MATERIAL FOR DEPOSIT

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SOME SIXTY NEW SPACE GROUP CORRECTIONS

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SYNOPSIS

Some sixty examples of crystal structures are presented which can be better described in space groups different from those used in the original publications.

ABSTRACT.

Some sixty examples of crystal structures are presented which can be better described in space groups of higher symmetry than used in the original publications. These are divided into three categories — (A) incorrect Laue group (33 examples), (B) omission of a center of symmetry (22 examples), (C) omission of a center of symmetry coupled with a failure to recognize systematic absences (9 examples). Category A errors do not lead to systematic errors in atomic coordinates but these do accompany the two other types of error. 19 of the current set of examples have publication dates 1996 or later. Critical scrutiny on the part of authors, editors, and referees is needed to eliminate such errors in order not to impair the role of crystal structure analysis as the chemical court of last resort.

Tables of Revised Coordinates in Corrected Space Groups.

Note that minor adjustments have been made in cell dimensions so that these conform to the revised Laue symmetry of the crystals.

CATEGORY A. Change in Laue Group

Table 1S. Refcode not yet assigned. (β-cyclodextrin)$_2$. [tridecanoic acid].19.5H$_2$O ($C_{42}H_{70}O_{35}$)$_2$.($C_{13}H_{26}O_2$).19.5H$_2$O. Makedonopoulou, S., Papaionnou, J., Argyroglou, J. & Mavridis, I. M. (2000). J. Inclus. Phenom. Macrocyc. Chem. 36, 191–215.
Revised space group *C*2. CELL: 19.363 24.597 15.937 Å, 108.95°.

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Cyclodextrin molecule	x	y	z	
CA11	0.0568	0.1987	0.2532	
CA21	0.0949	0.2045	0.1866	
OA21	0.0438	0.2157	0.1012	
CA31	0.1382	0.1533	0.1846	
OA31	0.1796	0.1614	0.1245	
CA41	0.1893	0.1426	0.2760	
CA51	0.1478	0.1378	0.3404	
OA41	0.2273	0.0922	0.2728	
OA51	0.1045	0.1858	0.3386	
CA61	0.1934	0.1296	0.4367	
OA61	0.2386	0.1709	0.4708	
CA12	0.3052	0.0906	0.3105	
CA22	0.3341	0.0693	0.2414	
OA22	0.3129	0.1023	0.1636	
CA32	0.3110	0.0097	0.2208	
OA32	0.3427	-0.0120	0.1582	
CA42	0.3345	-0.0202	0.3047	
CA52	0.3048	0.0025	0.3716	
OA42	0.3050	-0.0762	0.2834	
OA52	0.3264	0.0594	0.3864	
CA62	0.3272	-0.0236	0.4602	
OA62	0.4024	-0.0258	0.4989	
CA13	0.3540	-0.1215	0.3090	
CA23	0.3377	-0.1562	0.2271	
OA23	0.3515	-0.1286	0.1568	
CA33	0.2600	-0.1774	0.2016	
OA33	0.2461	-0.2143	0.1290	
OA43	0.1720	-0.2193	0.2548	
CB43	-0.2505	-0.2064	-0.2806	
CA53	0.2720	-0.1711	0.3626	
OA53	0.3446	-0.1500	0.3795	
CA63	0.2742	-0.2020	0.4469	
OA63	0.3257	-0.2455	0.4648	
CA14	0.1516	-0.2729	0.2697	
CA24	0.1006	-0.2943	0.1852	
OA24	0.1344	-0.2942	0.1177	
CA34	0.0298	-0.2630	0.1566	
OA34	-0.0202	-0.2870	0.0776	
CA44	-0.0034	-0.2623	0.2306	
CA54	0.0512	-0.2402	0.3134	
OA44	-0.0687	-0.2308	0.2036	
OA54	0.1174	-0.2721	0.3370	
CA64	0.0225	-0.2450	0.3916	

OA64	0.0028	-0.2928	0.4096	Pops= 0.66, 0.60
OA64	0.0748	-0.2318	0.4700	Pops= 0.34, 0.40
CA15	-0.1343	-0.2554	0.2076	
CA25	-0.1926	-0.2469	0.1197	
OA25	-0.1724	-0.2700	0.0494	
CA35	-0.2069	-0.1868	0.1052	
OA35	-0.2667	-0.1778	0.0250	
CA45	-0.2284	-0.1643	0.1822	
CA55	-0.1682	-0.1755	0.2699	
OA45	-0.2330	-0.1058	0.1690	
OA55	-0.1541	-0.2333	0.2777	
CA65	-0.1944	-0.1631	0.3484	
OA65	-0.2548	-0.1945	0.3508	Pops= 0.72, 1.0
OA65	-0.1470	-0.1755	0.4276	Unpaired; Pop = 0.28
CA16	-0.2989	-0.0788	0.1716	
CA26	-0.3270	-0.0447	0.0910	
OA26	-0.3428	-0.0766	0.0118	
CA36	-0.2740	0.0002	0.0910	
OA36	-0.3038	0.0348	0.0160	
CA46	-0.2578	0.0324	0.1752	
CA56	-0.2318	-0.0042	0.2561	
OA46	-0.2008	0.0707	0.1780	
OA56	-0.2832	-0.0476	0.2493	
CA66	-0.2300	0.0250	0.3390	
OA66	-0.3002	0.0432	0.3395	Pops= 0.69, 0.76
OA66	-0.1832	-0.0068	0.4130	Pops= 0.31, 0.24
CA17	-0.2160	0.1280	0.1865	
CA27	-0.1973	0.1572	0.1131	
OA27	-0.2441	0.1397	0.0278	
CA37	-0.1189	0.1506	0.1228	
OA37	-0.1007	0.1802	0.0550	
CA47	-0.0735	0.1708	0.2128	
CA57	-0.0934	0.1424	0.2856	
OA47	0.0028	0.1566	0.2253	
OA57	-0.1718	0.1478	0.2692	
CA67	-0.0577	0.1670	0.3768	
OA67	-0.0693	0.2244	0.3786	

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Water molecules	x	y	z	
61A1	-0.1488	-0.2898	0.4350	Pops. = 0.41, 0.45
61A2	-0.1325	-0.3825	-0.4275	Pops. = 0.74, 0.92
62A1	0.4184	-0.0440	-0.3218	Pops. = 0.84, 0.88

65A	-0.3947	-0.1542	0.3025	Pops. = 1.0, 1.0
67A	0.0447	0.2988	0.4188	Pops. = 0.98, 1.0
21A	0.0900	0.3004	0.0246	Pops. = 0.94, 0.80
22A2	-0.0611	-0.3941	0.1265	Pops. = 0.61, 0.56
23A	0.4844	-0.1640	0.1518	Pops. = 0.95, 1.0
24A	0.5840	0.1050	0.0450	Pops. = 0.63, 0.59
26A2	0.5082	-0.0728	-0.0435	Pops. = 0.49 0.39,
62A2	0.0000	0.3898	0.5000	Pop. = 0.94
62B2	-0.5000	0.0635	0.5000	Pop. = 0.68
64A	-0.4795	0.0910	0.3746	Unpaired; pop. = 0.35
32A	-0.5210	-0.0375	0.0956	Unpaired; pop. = 0.16
32B	-0.4890	-0.0215	-0.1434	Unpaired; pop. = 0.50
W2	-0.4915	0.0010	0.1706	Unpaired; pop. = 0.59
W3	-0.5705	0.1030	0.0176	Unpaired; pop. = 0.50
W4	-0.4395	0.0680	0.2806	Unpaired; pop. = 0.41

Tridecanoic acid molecules (disordered and constrained; no pairing).

	x	y	z
O2A	0.0095	-0.0120	0.3856
O1A	0.0425	-0.0930	0.4286
C1A	0.0285	-0.0580	0.3696
C2A	0.0295	-0.0720	0.2776
C3A	0.0585	-0.0220	0.2386
C4A	0.0665	-0.0360	0.1486
C5A	-0.0015	-0.0660	0.0926
C6A	-0.0600	-0.0235	0.0446
C7A	-0.1215	-0.0510	-0.0294
C8A	-0.1065	-0.0450	-0.1174
C9A	-0.0375	-0.0780	-0.1134
C10A	0.0020	-0.0505	-0.1724
C11A	-0.0545	-0.0200	-0.2464
C12A	-0.0550	-0.0425	-0.3374
C13A	-0.1265	-0.0260	-0.4094
O1B	0.0315	-0.0690	-0.4234
O2B	-0.0415	-0.0030	-0.4734
C1B	-0.0170	-0.0385	-0.4184
C2B	-0.0440	-0.0435	-0.3384
C3B	0.0045	-0.0830	-0.2704
C4B	0.0020	-0.0675	-0.1784
C5B	0.0760	-0.0785	-0.1104
C6B	0.0665	-0.0830	-0.0194
C7B	-0.0130	-0.0695	-0.0284
C8B	-0.0250	-0.0805	0.0606

C9B	0.0460	-0.0685	0.1366
C10B	0.0300	-0.0255	0.1976
C11B	0.0305	-0.0520	0.2856
C12B	0.0980	-0.0325	0.3616
C13B	0.1275	-0.0800	0.4266

C2 axis, cyclodextrin molecule only:
Coords: 0.5725, 0.0000, 0.4776
Rms dev: 0.0005, 0.0006, 0.0006

All paired atoms:
C2 axis: 0.5725, 0.0001, 0.4774
Rms dev: 0.0010, 0.0009, 0.0013

Cell transformation from P1: (1,1,0), (-1,1,0), (0,0,1)
New angles: alpha = 89.99, gamma = 90.02

Table 2S. Refcode not yet assigned. (β-cyclodextrin)$_2$. [(Z)-tetradec-7-enoic acid]. 14.9H_2O. ($C_{42}H_{70}O_{35}$)$_2$.($C_{14}H_{26}O_2$).14.9H_2O. Makedonopoulou, S., Papaionnou, J., Argyroglou, J. & Mavridis, I. M. (2000). J. Inclus. Phenom. Macrocyc. Chem. 36, 191–215.

Revised space group *C*2. CELL 19.316 24.564 15.935 Å, 108.90°.

Cyclodextrin molecule	x	y	z
CA11	0.0564	0.1932	0.2534
CA21	0.0950	0.1989	0.1858
OA21	0.0438	0.2099	0.1014
CA31	0.1387	0.1471	0.1836
OA31	0.1800	0.1552	0.1237
CA41	0.1902	0.1368	0.2754
CA51	0.1473	0.1316	0.3410
OA41	0.2280	0.0868	0.2726
OA51	0.1059	0.1806	0.3388
CA61	0.1936	0.1232	0.4355
OA61	0.2405	0.1649	0.4692
CA12	0.3054	0.0864	0.3092
CA22	0.3344	0.0634	0.2402
OA22	0.3138	0.0965	0.1629
CA32	0.3112	0.0048	0.2212
OA32	0.3432	-0.0184	0.1580
CA42	0.3347	-0.0269	0.3061
CA52	0.3058	-0.0029	0.3722

OA42	0.3055	-0.0823	0.2844
OA52	0.3283	0.0533	0.3864
CA62	0.3302	-0.0290	0.4620
OA62	0.4032	-0.0312	0.4985
CA13	0.3537	-0.1266	0.3086
CA23	0.3376	-0.1636	0.2263
OA23	0.3509	-0.1348	0.1564
CA33	0.2600	-0.1832	0.2015
OA33	0.2447	-0.2205	0.1296
CA43	0.2494	-0.2127	0.2806
CA53	0.2718	-0.1771	0.3637
OA43	0.1720	-0.2250	0.2554
OA53	0.3447	-0.1564	0.3802
CA63	0.2736	-0.2062	0.4462
OA63	0.3248	-0.2512	0.4649
CA14	0.1520	-0.2784	0.2705
CA24	0.1009	-0.3003	0.1840
OA24	0.1350	-0.2998	0.1184
CA34	0.0291	-0.2691	0.1569
OA34	-0.0210	-0.2922	0.0770
CA44	-0.0038	-0.2696	0.2300
CA54	0.0502	-0.2470	0.3124
OA44	-0.0692	-0.2375	0.2036
OA54	0.1170	-0.2786	0.3372
CA64	0.0230	-0.2480	0.3922
OA64	0.0038	-0.3012	0.4080
CA15	-0.1338	-0.2618	0.2079
CA25	-0.1933	-0.2527	0.1204
OA25	-0.1723	-0.2770	0.0491
CA35	-0.2082	-0.1930	0.1041
OA35	-0.2670	-0.1837	0.0240
CA45	-0.2289	-0.1698	0.1819
CA55	-0.1700	-0.1824	0.2696
OA45	-0.2342	-0.1122	0.1686
OA55	-0.1552	-0.2398	0.2774
CA65	-0.1942	-0.1687	0.3485
OA65	-0.2562	-0.2010	0.3482
CA16	-0.2999	-0.0856	0.1722
CA26	-0.3272	-0.0508	0.0894
OA26	-0.3428	-0.0829	0.0106
CA36	-0.2741	-0.0056	0.0904
OA36	-0.3029	0.0288	0.0155
CA46	-0.2591	0.0274	0.1753
CA56	-0.2333	-0.0093	0.2568
OA46	-0.2016	0.0651	0.1784
OA56	-0.2852	-0.0540	0.2478
CA66	-0.2292	0.0191	0.3402
OA66	-0.3038	0.0384	0.3332

CA17	-0.2145	0.1219	0.1871
CA27	-0.1975	0.1514	0.1125
OA27	-0.2443	0.1339	0.0285
CA37	-0.1192	0.1447	0.1226
OA37	-0.1007	0.1752	0.0546
CA47	-0.0729	0.1645	0.2128
CA57	-0.0940	0.1370	0.2860
OA4 7	0.0027	0.1507	0.2250
OA57	-0.1724	0.1413	0.2688
CA67	-0.0576	0.1606	0.3782
OA67	-0.0694	0.2187	0.3785

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Water molecules	x	y	z	
61A1	0.3565	0.2020	0.4363	Pops: 0.40, 0.41
61A2	0.3720	0.1112	-0.4300	Pops: 0.35, 0.39
62A1	-0.0794	0.4498	-0.3218	Pops: 0.52, 0.57
64A	-0.4738	0.1022	0.3482	Pops: 0.13, 0.24
65A	0.1035	0.3398	0.2994	Pops: 0.80, 0.85
67A	0.0462	0.2924	0.4208	Pops: 1.0, 1.0
21A1	0.0884	0.2944	0.0240	Pops: 1.0, 0.70
22A	0.4331	0.1000	0.1064	Pops: 0.31, 0.39
23A	-0.0193	0.3236	0.1570	Pops: 0.59, 0.40
24A	-0.4155	0.1007	0.0463	Pops: 0.51, 0.50
26A1	0.5220	-0.0531	-0.0903	Pops: 0.25, 0.23
26A2	0.5046	-0.0910	-0.0362	Pops: 0.31, 0.23
W1	0.4778	0.0112	-0.1723	Pops: 0.17, 0.14
32A	-0.5170	-0.0256	0.1396	Pops: 0.26, 0.28
62A2	0.0	0.3833	0.5	Pop: 1.0
21A2	-0.0473	-0.4013	0.1464	Unpaired; pop = 0.26
23B2	0.5065	-0.1564	-0.1345	Unpaired; pop = 0.27
62B2	0.0901	-0.4387	-0.5012	Unpaired; pop = 0.37

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Tetradecenoic acid molecule	x	y	z
O1A	-0.060	-0.078	-0.474
O2A	-0.043	0.007	-0.448
C1A	-0.062	-0.038	-0.428
C2A	-0.090	-0.043	-0.350
C3A	-0.030	-0.069	-0.278

C4A	-0.009	-0.038	-0.192
C5A	0.023	-0.076	-0.115
C6A	-0.037	-0.112	-0.100
C7A	-0.098	-0.075	-0.090
C8A	-0.100	-0.063	-0.010
C9A	-0.051	-0.093	0.069
C10A	-0.020	-0.072	0.143
C11A	0.002	-0.040	0.210
C12A	0.050	-0.070	0.294
C13A	0.088	-0.031	0.366
C14A	0.119	-0.062	0.452

C2 axis, cyclodextrin molecule only:
Coords: 0.572121-0.000017 0.482157
rms dev. 0.000354 0.000212 0.000274

C2 axis, all paired atoms:
Coords: 0.573172 0.000050 0.482219
rms dev. 0.005119 0.001623 0.002762

Cell transformation: (1,1,0), (-1,1,0), (0,0,1)
New angles: alpha = 89.99, gamma = 90.01

Table 3S. LEKKUH.. 1,7,13,19,25-Pentathio[1.5](2,5)-thiophenophane $C_{20}H_{10}S_{10}$. Katano, N., Sugihara, Y., Ishii, A. & Nakayama, J. (1998). Bull. Chem. Soc. Jpn. 71, 2695-2700.
Revised space group P2(1)/c, transformation from P1-bar: (1,0,0), (0,0,1), (0,-1,0).
CELL 6.044 22.726 17.025 Å, 94.033°

Atom	x	y	z
S2	-0.4502	0.6262	0.1688
S3	0.1088	0.3968	0.2452
S4	-0.2289	0.3510	0.1222
S7	-0.4455	0.4680	0.1573
S8	0.1029	0.6935	0.2668
S10	0.1562	0.5398	0.4337
S14	0.2968	0.6682	0.4324
S16	-0.2435	0.7480	0.1542
S17	0.2743	0.4106	0.4172
S19	-0.8532	0.5468	0.1386
C25	0.3392	0.5941	0.4088
C27	-0.4436	0.4024	0.1071
C30	0.3312	0.4858	0.4030
C33	-0.1426	0.3635	0.2212

C29	-0.6473	0.7081	0.0884
C28	-0.6918	0.4893	0.1063
C37	-0.7038	0.6104	0.1197
C40	-0.4611	0.6980	0.1351
C41	0.0770	0.6916	0.3654
C35	-0.6198	0.3974	0.0551
C36	0.0648	0.3938	0.3434
C39	0.5176	0.5710	0.3791
C50	-0.1316	0.3683	0.3558
C43	-0.7857	0.6580	0.0796
C44	-0.7618	0.4470	0.0542
C54	0.5160	0.5094	0.3762
C48	-0.1458	0.7288	0.2505
C59	-0.2504	0.3512	0.2856
C60	-0.2406	0.7389	0.3178
C53	-0.1138	0.7173	0.3848

Table 4S. PENNAX *Meso*-tetraphenylporphrinatothallium(III) cyanide $C_{45}H_{28}N_5Tl$ Tl(tpp) CN (Lee, W.–B., Suen, S.–C., Jong, T.–T., Hong, F.–E., Chen, J.–H., Lin, H.–J.& Hwang, L.–P. (1993). J. Organomet. Chem., 450, 63–66).
The coordinates, averaged over the two molecules, are given in terms of molecule I (Tl1...) in $P2_1/n$, 10.003(3) 16.231(7) 21.277(8) Å, 90.57(3) °. $Z = 4$.

Atom	x	y	z
Tl1 Tl	0.33295	0.68420	0.15235
C1 C	0.1340	0.7362	0.1727
N1 N	0.0418	0.7576	0.1830
C2 C	0.3382	0.5150	0.2330
C3 C	0.3020	0.4304	0.2300
C4 C	0.2682	0.4142	0.1688
C5 C	0.2795	0.4900	0.1342
N2 N	0.3247	0.5496	0.1745
C6 C	0.2629	0.4985	0.0680
C7 C	0.2090	0.4244	0.0339
C8 C	0.2844	0.3829	-0.0114
C9 C	0.2332	0.3186	-0.0477
C10 C	0.1068	0.2946	-0.0380
C11 C	0.0264	0.3345	0.0062
C12 C	0.0810	0.3982	0.0411
C13 C	0.2982	0.5666	0.0324
C14 C	0.2920	0.5724	-0.0360
C15 C	0.3413	0.6434	-0.0523
C16 C	0.3780	0.6886	0.0038

C17 C	0.4395	0.7681	0.0057
C18 C	0.4653	0.8039	-0.0581
C19 C	0.3646	0.8424	-0.0912
C20 C	0.3851	0.8683	-0.1529
C21 C	0.5077	0.8592	-0.1794
C22 C	0.6072	0.8210	-0.1465
C23 C	0.5900	0.7950	-0.0846
N3 N	0.4587	0.6896	0.2398
C24 C	0.4886	0.8079	0.0600
C25 C	0.5611	0.8825	0.0588
C26 C	0.5936	0.8988	0.1218
C27 C	0.5402	0.8356	0.1596
N4 N	0.4758	0.7791	0.1208
C28 C	0.5584	0.8268	0.2248
C29 C	0.6354	0.8938	0.2580
C30 C	0.5734	0.9642	0.2794
C31 C	0.6454	1.0291	0.3080
C32 C	0.7810	1.0171	0.3144
C33 C	0.8424	0.9498	0.2926
C34 C	0.7687	0.8882	0.2665
C35 C	0.5203	0.7608	0.2614
C36 C	0.5422	0.7506	0.3284
C37 C	0.4984	0.6776	0.3448
C38 C	0.4412	0.6364	0.2902
N5 N	0.3498	0.6383	0.0548
C39 C	0.3900	0.5553	0.2874
C40 C	0.2980	0.4394	0.4343
C41 C	0.2836	0.4838	0.3792
C42 C	0.3994	0.5049	0.3452
C43 C	0.5204	0.4794	0.3690
C44 C	0.5292	0.4332	0.4223
C45 C	0.4175	0.4139	0.4560

Table 5S. RIJQOQ. $C_{25}H_{36}BrCrNO_2P_2$. Filippou, A. C., Wossner, D., Kociok-Kohn, G., Hinz, I. & Gruber, L. J. Organomet. Chem., 1997, 532, 207-218. Revised coordinates in space group $P2_1/n$, $Z = 4$, with cell dimensions 10.084(2) 17.351(3)16.340(3) Å, 90.02(2)°.

Atom	x	y	z
Cr1	0.42668	0.24162	0.08906
Br1	0.26543	0.32773	0.00321
C1	0.2924	0.2462	0.1678

O1	0.2095	0.2455	0.2155
C2	0.3516	0.1540	0.0467
O2	0.3080	0.0958	0.0258
C3	0.5207	0.1800	0.1496
N1	0.5797	0.1286	0.1958
C4	0.5094	0.0870	0.2630
C5	0.4750	0.1405	0.3328
C6	0.3898	0.0443	0.2312
C7	0.7172	0.1044	0.1756
C8	0.8107	0.1196	0.2464
C9	0.7196	0.0206	0.1494
P1	0.55616	0.24528	-0.03626
C10	0.5976	0.3386	-0.0816
C11	0.4693	0.2006	-0.1226
C12	0.7146	0.1944	-0.0363
C13	0.7218	0.1158	-0.0522
C14	0.8419	0.0771	-0.0488
C15	0.9553	0.1154	-0.0276
C16	0.9498	0.1930	-0.0114
C17	0.8310	0.2321	-0.0161
P2	0.51873	0.35447	0.15320
C18	0.4288	0.4442	0.1415
C19	0.5236	0.3461	0.2641
C20	0.6896	0.3830	0.1338
C21	0.7914	0.3376	0.1617
C22	0.9236	0.3560	0.1444
C23	0.9506	0.4204	0.0995
C24	0.8519	0.4666	0.0727
C25	0.7218	0.4489	0.0899

Table 6S. CICTUD. {[(tpa)Ni(II)(μ-OH)$_2$Ni(II)(tpa)](ClO$_4$)$_2$].2MeOH} $C_{38}H_{46}Ni_2Cl_2O_{10}N_8$. Ito, M., Sakai, K., Tsubomura, T. & Takita, Y. (1999). Bull. Chem. Soc. Jpn. 72, 239–247. tpa is tris(2-pyridylmethane)amine.
Revised coordinates in space group *C2/c*, *Z* = 4; 22.946 14.728 14.679 Å, 116.33°; transformation matrix (012, 010, 100).

Atom	x	y	z
Ni	0.2388	0.2788	0.0916
Cl1	0.0	0.7990	0.25
Cl2	0.0	0.7301	0.75
O1	0.3061	0.2029	0.0663
O3	0.1595	0.5408	0.3400
O7	-0.0002	0.6736	0.6698

O9	-0.0548	0.7426	0.1890
O11	0.0162	0.8556	0.1846
O13	-0.0572	0.7865	0.7106
N1	0.1684	0.3541	0.1192
N2	0.2801	0.4105	0.1123
N3	0.2844	0.2699	0.2510
N4	0.1727	0.1734	0.0848
C1	0.1710	0.4460	0.0850
C2	0.2400	0.4754	0.1132
C3	0.2592	0.5642	0.1350
C4	0.3212	0.5888	0.1555
C5	0.3642	0.5208	0.1561
C6	0.3402	0.4341	0.1343
C7	0.1858	0.3508	0.2314
C8	0.2505	0.3105	0.2953
C9	0.2775	0.3140	0.4025
C10	0.3362	0.2788	0.4596
C11	0.3710	0.2370	0.4140
C12	0.3430	0.2355	0.3084
C13	0.1072	0.3092	0.0592
C14	0.1148	0.2088	0.0735
C15	0.0665	0.1510	0.0727
C16	0.0785	0.0590	0.0856
C17	0.1378	0.0258	0.0970
C18	0.1828	0.0842	0.0964
C37	0.0890	0.5280	0.2860

Table 7S. DEMWOH Bis(benzonitrile-N)-tetrakis(μ^2-trichloroacetato-O,O')di-copper(II). Nakashima, M., Mikuriya, M. & Muto, Y. (1985). Bull.Chem. Soc. Jpn. 58, 968–973.
Revised coordinates in C2/c; transformation matrix [201], [00-1], [-1,1,0]; Z = 4; 23.468 10.130 18.911 Å, 126.34°.

Atom pair	x	y	z
Cu1	0.0366	0.0805	-0.0180
Cl1,7	0.2144	-0.0888	0.2934
Cl2,8	0.1172	0.0324	0.3188
Cl3,9	0.1968	0.1917	0.2796
Cl4,10	0.0891	-0.4594	0.0222
Cl5,11	0.1648	-0.2913	-0.0154
Cl6,12	0.0208	-0.3465	-0.1474
O1,6	-0.0455	0.0491	-0.1396
O2,5	0.1055	0.0812	0.1102

O3,8	-0.0158	0.2200	-0.0064
O4,7	0.0756	-0.0880	-0.0234
N1,2	0.0888	0.2064	-0.0540
C1,12	0.0949	0.0231	0.1595
C2,13	0.1518	0.0409	0.2576
C3,14	0.0562	-0.1970	-0.0144
C4,15	0.0826	-0.3193	-0.0360
C5,16	0.1118	0.2647	-0.0816
C6,17	0.1416	0.3380	-0.1179
C7,18	0.2064	0.3971	-0.0610
C8,19	0.2362	0.4613	-0.0974
C9,20	0.2017	0.4669	-0.1818
C10,21	0.1367	0.4158	-0.2408
C11,22	0.1040	0.3414	-0.2082

Table 8S. FIYGOJ Catena(bis((μ^2-thiocyanato-N,S)-2-methylpyridyl)cadmium(II)-catena(bis-((μ^{2}thiocyanato-N,S)-α-picolyl)cadmium(II)) $(C_{28}H_{28}Cd_2N_8S_4)_n$ (Taniguchi, Sugita & Ouchi, 1987).
Revised coordinates in *C*2/*c*; *Z* = 4; 20.103 9.299 20.023 Å,116.92°; transformation matrix (201; 00,-1; -1,1,0).

Atom	x	y	z
Cd1	0.25	0.25	0.5
Cd3	0.0	-0.0244	0.25
S1	-0.2736	0.0246	0.0744
S2	0.0218	0.1945	0.1668
N1	-0.1281	-0.0114	0.1856
N2	-0.1250	0.2533	0.0672
C1	-0.1878	0.0030	0.1400
C2	-0.0646	0.2278	0.1081
N5	-0.0112	-0.1923	0.3336
C5	-0.0674	-0.1622	0.3512
C6	-0.0856	-0.2460	0.3960
C7	-0.0457	-0.3684	0.4242
C8	0.0125	-0.4010	0.4082
C9	0.0285	-0.3119	0.3624
C10	0.0904	-0.3508	0.3436
N7	0.2526	0.4161	0.4018
C17	0.2038	0.3742	0.3319
C18	0.1944	0.4479	0.2685
C19	0.2358	0.5691	0.2764
C20	0.2855	0.6123	0.3467
C21	0.2932	0.5358	0.4088

C22	0.3481	0.5830	0.4858

Table 9S. KUSLUF (at 297 K) Tetrakis(hexylthio)tetrathiafulvalene (Nakano, C., Mori, T., Imaeda, K., Yasuoka, N., Maruyama, Y., Inokuchi, H., Iwasawa, N. & Saito, G. (1992). Bull. Chem. Soc. Jpn. 65, 1878–1883).
Revised coordinates in *C*2/*c*. Transformation matrix (021, 001, 100); $Z = 4$; 36.620 5.498 18.470 Å, 93.31°.

Atom	x	y	z
S1	0.2888	-0.0435	0.5274
S2	0.2552	0.1301	0.3878
S3	0.3349	-0.4172	0.4602
S4	0.2949	-0.2374	0.3010
C1	0.2595	0.1654	0.4828
C2	0.3035	-0.1799	0.4486
C3	0.2879	-0.1015	0.3844
C4	0.3758	-0.2452	0.4912
C5	0.3902	-0.0903	0.4404
C6	0.4256	0.0328	0.4653
C7	0.4418	0.1646	0.4070
C8	0.4768	0.2512	0.4168
C9	0.4926	0.3780	0.3666
C10	0.3040	0.0216	0.2426
C11	0.3392	0.1578	0.2647
C12	0.3492	0.3313	0.2033
C13	0.3835	0.4784	0.2254
C14	0.3941	0.6538	0.1646
C15	0.4270	0.8080	0.1880

Table 10S. RICLOE (μ^2-2-Aminophenylthiolato)-(μ^2-hydrido)-decacarbonyl-tri-osmium $C_{16}H_7NO_{10}Os_3S$. Cabeza *et al.*, (1996).
Revised coordinates in *C*2/*c*; transformation matrix (-120, 100, 00-1), no origin shift); $Z = 8$; 25.815 8.670 19.420 Å, 99.50°.

Paired Atoms	<x>	<y>	<z>
Os1,4	-0.1424	0.0840	0.2204
Os2,6	-0.1144	0.0943	0.0840
Os3,5	-0.1852	0.3194	0.1237

S1,2	-0.0935	0.3582	0.1166
N1,2	-0.0164	0.6136	0.1296
O1,11	-0.0520	0.3024	0.2770
O2,13	-0.1906	0.1252	0.3525
O3,12	-0.0806	-0.2096	0.2668
O4,14	-0.2398	-0.1039	0.1566
O5,19	-0.0943	0.0981	-0.0663
O6,18	-0.1579	-0.2316	0.0654
O7,20	-0.0040	-0.0084	0.1450
O8,16	-0.2960	0.2196	0.1362
O9,15	-0.2349	0.5354	0.0071
O10,17	-0.1826	0.5567	0.2388
C1,17	-0.0845	0.2233	0.2537
C2,19	-0.1725	0.1150	0.3028
C3,18	-0.1027	-0.1005	0.2500
C4,20	-0.2032	-0.0345	0.1792
C5,25	-0.1024	0.1052	-0.0100
C6,24	-0.1423	-0.1102	0.0717
C7,26	-0.0457	0.0254	0.1221
C8,22	-0.2548	0.2533	0.1318
C9,21	-0.2135	0.4569	0.0492
C10,23	-0.1838	0.4642	0.1950
C11,27	-0.0823	0.4809	0.0474
C12,28	-0.0436	0.5926	0.0638
C13,29	-0.0338	0.6951	0.0126
C14,30	-0.0625	0.6826	-0.0546
C15,31	-0.1006	0.5706	-0.0704
C16,32	-0.1096	0.4726	-0.0197

Table 11S. TILMEG. [Nd(η^3-C_3H_5)$_3$.(μ-$C_4H_8O_2$)]; $C_{13}H_{23}O_2Nd$. Taube, R., Windisch, H., Maiwald, S., Hemling, H. & Schumann, H. (1996). J. Organomet. Chem. 513, 49–61.
Revised coordinates in *C2/c*, $Z = 4$, (14.223 7.813 13.813 Å, 111.26°); transformation matrix (-120; -100; 0,-11); shift of origin $\Delta x = 0$, $\Delta y = 0.1595$, $\Delta z = 1/4$).

Atom	x	y	z
Nd	0	0.34054	0.25
O1	0.1678	0.2675	0.4022
C1	0.1882	0.1095	0.4611
C2	0.2630	0.3572	0.4251
C5	0.0752	0.0835	0.1680
C6	0.0686	0.2204	0.1000
C7	0.1150	0.3747	0.1277

C11	0.0779	0.6527	0.3259
C12	0.0	0.6874	0.25

Table 12S. VEWPOC10 Bis(5-chloro-o-(salicylideneaminomethyl)phenolato-O,O',N)manganese(IV) tetrahydrofuran solvate $C_{28}H_{20}Cl_2MnN_2O_4.2(C_4H_8O)$ (Mikuriya, M., DaiJie, Kakuta, Y. & Tokii, T. (1993). Bull. Chem. Soc. Jpn. 66, 1132–1139).
Transformed coordinates in *C2/c*. Transformation matrix (201, 001, -1-1-1); origin shift $\Delta x = 0$, $\Delta y = 005283$, $\Delta z = 1/4$); $Z = 4$; 23.000 8.568 18.991 Å, 114.36°.

Atom	x	y	z
Mn	0.0	0.05283	0.25
Cl1	-0.21734	0.66818	0.19968
O1	-0.0096	0.2086	0.3150
O2	0.0063	-0.1024	0.1822
O5	-0.2789	0.0758	0.0562
N1	-0.0946	0.0418	0.1916
C1	-0.0568	0.3153	0.2884
C2	-0.0440	0.4750	0.2998
C3	-0.0934	0.5819	0.2728
C4	-0.1552	0.5315	0.2349
C5	-0.1697	0.3744	0.2228
C6	-0.1204	0.2665	0.2496
C7	-0.1321	0.0950	0.2344
C8	-0.1241	-0.0033	0.1212
C9	-0.0936	-0.0630	0.0744
C10	-0.1302	-0.0840	-0.0054
C11	-0.1032	-0.1465	-0.0514
C12	-0.0400	-0.1911	-0.0190
C13	-0.0030	-0.1751	0.0588
C14	-0.0294	-0.1102	0.1072
C29	-0.3257	0.0864	0.0782
C30	-0.3858	0.1004	0.0082
C31	-0.3704	0.0388	-0.0518
C32	-0.3028	0.0399	-0.0196

Table 13S. WABKOZ $Rh(C_6H_5)Cl_2(PPh_3)_2$, Fawcett, J., Holloway, J. H. & Saunders, G. C. Inorg. Chim. Acta, 1992, 202, 111-113.

Revised coordinates in *C2/c*; (*Z* = 4; 12.99 13.93 20.11 Å, 94.0)° (transformation matrix is (-1,-1, 0; 1,-1, 0; 011), origin shift 1/4, 1/4, 0).

Atom	x	y	z
Rh	0.0000	0.2740	0.2500
Cl1	-0.1629	0.2575	0.2936
P1	0.0940	0.2650	0.3552
C1	0.0000	0.4186	0.2500
C2	0.0604	0.4686	0.2070
C3	0.0604	0.5688	0.2070
C4	0.0000	0.6188	0.2500
C11	0.1363	0.1404	0.3696
C12	0.1372	0.0760	0.3166
C13	0.1714	-0.0188	0.3270
C14	0.2040	-0.0492	0.3900
C15	0.2011	0.0133	0.4434
C16	0.1680	0.1082	0.4334
C21	0.2121	0.3399	0.3634
C22	0.2032	0.4391	0.3558
C23	0.2915	0.4963	0.3594
C24	0.3886	0.4544	0.3706
C25	0.3975	0.3552	0.3783
C26	0.3092	0.2979	0.3746
C31	0.0250	0.2905	0.4302
C32	0.0515	0.3664	0.4731
C33	-0.0034	0.3817	0.5293
C34	-0.0849	0.3210	0.5424
C35	-0.1114	0.2451	0.4994
C36	-0.0565	0.2298	0.4432

Table 14S. YATZOI10 $[Ni_4(L)_2(pz)_2(CH_3OH)]$ where H3L is 2,6-bis(salicylideneaminomethyl)-4-methylphenol and Hpz is pyrazole (Mikuriya, M., Nakadera, K. & Kotera, T. (1996). Bull. Chem. Soc. Jpn. 69, 399–405.
Transformed coordinates in *C2/c*. Transformation matrix [(1,-1,0), (-1,-1,0), (-1,0,-1)]; *Z* = 4; 22.177 13.638 18.663 Å, 119.12°.

Atom	x	y	z
Ni1	0.2305	0.0777	0.3406
Ni2	0.0703	0.0844	0.3246
O1	0.3072	0.0024	0.3630

O2	0.1564	0.1481	0.3348
O3	-0.0234	0.0412	0.2999
O7	0.0	0.2234	0.25
N1	0.2525	0.1821	0.2900
N2	0.0836	0.1550	0.4276
N3	0.1963	-0.0298	0.3741
N7	-0.1312	-0.0326	0.1345
C1	0.1678	0.2427	0.3560
C2	0.1849	0.3077	0.3093
C3	0.1892	0.4058	0.3245
C4	0.1792	0.4428	0.3855
C5	0.1647	0.3813	0.4354
C6	0.1602	0.2804	0.4208
C7	0.1808	0.5528	0.3995
C8	0.1978	0.2592	0.2465
C9	0.3125	0.1970	0.2895
C10	0.3670	0.1185	0.3300
C11	0.4295	0.1700	0.3225
C12	0.4798	0.0892	0.3575
C13	0.4800	0.0095	0.3880
C14	0.4218	-0.0432	0.3985
C15	0.3645	0.0405	0.3600
C16	0.1496	0.2088	0.4756
C17	0.0397	0.1562	0.4544
C18	-0.0260	0.1047	0.4180
C19	-0.0605	0.1115	0.4660
C20	-0.1210	0.0540	0.4405
C21	-0.1420	-0.0090	0.3760
C22	-0.1100	-0.0150	0.3275
C23	-0.0511	0.0460	0.3482
C24	0.2252	-0.1202	0.3940
C25	0.1778	-0.1768	0.3965
C26	0.1148	-0.1278	0.3770
C53	0.0	0.3175	0.25

Table 15S. TUMLES $C_{27}H_{24}N_3O_2Ir.2H_2O$. Urban, R., Krämer, R., Mihan, S., Polborn, K., Wagner, B. & Beck,W. (1996). J. Organomet. Chem., 517, 191–200. Revised coordinates in space group $P2_12_12_1$. New cell is essentially unchanged at 10.322(3) 17.864(5) 13.005(6) Å, $\beta = 90.00°$ $Z = 4$ but origin must be shifted by 0.3446 in y and 0.25 in z.

Atom	x	y	z
Ir2	0.2838	-0.1510	0.6798

O1	0.4368	-0.1665	0.5683
O2	0.4772	-0.1996	0.4066
O5	0.3204	-0.5885	-0.0427
N4	0.3138	-0.2578	0.7336
N5	0.2572	-0.0407	0.6454
N6	0.1728	-0.1884	0.5464
C1	0.4014	-0.1276	0.7962
C2	0.4520	-0.0578	0.8302
C3	0.5383	-0.0544	0.9085
C4	0.5867	-0.1164	0.9584
C5	0.5404	-0.1837	0.9280
C6	0.4528	-0.1932	0.8482
C7	0.4000	-0.2625	0.8158
C8	0.4306	-0.3318	0.8564
C9	0.3732	-0.3960	0.8219
C10	0.2862	-0.3905	0.7411
C11	0.2576	-0.3200	0.7000
C12	0.1297	-0.1290	0.7650
C13	0.0517	-0.1774	0.8230
C14	-0.0553	-0.1542	0.8744
C15	-0.0836	-0.0768	0.8816
C16	-0.0109	-0.0280	0.8252
C17	0.0933	-0.0530	0.7684
C18	0.1652	-0.0055	0.6966
C19	0.1387	0.0698	0.6774
C20	0.2044	0.1066	0.5994
C21	0.2966	0.0688	0.5475
C22	0.3224	-0.0037	0.5696
C23	0.4014	-0.1928	0.4791
C24	0.2642	-0.2212	0.4684
C25	0.2045	-0.2048	0.3649
C26	0.1384	-0.1364	0.3802
C27	0.0877	-0.1340	0.4860
O5	0.3204	-0.5885	0.9573
O7	0.2540	-0.5846	0.8672

Table 16S. CECMAY10 Complex of hexakis(2,3,6-tri-O-methyl)-alpha-cyclodextrin with (S)-mandelic acid ($C_{54}H_{96}O_{30}.C_8H_8O_3.3H_2O$)
(Harata, K., Uekama, K., Otagiri, M. & Hirayama, F. (1987). Bull. Chem. Soc. Jpn. 60, 497–502).
Revised coordinates in $C222_1$; $Z = 4$, 15.571, 21.116, 23.187; transformation matrix (101; 10-1; 010).

Equivalent atoms	x	y	z
hexakis(2,3,6-tri-O-methyl)-alpha-cyclodextrin			
C1,28	0.3056	0.2412	0.3254
C2,29	0.3685	0.2869	0.2937
C3,30	0.3277	0.3122	0.2392
C4,31	0.2916	0.2584	0.2012
C5,32	0.2384	0.2124	0.2360
C6,33	0.2204	0.1498	0.2032
C7,34	0.4446	0.3244	0.3782
C8,35	0.3872	0.4136	0.2121
C9,36	0.1398	0.0556	0.2120
O1,16	0.3932	0.3389	0.3284
O2,17	0.3894	0.3456	0.2057
O3,18	0.2378	0.2879	0.1592
O4,19	0.2846	0.1926	0.2874
O5,20	0.1534	0.1180	0.2332
C10,37	0.0594	0.2806	0.4772
C11,38	0.1324	0.3300	0.4806
C12,39	0.1739	0.3360	0.4201
C13,40	0.2028	0.2698	0.4008
C14,41	0.1268	0.2230	0.4022
C15,42	0.1501	0.1547	0.3875
C16,43	0.1372	0.4166	0.5465
C17,44	0.2439	0.4306	0.3880
C18,45	0.2493	0.0712	0.4047
O6,21	0.0984	0.3900	0.4982
O7,22	0.2459	0.3770	0.4252
O8,23	0.2338	0.2782	0.3424
O9,24	0.0943	0.2215	0.4603
O10,25	0.2237	0.1350	0.4192
C19,46	-0.2597	0.2820	0.3995
C20,47	-0.2353	0.3415	0.4317
C21,48	-0.1380	0.3517	0.4278
C22,49	-0.0932	0.2934	0.4520
C23,50	-0.1266	0.2314	0.4256
C24,51	-0.0978	0.1729	0.4596
C25,52	-0.3526	0.4136	0.4400
C26,53	-0.0702	0.4538	0.4245
C27,54	-0.0861	0.0638	0.4562
O11,26	-0.2774	0.3968	0.4102
O12,27	-0.1141	0.4059	0.4599
O13,28	-0.0036	0.3021	0.4386
O14,29	-0.2189	0.2300	0.4248
O15,30	-0.1068	0.1195	0.4240

S-mandelic acid (disordered around C_2 axis at (0,y,1/4)			
C55	0.0	0.4896	0.25
C56,60	0.0793	0.4614	0.2473
C57,59	0.0778	0.3971	0.2468
C58	0.0	0.3557	0.25
C61*	-0.0102	0.5788	0.2223
C62*	-0.0120	0.5926	0.2834
O34,36	-0.0621	0.5801	0.3060
O35*	0.0	0.6277	0.25
Water oxygens			
O31	0.0	0.1923	0.25
O32,33	-0.4407	0.1306	0.0772

* half populated.

Table 17S. JIGREW O-Methyl-neopyrrolomycin ($C_{11}H_6Cl_5NO$) Nogami, T., Shigihara, Y., Matsuda, N., Takahashi, Y., Naganawa, H., Nakamura, H., Hamada, M., Muraoka, Y., Takita, T., Iitaka, Y. & Takeuchi, T. (1990). J. Antibiot., 43, 1192–1194.
Coordinates for JIGREW in space group $C222_1$, cell dimensions 7.246 15.512 23.838 Å; transformation matrix [001], [201], [010].

Atom	x	y	z
Cl1	0.18967	0.55534	0.67756
Cl2	0.28211	0.62799	0.79602
Cl3	0.29675	0.82764	0.81426
Cl4	0.20274	0.58655	0.44433
Cl5	0.46224	0.64422	0.55965
C1	0.1720	0.7194	0.6440
C2	0.2036	0.6640	0.6880
C3	0.2477	0.6968	0.7411
C4	0.2528	0.7853	0.7488
C5	0.2254	0.8423	0.7045
C6	0.1847	0.8091	0.6517
C7	0.1725	0.9494	0.6104
C8	-0.0616	0.6895	0.5704
C9	-0.0591	0.6541	0.5164
C10	0.1257	0.6328	0.5045
C11	0.2319	0.6540	0.5494
O1	0.1580	0.8576	0.6053
N1	0.1175	0.6885	0.5903

Table 18S. VOGLUY (Hydrogen-tris(3,5-dimethylpyrazolyl)borate-N,N',N'')-(μ^2-carbonato-O,O,O',O'')- di-copper(II) $C_{31}H_{44}B_2Cu_2N_{12}O_3$ (Kitajima, N., Koda, T., Hashimoto, S., Kitagawa, T. & Moro-oka, Y. (1991). *J. Am. Chem. Soc.*, **113**, 5664–5671.
Revised coordinates in $Cmc2_1$. CELL 13.498 8.835 31.008 Å. Transformation matrix [-101], [101], [010].

Atom	x	y	z
Cu1	0.0	0.37292	0.11598
Cu2	0.0	0.30570	0.24813
O1	0.0	0.3214	0.18296
O2	0.0	0.5430	0.15391
O3	0.0	0.5050	0.22533
N1	0.0	0.4728	0.06051
N2	0.1080	0.2246	0.09685
N4	0.0	0.0930	0.25948
N5	0.1092	0.3394	0.29609
N7	0.0	0.3789	0.02579
N8	0.0932	0.1632	0.05770
N10	0.0	0.0438	0.30213
N11	0.0944	0.2657	0.33389
B1	0.0	0.2076	0.03164
B2	0.0	0.1660	0.33987
C1	0.0	0.4625	0.18754
C2	0.0	0.7560	0.07701
C3	0.0	0.6200	0.04554
C4	0.0	0.6094	0.00175
C5	0.0	0.4650	-0.01115
C6	0.0	0.3962	-0.05560
C7	0.2387	0.2290	0.15554
C8	0.1981	0.1749	0.11128
C9	0.2382	0.0808	0.08153
C10	0.1738	0.0733	0.04800
C11	0.1817	-0.0138	0.00474
C17	0.0	-0.0346	0.18716
C18	0.0	-0.0350	0.23599
C19	0.0	-0.1604	0.26366
C20	0.0	-0.1094	0.30421
C21	0.0	-0.1936	0.34716
C22	0.2290	0.5212	0.26302
C23	0.1894	0.4252	0.30109
C24	0.2286	0.4059	0.34196
C25	0.1656	0.3050	0.36212
C26	0.1688	0.2394	0.40800

Table 19S. WIFFOG bis-[(η^5-pentamethylcyclopentadienyl)-tetrahydroborato]-uranium(IV) [$U(C_5Me_5)_2.(BH_4)_2$] (Gradoz *et al.* (1994)).
Revised coordinates in space group *Fmm*2; the new cell (17.639 15.172 8.187 Å, Z = 4) is defined by the vectors [102], [010], [-100].

Atom	x	y	z
U	0.0000	0.0000	0.0000
C1, 7	0.1553	0.0000	0.0043
C2, 8	0.1380	0.0735	-0.0800
C3, 9	0.1058	0.0470	-0.2253
C4, 10	0.1970	0.0000	0.1765
C5, 11	0.1580	0.1690	-0.0555
C6, 12	0.0928	0.1030	-0.3898
B	0.0000	0.1320	0.2000

Table 20S. AZPADO. 1,3,5-Triaza-7-phospha-adamantane-7-oxide. $C_6H_{12}N_3OP$.
Jogun, K. H., Stezowski, J. J., Fluck, E. & Weidlein, J. (1978). Phosphorus and Sulfur, 4, 199–204.
Revised space group *R*3*m*. CELL 5.8847 5.8847 5.8847 Å, 104.09 104.09 104.09

Atom	x	y	z
P	0.0	0.0	0.0
O	-0.2022	-0.2022	-0.2022
C1	0.0154	0.0154	0.3158
N	0.2272	0.2272	0.4920
C2	0.2050	0.4614	0.4614
H1	-0.1353	0.0306	0.3439
H2	0.0238	0.4585	0.4585
H3	0.3402	0.5878	0.5878

Table 21S. AZPADS. 1,3,5-Triaza-7-phospha-adamantane-7-sulfide. $C_6H_{12}N_3SP$.
Jogun, K. H., Stezowski, J. J., Fluck, E. & Weidlein, J. (1978). Phosphorus and Sulfur, 4, 199–204.
Revised space group *R*3*m*. CELL 6.0482 6.0482 6.0482 Å, 100.90 100.90 100.90°.

Atom	x	y	z
P	0.0	0.0	0.0
S	0.2370	0.2370	0.2370
C1	-0.0018	-0.0018	-0.3040
N	-0.1914	-0.1914	-0.4576
C2	-0.1620	-0.4191	-0.4191
H1	0.1566	-0.0202	-0.3273
H2	-0.0077	-0.4342	-0.4342
H3	-0.2699	-0.5369	-0.5369

Table 22S. No refcode because the compound is inorganic. $LiNa_3(MoO_4)_3.6H_2O$, Makitova, D. D., Tkachev, V. V., Mizoev, R. S. & Karov, Z. G. Koord. Khim. 15(10), 1334–1339 (1989). Russ. J. Coord. Chem. 15, 761–765. Chem. Abstr. 112, 228536w (1990).
Revised coordinates in *R*3*c* (no. 161), (8.735 8.732 31.163 Å, 90.00 90.01 119.99°; $Z = 6$; the new (obverse hexagonal) cell is defined by the vectors [1/2, 0, 1/2], [0, 0, -1], [2, -3, 0].

Atom	x	y	z
Mo1	0.0	0.0	0.09267
Mo2	0.0	0.0	0.84499
O1	0.0	0.0	0.0355
O2	-0.1514	0.0620	0.1110
O5	0.4632	0.3028	0.1974
O8	0.0	0.0	0.7898
Ow1	0.7121	0.1506	0.0417
Ow2	0.5494	0.6301	0.1197
Li	0.0	0.0	0.7272
Na	0.2939	0.4053	0.15846

Table 23S. NEGXOM Di-potassium *trans*-(dichloro-bis(glutarimidato)-palladium(II)) hydrate; *trans*-$K_2[Pd(C_5H_6NO_2)_2Cl_2].4.5H_20$. (Michalska, D., Morzyk, B., Wojciechowski, W. & Glowiak, T. (1996). *Inorg. Chim. Acta*, **248**, 159-166).
Revised coordinates in space group *Pccn* Transformation matrix [101],[010],[001]; orthorhombic cell 15.533 16.225 7.932 Å,

Atom	x	y	z

Pd	0.5	0.0	0.0
Cl	0.9452	-0.0631	0.7396
O1	0.3170	0.0086	0.1332
O2	0.5570	0.1662	0.1504
N	0.4390	0.0844	0.1475
C1	0.3562	0.0694	0.1908
C2	0.3113	0.1264	0.3108
C3	0.3536	0.1981	0.3570
C4	0.4427	0.2078	0.3337
C5	0.4838	0.1512	0.2028
K	0.7902	0.0828	0.6592
O5*	0.8570	0.1896	0.2988
O7*	0.6269	0.0758	0.5002
O9*	0.75	0.25	0.4830

* Oxygen of water molecule.

Table 24S. YIVWOP. μ-Hydroxy-cyclooctadien(1,5)-rhodium(I)-Dimer [(μ-OH)Rh(COD-1,5)]$_2$ [$C_{16}H_{26}O_2Rh_2$] at 173 K. Selent, D. & Ramm, M. (1995). J. Organomet. Chem. 485, 135–140.
Revised space group I4(1)/a; CELL 22.409 22.409 12.216 Å. Transformation matrix [001], [101], [010].

Atom Pair	x	y	z
Rh1,4	0.36956	0.30616	0.22872
Rh2,3	0.34542	0.31556	0.45944
O1,4	0.3092	0.2637	0.3328
O2,3	0.4189	0.2914	0.3676
C1,27	0.4418	0.3278	0.1279
C2,28	0.4187	0.3792	0.1770
C3,25	0.3295	0.2876	0.0792
C4,26	0.3056	0.3410	0.1206
C5,30	0.4312	0.3126	0.0081
C6,29	0.3741	0.2847	-0.0148
C7,32	0.3790	0.4246	0.1212
C8,31	0.3221	0.4020	0.0792
C9,19	0.3922	0.3536	0.5915
C10,20	0.3770	0.3977	0.5140
C11,17	0.2821	0.2986	0.5806

C12,18	0.2636	0.3483	0.5204
C13,22	0.3622	0.3451	0.7002
C14,21	0.3098	0.3000	0.6938
C15,24	0.3255	0.4413	0.5236
C16,23	0.2686	0.4119	0.5654

Table 25S. TONWUO. Catena-(tetrakis(μ^2-1,4-diazoniabicyclo(2.2.2)octane-1,4-dipropianato)di-zinc(II) tetraperchlorate. $(C_{48}H_{80}N_8O_{16}Zn_2)^{4+}4(ClO_4)^-$. Wei, P.-R., Wu, B.-M., Leung, W.-P. & Mak, T. C. W. (1996). Polyhedron, 15, 4041–4046. Revised coordinates in space group I4(1)/acd; CELL 19.265 19.265 15.913. Transformation matrix: (101), (010), (001).

Related atoms	x	y	z
Zn	0.5	0.25	-0.125
N1,2,3,4	0.7037	0.3135	-0.4426
O1,3,5,7	0.5962	0.2399	-0.1786
O2,4,6,8	0.5450	0.3142	-0.2618
C1,7,13,24	0.5953	0.2783	-0.2413
C2,8,14,23	0.6594	0.2790	-0.2969
C3,9,15,22	0.6444	0.3161	-0.3791
C4,10,16,17	0.7198	0.2401	-0.4694
C5,11,19,20	0.6797	0.3525	-0.5170
C6,12,18,21	0.7686	0.3454	-0.4103
Cl	0.6924	0.4424	-0.125
O9,12'	0.6680	0.4260	-0.2064
O10,11'	0.6868	0.3841	-0.0728
O11,9'	0.6458	0.4945	-0.0927
O12,10'	0.7578	0.4731	-0.1240

Table 26S. PYRDNO10 Pyridine N-oxide. C_5H_5NO Ülkü, D., Huddle, B. P. & Morrow, J. C. (1971). *Acta Cryst.* B**27**, 432–436.

CELL: 5.816 5.816 13.747 Å, $Z = 4$; space group $P4_12_12$.

Atom	x	y	z	Ueq
O1	0.1757(7)	0.1757(7)	0	0.0594(19)

N1	0.0140(8)	0.0140(8)	0	0.0379(16)
C2	0.0420(9)	-0.17540(11)	0.0553(4)	0.0439(14)
C3	-0.1242(10)	-0.3426(10)	0.0554(4)	0.0476(16)
C4	-0.3196(11)	-0.3196(11)	0	0.0499(21)
H2	0.1930(111)	-0.1698(105)	0.0920(48)	0.0573(164)
H3	-0.0914(76)	-0.4784(108)	0.1071(45)	0.0484(166)
H4	-0.4246(177)	-0.4246(177)	0	0.1785(754)

Table 27S. ROBJEX 2,2'-(Methylenedioxy)-bis(phenyl-isocyanide) $C_{15}H_{10}N_2O_2$. F.E.Hahn, M.Tamm, L.Imhof, T.Lugger J. Organomet. Chem., (1996) 526, 149–155.
Revised coordinates in space group $P4_12_12$, Z = 4; 9.591 13.431 Å).

Atom Pairs	x	y	z
O1,2	0.4290	0.4894	0.3269
N1,2	0.2503	0.5012	0.4770
C1,15	0.1704	0.4120	0.4826
C2,10	0.3502	0.6057	0.4688
C3,9	0.4442	0.6097	0.3899
C4,14	0.5428	0.7043	0.3816
C5,13	0.5496	0.8088	0.4524
C6,12	0.4566	0.8128	0.5304
C7,11	0.3560	0.7118	0.5384
C8	0.5280	0.4720	0.25

Table 28S. JUNNAH. Bis[cis-cyclohexane tris(methylamine)zinc bis(trifluoromethyl-sulfonate). $[(C_6H_9(NH_2)_3]\ Zn(CF_3SO_3)_2$. $C_{14}H_{30}F_6N_6O_6S_2Zn$. U. Brand & H. Vahrenkamp, (1992). Inorg. Chim. Acta, 198–200, 663–669.
Revised coordinates in space group P2(1)3.
CELL 13.6054.

Atom	x	y	z
Zn	0.35682	0.35682	0.35682
N1	0.4974	0.3167	0.4230
N2	0.2908	0.2148	0.3961
C1	0.5451	0.3924	0.4839
C2	0.5704	0.4819	0.4236
C7	0.2303	0.1665	0.3198
C8	0.2936	0.1403	0.2301

S1	-0.03166	-0.03166	-0.03166
S2	0.77778	0.77778	0.77778
O1	0.0306	-0.0648	-0.1095
O2	0.7584	0.7427	0.8743
C17	0.0601	0.0601	0.0601
C18	0.6974	0.6974	0.6974
F1	0.0612	0.1267	0.0018
F2	0.7249	0.6065	0.7094

Transformation from R3: (2/3,1/3,1/3); (-1/3,1/3,1/3); (-1/3,-2/3,1/3)
New cell angles: 89.96 deg.

Table 29S. TAZPAD 1,3,5-Triaza-7-phospha-adamantane $C_6H_{12}N_3P$. Fluck, E., Förster, J.-E., Weidlein, J. & Hädicke, E. (1977). Z. Naturforsch. 32b, 499-506.
Revised space group: R3m (original structure, in R3, had hexagonal setting)
Cell 6.024 6.024 6.024 105.94 105.94 105.94

Atom	x	y	z
P	0.0	0.0	0.0
C1	0.0402	0.0402	0.3272
N	0.2577	0.2577	0.5136
C2	0.2413	0.4880	0.4881
H1	-0.1246	0.0586	0.3544
H2	0.0738	0.5073	0.5073
H3	0.4020	0.6380	0.6380

Table 30S. POJKAA *trans*-$[Pt(CF_3)\{N{=}C(Ph)OCH_2CH_2CH_2\}(PPh_3)_2]BF_4 \cdot [PtC_{45.8}H_{41}F_{6.4}NOBP_2]Cl_{0.2}$, Michelin, R. A., Belluco, U., Mozzon, M., Berin, P., Bertani, R., Benetello, F., Bombieri, G. & Angelici, R. J. (1994). Inorg. Chim. Acta, 220, 21-33.
Reported in P-3 with a = 22.590(4), c = 15.970(3) Å, $Z = 6$. Revised to $P6_3/m$ with cell unchanged.

Atom	x	y	z
Pt	0.3117	0.3750	0.2500
P1	0.3055	0.3662	0.1036
F1	0.2020	0.3920	0.1890
F3	0.1660	0.3060	0.2500
O	0.5157	0.4078	0.2500
N	0.4005	0.3693	0.2500

C(Cl)	0.2149	0.3758	0.2500
C1	0.4620	0.4180	0.2500
C2	0.4440	0.2890	0.2500
C3	0.5060	0.3410	0.2500
C4	0.3850	0.2980	0.2500
C5	0.4847	0.4930	0.2500
C6	0.4430	0.5200	0.2500
C7	0.4680	0.5910	0.2500
C8	0.5350	0.6310	0.2500
C9	0.5810	0.6050	0.2500
C10	0.5540	0.5360	0.2500
C11	0.3124	0.4400	0.0465
C12	0.3160	0.4360	-0.0445
C13	0.3220	0.4960	-0.0850
C14	0.3290	0.5525	-0.0425
C15	0.3230	0.5520	0.0415
C16	0.3155	0.4945	0.0875
C17	0.2235	0.2881	0.0770
C18	0.1870	0.2895	0.0055
C19	0.1020	0.1745	0.0495
C20	0.1230	0.2245	-0.0060
C21	0.1365	0.1720	0.1180
C22	0.2025	0.2345	0.1330
C23	0.3727	0.3561	0.0525
C24	0.4376	0.4116	0.0510
C25	0.4900	0.4045	0.0125
C26	0.4770	0.3440	-0.0225
C27	0.4125	0.2865	-0.0215
C28	0.3565	0.2915	0.0175

Table 31S. FABTAD10. Carbon tetrachloride–thiourea (1/3) Adduct at 170 K. $CCl_4.3[SC(NH_2)_2]$. Fait, J. F., Fitzgerald, A., Caughlan, C. N. & McCandless, F. P. (1991). Acta Cryst. C47 332–337. Note that the CCl_4 molecule is disordered. $Z = 6$,[1] 15.53(4), 12.529(9) Å),

Atom pair	x	y	z
C2	0	0	0.75
Cl1	0.1042	0.1042	0.75
Cl2,3	0.0787	0.0732	0.6386
S1	0.3734	0.333	0.5833
N1,2	0.2074	0.3097	0.4951
C1	0.2264	0.2959	0.4364

[1] Misprinted as $Z = 18$ in the paper.

Table 32S. FISMUP Adamantane-1,3-diol. $C_{10}H_{14}O_2$. Prozorovskii, A. E.,Tafeenko, V. A., Rybakov, V. B.,Shokova, E. A. & Kovalev, V. V. (1987). J. Struct. Chem, USSR, 28, 243–251.
Revised space group $P6_3/mcm$. CELL 11.885 10.939.

Atom, Wyckoff position	x	y	z
O1 12(k)	0.7751	0.0	0.9737
C1 12(k)	0.7052	0.0	0.8645
C2 6(g)	0.7817	0.0	0.75
C4 24(l)	0.6933	0.1227	0.8650
C5 12(j)	0.6195	0.1217	0.75
C6 6(g)	0.4823	0.0	0.75

CATEGORY B.

Table 33S. YOJBUU Bis(ethylenediammonium) hexachlororuthenate(III) monochloride monohydrate (Balakaeva, T. A., Gorbunova, Yu. E., Kurbakova, A. P., Mikhailov, Yu. N. & Efimenko, I. A. (1994). Russ. J. Coord. Chem. 20, 888–892; Koord. Khim. 20(12), 939–942; Chem. Abstr. 123, 186807e (1995).
Revised coordinates in space group P2(1)/m, , $Z = 2$ (10.393(2) 10.031(2) 8.089(1) Å, $\beta = 90.66°$.

Atom	x	y	z
Ru1	0.2543	0.25	0.0054
Cl1	0.2216	0.25	-0.2844
Cl2	0.2882	0.25	0.2956
Cl3	0.2530	0.4862	0.0088
Cl5	0.4815	0.25	-0.0382
Cl6	0.0287	0.25	0.0423
Cl7	0.7332	0.25	-0.6320
O1	0.834	0.25	-0.279
N1	0.476	-0.026	-0.269
N3	-0.003	0.512	0.270
C1	0.486	0.045	-0.430
C2	0.023	0.459	0.434

Table 34S. HEFSIU $Na_4[HO(O_2N)C_6H_3SO_3]_4.2H_2O$, Shubnell, A. J., Kosnic, E. J. & Squattrito, P.J. (1994). Inorg. Chim. Acta, 216, 101–112.
Revised space group P2/c; CELL 8.293 16.580 13.465 Å, 90.29°.

Atom pair	x	y	z
S1,4	0.2974	0.3894	0.1157
S2,3	-0.2290	0.6307	0.3527
Na1	0.0	0.5	0.0
Na2,3	-0.4020	0.5569	0.1166
Na4	0.0	0.4947	0.25
O1,19	0.1860	0.4010	0.1970
O2,20	0.2210	0.4020	0.0195
O3,21	0.4450	0.4340	0.1235
O4,22	0.4640	0.0430	0.1245
O5,23	0.8195	0.2150	0.1095
O6,24	0.7595	0.0895	0.1155
O7,14	-0.0870	0.5825	0.3720
O8,13	-0.3510	0.6215	0.4290
O9,15	-0.2920	0.6193	0.2530
O10,16	-0.0345	0.9730	0.3815
O11,17	0.3095	0.7915	0.3900
O12,18	0.2585	0.9205	0.3925
O25,26	0.2010	0.4425	0.3930
N1,4	0.720	0.162	0.114
N2,3	0.215	0.848	0.386
C1,19	0.350	0.286	0.122
C2,24	0.512	0.263	0.116
C3,23	0.552	0.182	0.118
C4,22	0.431	0.124	0.125
C5,21	0.270	0.147	0.130
C6,20	0.230	0.229	0.130
C7,13	-0.164	0.732	0.364
C8,18	-0.002	0.751	0.374
C9,17	0.046	0.832	0.380
C10,16	-0.070	0.893	0.376
C11,15	-0.232	0.873	0.365
C12,14	-0.280	0.792	0.359

Table 35S. RACFEG. catena-(bis(Tetramethylammonium) (hexa(μ^2-cyano)-di-iodo-tri-cadmium) tetrachloroethene clathrate). {n($C_6Cd_3I_2N_6^{2-}$), 2n($C_4H_{12}N^+$),

n(C_2Cl_4)}. Kitazawa,, T., Nishikiori, S. & Iwamoto, T. (1992). Materials Science Forum, 91–93, 257–264.
Revised space group C2/m. CELL 15.467 8.541 12.840 Å 92.01°.

Atom	x	y	z
Cd1 (tetrahedral)	-0.3290	0.0	-0.6932
Cd3 (octahedral)	0.0	0.0	0.5
I1*	-0.3608	0.0	-0.9014
N1	-0.120	0.0	-0.614
C1	-0.188	0.0	-0.644
N3	-0.070	0.191	-0.410
C3	0.394	-0.208	-0.376
N5	-0.343	0.0	-0.251
C5**	-0.384	0.150	-0.202
C6 **	-0.292	0.123	-0.198
C7 **	-0.342	0.038	-0.378
Cl1	-0.1359	0.0	0.0270
Cl3	0.0300	0.0	0.1628
C11	-0.028	0.0	-0.020

* Occupancy 0.876(2); ** Occupancy 0.67

Table 36S. . CHXCUB. bis(cis-1,3-Cyclohexanediamine-N,N')-copper(ii) dinitrate $C_{12}H_{28}CuN_4^{2+}$,2(NO_3^-) (Kamisawa, K., Matsumoto, K., Ooi, S., Saito, R. & Kidani, Y. (1981). Bull.Chem.Soc.Jpn., 54, 1072–1076).
Revised coordinates in space group C2/m, $Z = 2$; 10.059(3) 9.278(3) 10.428(3) Å, β = 117.12(4)°,

Atom	x	y	z
Cu1	0.0	0.0	0.0
N1	0.0342	0.1572	0.1444
C1	0.0812	0.0	0.3535
C2	0.1263	0.1362	0.3032
C3	0.2914	0.1342	0.3408
C4	0.3355	0.0	0.2882
N3	0.1828	0.5	0.1073
O1	0.1355	0.5	0.1962
O2	0.2070	0.3831	0.0614

Table 37S. FOHDUB. Bis(μ^2-Carbonyl)-(η^5-cyclopentadienyl)-(η^5-pentamethyl-cyclopentadienyl)-cobalt-iridium $C_{17}H_2$ $CoIrO_2$. Horlein, R., Herrmann, W. A., Barnes, C. E., , Weber, C., Kruger, C., ,Ziegler, M. L., & Zahn, T. (1987). J. Organomet. Chem., 321, 257–272.
Revised coordinates in space group C2/m; 17.305(5) 9.299(2) 10.2970(7) Å, 93.700(7)°).

Atom	x	y	z
Ir1	-0.3328	0.0	-0.2539
Co1	-0.2244	0.0	-0.0900
O1	-0.1734	0.0	-0.3474
O2	-0.3740	0.0	0.0232
C1	-0.2232	0.0	-0.2672
C2	-0.3293	0.0	-0.0664
C5	-0.4984	0.1686	-0.2224
C6	-0.3880	0.2778	-0.4367
C7	-0.3287	0.0	-0.5785
C11	-0.4541	0.0750	-0.3056
C21	-0.4038	0.1223	-0.4028
C31	-0.3702	0.0	-0.4674
C110	-0.1850	0.0781	0.0876
C120	-0.1326	0.1200	-0.0052
C130	-0.1038	0.0	-0.0584

Table 38S. KOYXOL. Bis-guanidinium hexafluorotitanium. $[C(NH_2)_3]_2TiF_6$. Calov, U., Schneider, M. & Leibnitz; P. (1991). Z. anorg. allgem. Chem. 604, 77–83.
Revised space group C2/m. CELL 12.869 7.378 6.243 Å, 114.45°.

Atom	x	y	z
Ti1	0.0	0.5	0.0
F1	0.1572	0.5	0.1721
F3	0.0160	0.3218	-0.1938
N1	0.2230	0.3442	-0.2762
N2	0.3784	0.5	-0.2709
C2	0.2748	0.5	-0.2728

Table 39S. PASQAB. C60-fullerene 5,6,11,12-tetrahydro-5,12(1',2'):6,11(1",2")-dibenzenodibenzo(a,e)cyclo-octene benzene solvate. C_{60}, $C_{28}H_{20}$, $3(C_6H_6)$
Konarev, D. V., Valeev, E. F., Slovokhotov, Y. L., Shul'ga, Y. M. & Lyubovskaya, R. N. (1997). J. Chem. Res.(S), 442–443..
Revised coordinates in space group C2/m; CELL 13.260 15.177 15.764 Å, 110.970°.

Atom	x	y	z
C1	0.1194	0.0	-0.0046
C2	0.0132	0.0	-0.0965
C3	-0.0562	0.0811	-0.1036
C4	-0.0554	0.1538	-0.1570
C5	-0.1210	0.2246	-0.1600
C6	-0.1886	0.2242	-0.1114
C7	-0.1896	0.1517	-0.0571
C8	-0.1229	0.0802	-0.0531
C17	1.0691	0.0455	0.6574
C18	1.1490	0.0901	0.7235
C19	1.2271	0.0446	0.7904
C23	0.5636	0.0	-0.0516
C24	0.5304	0.0767	-0.0258
C27	-0.7633	0.0	0.5006
C28	-0.7016	0.0	0.5980
C29	-0.6410	0.0770	0.6352
C30	-0.5362	0.0516	0.7019
C31	0.5429	0.0946	0.7136
C32	0.6456	0.0492	0.7272
C33	0.7038	0.0904	0.6880
C34	0.7606	0.0484	0.6468
C35	0.7639	0.0764	0.5544
C45	-0.7132	0.1440	0.4767
C46	-0.6516	0.1486	0.5759
C47	-0.5540	0.1988	0.5880
C48	-0.4638	0.1703	0.6566
C49	-0.3597	0.1715	0.6372
C50	-0.3503	0.1934	0.5703
C57	-0.5506	0.2268	0.5061

Table 40S. VOKKIP. catena-(Potassium cyanurate monohydrate). $KC_3H_2N_3O_3$, H_2O. T.F.Sysoeva, ,M.Z.Branzburg, M.Z.Gurevich, & Z.A.Starikova, Zh.Strukt.Khim., 31, 90-96,(1990); J. Struct. Chem. 31, 602–608 (1990).
Revised space group *C2/m*. CELL 11.044(3) 16.390(3) 7.199(2) Å, 103.80(2)°.

Atom	x	y	z	Wyckoff position and symmetry
K1	0.0758	0.0	-0.2548	4i m
K3	-0.4194	0.0	0.2584	4i m
water				
O1	-0.1933	0.0	-0.4478	4i m
O2	0.3044	0.0	0.0355	4i m
Cyanurate I				
O7	0.5	0.1040	0.5	4h 2
N2	0.5	0.3505	0.5	4h 2
C3	0.5	0.1790	0.5	4h 2
O5	-0.1936	-0.1572	0.3014	8j 1
N1	-0.0984	-0.2760	0.4040	8j 1
C1	-0.0993	-0.1915	0.4000	8j 1
Cyanurate II				
O10	0.5	0.1266	0.	4h 2
N5	0.5	0.3728	0.	4h 2
C6	0.5	0.2011	0.	4h 2
O8	-0.1968	-0.1350	-0.1891	8j 1
N4	-0.0994	-0.2536	-0.0953	8j 1
C4	-0.1002	-0.1696	-0.0951	8j 1

Table 41S. POWYUV; tetrakis(dimethyldithiocarbamato)-tungsten(v) 7,7,8,8-tetracyanoquinodimethanideC12 H24 N4 S8 W1 1+, C12 H4 N4 1-

Le Stang, S., Conan, F., Sala Pala, J., Le Mest, Y., Garland, M. T., Baggio, R., Faulques, E.,, Lebl, A., Molinie, P. & Toupet. L. J. Chem. Soc., Dalton Trans., 489, 1998

Revised space group *C*2/*c*; CELL 12.894 18.666 14.059 Å, 91.11°.

Atom	x	y	z
W1	0.0	1.1776	0.25
S1	-0.0558	1.0664	0.3394
S2	-0.0838	1.2076	0.4036
S3	0.1027	1.2888	0.2937
S4	0.1659	1.1482	0.3365
C1	-0.1070	1.1194	0.4260
C2	0.1996	1.2365	0.3408
C5	-0.6054	1.0629	0.1550
C7	-0.5518	1.0316	0.0772
C8	-0.5326	0.9576	0.0740
C9	-0.4826	0.9268	-0.0003

C13	-0.1758	1.0176	0.5108
C14	-0.2018	1.1440	0.5690
C15	0.3159	1.3370	0.3704
C16	0.3686	1.2135	0.4116
C21	-0.6198	1.1376	0.1632
C22	-0.6480	1.0190	0.2268
N1	-0.1588	1.0948	0.4988
N2	0.2888	1.2612	0.3743
N5	-0.6269	1.1988	0.1676
N6	-0.6830	0.9820	0.2816

Table 42S. RIDPID Aizawa, S., Yagu, T., Kato, K. & Funahashi, S. (1995). Anal. Sci. 11, 557–562.
Revised coordinates in *C2/c*; CELL 9.941(7) 14.48(1) 18.55(1) Å, 101.98(3)°, $Z = 4$

Atom	x	y	z
Ni	0.0	0.33546	0.25
S1	-0.2018	0.4906	0.14112
F1	-0.4592	0.5100	0.0780
F2	-0.4238	0.5125	0.1927
F3	-0.4137	0.3856	0.1354
O1	-0.1401	0.4449	0.2093
O2	-0.1868	0.5893	0.1420
O3	-0.1782	0.4470	0.0758
N1	0.0686	0.3293	0.1532
N2	-0.1338	0.2398	0.1932
C1	0.1719	0.3804	0.1363
C2	0.2027	0.3786	0.0668
C3	0.1299	0.3206	0.0143
C4	0.0284	0.2656	0.0320
C5	-0.0025	0.2730	0.1021
C6	-0.1175	0.2222	0.1241
C7	-0.2035	0.1624	0.0776
C8	-0.3102	0.1210	0.1032
C9	-0.3258	0.1373	0.1738
C10	-0.2367	0.1986	0.2174
C21	-0.3834	0.4740	0.1374

Table 43S. ZAWSUL (N,N'-Dibenzyl-N,N'-di(quinoline-2-methyl))-1,2-ethylenediamine at 173 K; $C_{36}H_{34}N_4$; Rieger, B. Abu–Surrah, A. S., Fawzi, R. & Steiman, M. (1995). J. Organomet. Chem., 497, 73–79.
Revised coordinates in space group *C2/c*, $Z = 4$, CELL 30.834(6) 6.361(1) 17.283(3) Å, 123.26(3)°;

Paired atoms	x(C2/c)	y(C2/c)	z(C2/c)
N1,3	0.0519	0.1560	-0.0014
N2,4	0.1672	0.1684	0.2309
C1,2	0.0189	0.0860	0.0309
C3,20	-0.0991	-0.2549	-0.0748
C4,21	-0.1369	-0.0984	-0.1455
C5,22	-0.1403	0.1089	-0.1182
C6,23	-0.1771	0.2424	-0.1829
C7,24	-0.2104	0.1739	-0.2745
C8,25	-0.2495	0.3055	-0.3453
C9,26	-0.2810	0.2280	-0.4338
C10,27	-0.2749	0.0222	-0.4549
C11,28	-0.2372	-0.1079	-0.3877
C12,29	-0.2043	-0.0348	-0.2961
C13,30	-0.0240	-0.3004	0.0802
C14,31	-0.0543	-0.3485	0.1233
C15,36	-0.0616	-0.5534	0.1411
C16,35	-0.0885	-0.5951	0.1828
C17,34	-0.1099	-0.4363	0.2044
C18,33	-0.1030	-0.2307	0.1864
C19,32	-0.0753	-0.1874	0.1471

Table 44S. ZEDCUG Hexa-t-butyl 1,2,4,5-benzenehexacarboxylate (C36 H54 O12) (Yasuda, M., Kuwamura, G., Nakazono, T., Shima, K., Inoue, Y., Yamasaki, N. & Tai, A. (1994). Bull. Chem. Soc. Jpn. 67, 505–510).
Revised coordinates in space group *C*2/*c*; 16.632(0) 14.074(5) 16.872(4) Å, 92.98(1)°, $Z = 4$.

Atom	x	y	z
O1 O	0.3752	0.2886	0.1571
O2 O	0.5092	0.2560	0.1599
O5 O	0.6986	0.5072	0.3508
O6 O	0.6088	0.4684	0.4418
O7 O	0.5832	0.6782	0.3765
O8 O	0.5933	0.7110	0.2463
C1 C	0.4696	0.3974	0.2183
C3 C	0.5628	0.4832	0.3088
C4 C	0.5325	0.5678	0.2786
C7 C	0.4440	0.3065	0.1760
C8 C	0.5042	0.1730	0.1042
C9 C	0.4729	0.2072	0.0220

C10 C	0.5925	0.1410	0.1055
C11 C	0.4478	0.0976	0.1397
C17 C	0.6329	0.4866	0.3696
C18 C	0.6653	0.4754	0.5146
C19 C	0.6090	0.4560	0.5812
C20 C	0.7306	0.3974	0.5072
C21 C	0.7002	0.5778	0.5174
C22 C	0.5718	0.6608	0.3069
C23 C	0.6480	0.7977	0.2590
C24 C	0.6536	0.8302	0.1720
C25 C	0.7306	0.7566	0.2950
C26 C	0.6108	0.8706	0.3128
H1 HS	0.470	0.155	-0.014
H2 HS	0.421	0.234	0.026
H3 HS	0.508	0.254	0.003
H4 HS	0.597	0.087	0.072
H5 HS	0.625	0.190	0.088
H6 HS	0.610	0.124	0.158
H7 HS	0.444	0.044	0.106
H8 HS	0.470	0.079	0.190
H9 HS	0.397	0.124	0.145
H19 HS	0.638	0.458	0.631
H20 HS	0.568	0.502	0.580
H21 HS	0.586	0.396	0.574
H22 HS	0.767	0.400	0.552
H23 HS	0.706	0.336	0.504
H24 HS	0.759	0.409	0.461
H25 HS	0.736	0.584	0.562
H26 HS	0.728	0.590	0.471
H27 HS	0.658	0.622	0.520
H28 HS	0.686	0.884	0.170
H29 HS	0.676	0.781	0.142
H30 HS	0.602	0.844	0.150
H31 HS	0.767	0.807	0.304
H32 HS	0.722	0.725	0.344
H33 HS	0.752	0.714	0.258
H34 HS	0.645	0.924	0.320
H35 HS	0.560	0.890	0.290
H36 HS	0.604	0.843	0.362

Table 45S. Refcode not yet assigned. 6,12-Dioxaanthracene[2] $C_{20}H_{10}O_2$. Asari, T., Kobayashi, N., Naito, T. & Inabe. T. (2001). Bull. Soc. Chem. Jpn. 74, 53–58.

CELL. Space group *C*2/*c* (*Z* = 4; 15.928(3) 4.983(3) 16.170(3) Å β = 91.33(2) °)

[2] Alternative name *peri*-xanthenoxanthene, hence the acronym PXX (Hjorth *et al.*, 1994)

Atom Pair	x	y	z
O(1), (2)	0.0929	0.2279	-0.0225
C(1), (12)	0.1464	0.3818	0.0274
C(2), (13)	0.1113	0.5764	0.0790
C(3), (14)	0.1628	0.7309	0.1283
C(4), (15)	0.2515	0.7007	0.1296
C(5), (16)	0.3079	0.8535	0.1795
C(6), (17)	0.3921	0.8065	0.1762
C(7), (18)	0.4260	0.6095	0.1241
C(8), (19)	0.3727	0.4621	0.0747
C(9), (20)	0.2851	0.5030	0.0771
C(10), (11)	0.2315	0.3471	0.0263

Table 46S. No REFCODE because compound is inorganic. Mo3FeS4(H2O)(NH3)9Cl4. Shibahara, T., Sakane, G., Naruse, Y., Taya, K., Akashi, H., Ichimura, A. & Adachi, H. (1996). Bull. Chem. Soc. Jpn. 68, 2769-2782. Revised coordinates in space group *Pnma*; 9.208 14.948 16.233 Å; $Z = 4$.

Atom	x	y	z
Mo1	0.19940	0.34306	0.08195
Mo2	0.18268	0.25	-0.06719
Fe	-0.0387	0.25	0.03948
S1	0.3808	0.25	0.0251
S2	0.0370	0.3730	-0.0267
S4	0.0563	0.25	0.1670
N11	0.0825	0.4551	0.1500
N12	0.3385	0.4580	0.0376
N13	0.3525	0.3630	0.1885
N21	0.0394	0.25	-0.1813
N22	0.3130	0.1565	-0.1455
Cl1	0.6882	0.4318	0.1414
Cl3	0.3205	0.6284	0.1630
O	-0.2585	0.25	0.0304

Table 47S. FOZPAL Pentacarbonyl(phenylisocyanide)rhenium Tetrafluoroborate.$ReC_{12}H_5NO_5BF_4$. Steil, P., Nagel, U. & Beck, W. J. Organometall. Chem. 339 (1988). 111–124.
Revised coordinates in space group *Pnma*. CELL 15.412 7.668 13.038 Å.

Atom	x	y	z
Re1	0.1256	0.75	0.6539
C1	0.0368	0.9340	0.6523
O1	-0.0146	1.0368	0.6114
C3	0.2132	0.9386	0.6885
O3	0.2627	1.0429	0.7068
C5	0.1603	0.75	0.5050
O5	0.1777	0.75	0.4207
C6	0.0825	0.75	0.8047
N1	0.0547	0.75	0.8856
C7	0.0703	0.75	1.0685
C8	0.0341	0.75	1.1666
C9	-0.0541	0.75	1.1795
C10	-0.1062	0.75	1.0944
C11	-0.0701	0.75	0.9963
C12	0.0181	0.75	0.9833
B1	0.3057	0.75	0.9484
F1	.03693	0.75	1.0217
F2	0.2551	0.6042	0.9609
F4	0.3452	0.75	0.8533

Coord xxxx -0.000760 0.753320 -0.003520
Xxxx 0.005915 0.006142 0.007610

Table 48S. KISNAB. Dichloro(6,13-(bis-2-hydroxyethyl)-6H,13H-tripyrido-[*cd,fg,lm*]-[1,2,4,7,9,10]heptaaza-pentadecine)iron(III) chloride. Constable, E. C., Khan, M. S., Lewis, J., Liptrot, M. C.& Raithby, P. R. (1991). Inorg. Chim. Acta, 181, 207–212.
Revised coordinates in *Pnma*.; (CELL 15.494(8) 12.229(6) 12.873(6) Å, $Z = 4$).

Atom pair	<x>	<y>	<z>
Fe1	0.3320	0.25	0.6342
N1	0.1960	0.25	0.6142
C1,5	0.1542	0.1542	0.6059
C2,4	0.0646	0.1514	0.5945
C3	0.0216	0.25	0.5887

C6,22	0.2086	0.4437	0.6105
C7,23	0.1720	0.5538	0.5804
N2,7	0.2883	0.4221	0.6331
N3,6	0.3494	0.5050	0.6410
C8,20	0.3326	0.5964	0.7154
C9,21	0.3367	0.5628	0.8287
O1,2	0.4225	0.5370	0.8594
N4,5	0.4420	0.3549	0.6361
C10,19	0.4328	0.4643	0.6383
C11,18	0.5053	0.5331	0.6326
C12,17	0.5853	0.4870	0.6263
C13,16	0.5948	0.3744	0.6247
C14,15	0.5213	0.3107	0.6291
Cl1	0.3380	0.25	0.4510
Cl2	0.3121	0.25	0.8146
Cl3	0.4810	0.25	0.1796

Table 49S. YUFXIG [$(CO)_6Fe_2(\mu\text{-}SeCH_3)_2$]. Mathur, P., Trivedi, R., Hossain, M. Md., Tavale, S. S. & Puranik, V. G. (1995). J. Organomet. Chem., 491, 291–294. Revised coordinates in *Pnma*, (CELL 18.344(3) 10.544(1) 7.202(1)).

Atom	x	y	z
Se1	0.0776	0.1092	0.0936
Fe1	0.0586	0.25	0.3476
Fe2	0.1760	0.25	0.1547
O1	0.096	0.452	0.614
O2	-0.103	0.25	0.359
O4	0.262	0.056	0.340
O5	0.251	0.25	-0.205
C1	0.078	0.372	0.516
C2	-0.040	0.25	0.358
C4	0.228	0.124	0.268
C5	0.221	0.25	-0.072
C7	0.097	-0.066	0.190

Table 50S. ZUFDIN. $[Ni_2(cyclam)_2\text{-}p\text{-}xyl]ClO_4.2H_2O$, $(cyclam)_2$-*p*-xyl is α,α'-bis(1,4,8,11-tetraazacyclotetradecan-6-yl)-*p*-xylene). Kido, H., Takada, M., Suwabe, M., Yamaguchi, T. & Ito, T. (1995). Inorg. Chim. Acta, 228, 133–138. Revised coordinates in space group $P4_2/m$ (no. 84), ($Z = 2$, 15.251(2) 9.821(2) Å).

Atom	x	y	z
Ni1	0.73901	0.18757	0.0
N1	0.7435	0.1010	-0.1438
N2	0.7352	0.2750	-0.1422
C1	0.7153	0.1442	-0.272
C2	0.7570	0.2332	-0.274
C3	0.7876	0.3571	-0.126
C4	0.7644	0.4068	0.0
C8	0.6966	0.0151	0.126
C9	0.7252	-0.0325	0.0
C11	0.8083	0.4978	0.0
C12	0.9075	0.4985	0.0
C13	0.9542	0.4994	0.120

Table 51S. LAKRIY Joachim, J. E., Apostolidis, C., Kanellakopulos, B., Maier, R., Marques, N., Meyer, D., Pires de Matos, ,A., Nuber, B., Rebizant, J. & Ziegler, M. L. (1993). J. Organomet. Chem. 448, 119–129.
Revised coordinates in space group P3bar; $Z = 1$ (11.522(4) 7.933(3) Å.

Atom Pair	x	y	z
Mn1,2	0.6667	0.3333	0.2730
C1,12	0.6666	0.4571	0.4008
O1,12	0.6640	0.5426	0.4832
N1,12	0.5244	0.3312	0.1118
N2,22	0.5389	0.3278	-0.0572
C4,42	0.4086	0.3296	0.1367
C5,52	0.3512	0.3251	-0.0060
C6,62	0.4331	0.3244	-0.1320
B1,2	0.6667	0.3333	-0.1260

Table 52S. LAKROE Joachim, J. E., Apostolidis, C., Kanellakopulos, B., Maier, R., Marques, N., Meyer, D., Pires de Matos, ,A., Nuber, B., Rebizant, J. & Ziegler, M. L. (1993). J. Organomet. Chem. 448, 119–129.
Revised coordinates in space group P3bar; $Z = 1$ (11.464(4) 8.091(3) Å).

Atom pair	x	y	z
Tc1,2	0.6667	0.3333	0.2790
C1,12	0.6642	0.4672	0.4124
O 1,12	0.6705	0.5533	0.4930
N1,12	0.5194	0.3313	0.1102
N2,22	0.5387	0.3271	-0.0568
C2,22	0.4016	0.3279	0.1285
C3,32	0.3453	0.3210	-0.0240
C4,42	0.4329	0.3214	-0.1405
B1,2	0.6667	0.3333	-0.1280

Table 53S. ZATGIK $In(DEHP)_3$, $C_{27}H_{42}N_3O_9In$, Ma, R., Reibenspies, J. J. & Martell, A. E. Inorg. Chim. Acta, 1994, 223, 21-29.
Revised coordinates in space group R3bar; a = 15.447(3)[3], c = 23.026(5) Å, Z = 6 units of $C_{27}H_{36}N_3O_6In$. $3H_2O$. Origin has been shifted to 0, 0, -0.460.

Atom	x	y	z
In	0.0000	0.0000	0.1668
O1	0.0940	-0.0374	0.2172
O2	0.1307	0.0518	0.1125
O5	0.5579	0.2195	0.0068
O6	0.0823	0.1748	0.0052
N1	0.3493	0.0254	0.1947
C1	0.1836	-0.0036	0.1934
C2	0.2579	-0.0119	0.2208
C3	0.3656	0.0674	0.1420
C4	0.2950	0.0752	0.1126
C5	0.2013	0.0427	0.1370
C6	0.2395	-0.0596	0.2789
C7	0.2628	0.0108	0.3280
C8	0.4323	0.0192	0.2222
C9	0.4330	-0.0739	0.2042

Table 54S. PAMCOV [Tris(ruthenium(III))(mu3-O)hexatris(mu-benzoate)tris(N-pyridine)]-(hexafluorophosphate) (Abe, M., Sasaki, Y., Yamaguchi, T. & Ito, T. (1992). Bull. Chem. Soc. Jpn., 65, 1585–1590).
Revised coordinates in space group P6(3)/m; (13.619(6) 19.204(9) Å, Z = 2)

[3] The calculated volume shows that the value of 15.477(3) Å given for b in Table 1 is a misprint.

Atom	x(P6(3)/m)	y(P6(3)/m)	z(P6(3)/m)
Ru	0.5099	0.2965	1/4
P	0	0	1/2
O1	2/3	1/3	1/4
F1,2	0.1100	0.0449	0.4525
O2,4	0.5315	0.4117	0.1772
O3,5	0.7146	0.5389	0.1761
N	0.3370	0.2559	1/4
C17	0.1131	0.2043	1/4
C15,19	0.2835	0.2437	0.1886
C16,18	0.1698	0.2180	0.1885
C1,8	0.6149	0.5022	0.1570
C2,9	0.5925	0.5718	0.1060
C3,10	0.6845	0.6678	0.0752
C4,11	0.6620	0.7312	0.0259
C5,12	0.5510	0.6992	0.0076
C6,13	0.4611	0.6051	0.0394
C7,14	0.4798	0.5394	0.0895

Category C. Add center of symmetry and systematic absences.

Table 55S. KERGET. cis-transoid-cis-Cyclobuta(1,2-a;3,4-a')di-indene C_{18} H_{16}. Shima, K., Kimura, J., Yoshida, K., Yasuda, M., Imada K. & Chyongjin Pac. (1989). Bull. Chem. Soc. Jpn., 62, 1934–1942.
Revised coordinates in $P2_1/n$. CELL 7.162 6.320 13.647Å, 97.60°.

Atom	x	y	z
C1	0.4091	0.0815	0.0482
C2	0.3932	-0.1230	-0.0170
C5	0.0008	0.1839	-0.1501
C6	-0.0668	0.0555	-0.2296
C7	0.0121	-0.1380	-0.2412
C8	0.1615	-0.2080	-0.1752
C9	0.2314	-0.0816	-0.0958
C10	0.1514	0.1168	-0.0835
C17	0.2464	0.2284	0.0062

Table 56S. LEVJUR $(C_5Me_5)Ta(S\text{–}t\text{-}Bu)_3(O\text{–}n\text{-}Bu)$; Tatsumi, K., Tahara, A. & Nakamura, A. (1994). J. Organomet. Chem. 471, 111–115.
Revised coordinates in space group is *P*2/*c*; CELL 9.134 12.078 27.740 Å, 92.39°.

Atom Pair	x	y	z
Ta1,2	0.13368	0.23852	0.62278
S1,4	0.1434	0.0368	0.6376
S2,5	0.2901	0.1695	0.5600
S3,6	0.2428	0.4226	0.6136
O1,2	0.1744	0.2543	0.6894
C1,27	-0.062	0.3492	0.5780
C2,28	-0.099	0.3361	0.6309
C3,29	-0.128	0.2220	0.6384
C4,30	-0.112	0.1658	0.5944
C5,31	-0.070	0.2454	0.5575
C6,32	-0.051	0.455	0.5541
C7,33	-0.112	0.429	0.6654
C8,34	-0.172	0.170	0.6810
C9,35	-0.162	0.050	0.5819
C10,36	-0.060	0.222	0.5063
C11,41	0.320	-0.036	0.6514
C12,40	0.352	-0.104	0.6104
C13,39	0.294	-0.110	0.6932
C14,38	0.449	0.044	0.6637
C15,41	0.403	0.255	0.5198
C16,42	0.314	0.344	0.4938
C17,44	0.530	0.303	0.5457
C18,43	0.454	0.170	0.4813
C19,45	0.380	0.462	0.6606
C20,48	0.486	0.366	0.6768
C21,47	0.302	0.508	0.7034
C22,46	0.468	0.557	0.6392
C23,49	0.190	0.198	0.7358
C24,50	0.133	0.262	0.7746
C25,51	0.152	0.196	0.8244
C26,52	0.114	0.256	0.8642

Table 57S. ZEDDAN Tetra-t-butylbenzenetetracarboxylate (Yasuda, M., Kuwamura, G., Nakazono, T., Shima, K., Inoue, Y., Yamasaki, N. & Tai, A. (1994). Bull. Chem. Soc. Jpn. 67, 505-510).
Revised coordinates in space group P2(1)/c. $Z = 2$, (11.696(3) 10.450(5) 11.176(5) Å, 95.14(2)°).

Atom	x(P2(1)/c)Avg	y(P2(1)/c)Avg	z(P2(1)/c)Avg
O1,5	0.1773	-0.0462	-0.2527
O2,6	0.2638	0.0946	-0.1204
O3,7	-0.0172	-0.2800	-0.2037
O4,8	0.1553	-0.2680	-0.0949
C1,4	0.0898	0.0051	-0.0743
C2,5	0.0251	-0.1058	-0.0684
C3,6	-0.0649	-0.1107	0.0053
C7,17	0.1809	0.0135	-0.1607
C8,18	0.3617	0.1200	-0.1918
C9,21	0.3181	0.1841	-0.3095
C10,19	0.4324	0.2131	-0.1123
C11,20	0.4270	-0.0008	-0.2085
C12,22	0.0506	-0.2274	-0.1339
C13,23	0.2040	-0.3883	-0.1393
C14,26	0.2133	-0.3779	-0.2732
C15,25	0.3212	-0.3903	-0.0700
C16,24	0.1310	-0.5005	-0.1053

Table 58S. CADKUN. (N,N'-dibenzyl-4-methyl-4-azaheptane-1,7-diamine)-(dimethylformamide)$(BF_4)_2$; $PdF_8ON_4C_{24}B_2H_{38}$; (Yagyu, Aizawa & Funahashi, 1998).
Revised coordinates in space group $P2_1/n$, , ($Z = 4$; 21.173(4) 13.096(2) 10.826(2) Å, 102.07(1)°).

Atom	x	y	z
Pd1,2	0.12471	0.24652	0.35544
O1,2	0.1727	0.3029	0.5230
N1,5	0.0471	0.2511	0.4435
C22,46	0.2125	0.0075	0.6090
N4,8	0.2377	0.3064	0.7145
C23,47	0.2151	0.4055	0.7465
C24.48	0.2832	0.2535	0.8130
N2,6	0.0718	0.2092	0.1785
N3,7	0.2146	0.2530	0.3045
C11,35	0.0510	0.3077	0.1095
C1,25	0.0054	0.3863	0.6660
C2,26	-0.0365	0.4054	0.7490
C3,27	-0.1026	0.4186	0.7025

C4,28	-0.1253	0.4115	0.5715
C5,29	-0.0849	0.3911	0.4895
C6,30	-0.0200	0.3774	0.5355
C7,31	0.0254	0.3605	0.4455
C8,32	-0.0081	0.1804	0.3985
C9,33	-0.0332	0.1864	0.2584
C10,34	0.0121	0.1472	0.1810
C14,38	0.2240	0.1834	0.2015
C13,37	0.1722	0.1885	0.0835
C12,36	0.1072	0.1464	0.1025
C15,39	0.2290	0.3617	0.2810
C16,40	0.2953	0.3770	0.2495
C17,45	0.2990	0.4206	0.1350
C18,44	0.3569	0.4355	0.0910
C19,43	0.4132	0.4010	0.1755
C20,42	0.4108	0.3575	0.2975
C21,41	0.3505	0. 3466	0.3295
B3	0.6084	0.4107	0.243
B2	0.1414	0.5810	-0.045
F11	0.5744	0.4488	0.320
F12	0.5886	0.4475	0.131
F9	0.6692	.4295	0.285
F10	0.6038	0.3094	0.244
F5	0.1976	0.6221	0.010
F6	0.1313	0.5848	-0.172
F7	0.0918	0.6350	-0.016
F8	0.1392	0.4839	-0.002

Table 59S. KUSLOZ. Bis(2-(dimethylphosphino)ethane-1-thiolato)Ni(II). $C_8H_{20}NiP_2S_2$. (Kita, M., Yamamoto, T., Kashiwabara, K. & Fujita, J. Bull. Chem. Soc. Jpn. 65, 2272–2274).
Revised coordinates in space group P2(1)/n. CELL 5.897 10.578 10.895 Å, 92.83°.

Atom Pair	x	y	z
Ni	0.0	0.0	0.0
S1,2	0.0560	-0.0614	0.1898
P1,2	-0.1474	0.1732	0.0661
C1,5	-0.4553	0.1776	0.0532
C2,6	-0.0638	0.3248	0.0022
C3,7	-0.0732	0.1877	0.2301
C4,8	-0.0894	0.0548	0.2830

Table 60S. TOSSAV (Aizawa, S., Natsume, T., Hatano, K. & Funahashi, S. (1996). Inorg. Chim. Acta 248, 215–224.
Revised coordinates in space group P2(1)/c, , Z = 4 (cell dimensions 18.377(4) 7.563(2) 15.642(4) Å, 92.923 (9)°).

Atom	x	y	z
Sn1	0.09801	0.0996	-0.06740
Sn2	0.39984	-0.1362	0.03152
O1	0.0461	0.0815	0.0682
O2	0.0318	0.2275	0.1894
O3	0.1902	0.2005	-0.1306
O4	0.2783	0.4010	-0.1340
O5	0.4700	0.1145	0.0662
O6	0.5080	0.2910	0.1738
O7	0.3030	-0.2740	0.0626
O8	0.2292	-0.3540	0.1630
O17	0.0716	0.0135	-0.2053
O18	0.3945	-0.3905	-0.0608
O21	-0.1310	0.1270	-0.2360
N1	0.1772	0.2400	0.0396
N2	0.3480	0.0190	0.1486
C1	0.1285	-0.1680	-0.0490
C2	0.0292	0.3215	-0.0899
C3	0.0662	0.1950	0.1238
C4	0.1337	0.3045	0.1122
C5	0.2290	0.3270	-0.0980
C6	0.2120	0.3850	-0.0073
C7	0.2301	0.1010	0.0676
C8	0.2968	0.1645	0.1230
C9	0.3613	-0.0020	-0.0793
C10	0.4729	-0.2935	0.1075
C11	0.4670	0.1770	0.1432
C12	0.4104	0.0960	0.1992
C13	0.2777	-0.2585	0.1370
C14	0.3116	-0.1220	0.1967

Table 61S. VOZVIP 6-Methyl-4-(morpholinomethyl)-2H-1-benzothiopyran-2-one C15 H17 N1 O2 S1 (Nakazumi, H., Kobara, Y. & Kitao, T. (1992). J. Heterocycl. Chem., 29, 135–139).
Revised coordinates in space group P2(1)/c. CELL 11.336 16.871 7.287 Å, 80.748°.

Atom	x	y	z
S1	0.0682	-0.1849	0.2276
C1	0.0495	-0.0815	0.2360
C2	-0.0660	-0.0498	0.3180
C3	-0.1640	-0.0916	0.3890
C4	-0.1710	-0.1782	0.3900
C5	-0.2765	-0.2181	0.4605
C6	-0.2840	-0.3002	0.4600
C7	-0.1830	-0.3440	0.3910
C8	-0.0770	-0.3070	0.3215
C9	-0.0715	-0.2242	0.3200
O1	0.1351	-0.0405	0.1720
C10	-0.2750	-0.0460	0.4800
N1	-0.2726	0.0380	0.4250
C11	-0.3080	0.0478	0.2440
C12	-0.3075	0.1356	0.1925
O2	-0.3840	0.1793	0.3285
C13	-0.3470	0.1706	0.5040
C14	-0.3495	0.0844	0.5718
C15	-0.4010	-0.3403	0.5315

Table 62S. NALCIM (μ^2-α,α'-bis((Di-2-pyridyl)methylamino)-*m*-xylene)-bis(μ^2-hydroxo)-(μ^2-perchlorato-O,O')-di-copper(ii) perchlorate monohydrate $[C_{30}H_{26}ClCu_2N_6O_6]^+[ClO_4]^-\cdot H_2O$. Garcia, A. M., Manzur, J., Garland, M. T., Baggio, R., Gonzalez, O., Pena, O. & Spodine, E. (1996). Inorg. Chim. Acta, 248, 247–255, Revised coordinates in space group *Pnma*. CELL 16.763 14.188 14.275Å.

Atom	x	y	z
Cu1	0.7220	0.3517	0.3882
O1	0.6515	0.25	0.3599
O2	0.7915	0.25	0.4267
O3	0.0859	0.75	0.4074
N1	0.7962	0.4550	0.4282
N2	0.6406	0.4520	0.3556
N5	0.7700	0.4293	0.2400
C1	0.8391	0.4546	0.5072
C2	0.8887	0.5278	0.5330
C3	0.8958	0.6024	0.4724

C4	0.8532	0.6038	0.3896
C5	0.8037	0.5288	0.3695
C6	0.7544	0.5225	0.2817
C7	0.6669	0.5254	0.3047
C8	0.6159	0.5954	0.2750
C9	0.5369	0.5910	0.2996
C10	0.5104	0.5164	0.3530
C11	0.5630	0.4469	0.3798
C23	0.7962	0.4247	0.1564
C24	0.8134	0.3346	0.1102
C25	0.8508	0.3338	0.0238
C26	0.8707	0.25	-0.0188
C30	0.7938	0.25	0.1513
75% perchlorate			
Cl1	0.6717	0.25	0.6277
O4	0.7508	0.25	0.6643
O7	0.6152	0.25	0.7029
O56	0.6600	0.1676	0.5720
25% perchlorate			
Cl1A	0.6494	0.25	0.6138
O4 A	0.7244	0.25	0.6581
O7A	0.5908	0.25	0.6844
O56A	0.6415	0.1699	0.6573
Other perchlorate			
Cl3 (100%)	1.0054	-0.25	0.6763
60% oxygens			
O19	0.9215	-0.25	0.6635
O17	1.0261	-0.25	0.7692
O168	1.0368	-0.1733	0.6364
40% oxygens			
O19A	1.0309	-0.25	0.5804
O17A	0.9254	-0.25	0.6820
O168A	1.0324	-0.1743	0.7192

Table 63S. DIXVOV. Trichloro-bis(3-methylimidazole-2-thione-S)Sb(III) (Berges, P., Hinrichs, W., Kopf, J., Mandak, D. & Klar, G. (1985). J. Chem. Res. (S), 218--219.

Revised coordinates in space group *Pbca*, $Z = 4$, 9.738(2) 23.630(7) 13.584(4) Å, Note that the s.u.s of the coordinates were obtained from a least squares refinement in

the revised space group *Pbca* using the intensities measured in the original structure determination.

Atom	x	y	z
Sb	10314(1)	48869(2)	51680(3)
Cl1	11773(7)	33423(10)	38816(17)
Cl2	17003(7)	43506(11)	71749(15)
CL3	9484(6)	68289(10)	60508(15)
S1	18787(6)	53333(10)	37195(15)
N11	17797(18)	73251(35)	33308(47)
N12	23990(17)	69427(31)	48829(47)
C11	20164(21)	65681(39)	40168(55)
C12	23983(26)	79577(41)	47373(72)
C13	20170(28)	81824(45)	37854(76)
C14	27867(28)	63859(54)	57469(66)
S2	2843(7)	55673(11)	31646(15)
N21	516(21)	38157(38)	19125(50)
N22	6464(18)	46916(34)	7996(45)
C21	3321(21)	46914(40)	19292(56)
C22	5760(25)	38348(42)	634(65)
C23	2032(28)	32873(45)	7884(69)
C24	10170(29)	54746(41)	3953(62)