Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters for non-*H *atoms*

$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	y	z	U_{eq}(Å^2)
Fe	0·2604 (1)	0·23211 (6)	0·42096 (7)	0·048
B	0·6478 (8)	0·1967 (5)	0·4816 (5)	0·035
C(11)	0·6388 (6)	0·1535 (5)	0·3837 (4)	0·038
C(12)	0·6773 (7)	0·1989 (5)	0·3150 (6)	0·049
C(13)	0·6778 (8)	0·1607 (6)	0·2337 (6)	0·060
C(14)	0·6410 (8)	0·0758 (7)	0·2156 (5)	0·059
C(15)	0·6028 (8)	0·0277 (5)	0·2810 (6)	0·062
C(16)	0·6036 (7)	0·0660 (5)	0·3624 (5)	0·052
C(21)	0·7203 (8)	0·2929 (4)	0·4930 (5)	0·039
C(22)	0·8530 (8)	0·3138 (5)	0·5573 (5)	0·042
C(23)	0·9104 (7)	0·3964 (6)	0·5680 (5)	0·051
C(24)	0·837 (1)	0·4646 (5)	0·5149 (6)	0·062
C(25)	0·7059 (9)	0·4469 (5)	0·4504 (5)	0·055
C(26)	0·6520 (8)	0·3635 (6)	0·4402 (5)	0·050
C(31)	0·7447 (7)	0·1314 (4)	0·5621 (5)	0·037
C(32)	0·7136 (7)	0·1133 (5)	0·6429 (5)	0·046
C(33)	0·806 (1)	0·0621 (5)	0·7109 (5)	0·051
C(34)	0·9352 (9)	0·0314 (5)	0·6996 (5)	0·048
C(35)	0·9702 (7)	0·0476 (5)	0·6213 (6)	0·051
C(36)	0·8750 (8)	0·0978 (5)	0·5529 (4)	0·040
C(41)	0·4826 (7)	0·2024 (5)	0·4982 (4)	0·035
C(42)	0·3858 (8)	0·1295 (4)	0·4860 (4)	0·040
C(43)	0·2530 (8)	0·1304 (5)	0·5065 (5)	0·053
C(44)	0·2065 (8)	0·2066 (7)	0·5395 (5)	0·069
C(45)	0·2935 (9)	0·2810 (5)	0·5514 (5)	0·061
C(46)	0·4297 (7)	0·2786 (5)	0·5302 (4)	0·042
C(51)	0·201 (1)	0·1902 (6)	0·2894 (5)	0·071
C(52)	0·073 (1)	0·2084 (9)	0·3155 (7)	0·086
C(53)	0·082 (1)	0·2972 (8)	0·3406 (7)	0·083
C(54)	0·211 (1)	0·3318 (6)	0·3306 (7)	0·075
C(55)	0·2847 (9)	0·2667 (9)	0·2979 (5)	0·073

C—C distances [1·40 (1) Å] is also found. The C—C bond distances average 1·39 (1) Å in the other three phenyl rings.

The Fe atom is 1·537 Å from the plane defined by atoms C(41)–C(46). The angle between the planes defined by the cyclopentadienyl and phenyl rings is 2·28°. Both rings are planar to within 0·013 Å.

Table 2. *Selected interatomic distances* (Å)

Fe—C(41)	2·156 (6)	Fe—C(51)	2·042 (8)
Fe—C(42)	2·060 (6)	Fe—C(52)	2·064 (8)
Fe—C(43)	2·062 (7)	Fe—C(53)	2·050 (8)
Fe—C(44)	2·072 (7)	Fe—C(54)	2·035 (8)
Fe—C(45)	2·081 (7)	Fe—C(55)	2·045 (8)
Fe—C(46)	2·090 (6)		
Fe—Cent4*	1·537	Fe—Cent5	1·660
B—C(11)	1·63 (1)	B—C(21)	1·63 (1)
B—C(31)	1·65 (1)	B—C(41)	1·67 (1)

* Cent4 is the centroid of the plane defined by atoms C(41)–C(46), Cent5 by atoms C(51)–C(55).

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Tris(2,6-dimethyl-4*H*-pyran-4-one)dinitratocadmium(II), $[Cd(NO_3)_2(C_7H_8O_2)_3]$

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Abstract. $M_r = 608·8$, monoclinic, $P2_1/n$, $a = 19·372\ (5)$, $b = 11·345\ (4)$, $c = 23·023\ (5)$ Å, $\beta = 93·77\ (5)°$, $V = 5048·9$ Å^3, $Z = 8$, $D_m = 1·60\ (1)$, $D_x = 1·602$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 0·93$ mm^{-1}, $F(000) = 2464$, $T = 293$ K, $R = 0·061$ for 7325 observed reflexions ($I > \sigma I$). The structure comprises two discrete non-equivalent molecules in each of which cadmium is seven-coordinated, to three oxygen atoms of the dimethyl-4-pyrone ligands, and bidentately to four oxygen atoms of two nitrato groups. The pyrone rings are planar and there are no strong intermolecular interactions.

0108-2701/84/071161-04$01.50

Introduction. The material was originally prepared by Drs E. Briggs and A. E. Hill of the Chemistry Department in the City of London Polytechnic (Hill, 1971) as part of a research project to investigate the protective properties of compounds of this class against the corrosion of steel. The molecular formula and the atomic numbering used are shown in Fig. 1.

Experimental. Equidimensional crystals (*ca* 0·2 mm) by reacting hot solutions of cadmium nitrate and 2,6-dimethyl-4-pyrone in 2,2-dimethoxypropane and cooling during addition of ethyl acetate, density by flotation in carbon tetrachloride/methylene bromide, lattice parameters initially from zero-level Weissenberg photographs and refined on the diffractometer, 7438 measured reflexions of which 113 considered unobserved; absences $0k0$ for k odd and $h0l$ for $h + l$ odd, intensities on an Enraf–Nonius CAD-4 diffractometer at Queen Mary College with crystal enclosed in sealed glass tube, corrections made for Lp effects and for fading (maximum 8%; 3 standard reflections monitored) owing to deterioration of crystals, but not for absorption or extinction, index range h 0 to 21, k 0 to 12, l 0 to ± 25, $2\theta_{\max} = 120°$; structure solved from Patterson and successive Fourier syntheses; refinement on F by least squares using initially $B_{\rm iso}$ and $w^{1/2} = 1/F_o$, and finally B_{ij} until all shifts were $< 0·1\sigma$, approximate H positions determined from difference syntheses but included in structure factor calculations in idealized positions with $B_{\rm iso} = 5·0$ Å^2 without refining, $\Delta\rho$ in final difference synthesis generally within $\pm 0·4$ e Å^{-3} but down to $-0·9$ e Å^{-3} in regions around Cd atoms, $R_w = 0·16$, scattering factors from *International Tables for X-ray Crystallography* (1962), computer programs of the *NRC* series (Ahmed, Hall, Pippy & Huber, 1970) used on our DEC-10 computer.

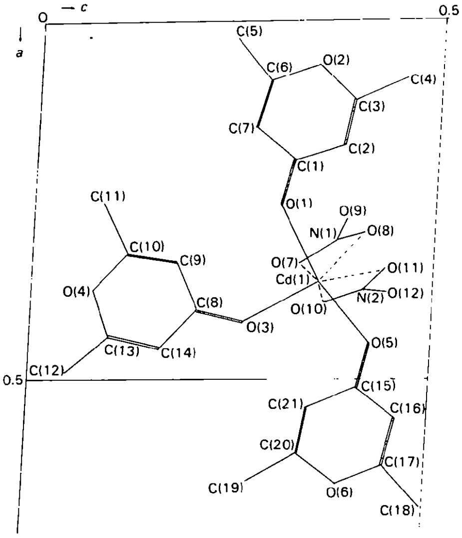

Fig. 1. Projection of part of the unit cell on (010) showing one of the molecules and the atomic numbering used. Atoms of the second molecule are numbered C(n + 21), N(n + 2), O(n + 12).

Table 1. *Final atomic parameters and e.s.d.'s*

$$B_{\rm eq} = \tfrac{4}{3}\left(\frac{\beta_{11}}{a^{*2}} + \frac{\beta_{22}}{b^{*2}} + \frac{\beta_{33}}{c^{*2}}\right).$$

	x	y	z	$B_{\rm eq}$(Å^2)
Cd(1)	0·38279 (2)	0·37833 (3)	0·35515 (1)	3·08 (1)
Cd(2)	0·36140 (2)	0·08814 (3)	0·84911 (1)	3·40 (1)
C(1)	0·2175 (2)	0·2964 (4)	0·3313 (2)	2·59 (8)
C(2)	0·2013 (3)	0·2889 (5)	0·3905 (2)	3·43 (9)
C(3)	0·1385 (3)	0·2506 (5)	0·4035 (2)	3·62 (8)
C(4)	0·1133 (4)	0·2377 (8)	0·4640 (2)	5·81 (13)
C(5)	0·0439 (3)	0·1839 (7)	0·2664 (3)	4·66 (11)
C(6)	0·1051 (2)	0·2250 (4)	0·3052 (2)	2·87 (8)
C(7)	0·1664 (3)	0·2604 (4)	0·2873 (2)	3·48 (8)
C(8)	0·4089 (3)	0·3751 (5)	0·2133 (2)	4·14 (9)
C(9)	0·3410 (3)	0·4117 (5)	0·1923 (2)	4·07 (10)
C(10)	0·3235 (3)	0·4283 (4)	0·1351 (2)	3·75 (9)
C(11)	0·2532 (3)	0·4651 (6)	0·1095 (3)	5·18 (11)
C(12)	0·4779 (4)	0·3592 (8)	0·0598 (3)	7·94 (13)
C(13)	0·4356 (4)	0·3739 (5)	0·1118 (2)	4·23 (10)
C(14)	0·4556 (3)	0·3589 (5)	0·1682 (2)	3·53 (8)
C(15)	0·5312 (2)	0·4966 (5)	0·3960 (2)	3·22 (8)
C(16)	0·5783 (3)	0·5446 (5)	0·4402 (2)	4·10 (8)
C(17)	0·6399 (3)	0·5854 (5)	0·4255 (3)	4·35 (10)
C(18)	0·6967 (3)	0·6387 (6)	0·4649 (3)	4·59 (11)
C(19)	0·6440 (4)	0·5548 (7)	0·2668 (3)	6·16 (13)
C(20)	0·6144 (3)	0·5469 (5)	0·3260 (2)	4·15 (9)
C(21)	0·5531 (3)	0·5006 (4)	0·3378 (2)	3·40 (8)
C(22)	0·2224 (2)	0·1895 (4)	0·9056 (2)	2·99 (7)
C(23)	0·1811 (3)	0·2095 (5)	0·9537 (2)	4·09 (9)
C(24)	0·1183 (3)	0·2598 (6)	0·9476 (2)	5·07 (11)
C(25)	0·0709 (5)	0·2874 (8)	0·9946 (3)	7·08 (15)
C(26)	0·0907 (4)	0·3155 (7)	0·7899 (3)	5·35 (14)
C(27)	0·1282 (3)	0·2747 (4)	0·8456 (2)	3·46 (8)
C(28)	0·1908 (3)	0·2237 (4)	0·8507 (2)	4·12 (8)
C(29)	0·3126 (3)	0·0988 (6)	0·7078 (2)	4·18 (9)
C(30)	0·2608 (3)	0·0627 (6)	0·6650 (2)	4·26 (10)
C(31)	0·2732 (3)	0·0474 (5)	0·6091 (2)	4·16 (9)
C(32)	0·2242 (5)	0·0080 (8)	0·5596 (3)	7·37 (17)
C(33)	0·4541 (4)	0·1190 (8)	0·5968 (3)	7·86 (15)
C(34)	0·3900 (4)	0·1038 (5)	0·6299 (3)	4·75 (11)
C(35)	0·3783 (4)	0·1213 (6)	0·6862 (2)	5·27 (11)
C(36)	0·5181 (2)	−0·0011 (4)	0·8232 (2)	2·99 (8)
C(37)	0·5418 (2)	−0·0183 (5)	0·8830 (2)	3·97 (9)
C(38)	0·6055 (3)	−0·0573 (4)	0·8994 (2)	3·52 (8)
C(39)	0·6353 (3)	−0·0768 (7)	0·9610 (2)	4·96 (11)
C(40)	0·6875 (4)	−0·1086 (6)	0·7642 (3)	4·70 (11)
C(41)	0·6310 (2)	−0·0732 (4)	0·8018 (2)	2·91 (8)
C(42)	0·5680 (3)	−0·0335 (5)	0·7837 (2)	3·94 (9)
N(1)	0·3291 (3)	0·6013 (4)	0·3776 (2)	3·30 (8)
N(2)	0·4014 (3)	0·1562 (4)	0·4076 (2)	4·38 (9)
N(3)	0·3540 (3)	−0·1540 (5)	0·8726 (3)	5·13 (11)
N(4)	0·4250 (3)	0·2940 (4)	0·8937 (2)	4·06 (9)
O(1)	0·2760 (2)	0·3304 (3)	0·3144 (2)	3·72 (6)
O(2)	0·0895 (2)	0·2176 (3)	0·3616 (1)	3·46 (6)
O(3)	0·4283 (2)	0·3599 (4)	0·2664 (2)	5·03 (8)
O(4)	0·3695 (2)	0·4082 (4)	0·0944 (2)	4·37 (7)
O(5)	0·4739 (2)	0·4574 (4)	0·4106 (2)	4·80 (7)
O(6)	0·6592 (2)	0·5884 (3)	0·3698 (2)	3·68 (7)
O(7)	0·3572 (3)	0·5771 (4)	0·3329 (2)	5·87 (8)
O(8)	0·3224 (2)	0·5224 (4)	0·4123 (2)	4·99 (8)
O(9)	0·3096 (4)	0·7009 (5)	0·3869 (3)	7·06 (13)
O(10)	0·4183 (3)	0·1738 (4)	0·3582 (2)	6·04 (10)
O(11)	0·3743 (3)	0·2399 (4)	0·4321 (2)	6·24 (9)
O(12)	0·4077 (3)	0·0628 (5)	0·4332 (3)	6·95 (12)
O(13)	0·2808 (2)	0·1415 (4)	0·9111 (2)	4·18 (7)
O(14)	0·0926 (2)	0·2927 (3)	0·8941 (2)	3·90 (7)
O(15)	0·3029 (2)	0·1162 (4)	0·7609 (2)	4·91 (8)
O(16)	0·3376 (3)	0·0668 (4)	0·5922 (2)	5·46 (9)
O(17)	0·4596 (2)	0·0348 (4)	0·8057 (2)	4·86 (7)
O(18)	0·6498 (2)	−0·0870 (3)	0·8588 (2)	3·94 (6)
O(19)	0·3254 (3)	−0·1125 (5)	0·8292 (2)	5·39 (10)
O(20)	0·3588 (4)	−0·2600 (5)	0·8842 (3)	7·60 (13)
O(21)	0·3814 (2)	−0·0840 (4)	0·9084 (2)	4·43 (8)
O(22)	0·3900 (3)	0·2900 (5)	0·8478 (2)	6·15 (10)
O(23)	0·4354 (2)	0·2025 (4)	0·9205 (2)	4·70 (8)
O(24)	0·4459 (4)	0·3889 (5)	0·9108 (3)	7·71 (13)

Table 2. *Bond lengths* (Å) *and selected inter-bond angles* (°)

Angles subtended at Cd(1) and Cd(2) have been deposited (see deposition footnote).

Cd(1)–O(1)	2·281 (4)	Cd(2)–O(13)	2·267 (4)
Cd(1)–O(3)	2·287 (4)	Cd(2)–O(15)	2·282 (4)
Cd(1)–O(5)	2·292 (4)	Cd(2)–O(17)	2·287 (4)
Cd(1)–O(7)	2·357 (4)	Cd(2)–O(19)	2·416 (5)
Cd(1)–O(8)	2·444 (4)	Cd(2)–O(21)	2·400 (4)
Cd(1)–O(10)	2·420 (5)	Cd(2)–O(22)	2·357 (6)
Cd(1)–O(11)	2·382 (5)	Cd(2)–O(23)	2·476 (4)
O(1)–C(1)	1·280 (6)	O(13)–C(22)	1·254 (6)
C(1)–C(2)	1·421 (6)	C(22)–C(23)	1·427 (7)
C(1)–C(7)	1·429 (7)	C(22)–C(28)	1·420 (6)
C(2)–C(3)	1·343 (7)	C(23)–C(24)	1·343 (9)
C(3)–C(4)	1·514 (8)	C(24)–C(25)	1·497 (10)
C(3)–O(2)	1·362 (6)	C(24)–O(14)	1·351 (7)
O(2)–C(6)	1·355 (5)	O(14)–C(27)	1·365 (6)
C(5)–C(6)	1·511 (8)	C(26)–C(27)	1·504 (8)
C(6)–C(7)	1·343 (7)	C(27)–C(28)	1·343 (7)
O(3)–C(8)	1·268 (6)	O(15)–C(29)	1·264 (6)
C(8)–C(9)	1·433 (9)	C(29)–C(30)	1·421 (8)
C(8)–C(14)	1·434 (7)	C(29)–C(35)	1·420 (9)
C(9)–C(10)	1·350 (7)	C(30)–C(31)	1·336 (7)
C(10)–C(11)	1·508 (8)	C(31)–C(32)	1·502 (10)
C(10)–O(4)	1·354 (7)	C(31)–O(16)	1·349 (8)
O(4)–C(13)	1·371 (8)	O(16)–C(34)	1·358 (9)
C(12)–C(13)	1·504 (10)	C(33)–C(34)	1·510 (11)
C(13)–C(14)	1·341 (7)	C(34)–C(35)	1·346 (9)
O(5)–C(15)	1·261 (6)	O(17)–C(36)	1·247 (6)
C(15)–C(16)	1·430 (7)	C(36)–C(37)	1·435 (7)
C(15)–C(21)	1·432 (7)	C(36)–C(42)	1·419 (7)
C(16)–C(17)	1·342 (8)	C(37)–C(38)	1·343 (7)
C(17)–C(18)	1·508 (9)	C(38)–C(39)	1·513 (7)
C(17)–O(6)	1·360 (8)	C(38)–O(18)	1·352 (6)
O(6)–C(20)	1·370 (7)	O(18)–C(41)	1·347 (6)
C(19)–C(20)	1·516 (9)	C(40)–C(41)	1·494 (8)
C(20)–C(21)	1·343 (8)	C(41)–C(42)	1·342 (7)
N(1)–O(7)	1·226 (7)	N(3)–O(19)	1·206 (8)
N(1)–O(8)	1·213 (6)	N(3)–O(20)	1·234 (8)
N(1)–O(9)	1·215 (8)	N(3)–O(21)	1·239 (7)
N(2)–O(10)	1·220 (7)	N(4)–O(22)	1·217 (7)
N(2)–O(11)	1·239 (7)	N(4)–O(23)	1·218 (6)
N(2)–O(12)	1·215 (8)	N(4)–O(24)	1·208 (8)

Cd(1)–O(1)–C(1)	138·1 (3)	Cd(2)–O(13)–C(22)	134·9 (3)
Cd(1)–O(3)–C(8)	137·9 (4)	Cd(2)–O(15)–C(29)	137·9 (4)
Cd(1)–O(5)–C(15)	130·4 (3)	Cd(2)–O(17)–C(36)	135·2 (3)
C(2)–C(1)–C(7)	118·4 (4)	C(23)–C(22)–C(28)	114·6 (4)
C(2)–C(1)–O(1)	124·4 (4)	C(23)–C(22)–O(13)	122·5 (5)
C(7)–C(1)–O(1)	117·1 (4)	C(28)–C(22)–O(13)	122·8 (4)
C(1)–C(2)–C(3)	119·6 (5)	C(22)–C(23)–C(24)	122·4 (5)
C(2)–C(3)–C(4)	126·1 (5)	C(23)–C(24)–C(25)	127·4 (6)
C(2)–C(3)–O(2)	122·0 (5)	C(23)–C(24)–O(14)	119·3 (5)
C(4)–C(3)–O(2)	111·9 (5)	C(25)–C(24)–O(14)	113·3 (5)
C(3)–O(2)–C(6)	118·2 (4)	C(24)–O(14)–C(27)	122·0 (4)
C(5)–C(6)–C(7)	125·9 (5)	C(26)–C(27)–C(28)	126·2 (5)
C(5)–C(6)–O(2)	109·3 (4)	C(26)–C(27)–O(14)	114·2 (5)
C(7)–C(6)–O(2)	124·7 (4)	C(28)–C(27)–O(14)	119·6 (4)
C(1)–C(7)–C(6)	116·9 (4)	C(22)–C(28)–C(27)	122·0 (4)
C(9)–C(8)–C(14)	113·7 (5)	C(30)–C(29)–C(35)	114·7 (5)
C(9)–C(8)–O(3)	124·9 (5)	C(30)–C(29)–O(15)	125·0 (5)
C(14)–C(8)–O(3)	121·3 (5)	C(35)–C(29)–O(15)	120·2 (5)
C(8)–C(9)–C(10)	122·3 (5)	C(29)–C(30)–C(31)	122·9 (6)
C(9)–C(10)–C(11)	125·6 (5)	C(30)–C(31)–C(32)	128·6 (6)
C(9)–C(10)–O(4)	121·1 (5)	C(30)–C(31)–O(16)	119·0 (5)
C(11)–C(10)–O(4)	113·3 (5)	C(32)–C(31)–O(16)	112·4 (5)
C(10)–O(4)–C(13)	119·4 (4)	C(31)–O(16)–C(34)	122·1 (5)
C(12)–C(13)–C(14)	128·2 (6)	C(33)–C(34)–C(35)	131·7 (7)
C(12)–C(13)–O(4)	110·3 (5)	C(33)–C(34)–O(16)	108·5 (6)
C(14)–C(13)–O(4)	121·6 (5)	C(35)–C(34)–O(16)	119·8 (6)
C(8)–C(14)–C(13)	121·9 (5)	C(29)–C(35)–C(34)	121·4 (6)
C(16)–C(15)–C(21)	116·1 (4)	C(37)–C(36)–C(42)	113·1 (4)
C(16)–C(15)–O(5)	118·4 (5)	C(37)–C(36)–O(17)	125·5 (5)
C(21)–C(15)–O(5)	125·5 (5)	C(42)–C(36)–O(17)	121·4 (4)
C(15)–C(16)–C(17)	119·2 (5)	C(36)–C(37)–C(38)	122·9 (5)
C(16)–C(17)–C(18)	127·8 (6)	C(37)–C(38)–C(39)	126·7 (5)
C(16)–C(17)–O(6)	123·5 (5)	C(37)–C(38)–O(18)	120·2 (5)
C(18)–C(17)–O(6)	108·8 (5)	C(39)–C(38)–O(18)	113·0 (4)
C(17)–O(6)–C(20)	118·9 (4)	C(38)–O(18)–C(41)	120·0 (4)
C(19)–C(20)–C(21)	126·6 (5)	C(40)–C(41)–C(42)	126·6 (5)
C(19)–C(20)–O(6)	112·5 (5)	C(40)–C(41)–O(18)	111·8 (4)
C(21)–C(20)–O(6)	120·8 (5)	C(42)–C(41)–O(18)	121·6 (4)
C(15)–C(21)–C(20)	121·4 (5)	C(36)–C(42)–C(41)	122·1 (5)
O(7)–N(1)–O(8)	117·4 (5)	O(19)–N(3)–O(20)	125·7 (6)
O(7)–N(1)–O(9)	121·1 (6)	O(19)–N(3)–O(21)	117·1 (6)

Table 2 (*cont.*)

O(8)–N(1)–O(9)	121·5 (5)	O(20)–N(3)–O(21)	117·2 (6)
O(10)–N(2)–O(11)	116·6 (5)	O(22)–N(4)–O(23)	118·2 (5)
O(10)–N(2)–O(12)	124·7 (6)	O(22)–N(4)–O(24)	118·2 (6)
O(11)–N(2)–O(12)	118·7 (6)	O(23)–N(4)–O(24)	123·6 (6)

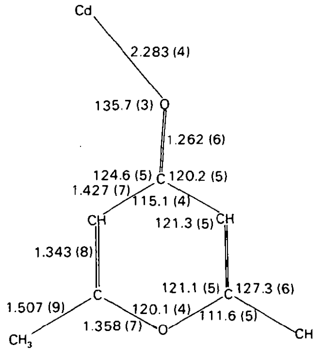

Fig. 2. 2,6-Dimethyl-4-pyrone ring showing averaged bond lengths (Å) and angles (°).

Discussion. The final atomic coordinates and equivalent isotropic temperature parameters are given in Table 1.* Bond lengths and inter-bond angles are given in Table 2.

Although prepared in the same way as the copper and zinc compounds, this cadmium compound is different in composition, probably because of the greater size of the Cd atom. Three 2,6-dimethyl-4-pyrone ligands coordinate to the metal instead of two, and the two nitrato groups are bidentate in coordination whereas in the Cu and Zn compounds they are unidentate (Brown & Lewis, 1984*a*,*b*). These differences confer seven-coordination on the Cd whereas the Cu and Zn are both four-coordinated. Seven O atoms lie at the corners of a slightly distorted pentagonal bipyramid around each of the two Cd atoms (Fig. 1), in each of which four nitrato O atoms and one 4-pyrone O atom form the equatorial plane and the two other 4-pyrone O atoms lie at the apices. The mean Cd—O distance for the 2,6-dimethyl-4-pyrone ligands is 2·283 (4) Å, while the distance for the nitrato oxygens is 2·406 (5) Å.

The six 4-pyrone rings are each closely planar, the r.m.s. deviation being 0·009 Å, with the maximum 0·018 (6) Å. The substituent oxygen and two methyl carbon atoms also lie in the plane of the rings. Mean dimensions are shown in Fig. 2. The four nitrate groups are also planar, the N atoms lying 0·006 (5), 0·011 (6),

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, angles subtended at Cd(1) and Cd(2) and least-squares-planes' information have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39356 (47 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0·002 (6) and 0·012 (5) Å out of the planes of the O atoms.

A similar structural arrangement to this has been observed in dinitratotris(pyridine)Cd^{II} (Cameron, Taylor & Nuttall, 1972) and also in aquadinitratobis(quinoline)Cd^{II} (Cameron, Taylor & Nuttall, 1973). The only structural results for 2,6-dimethyl-4-pyrone compounds are for the hydrobromide monohydrate (Hope, 1965) determined with limited X-ray data, dinitratobis(2,6-dimethyl-4-pyrone)zinc (Brown & Lewis, 1984*a*) and dinitratobis(2,6-dimethyl-4-pyrone)copper (Brown & Lewis, 1984*b*).

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Structures of *cis*-Dichloro(methanol)(salicylaldehyde benzoylhydrazonato)iron(III), [$FeCl_2(C_{14}H_{11}N_2O_2)(CH_4O)$], and Chloro(salicylaldehyde benzoylhydrazonato)copper(II) Monohydrate, [$CuCl(C_{14}H_{11}N_2O_2)$].H_2O

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Abstract. [$FeCl_2$(Hsbh)(CH_3OH)] (*A*) (H_2sbh is *s*alicylaldehyde *b*enzoyl*h*ydrazone): $M_r = 398{\cdot}0$, triclinic, $P\overline{1}$, $a = 6{\cdot}665$ (2), $b = 13{\cdot}818$ (6), $c = 10{\cdot}122$ (4) Å, $\alpha = 108{\cdot}40$ (2), $\beta = 73{\cdot}23$ (2), $\gamma = 103{\cdot}32$ (2)°, $V = 837$ Å^3, $Z = 2$, $D_x = 1{\cdot}580$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 12{\cdot}5$ cm^{-1}, $F(000) = 406$, room temperature. [CuCl(Hsbh)].H_2O (*B*): $M_r = 356{\cdot}3$, monoclinic, $P2_1/a$, $a = 16{\cdot}201$ (21), $b = 7{\cdot}107$ (10), $c = 12{\cdot}540$ (18) Å, $\beta = 89{\cdot}87$ (9)°, $V = 1444$ Å^3, $Z = 4$, $D_x = 1{\cdot}64$ g cm^{-3}, $\mu = 17{\cdot}7$ cm^{-1}, $F(000) = 724$, room temperature. For (*A*), 3740 observations gave $R = 0{\cdot}043$ and $wR = 0{\cdot}036$. For (*B*), 1250 observations gave $R = 0{\cdot}091$ and $wR = 0{\cdot}065$. The Cu coordination in (*B*) is square-planar, with Cl^- and O(1), O(2), and N(2) of Hsbh$^-$; the Fe in (*A*) is octahedral, with axial Cl^- and CH_3OH in addition to Cl^-, O(1), O(2), and N(2) as in (*B*). The uncoordinated hydrazidic nitrogen, N(1), remains protonated in both.

Introduction. H_2sbh is a potentially tridentate chelating agent formed by the Schiff-base condensation of salicylaldehyde with benzoyl hydrazide. This agent produces a variety of biological responses, both in animals (Johnson, Pippard, Murphy & Rose, 1982), microorganisms (Dimmock, Baker & Taylor, 1972), and cultured cells (Ponka, Borova, Neuwirt, Fuchs & Necas, 1979; Johnson, Murphy, Rose, Goodwin & Pickart, 1982), which appear to be associated with its ability to chelate essential metal ions *in vivo*. Crystallographic studies of complexes (*A*) and (*B*), formed by H_2sbh with the common essential metals iron and copper, were therefore undertaken (preliminary communication: Aruffo, Murphy, Johnson, Rose & Schomaker, 1982) as part of our attempts to understand its biological properties. Although various transition-metal complexes of Hsbh$^-$ have been described, we know of no other Hsbh$^-$ crystal structures.§

Experimental. Crystals of (*A*) were obtained by mixing equimolar quantities of H_2sbh and $FeCl_3.6H_2O$ in methanol. The resulting solution was filtered; on

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§ Hsbh$^-$: monoanion of H_2sbh (the H_2 here signifying the two acidic hydrogens).

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