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Cavity-directed Synthesis of Labile Silanol Oligomers within Self-assembled Coordination Cages

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Contents

- X-ray crystal data of **1•4**.
- X-ray crystal data of **2•5a**.
- X-ray crystal data of **2•5b**.

Table 1. Crystal data and structure refinement for **1•4**.

Identification code	yoshi41	
Empirical formula	C82 H146 N36 O61 Pd6 Si	
Formula weight	3278.84	
Temperature	105(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.4526(12) Å	α = 93.6500(10)°.
	b = 17.9866(12) Å	β = 97.5560(10)°.
	c = 23.8334(16) Å	γ = 101.6860(10)°.
Volume	7231.4(8) Å ³	
Z	2	
Density (calculated)	1.506 Mg/m ³	
Absorption coefficient	0.835 mm ⁻¹	
F(000)	3336	
Crystal size	0.40 x 0.40 x 0.50 mm ³	
Theta range for data collection	1.16 to 20.82°.	
Index ranges	-16 ≤ h ≤ 17, -17 ≤ k ≤ 14, -23 ≤ l ≤ 23	
Reflections collected	26188	
Independent reflections	15040 [R(int) = 0.0328]	
Completeness to theta = 20.82°	99.4 %	
Absorption correction	Empirical (SADABS)	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15040 / 0 / 1462	
Goodness-of-fit on F ²	2.416	
Final R indices [I > 2σ(I)]	R1 = 0.0885, wR2 = 0.2751	
R indices (all data)	R1 = 0.0997, wR2 = 0.2888	
Largest diff. peak and hole	2.010 and -1.486 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **1•4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	O(5)	2268(6)	636(6)	3715(4)	68(3)
Pd(1)	-543(1)	2499(1)	423(1)	28(1)	O(005)	-4422(8)	-3039(8)	3635(6)	115(4)
Pd(2)	754(1)	-1165(1)	2869(1)	30(1)	O(006)	-4770(9)	-3317(8)	2787(6)	119(4)
Pd(3)	-13(1)	3780(1)	3626(1)	45(1)	O(6)	-2477(17)	4166(17)	1029(11)	261(12)
Pd(4)	-4514(1)	-3746(1)	1569(1)	46(1)	O(7)	-5794(6)	-1868(6)	3613(4)	83(3)
Pd(5)	-5183(1)	1338(1)	2176(1)	28(1)	O(007)	-2301(9)	2561(8)	4465(6)	117(4)
Pd(6)	-3775(1)	-2164(1)	4715(1)	38(1)	O(008)	-2938(10)	2015(10)	3677(7)	148(6)
Si(1)	-2270(2)	-1813(2)	346(1)	30(1)	O(8)	-3770(7)	3685(7)	-308(5)	94(3)
O(1)	-6239(5)	767(5)	3485(4)	57(2)	O(009)	-3565(10)	2195(9)	4367(6)	135(5)
O(001)	-729(5)	2697(5)	2084(3)	49(2)	O(9)	-1217(8)	-5337(8)	712(6)	122(5)
O(2)	-1416(5)	-1015(5)	-956(3)	57(2)	O(010)	-6388(7)	-1906(6)	1604(5)	87(3)
O(002)	153(10)	3674(10)	2402(7)	153(6)	O(10)	1656(8)	-1784(8)	4299(6)	119(4)
O(3)	-4066(5)	-1892(5)	-776(3)	56(2)	O(011)	-6028(7)	-1171(7)	2413(5)	92(3)
O(003)	2(10)	3349(10)	1594(7)	144(6)	O(11)	-2365(8)	-5166(8)	-152(5)	107(4)
O(4)	1469(5)	2355(5)	1544(3)	53(2)	O(012)	-6110(10)	-2426(10)	2364(7)	151(6)
O(004)	-3690(5)	-2494(5)	3062(3)	49(2)	O(12)	-4949(8)	2058(8)	3534(6)	117(4)

O(013)	-7862(9)	-425(9)	827(6)	133(5)	C(6C)	-4632(6)	-90(6)	1967(5)	30(3)
O(13)	-7152(9)	-3141(9)	3755(6)	135(5)	C(7A)	-249(6)	462(6)	1973(4)	28(3)
O(014)	-8651(10)	-306(9)	1420(6)	134(5)	C(7D)	-3117(5)	2365(5)	1471(4)	22(2)
O(14)	3238(9)	-1764(9)	4564(6)	130(5)	C(7C)	-4352(6)	-749(6)	2085(4)	30(3)
O(015)	-7725(10)	-904(9)	1656(7)	139(5)	C(7B)	-1507(7)	-2682(6)	2622(4)	30(3)
O(15)	3327(8)	5158(8)	4847(5)	114(4)	C(8A)	-410(5)	944(5)	2396(4)	20(2)
O(016)	-373(7)	-1894(7)	1307(5)	98(4)	C(8D)	-2668(6)	2840(6)	1937(5)	31(3)
O(16)	-3130(10)	-4052(10)	3585(7)	145(6)	C(8B)	-1755(7)	-2635(6)	3145(4)	31(3)
O(017)	513(9)	-2057(9)	807(6)	127(5)	C(8C)	-4087(6)	-818(6)	2651(4)	25(2)
O(17)	-6266(10)	-3924(10)	3122(7)	150(6)	C(9A)	-249(5)	829(6)	2960(4)	26(3)
O(018)	674(8)	-2164(8)	1708(5)	111(4)	C(9B)	-1283(6)	-2156(6)	3592(4)	31(3)
O(18)	370(10)	-2976(10)	4346(7)	154(6)	C(9D)	-2931(6)	2885(6)	2454(4)	27(3)
O(019)	-4710(5)	3028(6)	534(4)	67(3)	C(9C)	-4110(6)	-245(6)	3074(4)	33(3)
O(19)	-5935(10)	-4927(10)	3908(7)	157(6)	C(10B)	-561(6)	-1756(6)	3499(4)	30(3)
O(020)	-4054(8)	4155(8)	934(5)	112(4)	C(10A)	66(5)	200(6)	3092(4)	25(2)
O(20)	-7922(11)	-2843(11)	1466(8)	168(7)	C(10D)	-3667(6)	2454(6)	2501(4)	28(3)
O(021)	-4939(12)	3465(12)	1346(9)	175(7)	C(10C)	-4398(6)	377(6)	2920(4)	30(3)
O(21)	1596(15)	4575(14)	1849(10)	221(9)	C(11A)	-226(6)	2128(6)	3364(4)	28(3)
O(022)	854(8)	3614(8)	4928(5)	107(4)	C(11B)	-2331(6)	-2154(6)	4208(4)	30(3)
O(22)	83(13)	5850(13)	1047(9)	200(8)	C(11C)	-3908(6)	-1020(7)	3906(4)	30(3)
O(023)	1649(9)	3968(8)	5734(6)	121(5)	C(11D)	-1643(6)	3433(6)	3051(4)	29(3)
O(024)	2108(10)	3841(10)	4906(7)	145(6)	C(11)	408(7)	3987(8)	380(7)	67(4)
O(025)	-1591(5)	-1349(5)	7362(4)	62(2)	C(12A)	-395(6)	1359(6)	3421(4)	26(3)
O(026)	-1581(5)	-1882(5)	6521(4)	63(2)	C(12B)	-1534(6)	-2095(6)	4168(4)	31(3)
O(027)	-1342(6)	-2481(6)	7278(4)	81(3)	C(12D)	-2440(6)	3376(6)	2956(4)	30(3)
O(028)	-5680(14)	554(13)	875(9)	190(8)	C(12C)	-3813(6)	-318(6)	3680(4)	32(3)
O(029)	-5659(13)	-324(13)	292(9)	193(8)	C(12)	925(8)	3457(7)	252(7)	63(4)
O(030)	-4926(13)	692(13)	205(10)	194(8)	C(13C)	-3404(8)	325(7)	4050(5)	52(4)
O(101)	-1336(4)	-1853(4)	345(3)	36(2)	C(13A)	-721(6)	1119(6)	3893(4)	25(2)
O(102)	-2810(4)	-2627(4)	475(3)	40(2)	C(13D)	-2786(8)	3766(6)	3344(5)	41(3)
O(103)	-2539(4)	-1574(4)	-289(3)	37(2)	C(13B)	-998(6)	-1962(7)	4684(5)	39(3)
C(1A)	-713(6)	826(6)	236(4)	31(3)	C(14D)	-2291(10)	4184(7)	3807(5)	58(4)
C(1D)	-2238(7)	2163(7)	-87(4)	39(3)	C(14C)	-3094(9)	234(8)	4584(5)	60(4)
C(1C)	-4454(6)	-2528(7)	791(5)	35(3)	C(14A)	-852(6)	1645(6)	4297(4)	30(3)
C(1B)	-3011(7)	-4013(6)	1214(5)	36(3)	C(14B)	-1270(6)	-1901(7)	5190(4)	38(3)
C(2A)	-707(5)	96(6)	364(4)	29(3)	C(15C)	-3246(8)	-495(7)	4776(5)	48(3)
C(2C)	-4435(6)	-1794(8)	647(5)	45(3)	C(15D)	-1492(8)	4218(7)	3876(5)	45(3)
C(2D)	-3061(7)	2003(7)	-95(5)	44(3)	C(15A)	-653(7)	2419(7)	4207(5)	41(3)
C(2B)	-2210(8)	-3940(6)	1235(4)	42(3)	C(15B)	-2085(6)	-1978(6)	5204(5)	36(3)
C(3A)	-545(6)	-40(6)	929(4)	28(3)	C(21)	2465(8)	-993(8)	2978(6)	65(4)
C(3D)	-3356(6)	2079(6)	401(4)	32(3)	C(22)	2118(7)	-1828(8)	2814(7)	64(4)
C(3C)	-4401(6)	-1221(7)	1055(5)	40(3)	C(31)	1597(10)	4488(11)	3578(11)	120(8)
C(3B)	-1715(7)	-3520(6)	1691(5)	37(3)	C(32)	1201(13)	5052(11)	3475(14)	175(14)
C(4C)	-4374(6)	-1337(6)	1626(4)	28(3)	C(41)	-6097(14)	-4665(12)	1573(11)	124(8)
C(4A)	-408(5)	570(6)	1357(4)	24(2)	C(42)	-5586(13)	-4992(9)	1894(8)	95(6)
C(4D)	-2841(6)	2285(5)	914(4)	23(2)	C(51)	-6882(7)	1137(10)	2016(6)	66(5)
C(4B)	-2021(7)	-3155(6)	2114(4)	33(3)	C(52)	-6576(7)	1949(9)	2197(6)	60(4)
C(5A)	-428(5)	1295(6)	1192(4)	21(2)	C(61)	-4750(9)	-3385(12)	5160(9)	129(10)
C(5D)	-2040(6)	2394(5)	890(4)	26(2)	C(62)	-5301(9)	-3090(9)	4784(8)	88(6)
C(5C)	-4396(6)	-2109(6)	1740(4)	32(3)	C(101)	-2382(6)	-1088(5)	904(4)	28(3)
C(5B)	-2834(7)	-3233(6)	2053(4)	34(3)	C(102)	-2228(6)	-1173(6)	1466(5)	34(3)
C(6A)	68(5)	-147(5)	2143(4)	22(2)	C(103)	-2255(6)	-606(5)	1919(4)	25(2)
C(6B)	-784(7)	-2261(6)	2563(5)	33(3)	C(104)	-2108(6)	-722(6)	2496(4)	33(3)
C(6D)	-3855(6)	1942(6)	1562(4)	26(2)	C(105)	-2162(6)	-171(6)	2897(5)	37(3)

C(106)	-2340(6)	528(6)	2745(5)	35(3)	N(004)	-6167(9)	-1773(10)	2158(6)	94(4)
C(107)	-2485(6)	649(7)	2187(5)	44(3)	N(005)	-8141(8)	-487(7)	1387(5)	66(3)
C(108)	-2444(6)	87(6)	1753(5)	31(3)	N(006)	281(7)	-2045(6)	1233(5)	54(3)
C(109)	-2602(6)	182(6)	1169(5)	36(3)	N(007)	-4595(9)	3546(9)	905(7)	96(4)
C(110)	-2568(6)	-375(6)	765(5)	32(3)	N(008)	1541(11)	3851(10)	5174(8)	114(5)
N(1D)	-1730(5)	2335(5)	396(4)	33(2)	N(009)	-1502(7)	-1915(7)	7078(5)	64(3)
N(001)	-244(6)	3219(6)	2019(4)	47(3)	N(010)	-5266(9)	498(8)	601(6)	81(4)
N(1A)	-569(5)	1425(5)	641(3)	25(2)	N(11)	-416(5)	3583(6)	201(5)	47(3)
N(1B)	-3328(6)	-3665(5)	1611(4)	35(2)	N(12)	650(5)	2709(5)	474(4)	32(2)
N(1C)	-4438(5)	-2676(5)	1350(4)	33(2)	N(21)	1832(5)	-560(6)	2752(4)	39(2)
N(002)	-4265(6)	-2976(5)	3148(4)	39(2)	N(22)	1339(6)	-2015(6)	3008(4)	44(2)
N(2A)	222(5)	-283(5)	2692(3)	25(2)	N(31)	1145(6)	3749(6)	3720(5)	65(3)
N(2B)	-312(5)	-1808(5)	2992(4)	29(2)	N(32)	357(8)	4879(6)	3487(6)	76(4)
N(2D)	-4119(5)	2003(5)	2057(3)	27(2)	N(41)	-5723(7)	-3855(7)	1544(6)	86(5)
N(2C)	-4662(5)	452(5)	2371(4)	28(2)	N(42)	-4715(9)	-4812(6)	1771(6)	86(5)
N(3B)	-2609(5)	-2092(5)	4713(4)	30(2)	N(51)	-6270(5)	702(6)	2251(4)	40(2)
N(003)	-2917(9)	2272(8)	4173(6)	82(4)	N(52)	-5772(5)	2175(6)	2034(4)	41(2)
N(3A)	-338(5)	2657(5)	3754(4)	36(2)	N(61)	-3942(6)	-3208(6)	4998(5)	59(3)
N(3C)	-3647(5)	-1108(5)	4443(4)	32(2)	N(62)	-4954(6)	-2282(8)	4711(5)	69(4)
N(3D)	-1172(6)	3832(5)	3510(4)	36(2)					

Table 3. Bond lengths [Å] and angles [°] for **1•4**.

Pd(1)-N(1A)	2.025(8)	O(002)-N(001)	1.221(18)	C(1A)-N(1A)	1.362(14)
Pd(1)-N(1D)	2.025(9)	O(003)-N(001)	1.169(17)	C(1A)-C(2A)	1.368(15)
Pd(1)-N(12)	2.025(8)	O(004)-N(002)	1.234(11)	C(1D)-N(1D)	1.336(14)
Pd(1)-N(11)	2.030(9)	O(005)-N(002)	1.235(15)	C(1D)-C(2D)	1.403(16)
Pd(2)-N(22)	2.024(10)	O(006)-N(002)	1.186(15)	C(1C)-N(1C)	1.372(14)
Pd(2)-N(21)	2.037(9)	O(007)-N(003)	1.202(16)	C(1C)-C(2C)	1.381(17)
Pd(2)-N(2A)	2.032(8)	O(008)-N(003)	1.236(18)	C(1B)-N(1B)	1.340(14)
Pd(2)-N(2B)	2.050(9)	O(009)-N(003)	1.261(18)	C(1B)-C(2B)	1.370(17)
Pd(3)-N(32)	2.015(11)	O(010)-N(004)	1.318(16)	C(2A)-C(3A)	1.388(14)
Pd(3)-N(31)	2.015(11)	O(011)-N(004)	1.172(17)	C(2C)-C(3C)	1.359(17)
Pd(3)-N(3D)	2.027(9)	O(012)-N(004)	1.32(2)	C(2D)-C(3D)	1.360(15)
Pd(3)-N(3A)	2.038(9)	O(013)-N(005)	1.481(18)	C(2B)-C(3B)	1.371(16)
Pd(4)-N(42)	1.981(11)	O(014)-N(005)	1.019(16)	C(3A)-C(4A)	1.409(14)
Pd(4)-N(1C)	2.009(9)	O(015)-N(005)	1.288(18)	C(3D)-C(4D)	1.400(14)
Pd(4)-N(1B)	2.035(10)	O(016)-N(006)	1.256(14)	C(3C)-C(4C)	1.386(15)
Pd(4)-N(41)	2.072(12)	O(017)-N(006)	1.143(16)	C(3B)-C(4B)	1.390(15)
Pd(5)-N(52)	2.011(9)	O(018)-N(006)	1.298(15)	C(4C)-C(5C)	1.425(15)
Pd(5)-N(2C)	2.037(8)	O(019)-N(007)	1.209(16)	C(4C)-C(7C)	1.464(15)
Pd(5)-N(51)	2.045(9)	O(020)-N(007)	1.284(18)	C(4A)-C(5A)	1.391(14)
Pd(5)-N(2D)	2.059(8)	O(021)-N(007)	1.28(2)	C(4A)-C(7A)	1.490(14)
Pd(6)-N(61)	2.014(10)	O(022)-N(008)	1.241(19)	C(4D)-C(5D)	1.382(14)
Pd(6)-N(3B)	2.015(8)	O(023)-N(008)	1.320(19)	C(4D)-C(7D)	1.479(14)
Pd(6)-N(3C)	2.025(9)	O(024)-N(008)	1.25(2)	C(4B)-C(5B)	1.384(16)
Pd(6)-N(62)	2.023(10)	O(025)-N(009)	1.233(13)	C(4B)-C(7B)	1.506(16)
Si(1)-O(103)	1.635(8)	O(026)-N(009)	1.323(13)	C(5A)-N(1A)	1.349(12)
Si(1)-O(102)	1.644(8)	O(027)-N(009)	1.219(14)	C(5D)-N(1D)	1.363(13)
Si(1)-O(101)	1.646(8)	O(028)-N(010)	1.05(2)	C(5C)-N(1C)	1.319(13)
Si(1)-C(101)	1.860(11)	O(029)-N(010)	1.59(2)	C(5B)-N(1B)	1.356(13)
O(001)-N(001)	1.163(12)	O(030)-N(010)	1.21(2)	C(6A)-N(2A)	1.349(12)

C(6A)-C(7A)	1.384(14)	C(11A)-N(3A)	1.347(13)	C(21)-C(22)	1.508(19)
C(6B)-N(2B)	1.338(14)	C(11A)-C(12A)	1.374(15)	C(21)-N(21)	1.537(15)
C(6B)-C(7B)	1.363(15)	C(11B)-N(3B)	1.361(13)	C(22)-N(22)	1.474(16)
C(6D)-N(2D)	1.330(13)	C(11B)-C(12B)	1.391(15)	C(31)-C(32)	1.36(3)
C(6D)-C(7D)	1.407(14)	C(11C)-N(3C)	1.331(13)	C(31)-N(31)	1.49(2)
C(6C)-N(2C)	1.339(14)	C(11C)-C(12C)	1.390(15)	C(32)-N(32)	1.45(3)
C(6C)-C(7C)	1.402(15)	C(11D)-N(3D)	1.347(13)	C(41)-C(42)	1.35(3)
C(7A)-C(8A)	1.382(14)	C(11D)-C(12D)	1.362(15)	C(41)-N(41)	1.48(2)
C(7D)-C(8D)	1.399(14)	C(11)-N(11)	1.467(16)	C(42)-N(42)	1.56(2)
C(7C)-C(8C)	1.387(14)	C(11)-C(12)	1.484(18)	C(51)-C(52)	1.47(2)
C(7B)-C(8B)	1.376(15)	C(12A)-C(13A)	1.382(14)	C(51)-N(51)	1.518(16)
C(8A)-C(9A)	1.373(13)	C(12B)-C(13B)	1.419(15)	C(52)-N(52)	1.489(15)
C(8D)-C(9D)	1.373(14)	C(12D)-C(13D)	1.397(16)	C(61)-C(62)	1.43(2)
C(8B)-C(9B)	1.386(15)	C(12C)-C(13C)	1.413(16)	C(61)-N(61)	1.49(2)
C(8C)-C(9C)	1.406(15)	C(12)-N(12)	1.489(15)	C(62)-N(62)	1.487(18)
C(9A)-C(10A)	1.391(14)	C(13C)-C(14C)	1.349(17)	C(101)-C(102)	1.357(14)
C(9A)-C(12A)	1.490(14)	C(13A)-C(14A)	1.380(14)	C(101)-C(110)	1.433(15)
C(9B)-C(10B)	1.370(15)	C(13D)-C(14D)	1.381(18)	C(102)-C(103)	1.449(14)
C(9B)-C(12B)	1.499(15)	C(13B)-C(14B)	1.358(15)	C(103)-C(104)	1.401(14)
C(9D)-C(10D)	1.384(15)	C(14D)-C(15D)	1.370(18)	C(103)-C(108)	1.419(15)
C(9D)-C(12D)	1.494(15)	C(14C)-C(15C)	1.402(18)	C(104)-C(105)	1.359(15)
C(9C)-C(10C)	1.369(15)	C(14A)-C(15A)	1.402(16)	C(105)-C(106)	1.413(16)
C(9C)-C(12C)	1.493(15)	C(14B)-C(15B)	1.407(15)	C(106)-C(107)	1.360(16)
C(10B)-N(2B)	1.341(13)	C(15C)-N(3C)	1.330(15)	C(107)-C(108)	1.418(16)
C(10A)-N(2A)	1.341(13)	C(15D)-N(3D)	1.329(15)	C(108)-C(109)	1.410(15)
C(10D)-N(2D)	1.345(13)	C(15A)-N(3A)	1.331(14)	C(109)-C(110)	1.361(15)
C(10C)-N(2C)	1.354(13)	C(15B)-N(3B)	1.363(13)		
N(1A)-Pd(1)-N(1D)	90.6(3)	N(2C)-Pd(5)-N(51)	91.1(4)	C(2C)-C(3C)-C(4C)	122.5(11)
N(1A)-Pd(1)-N(12)	91.2(3)	N(52)-Pd(5)-N(2D)	93.2(3)	C(2B)-C(3B)-C(4B)	120.4(11)
N(1D)-Pd(1)-N(12)	177.3(4)	N(2C)-Pd(5)-N(2D)	91.5(3)	C(3C)-C(4C)-C(5C)	113.9(10)
N(1A)-Pd(1)-N(11)	175.1(3)	N(51)-Pd(5)-N(2D)	176.6(3)	C(3C)-C(4C)-C(7C)	125.2(10)
N(1D)-Pd(1)-N(11)	94.3(4)	N(61)-Pd(6)-N(3B)	93.4(4)	C(5C)-C(4C)-C(7C)	120.9(9)
N(12)-Pd(1)-N(11)	83.9(4)	N(61)-Pd(6)-N(3C)	177.7(4)	C(5A)-C(4A)-C(3A)	118.2(9)
N(22)-Pd(2)-N(21)	84.1(4)	N(3B)-Pd(6)-N(3C)	88.7(3)	C(5A)-C(4A)-C(7A)	119.4(9)
N(22)-Pd(2)-N(2A)	176.0(4)	N(61)-Pd(6)-N(62)	84.5(5)	C(3A)-C(4A)-C(7A)	122.4(9)
N(21)-Pd(2)-N(2A)	92.4(3)	N(3B)-Pd(6)-N(62)	177.6(5)	C(5D)-C(4D)-C(3D)	117.2(9)
N(22)-Pd(2)-N(2B)	93.8(4)	N(3C)-Pd(6)-N(62)	93.4(4)	C(5D)-C(4D)-C(7D)	119.6(9)
N(21)-Pd(2)-N(2B)	177.9(3)	O(103)-Si(1)-O(102)	112.5(4)	C(3D)-C(4D)-C(7D)	123.1(9)
N(2A)-Pd(2)-N(2B)	89.7(3)	O(103)-Si(1)-O(101)	103.4(4)	C(5B)-C(4B)-C(3B)	117.4(10)
N(32)-Pd(3)-N(31)	84.9(5)	O(102)-Si(1)-O(101)	112.3(4)	C(5B)-C(4B)-C(7B)	119.8(10)
N(32)-Pd(3)-N(3D)	93.6(4)	O(103)-Si(1)-C(101)	110.9(4)	C(3B)-C(4B)-C(7B)	122.8(11)
N(31)-Pd(3)-N(3D)	178.2(4)	O(102)-Si(1)-C(101)	106.2(4)	N(1A)-C(5A)-C(4A)	122.0(9)
N(32)-Pd(3)-N(3A)	177.2(5)	O(101)-Si(1)-C(101)	111.7(4)	N(1D)-C(5D)-C(4D)	123.8(9)
N(31)-Pd(3)-N(3A)	92.5(4)	N(1A)-C(1A)-C(2A)	122.6(9)	N(1C)-C(5C)-C(4C)	124.7(9)
N(3D)-Pd(3)-N(3A)	88.9(4)	N(1D)-C(1D)-C(2D)	122.4(10)	N(1B)-C(5B)-C(4B)	122.5(10)
N(42)-Pd(4)-N(1C)	173.8(5)	N(1C)-C(1C)-C(2C)	119.7(10)	N(2A)-C(6A)-C(7A)	123.3(9)
N(42)-Pd(4)-N(1B)	93.7(5)	N(1B)-C(1B)-C(2B)	122.5(10)	N(2B)-C(6B)-C(7B)	122.5(10)
N(1C)-Pd(4)-N(1B)	92.5(3)	C(1A)-C(2A)-C(3A)	118.8(10)	N(2D)-C(6D)-C(7D)	122.0(10)
N(42)-Pd(4)-N(41)	84.7(6)	C(3C)-C(2C)-C(1C)	120.2(11)	N(2C)-C(6C)-C(7C)	123.1(9)
N(1C)-Pd(4)-N(41)	89.2(5)	C(3D)-C(2D)-C(1D)	119.1(10)	C(8A)-C(7A)-C(6A)	116.8(9)
N(1B)-Pd(4)-N(41)	178.2(5)	C(1B)-C(2B)-C(3B)	118.9(11)	C(8A)-C(7A)-C(4A)	123.1(9)
N(52)-Pd(5)-N(2C)	174.4(3)	C(2A)-C(3A)-C(4A)	119.5(10)	C(6A)-C(7A)-C(4A)	120.0(9)
N(52)-Pd(5)-N(51)	84.3(4)	C(2D)-C(3D)-C(4D)	120.0(10)	C(8D)-C(7D)-C(6D)	116.2(9)

C(8D)-C(7D)-C(4D)	123.1(9)	N(3C)-C(15C)-C(14C)	122.5(10)	C(6D)-N(2D)-C(10D)	120.5(9)
C(6D)-C(7D)-C(4D)	120.7(9)	N(3D)-C(15D)-C(14D)	121.1(11)	C(6D)-N(2D)-Pd(5)	120.3(7)
C(6C)-C(7C)-C(8C)	116.8(10)	N(3A)-C(15A)-C(14A)	122.4(10)	C(10D)-N(2D)-Pd(5)	119.0(7)
C(6C)-C(7C)-C(4C)	120.1(9)	N(3B)-C(15B)-C(14B)	120.7(10)	C(6C)-N(2C)-C(10C)	119.4(9)
C(8C)-C(7C)-C(4C)	123.1(10)	C(22)-C(21)-N(21)	106.6(10)	C(6C)-N(2C)-Pd(5)	120.7(6)
C(6B)-C(7B)-C(8B)	118.2(10)	N(22)-C(22)-C(21)	108.3(11)	C(10C)-N(2C)-Pd(5)	119.7(7)
C(6B)-C(7B)-C(4B)	119.6(10)	C(32)-C(31)-N(31)	118.1(17)	C(11B)-N(3B)-C(15B)	118.8(9)
C(8B)-C(7B)-C(4B)	122.1(10)	C(31)-C(32)-N(32)	117.3(16)	C(11B)-N(3B)-Pd(6)	119.4(7)
C(9A)-C(8A)-C(7A)	121.4(9)	C(42)-C(41)-N(41)	108.9(17)	C(15B)-N(3B)-Pd(6)	121.9(7)
C(9D)-C(8D)-C(7D)	121.7(9)	C(41)-C(42)-N(42)	116.0(15)	O(007)-N(003)-O(008)	121.2(17)
C(7B)-C(8B)-C(9B)	120.1(10)	C(52)-C(51)-N(51)	108.1(10)	O(007)-N(003)-O(009)	121.3(16)
C(7C)-C(8C)-C(9C)	120.3(10)	C(51)-C(52)-N(52)	108.4(11)	O(008)-N(003)-O(009)	117.5(16)
C(8A)-C(9A)-C(10A)	117.8(9)	C(62)-C(61)-N(61)	111.5(12)	C(15A)-N(3A)-C(11A)	118.2(10)
C(8A)-C(9A)-C(12A)	121.9(9)	C(61)-C(62)-N(62)	109.1(12)	C(15A)-N(3A)-Pd(3)	123.1(8)
C(10A)-C(9A)-C(12A)	120.3(9)	C(102)-C(101)-C(110)	116.0(10)	C(11A)-N(3A)-Pd(3)	118.7(7)
C(10B)-C(9B)-C(8B)	118.0(10)	C(102)-C(101)-Si(1)	122.1(8)	C(15C)-N(3C)-C(11C)	118.2(10)
C(10B)-C(9B)-C(12B)	120.5(9)	C(110)-C(101)-Si(1)	121.7(8)	C(15C)-N(3C)-Pd(6)	121.4(7)
C(8B)-C(9B)-C(12B)	121.4(10)	C(101)-C(102)-C(103)	124.6(10)	C(11C)-N(3C)-Pd(6)	120.2(8)
C(8D)-C(9D)-C(10D)	117.9(10)	C(104)-C(103)-C(108)	120.5(9)	C(15D)-N(3D)-C(11D)	118.6(10)
C(8D)-C(9D)-C(12D)	121.7(9)	C(104)-C(103)-C(102)	122.8(9)	C(15D)-N(3D)-Pd(3)	123.1(8)
C(10D)-C(9D)-C(12D)	120.3(9)	C(108)-C(103)-C(102)	116.7(9)	C(11D)-N(3D)-Pd(3)	118.2(7)
C(10C)-C(9C)-C(8C)	119.0(9)	C(105)-C(104)-C(103)	119.5(10)	O(011)-N(004)-O(012)	126.7(17)
C(10C)-C(9C)-C(12C)	121.2(10)	C(104)-C(105)-C(106)	121.2(11)	O(011)-N(004)-O(010)	125.0(16)
C(8C)-C(9C)-C(12C)	119.9(9)	C(107)-C(106)-C(105)	119.9(10)	O(012)-N(004)-O(010)	108.2(15)
N(2B)-C(10B)-C(9B)	122.1(10)	C(106)-C(107)-C(108)	120.8(11)	O(014)-N(005)-O(015)	137.3(18)
N(2A)-C(10A)-C(9A)	122.4(9)	C(109)-C(108)-C(103)	119.2(9)	O(014)-N(005)-O(013)	115.5(16)
N(2D)-C(10D)-C(9D)	121.6(9)	C(109)-C(108)-C(107)	122.8(10)	O(015)-N(005)-O(013)	105.5(13)
N(2C)-C(10C)-C(9C)	121.5(10)	C(103)-C(108)-C(107)	118.0(10)	O(017)-N(006)-O(016)	124.7(14)
N(3A)-C(11A)-C(12A)	123.4(10)	C(110)-C(109)-C(108)	121.2(10)	O(017)-N(006)-O(018)	124.0(14)
N(3B)-C(11B)-C(12B)	123.1(9)	C(109)-C(110)-C(101)	122.4(10)	O(016)-N(006)-O(018)	111.3(12)
N(3C)-C(11C)-C(12C)	123.7(10)	C(1D)-N(1D)-C(5D)	117.3(9)	O(019)-N(007)-O(020)	124.1(16)
N(3D)-C(11D)-C(12D)	123.2(10)	C(1D)-N(1D)-Pd(1)	123.1(7)	O(019)-N(007)-O(021)	120.3(18)
N(11)-C(11)-C(12)	107.8(12)	C(5D)-N(1D)-Pd(1)	119.6(7)	O(020)-N(007)-O(021)	114.9(17)
C(11A)-C(12A)-C(13A)	117.9(9)	O(001)-N(001)-O(003)	126.2(13)	O(024)-N(008)-O(022)	119.7(19)
C(11A)-C(12A)-C(9A)	118.4(9)	O(001)-N(001)-O(002)	124.6(13)	O(024)-N(008)-O(023)	121.4(19)
C(13A)-C(12A)-C(9A)	123.6(9)	O(003)-N(001)-O(002)	108.8(15)	O(022)-N(008)-O(023)	117.7(18)
C(11B)-C(12B)-C(13B)	117.1(10)	C(5A)-N(1A)-C(1A)	118.8(8)	O(027)-N(009)-O(025)	124.3(12)
C(11B)-C(12B)-C(9B)	119.2(9)	C(5A)-N(1A)-Pd(1)	120.3(7)	O(027)-N(009)-O(026)	119.5(12)
C(13B)-C(12B)-C(9B)	123.7(10)	C(1A)-N(1A)-Pd(1)	120.8(7)	O(025)-N(009)-O(026)	116.1(11)
C(11D)-C(12D)-C(13D)	118.6(10)	C(1B)-N(1B)-C(5B)	118.4(10)	O(028)-N(010)-O(030)	151(2)
C(11D)-C(12D)-C(9D)	120.1(9)	C(1B)-N(1B)-Pd(4)	122.6(8)	O(028)-N(010)-O(029)	99.8(19)
C(13D)-C(12D)-C(9D)	121.2(10)	C(5B)-N(1B)-Pd(4)	119.0(8)	O(030)-N(010)-O(029)	93.0(16)
C(11C)-C(12C)-C(13C)	116.8(10)	C(5C)-N(1C)-C(1C)	119.0(10)	C(11)-N(11)-Pd(1)	108.9(7)
C(11C)-C(12C)-C(9C)	122.0(10)	C(5C)-N(1C)-Pd(4)	120.4(7)	C(12)-N(12)-Pd(1)	109.0(7)
C(13C)-C(12C)-C(9C)	121.2(10)	C(1C)-N(1C)-Pd(4)	120.5(8)	C(21)-N(21)-Pd(2)	108.4(8)
C(11)-C(12)-N(12)	110.2(10)	O(006)-N(002)-O(005)	114.1(12)	C(22)-N(22)-Pd(2)	110.1(8)
C(14C)-C(13C)-C(12C)	119.7(11)	O(006)-N(002)-O(004)	124.7(11)	C(31)-N(31)-Pd(3)	108.6(10)
C(14A)-C(13A)-C(12A)	120.2(10)	O(005)-N(002)-O(004)	120.1(11)	C(32)-N(32)-Pd(3)	110.5(10)
C(14D)-C(13D)-C(12D)	117.3(12)	C(6A)-N(2A)-C(10A)	118.2(8)	C(41)-N(41)-Pd(4)	109.4(13)
C(14B)-C(13B)-C(12B)	120.2(10)	C(6A)-N(2A)-Pd(2)	118.0(6)	C(42)-N(42)-Pd(4)	105.7(10)
C(13D)-C(14D)-C(15D)	121.1(12)	C(10A)-N(2A)-Pd(2)	123.6(7)	C(51)-N(51)-Pd(5)	107.2(8)
C(13C)-C(14C)-C(15C)	118.9(12)	C(6B)-N(2B)-C(10B)	119.0(9)	C(52)-N(52)-Pd(5)	109.2(7)
C(13A)-C(14A)-C(15A)	117.9(10)	C(6B)-N(2B)-Pd(2)	120.7(7)	C(61)-N(61)-Pd(6)	107.7(9)
C(13B)-C(14B)-C(15B)	120.0(10)	C(10B)-N(2B)-Pd(2)	120.3(7)	C(62)-N(62)-Pd(6)	108.8(10)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1•4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pd(1)	25(1)	30(1)	34(1)	7(1)	12(1)	13(1)
Pd(2)	30(1)	29(1)	35(1)	2(1)	7(1)	16(1)
Pd(3)	47(1)	25(1)	54(1)	-2(1)	-14(1)	7(1)
Pd(4)	53(1)	29(1)	50(1)	-12(1)	14(1)	-9(1)
Pd(5)	19(1)	37(1)	33(1)	15(1)	8(1)	9(1)
Pd(6)	28(1)	48(1)	39(1)	23(1)	5(1)	6(1)
Si(1)	29(2)	24(2)	38(2)	5(1)	12(1)	5(1)
C(1A)	24(6)	39(8)	32(6)	18(6)	7(5)	8(5)
C(1D)	44(8)	53(8)	23(6)	2(5)	13(6)	16(6)
C(1C)	25(6)	46(8)	33(7)	-12(6)	-4(5)	10(5)
C(1B)	56(9)	19(7)	29(6)	-3(5)	-2(6)	2(6)
C(2A)	17(6)	33(7)	33(7)	-12(5)	7(5)	-2(5)
C(2C)	29(7)	75(11)	30(7)	0(7)	4(5)	11(6)
C(2D)	37(8)	64(9)	37(7)	5(6)	1(6)	24(6)
C(2B)	76(10)	27(7)	25(6)	-2(5)	2(6)	23(6)
C(3A)	23(6)	32(7)	33(7)	11(5)	10(5)	7(5)
C(3D)	23(6)	41(7)	35(7)	8(5)	11(5)	7(5)
C(3C)	27(6)	51(8)	48(8)	23(7)	15(5)	13(6)
C(3B)	47(7)	27(7)	44(7)	16(6)	16(6)	17(6)
C(4C)	22(6)	40(8)	25(6)	15(5)	5(4)	6(5)
C(4A)	15(5)	24(7)	32(6)	-9(5)	8(4)	2(4)
C(4D)	24(6)	16(6)	33(6)	3(5)	7(5)	11(5)
C(4B)	56(8)	17(6)	35(7)	14(5)	12(6)	20(6)
C(5A)	29(6)	22(7)	19(6)	4(4)	12(4)	13(5)
C(5D)	26(6)	21(6)	34(6)	9(5)	10(5)	10(5)
C(5C)	28(6)	44(8)	24(6)	3(6)	1(5)	9(5)
C(5B)	51(8)	18(6)	31(6)	-3(5)	-1(6)	11(5)
C(6A)	25(6)	18(6)	23(6)	1(5)	4(4)	8(5)
C(6B)	41(7)	29(7)	36(7)	10(6)	8(6)	18(6)
C(6D)	24(6)	27(6)	33(6)	15(5)	10(5)	11(5)
C(6C)	20(6)	32(7)	35(6)	15(6)	-7(5)	5(5)
C(7A)	22(6)	35(7)	28(6)	1(5)	11(5)	3(5)
C(7D)	21(6)	12(6)	34(6)	1(5)	1(5)	8(5)
C(7C)	20(6)	35(7)	34(7)	7(5)	8(5)	-3(5)
C(7B)	50(8)	13(6)	32(7)	5(5)	3(5)	17(6)
C(8A)	16(5)	16(6)	26(6)	3(5)	3(4)	1(4)
C(8D)	25(6)	25(7)	55(8)	20(6)	24(6)	11(5)
C(8B)	41(7)	24(6)	30(7)	8(5)	2(5)	11(5)
C(8C)	26(6)	28(6)	21(6)	2(5)	5(4)	3(5)
C(9A)	12(5)	31(7)	34(7)	0(5)	5(4)	1(5)
C(9B)	39(7)	24(6)	35(7)	4(5)	1(5)	20(6)
C(9D)	26(6)	20(6)	41(7)	3(5)	10(5)	15(5)
C(9C)	22(6)	37(7)	42(7)	14(6)	12(5)	3(5)
C(10B)	38(7)	17(6)	34(7)	5(5)	8(5)	4(5)
C(10A)	18(5)	29(7)	30(6)	10(5)	6(4)	7(5)
C(10D)	35(7)	21(6)	35(6)	4(5)	14(5)	14(5)
C(10C)	29(6)	38(7)	26(6)	2(5)	3(5)	12(5)

C(11A)	38(6)	20(7)	27(6)	-4(5)	1(5)	13(5)
C(11B)	28(7)	22(6)	35(7)	9(5)	-5(5)	1(5)
C(11C)	15(5)	43(8)	36(7)	7(5)	4(5)	11(5)
C(11D)	37(7)	14(6)	37(7)	0(5)	13(6)	3(5)
C(11)	38(8)	64(10)	114(12)	52(9)	27(8)	24(7)
C(12A)	29(6)	31(7)	20(6)	-5(5)	-3(5)	21(5)
C(12B)	42(7)	21(6)	31(6)	2(5)	5(5)	7(5)
C(12D)	39(7)	24(6)	33(6)	8(5)	9(5)	14(5)
C(12C)	39(7)	27(7)	33(6)	6(6)	6(5)	14(5)
C(12)	55(9)	29(8)	118(12)	11(8)	37(8)	17(7)
C(13C)	81(10)	29(8)	47(8)	8(6)	-9(7)	27(7)
C(13A)	24(6)	20(6)	34(6)	9(5)	1(5)	14(5)
C(13D)	61(8)	28(7)	41(7)	13(6)	24(7)	14(6)
C(13B)	26(6)	47(8)	43(8)	11(6)	-1(6)	7(6)
C(14D)	107(13)	35(8)	41(8)	-7(6)	13(8)	35(8)
C(14C)	83(10)	48(10)	50(9)	1(7)	-7(7)	27(8)
C(14A)	24(6)	33(7)	35(6)	3(6)	6(5)	10(5)
C(14B)	31(7)	58(8)	23(6)	2(5)	-2(5)	12(6)
C(15C)	69(9)	51(9)	26(6)	3(7)	1(6)	18(7)
C(15D)	63(9)	37(8)	40(7)	-6(6)	-5(6)	31(7)
C(15A)	48(7)	48(9)	32(7)	-7(6)	2(6)	27(6)
C(15B)	40(8)	31(7)	34(7)	1(5)	4(6)	2(5)
C(21)	40(8)	67(11)	89(11)	-10(8)	-7(7)	31(7)
C(22)	29(7)	71(11)	103(11)	5(9)	17(7)	31(7)
C(31)	55(11)	85(15)	220(20)	63(15)	10(13)	-2(10)
C(32)	104(18)	54(14)	330(40)	71(18)	-50(20)	-22(13)
C(41)	118(18)	89(16)	140(20)	33(15)	22(15)	-32(14)
C(42)	143(18)	32(9)	87(12)	10(9)	33(12)	-45(11)
C(51)	17(7)	130(16)	62(9)	37(9)	9(6)	29(8)
C(52)	38(8)	81(12)	83(10)	49(9)	25(7)	35(8)
C(61)	51(10)	142(18)	176(19)	134(16)	-27(11)	-31(11)
C(62)	51(9)	73(12)	137(15)	62(11)	11(10)	-11(8)
C(101)	24(6)	16(6)	44(7)	13(5)	8(5)	-1(5)
C(102)	22(6)	34(7)	51(8)	13(6)	9(5)	14(5)
C(103)	25(6)	15(6)	37(7)	-3(5)	8(5)	5(5)
C(104)	25(6)	34(7)	44(7)	3(6)	13(5)	12(5)
C(105)	26(6)	38(8)	45(7)	-3(6)	1(5)	7(5)
C(106)	27(6)	28(7)	46(8)	-9(5)	0(5)	6(5)
C(107)	29(7)	31(7)	69(9)	5(7)	5(6)	1(5)
C(108)	18(6)	26(7)	47(7)	-5(6)	2(5)	5(5)
C(109)	32(6)	23(7)	63(9)	22(6)	24(6)	15(5)
C(110)	25(6)	36(7)	36(6)	3(6)	7(5)	8(5)
N(1D)	34(5)	40(6)	33(6)	-1(4)	18(5)	18(4)
N(1A)	30(5)	17(5)	34(6)	1(4)	10(4)	12(4)
N(1B)	57(6)	17(5)	32(5)	10(4)	6(5)	7(5)
N(1C)	27(5)	41(6)	27(5)	-3(5)	-1(4)	0(4)
N(2A)	23(5)	22(5)	33(5)	-1(4)	9(4)	10(4)
N(2B)	37(5)	14(5)	38(6)	2(4)	5(5)	11(4)
N(2D)	27(5)	32(6)	31(5)	19(4)	13(4)	16(4)
N(2C)	22(5)	32(6)	35(6)	15(5)	9(4)	7(4)
N(3B)	32(5)	29(6)	31(5)	7(4)	10(5)	5(4)
N(3A)	39(6)	30(6)	38(6)	4(5)	0(5)	9(4)
N(3C)	36(5)	38(6)	29(6)	11(5)	10(4)	15(5)
N(3D)	50(6)	20(5)	40(6)	1(5)	-2(5)	17(5)

N(11)	33(6)	47(7)	71(7)	25(5)	16(5)	16(5)
N(12)	27(5)	37(6)	36(5)	7(4)	11(4)	13(4)
N(21)	27(5)	55(7)	38(5)	1(5)	5(4)	15(5)
N(31)	62(7)	34(7)	87(8)	8(6)	-19(6)	0(6)
N(32)	79(10)	35(7)	102(10)	7(6)	-15(7)	2(6)
N(41)	63(8)	59(9)	120(11)	-36(8)	34(8)	-27(7)
N(42)	143(13)	22(7)	99(10)	-2(6)	67(9)	4(7)
N(51)	24(5)	62(7)	38(5)	17(5)	7(4)	10(5)
N(52)	29(5)	57(7)	43(6)	17(5)	9(4)	18(5)
N(61)	51(7)	50(7)	65(7)	32(6)	-10(5)	-10(6)
N(62)	38(6)	113(11)	53(7)	29(7)	8(5)	3(7)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1•4**.

	x	y	z	U(eq)					
H(1AA)	-820	916	-144	37	H(12B)	916	3384	-156	76
H(1DA)	-2040	2148	-430	46	H(13A)	-3349	811	3926	62
H(1CA)	-4478	-2920	512	43	H(13B)	-853	601	3939	30
H(1BA)	-3346	-4315	913	44	H(13C)	-3328	3745	3294	49
H(2AA)	-809	-302	77	35	H(13D)	-459	-1915	4676	47
H(2CA)	-4446	-1692	268	54	H(14A)	-2503	4447	4075	70
H(2DA)	-3400	1848	-436	53	H(14B)	-2784	647	4820	72
H(2BA)	-2006	-4171	946	50	H(14C)	-1065	1491	4620	36
H(3AA)	-528	-530	1025	34	H(14D)	-917	-1810	5527	45
H(3DA)	-3900	1993	399	39	H(15A)	-3059	-551	5152	58
H(3CA)	-4395	-732	947	48	H(15B)	-1169	4517	4185	54
H(3BA)	-1172	-3479	1717	44	H(15C)	-745	2779	4473	50
H(5AA)	-342	1701	1471	26	H(15D)	-2269	-1951	5552	43
H(5DA)	-1692	2514	1229	31	H(21A)	2943	-834	2811	78
H(5CA)	-4380	-2221	2116	38	H(21B)	2596	-893	3388	78
H(5BA)	-3049	-2979	2324	40	H(22A)	2059	-1938	2405	77
H(6AA)	180	-479	1866	26	H(22B)	2464	-2133	2991	77
H(6BA)	-612	-2291	2210	40	H(31A)	2023	4680	3890	144
H(6DA)	-4167	1609	1266	31	H(31B)	1839	4387	3245	144
H(6CA)	-4805	-26	1590	35	H(32A)	1288	5214	3103	210
H(8AA)	-633	1354	2297	24	H(32B)	1438	5483	3751	210
H(8DA)	-2178	3134	1895	38	H(41A)	-6580	-4700	1740	148
H(8BA)	-2240	-2925	3200	37	H(41B)	-6231	-4928	1194	148
H(8CA)	-3894	-1244	2750	30	H(42A)	-5780	-5540	1840	114
H(10A)	-234	-1440	3797	35	H(42B)	-5586	-4832	2290	114
H(10B)	171	111	3472	30	H(51A)	-6978	1056	1604	79
H(10C)	-3855	2475	2848	34	H(51B)	-7377	960	2157	79
H(10D)	-4414	758	3199	36	H(52A)	-6549	2040	2605	72
H(11A)	-24	2292	3041	34	H(52B)	-6924	2248	2015	72
H(11B)	-2692	-2240	3875	36	H(61A)	-4927	-3933	5151	155
H(11C)	-4167	-1452	3668	37	H(61B)	-4732	-3166	5545	155
H(11D)	-1412	3185	2785	35	H(62A)	-5792	-3121	4940	106
H(11E)	495	4146	784	80	H(62B)	-5418	-3389	4418	106
H(11F)	525	4438	177	80	H(10E)	-2095	-1626	1568	41
H(12A)	1466	3676	425	76	H(10F)	-1974	-1173	2603	39
H(10G)	-2081	-256	3279	44	H(10H)	-2359	905	3025	42

H(10I)	-2612	1106	2088	53					
H(10J)	-2731	633	1059	43					
H(11I)	-2669	-289	384	38					
H(11G)	-542	3578	-178	57					
H(11H)	-742	3823	369	57					
H(12C)	873	2720	838	38					
H(12D)	794	2337	268	38					
H(21C)	1842	-506	2380	47	H(32C)	243	5183	3765	91
H(21D)	1928	-92	2939	47	H(41B)	-5820	-3567	1839	104
H(22C)	1404	-2080	3381	53	H(41C)	-5929	-3691	1220	104
H(22D)	1053	-2453	2819	53	H(42B)	-4653	-5132	1482	103
H(31B)	1312	3670	4081	78	H(42C)	-4379	-4860	2081	103
H(31C)	1221	3365	3488	78	H(51C)	-6351	242	2055	49
H(32B)	101	4970	3154	91	H(51D)	-6305	633	2619	49
H(32C)	243	5183	3765	91	H(52C)	-5508	2610	2240	49
H(41B)	-5820	-3567	1839	104	H(52D)	-5813	2259	1664	49
H(32B)	101	4970	3154	91	H(61C)	-3897	-3556	4723	71
					H(61D)	-3577	-3215	5300	71
					H(62C)	-5046	-1974	4996	83
					H(62D)	-5179	-2152	4381	83

Table 1. Crystal data and structure refinement for **2•5a**.

Identification code	yoshi35	
Empirical formula	C104 H154 N48 O61 Pd6 Si2	
Formula weight	3747.33	
Temperature	105(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 17.124(3) Å	$\alpha = 90^\circ$.
	b = 44.546(8) Å	$\beta = 101.217(3)^\circ$.
	c = 20.284(4) Å	$\gamma = 90^\circ$.
Volume	15178(5) Å ³	
Z	4	
Density (calculated)	1.640 Mg/m ³	
Absorption coefficient	0.817 mm ⁻¹	
F(000)	7624	
Crystal size	0.40 x 0.40 x 0.20 mm ³	
Theta range for data collection	1.50 to 20.80°.	
Index ranges	-17<=h<=16, -44<=k<=44, -13<=l<=20	
Reflections collected	52051	
Independent reflections	15820 [R(int) = 0.0788]	
Completeness to theta = 20.80°	99.8 %	
Absorption correction	Empirical(SADABS)	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15820 / 0 / 957	
Goodness-of-fit on F ²	2.714	
Final R indices [I>2sigma(I)]	R1 = 0.1304, wR2 = 0.3564	
R indices (all data)	R1 = 0.1481, wR2 = 0.3654	
Largest diff. peak and hole	1.936 and -1.853 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² $\times 10^3$) for **2•5a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)					
Pd(1)	-3881(1)	2614(1)	-793(1)	23(1)	N(2B)	-8913(8)	4113(3)	1949(7)	23(3)
Pd(2)	-8652(1)	3799(1)	2694(1)	27(1)	N(2C)	-3942(8)	3986(3)	992(7)	24(3)
Pd(3)	-2873(1)	3938(1)	697(1)	29(1)	N(3C)	-5031(8)	2638(3)	-693(7)	17(3)
Pd(4)	-10587(1)	2857(1)	-2564(1)	28(1)	N(003)	-6960(10)	2935(4)	-6761(8)	40(4)
Pd(5)	-5134(1)	3776(1)	-5760(1)	38(1)	N(3B)	-10354(9)	3026(3)	-1608(7)	30(4)
Pd(6)	-10641(1)	4446(1)	-3674(1)	46(1)	N(3D)	-4124(8)	2768(3)	-1745(7)	17(3)
N(001)	-672(13)	4236(5)	2369(11)	71(6)	N(3A)	-5632(9)	3470(3)	-5224(7)	30(4)
N(1D)	-4938(9)	4050(3)	-4949(8)	34(4)	N(004)	-4085(11)	2957(4)	1409(9)	51(5)
N(1A)	-9572(10)	4347(4)	-3924(8)	38(4)	N(4A)	-7433(9)	3186(3)	-3807(7)	28(4)
N(1C)	-8423(8)	3485(3)	2027(7)	24(3)	N(4C)	-6773(8)	3066(3)	622(7)	22(3)
N(1B)	-10153(10)	4558(4)	-2737(8)	38(4)	N(4B)	-9790(8)	3829(3)	-22(7)	26(4)
N(002)	-2149(10)	3344(4)	-1004(8)	40(4)	N(4D)	-4129(9)	4133(3)	-2574(7)	28(4)
N(2A)	-9429(9)	2844(3)	-2629(7)	26(4)	N(005)	-6694(14)	4157(5)	2732(12)	72(6)
N(2D)	-3282(8)	4167(3)	-160(7)	22(3)	N(5D)	-3961(8)	3685(3)	-1920(7)	25(3)
					N(5A)	-8419(9)	3526(3)	-3587(7)	30(4)
					N(5C)	-6432(9)	3518(3)	1187(8)	32(4)
					N(5B)	-10028(8)	3935(3)	-1197(7)	24(3)

N(006)	-10840(10)	2713(4)	1560(9)	41(4)	O(018)	-10715(9)	2652(3)	1004(7)	50(4)
N(6D)	-4358(9)	3657(3)	-3097(7)	30(4)	O(19W)	-9755(19)	3098(7)	3284(16)	162(11)
N(6C)	-5600(8)	3323(3)	493(7)	26(4)	O(019)	-12883(17)	3698(7)	-3994(15)	140(9)
N(6A)	-7520(9)	3676(3)	-4246(7)	29(4)	O(20W)	-12310(30)	3668(11)	3840(20)	250(20)
N(6B)	-9681(9)	4325(3)	-424(7)	30(4)	O(020)	-12696(14)	3328(5)	-3245(12)	110(7)
N(007)	-13080(20)	3420(7)	-3893(17)	119(10)	O(021)	-13507(12)	3279(4)	-4330(10)	89(6)
N(008)	-11452(11)	4527(4)	-437(10)	54(5)	O(022)	-11320(9)	4513(3)	201(8)	59(4)
N(009)	-9862(13)	5372(5)	-4291(10)	63(6)	O(023)	-11494(11)	4770(4)	-750(9)	76(5)
N(010)	-4703(15)	1806(6)	231(12)	83(7)	O(024)	-11513(10)	4295(4)	-761(8)	65(4)
N(011)	-4050(20)	4840(9)	-6250(20)	151(13)	O(025)	-10292(11)	5170(4)	-4095(9)	75(5)
N(11)	-3533(9)	2474(3)	191(8)	31(4)	O(026)	-9180(11)	5311(4)	-4352(9)	78(5)
N(12)	-2702(8)	2601(3)	-830(7)	23(3)	O(027)	-10125(10)	5634(4)	-4437(9)	71(5)
N(21)	-8839(10)	4070(4)	3455(9)	45(4)	O(028)	-4046(12)	1859(4)	75(10)	82(5)
N(22)	-8390(11)	3495(4)	3424(10)	56(5)	O(029)	-5046(17)	2023(7)	426(14)	139(9)
N(31)	-2356(10)	3708(4)	1528(9)	45(4)	O(030)	-4839(16)	1510(6)	128(14)	131(9)
N(32)	-1820(9)	3866(3)	398(8)	32(4)	O(031)	-4613(19)	4709(7)	-6692(15)	145(10)
N(41)	-10893(9)	2682(3)	-3528(8)	34(4)	O(032)	-3836(16)	4752(6)	-5657(14)	122(8)
N(42)	-11765(8)	2828(3)	-2574(7)	21(3)	O(033)	-3820(19)	5093(7)	-6448(16)	149(10)
N(51)	-5271(10)	3496(4)	-6582(9)	47(5)	O(034)	-2530(30)	4330(13)	2400(30)	300(30)
N(52)	-4604(11)	4048(4)	-6324(9)	51(5)	O(036)	-2420(50)	4493(19)	3150(40)	430(40)
N(61)	-11271(12)	4341(5)	-4622(11)	66(6)	O(100)	-7989(14)	5049(5)	-966(12)	110(7)
N(62)	-11713(10)	4562(4)	-3465(9)	46(5)	O(101)	-7629(11)	4804(4)	280(9)	75(5)
Si(2)	-5751(4)	4720(2)	-694(3)	56(2)	O(102)	-6568(11)	4833(4)	-517(9)	80(5)
Si(1)	-7491(4)	4788(2)	-513(4)	67(2)	O(103)	-5366(9)	5011(3)	-997(8)	59(4)
O(1W)	-1717(12)	2991(5)	2826(10)	93(6)	O(104)	-5181(11)	4595(4)	-4(10)	82(5)
O(001)	-758(12)	3952(5)	2470(10)	91(6)	C(1C)	-9002(11)	3270(4)	1826(9)	27(4)
O(2W)	-4764(10)	5043(3)	-2100(8)	62(4)	C(1B)	-9933(12)	4856(5)	-2576(10)	41(5)
O(002)	-845(13)	4336(5)	1728(11)	101(7)	C(1D)	-5062(13)	4348(5)	-5002(11)	48(6)
O(3W)	-10721(9)	2075(3)	-2885(7)	53(4)	C(1A)	-9193(13)	4589(5)	-4128(11)	44(5)
O(003)	-325(10)	4392(4)	2786(9)	66(5)	C(2A)	-8408(12)	4555(5)	-4267(10)	43(5)
O(4W)	-11720(10)	5251(4)	-3706(8)	66(5)	C(2C)	-8883(10)	3043(4)	1369(9)	26(4)
O(004)	-2248(10)	3235(4)	-461(8)	67(5)	C(2D)	-4965(12)	4533(5)	-4440(10)	42(5)
O(5W)	-12058(11)	4366(4)	-2184(9)	73(5)	C(2B)	-9686(14)	4951(5)	-1919(12)	54(6)
O(005)	-1980(8)	3611(3)	-1013(7)	42(3)	C(3C)	-8184(11)	3048(4)	1130(9)	32(5)
O(6W)	-6744(11)	4701(4)	1589(9)	74(5)	C(3B)	-9695(12)	4757(4)	-1411(10)	37(5)
O(006)	-2204(8)	3177(3)	-1492(7)	40(3)	C(3A)	-8098(13)	4265(5)	-4249(11)	47(6)
O(7W)	-13122(12)	5194(4)	-4727(10)	86(6)	C(3D)	-4678(12)	4420(5)	-3801(10)	43(5)
O(007)	-6392(10)	2751(3)	-6670(8)	59(4)	C(4C)	-7613(10)	3268(4)	1343(9)	27(4)
O(8W)	-6936(13)	4191(5)	4440(10)	94(6)	C(4B)	-9911(12)	4445(5)	-1560(10)	41(5)
O(008)	-6852(9)	3215(3)	-6732(7)	52(4)	C(4D)	-4562(10)	4110(4)	-3748(9)	26(4)
O(9W)	-12049(14)	3762(5)	-2400(12)	112(7)	C(4A)	-8476(10)	4034(4)	-4015(9)	27(4)
O(009)	-7682(10)	2852(3)	-6878(8)	63(4)	C(5B)	-10099(12)	4363(5)	-2216(10)	41(5)
O(10W)	-10624(13)	3638(5)	-3060(11)	96(6)	C(5D)	-4649(12)	3933(4)	-4339(10)	40(5)
O(010)	-3566(13)	3058(5)	1133(10)	93(6)	C(5C)	-7743(10)	3489(4)	1790(9)	24(4)
O(11W)	-12758(15)	4907(6)	-2534(13)	123(8)	C(5A)	-9244(12)	4071(4)	-3874(10)	36(5)
O(011)	-4279(12)	3111(4)	1878(10)	83(5)	C(6C)	-6894(11)	3292(4)	1018(9)	29(5)
O(12W)	-6161(13)	4930(5)	3670(11)	100(6)	C(6D)	-4329(12)	3962(4)	-3101(10)	37(5)
O(012)	-4480(9)	2742(3)	1209(8)	55(4)	C(6A)	-8114(10)	3730(4)	-3954(9)	25(4)
O(13W)	-3575(14)	3295(5)	-24(12)	115(8)	C(6B)	-9881(10)	4217(4)	-1045(9)	28(4)
O(013)	-6110(15)	4349(5)	2922(12)	116(8)	C(7D)	-3344(11)	4467(4)	-180(9)	28(4)
O(14W)	-2918(14)	3405(5)	2573(11)	104(7)	C(7B)	-8699(11)	4402(4)	2076(10)	35(5)
O(014)	-6806(12)	3963(4)	3150(10)	86(6)	C(7A)	-8989(12)	2608(4)	-2370(10)	35(5)
O(15W)	-6168(17)	1318(6)	613(14)	133(9)	C(7C)	-4119(11)	4245(4)	1292(9)	29(4)
O(015)	-6996(10)	4168(4)	2136(8)	63(4)	C(8A)	-8215(12)	2568(5)	-2488(10)	41(5)
O(16W)	-6960(18)	1799(6)	-180(15)	144(10)	C(8C)	-4860(12)	4278(4)	1481(10)	41(5)
O(016)	-11267(12)	2541(4)	1825(10)	88(6)	C(8B)	-8848(13)	4622(5)	1559(11)	46(6)
O(17W)	-10936(18)	3884(7)	3787(15)	146(10)	C(8D)	-3577(12)	4626(5)	-756(10)	42(5)
O(017)	-10550(9)	2926(3)	1874(8)	54(4)	C(9A)	-7907(11)	2781(4)	-2857(9)	27(4)
O(18W)	-13160(19)	3911(7)	-5300(15)	151(10)	C(9C)	-5416(13)	4049(5)	1365(11)	44(5)

C(9D)	-3783(11)	4472(4)	-1359(9)	30(5)	C(18D)	-4141(10)	3539(4)	-2489(8)	22(4)
C(9B)	-9141(12)	4536(4)	936(10)	37(5)	C(18C)	-6128(11)	3092(4)	381(9)	29(5)
C(10A)	-8364(10)	3017(4)	-3120(9)	26(4)	C(18B)	-9992(11)	3744(4)	-666(9)	30(5)
C(10B)	-9338(10)	4234(4)	793(9)	24(4)	C(18A)	-7179(10)	3398(4)	-4162(9)	26(4)
C(10C)	-5199(10)	3784(4)	1068(8)	19(4)	C(21)	-8228(15)	3639(6)	4099(13)	63(7)
C(10D)	-3751(11)	4164(4)	-1354(9)	33(5)	C(22)	-8831(14)	3862(5)	4068(12)	52(6)
C(11B)	-9225(10)	4040(4)	1306(9)	26(4)	C(31)	-1744(13)	3506(5)	1337(11)	49(6)
C(11D)	-3470(10)	4010(4)	-752(9)	26(4)	C(32)	-1262(15)	3690(5)	916(12)	59(6)
C(11C)	-4494(11)	3765(4)	884(9)	26(4)	C(41)	-11752(12)	2718(5)	-3760(10)	41(5)
C(11A)	-9125(11)	3059(4)	-2987(9)	31(5)	C(42)	-12138(12)	2640(5)	-3169(11)	43(5)
C(11)	-2646(13)	2520(5)	397(11)	45(5)	C(51)	-5027(14)	3665(5)	-7131(11)	52(6)
C(12D)	-3953(11)	3987(4)	-1990(9)	30(5)	C(52)	-4369(15)	3871(5)	-6870(12)	59(6)
C(12A)	-8050(10)	3264(4)	-3514(9)	27(4)	C(61)	-12125(17)	4477(6)	-4691(14)	74(8)
C(12C)	-5746(10)	3519(4)	907(8)	22(4)	C(62)	-12365(16)	4426(6)	-3979(14)	72(8)
C(12B)	-9639(11)	4126(4)	80(9)	28(4)	C(100)	-7786(16)	4429(6)	-907(14)	69(7)
C(12)	-2276(13)	2436(5)	-207(11)	49(6)	C(101)	-7781(18)	4170(7)	-484(15)	86(9)
C(13D)	-4242(10)	2602(3)	-2318(8)	18(4)	C(102)	-7939(14)	3872(5)	-764(12)	55(6)
C(13A)	-5260(11)	3204(4)	-5115(9)	31(5)	C(103)	-7947(13)	3633(5)	-364(11)	46(6)
C(13C)	-5608(12)	2448(4)	-1017(10)	35(5)	C(104)	-8065(17)	3350(6)	-606(14)	74(8)
C(13B)	-10311(11)	2813(4)	-1106(9)	28(4)	C(105)	-8209(16)	3311(6)	-1354(13)	70(7)
C(14C)	-6383(12)	2463(4)	-918(10)	35(5)	C(106)	-8199(15)	3548(6)	-1768(12)	60(7)
C(14B)	-10173(10)	2911(4)	-431(9)	26(4)	C(107)	-8039(14)	3840(5)	-1472(12)	56(6)
C(14D)	-4305(11)	2711(4)	-2940(9)	30(5)	C(108)	-8041(15)	4099(6)	-1888(13)	65(7)
C(14A)	-5466(11)	2991(4)	-4663(9)	33(5)	C(109)	-7896(15)	4385(6)	-1599(13)	65(7)
C(15D)	-4289(11)	3019(4)	-3007(9)	28(4)	C(110)	-5873(14)	4402(5)	-1282(12)	53(6)
C(15C)	-6594(11)	2672(4)	-452(10)	34(5)	C(111)	-5830(15)	4110(5)	-1042(12)	61(7)
C(15A)	-6089(12)	3067(4)	-4342(10)	36(5)	C(112)	-5896(13)	3867(5)	-1509(11)	47(6)
C(15B)	-10057(11)	3203(4)	-280(9)	31(5)	C(113)	-5902(15)	3559(5)	-1290(12)	59(7)
C(16C)	-5976(10)	2857(4)	-114(9)	23(4)	C(114)	-5991(13)	3328(5)	-1722(11)	51(6)
C(16A)	-6476(10)	3329(4)	-4487(8)	22(4)	C(115)	-6100(14)	3380(5)	-2406(12)	57(6)
C(16D)	-4184(10)	3204(4)	-2443(8)	21(4)	C(116)	-6151(13)	3669(5)	-2647(11)	44(5)
C(16B)	-10075(10)	3430(4)	-810(9)	24(4)	C(117)	-6075(13)	3911(5)	-2225(11)	48(6)
C(17C)	-5224(10)	2839(4)	-262(8)	22(4)	C(118)	-6093(15)	4203(6)	-2463(13)	65(7)
C(17D)	-4115(11)	3076(4)	-1834(9)	30(5)	C(119)	-5990(16)	4452(6)	-2003(14)	69(7)
C(17A)	-6236(11)	3537(4)	-4908(9)	33(5)					
C(17B)	-10247(10)	3317(4)	-1453(9)	26(4)					

Table 3. Bond lengths [Å] and angles [°] for **2•5a**.

Pd(1)-N(3D)	2.016(13)	Pd(5)-N(1D)	2.021(15)	N(1B)-C(1B)	1.40(3)
Pd(1)-N(3C)	2.021(13)	Pd(5)-N(3A)	2.031(15)	N(002)-O(005)	1.229(19)
Pd(1)-N(12)	2.036(14)	Pd(5)-N(51)	2.060(18)	N(002)-O(006)	1.226(19)
Pd(1)-N(11)	2.064(15)	Pd(6)-N(1B)	1.985(16)	N(002)-O(004)	1.24(2)
Pd(2)-N(22)	1.990(19)	Pd(6)-N(62)	2.029(17)	N(2A)-C(7A)	1.34(2)
Pd(2)-N(21)	2.035(17)	Pd(6)-N(1A)	2.041(16)	N(2A)-C(11A)	1.37(2)
Pd(2)-N(2B)	2.043(14)	Pd(6)-N(61)	2.07(2)	N(2D)-C(7D)	1.34(2)
Pd(2)-N(1C)	2.035(14)	N(001)-O(003)	1.16(2)	N(2D)-C(11D)	1.37(2)
Pd(3)-N(2D)	2.020(13)	N(001)-O(001)	1.29(3)	N(2B)-C(11B)	1.35(2)
Pd(3)-N(31)	2.025(17)	N(001)-O(002)	1.35(3)	N(2B)-C(7B)	1.35(2)
Pd(3)-N(32)	2.037(15)	N(1D)-C(5D)	1.34(2)	N(2C)-C(11C)	1.35(2)
Pd(3)-N(2C)	2.045(14)	N(1D)-C(1D)	1.35(3)	N(2C)-C(7C)	1.37(2)
Pd(4)-N(2A)	2.014(14)	N(1A)-C(5A)	1.35(2)	N(3C)-C(17C)	1.34(2)
Pd(4)-N(42)	2.018(13)	N(1A)-C(1A)	1.36(3)	N(3C)-C(13C)	1.37(2)
Pd(4)-N(3B)	2.043(15)	N(1C)-C(5C)	1.34(2)	N(003)-O(007)	1.26(2)
Pd(4)-N(41)	2.076(15)	N(1C)-C(1C)	1.38(2)	N(003)-O(008)	1.26(2)
Pd(5)-N(52)	2.000(18)	N(1B)-C(5B)	1.36(3)	N(003)-O(009)	1.27(2)

N(3B)-C(17B)	1.34(2)	N(12)-C(12)	1.52(3)	C(10C)-C(11C)	1.33(2)
N(3B)-C(13B)	1.38(2)	N(21)-C(22)	1.55(3)	C(10C)-C(12C)	1.50(2)
N(3D)-C(13D)	1.36(2)	N(22)-C(21)	1.49(3)	C(10D)-C(11D)	1.40(3)
N(3D)-C(17D)	1.38(2)	N(31)-C(31)	1.49(3)	C(10D)-C(12D)	1.49(3)
N(3A)-C(13A)	1.35(2)	N(32)-C(32)	1.50(3)	C(11)-C(12)	1.53(3)
N(3A)-C(17A)	1.35(2)	N(41)-C(41)	1.46(3)	C(13D)-C(14D)	1.34(2)
N(004)-O(012)	1.20(2)	N(42)-C(42)	1.51(3)	C(13A)-C(14A)	1.41(3)
N(004)-O(010)	1.22(2)	N(51)-C(51)	1.47(3)	C(13C)-C(14C)	1.38(3)
N(004)-O(011)	1.27(2)	N(52)-C(52)	1.48(3)	C(13B)-C(14B)	1.41(3)
N(4A)-C(18A)	1.32(2)	N(61)-C(61)	1.57(3)	C(14C)-C(15C)	1.42(3)
N(4A)-C(12A)	1.35(2)	N(62)-C(62)	1.50(3)	C(14B)-C(15B)	1.34(3)
N(4C)-C(18C)	1.30(2)	Si(2)-O(102)	1.59(2)	C(14D)-C(15D)	1.38(3)
N(4C)-C(6C)	1.33(2)	Si(2)-O(103)	1.627(17)	C(14A)-C(15A)	1.39(3)
N(4B)-C(12B)	1.35(2)	Si(2)-O(104)	1.64(2)	C(15D)-C(16D)	1.39(2)
N(4B)-C(18B)	1.34(2)	Si(2)-C(110)	1.83(2)	C(15C)-C(16C)	1.41(3)
N(4D)-C(6D)	1.30(2)	Si(1)-O(102)	1.59(2)	C(15A)-C(16A)	1.34(3)
N(4D)-C(12D)	1.33(2)	Si(1)-O(100)	1.62(2)	C(15B)-C(16B)	1.47(3)
N(005)-O(015)	1.22(2)	Si(1)-O(101)	1.67(2)	C(16C)-C(17C)	1.38(2)
N(005)-O(014)	1.25(3)	Si(1)-C(100)	1.82(3)	C(16C)-C(18C)	1.50(3)
N(005)-O(013)	1.31(3)	C(1C)-C(2C)	1.41(3)	C(16A)-C(17A)	1.38(3)
N(5D)-C(18D)	1.31(2)	C(1B)-C(2B)	1.38(3)	C(16A)-C(18A)	1.51(2)
N(5D)-C(12D)	1.36(2)	C(1D)-C(2D)	1.39(3)	C(16D)-C(17D)	1.35(2)
N(5A)-C(12A)	1.32(2)	C(1A)-C(2A)	1.43(3)	C(16D)-C(18D)	1.50(2)
N(5A)-C(6A)	1.34(2)	C(2A)-C(3A)	1.39(3)	C(16B)-C(17B)	1.37(2)
N(5C)-C(6C)	1.29(2)	C(2C)-C(3C)	1.38(3)	C(16B)-C(18B)	1.43(3)
N(5C)-C(12C)	1.40(2)	C(2D)-C(3D)	1.39(3)	C(21)-C(22)	1.42(3)
N(5B)-C(6B)	1.31(2)	C(2B)-C(3B)	1.35(3)	C(31)-C(32)	1.54(3)
N(5B)-C(18B)	1.36(2)	C(3C)-C(4C)	1.39(3)	C(41)-C(42)	1.52(3)
N(006)-O(017)	1.20(2)	C(3B)-C(4B)	1.45(3)	C(51)-C(52)	1.47(3)
N(006)-O(018)	1.22(2)	C(3A)-C(4A)	1.35(3)	C(61)-C(62)	1.59(4)
N(006)-O(016)	1.25(2)	C(3D)-C(4D)	1.40(3)	C(100)-C(109)	1.40(4)
N(6D)-C(18D)	1.33(2)	C(4C)-C(5C)	1.38(2)	C(100)-C(101)	1.44(4)
N(6D)-C(6D)	1.36(2)	C(4C)-C(6C)	1.51(3)	C(101)-C(102)	1.45(4)
N(6C)-C(12C)	1.27(2)	C(4B)-C(5B)	1.36(3)	C(102)-C(103)	1.34(3)
N(6C)-C(18C)	1.36(2)	C(4B)-C(6B)	1.45(3)	C(102)-C(107)	1.42(3)
N(6A)-C(6A)	1.29(2)	C(4D)-C(5D)	1.42(3)	C(103)-C(104)	1.35(3)
N(6A)-C(18A)	1.36(2)	C(4D)-C(6D)	1.46(3)	C(104)-C(105)	1.50(4)
N(6B)-C(6B)	1.33(2)	C(4A)-C(5A)	1.41(3)	C(105)-C(106)	1.35(3)
N(6B)-C(12B)	1.34(2)	C(4A)-C(6A)	1.49(3)	C(106)-C(107)	1.43(3)
N(007)-O(021)	1.21(3)	C(7D)-C(8D)	1.36(3)	C(107)-C(108)	1.43(3)
N(007)-O(019)	1.31(4)	C(7B)-C(8B)	1.42(3)	C(108)-C(109)	1.40(3)
N(007)-O(020)	1.41(4)	C(7A)-C(8A)	1.40(3)	C(110)-C(111)	1.39(3)
N(008)-O(024)	1.22(2)	C(7C)-C(8C)	1.40(3)	C(110)-C(119)	1.46(3)
N(008)-O(023)	1.25(2)	C(8A)-C(9A)	1.38(3)	C(111)-C(112)	1.43(3)
N(008)-O(022)	1.27(2)	C(8C)-C(9C)	1.38(3)	C(112)-C(117)	1.44(3)
N(009)-O(026)	1.23(2)	C(8B)-C(9B)	1.32(3)	C(112)-C(113)	1.44(3)
N(009)-O(027)	1.26(2)	C(8D)-C(9D)	1.39(3)	C(113)-C(114)	1.34(3)
N(009)-O(025)	1.27(2)	C(9A)-C(10A)	1.35(2)	C(114)-C(115)	1.38(3)
N(010)-O(029)	1.23(3)	C(9C)-C(10C)	1.41(3)	C(115)-C(116)	1.38(3)
N(010)-O(028)	1.25(3)	C(9D)-C(10D)	1.37(3)	C(116)-C(117)	1.37(3)
N(010)-O(030)	1.35(3)	C(9B)-C(10B)	1.40(3)	C(117)-C(118)	1.38(3)
N(011)-O(032)	1.25(4)	C(10A)-C(11A)	1.39(3)	C(118)-C(119)	1.44(4)
N(011)-O(033)	1.29(4)	C(10A)-C(12A)	1.52(3)		
N(011)-O(031)	1.32(4)	C(10B)-C(11B)	1.34(2)		
N(11)-C(11)	1.51(3)	C(10B)-C(12B)	1.51(2)		
		N(3D)-Pd(1)-N(11)	174.8(6)	N(22)-Pd(2)-N(2B)	179.5(7)
N(3D)-Pd(1)-N(3C)	93.1(5)	N(3C)-Pd(1)-N(11)	91.4(6)	N(21)-Pd(2)-N(2B)	96.3(6)
N(3D)-Pd(1)-N(12)	89.7(5)	N(12)-Pd(1)-N(11)	85.7(6)	N(22)-Pd(2)-N(1C)	89.1(7)
N(3C)-Pd(1)-N(12)	176.2(5)	N(22)-Pd(2)-N(21)	83.4(7)	N(21)-Pd(2)-N(1C)	172.5(6)

N(2B)-Pd(2)-N(1C)	91.2(5)	C(13C)-N(3C)-Pd(1)	123.1(11)	C(61)-N(61)-Pd(6)	107.7(15)
N(2D)-Pd(3)-N(31)	174.3(6)	O(007)-N(003)-O(008)	122.3(17)	C(62)-N(62)-Pd(6)	109.6(14)
N(2D)-Pd(3)-N(32)	90.1(6)	O(007)-N(003)-O(009)	122.4(17)	O(102)-Si(2)-O(103)	105.8(10)
N(31)-Pd(3)-N(32)	84.3(6)	O(008)-N(003)-O(009)	115.3(16)	O(102)-Si(2)-O(104)	108.5(10)
N(2D)-Pd(3)-N(2C)	91.0(5)	C(17B)-N(3B)-C(13B)	120.3(15)	O(103)-Si(2)-O(104)	112.0(10)
N(31)-Pd(3)-N(2C)	94.6(6)	C(17B)-N(3B)-Pd(4)	124.8(12)	O(102)-Si(2)-C(110)	113.4(10)
N(32)-Pd(3)-N(2C)	177.1(6)	C(13B)-N(3B)-Pd(4)	114.9(11)	O(103)-Si(2)-C(110)	111.8(10)
N(2A)-Pd(4)-N(42)	173.1(5)	C(13D)-N(3D)-C(17D)	115.5(14)	O(104)-Si(2)-C(110)	105.5(10)
N(2A)-Pd(4)-N(3B)	93.5(6)	C(13D)-N(3D)-Pd(1)	127.1(10)	O(102)-Si(1)-O(100)	108.7(12)
N(42)-Pd(4)-N(3B)	92.5(6)	C(17D)-N(3D)-Pd(1)	117.2(11)	O(102)-Si(1)-O(101)	109.0(10)
N(2A)-Pd(4)-N(41)	89.9(6)	C(13A)-N(3A)-C(17A)	119.8(15)	O(100)-Si(1)-O(101)	111.0(11)
N(42)-Pd(4)-N(41)	84.1(6)	C(13A)-N(3A)-Pd(5)	116.5(12)	O(102)-Si(1)-C(100)	107.4(11)
N(3B)-Pd(4)-N(41)	176.6(6)	C(17A)-N(3A)-Pd(5)	123.1(12)	O(100)-Si(1)-C(100)	108.3(12)
N(52)-Pd(5)-N(1D)	94.5(7)	O(012)-N(004)-O(010)	124(2)	O(101)-Si(1)-C(100)	112.3(11)
N(52)-Pd(5)-N(3A)	175.2(7)	O(012)-N(004)-O(011)	118(2)	Si(1)-O(102)-Si(2)	151.3(13)
N(1D)-Pd(5)-N(3A)	89.4(6)	O(010)-N(004)-O(011)	118(2)	N(1C)-C(1C)-C(2C)	120.2(16)
N(52)-Pd(5)-N(51)	84.1(7)	C(18A)-N(4A)-C(12A)	115.1(15)	C(2B)-C(1B)-N(1B)	122.1(19)
N(1D)-Pd(5)-N(51)	177.0(7)	C(18C)-N(4C)-C(6C)	114.0(15)	N(1D)-C(1D)-C(2D)	121.9(19)
		C(12B)-N(4B)-C(18B)	115.4(15)	N(1A)-C(1A)-C(2A)	119.7(18)
		C(6D)-N(4D)-C(12D)	115.2(15)	C(3A)-C(2A)-C(1A)	117.5(19)
N(3A)-Pd(5)-N(51)	91.9(6)	O(015)-N(005)-O(014)	127(2)	C(3C)-C(2C)-C(1C)	117.9(16)
N(1B)-Pd(6)-N(62)	88.1(7)	O(015)-N(005)-O(013)	115(2)	C(1D)-C(2D)-C(3D)	121.1(19)
N(1B)-Pd(6)-N(1A)	93.5(6)	O(014)-N(005)-O(013)	117(2)	C(3B)-C(2B)-C(1B)	120(2)
N(62)-Pd(6)-N(1A)	176.9(7)	C(18D)-N(5D)-C(12D)	114.1(15)	C(2C)-C(3C)-C(4C)	120.5(17)
N(1B)-Pd(6)-N(61)	173.6(8)	C(12A)-N(5A)-C(6A)	115.5(15)	C(2B)-C(3B)-C(4B)	119.6(19)
N(62)-Pd(6)-N(61)	85.5(8)	C(6C)-N(5C)-C(12C)	114.7(15)	C(4A)-C(3A)-C(2A)	121(2)
N(1A)-Pd(6)-N(61)	92.9(7)	C(6B)-N(5B)-C(18B)	115.8(15)	C(2D)-C(3D)-C(4D)	116.6(18)
O(003)-N(001)-O(001)	122(2)	O(017)-N(006)-O(018)	122.9(18)	C(5C)-C(4C)-C(3C)	120.6(16)
O(003)-N(001)-O(002)	119(2)	O(017)-N(006)-O(016)	118.3(18)	C(5C)-C(4C)-C(6C)	119.1(15)
O(001)-N(001)-O(002)	118(2)	O(018)-N(006)-O(016)	118.8(18)	C(3C)-C(4C)-C(6C)	119.8(16)
C(5D)-N(1D)-C(1D)	118.5(17)	C(18D)-N(6D)-C(6D)	113.4(15)	C(5B)-C(4B)-C(3B)	117.6(19)
C(5D)-N(1D)-Pd(5)	119.3(13)	C(12C)-N(6C)-C(18C)	115.0(15)	C(5B)-C(4B)-C(6B)	119.1(18)
C(1D)-N(1D)-Pd(5)	122.1(13)	C(6A)-N(6A)-C(18A)	117.7(15)	C(3B)-C(4B)-C(6B)	123.2(18)
C(5A)-N(1A)-C(1A)	121.9(17)	C(6B)-N(6B)-C(12B)	116.6(15)	C(3D)-C(4D)-C(5D)	119.7(17)
C(5A)-N(1A)-Pd(6)	124.1(13)	O(021)-N(007)-O(019)	121(3)	C(3D)-C(4D)-C(6D)	121.9(17)
C(1A)-N(1A)-Pd(6)	113.9(13)	O(021)-N(007)-O(020)	129(3)	C(5D)-C(4D)-C(6D)	118.4(16)
C(5C)-N(1C)-C(1C)	121.6(14)	O(019)-N(007)-O(020)	110(3)	C(3A)-C(4A)-C(5A)	120.9(17)
C(5C)-N(1C)-Pd(2)	121.5(11)	O(024)-N(008)-O(023)	118.1(19)	C(3A)-C(4A)-C(6A)	120.2(17)
C(1C)-N(1C)-Pd(2)	116.9(11)	O(024)-N(008)-O(022)	119.2(19)	C(5A)-C(4A)-C(6A)	118.7(16)
C(5B)-N(1B)-C(1B)	116.7(17)	O(023)-N(008)-O(022)	122.7(19)	N(1B)-C(5B)-C(4B)	124.0(19)
C(5B)-N(1B)-Pd(6)	122.4(13)	O(026)-N(009)-O(027)	119(2)	N(1D)-C(5D)-C(4D)	121.5(17)
C(1B)-N(1B)-Pd(6)	120.4(13)	O(026)-N(009)-O(025)	119(2)	N(1C)-C(5C)-C(4C)	119.2(15)
O(005)-N(002)-O(006)	123.9(16)	O(027)-N(009)-O(025)	122(2)	N(1A)-C(5A)-C(4A)	118.9(17)
O(005)-N(002)-O(004)	117.6(17)	O(029)-N(010)-O(028)	116(3)	N(5C)-C(6C)-N(4C)	126.4(17)
O(006)-N(002)-O(004)	118.5(17)	O(029)-N(010)-O(030)	137(3)	N(5C)-C(6C)-C(4C)	116.8(16)
C(7A)-N(2A)-C(11A)	121.1(16)	O(028)-N(010)-O(030)	106(2)	N(4C)-C(6C)-C(4C)	116.7(15)
C(7A)-N(2A)-Pd(4)	118.9(12)	O(032)-N(011)-O(033)	121(4)	N(4D)-C(6D)-N(6D)	125.6(17)
C(11A)-N(2A)-Pd(4)	119.7(12)	O(032)-N(011)-O(031)	124(4)	N(4D)-C(6D)-C(4D)	117.3(16)
C(7D)-N(2D)-C(11D)	118.6(14)	O(033)-N(011)-O(031)	114(4)	N(6D)-C(6D)-C(4D)	117.1(17)
		C(11)-N(11)-Pd(1)	108.2(12)	N(6A)-C(6A)-N(5A)	123.6(16)
C(7D)-N(2D)-Pd(3)	123.0(11)	C(12)-N(12)-Pd(1)	107.6(11)	N(6A)-C(6A)-C(4A)	118.9(15)
C(11D)-N(2D)-Pd(3)	118.4(11)	C(22)-N(21)-Pd(2)	105.8(12)	N(5A)-C(6A)-C(4A)	117.5(15)
C(11B)-N(2B)-C(7B)	117.0(15)	C(21)-N(22)-Pd(2)	111.6(14)	N(6B)-C(6B)-N(5B)	125.0(16)
C(11B)-N(2B)-Pd(2)	122.7(11)	C(31)-N(31)-Pd(3)	107.7(13)	N(6B)-C(6B)-C(4B)	113.3(16)
C(7B)-N(2B)-Pd(2)	120.0(12)	C(32)-N(32)-Pd(3)	110.7(13)	N(5B)-C(6B)-C(4B)	121.6(16)
C(11C)-N(2C)-C(7C)	118.7(15)	C(41)-N(41)-Pd(4)	108.4(12)	N(2D)-C(7D)-C(8D)	123.7(17)
C(11C)-N(2C)-Pd(3)	120.7(11)	C(42)-N(42)-Pd(4)	108.1(11)	N(2B)-C(7B)-C(8B)	121.0(17)
C(7C)-N(2C)-Pd(3)	120.6(11)	C(51)-N(51)-Pd(5)	107.5(13)	N(2A)-C(7A)-C(8A)	120.8(17)
C(17C)-N(3C)-C(13C)	118.8(14)	C(52)-N(52)-Pd(5)	109.0(14)	N(2C)-C(7C)-C(8C)	119.9(16)
C(17C)-N(3C)-Pd(1)	118.1(11)				

C(9A)-C(8A)-C(7A)	118.6(18)	N(3C)-C(13C)-C(14C)	121.7(17)	N(31)-C(31)-C(32)	107.7(18)
C(9C)-C(8C)-C(7C)	120.6(18)	N(3B)-C(13B)-C(14B)	118.5(16)	N(32)-C(32)-C(31)	109.4(19)
C(9B)-C(8B)-C(7B)	118.8(19)	C(13C)-C(14C)-C(15C)	120.2(18)	N(41)-C(41)-C(42)	106.7(17)
C(7D)-C(8D)-C(9D)	118.9(18)	C(15B)-C(14B)-C(13B)	120.7(17)	C(41)-C(42)-N(42)	108.9(16)
C(10A)-C(9A)-C(8A)	119.7(17)	C(13D)-C(14D)-C(15D)	117.1(17)	C(52)-C(51)-N(51)	111.0(19)
C(8C)-C(9C)-C(10C)	117.3(19)	C(15A)-C(14A)-C(13A)	116.7(17)	C(51)-C(52)-N(52)	107.5(19)
C(10D)-C(9D)-C(8D)	119.0(18)	C(14D)-C(15D)-C(16D)	120.7(16)	N(61)-C(61)-C(62)	105(2)
C(8B)-C(9B)-C(10B)	120.6(19)	C(16C)-C(15C)-C(14C)	116.3(17)	N(62)-C(62)-C(61)	107(2)
C(9A)-C(10A)-C(11A)	121.3(16)	C(16A)-C(15A)-C(14A)	119.9(18)	C(109)-C(100)-C(101)	118(2)
C(9A)-C(10A)-C(12A)	122.1(16)	C(14B)-C(15B)-C(16B)	121.2(17)	C(109)-C(100)-Si(1)	123(2)
C(11A)-C(10A)-C(12A)	116.3(15)	C(17C)-C(16C)-C(15C)	120.2(16)	C(101)-C(100)-Si(1)	118(2)
C(11B)-C(10B)-C(9B)	117.6(16)	C(17C)-C(16C)-C(18C)	118.4(15)	C(100)-C(101)-C(102)	122(3)
C(11B)-C(10B)-C(12B)	120.7(15)	C(15C)-C(16C)-C(18C)	121.3(16)	C(103)-C(102)-C(107)	121(2)
C(9B)-C(10B)-C(12B)	121.7(16)	C(15A)-C(16A)-C(17A)	121.7(17)	C(103)-C(102)-C(101)	121(2)
C(11C)-C(10C)-C(9C)	120.3(16)	C(15A)-C(16A)-C(18A)	118.9(16)	C(107)-C(102)-C(101)	118(2)
C(11C)-C(10C)-C(12C)	116.5(14)	C(17A)-C(16A)-C(18A)	119.3(15)	C(104)-C(103)-C(102)	123(2)
C(9C)-C(10C)-C(12C)	123.1(16)	C(17D)-C(16D)-C(15D)	118.4(16)	C(103)-C(104)-C(105)	117(2)
C(9D)-C(10D)-C(11D)	120.2(17)	C(17D)-C(16D)-C(18D)	119.0(15)	C(106)-C(105)-C(104)	121(2)
C(9D)-C(10D)-C(12D)	121.2(17)	C(15D)-C(16D)-C(18D)	122.6(15)	C(105)-C(106)-C(107)	118(2)
C(11D)-C(10D)-C(12D)	118.5(16)	C(17B)-C(16B)-C(18B)	123.0(16)	C(102)-C(107)-C(108)	120(2)
C(10B)-C(11B)-N(2B)	124.7(16)	C(17B)-C(16B)-C(15B)	114.4(15)	C(102)-C(107)-C(106)	119(2)
N(2D)-C(11D)-C(10D)	119.6(15)	C(18B)-C(16B)-C(15B)	122.4(16)	C(108)-C(107)-C(106)	120(2)
C(10C)-C(11C)-N(2C)	123.2(15)	N(3C)-C(17C)-C(16C)	122.8(15)	C(109)-C(108)-C(107)	120(2)
N(2A)-C(11A)-C(10A)	118.3(16)	C(16D)-C(17D)-N(3D)	122.7(16)	C(100)-C(109)-C(108)	122(2)
N(11)-C(11)-C(12)	107.2(17)	N(3A)-C(17A)-C(16A)	119.6(16)	C(111)-C(110)-C(119)	119(2)
N(4D)-C(12D)-N(5D)	124.7(16)	N(3B)-C(17B)-C(16B)	124.9(16)	C(111)-C(110)-Si(2)	120.3(18)
N(4D)-C(12D)-C(10D)	119.2(16)	N(5D)-C(18D)-N(6D)	126.9(16)	C(119)-C(110)-Si(2)	120.9(18)
N(5D)-C(12D)-C(10D)	116.1(16)	N(5D)-C(18D)-C(16D)	116.5(15)	C(110)-C(111)-C(112)	119(2)
N(5A)-C(12A)-N(4A)	125.1(16)	N(6D)-C(18D)-C(16D)	116.3(15)	C(111)-C(112)-C(117)	123(2)
N(5A)-C(12A)-C(10A)	119.2(15)	N(4C)-C(18C)-N(6C)	126.1(16)	C(111)-C(112)-C(113)	121(2)
N(4A)-C(12A)-C(10A)	115.5(15)	N(4C)-C(18C)-C(16C)	117.5(15)	C(117)-C(112)-C(113)	115(2)
N(6C)-C(12C)-N(5C)	123.6(15)	N(6C)-C(18C)-C(16C)	116.2(15)	C(114)-C(113)-C(112)	122(2)
N(6C)-C(12C)-C(10C)	119.4(15)	N(4B)-C(18B)-N(5B)	124.0(16)	C(113)-C(114)-C(115)	120(2)
N(5C)-C(12C)-C(10C)	116.8(14)	N(4B)-C(18B)-C(16B)	118.1(16)	C(114)-C(115)-C(116)	120(2)
N(4B)-C(12B)-N(6B)	123.1(16)	N(5B)-C(18B)-C(16B)	117.4(16)	C(117)-C(116)-C(115)	122(2)
N(4B)-C(12B)-C(10B)	118.3(15)	N(4A)-C(18A)-N(6A)	122.9(16)	C(116)-C(117)-C(118)	122(2)
N(6B)-C(12B)-C(10B)	118.4(15)	N(4A)-C(18A)-C(16A)	117.8(15)	C(116)-C(117)-C(112)	120(2)
N(12)-C(12)-C(11)	109.9(17)	N(6A)-C(18A)-C(16A)	119.3(15)	C(118)-C(117)-C(112)	118(2)
C(14D)-C(13D)-N(3D)	125.5(15)	C(22)-C(21)-N(22)	105(2)	C(117)-C(118)-C(119)	120(2)
N(3A)-C(13A)-C(14A)	122.1(17)	C(21)-C(22)-N(21)	110.3(19)	C(110)-C(119)-C(118)	121(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2•5a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	27(1)	25(1)	19(1)	1(1)	8(1)	3(1)
Pd(2)	30(1)	35(1)	18(1)	-5(1)	7(1)	2(1)
Pd(3)	27(1)	39(1)	20(1)	-2(1)	4(1)	0(1)
Pd(4)	24(1)	42(1)	18(1)	0(1)	3(1)	0(1)
Pd(5)	38(1)	59(1)	18(1)	5(1)	6(1)	1(1)
Pd(6)	45(1)	63(1)	32(1)	11(1)	11(1)	15(1)
Si(2)	52(4)	67(5)	52(4)	-3(4)	12(3)	-17(3)

Si(1)	53(4)	62(5)	87(6)	-4(4)	13(4)	-2(4)
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Table 1. Crystal data and structure refinement for **2•5b**.

Identification code	kusu102	
Empirical formula	C108 H130 N48 O51 Pd6 Si2	
Formula weight	3611.18	
Temperature	105(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P4(3)2(1)2	
Unit cell dimensions	a = 24.2902(11) Å	$\alpha = 90^\circ$.
	b = 24.2902(11) Å	$\beta = 90^\circ$.
	c = 28.0015(17) Å	$\gamma = 90^\circ$.
Volume	16521.3(15) Å ³	
Z	4	
Density (calculated)	1.452 Mg/m ³	
Absorption coefficient	0.743 mm ⁻¹	
F(000)	7304	
Crystal size	0.60 x 0.50 x 0.50 mm ³	
Theta range for data collection	1.68 to 20.80°	
Index ranges	-24 ≤ h ≤ 24, -20 ≤ k ≤ 24, -24 ≤ l ≤ 27	
Reflections collected	59909	
Independent reflections	8627 [R(int) = 0.0440]	
Completeness to theta = 20.80°	99.9 %	
Absorption correction	Empirical (SADABS)	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8627 / 0 / 810	
Goodness-of-fit on F ²	2.190	
Final R indices [I > 2σ(I)]	R1 = 0.0962, wR2 = 0.2546	
R indices (all data)	R1 = 0.1073, wR2 = 0.2641	
Absolute structure parameter	0.04(7)	
Largest diff. peak and hole	1.250 and -0.863 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **2•5b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	N(8)	-1380(5)	8159(5)	-2253(4)	55(3)
					N(9)	-2571(5)	5571(7)	-1750(6)	71(4)
Pd(1)	-5064(1)	10367(1)	-265(1)	67(1)	N(10)	-524(4)	6979(5)	-1089(4)	46(3)
Pd(2)	-1923(1)	8241(1)	-2793(1)	78(1)	N(11)	-1327(5)	6687(5)	-1485(4)	50(3)
Pd(3)	-3233(1)	5800(1)	-2140(1)	111(1)	N(12)	-876(6)	6074(6)	-981(5)	67(4)
Si(1)	-418(7)	9082(7)	-429(5)	203(5)	N(13)	-5829(6)	10409(6)	-569(6)	94(5)
N(001)	-3099(6)	4886(6)	-375(5)	74(4)	N(14)	-5178(7)	11160(6)	-167(7)	96(5)
N(1)	-5050(5)	9531(5)	-336(4)	58(3)	N(15)	-1456(6)	7762(8)	-3212(5)	96(5)
N(2)	-2420(5)	8710(7)	-2359(4)	72(4)	N(16)	-2397(9)	8304(11)	-3388(6)	138(9)
N(002)	-6671(13)	8697(13)	696(11)	154(9)	N(17)	-2951(8)	5414(13)	-2729(8)	187(15)
N(3)	-3559(5)	6178(8)	-1572(6)	81(5)	N(18)	-3891(10)	5952(19)	-2521(10)	240(20)
N(4)	-3897(5)	8718(6)	-1219(5)	66(4)	C(1)	-5380(7)	9223(7)	-93(5)	61(4)
N(5)	-3493(5)	7883(6)	-1470(5)	65(4)	C(2)	-5371(6)	8679(7)	-79(6)	57(4)
N(6)	-4231(4)	7875(5)	-919(4)	50(3)	C(3)	-4989(6)	8411(7)	-354(5)	63(5)
N(7)	350(6)	5709(6)	-33(6)	73(4)	C(4)	-4647(5)	8716(7)	-647(5)	49(4)

C(5)	-4685(7)	9285(6)	-621(5)	52(4)	C(40)	-2170(11)	7890(20)	-3763(7)	260(30)
C(6)	-4236(6)	8409(7)	-938(5)	57(4)	C(41)	-3420(20)	5620(30)	-3127(13)	300(40)
C(7)	-2405(6)	9254(7)	-2368(6)	70(5)	C(42)	-3885(19)	5690(30)	-2930(20)	300(40)
C(8)	-2732(7)	9555(8)	-2062(8)	91(7)	C(100)	-1224(6)	8136(7)	-474(6)	131(9)
C(9)	-3111(7)	9315(8)	-1782(7)	89(6)	C(101)	-1047(6)	8657(8)	-612(8)	143(10)
C(10)	-3147(7)	8751(8)	-1773(6)	75(5)	C(102)	-1381(9)	8983(6)	-899(8)	161(12)
C(11)	-2799(7)	8451(8)	-2096(6)	70(5)	C(103)	-1891(8)	8789(7)	-1048(6)	139(9)
C(12)	-3564(6)	8421(7)	-1476(6)	57(4)	C(104)	-2068(5)	8269(7)	-910(6)	133(9)
C(13)	-3825(8)	5922(8)	-1236(10)	100(8)	C(105)	-1734(6)	7942(5)	-623(5)	76(5)
C(14)	-4056(9)	6174(7)	-834(8)	90(6)	C(106)	-1900(7)	7437(7)	-498(6)	66(4)
C(15)	-4094(6)	6727(7)	-830(8)	74(5)	C(107)	-2391(9)	7163(9)	-632(7)	90(6)
C(16)	-3834(6)	7005(7)	-1174(6)	63(4)	C(108)	-2519(9)	6598(10)	-521(8)	102(7)
C(17)	-3583(5)	6712(8)	-1540(6)	62(4)	C(109)	-2162(7)	6307(7)	-243(7)	74(5)
C(18)	-3847(6)	7629(6)	-1198(6)	55(4)	C(110)	-1650(10)	6601(10)	-115(8)	110(7)
C(19)	710(8)	6121(8)	110(9)	96(7)	C(111)	-1568(10)	7107(11)	-208(9)	112(7)
C(20)	697(8)	6631(7)	-18(7)	77(5)	O(1)	-2649(5)	4719(5)	-274(4)	83(3)
C(21)	284(7)	6773(7)	-391(5)	65(4)	O(2)	-3330(7)	5293(7)	-188(6)	120(5)
C(22)	-69(6)	6358(8)	-537(6)	64(4)	O(3)	-3367(6)	4630(6)	-692(5)	101(4)
C(23)	-19(6)	5830(6)	-359(6)	56(4)	O(4)	-6612(10)	8799(10)	264(10)	176(8)
C(24)	-513(6)	6484(7)	-899(6)	58(4)	O(5)	-6374(12)	8356(12)	831(9)	185(9)
C(25)	-1007(7)	8552(6)	-2141(5)	56(4)	O(6)	-7059(12)	8990(11)	924(10)	186(9)
C(26)	-620(7)	8514(6)	-1813(6)	62(4)	O(8W)	-2020(50)	10600(50)	-2950(40)	650(70)
C(27)	-576(7)	8026(6)	-1567(5)	58(4)	O(9W)	-1113(19)	9970(20)	-2393(17)	316(19)
C(28)	-960(6)	7620(7)	-1655(6)	59(4)	O(10W)	-6654(9)	9906(9)	62(8)	157(7)
C(29)	-1346(6)	7691(7)	-2010(5)	53(4)	O(11W)	-2082(12)	7153(12)	-4891(10)	207(10)
C(30)	-928(6)	7058(5)	-1398(4)	40(3)	O(12W)	-4451(13)	4857(13)	-401(10)	219(11)
C(31)	-2535(8)	5078(9)	-1553(7)	82(6)	O(13W)	-1270(20)	9660(20)	-3206(18)	340(20)
C(32)	-2096(9)	4933(10)	-1262(7)	93(6)	O(14W)	-1080(20)	7490(20)	-4807(18)	330(20)
C(33)	-1676(8)	5263(7)	-1155(6)	69(5)	O(15W)	-730(20)	8020(20)	-5130(20)	360(30)
C(34)	-1714(6)	5780(7)	-1379(6)	62(4)	O(16W)	200(30)	8950(40)	1570(30)	470(40)
C(35)	-2176(8)	5933(7)	-1669(6)	71(5)	O(17W)	-8430(30)	7880(30)	1560(20)	420(30)
C(36)	-1273(6)	6203(6)	-1279(5)	47(4)	O(100)	-205(11)	8673(12)	-299(9)	175(8)
C(37)	-6017(12)	10986(12)	-510(14)	181(18)	O(101)	-203(17)	9638(17)	-924(13)	279(16)
C(38)	-5671(14)	11336(10)	-420(20)	280(30)	O(102)	-555(9)	9445(9)	0	153(10)
C(39)	-1638(9)	7809(16)	-3711(8)	152(14)					

Table 3. Bond lengths [Å] and angles [°] for **2•5b**.

Pd(1)-N(14)	1.966(14)	Si(1)-C(101)	1.91(2)	N(4)-C(12)	1.30(2)
Pd(1)-N(1)	2.039(13)	Si(1)-O(101)	2.00(4)	N(4)-C(6)	1.36(2)
Pd(1)-N(13)	2.048(13)	N(001)-O(1)	1.199(17)	N(5)-C(18)	1.30(2)
Pd(1)-N(7)#1	2.053(15)	N(001)-O(3)	1.265(18)	N(5)-C(12)	1.32(2)
Pd(2)-N(15)	2.005(16)	N(001)-O(2)	1.251(19)	N(6)-C(6)	1.30(2)
Pd(2)-N(8)	2.016(12)	N(1)-C(1)	1.29(2)	N(6)-C(18)	1.354(19)
Pd(2)-N(16)	2.033(17)	N(1)-C(5)	1.334(19)	N(7)-C(23)	1.31(2)
Pd(2)-N(2)	2.058(14)	N(2)-C(7)	1.32(2)	N(7)-C(19)	1.39(2)
Pd(3)-N(18)	1.96(3)	N(2)-C(11)	1.34(2)	N(7)-Pd(1)#1	2.053(15)
Pd(3)-N(3)	2.000(15)	N(002)-O(5)	1.16(3)	N(8)-C(29)	1.325(19)
Pd(3)-N(17)	2.017(16)	N(002)-O(4)	1.24(3)	N(8)-C(25)	1.35(2)
Pd(3)-N(9)	2.024(15)	N(002)-O(6)	1.34(3)	N(9)-C(35)	1.32(2)
Si(1)-O(100)	1.18(3)	N(3)-C(13)	1.30(3)	N(9)-C(31)	1.32(3)
Si(1)-O(102)	1.528(17)	N(3)-C(17)	1.30(2)	N(10)-C(24)	1.315(19)

N(10)-C(30)	1.323(17)	C(10)-C(12)	1.54(2)	C(34)-C(36)	1.51(2)
N(11)-C(36)	1.316(18)	C(13)-C(14)	1.40(3)	C(37)-C(38)	1.22(3)
N(11)-C(30)	1.346(18)	C(14)-C(15)	1.35(2)	C(39)-C(40)	1.31(3)
N(12)-C(36)	1.31(2)	C(15)-C(16)	1.34(2)	C(41)-C(42)	1.27(6)
N(12)-C(24)	1.35(2)	C(16)-C(17)	1.39(2)	C(100)-C(101)	1.3900
N(13)-C(37)	1.48(3)	C(16)-C(18)	1.52(2)	C(100)-C(105)	1.3900
N(14)-C(38)	1.46(3)	C(19)-C(20)	1.29(2)	C(101)-C(102)	1.3900
N(15)-C(39)	1.47(3)	C(20)-C(21)	1.49(2)	C(102)-C(103)	1.3900
N(16)-C(40)	1.56(4)	C(21)-C(22)	1.38(2)	C(103)-C(104)	1.3900
N(17)-C(41)	1.67(5)	C(22)-C(23)	1.38(2)	C(104)-C(105)	1.3900
N(18)-C(42)	1.31(7)	C(22)-C(24)	1.51(2)	C(105)-C(106)	1.34(2)
C(1)-C(2)	1.32(2)	C(25)-C(26)	1.32(2)	C(106)-C(111)	1.40(3)
C(2)-C(3)	1.37(2)	C(26)-C(27)	1.37(2)	C(106)-C(107)	1.42(3)
C(3)-C(4)	1.38(2)	C(27)-C(28)	1.38(2)	C(107)-C(108)	1.44(3)
C(4)-C(5)	1.39(2)	C(28)-C(29)	1.38(2)	C(108)-C(109)	1.36(3)
C(4)-C(6)	1.49(2)	C(28)-C(30)	1.54(2)	C(109)-C(110)	1.48(3)
C(7)-C(8)	1.38(3)	C(31)-C(32)	1.39(3)	C(110)-C(111)	1.27(3)
C(8)-C(9)	1.34(2)	C(32)-C(33)	1.33(3)	O(102)-Si(1)#1	1.528(17)
C(9)-C(10)	1.37(3)	C(33)-C(34)	1.41(2)		
C(10)-C(11)	1.44(2)	C(34)-C(35)	1.43(2)		
N(14)-Pd(1)-N(1)	172.4(6)	O(5)-N(002)-O(4)	113(3)	N(1)-C(5)-C(4)	121.5(14)
N(14)-Pd(1)-N(13)	83.2(6)	O(5)-N(002)-O(6)	131(3)	N(6)-C(6)-N(4)	124.6(13)
N(1)-Pd(1)-N(13)	91.3(5)	O(4)-N(002)-O(6)	116(3)	N(6)-C(6)-C(4)	119.0(14)
N(14)-Pd(1)-N(7)#1	95.3(6)	C(13)-N(3)-C(17)	113.9(15)	N(4)-C(6)-C(4)	116.4(15)
N(1)-Pd(1)-N(7)#1	90.3(5)	C(13)-N(3)-Pd(3)	123.6(14)	N(2)-C(7)-C(8)	120.1(15)
N(13)-Pd(1)-N(7)#1	178.2(7)	C(17)-N(3)-Pd(3)	121.9(14)	C(9)-C(8)-C(7)	121.8(19)
N(15)-Pd(2)-N(8)	90.6(5)	C(12)-N(4)-C(6)	112.8(14)	C(8)-C(9)-C(10)	119.3(16)
N(15)-Pd(2)-N(16)	83.3(8)	C(18)-N(5)-C(12)	112.9(13)	C(9)-C(10)-C(11)	117.2(14)
N(8)-Pd(2)-N(16)	173.4(7)	C(6)-N(6)-C(18)	115.0(12)	C(9)-C(10)-C(12)	125.0(15)
N(15)-Pd(2)-N(2)	178.0(7)	C(23)-N(7)-C(19)	117.9(16)	C(11)-C(10)-C(12)	117.6(17)
N(8)-Pd(2)-N(2)	89.8(5)	C(23)-N(7)-Pd(1)#1	120.1(11)	N(2)-C(11)-C(10)	120.8(17)
N(16)-Pd(2)-N(2)	96.3(7)	C(19)-N(7)-Pd(1)#1	122.0(13)	N(4)-C(12)-N(5)	128.7(14)
N(18)-Pd(3)-N(3)	91.4(8)	C(29)-N(8)-C(25)	116.5(13)	N(4)-C(12)-C(10)	114.7(15)
N(18)-Pd(3)-N(17)	85.5(9)	C(29)-N(8)-Pd(2)	120.6(11)	N(5)-C(12)-C(10)	115.9(15)
N(3)-Pd(3)-N(17)	176.6(7)	C(25)-N(8)-Pd(2)	122.7(10)	N(3)-C(13)-C(14)	124.9(17)
N(18)-Pd(3)-N(9)	174.9(13)	C(35)-N(9)-C(31)	118.9(17)	C(15)-C(14)-C(13)	118.2(19)
N(3)-Pd(3)-N(9)	90.6(6)	C(35)-N(9)-Pd(3)	119.2(14)	C(16)-C(15)-C(14)	117.7(18)
N(17)-Pd(3)-N(9)	92.4(7)	C(31)-N(9)-Pd(3)	121.8(12)	C(15)-C(16)-C(17)	118.7(17)
O(100)-Si(1)-O(102)	109.8(18)	C(24)-N(10)-C(30)	114.4(12)	C(15)-C(16)-C(18)	121.9(15)
O(100)-Si(1)-C(101)	88.8(18)	C(36)-N(11)-C(30)	116.5(12)	C(17)-C(16)-C(18)	119.2(16)
O(102)-Si(1)-C(101)	110.4(16)	C(36)-N(12)-C(24)	114.2(14)	N(3)-C(17)-C(16)	125.5(17)
O(100)-Si(1)-O(101)	132(2)	C(37)-N(13)-Pd(1)	106.2(12)	N(5)-C(18)-N(6)	125.7(14)
O(102)-Si(1)-O(101)	102.2(17)	C(38)-N(14)-Pd(1)	109.5(15)	N(5)-C(18)-C(16)	119.0(13)
C(101)-Si(1)-O(101)	112.8(15)	C(39)-N(15)-Pd(2)	109.9(13)	N(6)-C(18)-C(16)	115.3(14)
O(1)-N(001)-O(3)	117.9(16)	C(40)-N(16)-Pd(2)	107.7(14)	C(20)-C(19)-N(7)	126.8(19)
O(1)-N(001)-O(2)	125.3(16)	C(41)-N(17)-Pd(3)	100(2)	C(19)-C(20)-C(21)	115.6(17)
O(3)-N(001)-O(2)	116.8(16)	C(42)-N(18)-Pd(3)	112(3)	C(22)-C(21)-C(20)	117.3(15)
C(1)-N(1)-C(5)	117.9(14)	N(1)-C(1)-C(2)	125.8(15)	C(23)-C(22)-C(21)	120.9(14)
C(1)-N(1)-Pd(1)	121.0(11)	C(1)-C(2)-C(3)	118.1(16)	C(23)-C(22)-C(24)	119.6(16)
C(5)-N(1)-Pd(1)	121.0(10)	C(2)-C(3)-C(4)	119.0(16)	C(21)-C(22)-C(24)	119.5(16)
C(7)-N(2)-C(11)	120.2(14)	C(3)-C(4)-C(5)	117.6(13)	N(7)-C(23)-C(22)	121.3(15)
C(7)-N(2)-Pd(2)	121.6(11)	C(3)-C(4)-C(6)	117.3(15)	N(10)-C(24)-N(12)	126.4(15)
C(11)-N(2)-Pd(2)	117.9(13)	C(5)-C(4)-C(6)	124.9(14)	N(10)-C(24)-C(22)	118.1(14)

N(12)-C(24)-C(22)	115.5(16)	C(35)-C(34)-C(36)	118.9(16)	C(102)-C(103)-C(104)	120.0
C(26)-C(25)-N(8)	126.0(14)	N(9)-C(35)-C(34)	119.6(16)	C(105)-C(104)-C(103)	120.0
C(25)-C(26)-C(27)	117.8(14)	N(12)-C(36)-N(11)	124.5(13)	C(106)-C(105)-C(104)	119.9(14)
C(26)-C(27)-C(28)	118.4(14)	N(12)-C(36)-C(34)	118.4(14)	C(106)-C(105)-C(100)	120.1(14)
C(29)-C(28)-C(27)	119.9(15)	N(11)-C(36)-C(34)	117.0(15)	C(104)-C(105)-C(100)	120.0
C(29)-C(28)-C(30)	118.8(14)	C(38)-C(37)-N(13)	118(2)	C(105)-C(106)-C(111)	120.3(18)
C(27)-C(28)-C(30)	121.0(14)	C(37)-C(38)-N(14)	117(2)	C(105)-C(106)-C(107)	128.0(16)
N(8)-C(29)-C(28)	121.3(15)	C(40)-C(39)-N(15)	114(2)	C(111)-C(106)-C(107)	111.7(18)
N(10)-C(30)-N(11)	123.7(12)	C(39)-C(40)-N(16)	112(3)	C(106)-C(107)-C(108)	124.9(19)
N(10)-C(30)-C(28)	118.0(12)	C(42)-C(41)-N(17)	111(4)	C(109)-C(108)-C(107)	119(2)
N(11)-C(30)-C(28)	118.2(12)	C(41)-C(42)-N(18)	117(5)	C(108)-C(109)-C(110)	115.0(19)
N(9)-C(31)-C(32)	121.8(18)	C(101)-C(100)-C(105)	120.0	C(111)-C(110)-C(109)	123(2)
C(33)-C(32)-C(31)	125(2)	C(100)-C(101)-C(102)	120.0	C(110)-C(111)-C(106)	126(2)
C(32)-C(33)-C(34)	112.7(19)	C(100)-C(101)-Si(1)	131.5(13)	Si(1)#1-O(102)-Si(1)	150(3)
C(33)-C(34)-C(35)	122.3(15)	C(102)-C(101)-Si(1)	108.2(13)		
C(33)-C(34)-C(36)	118.6(15)	C(103)-C(102)-C(101)	120.0		

Symmetry transformations used to generate equivalent atoms:

#1 y-1,x+1,-z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2•5b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pd(1)	65(1)	57(1)	78(1)	-2(1)	-22(1)	5(1)
Pd(2)	59(1)	120(1)	56(1)	20(1)	8(1)	28(1)
Pd(3)	54(1)	154(2)	124(1)	-82(1)	-12(1)	1(1)
N(1)	39(7)	74(9)	61(7)	-20(8)	-3(6)	-11(7)
N(2)	48(8)	110(14)	59(8)	44(8)	24(7)	26(8)
N(3)	14(7)	86(12)	142(14)	-38(11)	23(8)	-13(7)
N(4)	49(8)	72(9)	77(9)	16(8)	15(7)	16(7)
N(5)	50(8)	56(10)	88(10)	19(7)	8(7)	11(7)
N(6)	30(6)	43(8)	75(8)	15(6)	6(6)	10(6)
N(7)	44(8)	69(9)	105(10)	-3(8)	5(8)	-3(7)
N(8)	58(8)	52(8)	56(7)	13(7)	9(6)	13(7)
N(9)	48(8)	58(10)	106(11)	-51(9)	0(7)	-15(7)
N(10)	26(6)	56(8)	56(7)	9(6)	0(6)	7(5)
N(11)	52(8)	61(9)	36(6)	-9(6)	8(5)	23(7)
N(12)	54(9)	74(10)	73(9)	5(7)	14(8)	20(8)
N(13)	75(10)	74(10)	132(13)	-13(10)	-55(10)	17(8)
N(14)	94(11)	45(8)	149(15)	14(9)	-12(11)	14(7)
N(15)	37(8)	161(17)	89(11)	0(11)	5(8)	13(9)
N(16)	113(15)	220(30)	78(11)	33(14)	-13(11)	46(16)
N(17)	73(12)	320(40)	160(20)	-170(20)	-7(13)	32(16)
N(18)	83(16)	470(60)	160(20)	-200(30)	-12(16)	10(20)
C(1)	67(11)	58(12)	59(9)	-20(8)	2(8)	1(9)
C(2)	35(8)	65(12)	72(10)	-9(8)	-6(8)	-13(8)
C(3)	54(10)	86(12)	50(9)	-26(8)	-14(8)	26(9)
C(4)	16(7)	95(13)	36(7)	17(8)	-1(6)	10(7)
C(5)	73(11)	35(9)	49(8)	12(7)	-11(8)	2(8)
C(6)	35(8)	82(14)	54(9)	8(9)	7(7)	27(8)

C(7)	49(10)	65(12)	97(13)	48(10)	-14(9)	-6(9)
C(8)	45(10)	87(13)	139(17)	29(13)	52(12)	30(10)
C(9)	69(12)	84(15)	114(14)	29(12)	51(11)	43(10)
C(10)	54(10)	88(14)	84(11)	54(10)	29(9)	25(9)
C(11)	62(11)	79(12)	67(10)	2(9)	6(9)	35(9)
C(12)	31(8)	69(12)	72(11)	21(9)	0(8)	5(8)
C(13)	38(11)	51(11)	210(30)	-37(15)	-5(14)	-8(9)
C(14)	103(15)	43(12)	124(16)	34(11)	27(13)	25(10)
C(15)	32(9)	58(12)	131(16)	-24(11)	1(9)	4(8)
C(16)	39(9)	78(12)	71(10)	-17(10)	11(8)	-7(9)
C(17)	21(8)	89(14)	76(11)	-1(10)	9(7)	6(8)
C(18)	36(9)	55(10)	73(10)	-3(8)	1(8)	7(8)
C(19)	69(13)	54(13)	160(20)	2(12)	-33(13)	-3(10)
C(20)	72(12)	52(12)	109(14)	4(10)	-9(11)	5(9)
C(21)	80(11)	55(9)	62(9)	14(8)	-10(9)	-5(9)
C(22)	41(9)	88(14)	64(9)	-6(9)	6(8)	19(9)
C(23)	39(9)	52(10)	78(10)	-7(8)	-3(8)	12(7)
C(24)	55(10)	53(10)	65(9)	-13(8)	2(8)	-17(8)
C(25)	77(11)	45(9)	46(9)	9(7)	16(9)	15(9)
C(26)	68(11)	38(9)	79(11)	-20(8)	-15(10)	-9(8)
C(27)	68(11)	58(11)	47(8)	4(8)	-14(7)	4(9)
C(28)	38(9)	63(11)	75(11)	-10(9)	25(9)	13(8)
C(29)	26(8)	77(12)	55(9)	-12(9)	13(7)	11(7)
C(30)	53(9)	27(7)	39(7)	-11(6)	-9(7)	-10(7)
C(31)	77(14)	77(16)	92(13)	-25(12)	30(12)	-41(11)
C(32)	87(15)	124(18)	67(11)	-13(12)	30(11)	-28(15)
C(33)	73(12)	58(11)	76(11)	-18(9)	11(9)	-18(9)
C(34)	31(8)	67(12)	88(11)	-8(9)	21(8)	1(8)
C(35)	107(16)	41(9)	65(10)	-19(8)	17(10)	8(10)
C(36)	47(9)	30(8)	63(9)	-3(7)	19(8)	-3(7)
C(37)	130(20)	120(20)	290(40)	-110(20)	-140(30)	80(20)
C(38)	190(30)	42(13)	620(90)	40(30)	-290(50)	16(16)
C(39)	62(15)	300(40)	95(16)	-30(20)	-33(12)	80(19)
C(40)	110(20)	640(90)	35(11)	-60(20)	5(12)	140(30)
C(41)	220(50)	560(110)	120(30)	-110(40)	-90(30)	-80(60)
C(42)	110(30)	550(130)	230(60)	110(70)	0(40)	20(50)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2·5b**.

	x	y	z	U(eq)
H(13A)	-5812	10320	-881	112
H(13B)	-6062	10175	-423	112
H(14A)	-5218	11231	147	115
H(14B)	-4884	11348	-274	115
H(15A)	-1101	7865	-3188	115
H(15B)	-1483	7409	-3116	115
H(16A)	-2750	8224	-3318	166
H(16B)	-2382	8649	-3505	166

H(17A)	-2611	5529	-2808	224
H(17B)	-2950	5046	-2692	224
H(18A)	-4192	5853	-2354	283
H(18B)	-3913	6316	-2578	283
H(1A)	-5648	9399	89	74
H(2A)	-5616	8484	112	69
H(3A)	-4961	8029	-344	76
H(5B)	-4450	9500	-806	63
H(7A)	-2173	9433	-2582	84
H(8A)	-2688	9935	-2048	109
H(9A)	-3347	9528	-1597	107
H(11B)	-2838	8071	-2123	83
H(13B)	-3865	5542	-1265	119
H(14B)	-4179	5966	-577	108
H(15B)	-4295	6909	-595	88
H(17B)	-3418	6915	-1783	75
H(19A)	989	6019	319	115
H(20A)	931	6893	114	93
H(21A)	263	7125	-520	78
H(23A)	-251	5555	-473	68
H(25A)	-1025	8880	-2312	67
H(26A)	-384	8806	-1750	74
H(27A)	-294	7971	-1348	69
H(29A)	-1588	7406	-2081	64
H(31A)	-2811	4822	-1610	99
H(32A)	-2096	4581	-1133	111
H(33A)	-1389	5162	-954	83
H(35A)	-2197	6285	-1799	86
H(37A)	-6208	11093	-799	218
H(37B)	-6285	10993	-253	218
H(38A)	-5845	11626	-242	340
H(38B)	-5555	11495	-726	340
H(39A)	-1444	8114	-3859	182
H(39B)	-1535	7476	-3880	182
H(40A)	-2360	7538	-3729	312
H(40B)	-2242	8026	-4082	312
H(41A)	-3303	5958	-3275	356
H(41B)	-3454	5341	-3376	356
H(42A)	-4048	5327	-2877	356
H(42B)	-4120	5882	-3151	356

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SUPPORTING INFORMATION FOR REVIEWERS

Cavity-directed Synthesis of Labile Silanol Oligomers within Self-assembled Coordination Cages

Michito Yoshizawa, Takahiro Kusukawa, Makoto Fujita, Shigeru Sakamoto, and Kentaro Yamaguchi

Contents

- CSI-MS spectra of **1•4**.
- NMR spectra of **1•4** (^1H , ^{13}C , DEPT, ^{29}Si , HH-COSY, NOESY, CH-COSY).
- CSI-MS spectra of **2•5a**.
- NMR spectra of **2•5a** (^1H , ^{13}C , DEPT, ^{29}Si , HH-COSY, NOESY, CH-COSY).
- CSI-MS spectra of **2•5b**.
- NMR spectra of **2•5b** (^1H , ^{13}C , ^{29}Si , HH-COSY, CH-COSY).
- CSI-MS spectra of **3•6**.
- NMR spectra of **3•6** (^1H , ^{13}C , ^{29}Si , HH-COSY, CH-COSY).
- NMR spectra of **3•6** (^1H).

[Mass Spectrum]
 Date : 22-Sep-2000 12:25
 Data : 000322-001

Sample :

Note : -

Inlet : Direct

Spectrum Type : Normal Ion [MF-Linear]

RT : 12.13 min

BP : m/z 462.1714

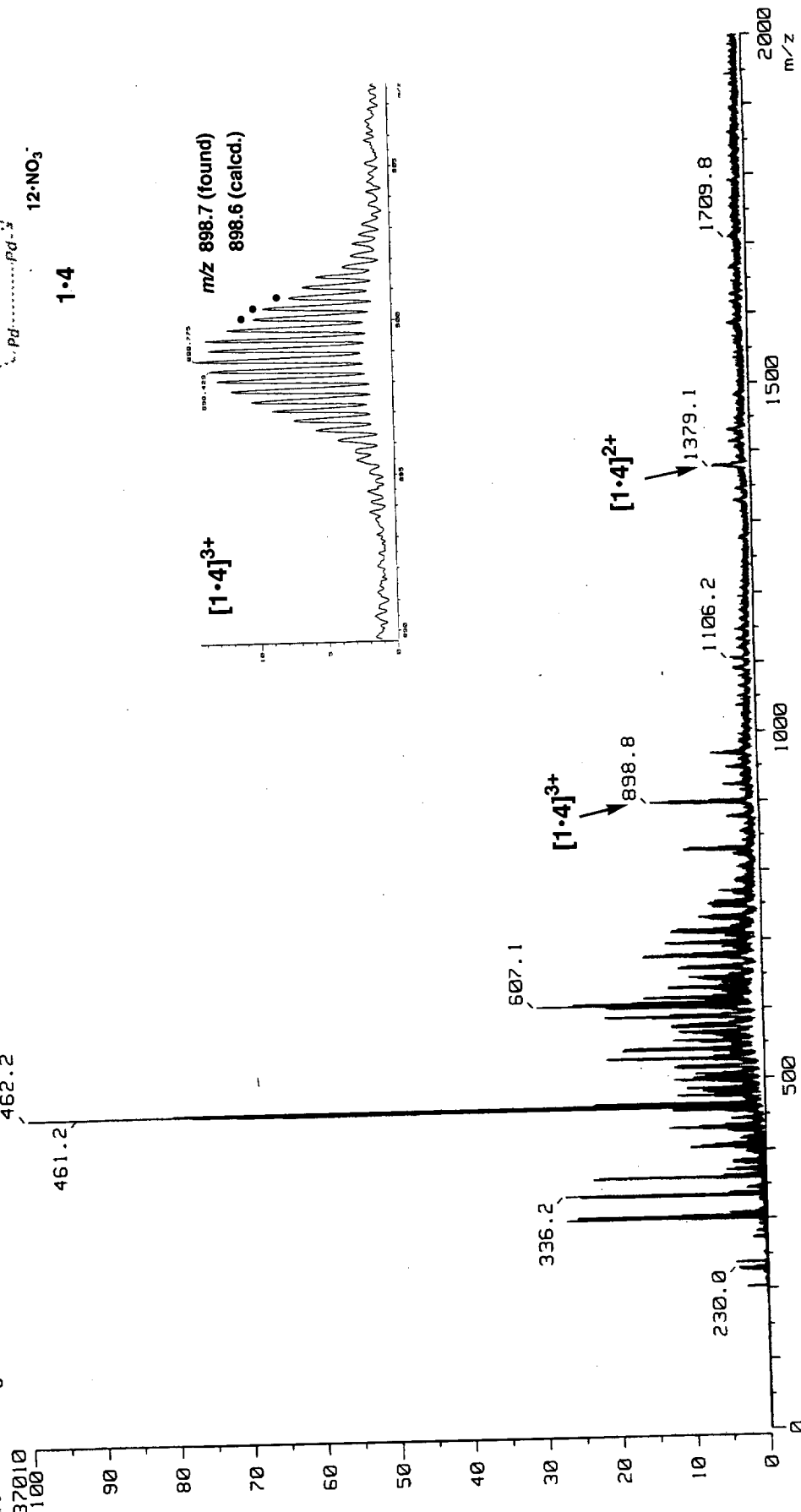
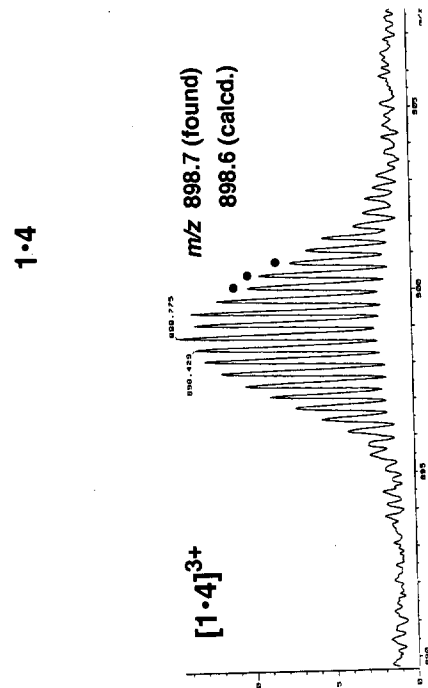
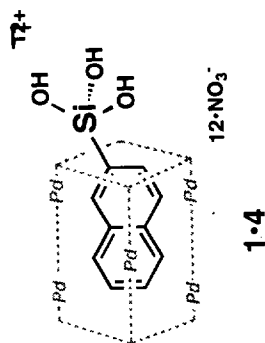
Output m/z range : 0.0000 to 2000.0000

44137010

Ion Mode : ESI+

Cut Level : 0.00 %

CSI MS (1) of 1•4



[Mass Spectrum J
 Date : 22-Sep-2000 12:25
 Data : 000922-001

Sample :

Note : -

Inlet : Direct

Spectrum Type : Normal Ion [MF-Linear]

RT : 12.13 min

BP : m/z 462.1714

Output m/z range : 278.9318 to 1017.8042

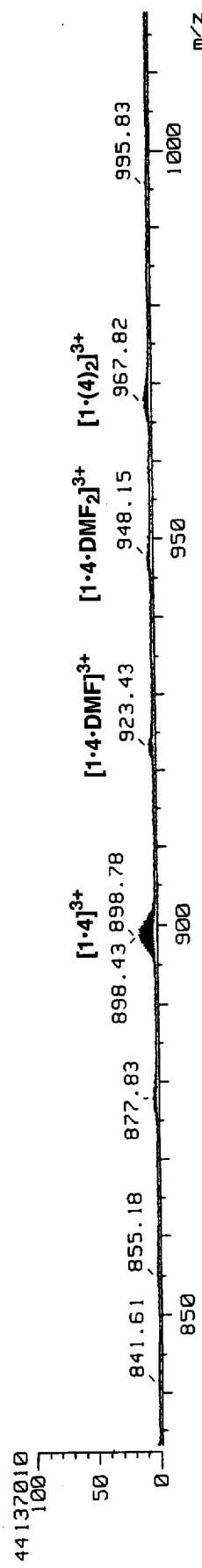
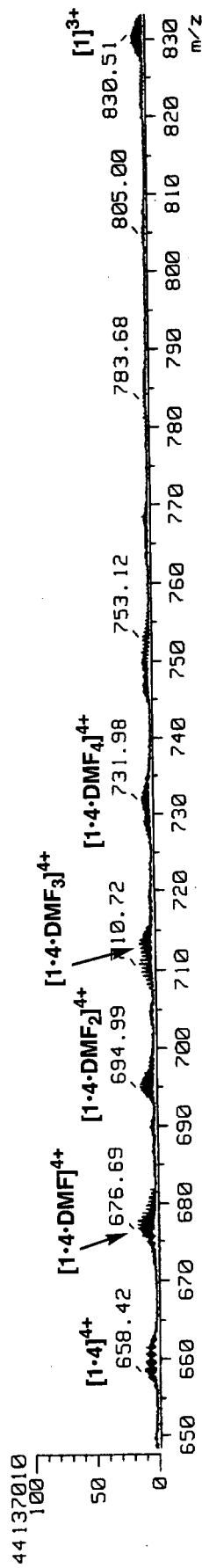
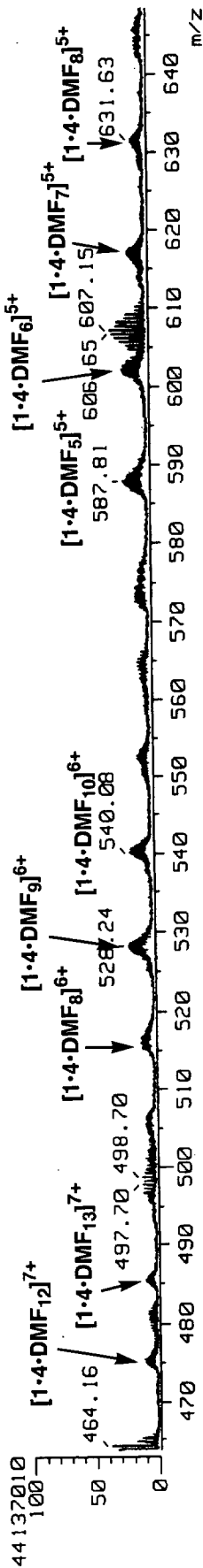
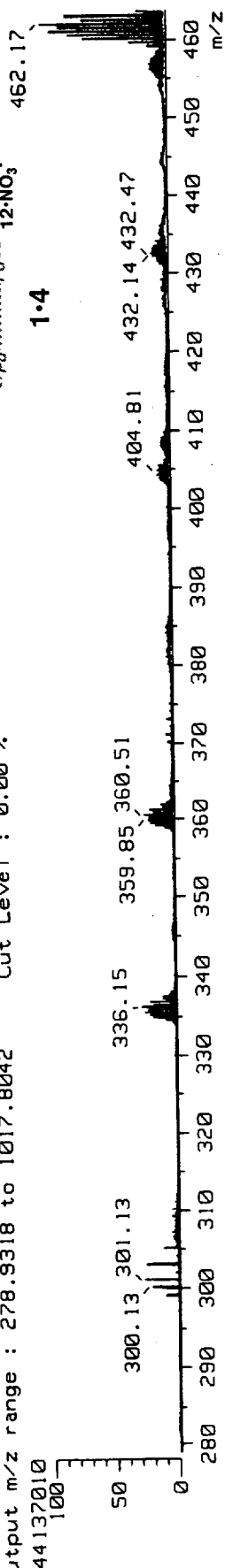
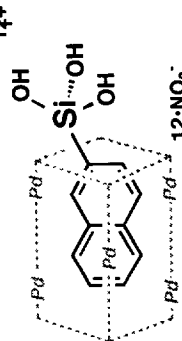
Ion Mode : ESI+

Scan# : (1,78)

Int. : 53.96

Cut Level : 0.00 %

CSI MS (2) of 1·4



¹H NMR(1) of 1•4

Current Data Parameters
 NAME Tube3
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

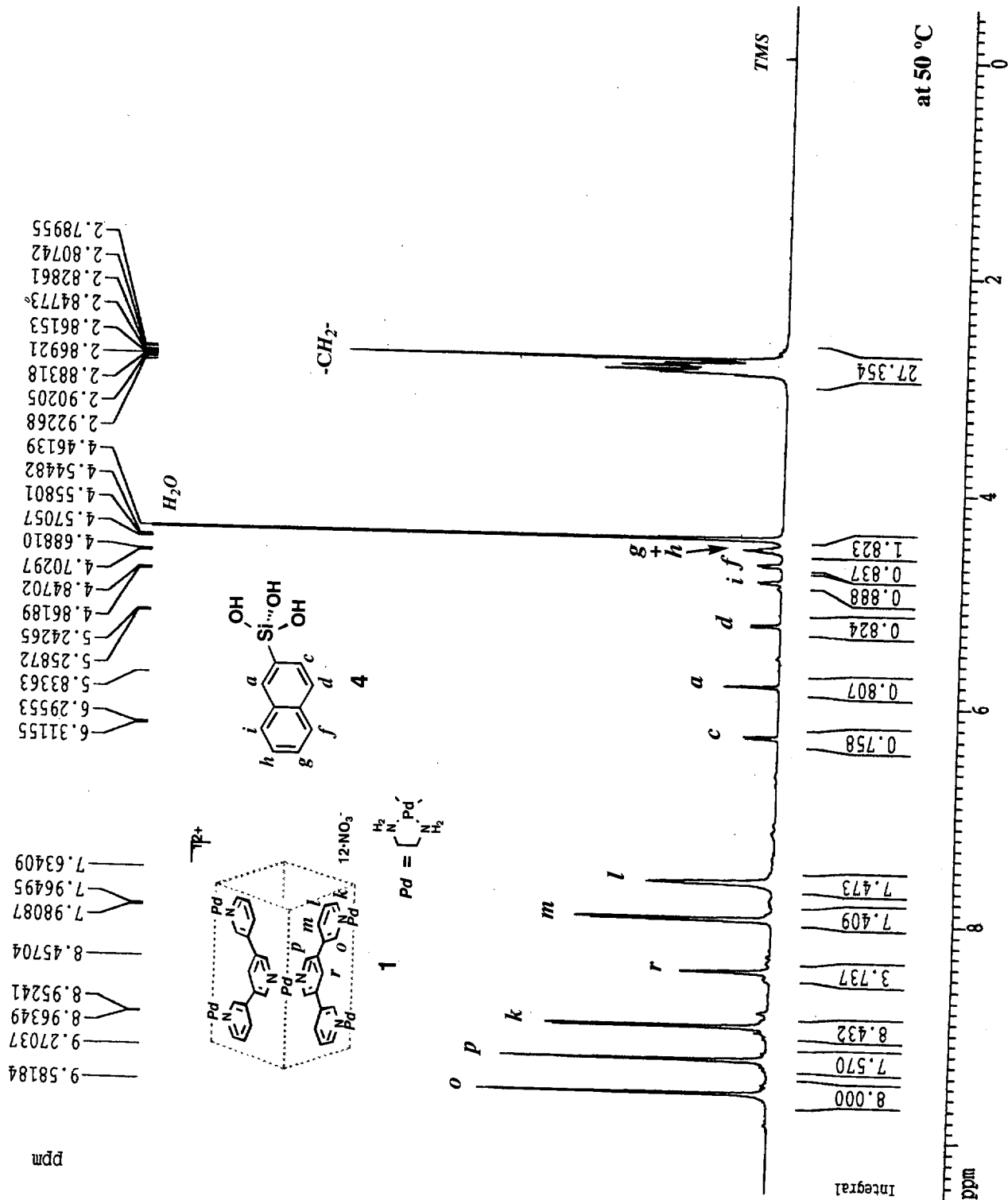
Date_ 20000912
 Time 10.42
 INSTRUM drx500
 PROBHD 5 mm BBI 1H-B
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 2
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 40.3
 DW 48.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.0000000 sec
 P1 8.40 usec
 SF01 500.1330885 MHz
 NUC1 1H
 PL1 -4.00 dB

F2 - Processing parameters

SI 16384
 SF 500.1301238 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 10.500 ppm
 F1 5251.37 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07156 Hz/cm



¹H NMR(2) of 1·4

Current Data Parameters
 NAME tube3
 EXPNO 298
 PROCNO 1

F2 - Acquisition Parameters

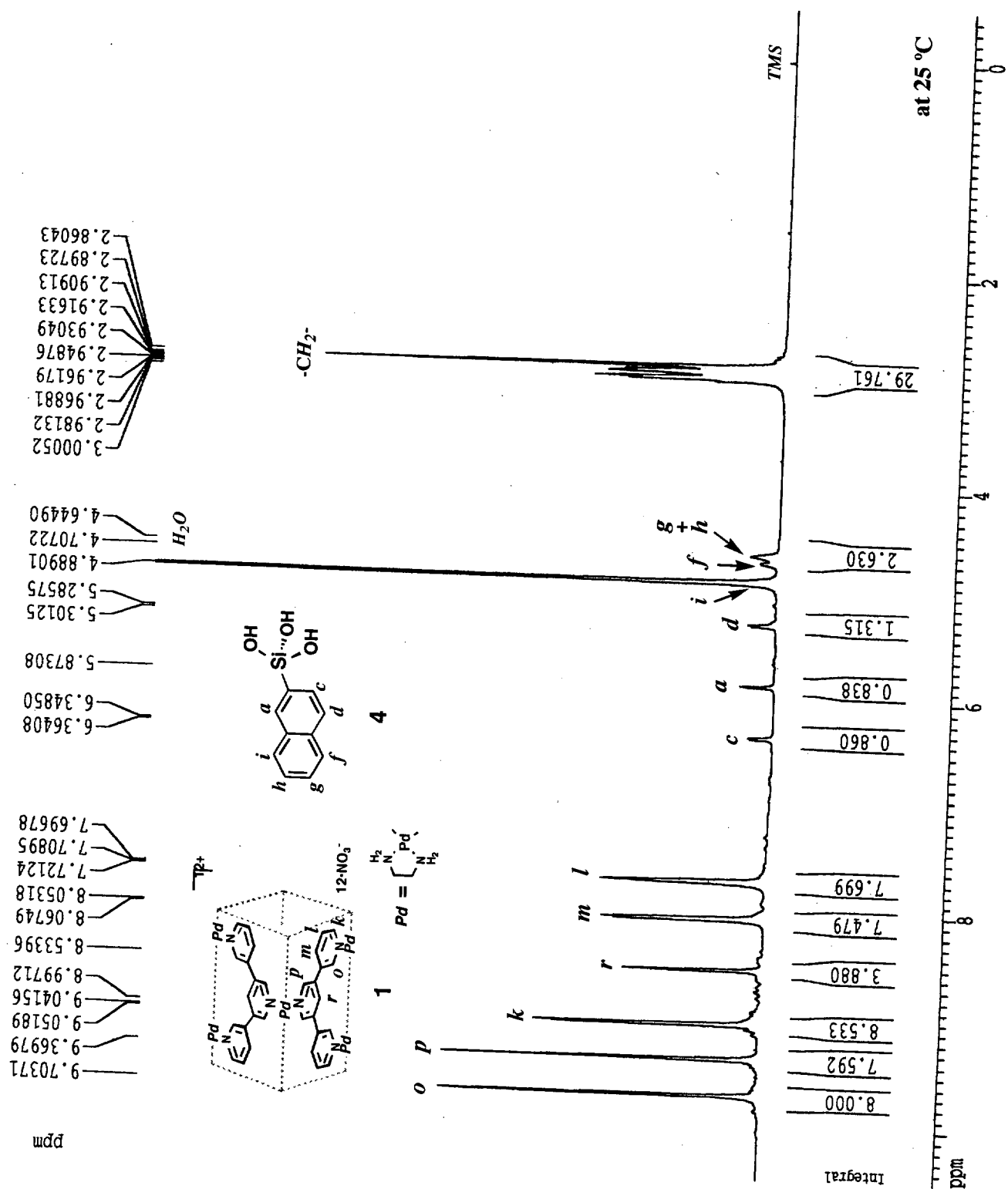
Date_ 20000912
 Time 11.27
 INSTRUM drx500
 PROBD 5 mm BBI 1H-B
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 2
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 35.9
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.40 usec
 SFO1 500.1330885 MHz
 NUC1 1H
 PL1 -4.00 dB

F2 - Processing parameters

SI 16384
 SF 500.1299050 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 10.500 ppm
 F1 5251.36 Hz
 F2P -0.500 ppm
 F2 -250.06 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07144 Hz/cm



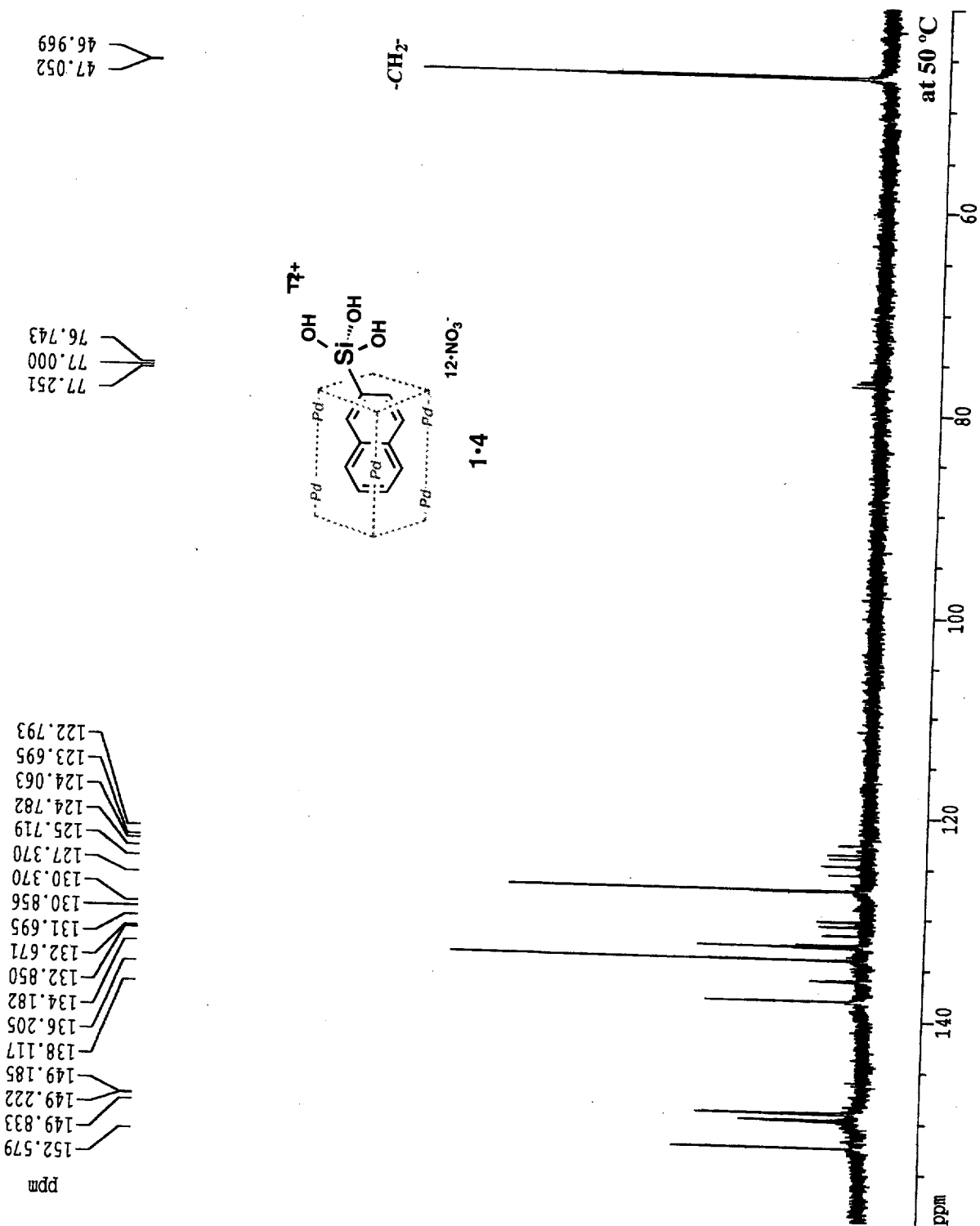
¹³C NMR(1) of 1·4

Current Data Parameters
 NAME tube3
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20000912
 Time 23.11
 INSTRUM drx500
 PROBHD 5 mm BBI 1H-B
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 13921
 DS 2
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 8192
 DW 12.600 usec
 DE 6.00 usec
 TE 300.0 K
 d11 0.03000000 sec
 d12 0.00002000 sec
 PL13 24.00 dB
 D1 2.00000000 sec
 CPDPRG2 waltz16
 RCPD2 100.00 usec
 SFO2 500.1320005 MHz
 NUC2 1H
 PL2 -1.00 dB
 PL12 24.00 dB
 P1 13.00 usec
 SFO1 125.7736214 MHz
 NUC1 13C
 PL1 -2.00 dB

F2 - Processing parameters
 SI 32768
 SF 125.7578091 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 FIP 160.000 ppm
 F1 20121.25 Hz
 F2P 40.000 ppm
 F2 5030.31 Hz
 PMCM 6.00000 ppm/cm
 HZCM 754.54688 Hz/cm



¹³C NMR(2) of 1·4

Current Data Parameters
tube# 7

EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20000912
Time 23.11

INSTRUM dirx500
PROBHD 5 mm BBI 1H-B

PULPROG zgpg30
TD 65536

SOLVENT D2O
NS 13921

DS 2
SWH 39682.539 Hz

FIDRES 0.605507 Hz
AQ 0.8258035 sec

RG 8192
DW 12.600 usec

DE 6.00 usec
TE 300.0 K

d11 0.03000000 sec
d12 0.00002000 sec

PL13 24.00 dB
DI 2.00000000 sec

CPDPRG2 waitz16
PCPD2 100.00 usec

SFO2 500.1320005 MHz
NUC2 1H

PL2 -1.00 dB
PL12 24.00 dB

P1 13.00 usec
SFO1 125.7736214 MHz

NUC1 13C
PL1 -2.00 dB

F2 - Processing parameters

SI 32768
SF 125.7578091 MHz

WDW NO
SSB 0

LB 0.00 Hz
GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 155.000 ppm

F1 19492.46 Hz
F2P 120.000 ppm

F2 15090.94 Hz
PPMCM 1.75000 ppm/cm

HZCM 220.07617 Hz/cm

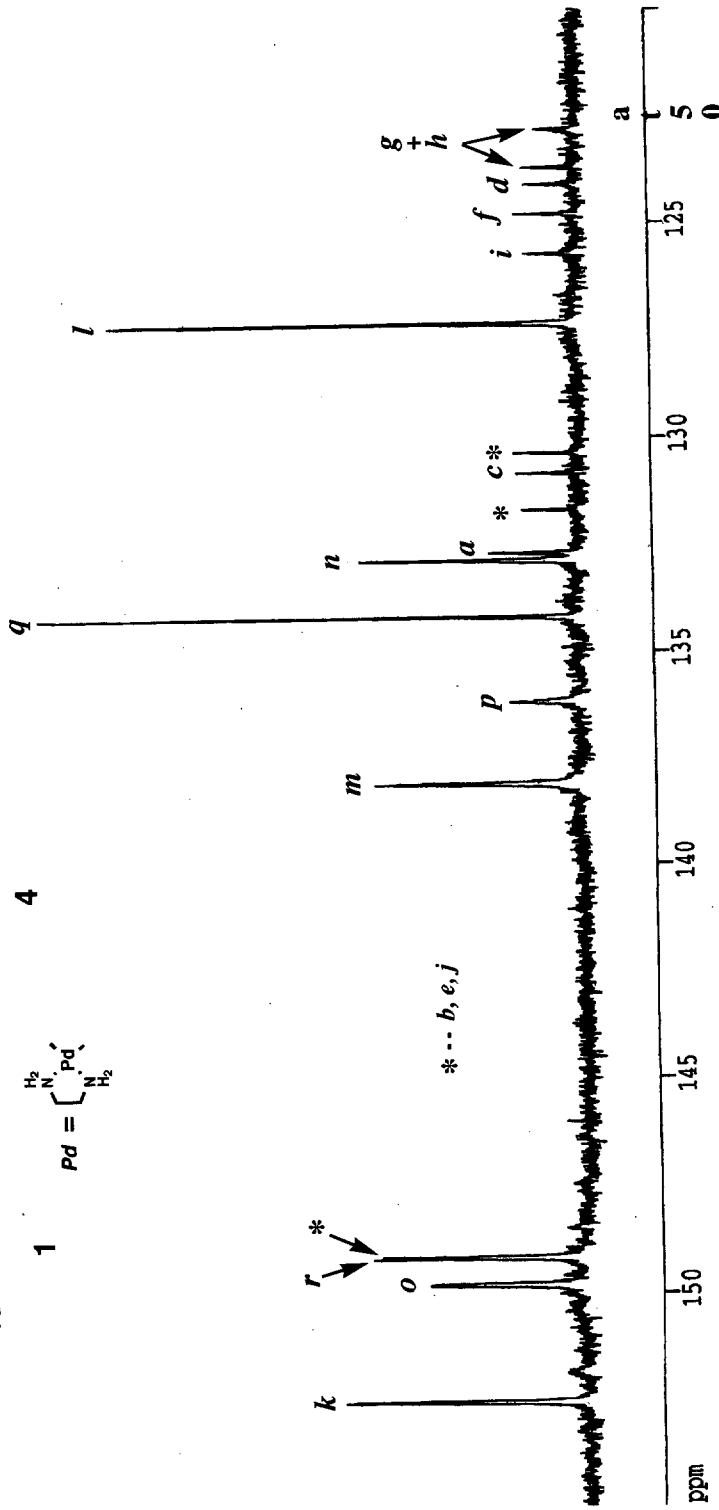
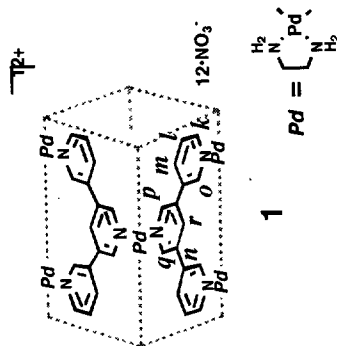
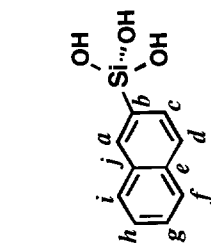
122.793
123.695
124.063
124.782
125.719
127.370

130.370
130.856
131.695
132.671
132.850
134.182

136.205
138.117

149.185
149.222
149.833
152.579

ppm



DEPT of 1·4

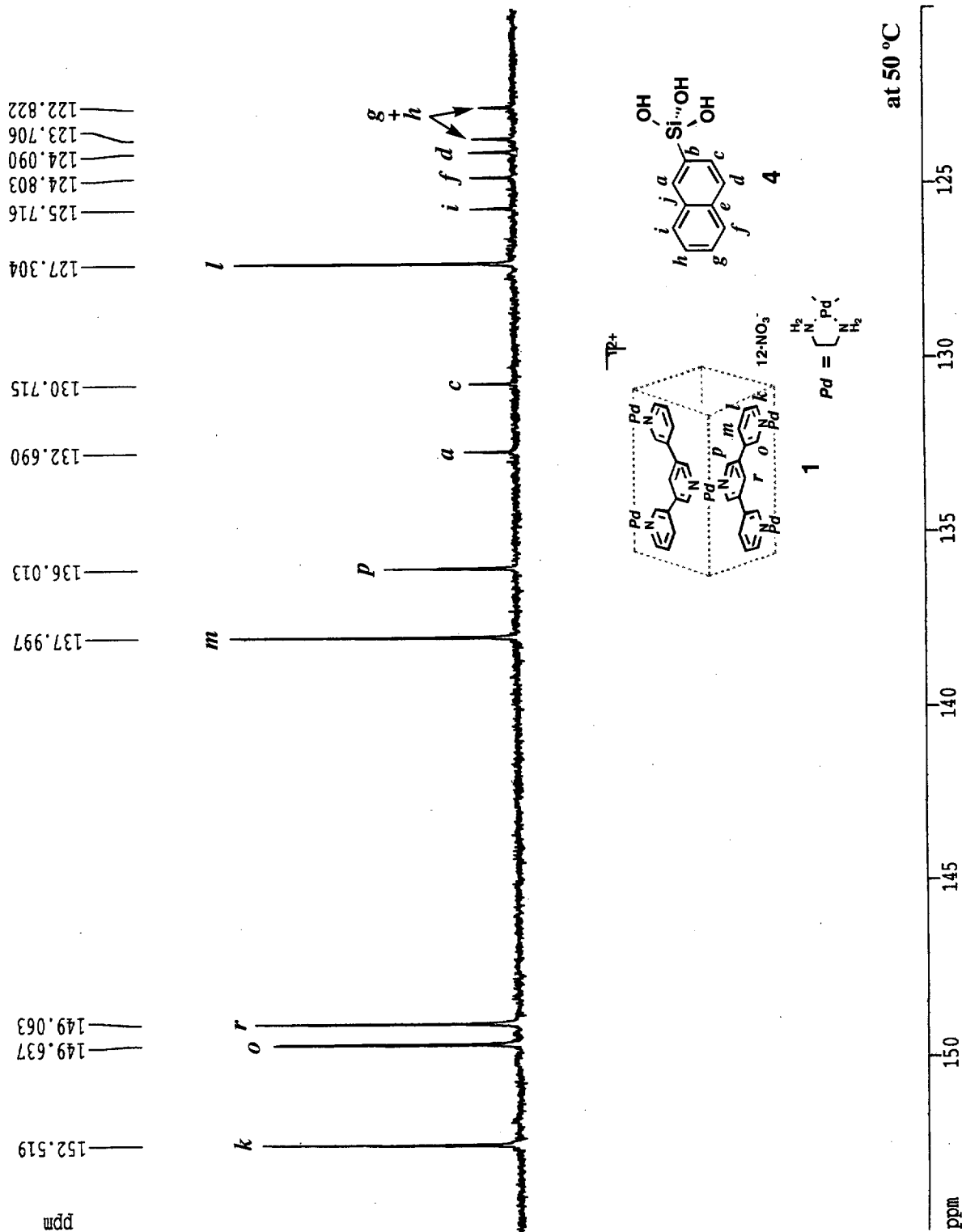
Current Data Parameters
 NAME tube4
 EXCNO 3
 PROCNO 1

P2 - Acquisition Parameters

Date_ 20001005
 Time 0.09
 INSTRUM drx500
 PROBRD 5 mm BBO BB-1
 PULPROG dept135
 TD 65536
 SOLVENT D2O
 NS 1079
 DS 4
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 8192
 DW 12.600 usec
 DE 6.00 usec
 TE 300.0 K
 P1 6.40 usec
 P2 12.80 usec
 P3 8.40 usec
 P4 16.80 usec
 CNST2 145.0000000
 d2 0.00344828 sec
 d12 0.0002000 sec
 DELTA 0.00000815 sec
 D1 2.00000000 sec
 PL2 4.00 dB
 SFO2 500.1320005 MHz
 NUC2 1H
 SFO1 125.7736214 MHz
 NUC1 13C
 PL1 2.00 dB
 PL12 16.00 dB
 CPDPRG2 waltz16
 PCPD2 81.00 usec

P2 - Processing parameters

SI 32768
 SF 125.7578355 MHz
 WDW DO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 ID NMR plot parameters
 CX 20.00 cm
 F1P 155.000 ppm
 F1 19492.46 Hz
 F2P 120.000 ppm
 F2 15090.94 Hz
 PPMCM 1.75000 ppm/cm
 HZCM 220.07622 Hz/cm



²⁹Si NMR of 1·4

Current Data Parameters
 NAME test
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001004
 Time 1.48

INSTRUM drx500
 PROBHD 5 mm BBO BB-1
 PULPROG dept45
 TD 65536
 SOLVENT CDC13
 NS 10383

DS 4
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 3649.1
 DM 12.600 usec
 DE 6.00 usec
 TE 300.0 K
 F1 7.50 usec
 P2 15.00 usec
 P3 7.60 usec
 P4 15.20 usec

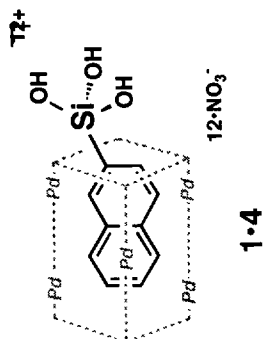
CNST2 20.0000000
 d2 0.02500000 sec
 d12 0.00002000 sec
 DELTA 0.00000955 sec
 D1 2.00000000 sec
 PL2 -4.00 dB
 SFO2 500.1320005 MHz

NUC2 ¹H
 SFO1 99.3617370 MHz
 NUC1 ²⁹Si
 PL1 2.00 dB
 PL12 16.00 dB
 CPDPRG2 waltz16
 PCPD2 81.00 usec

F2 - Processing parameters
 SI 32768
 SF 99.3617534 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

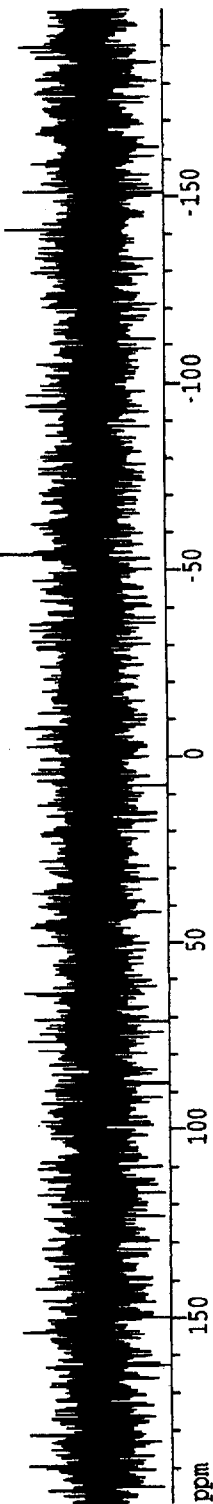
1D NMR plot parameters
 CX 20.00 cm
 FIP 199.522 ppm
 F1 19824.83 Hz
 F2P -199.853 ppm
 F2 -19857.71 Hz
 PPMCM 19.96872 ppm/cm
 HZCM 1984.12708 Hz/cm

54.318



at 25 °C

ppm



HH-COSY(1) of 1.4

Current Data Parameters
 NAME tubej
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20000911
 Time 23.36

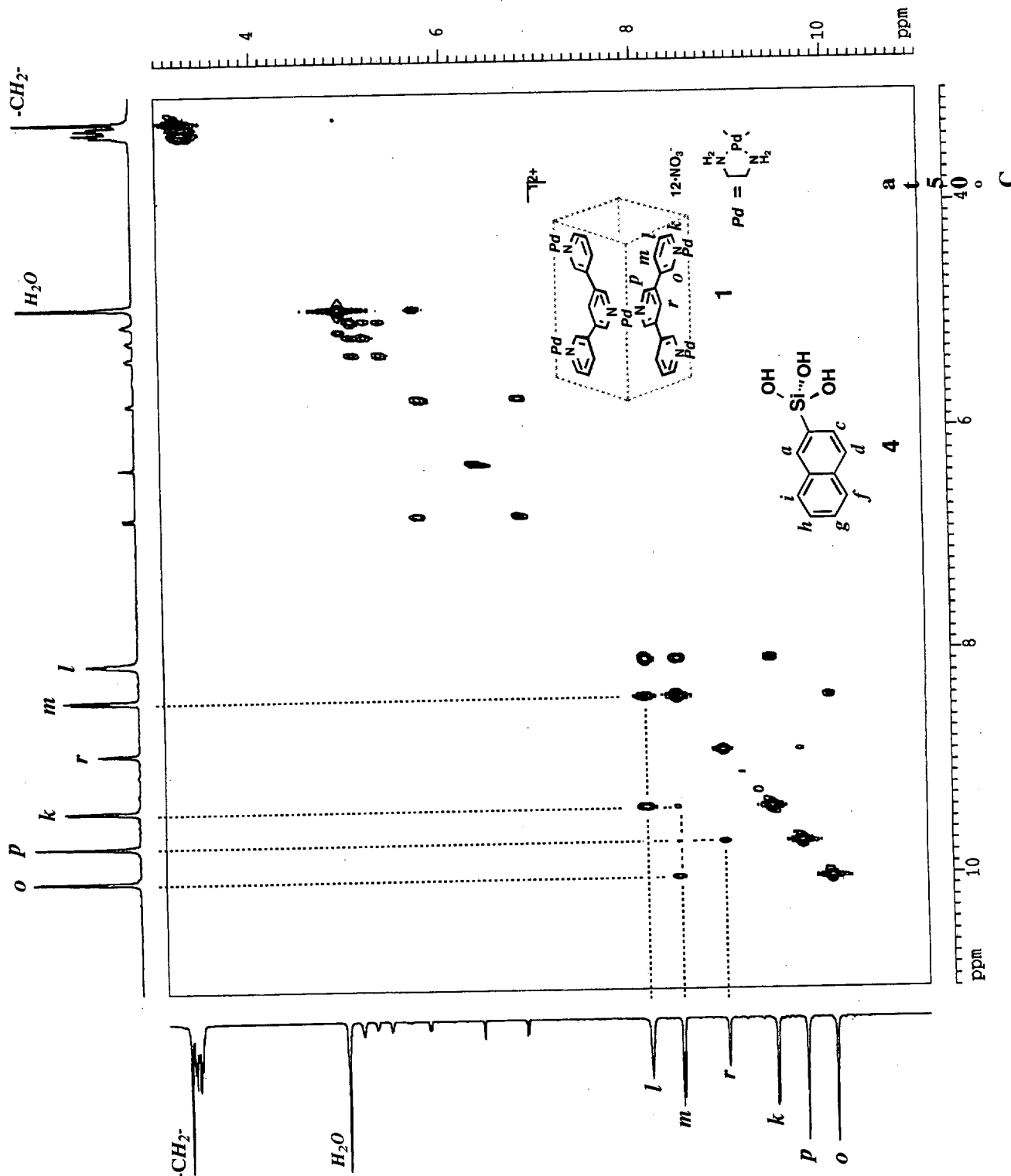
INSTRUM drx500
 PROBED 5 mm BBI IH-B
 PULPROG cosy90
 TD 2048
 SOLVENT D2O
 NS 64
 DS 4
 SWH 6510.417 Hz
 FIDRES 3.178914 Hz
 AQ 0.1573364 sec
 RG 512
 DW 76.800 usec
 DE 6.00 usec
 TE 300.0 K
 d0 0.0000300 sec
 P1 2.0000000 sec
 P1 7.10 usec
 SFO1 500.1324528 MHz
 NUC1 1H
 PL1 -1.00 dB
 INO 0.00015360 sec

F1 - Acquisition Parameters
 ND0 1
 TD 256
 SFO1 500.1325 MHz
 FIDRES 25.431314 Hz
 SW 13.017 ppm

F2 - Processing Parameters
 SI 1024
 SF 500.1299064 MHz
 SINE 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters
 SI 1024
 MC2 OP
 SP 500.1299195 MHz
 SINE 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 11.000 ppm
 F2LO 5501.43 Hz
 F2PHI 2.984 ppm
 F2HI 1497.34 Hz
 F1FLO 11.000 ppm
 F1LO 5501.43 Hz
 F1PHI 2.983 ppm
 F1HI 1497.01 Hz
 F2PPMCM 0.53374 ppm/cm
 F2HZCM 266.93948 Hz/cm
 F1PPMCM 0.53378 ppm/cm
 F1HZCM 266.96100 Hz/cm



HH-COSY(2) of 1.4

Current Data Parameters
 NAME EXPNO PROCNO
 tube3 2 1

F2 - Acquisition Parameters

Date_ 20000911
 Time 23.36
 INSTRUM drx500
 PROBD 5 mm BBI 1H-B
 PULPROG cosy90
 TD 2048
 SOLVENT D2O
 NS 64
 DS 4
 SWH 6510.417 Hz
 FIDRES 3.178914 Hz
 AQ 0.1573364 sec
 RG 512
 DM 76.800 usec
 DE 6.00 usec
 TE 300.0 K
 GC 0.0000300 sec
 DI 2.0000000 sec
 F1 7.10 usec
 SFO1 500.1324528 MHz
 NUC1 1H
 FL1 1.00 dB
 INO 0.00015360 sec

F1 - Acquisition Parameters

ND0 1
 TD 256
 SFO1 500.1325 MHz
 FIDRES 25.431314 Hz
 SN 13.017 ppm

F2 - Processing Parameters

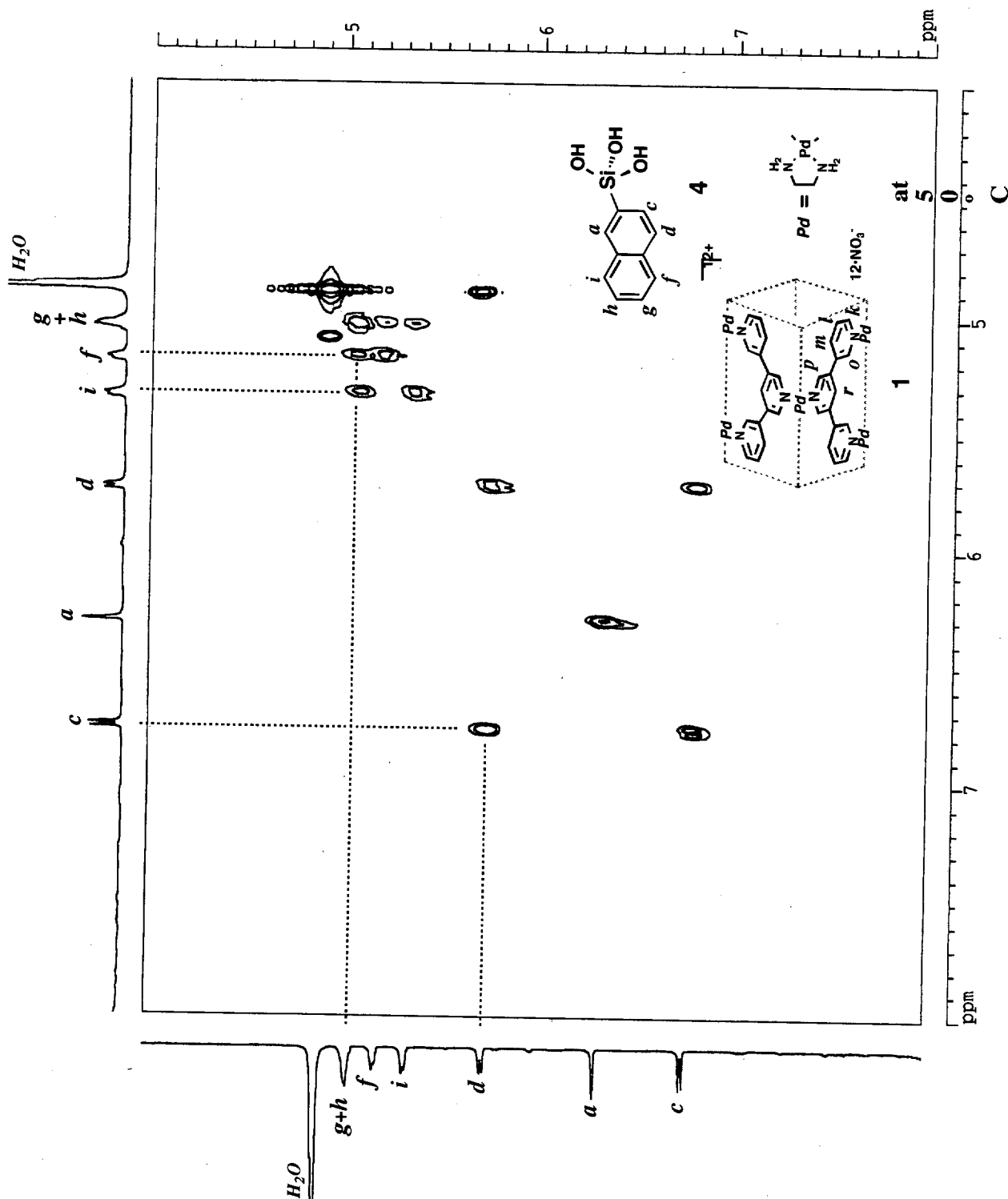
SI 1024
 SF 500.1299043 MHz
 SCA SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters

SI 1024
 SF 500.1298997 MHz
 SCA SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CY2 15.00 cm
 CX1 15.00 cm
 F2RLO 8.000 ppm
 F2LLO 4001.04 Hz
 F2H1 4.000 ppm
 F2H2 2000.52 Hz
 F1RLO 8.000 ppm
 F1LLO 4001.04 Hz
 F1H1 4.000 ppm
 F1H2 2000.52 Hz
 F2PRCM 0.26667 ppm/cm
 F2HZCM 133.36789 Hz/cm
 F1PRCM 0.26667 ppm/cm
 F1HZCM 133.36798 Hz/cm



CH-COSY of 1.4

Current Data Parameters
 NAME: 10
 PROCNO: 2

P2 - Acquisition Parameters

Date_: 20000913
 Time: 23.03
 INSTRUM: crys00
 PROBHD: 5 mm BB
 PULPROG: zgpg30
 TO: 1024
 SOLVENT: D2O
 NS: 128
 DS: 8
 SWH: 3156.566 Hz
 FIDRES: 1.082584 Hz
 AQ: 0.1622516 sec
 RG: 26008
 DM: 158.400 usec
 DE: 8.00 usec
 TE: 7.10 usec
 F2: 14.20 usec
 D0: 0.00000000 sec
 CHRG1: 145.00000000 sec
 CH2: 0.00148228 sec
 CH3: 0.00000000 sec
 CH4: 0.00000000 sec
 CH5: 1500.00 usec
 CH6: 0.00193528 sec
 CH7: 2.00000000 sec
 CH8: 500.132425 MHz
 P1: 1.00 dB
 P2: 2.00 dB
 P3: 13.00 usec
 SFO1: 125.775 MHz
 SFO2: 31.908421 Hz
 SFO3: 125.7750197 MHz
 D1: 0.00000000 sec
 D11: 0.00000000 sec
 D12: 15.00 dB
 CHRG2: gspg
 PCPD1: 75.00 usec
 INO: 0.0001520 sec

P1 - Acquisition Parameters

WDW: EM
 SSB: 0.00 Hz
 GB: 0
 PC: 1.00

P2 - Processing Parameters

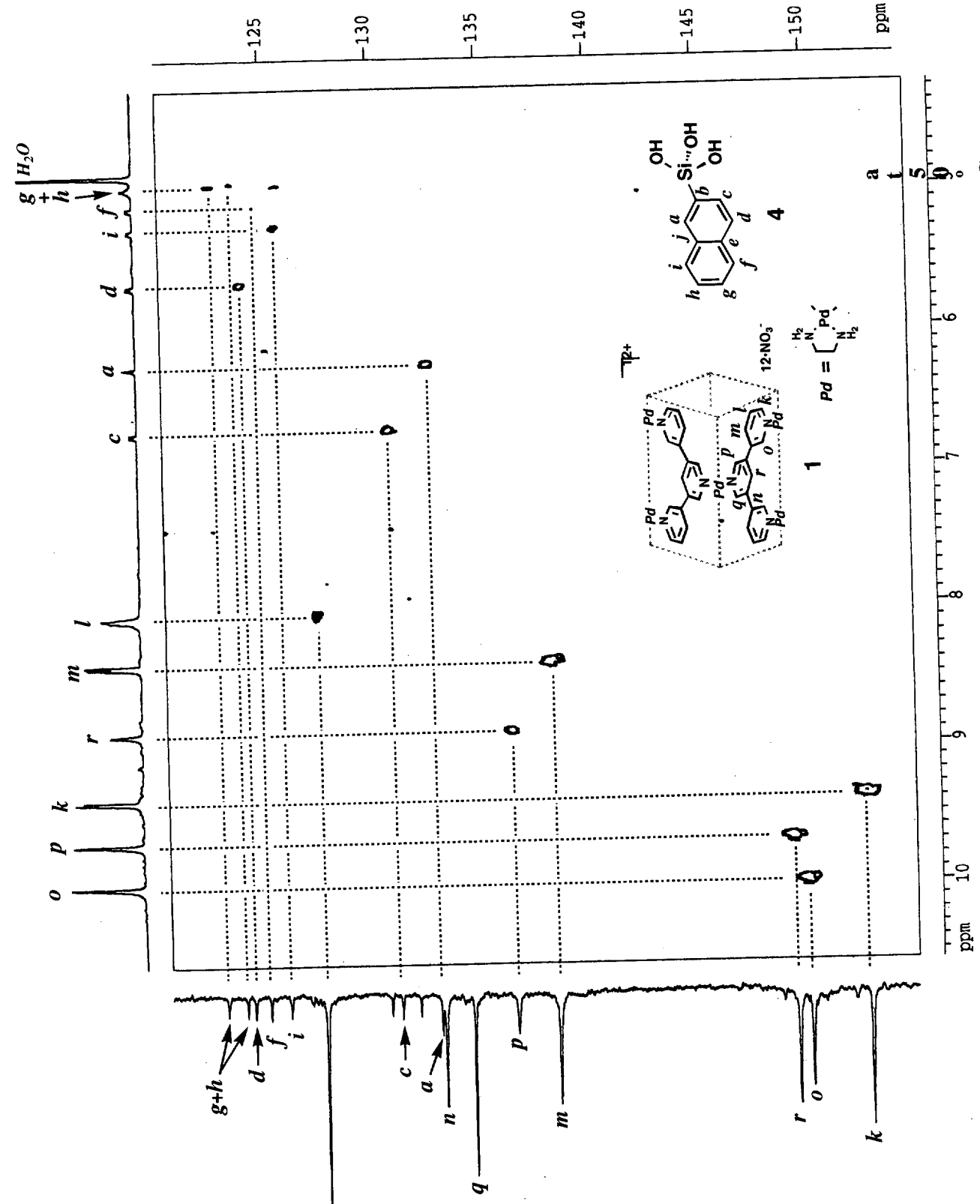
SI: 2048
 SF: 500.129192 MHz
 SFO: 8192
 GB: 0.00 Hz
 CB: 0
 PC: 1.00

P1 - Processing Parameters

SI: 1024
 SF: 125.775 MHz
 SFO: 8192
 GB: 0.00 Hz
 CB: 0
 PC: 1.00

2D NMR plot parameters

CK1: 15.00 cm
 F2H1O: 10.975 ppm
 F2H1: 44.283 ppm
 F1H1O: 2132.15 Hz
 F1H1: 154.757 ppm
 F1L1O: 19461.90 Hz
 F1L1: 120.244 ppm
 F1H1O: 0.44077 ppm/cm
 F1L1O: 210.43770 Hz/cm
 F1L1H1O: 2.30087 ppm/cm
 F1L1H1: 289.35196 Hz/cm



Atom Label	1D 1H NMR (ppm)	1D 13C NMR (ppm)	2D CH-COSY (ppm)
o	~10.0	~10.0	o
p	~9.5	~9.5	p
k	~8.5	~8.5	k
r	~7.5	~7.5	r
m	~6.5	~6.5	m
i	~5.5	~5.5	i
a	~5.0	~5.0	a
c	~4.5	~4.5	c
a	~4.0	~4.0	a
d	~3.5	~3.5	d
i	~3.0	~3.0	i
f	~2.5	~2.5	f
g	~2.0	~2.0	g
h	~1.5	~1.5	h
l	~10.0	~10.0	l
q	~9.5	~9.5	q
n	~8.5	~8.5	n
a	~7.5	~7.5	a
c	~6.5	~6.5	c
d	~5.5	~5.5	d
f	~4.5	~4.5	f
i	~3.5	~3.5	i
m	~2.5	~2.5	m
p	~1.5	~1.5	p
r	~1.0	~1.0	r
o	~0.5	~0.5	o
k	~0.0	~0.0	k

NOESY of 1.4

Current Data Parameters
 NAME tube4
 EXPNO 6
 PROCNO 1

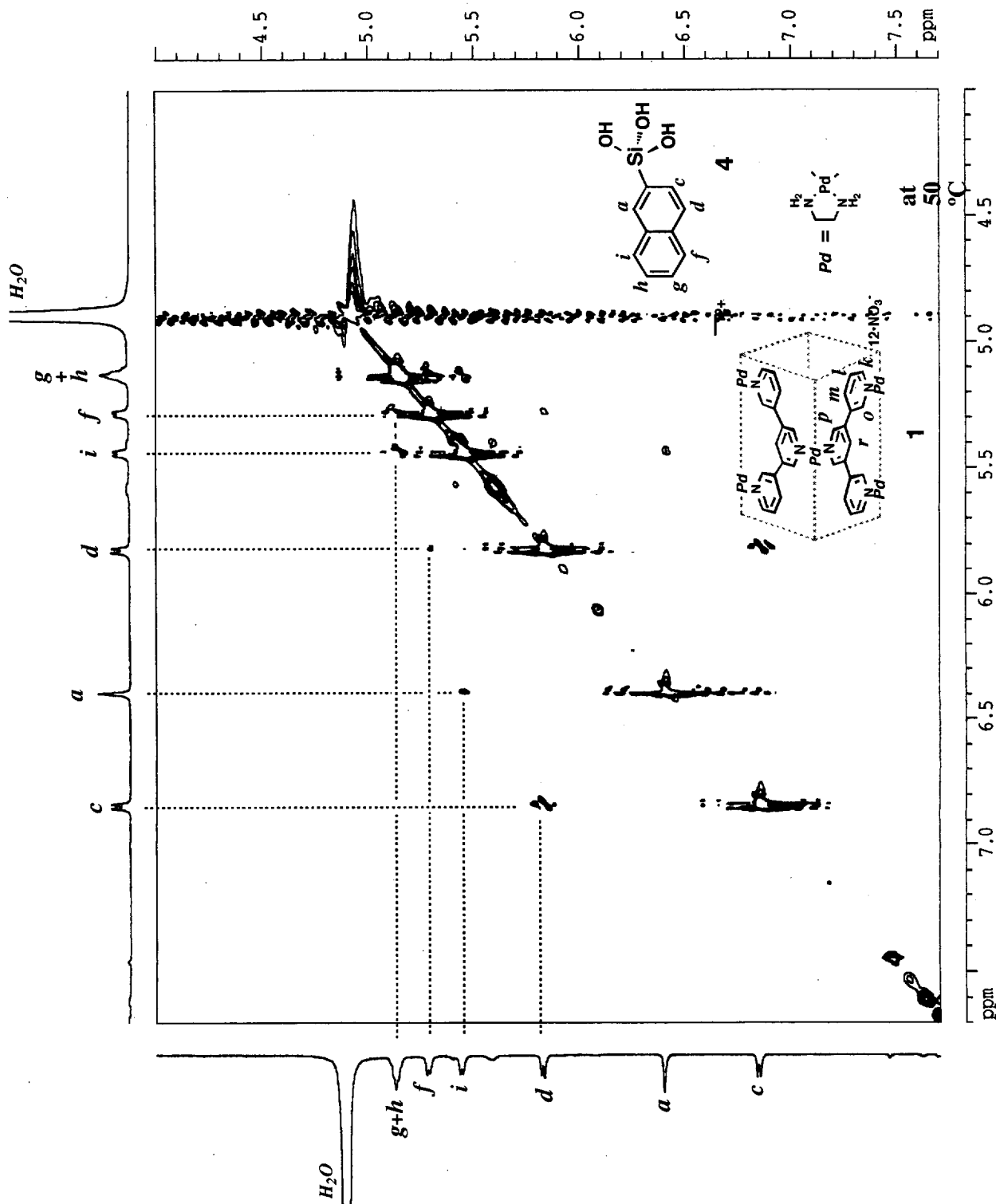
P2 - Acquisition Parameters
 Date_ 20001016
 Time 23.39
 INSTRUM drx500
 PROBHD 5 mm BBO BB-1
 PULPROG noesytp
 TD 2048
 SOLVENT D2O
 NS 32
 DS 4
 SWH 3125.000 Hz
 FIDRES 1.525879 Hz
 AQ 0.3277300 sec
 RG 728.1
 DM 160.000 usec
 DE 6.00 usec
 TE 300.0 K
 DO 0.0000300 sec
 D1 2.0000000 sec
 SFO1 500.132655 MHz
 H1 4.01 Hz
 F2 0.3000000 sec
 PR 0.0016000 sec
 LN0 0.0016000 sec

F1 - Acquisition Parameters
 NS0 481
 SFO1 500.1324 MHz
 FIDRES 6.496881 Hz
 SM 6.248 ppm

F2 - Processing Parameters
 SI 1024
 SF 500.1289082 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing Parameters
 SI 1024
 MC2 TPPI
 SF 500.1289879 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

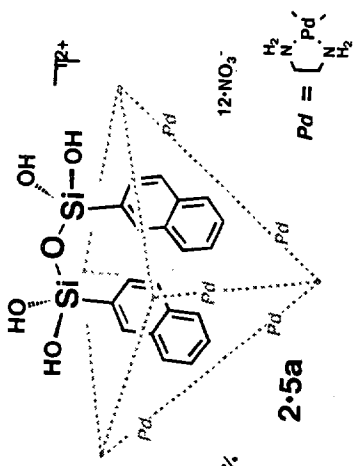
2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 FZPLO 7.700 ppm
 FZLO 3851.00 Hz
 FZPHI 3.998 ppm
 F2PHI 1999.41 Hz
 F1PLO 7.700 ppm
 F1LO 3851.00 Hz
 F1PHI 3.994 ppm
 F1H1 1997.51 Hz
 F2PMCK 0.24661 ppm/cm
 F1PMCK 123.43935 Hz/cm
 F1RPMCK 0.24707 ppm/cm
 F1RZCK 123.56632 Hz/cm



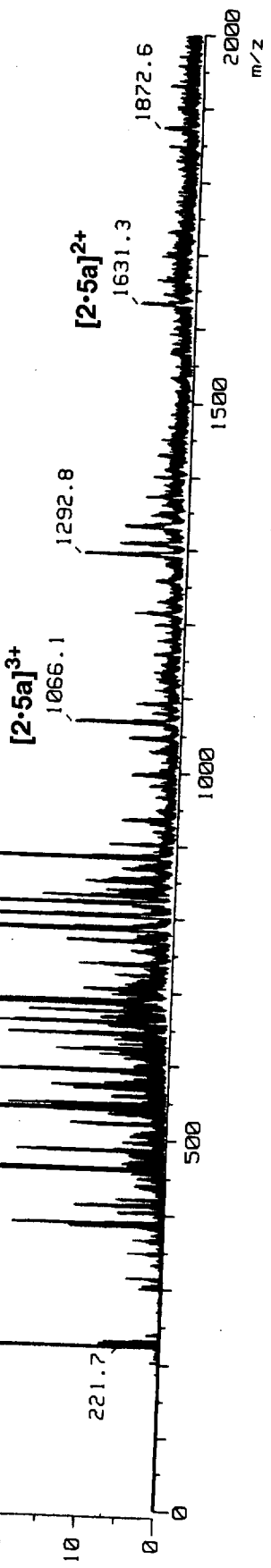
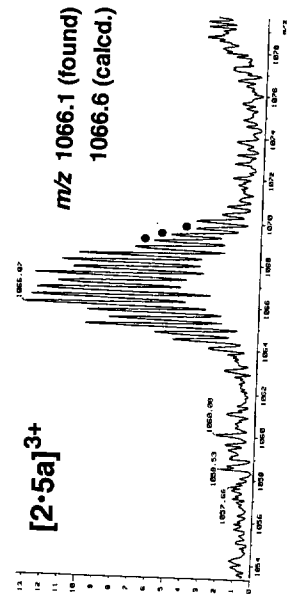
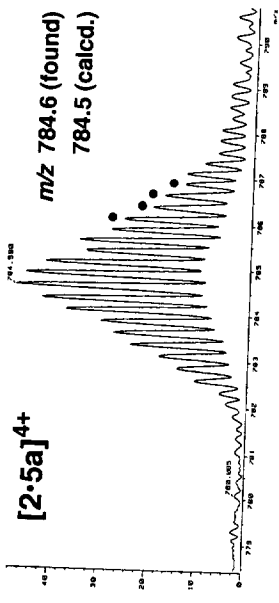
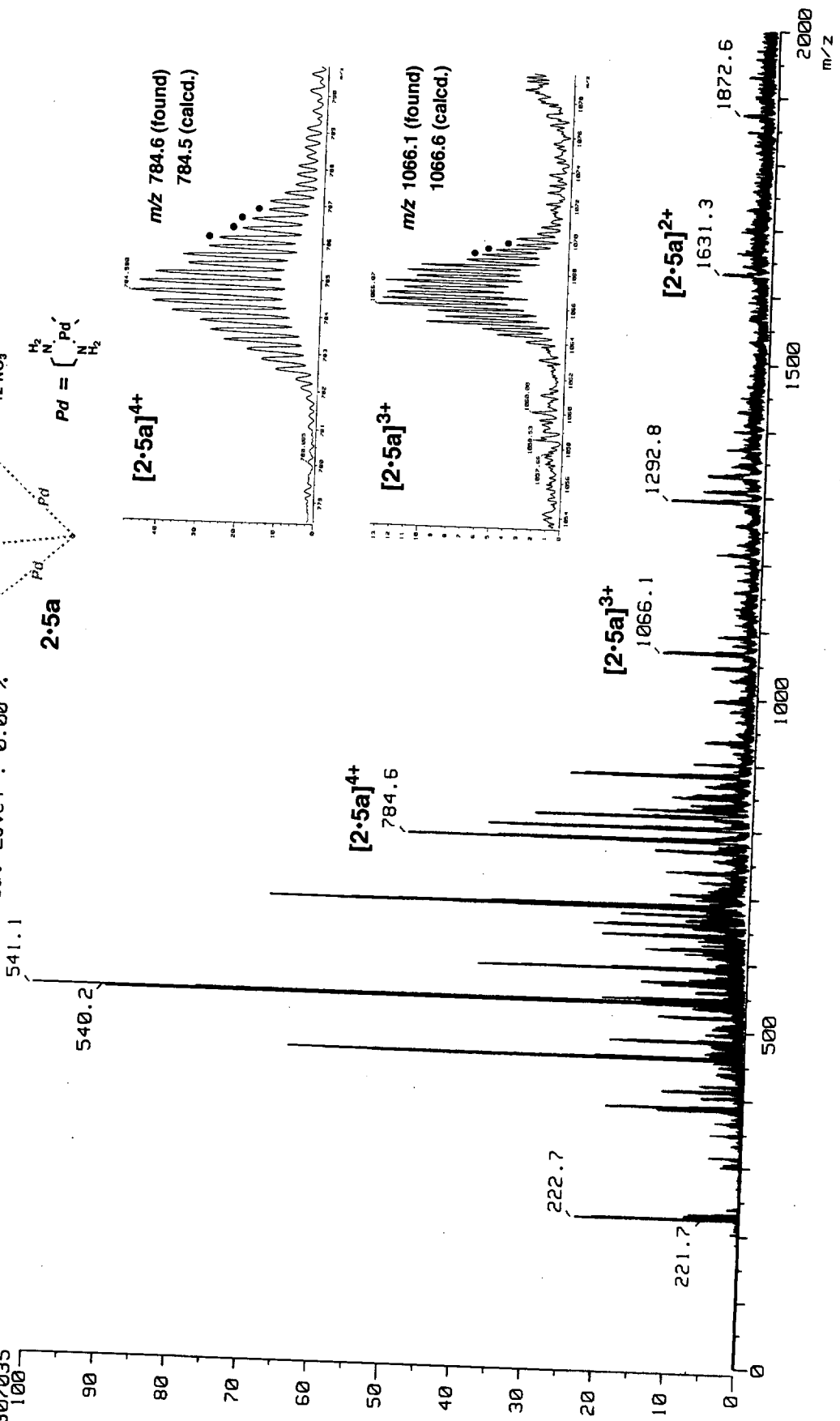
[Mass Spectrum]

Date : 22-Sep-2000 15:11
 Data : 000922-003
 Sample :
 Note : -
 Inlet : Direct
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 11.19 min
 Scan# : (1,72)
 BP : m/z 541.1498
 Int. : 14.98
 Output m/z range : 0.0000 to 2000.0000
 11307035

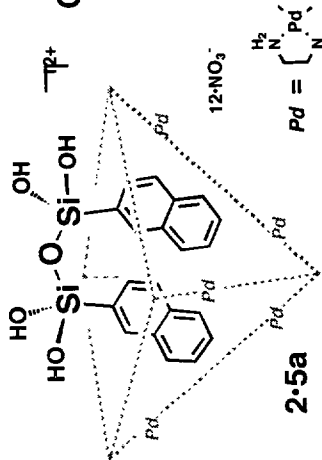
CSI MS (1) of 2-5a



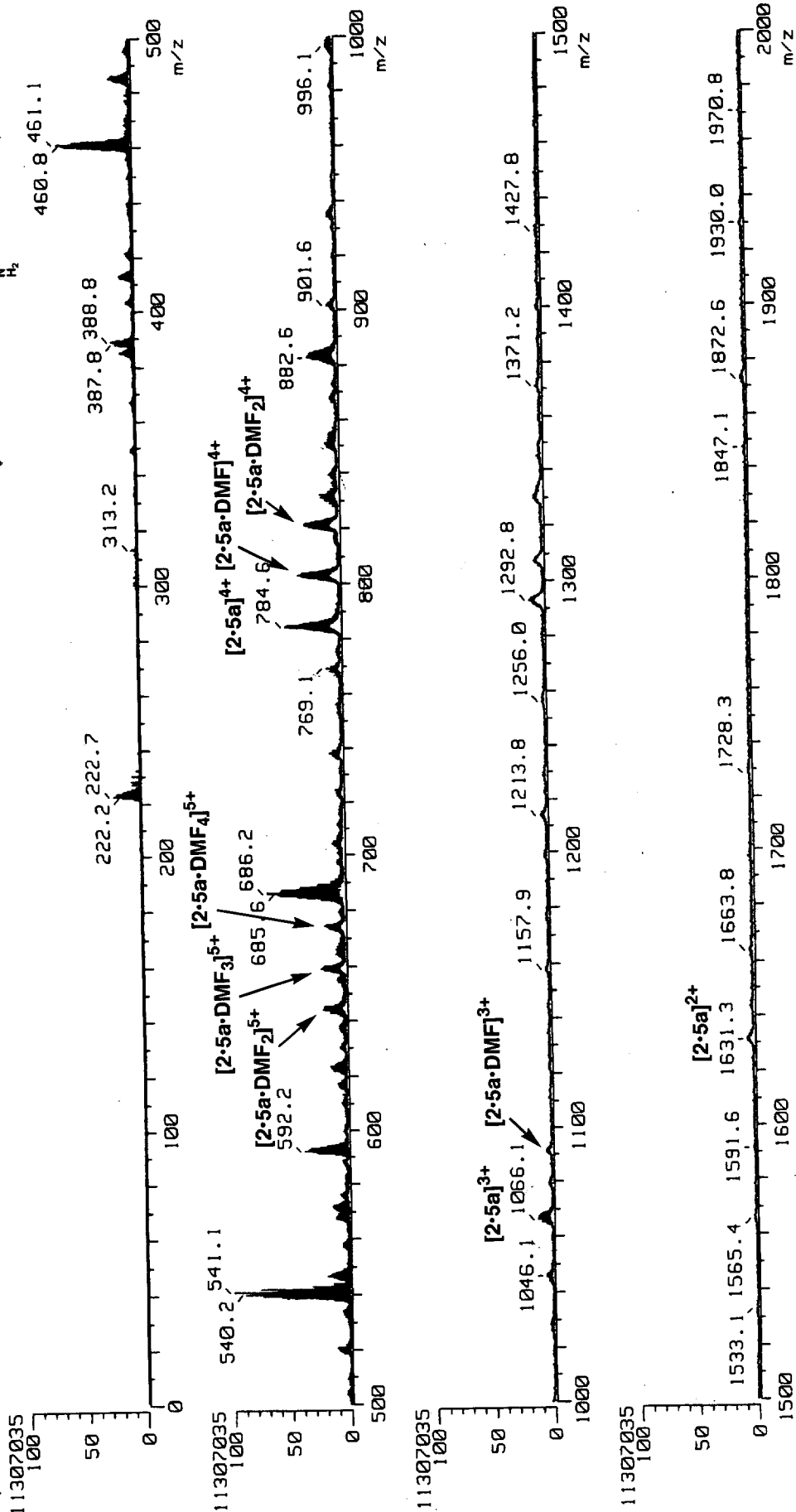
Cut Level : 0.00 %



CSI MS (2) of 2·5a



[Mass Spectrum 1
 Date : 22-Sep-2000 15:11
 Data : 000922-003
 Sample :
 Note : -
 Inlet : Direct
 Ion Mode : ESI+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 11.19 min
 Scan# : (1,72)
 BP : m/z 541.1498
 Int. : 14.98
 Output m/z range : 0.0000 to 2000.0000
 Cut Level : 0.00 %



¹H NMR(1) of 2.5a

Current Data Parameters
 NAME bow13
 EXPNO 2
 PROCNO 1

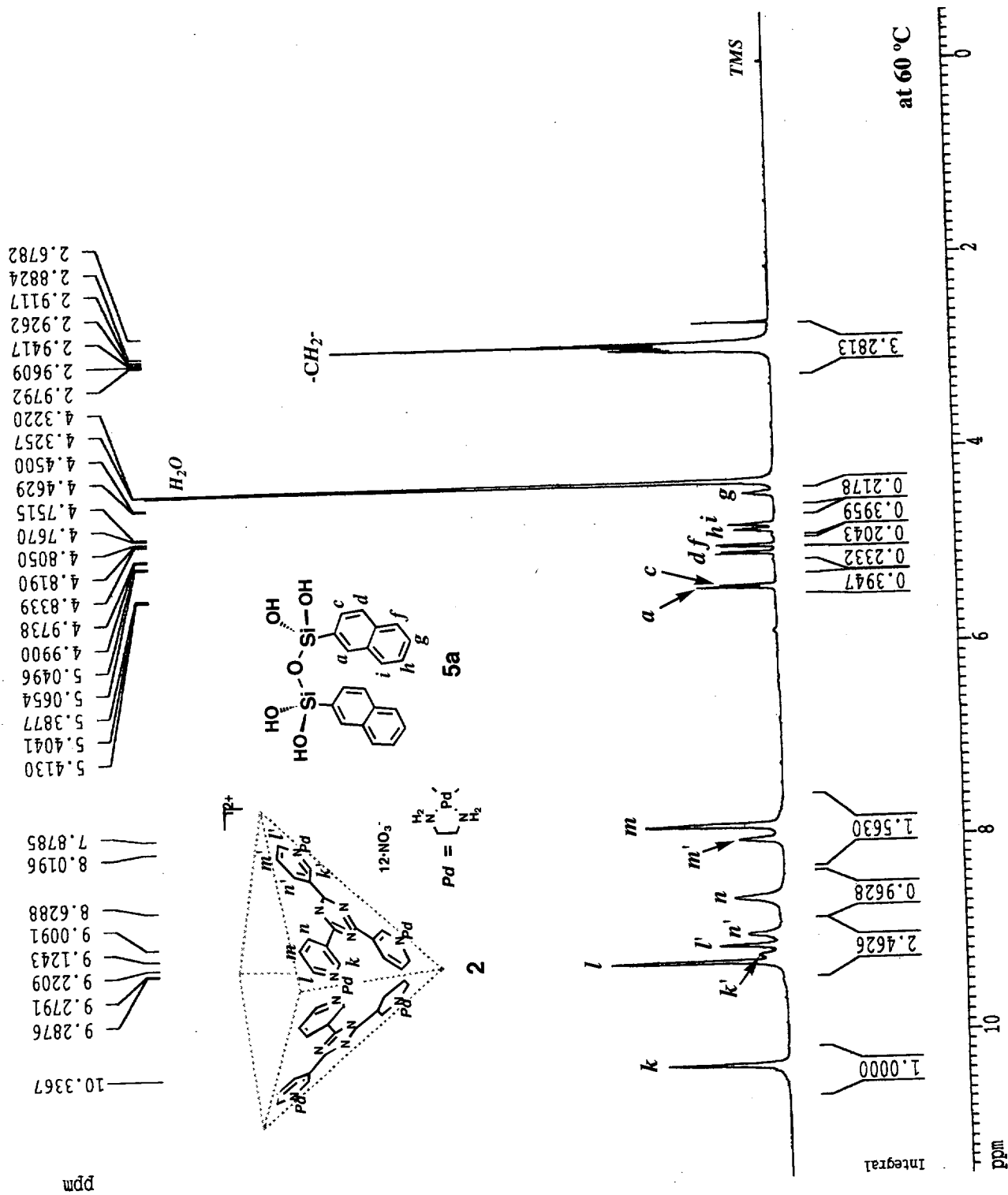
F2 - Acquisition Parameters

Date_ 20000908
 Time 0.06
 INSTRUM drx500
 PROBD 5 mm BBI 1H-B
 PULPROG zg30
 TD 32768
 SOLVENT D2O
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 71.8
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.40 usec
 SF01 500.1330885 MHz
 NUC1 1H
 PL1 -4.00 dB

F2 - Processing parameters

SI 16384
 SF 500.1301937 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.500 ppm
 F1 5751.50 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 300.07812 Hz/cm



¹H NMR(2) of 2·5a

Current Data Parameters
 NAME bow14
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001004
 Time 22.40
 INSTRUM drx500
 PROBED 5 mm BBO BB-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 90.5
 DM 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 P1 8.40 usec
 SFOL 500.1330885 MHz
 NUC1 1H
 PL1 -4.00 dB

F2 - Processing parameters
 SI 16384
 SF 500.1299838 MHz
 WDW HO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FLP 11.500 ppm
 F1 5751.49 Hz
 F2P -0.500 ppm
 F2 -250.06 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 300.07797 Hz/cm

