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Inorg. Chem., 1998, 37(6), 1347-1351, DOI:10.1021/ic970841f

Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Complex **I**.

Compound	**I**
formula	$C_{64}H_{32}N_{16}Nb \cdot I_3 \cdot 0.5I_2 \cdot 3.5C_{10}H_7Cl$
cryst habit	prism
cryst colour	black
fw	2194.8
cryst syst	triclinic
space group	$P\bar{1}$
cell parameters [a]	
a, Å	17.702(3)
b, Å	18.708(3)
c, Å	13.504(2)
α, deg	106.00(2)
β, deg	93.39(2)
γ, deg	83.26(1)
V, Å^3	4267.5(13)
Z	2
d_{calc}, Mg m^{-3}	1.708
cryst dimens, mm	0.21x0.26x0.56
linear abs coeff, cm^{-1}	17.35
diffractometer	Philips PW1100
diffraction geometry	equatorial
scan type	$\omega/2\theta$
scan speed deg min^{-1}	2-8
scan width, deg	1.20 + 0.35tgθ

Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Complex I (cont.).

compound	I
radiation	Graphite monochromated Mo Ka (λ = 0.71069 Å)
data collcn range of 2θ, deg	6-46
reflcns measd	$\pm$h, $\pm$k, l
unique total data	11865
criterion for obsn	$I > 2\sigma(I)$
unique obs data [$I>2\sigma(I)$]	6490
unique total data [I>0] (NO)	11764
no. of params refined (NV)	1055
overdetermn ratio (NO/NV)	11.2
transm factors	0.810-1.000
$R = \Sigma\lvert\Delta F\rvert / \Sigma\lvert F_o\rvert$	0.079 [b]
$wR2 = [\Sigma w\lvert\Delta F^2\rvert^2 / \Sigma w\lvert Fo^2\rvert^2]^{1/2}$	0.207 [c]
$GOF=[\Sigma w\lvert\Delta F^2\rvert^2 / (NO-NV)]^{1/2}$	0.997
largest shift/esd, final cycle	0.001
largest peak, e/Å^3	1.11 [d]

[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 collected at 295 K

[b] Calculated on the unique observed data [$I>2\sigma(I)$]

[c] Calculated on the unique total data with I>0

[d] Along the I1-I2 bond

Table S2. Fractional Atomic Coordinates ($x10^4$) for Complex **I**.

a. Cation

	Molecule A				*Molecule B*		
Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Nb1	2654.0(5)	2099.8(5)	4825.0(6)				
N1	1846(4)	2888(4)	4200(5)	N1	2705(4)	1079(4)	5393(5)
N2	670(4)	2269(5)	3967(6)	N2	1352(4)	897(4)	5385(6)
N3	1849(4)	1403(4)	3823(6)	N3	1601(4)	2224(4)	5675(5)
N4	2575(5)	297(5)	2819(6)	N4	1395(4)	3501(4)	6672(6)
N5	3358(4)	1306(4)	3533(6)	N5	2702(4)	3130(4)	6146(6)
N6	4524(4)	1923(4)	3706(6)	N6	4065(4)	3317(4)	6197(6)
N7	3361(4)	2792(4)	4286(5)	N7	3791(4)	1981(4)	5515(6)
N8	2575(4)	3892(4)	4164(6)	N8	4049(4)	731(4)	5675(6)
C1	1953(5)	3584(5)	4134(7)	C1	3334(5)	605(5)	5559(7)
C2	1209(5)	4014(6)	3985(8)	C2	3105(6)	-93(5)	5671(7)
C3	1036(6)	4726(6)	3874(9)	C3	3535(6)	-720(6)	5848(8)
C4	272(7)	4943(7)	3724(10)	C4	3142(8)	-1300(6)	5889(10)
C5	-276(7)	4462(8)	3657(10)	C5	2353(7)	-1283(6)	5753(11)
C6	-102(6)	3744(7)	3731(8)	C6	1939(6)	-649(6)	5593(9)
C7	656(6)	3542(6)	3906(7)	C7	2341(5)	-69(5)	5540(7)
C8	1041(5)	2809(6)	4014(7)	C8	2074(6)	687(5)	5424(7)
C11	1037(5)	1578(5)	4097(7)	C11	1097(5)	1627(5)	5281(8)
C12	649(6)	931(6)	3450(8)	C12	365(5)	1930(5)	5854(7)
C13	-117(6)	823(7)	3256(9)	C13	-261(6)	1581(6)	5903(9)
C14	-287(7)	149(8)	2631(12)	C14	-856(6)	2007(8)	6505(10)
C15	263(8)	-389(8)	2161(11)	C15	-806(6)	2751(7)	7011(10)
C16	1032(7)	-290(7)	2290(9)	C16	-159(6)	3081(6)	6998(9)
C17	1199(6)	397(6)	2955(8)	C17	432(5)	2653(6)	6398(7)
C18	1936(6)	700(6)	3208(7)	C18	1197(5)	2820(6)	6262(8)

Table S2. Fractional Atomic Coordinates ($x10^4$) for Complex **I** (cont.).

C21	3204(6)	620(5)	2941(7)	C21	2120(5)	3614(5)	6650(7)
C22	3871(5)	238(5)	2322(7)	C22	2377(5)	4330(5)	7235(7)
C23	3955(7)	-438(6)	1548(8)	C23	1988(6)	4955(6)	7887(8)
C24	4643(8)	-611(6)	1107(10)	C24	2420(7)	5526(6)	8385(9)
C25	5223(7)	-158(8)	1339(10)	C25	3194(7)	5482(6)	8237(10)
C26	5112(7)	514(6)	2088(9)	C26	3593(6)	4834(6)	7610(8)
C27	4429(6)	705(5)	2577(7)	C27	3144(5)	4268(5)	7116(8)
C28	4125(5)	1384(5)	3344(7)	C28	3389(6)	3514(5)	6430(7)
C31	4223(5)	2612(5)	4392(7)	C31	4287(5)	2582(5)	5548(8)
C32	4541(5)	3261(5)	4181(8)	C32	5053(5)	2288(5)	5903(7)
C33	5282(6)	3370(6)	4065(8)	C33	5704(6)	2651(6)	6201(8)
C34	5412(6)	4021(7)	3827(10)	C34	6318(6)	2239(7)	6586(9)
C35	4807(7)	4536(6)	3730(10)	C35	6264(6)	1513(7)	6648(9)
C36	4054(6)	4439(6)	3845(9)	C36	5615(6)	1177(6)	6351(8)
C37	3962(5)	3779(5)	4066(8)	C37	5026(5)	1586(5)	5985(7)
C38	3252(5)	3468(5)	4164(7)	C38	4234(5)	1403(5)	5705(7)

b. Anion

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
I1	2266.0(7)	6840.5(8)	6586.8(12)	I3	2861.6(9)	5746.4(7)	2214.1(13)
I2	2547.0(5)	6334.2(5)	4461.8(10)	I4	4429.5(9)	5204.2(7)	704.3(12)

c. Solvent Molecules of Crystallization

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
CL1	2330(6)	812(5)	8004(5)	C54	3115(13)	1378(16)	813(12)
CL2A	324(40)	1926(40)	1273(61)	C55	2332(13)	1526(11)	928(8)

Table S2. Fractional Atomic Coordinates ($x10^4$) for Complex I (cont.).

CL2B	4067(35)	1807(35)	960(53)	C56	2002(12)	2260(11)	1251(7)
CL2C	2345(26)	225(27)	170(39)	C57	1219(13)	2408(15)	1366(12)
CL2D	2482(28)	3504(29)	1675(44)	C58	767(12)	1822(20)	1158(13)
CL3	-628(13)	3309(12)	718(23)	C59	1098(17)	1087(18)	835(13)
CL4A	2010(12)	-1082(11)	-1364(16)	C60	1880(18)	939(12)	720(12)
CL4B	2936(23)	-1134(22)	-1498(30)	C61	207(12)	4903(15)	406(19)
CL4C	1427(39)	-1358(39)	-692(57)	C62	28(13)	4306(11)	730(17)
C41	2165(8)	1763(8)	8367(7)	C63	-619(15)	3955(9)	326(22)
C42	1432(7)	2100(12)	8606(8)	C64	-1058(11)	4180(13)	-450(19)
C43	1300(6)	2873(12)	8980(9)	C65	-879(7)	4784(12)	-767(13)
C44	1901(8)	3309(9)	9114(8)	C71	3424(12)	-1887(9)	-1267(11)
C45	2635(7)	2973(6)	8875(5)	C72	4176(12)	-2203(10)	-1355(14)
C46	2767(6)	2200(6)	8502(5)	C73	4467(9)	-2658(10)	-735(17)
C47	3500(7)	1863(7)	8262(7)	C74	4005(11)	-2797(8)	-26(14)
C48	4102(6)	2300(10)	8397(7)	C75	3253(11)	-2481(6)	62(9)
C49	3970(8)	3072(9)	8770(8)	C76	2962(10)	-2026(6)	-558(9)
C50	3236(9)	3409(6)	9010(8)	C77	2210(10)	-1710(8)	-470(14)
C51	2453(17)	2846(12)	1460(10)	C78	1748(11)	-1849(10)	238(17)
C52	3236(16)	2698(18)	1345(12)	C79	2039(14)	-2304(11)	859(14)
C53	3567(12)	1964(21)	1021(13)	C80	2791(15)	-2620(9)	771(10)

The site occupation factors for the A, B, C and D positions of CL2 are 0.25; for CL3 is 0.5; for the A, B and C positions of CL4 are 0.55, 0.25 and 0.20 respectively.

Table S3. Fractional Atomic Coordinates ($x10^4$) for Hydrogen Atoms for Complex **I**.

	Molecule A				*Molecule B*		
Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H3	1393	5054	3909	H3	4061	-743	5925
H4	129	5418	3673	H4	3424	-1746	5980
H5	-790	4619	3556	H5	2097	-1674	5757
H6	-478	3429	3664	H6	1405	-604	5540
H13	-494	1189	3563	H13	-314	1078	5558
H14	-788	24	2558	H14	-1295	1810	6573
H15	120	-814	1674	H15	-1223	3025	7379
H16	1411	-660	1997	H16	-124	3569	7387
H23	3569	-740	1368	H23	1474	4976	7970
H24	4732	-1075	623	H24	2186	5956	8846
H25	5679	-298	1015	H25	3459	5913	8579
H26	5511	795	2246	H26	4110	4776	7535
H33	5693	3008	4099	H33	5746	3142	6178
H34	5897	4147	3755	H34	6754	2489	6849
H35	4907	4961	3562	H35	6703	1228	6843
H36	3657	4779	3775	H36	5565	725	6429

Table S4. Anisotropic and Isotropic Thermal Parameters $U_{i,j}$ ($\times 10^4$ Å^2) for Complex **I**. $U_{i,j}$ are in the Form $\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{12}hka^*b^*+\ldots)]$

a. Cation

Molecule A

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	275(5)	330(5)	232(5)	92(4)	-6(4)	-23(4)
N1	322(45)	293(44)	279(44)	111(36)	-40(35)	-9(35)
N2	307(46)	516(55)	312(48)	57(42)	55(37)	-70(43)
N3	297(44)	332(46)	349(47)	179(40)	-57(36)	-30(36)
N4	360(51)	468(52)	437(55)	25(43)	-17(43)	-130(44)
N5	355(47)	322(46)	326(47)	139(39)	4(37)	34(37)
N6	329(46)	384(49)	382(50)	164(41)	1(39)	55(41)
N7	351(44)	280(43)	186(41)	96(34)	-47(33)	-10(34)
N8	331(49)	372(47)	535(57)	202(42)	26(41)	-67(41)
C1	422(62)	381(60)	217(54)	97(45)	-38(45)	46(50)
C2	360(60)	495(66)	376(62)	111(52)	-1(49)	16(52)
C3	477(71)	505(70)	804(90)	361(66)	-77(63)	-70(57)
C4	646(86)	554(77)	856(100)	354(73)	6(73)	156(68)
C5	518(77)	861(97)	696(90)	425(78)	-126(65)	43(72)
C6	357(65)	746(83)	519(73)	290(64)	-131(53)	-95(58)
C7	385(63)	622(72)	311(60)	142(53)	-36(48)	-139(56)
C8	238(53)	527(67)	335(60)	133(51)	-45(45)	-33(50)
C11	246(52)	516(65)	250(54)	63(48)	12(43)	-60(47)
C12	487(68)	523(69)	398(64)	205(55)	-132(54)	-212(58)
C13	516(74)	659(79)	514(74)	78(63)	-11(58)	-252(63)
C14	408(75)	957(109)	1038(117)	-73(94)	78(76)	-331(77)
C15	789(101)	755(96)	814(102)	-186(79)	108(82)	-430(83)
C16	623(82)	645(82)	607(82)	88(67)	124(65)	-159(66)
C17	524(69)	424(64)	392(64)	88(54)	-45(55)	-147(57)
C18	525(69)	447(65)	195(53)	85(49)	-19(49)	-127(55)
C21	450(65)	387(61)	251(56)	68(48)	-58(48)	115(52)
C22	394(60)	417(61)	286(57)	135(50)	23(47)	13(51)
C23	685(80)	400(65)	428(69)	25(55)	166(61)	104(58)
C24	933(104)	418(72)	599(86)	-90(62)	311(79)	219(72)
C25	518(78)	886(101)	548(82)	77(76)	267(66)	152(74)
C26	600(76)	576(75)	433(70)	116(61)	66(60)	36(61)
C27	420(62)	418(61)	313(58)	115(49)	119(50)	141(52)
C28	267(54)	411(61)	323(58)	84(49)	-28(45)	5(48)
C31	198(48)	315(54)	369(58)	120(47)	16(43)	25(41)
C32	252(55)	409(59)	428(63)	76(50)	-23(46)	-50(47)
C33	486(69)	493(68)	561(74)	211(58)	9(56)	-134(54)
C34	493(71)	657(81)	754(90)	359(71)	39(63)	-115(63)
C35	647(83)	478(72)	985(105)	394(72)	77(74)	-73(63)
C36	397(66)	593(74)	736(84)	369(66)	89(58)	-84(55)
C37	399(61)	449(63)	374(62)	149(52)	-28(49)	-44(52)
C38	325(57)	417(60)	306(57)	170(48)	1(45)	-87(48)
Molecule B						
N1	298(44)	333(44)	289(45)	99(37)	5(35)	-41(37)
N2	414(53)	422(51)	346(49)	108(40)	71(40)	-40(41)
N3	183(39)	322(44)	318(45)	141(37)	57(34)	21(35)

Table S4. Anisotropic and Isotropic Thermal Parameters $U_{i,j}$ ($x10^4$ Å^2) for Complex **I** (cont.).

N4	403(52)	375(50)	361(50)	76(40)	-10(39)	-88(40)
N5	303(44)	369(46)	276(45)	36(37)	63(37)	49(38)
N6	279(47)	395(49)	384(50)	179(41)	-125(39)	-62(38)
N7	255(42)	350(46)	342(47)	89(38)	6(36)	-52(36)
N8	377(50)	321(47)	355(49)	111(38)	16(39)	-24(38)
C1	374(62)	392(59)	293(58)	113(47)	-67(46)	-4(49)
C2	472(67)	352(58)	365(61)	154(49)	3(50)	-38(49)
C3	652(74)	357(61)	460(68)	184(53)	1(57)	60(56)
C4	790(93)	454(71)	714(89)	356(66)	45(71)	70(65)
C5	694(90)	487(74)	989(107)	421(74)	104(77)	-33(66)
C6	532(71)	484(69)	569(75)	127(59)	48(58)	-193(58)
C7	385(61)	390(59)	341(59)	150(48)	-4(47)	-53(48)
C8	423(64)	362(58)	231(55)	22(45)	47(46)	9(49)
C11	348(57)	438(61)	408(63)	227(51)	20(48)	-23(49)
C12	296(56)	475(65)	292(57)	130(50)	1(44)	25(48)
C13	387(65)	591(74)	646(81)	191(63)	133(58)	-57(57)
C14	427(71)	825(97)	812(95)	357(81)	109(67)	-106(67)
C15	457(72)	605(81)	694(86)	165(68)	178(63)	88(62)
C16	411(67)	540(72)	655(81)	165(63)	41(60)	28(58)
C17	352(60)	523(68)	288(58)	125(52)	15(47)	79(51)
C18	303(57)	467(67)	435(65)	301(56)	-8(49)	10(51)
C21	335(59)	349(57)	347(59)	126(48)	-30(47)	-53(47)
C22	346(58)	431(61)	208(52)	35(47)	-27(44)	-20(47)
C23	554(70)	411(65)	452(69)	-41(55)	-2(57)	-53(56)
C24	751(90)	421(69)	518(77)	-104(58)	-54(66)	-67(64)
C25	686(88)	484(74)	659(87)	-57(65)	-71(70)	-97(66)
C26	543(69)	497(68)	359(63)	124(55)	-119(54)	-35(57)
C27	424(64)	367(59)	378(61)	122(50)	-40(50)	-58(49)
C28	389(64)	353(58)	314(58)	141(47)	-184(48)	-154(49)
C31	324(54)	262(53)	431(62)	170(47)	-58(46)	10(43)
C32	321(57)	441(62)	341(59)	150(49)	-44(46)	-3(48)
C33	419(64)	553(69)	422(66)	163(55)	-7(52)	-40(55)
C34	356(63)	743(84)	582(77)	246(66)	-203(56)	-87(59)
C35	459(71)	685(81)	578(77)	338(66)	-38(58)	-16(61)
C36	338(61)	733(78)	390(64)	223(59)	-26(50)	-21(57)
C37	316(56)	489(64)	305(57)	191(50)	-33(46)	5(48)
C38	285(54)	374(59)	366(60)	181(48)	41(45)	60(46)

b. Anion

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	931(8)	1401(11)	1864(14)	1014(11)	-95(9)	-253(8)
I2	625(6)	635(6)	1923(13)	644(7)	-327(7)	-162(5)
I3	1744(14)	965(9)	1659(14)	364(9)	-376(11)	54(9)
I4	1775(14)	1100(10)	1465(13)	382(9)	-922(10)	-261(9)

c. Solvent Molecules of Crystallization

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
CL1	3796(118)	2131(75)	1033(47)	47(48)	90(58)	-1233(79)
CL3	1712(150)	2360(201)	3333(264)	-462(197)	-353(152)	713(146)

Table S4. Anisotropic and Isotropic Thermal Parameters $U_{i,j}$ ($x10^4$ Å^2) for Complex I (cont.).

C41	2426(243)	1879(211)	403(100)	311(123)	81(141)	209(191)
C42	1518(178)	3338(302)	564(122)	985(172)	60(119)	182(200)
C43	2069(236)	3664(330)	873(157)	1175(210)	302(159)	1086(242)
C44	1779(227)	3375(281)	1049(152)	1272(177)	340(165)	453(213)
C45	1725(185)	2446(218)	586(115)	832(144)	-50(125)	39(181)
C46	1145(132)	1568(159)	439(91)	464(107)	-84(90)	-366(120)
C47	1860(190)	1615(170)	362(89)	155(101)	-73(116)	25(153)
C48	1477(149)	1495(158)	352(84)	289(101)	-200(90)	-448(130)
C49	1947(209)	2706(247)	795(138)	954(162)	-540(144)	-1104(202)
C50	2176(218)	2086(193)	747(116)	857(126)	-635(142)	-1244(171)
C51	4094(305)	5017(327)	983(158)	1865(209)	789(215)	1917(294)
C52	3313(315)	5396(376)	656(140)	1745(215)	448(188)	1543(316)
C53	3881(321)	5339(334)	1280(178)	2398(227)	838(197)	1681(285)
C54	3632(358)	5188(364)	958(161)	1976(217)	517(223)	533(334)
C55	3896(330)	4725(326)	1190(168)	2160(223)	676(220)	328(305)
C56	3723(319)	5120(340)	1099(176)	2123(231)	582(212)	914(315)
C57	4480(389)	5775(388)	1005(174)	1598(245)	1195(254)	1851(366)
C58	4136(332)	4953(315)	1586(186)	2549(220)	1409(198)	2132(273)
C59	4354(398)	4075(336)	1509(208)	2012(238)	826(268)	1417(327)
C60	4128(379)	4010(319)	1474(186)	2118(214)	840(246)	442(321)
C61	2321(437)	1674(303)	2510(555)	-801(320)	1986(415)	-119(305)
C62	2602(403)	2387(403)	3594(504)	-478(354)	2403(394)	658(325)
C63	692(169)	4498(610)	2786(456)	-2834(433)	208(238)	488(298)
C64	1328(210)	2735(371)	1237(216)	-751(215)	62(172)	38(227)
C65	2371(298)	932(154)	1362(197)	-301(137)	1375(206)	19(169)
C71	2983(315)	1611(213)	2498(279)	414(208)	-965(263)	-151(239)
C72	2503(269)	1569(223)	2153(238)	399(181)	-958(215)	-750(201)
C73	2691(275)	1841(242)	2766(322)	-10(227)	-972(249)	-859(219)
C74	2881(289)	1438(180)	2111(244)	204(176)	-1572(230)	-994(204)
C75	3453(292)	1470(199)	1576(215)	-60(168)	-966(224)	-1019(214)
C76	3110(288)	1190(181)	1734(224)	52(164)	-670(221)	-492(199)
C77	3805(360)	1768(227)	1670(244)	-72(207)	-592(269)	-434(263)
C78	4136(342)	2166(272)	1859(289)	-940(232)	134(266)	-35(269)
C79	3821(343)	825(158)	2205(253)	148(162)	38(257)	-442(210)
C80	4153(364)	1698(225)	1615(230)	191(192)	-721(254)	-988(253)

Atom	U_{iso}	Atom	U_{iso}
CL2A	3841(244)	CL4A	2618(76)
CL2B	3537(228)	CL4B	2422(150)
CL2C	2927(198)	CL4C	3189(302)
CL2D	3031(187)		

Table S5. Bond Distances (Å) and Angles (°) for Complex **I**.

a. Cation

	Molecule A	*Molecule B*
Nb1 - N1	2.232(7)	2.237(8)
Nb1 - N3	2.190(7)	2.202(7)
Nb1 - N5	2.280(7)	2.243(7)
Nb1 - N7	2.186(8)	2.181(7)
N1 - C1	1.365(13)	1.387(11)
N1 - C8	1.450(11)	1.415(13)
N2 - C8	1.254(14)	1.295(12)
N2 - C11	1.428(13)	1.429(12)
N3 - C11	1.482(11)	1.475(12)
N3 - C18	1.345(12)	1.333(11)
N4 - C18	1.333(13)	1.321(13)
N4 - C21	1.309(14)	1.328(12)
N5 - C21	1.361(11)	1.367(11)
N5 - C28	1.428(12)	1.463(13)
N6 - C28	1.269(12)	1.243(12)
N6 - C31	1.429(10)	1.436(11)
N7 - C31	1.531(11)	1.496(13)
N7 - C38	1.311(13)	1.334(12)
N8 - C1	1.295(12)	1.307(12)
N8 - C38	1.357(11)	1.325(13)
C1 - C2	1.494(13)	1.460(15)
C2 - C3	1.378(17)	1.391(15)
C2 - C7	1.374(16)	1.351(14)
C3 - C4	1.385(16)	1.371(18)
C4 - C5	1.38(2)	1.396(19)
C5 - C6	1.37(2)	1.382(16)
C6 - C7	1.375(15)	1.385(16)
C7 - C8	1.498(16)	1.485(14)
C11 - C12	1.497(13)	1.518(12)
C11A - C11B	1.574(15)	
C12 - C13	1.393(15)	1.364(15)
C12 - C17	1.369(14)	1.365(13)
C13 - C14	1.366(18)	1.397(15)
C14 - C15	1.362(18)	1.382(18)
C15 - C16	1.390(19)	1.367(17)
C16 - C17	1.403(15)	1.392(13)
C17 - C18	1.468(15)	1.458(14)
C21 - C22	1.481(13)	1.464(12)
C22 - C23	1.400(12)	1.390(12)
C22 - C27	1.362(14)	1.364(13)
C23 - C24	1.353(18)	1.383(16)
C24 - C25	1.375(19)	1.386(18)
C25 - C26	1.381(16)	1.410(14)
C26 - C27	1.374(16)	1.394(14)
C27 - C28	1.468(11)	1.490(12)
C31 - C32	1.497(15)	1.505(13)
C31A - C31B	1.574(15)	
C32 - C33	1.375(14)	1.389(14)
C32 - C37	1.358(13)	1.355(14)

Table S5. Bond Distances (Å) and Angles (°) for Complex I (cont.).

C33 - C34	1.389(19)	1.415(16)
C34 - C35	1.380(16)	1.40(2)
C35 - C36	1.389(17)	1.361(16)
C36 - C37	1.377(16)	1.370(14)
C37 - C38	1.473(14)	1.485(13)
N5 - Nb1 - N7	73.9(3)	75.1(3)
N3 - Nb1 - N7	123.4(3)	123.5(3)
N3 - Nb1 - N5	74.3(3)	73.7(3)
N1 - Nb1 - N7	74.2(3)	74.4(3)
N1 - Nb1 - N5	110.2(3)	110.8(3)
N1 - Nb1 - N3	74.7(3)	74.4(3)
N7A - Nb1 - N7B	72.1(3)	
N7A - Nb1 - N5B	75.6(3)	
N7A - Nb1 - N3B	139.2(3)	
N7A - Nb1 - N1B	142.8(3)	
N5A - Nb1 - N7B	75.5(3)	
N5A - Nb1 - N5B	142.7(3)	
N5A - Nb1 - N3B	142.9(3)	
N5A - Nb1 - N1B	82.5(3)	
N3A - Nb1 - N7B	139.3(3)	
N3A - Nb1 - N5B	141.9(3)	
N3A - Nb1 - N3B	72.0(3)	
N3A - Nb1 - N1B	75.1(3)	
N1A - Nb1 - N7B	142.4(3)	
N1A - Nb1 - N5B	81.0(3)	
N1A - Nb1 - N3B	75.0(3)	
N1A - Nb1 - N1B	142.2(3)	
Nb1 - N1 - C8	123.5(6)	124.7(6)
Nb1 - N1 - C1	128.1(6)	129.2(6)
C1 - N1 - C8	107.0(8)	104.6(7)
C8 - N2 - C11	121.2(8)	119.8(8)
Nb1 - N3 - C18	131.9(7)	132.2(7)
Nb1 - N3 - C11	116.7(6)	115.6(6)
C11 - N3 - C18	107.4(8)	108.5(7)
C18 - N4 - C21	118.9(9)	118.6(8)
Nb1 - N5 - C28	124.2(6)	122.6(6)
Nb1 - N5 - C21	127.9(6)	129.4(6)
C21 - N5 - C28	106.8(8)	106.1(7)
C28 - N6 - C31	122.2(8)	120.4(8)
Nb1 - N7 - C38	134.0(6)	133.5(6)
Nb1 - N7 - C31	116.4(5)	116.6(6)
C31 - N7 - C38	106.2(7)	107.7(7)
C1 - N8 - C38	118.8(8)	119.4(8)
N1 - C1 - N8	130.2(9)	128.6(9)
N8 - C1 - C2	119.1(9)	120.3(8)
N1 - C1 - C2	110.7(8)	111.0(8)
C1 - C2 - C7	107.0(9)	108.0(8)
C1 - C2 - C3	131.4(9)	131.0(10)
C3 - C2 - C7	121.5(10)	121.0(9)
C2 - C3 - C4	115.9(10)	116.5(11)
C3 - C4 - C5	121.6(12)	123.1(11)
C4 - C5 - C6	122.6(12)	119.2(11)
C5 - C6 - C7	115.3(12)	117.4(10)
C2 - C7 - C6	123.1(11)	122.8(9)
C6 - C7 - C8	129.3(10)	130.9(9)

Table S5. Bond Distances (Å) and Angles (°) for Complex I (cont.).

C2 - C7 - C8	107.6(9)	106.1(8)
N2 - C8 - C7	121.4(9)	119.9(9)
N1 - C8 - C7	107.5(8)	110.0(8)
N1 - C8 - N2	131.1(9)	130.1(9)
N2 - C11 - N3	116.2(8)	118.2(8)
N3A - C11A- C11B	100.8(7)	
N2A - C11A- C11B	108.8(8)	
C12A- C11A- C11B	114.5(8)	
N3B - C11B- C11A		101.9(8)
N2B - C11B- C11A		107.9(8)
C12B- C11B- C11A		114.6(8)
N3 - C11 - C12	105.4(8)	104.0(7)
N2 - C11 - C12	111.0(8)	110.3(8)
C11 - C12 - C17	107.8(9)	107.7(8)
C11 - C12 - C13	132.0(10)	129.9(9)
C13 - C12 - C17	120.1(10)	122.3(9)
C12 - C13 - C14	117.6(11)	117.1(11)
C13 - C14 - C15	122.0(13)	120.6(10)
C14 - C15 - C16	122.3(13)	121.5(11)
C15 - C16 - C17	115.1(12)	117.4(11)
C12 - C17 - C16	122.8(10)	120.9(9)
C16 - C17 - C18	129.2(10)	131.0(10)
C12 - C17 - C18	107.9(10)	108.0(9)
N4 - C18 - C17	120.7(9)	120.0(9)
N3 - C18 - C17	110.9(9)	111.1(9)
N3 - C18 - N4	128.3(10)	128.9(8)
N4 - C21 - N5	130.3(10)	128.3(8)
N5 - C21 - C22	110.3(8)	112.0(8)
N4 - C21 - C22	119.4(9)	119.7(8)
C21 - C22 - C27	106.9(8)	106.5(8)
C21 - C22 - C23	130.6(9)	130.9(9)
C23 - C22 - C27	122.3(9)	122.3(9)
C22 - C23 - C24	115.2(10)	116.1(10)
C23 - C24 - C25	124.5(12)	122.1(11)
C24 - C25 - C26	118.6(12)	121.7(11)
C25 - C26 - C27	119.0(11)	115.0(10)
C22 - C27 - C26	120.3(9)	122.8(9)
C26 - C27 - C28	131.9(10)	128.3(9)
C22 - C27 - C28	107.7(9)	108.9(8)
N6 - C28 - C27	121.1(9)	121.6(9)
N5 - C28 - C27	108.3(8)	106.4(8)
N5 - C28 - N6	130.5(8)	131.9(9)
N7A - C31A- C31B	99.7(7)	
N6A - C31A- C31B	111.8(8)	
C32A- C31A- C31B	115.5(8)	
N7B - C31B- C31A		101.0(8)
N6B - C31B- C31A		108.6(8)
C32B- C31B- C31A		115.8(8)
N6 - C31 - N7	114.5(7)	117.7(8)
N7 - C31 - C32	103.9(7)	104.0(7)
N6 - C31 - C32	110.8(8)	109.8(8)
C31 - C32 - C37	109.5(8)	109.7(8)
C31 - C32 - C33	130.1(9)	129.2(9)
C33 - C32 - C37	120.4(9)	120.9(9)
C32 - C33 - C34	117.8(10)	115.5(10)
C33 - C34 - C35	119.8(11)	121.4(10)

Table S5. Bond Distances (Å) and Angles (°) for Complex **I** (cont.).

C34 - C35 - C36	123.4(11)	121.3(11)
C35 - C36 - C37	114.0(10)	116.4(10)
C32 - C37 - C36	124.6(9)	124.5(9)
C36 - C37 - C38	128.9(9)	128.7(9)
C32 - C37 - C38	106.5(8)	106.6(8)
N8 - C38 - C37	119.7(8)	119.8(8)
N7 - C38 - C37	113.6(8)	111.6(8)
N7 - C38 - N8	126.7(8)	128.5(8)

b. Anion

I1 - I2	2.818(2)	I3 ... I4	3.429(2)
I2 - I3	2.991(2)	I4 - I4'	2.752(2)

I1 - I2 - I3 178.1(1)

Prime denotes a transformation of 1-x, 1-y, -z.

c. Solvent Molecules of Crystallization

CL1 - C41	1.704(17)	C52 - C53	1.39(5)
CL2A - C57	1.89(8)	C53 - C54	1.39(5)
CL2A - C59	1.94(7)	C54 - C55	1.39(3)
CL2B - C52	2.06(7)	C55 - C56	1.39(3)
CL2B - C54	1.93(7)	C55 - C60	1.39(4)
CL2C - C60	1.51(5)	C56 - C57	1.39(3)
CL2D - C52	1.87(6)	C57 - C58	1.39(4)
CL3 - C63	1.45(4)	C58 - C59	1.39(5)
CL4A - C77	1.90(3)	C59 - C60	1.39(4)
CL4B - C71	1.66(5)	C61 - C62	1.38(4)
CL4C - C77	1.51(7)	C62 - C63	1.39(3)
CL4C - C78	1.78(9)	C63 - C64	1.40(4)
C41 - C42	1.389(19)	C64 - C65	1.39(4)
C41 - C46	1.392(19)	C71 - C72	1.39(3)
C42 - C43	1.39(3)	C71 - C76	1.39(3)
C43 - C44	1.39(2)	C72 - C73	1.39(3)
C44 - C45	1.390(18)	C73 - C74	1.39(3)
C45 - C46	1.390(15)	C74 - C75	1.39(3)
C45 - C50	1.39(2)	C75 - C76	1.389(19)
C46 - C47	1.390(16)	C75 - C80	1.39(3)
C47 - C48	1.39(2)	C76 - C77	1.39(2)
C48 - C49	1.39(2)	C77 - C78	1.39(3)
C49 - C50	1.39(2)	C78 - C79	1.39(3)
C51 - C52	1.39(4)	C79 - C80	1.39(3)
C51 - C56	1.39(3)		

CL1 - C41 - C46	120.4(11)	CL2A- C57 - C56	142(3)
CL1 - C41 - C42	119.5(12)	C56 - C57 - C58	120(2)
C42 - C41 - C46	119.9(13)	CL2A- C58 - C57	117(6)

Table S5. Bond Distances (Å) and Angles (°) for Complex I (cont.).

C41 - C42 - C43	120.0(12)	C57 - C58 - C59	120(2)
C42 - C43 - C44	120.0(13)	CL2A- C58 - C59	123(6)
C43 - C44 - C45	120.1(13)	C58 - C59 - C60	120(3)
C44 - C45 - C50	120.1(11)	CL2A- C59 - C60	140(3)
C44 - C45 - C46	119.9(12)	C55 - C60 - C59	120(2)
C46 - C45 - C50	120.0(11)	CL2C- C60 - C59	130(3)
C41 - C46 - C45	120.0(11)	CL2C- C60 - C55	109(3)
C45 - C46 - C47	120.0(10)	C61 - C62 - C63	120(2)
C41 - C46 - C47	119.9(11)	CL3 - C63 - C62	108.3(19)
C46 - C47 - C48	119.9(12)	C62 - C63 - C64	120(2)
C47 - C48 - C49	120.0(11)	CL3 - C63 - C64	131(2)
C48 - C49 - C50	120.0(13)	C63 - C64 - C65	119.9(19)
C45 - C50 - C49	120.0(12)	CL4B- C71 - C76	100.7(18)
CL2D- C51 - C56	148(3)	CL4B- C71 - C72	136(2)
CL2D- C51 - C52	92(3)	C72 - C71 - C76	120.0(16)
C52 - C51 - C56	120(2)	C71 - C72 - C73	120.1(18)
CL2B- C52 - C51	140(3)	C72 - C73 - C74	119.9(17)
C51 - C52 - C53	120(3)	C73 - C74 - C75	120.0(15)
CL2D- C52 - C53	160(3)	C74 - C75 - C80	120.0(14)
CL2B- C53 - C52	127(5)	C74 - C75 - C76	120.1(15)
C52 - C53 - C54	120(2)	C76 - C75 - C80	119.9(16)
CL2B- C53 - C54	113(5)	C71 - C76 - C75	119.9(15)
C53 - C54 - C55	120(2)	C75 - C76 - C77	120.1(13)
CL2B- C54 - C55	145(3)	C71 - C76 - C77	120.0(13)
C54 - C55 - C60	120(2)	CL4A- C77 - C76	109.5(13)
C54 - C55 - C56	120(2)	C76 - C77 - C78	120.0(16)
C56 - C55 - C60	120(2)	CL4A- C77 - C78	130.4(15)
C51 - C56 - C55	120(2)	C77 - C78 - C79	119.9(19)
C55 - C56 - C57	120.0(19)	C78 - C79 - C80	120.0(18)
C51 - C56 - C57	120.0(19)	C75 - C80 - C79	120.0(15)

Table S6. Relevant Structural Parameters within the Pc units in Complex I.[a]

a) dihedral angles between the isoindole units and the N_4 mean plane (°): [b]

N1,N2,C1..C8 ^ N_4	22.1(2) [23.2)2)]
N3,N4,C11..C18 ^ N_4,	23.0(2) [24.6(2)]
N5,N6,C21,C28 ^ N_4,	29.2(2) [23.5(2)]
N7,N8,C31,C38 ^ N_4,	26.7(2) [28.8(2)]

b) distances of the outmost carbon atoms of the isoindole units from the N_4 mean plane (Å):

C4...N_4,	1.850(13) [1.909(13)]	C5...N_4,	1.711(13) [1.695(14)]
C14...N_4,	0.883(16)[1.054(13)]	C15...N_4,	1.223(14) [1.383(13)]
C24...N_4,	2.390(13) [2.005(12)]	C25...N_4,	2.292(13) [1.848(13)]
C34...N_4,	1.077(13) [1.254(12)]	C35...N_4,	1.490(13) [1.681(12)]

[a] Values in square brackets refer to the B phtalocyanine unit.

[b] N_4 refers to the least-square mean plane through the N1, N3, N5, N7 nitrogen atoms.

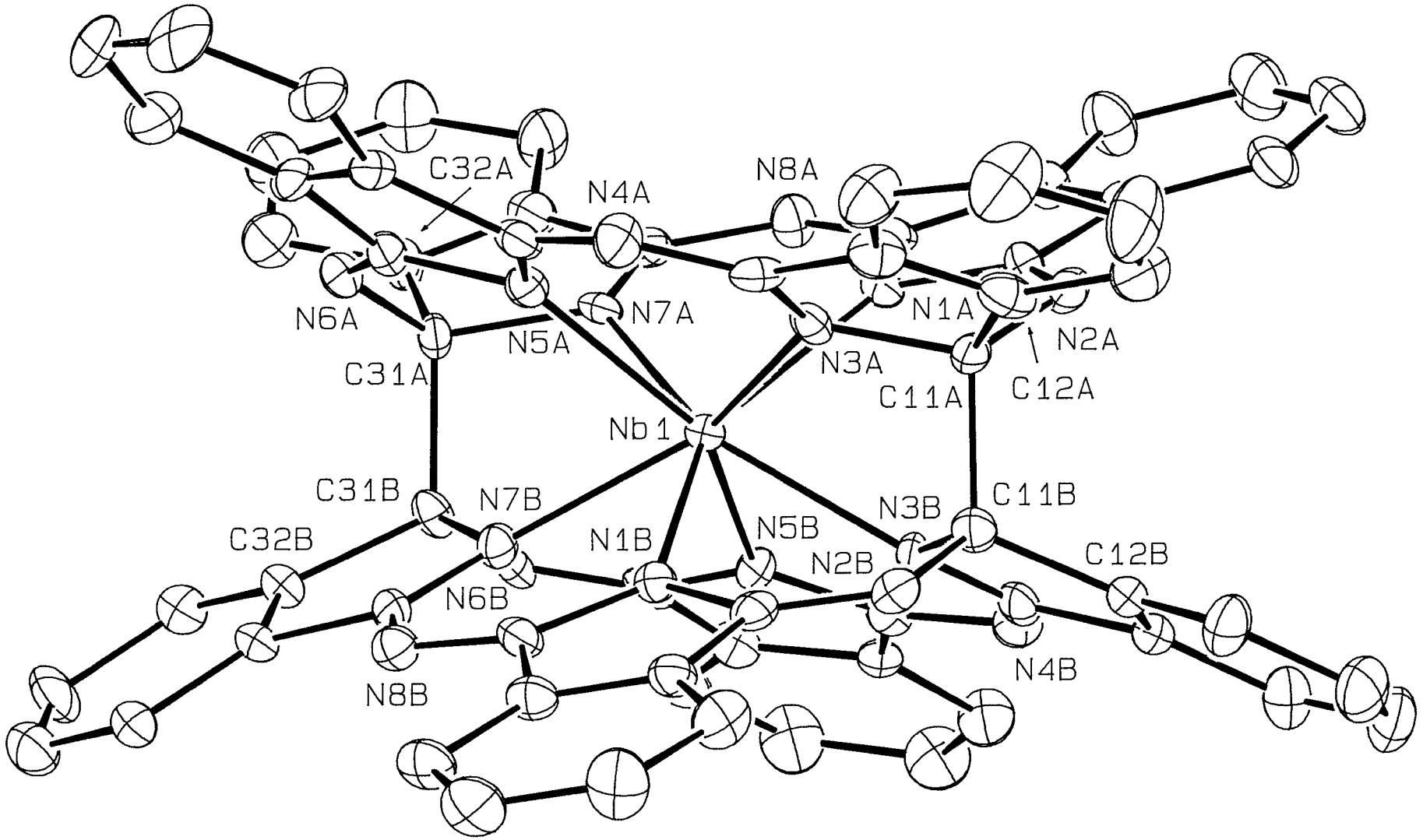
C32A
N4A
N8A
N6A
N5A
N7A
N1A
N2A
C31A
N3A
C11A
C12A
Nb1
C31B
N7B
N3B
C11B
C32B
N1B
N5B
N2B
C12B
N6B
N8B
N4B

Figure S1

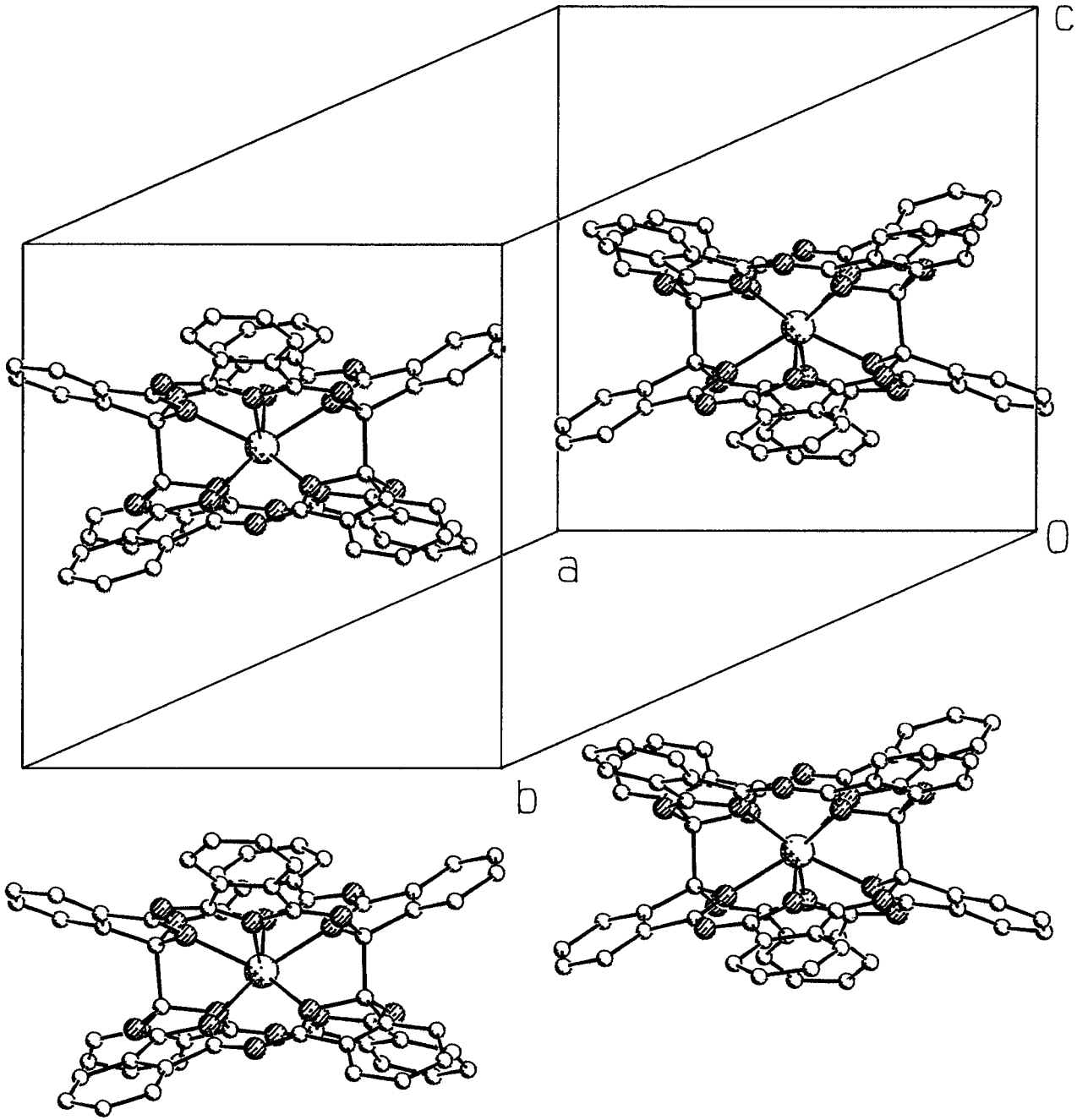

Figure S2