	- C16 -	N4	73.1(5)
N3	- Nb1 -	C16	69.3(3)	C15	- C16 -	C17	127.3(10)
N3	- Nb1 -	N5	88.9(3)	N4	- C16 -	C17	111.1(10)
N3	- Nb1 -	N4	89.6(3)	Nb1	- C16 -	C17	75.2(6)
N2	- Nb1 -	C43	77.4(3)	Nb1	- C17 -	C16	72.1(6)
N2	- Nb1 -	C38	82.6(3)	C16	- C17 -	C18	105.9(9)
N2	- Nb1 -	C19	150.0(3)	Nb1	- C17 -	C18	72.8(6)
N2	- Nb1 -	C18	152.3(3)	Nb1	- C18 -	C17	74.3(6)
N2	- Nb1 -	C17	154.3(3)	C17	- C18 -	C19	106.0(9)
N2	- Nb1 -	C16	152.5(3)	Nb1	- C18 -	C19	73.1(6)
N2	- Nb1 -	N5	82.6(3)	N4	- C19 -	C18	111.0(10)
N2	- Nb1 -	N4	148.2(3)	Nb1	- C19 -	C18	74.4(6)
N2	- Nb1 -	N3	83.7(3)	Nb1	- C19 -	N4	72.8(5)
N1	- Nb1 -	C43	75.0(3)	C18	- C19 -	C20	127.2(10)
N1	- Nb1 -	C38	79.0(3)	N4	- C19 -	C20	121.8(10)
N1	- Nb1 -	C19	68.2(3)	Nb1	- C19 -	C20	119.2(7)
N1	- Nb1 -	C18	82.8(3)	C1	- C20 -	C19	105.4(9)
N1	- Nb1 -	C17	115.4(3)	C19	- C20 -	C35	109.1(9)
N1	- Nb1 -	C16	119.5(3)	C19	- C20 -	C33	108.7(9)
N1	- Nb1 -	N5	111.8(3)	C1	- C20 -	C35	112.6(9)
N1	- Nb1 -	N4	90.1(3)	C1	- C20 -	C33	109.4(10)
N1	- Nb1 -	N3	153.4(3)	C33	- C20 -	C35	111.4(9)
N1	- Nb1 -	N2	82.5(3)	C5	- C21 -	C22	117.0(10)
Nb1	- N1 -	C4	129.5(7)	C5	- C23 -	C24	116.9(13)
Nb1	- N1 -	C1	122.0(6)	C10	- C25 -	C26	118.1(11)
C1	- N1 -	C4	106.8(8)	C10	- C27 -	C28	120.8(13)
Nb1	- N2 -	C9	120.5(6)	C15	- C29 -	C30B	104.1(13)
Nb1	- N2 -	C6	119.8(6)	C15	- C29 -	C30A	124.6(15)
C6	- N2 -	C9	105.1(7)	C15	- C31A-	C32A	115.5(14)
Nb1	- N3 -	C14	122.3(6)	C15	- C31B-	C32B	102(2)
Nb1	- N3 -	C11	130.4(6)	C20	- C33 -	C34	112.9(12)
C11	- N3 -	C14	106.4(8)	C20	- C35 -	C36	114.5(11)
Nb1	- N4 -	C19	74.7(5)	N5	- C38 -	C37	136.2(10)
Nb1	- N4 -	C16	74.8(5)	Nb1	- C38 -	C37	147.0(8)
C16	- N4 -	C19	105.9(9)	Nb1	- C38 -	N5	76.7(6)
Nb1	- N5 -	C39	156.9(7)	N5	- C39 -	C42	109.1(9)
Nb1	- N5 -	C38	70.1(6)	N5	- C39 -	C41	107.7(9)
C38	- N5 -	C39	132.1(9)	N5	- C39 -	C40	107.5(9)
C43	- N6 -	C44	178.2(11)	C41	- C39 -	C42	110.1(10)

Table S16. Bond distances (Å) and angles (°) for complex **6**.(cont.)

N1	- C1	- C20	119.9(9)	C40	- C39	- C42	110.6(9)
N1	- C1	- C2	108.1(10)	C40	- C39	- C41	111.7(10)
C2	- C1	- C20	131.9(11)	Nb1	- C43	- N6	177.9(9)
C1	- C2	- C3	107.6(12)	N6	- C44	- C47B	103.3(17)
C2	- C3	- C4	110.0(13)	N6	- C44	- C45B	102.0(16)
N1	- C4	- C3	107.5(10)	N6	- C44	- C46B	112.7(16)
C3	- C4	- C5	128.5(11)	N6	- C44	- C47A	102.7(15)
N1	- C4	- C5	123.6(9)	N6	- C44	- C46A	108.0(17)
C4	- C5	- C23	104.2(10)	N6	- C44	- C45A	108.9(15)
C4	- C5	- C21	108.8(9)	C45B	- C44	- C47B	115(2)
C4	- C5	- C6	114.8(9)	C46B	- C44	- C47B	114(2)
C21	- C5	- C23	108.2(10)	C46B	- C44	- C45B	110(2)
C6	- C5	- C23	107.5(10)	C46A	- C44	- C47A	113(2)
C6	- C5	- C21	112.8(10)	C45A	- C44	- C47A	113(2)
N2	- C6	- C5	121.8(9)	C45A	- C44	- C46A	111(2)

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Table S17. Bond distances (Å) and angles (°) for complex **9**.

Nb1 - O1	1.741(7)	C15 - C16	1.533(12)
Nb1 - N1	2.124(8)	C15 - C30	1.488(15)
Nb1 - N2	2.158(9)	C15 - C32	1.564(15)
Nb1 - N3	2.170(9)	C16 - C17	1.378(15)
Nb1 - N4	2.436(8)	C17 - C18	1.388(15)
Nb1 - C30	2.242(8)	C18 - C19	1.363(15)
LI1 - O1	1.923(19)	C18 - C34	1.552(18)
LI1 - O2	1.929(20)	C19 - C20	1.376(16)
LI1 - O3	1.939(24)	C20 - C21	1.508(13)
LI1 - O4	1.967(19)	C21 - C35	1.552(16)
O2 - C39A	1.524(32)	C21 - C37	1.569(15)
O2 - C39B	1.402(36)	C22 - C23	1.459(26)
O2 - C42	1.482(18)	C24 - C25	1.499(21)
O3 - C43	1.443(22)	C26 - C27	1.496(27)
O3 - C46	1.461(20)	C28 - C29	1.488(34)
O4 - C47	1.467(20)	C30 - C31	1.512(16)
O4 - C50	1.417(16)	C32 - C33	1.504(19)
N1 - C1	1.399(14)	C35 - C36	1.509(17)
N1 - C4	1.396(12)	C37 - C38	1.498(22)
N2 - C6	1.400(13)	C39A - C39B	0.720(46)
N2 - C9	1.374(14)	C39A - C40	1.576(40)
N3 - C11	1.388(15)	C39B - C40	1.493(36)
N3 - C14	1.398(13)	C40 - C41A	1.359(41)
N4 - C16	1.359(11)	C40 - C41B	1.663(53)
N4 - C20	1.363(12)	C41A - C42	1.636(36)
C1 - C2	1.368(15)	C41B - C42	1.397(47)
C1 - C21	1.514(15)	C43 - C44A	1.451(73)
C2 - C3	1.408(19)	C43 - C44B	1.573(52)
C3 - C4	1.371(16)	C44A - C45A	1.379(75)
C4 - C5	1.506(17)	C45A - C46	1.611(53)
C5 - C6	1.531(18)	C44B - C45B	1.600(61)
C5 - C22	1.583(18)	C45B - C46	1.495(55)
C5 - C24	1.571(15)	C47 - C48A	1.432(30)
C6 - C7	1.373(17)	C47 - C48B	1.621(38)
C7 - C8	1.365(20)	C48A - C49A	1.554(45)
C8 - C9	1.377(17)	C49A - C50	1.415(32)
C9 - C10	1.526(15)	C48B - C49B	1.387(53)
C10 - C11	1.489(17)	C49B - C50	1.717(36)
C10 - C26	1.517(26)	C61 - C63	1.488(42)
C10 - C28	1.580(19)	C61 - C64	1.460(45)
C11 - C12	1.375(15)	C61 - C65	1.493(40)
C12 - C13	1.400(21)	C62 - C64	1.479(45)
C13 - C14	1.367(16)	C62 - C65	1.505(40)
C14 - C15	1.503(15)	C63 - C64	1.496(45)

N4 - Nb1 - C30	67.4(3)	C11 - C10 - C28	108.3(10)
N3 - Nb1 - C30	71.0(3)	C11 - C10 - C26	110.4(11)
N3 - Nb1 - N4	83.9(3)	N3 - C11 - C10	124.5(9)
N2 - Nb1 - C30	140.9(3)	C10 - C11 - C12	125.1(10)
N2 - Nb1 - N4	133.8(3)	N3 - C11 - C12	110.4(10)
N2 - Nb1 - N3	78.7(3)	C11 - C12 - C13	106.9(10)
N1 - Nb1 - C30	133.7(3)	C12 - C13 - C14	107.5(11)
N1 - Nb1 - N4	78.9(3)	N3 - C14 - C13	110.1(9)
N1 - Nb1 - N3	137.1(3)	C13 - C14 - C15	136.3(10)
N1 - Nb1 - N2	85.5(3)	N3 - C14 - C15	113.6(8)

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Table S17. Bond distances (Å) and angles (°) for complex **9**. (cont.)

O1	- Nb1 -	C30	81.7(3)	C14	- C15 -	C32	111.9(8)
O1	- Nb1 -	N4	130.7(3)	C14	- C15 -	C30	104.5(8)
O1	- Nb1 -	N3	121.9(4)	C14	- C15 -	C16	105.1(8)
O1	- Nb1 -	N2	94.4(3)	C30	- C15 -	C32	116.6(8)
O1	- Nb1 -	N1	98.7(3)	C16	- C15 -	C32	110.9(8)
O3	- LI1 -	O4	99.7(9)	C16	- C15 -	C30	106.9(8)
O2	- LI1 -	O4	99.8(9)	N4	- C16 -	C15	114.2(8)
O2	- LI1 -	O3	126.6(10)	C15	- C16 -	C17	123.2(8)
O1	- LI1 -	O4	123.1(10)	N4	- C16 -	C17	122.6(8)
O1	- LI1 -	O3	102.8(9)	C16	- C17 -	C18	120.4(9)
O1	- LI1 -	O2	106.7(9)	C17	- C18 -	C34	121.6(10)
Nb1	- O1 -	LI1	168.7(7)	C17	- C18 -	C19	115.6(11)
LI1	- O2 -	C42	119.0(9)	C19	- C18 -	C34	122.8(11)
LI1	- O2 -	C39B	133.7(15)	C18	- C19 -	C20	123.9(11)
LI1	- O2 -	C39A	121.8(14)	N4	- C20 -	C19	119.5(9)
C39B	- O2 -	C42	106.9(15)	C19	- C20 -	C21	118.2(9)
C39A	- O2 -	C42	115.3(14)	N4	- C20 -	C21	122.0(8)
LI1	- O3 -	C46	119.3(10)	C1	- C21 -	C20	117.1(8)
LI1	- O3 -	C43	126.8(11)	C20	- C21 -	C37	109.5(8)
C43	- O3 -	C46	112.7(13)	C20	- C21 -	C35	107.2(8)
LI1	- O4 -	C50	121.5(10)	C1	- C21 -	C37	106.5(8)
LI1	- O4 -	C47	127.7(10)	C1	- C21 -	C35	108.5(9)
C47	- O4 -	C50	110.2(11)	C35	- C21 -	C37	107.6(8)
Nb1	- N1 -	C4	113.8(6)	C5	- C22 -	C23	120.3(12)
Nb1	- N1 -	C1	126.9(6)	C5	- C24 -	C25	113.8(10)
C1	- N1 -	C4	106.6(8)	C10	- C26 -	C27	113.0(16)
Nb1	- N2 -	C9	135.0(7)	C10	- C28 -	C29	115.3(13)
Nb1	- N2 -	C6	118.0(7)	Nb1	- C30 -	C15	107.6(6)
C6	- N2 -	C9	106.5(8)	C15	- C30 -	C31	116.5(8)
Nb1	- N3 -	C14	117.2(6)	Nb1	- C30 -	C31	110.0(6)
Nb1	- N3 -	C11	137.6(7)	C15	- C32 -	C33	112.7(10)
C11	- N3 -	C14	105.1(8)	C21	- C35 -	C36	114.3(9)
Nb1	- N4 -	C20	130.2(6)	C21	- C37 -	C38	113.6(11)
Nb1	- N4 -	C16	111.5(6)	O2	- C39A -	C40	97.4(20)
C16	- N4 -	C20	117.4(7)	O2	- C39B -	C40	107(2)
N1	- C1 -	C21	124.9(8)	C39B	- C40 -	C41B	97(2)
N1	- C1 -	C2	109.4(9)	C39A	- C40 -	C41A	110(2)
C2	- C1 -	C21	123.8(9)	C40	- C41A -	C42	106(2)
C1	- C2 -	C3	107.0(11)	C40	- C41B -	C42	103(3)
C2	- C3 -	C4	108.4(10)	O2	- C42 -	C41B	110(2)
N1	- C4 -	C3	108.5(9)	O2	- C42 -	C41A	99.2(15)
C3	- C4 -	C5	124.2(9)	O3	- C43 -	C44B	104.2(20)
N1	- C4 -	C5	127.0(9)	O3	- C43 -	C44A	105(3)
C4	- C5 -	C24	107.2(9)	C43	- C44A -	C45A	111(5)
C4	- C5 -	C22	107.7(9)	C44A	- C45A -	C46	108(4)
C4	- C5 -	C6	116.1(9)	C43	- C44B -	C45B	106(3)
C22	- C5 -	C24	106.9(10)	C44B	- C45B -	C46	104(3)
C6	- C5 -	C24	107.7(9)	O3	- C46 -	C45B	109.3(20)
C6	- C5 -	C22	110.8(11)	O3	- C46 -	C45A	99.5(19)
N2	- C6 -	C5	127.7(9)	O4	- C47 -	C48B	103.6(17)
C5	- C6 -	C7	124.2(10)	O4	- C47 -	C48A	108.3(17)
N2	- C6 -	C7	108.1(10)	C48A	- C49A -	C50	108.8(23)
C6	- C7 -	C8	108.3(10)	C47	- C48B -	C49B	112(3)

Table S17. Bond distances (Å) and angles (°) for complex **9**. (cont.)

C7	- C8	- C9	108.0(11)	C48B	- C49B	- C50	101(3)
N2	- C9	- C8	109.0(10)	O4	- C50	- C49B	105.1(14)
C8	- C9	- C10	124.2(10)	O4	- C50	- C49A	107.2(16)
N2	- C9	- C10	126.4(9)	C64	- C61	- C65	103(2)
C9	- C10	- C28	104.7(10)	C63	- C61	- C65	88(2)
C9	- C10	- C26	110.4(10)	C64	- C62	- C65	101(2)
C9	- C10	- C11	115.7(9)	C62	- C64	- C63	101(3)
C26	- C10	- C28	106.9(11)				

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Captions of the supplementary figures.

Figure S1. SCHAKAL perspective view of complex **3**. Disorder omitted for clarity.

Figure S2. SCHAKAL perspective view of complex **4**. Disorder omitted for clarity.

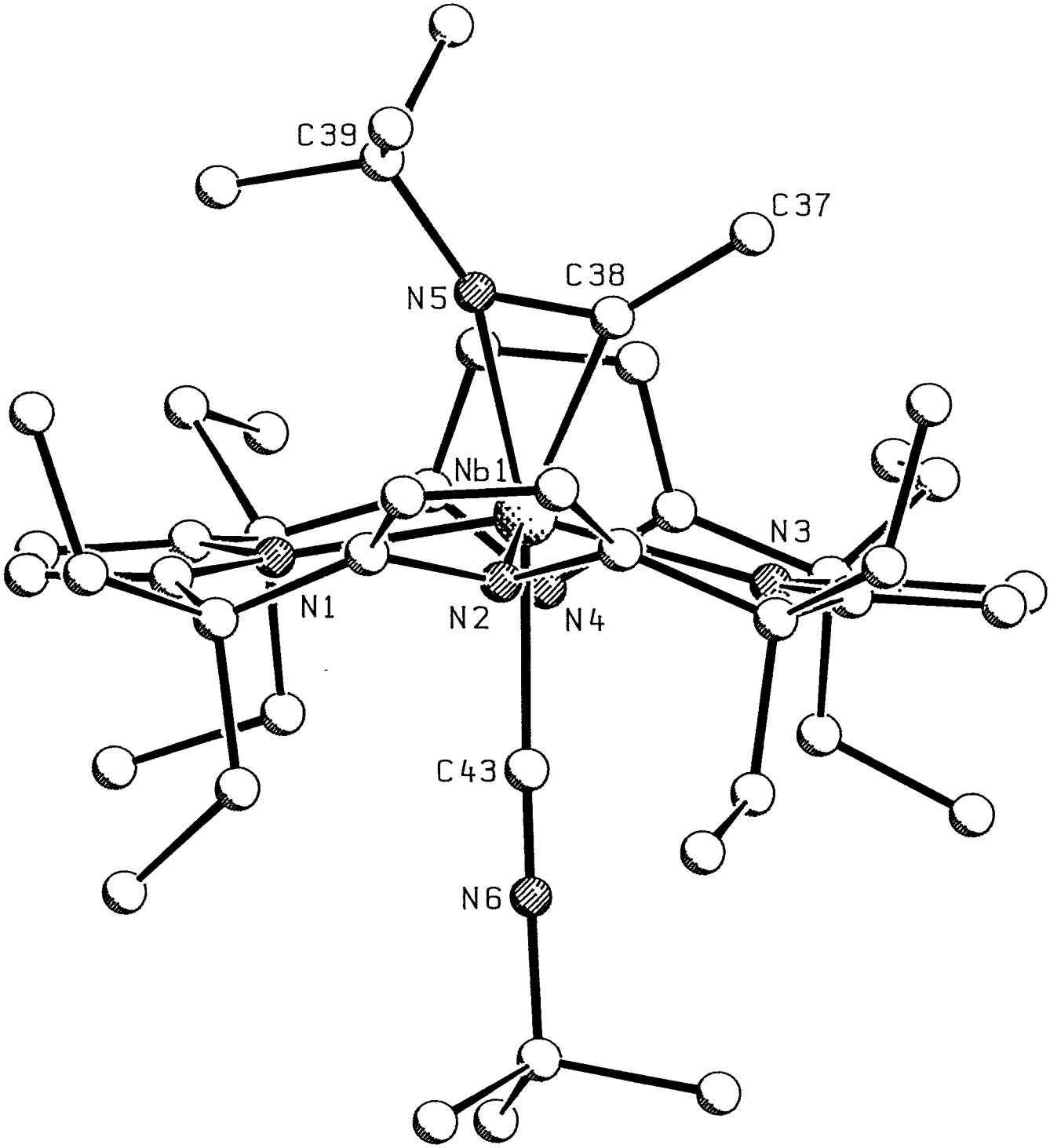

Figure 1

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Figure 2S