i $x-1,y,z$
ii $1-x,\bar{y},1-z$
iii $1-x,\bar{y},\bar{z}$
iv $\bar{x},\bar{y},\bar{z}$

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Crystal Structure of the Praseodymium β-Diketonate of 2,2,6,6-Tetramethyl-3,5-heptanedione, $Pr_2(thd)_6$

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The crystal structure of the β-diketonate with empirical formula $Pr[(CH_3)_3C.CO.CH.CO.C.(CH_3)_3]_3$ has been determined from 5373 intensities measured visually using the multiple-film Weissenberg technique at room temperature. The crystals are monoclinic with space group $P2_1/n$ and cell constants $a=22\cdot28$ (6), $b=28\cdot51$ (7), $c=12\cdot56$ (5) Å, and $\beta=105°\pm30'$. Observed and calculated densities are 1·20 and 1·19 g.cm^{-3} respectively, for $Z=8$, *i.e.* with two crystallographically independent formula units. Refinement by full-matrix least-squares including 9 layer-line scale factors and individual isotropic temperature factors (329 parameters) converged to a conventional R of 0·133. The asymmetric unit consists of a dimer $Pr_2(thd)_6$ in which each of the Pr atoms is surrounded by 7 oxygen atoms in positions consistent with maximum repulsion. Two of the oxygen atoms are shared equally between Pr atoms. Only the methyl groups of neighbouring dimers are in loose van der Waals contact as evidenced by exceptionally high temperature factors for the methyl carbon atoms. This is interpreted as symptomatic of the known volatility of the thd lanthanides.

Introduction

The β-diketone $[(CH_3)_3.C.CO]_2CH_2$, H(thd), forms volatile lanthanide complexes with the general empirical formula $Ln(thd)_3$ (Eisentraut & Sievers, 1965). These complexes have been the subject of several crystallographic studies (*e.g.* Chen, 1967; Mode & Smith, 1969) which established that the complexes of the lighter lanthanides (La to Dy) are monoclinic and that those of Ho to Lu are orthorhombic. Work in this laboratory has been confined to the study of the crystallography of the lighter series and the detailed analysis of two of the structure types encountered. Part of the work is described in this paper, a preliminary report having been published previously (Erasmus & Boeyens, 1969).

Crystallographic relationships

Sublimed samples of each of the La^{III} to Dy^{III} thd complexes were kindly supplied by Dr R. E. Sievers of Aerospace Research Laboratories, Dayton, Ohio. These were recrystallized from n-hexane, exposed to the atmosphere and found to constitute an isomorphous series with space group $P2_1/n$. The cell constants as determined from suitable oscillation, Weissenberg

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and precession photographs are summarized in Table 1. In the case of Dy and Eu, triclinic crystals of the monohydrates were found on the upper regions of the containers. Crystallographic data for these compounds are also listed in Table 1. A detailed analysis of the $Dy(thd)_3 . H_2O$ complex has been completed and will be reported shortly. To investigate possible isomorphism with the crystals from solution, crystals grown from the vapour were also investigated crystallographically. This study revealed that, apart from the general $P2_1/n$ type which appeared throughout the series, the Dy and Tb complexes also contained crystals of a less abundant orthorhombic phase. Crystal data for this phase are also listed in Table 1.

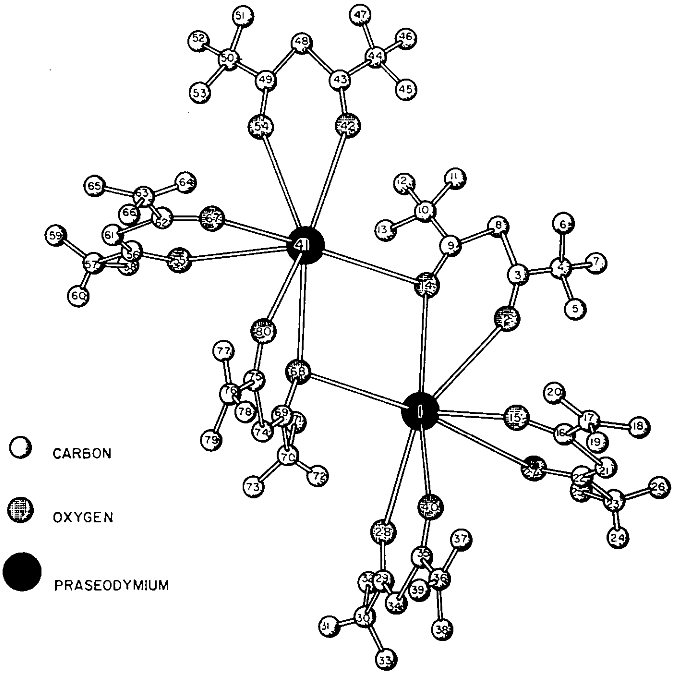

Fig. 1. Schematic diagram to show the structural formula and nomenclature used in the description of the $Pr_2(thd)_6$ dimer.

Determination of the structure

The praseodymium complex crystallizes from n-hexane as pale green crystals elongated along [001]. These crystals were found to decompose on X-irradiation even when sealed into thin-walled Lindemann glass capillaries. This phenomenon severely hampered data collection by counter methods and photographic methods were thus employed. No attempt was made to obtain highly accurate cell constants and the following values with their standard deviations were obtained from several sets of

Table 1. *Crystallographic relationships between crystals of the* thd *complexes of the lanthanides* La *to* Dy

Anhydrous complexes obtained from *n*-hexane. Space group $P2_1/n$, $Z=8$, $\beta=105°$.

Empirical formula	a	b	c	Volume/ formula unit	ϱ_{calc} (g.cm^{-3})	ϱ_{obs} (g.cm^{-3})
$La(thd)_3$	22·32 Å	28·59 Å	12·59 Å	970 Å^3	1·179	1·19
$Pr(thd)_3$	22·28	28·51	12·56	964	1·190	1·20
$Nd(thd)_3$	22·23	28·45	12·51	955	1·206	1·22
$Sm(thd)_3$	22·20	28·29	12·49	947	1·227	1·23
$Eu(thd)_3$	22·16	28·21	12·45	940	1·240	1·25
$Gd(thd)_3$	22·15	28·12	12·44	936	1·255	1·25
$Tb(thd)_3$	22·16	28·03	12·45	934	1·260	1·26
$Dy(thd)_3$	22·11	28·04	12·43	930	1·271	1·26

Hydrated complexes from *n*-hexane. Space group $P\bar{1}$, $Z=2$.

Empirical formula	a	b	c	α	β	γ	Volume/ formula unit	ϱ_{calc} (g.cm^{-3})	ϱ_{obs} (g.cm^{-3})
$Eu(thd)_3 . H_2O$	14·23 Å	14·84 Å	11·66 Å	99·9°	109·8°	113·9°	988 Å^3	1·214	1·23
$Dy(thd)_3 . H_2O$	14·21	14·88	11·60	99·8	109·9	114·1	983	1·238	1·24

Orthorhombic ($Pmmn$ or $Pmn2_1$) crystals obtained from the vapour, $Z=2$.

Empirical formula	a	b	c	Volume/ formula unit	ϱ_{calc} (g.cm^{-3})	ϱ_{obs} (g.cm^{-3})
$Tb(thd)_3$	18·25 Å	10·05 Å	10·72 Å	984 Å^3	1·196	1·20
$Dy(thd)_3$	18·12	10·09	10·71	979	1·208	1·21

Table 2. *Fractional coordinates and isotropic temperature factors of the atoms in the asymmetric unit*

Estimated standard deviations are given after each value.

	Number	Ring	x	y	z	B
Pr	1		0·2706 (01)	0·0321 (01)	0·9529 (02)	3·05 (0·04) Å^2
O	2		0·3537 (10)	0·0661 (08)	0·8929 (22)	5·36 (0·51)
C	3		0·3647 (14)	0·0673 (11)	0·7984 (33)	4·46 (0·07)
C	4		0·4359 (14)	0·0748 (11)	0·8003 (31)	4·69 (0·72)
C	5		0·4749 (23)	0·0349 (18)	0·8734 (45)	10·18 (1·38)
C	6		0·4562 (20)	0·1214 (15)	0·8603 (40)	8·29 (1·15)

Table 2 (*cont.*)

	Number	Ring	*x*	*y*	*z*	*B*
C	7		0·4495 (22)	0·0730 (17)	0·6911 (45)	9·59 (1·34)
C	8	*A*	0·3191 (21)	0·0612 (15)	0·6866 (40)	8·25 (1·14)
C	9		0·2582 (13)	0·0597 (10)	0·6880 (28)	3·84 (0·64)
C	10		0·2111 (15)	0·0490 (12)	0·5790 (32)	5·26 (0·79)
C	11		0·2437 (20)	0·0349 (15)	0·4843 (39)	7·59 (1·03)
C	12		0·1632 (15)	0·0872 (11)	0·5335 (31)	5·23 (0·78)
C	13		0·1764 (17)	0·0016 (13)	0·5965 (34)	6·34 (0·91)
O	14		0·2294 (08)	0·0728 (06)	0·7638 (18)	3·66 (0·40)
O	15		0·2984 (08)	−0·0327 (07)	0·8534 (17)	4·20 (0·42)
C	16		0·2762 (16)	−0·0751 (12)	0·8264 (33)	5·65 (0·82)
C	17		0·3254 (18)	−0·1083 (14)	0·7889 (38)	7·04 (0·99)
C	18		0·3008 (21)	−0·1579 (17)	0·7813 (42)	9·24 (1·28)
C	19		0·3392 (23)	−0·0906 (18)	0·6851 (47)	10·30 (1·43)
C	20		0·3880 (21)	−0·1049 (16)	0·8834 (42)	8·90 (1·23)
C	21	*B*	0·2156 (13)	−0·0885 (10)	0·8275 (27)	3·72 (0·63)
C	22		0·1738 (13)	−0·0595 (10)	0·8524 (27)	3·61 (0·61)
C	23		0·1085 (17)	−0·0789 (13)	0·8495 (35)	5·98 (0·86)
C	24		0·0699 (27)	−0·0650 (21)	0·7350 (55)	12·90 (1·82)
C	25		0·0775 (36)	−0·0512 (28)	0·9270 (81)	18·13 (2·69)
C	26		0·1031 (34)	−0·1255 (28)	0·8569 (67)	16·41 (2·48)
O	27		0·1810 (09)	−0·0170 (06)	0·8887 (18)	4·08 (0·43)
O	28		0·2899 (10)	−0·0315 (08)	0·0873 (20)	5·21 (0·49)
C	29		0·3205 (15)	−0·0381 (12)	0·1882 (33)	5·26 (0·77)
C	30		0·3072 (18)	−0·0871 (14)	0·2348 (38)	6·78 (0·95)
C	31		0·2449 (27)	−0·0871 (20)	0·2594 (52)	12·00 (1·65)
C	32		0·3263 (28)	−0·1227 (22)	0·1734 (54)	12·94 (1·83)
C	33		0·3448 (29)	−0·0928 (22)	0·3571 (58)	13·50 (1·92)
C	34	*C*	0·3619 (15)	−0·0057 (11)	0·2503 (30)	4·85 (0·74)
C	35		0·3710 (13)	0·0413 (10)	0·2155 (28)	3·83 (0·64)
C	36		0·4162 (18)	0·0775 (14)	0·2863 (36)	6·62 (0·94)
C	37		0·4564 (20)	0·0994 (16)	0·2153 (40)	8·31 (1·15)
C	38		0·4634 (19)	0·0555 (15)	0·3888 (39)	7·84 (1·09)
C	39		0·3759 (18)	0·1156 (14)	0·3268 (36)	7·17 (1·01)
O	40		0·3400 (08)	0·0589 (06)	0·1246 (18)	3·77 (0·41)
Pr	41		0·1757 (01)	0·1466 (01)	0·7888 (02)	3·01 (0·04)
O	42		0·2411 (10)	0·1805 (07)	0·6839 (20)	5·05 (0·49)
C	43		0·2373 (13)	0·2096 (10)	0·6070 (28)	4·04 (0·65)
C	44		0·3013 (16)	0·2234 (12)	0·5908 (34)	5·91 (0·87)
C	45		0·3448 (17)	0·2403 (13)	0·6997 (35)	6·51 (0·93)
C	46		0·3306 (17)	0·1806 (13)	0·5455 (35)	6·54 (0·93)
C	47		0·2931 (19)	0·2657 (15)	0·4982 (39)	7·95 (1·11)
C	48	*D*	0·1815 (14)	0·2269 (10)	0·5381 (28)	4·20 (0·67)
C	49		0·1207 (13)	0·2127 (10)	0·5500 (29)	4·01 (0·65)
C	50		0·0624 (14)	0·2296 (11)	0·4644 (31)	4·72 (0·73)
C	51		0·0720 (21)	0·2654 (16)	0·3853 (42)	8·94 (1·23)
C	52		0·0275 (24)	0·1865 (19)	0·4183 (47)	10·76 (1·50)
C	53		0·0216 (22)	0·2551 (17)	0·5215 (44)	9·80 (1·36)
O	54		0·1137 (09)	0·1907 (07)	0·6322 (20)	4·92 (0·49)
O	55		0·0766 (10)	0·1077 (07)	0·7531 (19)	5·02 (0·49)
C	56		0·0216 (17)	0·1246 (13)	0·7525 (33)	5·91 (0·86)
C	57		−0·0319 (18)	0·0924 (14)	0·6887 (37)	6·59 (0·94)
C	58		−0·0149 (22)	0·0605 (17)	0·6009 (45)	9·75 (1·35)
C	59		−0·0895 (22)	0·1217 (16)	0·6242 (42)	9·16 (1·27)
C	60		−0·0519 (23)	0·0603 (18)	0·7699 (46)	10·29 (1·43)
C	61	*E*	0·0064 (16)	0·1667 (12)	0·8010 (32)	5·58 (0·82)
C	62		0·0541 (16)	0·1966 (12)	0·8624 (32)	5·35 (0·79)
C	63		0·0369 (16)	0·2428 (13)	0·9241 (34)	5·72 (0·84)
C	64		0·0543 (28)	0·2870 (22)	0·8681 (57)	13·77 (1·94)
C	65		−0·0352 (25)	0·2464 (20)	0·9159 (50)	11·75 (1·63)
C	66		0·0698 (21)	0·2397 (16)	0·0428 (44)	9·01 (1·24)
O	67		0·1119 (09)	0·1937 (07)	0·8728 (19)	4·72 (0·47)
O	68		0·2022 (09)	0·0982 (07)	0·9690 (19)	4·64 (0·46)
C	69		0·1955 (17)	0·1216 (13)	0·0635 (35)	6·05 (0·88)
C	70		0·1573 (15)	0·0957 (11)	0·1299 (32)	4·85 (0·74)
C	71		0·0911 (18)	0·0883 (14)	0·0539 (36)	7·03 (0·99)
C	72		0·1845 (19)	0·0463 (14)	0·1665 (37)	7·60 (1·06)
C	73		0·1591 (20)	0·1199 (16)	0·2343 (41)	8·35 (1·17)
C	74		0·2248 (14)	0·1645 (11)	0·0948 (29)	4·61 (0·72)
C	75	*F*	0·2551 (16)	0·1954 (12)	0·0316 (35)	5·50 (0·82)
C	76		0·2931 (15)	0·2408 (12)	0·0791 (32)	4·99 (0·75)

Table 2 (*cont.*)

	Number	Ring	*x*	*y*	*z*	*B*
C	77		0·2686 (20)	0·2828 (16)	0·0153 (41)	8·55 (1·18)
C	78		0·3601 (24)	0·2307 (18)	0·0731 (47)	10·74 (1·49)
C	79		0·2952 (22)	0·2455 (17)	0·2021 (45)	9·58 (1·35)
O	80		0·2539 (11)	0·1875 (08)	0·9310 (24)	6·25 (0·58)

Table 3. *Observed and calculated structure factors on an absolute scale*

0,	K,	0
2	267	252
6	315	-250
8	53	-81
10	221	-221
12	110	-77
14	66	-63
16	154	-148
18	170	-187
24	69	-80
26	65	76
28	97	95
32	50	40
34	52	72
1,	K,	0
1	58	46
2	446	-475
3	248	-265
4	69	78
5	35	30
6	277	-239
7	93	84
8	290	-258
10	91	-103
12	75	79
13	44	44
15	49	49
16	42	-35
17	48	-40
18	95	95
20	107	118
21	66	65
24	82	90
26	133	125
2,	K,	0
0	543	-625
1	210	-232
2	250	-258
3	53	47
4	93	-88
5	355	368
6	209	-193
7	62	73
8	43	43
9	35	-42
10	160	151
11	61	-53
12	104	110
14	73	61
15	111	-118
16	204	210
17	41	35
18	140	152
19	131	135
21	53	-44
23	69	-74
24	58	43
25	42	36
26	60	-48
28	75	-81
29	53	-51
32	45	-41
33	32	27
34	41	-58
3,	K,	0
1	31	33
2	69	69
3	228	254
4	76	67
5	56	48
6	162	152
7	221	-212
8	272	264
9	55	-23
10	120	121
11	47	39
12	43	38
13	176	-170
15	113	-117
16	30	-17
17	99	113
18	58	-54
19	70	-69
20	65	-62
21	99	-107
22	55	-59
23	40	39
24	53	-52
25	60	54
26	61	-65
27	43	-38
28	42	-31
31	57	69
34	28	20
4,	K,	0
0	186	184
1	128	109
2	102	96
3	548	472
4	267	247
5	306	-296
6	79	65
7	44	-42
8	125	-92
9	76	42
10	98	-86
11	122	-130
12	99	-83
13	102	-110
14	189	-193
15	137	146
16	120	-110
17	32	-19
18	82	-86
19	92	-90
20	90	-98
21	49	44
22	39	-26
23	57	65
24	54	43
28	48	28
29	57	73
30	55	56
32	39	42
33	31	-34
34	28	17
5,	K,	0
1	41	-32
3	203	-205
4	133	-131
5	95	-119
6	200	-203
7	140	139
8	85	-68
10	75	-84
12	266	-272
13	203	227
15	115	112
16	78	73
18	34	-29
19	94	92
20	37	33
21	77	78
22	98	124
24	59	64
25	49	-47
28	54	48
29	46	-34
31	51	-63
32	33	-37
6,	K,	0
0	64	72
1	62	-61
2	65	-52
4	211	-220
5	212	169
6	71	73
7	66	70
8	169	174
10	168	-161
11	119	125
12	92	99
13	86	78
14	201	195
18	35	39
20	132	139
21	55	-49
22	52	37
23	58	-44
24	64	-77
27	42	-23
29	39	-34
30	53	-69
32	32	-35
7,	K,	0
1	59	63
2	138	-112
3	95	91
4	111	119
5	128	120
6	353	324
7	91	94
9	62	-58
11	79	-76
12	266	266
13	79	-87
14	35	-35
15	79	-94
16	67	-67
17	138	-143
18	42	36
19	84	-85
21	46	-36
22	107	-125
24	55	-45
25	55	20
27	54	41
28	62	-53
29	50	35
30	37	-33
31	40	30
32	31	42
33	28	33
8,	K,	0
0	152	-153
1	77	-80
2	45	49
3	32	-17
4	155	146
5	68	52
6	34	41
7	43	-29
8	173	-170
9	214	-220
10	138	129
11	70	-69
12	53	-69
13	35	-32
14	136	-140
15	96	-93
16	44	33
19	115	117
20	88	-94
21	68	60
22	41	-27
23	42	34
24	49	71
25	73	69
27	48	28
30	41	52
32	35	34
9,	K,	0
1	176	-178
2	59	-51
3	97	-92
4	84	-89
5	88	-80
6	241	-209
7	230	-223
8	62	-77
9	32	40
10	37	-35
11	197	197
12	108	-111
14	56	49
15	100	100
16	35	40
17	169	178
18	44	-37
19	50	46
21	41	-39
22	84	75
23	49	57
24	43	37
27	72	-81
28	39	35
29	48	-38
10,	K,	0
0	67	-73
1	169	159
2	33	-31
3	157	159
4	59	-38
6	39	28
7	56	43
8	71	68
9	277	274
11	41	37
15	121	108
16	37	-24
17	66	-71
19	156	-160
21	54	-43
25	96	-110
27	46	-41
11,	K,	0
1	287	286
2	118	110
3	40	44
4	48	36
5	37	39
7	180	161
8	51	63
9	53	-63
11	152	-160
12	44	-37
14	41	45
15	62	-52
16	49	39
17	136	-143
19	53	-39
20	42	-30
23	43	-55
26	40	-37
27	67	78
29	34	35
12,	K,	0
0	89	97
1	115	-116
3	127	-119
4	120	-124
5	30	-32
6	76	88
7	123	-141
9	166	-171
10	83	-72
11	40	-41
14	85	84
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19	102	111
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7	96	-88
9	72	59
11	99	104
17	104	111
8,	K,	8
1	93	77
2	54	32
3	108	92
4	54	41
7	109	107
9	130	143
15	59	55
19	77	-85
9,	K,	8
1	114	94
4	65	-52
6	73	-58
7	66	66
9	58	-39
11	83	-89
17	85	-83
10,	K,	8
2	88	-66
3	66	-57
4	103	-79
7	89	-74
9	102	-89
14	81	69
11,	K,	8
2	76	-54
4	83	81
6	84	70
12	88	82
12,	K,	8
2	77	71
4	84	65
5	84	79
6	59	-43
14	75	-71
13,	K,	8
3	98	79
4	75	-61
6	66	-58
-1,	K,	8
1	44	-30
2	134	-138
3	139	-163
5	61	-55
6	49	-30
7	61	54
8	140	-148
10	91	-108
13	77	85
14	67	-54
15	107	105
18	74	56
20	76	62
-2,	K,	8
0	204	247
1	36	26
2	42	35
5	77	-80
6	125	125
7	50	-39
8	58	60
9	65	-73
10	134	-140
12	96	-92
14	52	-34
16	110	-112
18	99	-110
-3,	K,	8
1	69	65
2	126	166
3	31	39
4	37	-25
6	51	39
8	168	179
10	74	106
11	65	-44
12	48	-33
17	72	-56
18	81	-86
20	76	-85
-4,	K,	8
0	209	-260
1	78	80
2	72	-83
3	65	76
4	41	-32
5	48	-39
6	97	-109
7	49	44
9	64	61
10	116	117
12	[illegible]	51
15	53	61
16	97	103
18	102	118
19	58	-40
-5,	K,	8
1	82	-100
2	90	-90
3	96	119
4	42	-24
6	75	-79
7	86	-90
8	106	-122
9	60	35
10	68	-59
11	60	65
17	86	87
20	76	67
-6,	K,	8
0	127	121
1	87	-102
2	132	156
4	81	108
5	112	116
6	38	25
7	56	-53
9	116	-116
10	76	-62
11	60	54
12	69	-50
14	79	-74
15	62	-55
16	63	-57
18	81	-74
19	75	64
20	68	-63
-7,	K,	8
1	33	23
3	104	-116
4	104	120
6	95	97
7	107	114
8	55	41
10	65	62
11	73	-68
12	85	87
13	59	62
17	56	-65
21	59	56
22	82	-80
-8,	K,	8
2	109	-134
4	148	-167
5	90	-84
8	56	52
9	59	51
11	56	-50
12	84	81
13	52	-35
14	121	145
20	100	96
-9,	K,	8
1	38	45
2	88	82
3	51	43
4	89	-79
5	53	36
6	148	-160
7	57	-48
10	48	-39
12	136	-154
16	73	65
22	81	102
-10,	K,	8
1	58	55
2	91	96
3	54	58
4	133	148
7	59	48
8	67	-56
9	62	60
10	64	55
12	68	-57
14	135	-152
20	90	-93
-11,	K,	8
1	126	-132
2	62	-46
4	69	74
6	115	125
7	55	-40
9	65	52
11	68	68
12	130	125
17	90	106
22	78	-76
-12,	K,	8
1	113	-116
2	66	69
3	79	89
4	61	-55
7	64	-61
9	127	-128
14	81	82
15	75	-74
19	76	78
-13,	K,	8
1	151	170
6	51	-31
7	79	78
8	80	-75
11	98	-103
15	76	-65
17	106	-122
-14,	K,	8
0	86	85
1	86	84
7	76	65
9	133	135
10	64	-58
19	80	-74
-15,	K,	8
1	106	-109
2	121	122
4	54	41
5	63	-61
7	71	-54
8	79	70
11	67	66
12	58	-46
16	59	47
17	74	83
-16,	K,	8
0	110	-102
4	79	80
6	56	-49
7	80	-88
9	67	-49
10	82	81
11	68	-47
-17,	K,	8
1	87	89
2	101	-107
3	81	96
8	75	-63
12	59	53
13	76	-74
-18,	K,	8
0	58	53
5	117	112
7	59	57
11	76	74
-19,	K,	8
3	130	-123
7	59	53
-20,	K,	8
1	68	51
5	104	-108
7	66	-62
-21,	K,	8
2	57	17
3	96	81
-22,	K,	8
0	92	-83
5	62	58

measurements:

$a=22{\cdot}28\pm0{\cdot}06$, $b=28{\cdot}51\pm0{\cdot}07$, $c=12{\cdot}56\pm0{\cdot}05$ Å, $\beta=105\pm0{\cdot}5°$.

The conditions limiting possible reflexions: $h0l$ for $h+l=2n$ and $0k0$ for $k=2n$ uniquely define space group No. 14 (*International Tables for X-ray Crystallography*, 1965) in the setting $P2_1/n$. The measured density is 1·20

Table 3 (*cont.*)

18	68	-84
19	91	100
20	73	-88
22	58	60
24	67	-55
26	63	-76
27	55	-63
-6,	K,	2
0	316	-318
1	35	-32
2	62	86
3	52	-63
4	110	95
5	237	-231
6	139	-131
7	199	-204
8	110	-118
9	146	-148
10	112	119
11	117	-140
12	40	35
13	46	-50
14	74	-74
16	96	117
17	38	24
18	89	97
19	53	36
20	74	-96
21	68	82
23	60	82
24	61	78
25	68	67
26	74	-21
27	61	38
28	46	-44
-7,	K,	2
1	165	142
2	90	-79
3	294	295
4	47	56
5	42	34
6	87	92
7	91	-72
8	106	-123
9	28	28
10	38	-35
12	108	107
13	192	-191
15	89	-114
16	100	-122
17	39	-31
18	62	68
19	75	-85
20	56	30
21	75	-74
22	65	-69
23	61	30
24	55	26
25	56	52
26	73	56
27	47	26
-8,	K,	2
0	82	67
1	104	-93
3	55	29
4	101	-111
5	332	344
7	150	152
8	51	50
9	51	49
10	44	-40
11	136	150
12	33	-23
13	130	138
14	62	65
15	84	-89
16	50	-40
18	54	-50
19	61	39
20	51	54
21	81	-100
23	85	-116
24	62	-29
25	63	-26
27	46	-31
-9,	K,	2
1	102	-108
2	90	-69
3	279	-286
5	69	-74
6	40	-18
7	172	167
8	35	-19
9	40	-33
11	33	-24
13	153	169
15	134	153
16	46	29
17	53	-26
19	100	128
21	82	99
23	55	-42
25	48	-69
-10,	K,	2
0	244	219
1	36	27
2	76	72
4	29	-32
5	300	-314
6	39	34
7	84	-99
8	37	17
9	43	-18
10	76	-82
11	118	-120
12	47	-50
13	82	-77
14	50	19
15	61	62
16	58	-29
17	49	-23
18	62	-15
19	58	-54
21	94	117
23	108	118
24	48	-41
25	47	21
-11,	K,	2
1	39	32
2	165	160
3	207	203
4	40	-31
5	78	77
6	56	-54
7	75	-65
8	117	129
10	46	31
12	49	-53
13	129	-137
14	46	44
15	83	-99
16	65	53
17	56	-33
18	75	-93
19	77	-93
20	66	-29
21	61	-77
23	48	23
24	48	-26
25	47	39
26	58	-68
-12,	K,	2
0	238	-257
4	96	103
5	88	93
6	84	-91
7	69	77
8	51	-48
9	47	55
10	113	143
11	87	98
13	68	72
14	54	-43
16	76	94
17	45	-25
18	77	77
19	54	-35
20	61	-32
21	74	-76
22	48	19
23	55	-68
24	54	59
-13,	K,	2
1	145	-145
2	174	-150
3	35	-25
4	41	35
5	41	-51
7	57	-64
8	146	-160
9	38	20
10	79	-87
11	70	78
12	73	63
13	54	66
14	66	-70
15	76	83
16	58	-55
17	65	74
18	72	87
19	55	38
20	56	62
22	48	-25
23	47	22
24	46	38
-14,	K,	2
0	146	167
1	96	-109
2	37	35
3	64	-74
6	77	76
7	68	-68
8	39	39
9	138	-138
10	82	-96
15	59	-32
16	105	-122
18	80	-92
19	74	84
20	48	20
-15,	K,	2
1	135	148
2	75	73
3	60	-46
4	51	44
6	47	53
7	107	112
8	102	128
9	54	-47
10	66	68
11	73	-90
12	44	32
13	52	20
14	53	49
15	47	-23
16	61	18
17	81	-103
18	48	-63
20	55	-56
21	47	39
-16,	K,	2
0	71	-82
1	94	104
2	71	-73
3	83	85
4	64	-66
5	75	-68
6	42	-34
7	72	48
9	78	88
10	45	27
11	76	-38
12	59	44
14	72	91
15	67	70
16	62	68
18	48	37
19	80	-91
-17,	K,	2
1	86	-92
3	56	44
4	62	-84
6	99	-121
7	75	-88
8	52	-47
9	65	69
10	60	-63
11	47	38
12	79	-89
13	48	-31
16	48	42
17	68	72
-18,	K,	2
1	52	-48
2	64	76
3	52	-67
4	102	126
5	46	30
12	48	-50
14	86	-115
15	55	-29
16	47	-33
-19,	K,	2
2	54	-47
4	79	79
6	124	144
10	48	55
12	74	101
-20,	K,	2
2	48	-62
4	86	-121
5	56	26
8	56	41
9	48	-40
12	47	42
14	82	95
-21,	K,	2
1	56	53
3	48	-28
4	56	-51
6	62	-82
7	55	49
10	47	-46
11	46	-40
12	52	-69
13	44	29
-22,	K,	2
0	47	34
1	61	50
2	47	54
3	47	33
4	47	47
5	47	-38
9	52	66
0,	K,	3
1	124	-119
2	131	-119
3	189	164
4	84	67
5	73	76
6	286	282
7	105	-82
9	83	62
10	115	124
11	76	78
12	197	217
13	137	-153
14	36	-38
15	94	-93
16	71	-84
17	42	33
19	52	-63
20	67	-54
21	63	-55
22	114	-136
24	61	-51
28	52	-45
1,	K,	3
0	25	-17
1	43	-45
2	255	259
3	224	-207
4	284	281
5	95	-92
6	48	-29
7	137	-128
8	73	-80
9	87	-73
10	180	177
11	184	-172
12	126	-120
13	118	-123
14	197	-226
17	49	37
20	104	-112
21	75	85
23	73	76
24	75	81
25	54	38
27	53	34
2,	K,	3
1	105	-102
2	136	117
4	155	-154
5	31	-38
6	252	-227
7	143	-116
8	50	55
11	50	41
12	203	-212
13	88	101
14	48	35
15	89	102
16	91	101
17	83	84
18	51	-41
19	65	51
22	102	129
27	61	-53
28	52	52
3,	K,	3
0	65	66
1	193	183
2	76	-68
3	211	177
4	245	-205
5	36	41
6	77	72
7	248	239
8	38	36
9	182	183
10	73	-60
11	75	52
12	80	62
14	162	185
15	98	98
19	93	-110
20	84	95
21	58	-36
23	61	-38
24	62	-52
25	83	-99
27	61	-60
4,	K,	3
1	197	220
2	113	-108
3	43	-45
4	110	89
5	125	102
6	81	98
7	102	90
8	51	-34
9	185	-181
10	56	36
11	179	-163
12	103	105
15	53	-22
16	49	-40
17	171	-188
19	61	-55
21	50	38
22	60	-27
23	53	-50
27	68	91
28	50	-35
5,	K,	3
0	48	-23
1	240	-224
3	185	-164
5	98	85
7	286	-277
9	193	-196
11	46	-22
12	57	-54
14	52	-56
15	103	-137
16	50	-57
18	54	-45
19	106	128
21	59	35
25	83	-118
6,	K,	3
1	299	-293
2	49	-31
3	118	110
4	120	123
5	103	-95
6	78	70
7	113	-125
8	76	-69
9	116	115
10	82	-76
11	142	158
13	52	52
15	66	63
16	58	-56
17	144	164
18	48	43
19	57	62
22	53	-38
23	54	46
27	59	-85
7,	K,	3
0	161	-164
1	209	222
2	106	104
4	137	148
5	50	47
6	83	-75
7	100	111
8	80	-72
9	142	157
10	86	91
11	55	41
13	59	42
14	56	-53
15	75	71
16	53	44
18	75	60
19	65	-86
20	66	-72
21	74	-55
24	54	44
25	81	-96
27	50	-40
28	48	-35
8,	K,	3
1	194	203
2	143	135
3	77	82
4	90	-108
5	61	56
6	105	-109
8	67	63
9	38	-31
11	80	-80
12	84	-91
13	75	-78
14	45	26
15	82	-100
16	72	91
17	82	-75
18	65	-80
19	59	-71
20	52	-38
22	62	81
26	51	-35
27	49	41
28	46	37
9,	K,	3
0	134	119
1	46	27
2	81	-84
4	110	-127
5	112	-123
6	58	64
7	131	-135
8	77	78
9	81	-84
10	91	-77
11	74	-66
12	51	26
13	45	-46
14	92	96
15	55	30
16	63	-29
18	51	-39
20	81	90
21	76	84
23	70	85
24	53	-61
25	59	39
10,	K,	3
1	75	-91
2	77	-69
3	163	-203
4	80	99
5	97	-107
6	120	140
7	53	34
12	70	77
13	103	124
15	96	103
16	65	-45
18	52	34
19	53	72
21	63	80
22	54	-55
23	61	-32
25	58	-40
11,	K,	3
0	52	52
1	68	-83
2	53	45
3	47	-22
4	72	80
5	162	188
6	49	-42
7	98	102
11	78	107
12	55	-51
13	69	74
14	86	-86
15	77	-90
16	51	-45
21	70	83
23	67	-91
12,	K,	3
1	50	35
2	61	-48
3	150	177
4	56	-50
5	78	89
6	58	-59
7	78	-93
8	70	-81
10	73	-67
11	56	52
12	49	-35
13	89	-121
14	66	-25
15	67	-77
18	70	36
19	70	-61
20	62	37
21	68	-74
23	50	30
13,	K,	3
0	121	-141
2	76	-69
4	46	32
5	124	-159
6	54	-56
7	55	-65
8	48	-32
9	69	37
10	83	71
11	65	-77
12	59	52
13	67	-64
14	52	30
15	81	63
16	76	90
18	63	62
19	62	-26
20	61	-22
21	60	49
14,	K,	3
1	55	-48
2	105	116
3	55	-63
4	68	68
5	56	-33
7	57	51
8	114	153
9	50	26
10	66	64
12	52	-29
13	61	58
14	62	39
15	70	41
16	70	55
18	53	-69
19	61	43
20	59	-55
15,	K,	3
2	64	73
3	58	63
5	58	32
6	51	66
7	59	53
8	60	29
10	105	-129
12	69	-39
13	54	28
16	69	-90
18	60	-84
16,	K,	3
4	52	-44
7	53	41
8	81	-124
9	53	-40
10	62	-74
-1,	K,	3
2	178	-139
3	74	-52
4	287	-266
5	311	300
6	56	-51
7	102	100
8	70	75
9	74	-85
10	99	-96
11	160	167
12	110	112
13	99	95
14	97	116
15	109	-121
16	89	84
18	61	61
19	52	50
20	66	70
21	63	-67
23	73	-97
24	61	-42
25	54	23
-2,	K,	3
2	157	-134
3	202	-163
4	39	-18
5	195	-187
6	153	-157
7	210	179
8	156	-143
9	47	-59
10	252	-235
11	93	-94
12	102	-98
13	177	184
14	47	-36
15	66	58
16	46	45
17	81	-99
18	95	95
19	52	54
20	72	84
21	63	80
22	77	82
23	60	-29
24	75	68
25	54	-37
26	63	63
27	62	57
-3,	K,	3
0	303	285
2	159	147
4	35	21
5	170	-195
7	44	-53
8	105	101
9	188	166
10	92	-97
11	209	-200
12	98	-81
13	60	-60
14	36	-37
15	94	108
16	166	-184
17	59	30
18	99	-118
19	52	-55
21	63	66
23	67	58
24	68	-38
25	76	-40
26	63	31
28	52	53
-4,	K,	3
1	99	105
2	198	190
3	116	110
4	107	104
6	92	76
7	138	-127
8	342	329
9	86	77
10	312	283
11	37	44
12	51	-45
13	85	-97
14	84	112
15	65	-40
16	52	44
17	71	74
18	127	-146
20	104	-124
21	57	-31
24	81	-88
26	94	-112
27	69	-35
-5,	K,	3
0	260	-232
1	29	-20
2	83	-76
3	54	43
4	30	22
5	174	160
6	132	-153
7	45	-31
8	36	-38
9	92	-87
10	248	242
11	86	-83
12	78	96
13	41	-10
16	161	195
17	55	-22
18	133	158
20	48	-54
24	61	70
26	54	-37
28	51	-75
-6,	K,	3
1	151	-142
2	209	-222
3	31	-23
4	38	-46
6	185	-178
7	85	-78
8	405	-386
9	104	104
10	147	-155
11	44	38
12	54	73
13	48	-26
14	50	-48
15	46	-20
16	94	-101
18	101	107
19	60	-40
20	107	122
21	50	-51
24	76	87
26	76	105
-7,	K,	3
0	224	226
1	131	-139
2	137	112
3	26	-26
5	202	200
6	166	175
7	30	24
8	81	-72
9	49	33
10	151	-164
11	109	95
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21	54	-35
23	65	-60
24	64	66
26	68	-55
28	68	-70
4,	K,	5
1	32	37
2	215	209
3	127	109
4	87	75
6	72	64
7	61	-62
8	201	200
9	45	34
10	98	103
12	49	-44
13	101	-103
15	55	-45
16	63	62
18	73	-70
20	76	-81
21	71	-80
24	71	-68
26	80	-78
5,	K,	5
0	146	130
1	106	106
2	133	138
4	35	32
5	222	-206

g.cm^{-3} and the density calculated for $Z=8$ is 1·19 g.cm^{-3}.

Quasi-cylindrical specimens with radii less than 0·1 mm were used to record the intensities of the layer lines *hk*0 to *hk*8 (8500 possible reflexions) using Cu $K\alpha$ (Ni filter) radiation and standard multiple-film Weissenberg techniques. Measurements were done by visual comparison with standard strips and a total of 5373 measurable intensities were obtained. To relieve the computing load unobserved reflexions were not included in the analysis. As indicated by Dunning & Vand (1969) this should not influence the analysis drastically.

The usual Lp, spot shape, α_1–α_2 splitting and absorption corrections were applied using a program written for the IBM 360/40 computer by E. G. Boonstra. The various layer lines were placed on the same relative scale by allowing for factors such as crystal size, exposure time and equi-inclination angles.

A three-dimensional Patterson synthesis obtained using the 3000 most prominent reflexions yielded the coordinates of the two Pr atoms which were used to phase a three-dimensional Fourier synthesis using the same data. Series termination and weak scaling caused severe ripple in the Fourier function and only the atomic positions which were chemically meaningful, as judged from a preliminary three-dimensional model, were used in further Fourier cycles. All Fourier calculations were done using the centrosymmetric Fourier program written by P. Gantzel and H. Hope.

A trial structure of 80 non-hydrogen atoms was obtained and refined by full-matrix least-squares using the program *ORFLS* of Busing, Martin & Levy (1962) on an IBM 360/65 machine. The quantity minimized by this program is $\sum w(F_o-F_c)^2$. Equal weighting with $w=1$ was used for all reflexions. After refining all atomic and individual thermal parameters together with 9 layer-line scale factors for five cycles, all parameter shifts were less than 0·1 of their estimated standard deviations. At the termination of refinement the conventional $R=0{\cdot}133$. This accuracy was considered sufficient to establish the prominent structural features. Accurate bond lengths and angles must await completion of the refinement with counter data now in progress for the isomorphous Nd complex (Burns, 1969).

The final parameters with their estimated standard deviations are given in Table 2. The nomenclature is explained in Fig. 1. The observed and calculated structure factors on an absolute scale ($F_{000}=2440$, excluding H atoms) are listed in Table 3.

Description of the structure

The most striking feature of the structure is the occurrence of $Pr_2(thd)_6$ dimers which comprise the two formula units per asymmetric unit. This dimerization occurs because of the equal sharing of two of the oxygen atoms by praseodymium atoms. As a consequence each praseodymium atom is surrounded by seven oxygen atoms. This coordination geometry is illustrated in Fig. 2.

The coordination polyhedron is not simply octahedral with local distortions in the vicinity of the extra ligand. Apart from the slightly elongated bridge bonds and some molecular constraints, it has pure seven-coordination geometry. Gillespie (1960) described three possible seven-coordination geometries. The second of these, *i.e.* the so-called 1:4:2 type (distorted trigonal prism) is considered the most likely for the present structure since the polyhedron derives directly from the expected octahedral arrangement of the momoner. This geometry can be approximated (see Appendix) by considering six octahedral ligand atoms on the surface of a sphere as in Fig. 3. The introduction of a seventh ligand atom next to atom 6, using the nomenclature of Hush (1962), will leave only number 5 undisturbed and the four equatorial ligand atoms will move down along the surface of the sphere towards number 5 so as to create sufficient space for 7. Numbers 6 and 7 can now move apart by following the paths along the sphere indicated by dashed lines in the diagram. The most probable arrangement is obtained when the separation between

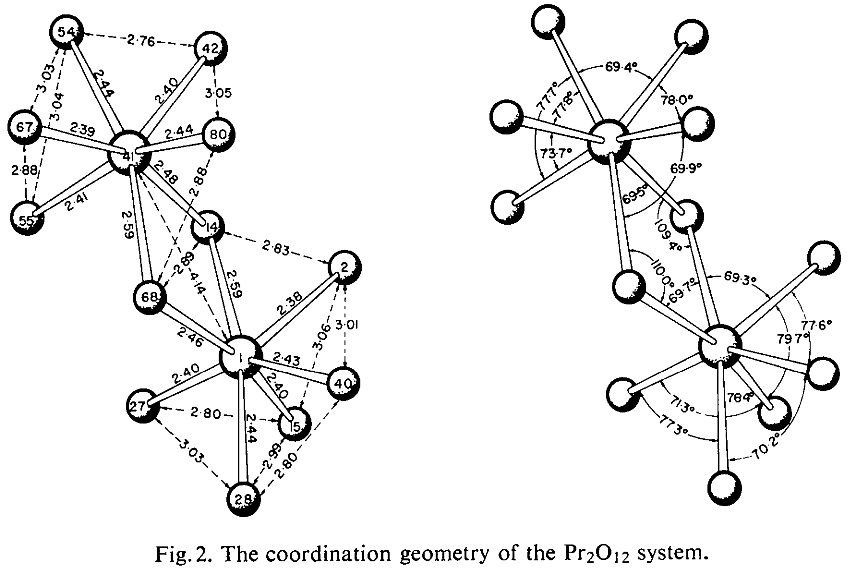

Fig. 2. The coordination geometry of the Pr_2O_{12} system.

equatorial atoms approaches the separation between 5 and any of the equatorial atoms as well as the separations between 1, 2 and 7 and also 3, 4 and 6. Each of the ligand atoms now has four nearest neighbours, except for 6 and 7 which have three each. The angle θ subtended at the centre by nearest neighbours is $\theta \simeq \frac{3}{7}\pi = 77{\cdot}14°$ and the separation d between nearest neighbours at a distance r from the central atom is $d = 2r \sin \theta/2$.

The average Pr–O distance (see Table 5) is 2·446 Å according to which neighbouring oxygen atoms should be 3·05 Å apart. Neighbouring oxygen atoms not involved in the bridging and not belonging to the same ligand are in fact an average distance of 3·03 Å apart, thus subtending an angle of 76·5°. Because of molecular constraint, those belonging to the same ligand are on the average 2·83 Å apart, thus subtending an angle of 70·4°.

Apart from the molecular constraint in the ligand, the bridge oxygen atoms are subject to an additional attraction through the bonding to the Pr atom to which they are not directly chelated. The relationship between a bridging oxygen atom and its neighbours is thus different in the two coordination spheres. In the sphere of the Pr to which it is directly chelated it has two neighbours, one of which is the other bridge oxygen atom, at the molecular distance of about 2·85 Å and two others at a separation of about 3·4 Å. In the sphere of the other Pr, it has one neighbour at 2·85, two at 3·4 and a fourth at about 4·5 Å.

The arrangement as predicted in Fig. 3 can nevertheless be recognized in both coordination spheres as shown in Tables 4, 5 and 6. The two polyhedra are in fact remarkably similar. The two bridging oxygen atoms are involved in one long Pr–O bond each. Surprisingly enough this is with the Pr atoms to which they are directly chelated.

Table 4. *Labelling of oxygen atoms in the polyhedra around* Pr(1) *and* Pr(41) *according to the notation of Fig.* 3

Fig. 3 notation	Pr(1)	Pr(41)
1	15	67
2	14	68
3	68	14
4	28	54
5	27	55
6	40	42
7	2	80

Table 5. *Observed* Pr–O *distances in the polyhedra around* Pr(1) *and* Pr(41) *according to the notation of Table* 4

($\sigma = 0{\cdot}02$ Å)

Oxygen	Pr(1)	Pr(2)
1	2·40	2·39
2	2·59	2·59
3	2·46	2·48
4	2·44	2·44
5	2·40	2·41
6	2·43	2·40
7	2·38	2·44

Table 6. *Geometry of the coordination polyhedra in the notation defined in Table* 4

Bond, $\sigma = 0{\cdot}03$ Å	Pr(1)	Pr(41)
1–2	3·43 Å	3·42 Å
2–3	2·89	2·89
3–4	4·44	4·55
4–1	2·99	3·03
1–5	2·80	2·88
2–5	3·33	3·37
3–5	3·43	3·52
4–5	3·03	3·04
1–7	3·06	3·06
2–7	2·83	2·88
3–6	3·38	3·26
4–6	2·80	2·76
6–7	3·01	3·05

Angle, $\sigma = 0{\cdot}8°$

O–Pr–O	Pr(1)	Pr(41)
1 2	86·8°	86·6°
2 3	69·7	69·5
3 4	130·0	135·2
4 1	76·4	77·8
1 5	71·3	73·7
2 5	83·5	84·7
3 5	89·7	91·9
4 5	77·3	77·7
1 7	79·7	78·6
2 7	69·3	69·9
3 6	87·3	83·7
4 6	70·2	69·4
6 7	77·6	78·0

Stereo diagrams displaying the three-dimensional configuration of the dimer are shown in Fig. 4. These were photographed and redrawn from an inch per Å

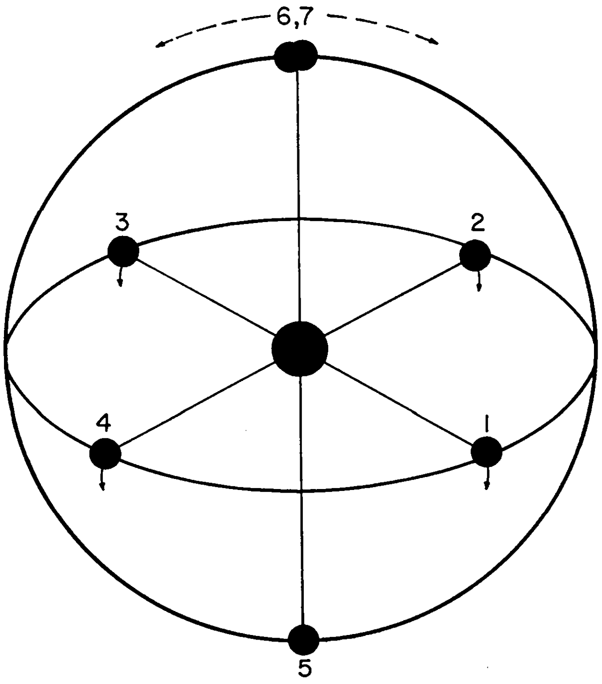

Fig. 3. Diagram to illustrate the seven-coordination geometry obtained by introducing an extra ligand in an octahedral coordination sphere.

model. Bond lengths and angles within the thd rings and their averages over chemically equivalent but crystallographically distinct bond lengths and angles are listed in Table 7. The bond lengths compare favourably with the values listed by Lingafelter & Braun (1966) in their survey of previously reported structures of monomeric acetylacetonato complexes. Notable exceptions are those bonds influenced by distortion effects. All of these are in the immediate vicinity of the bridging oxygen atoms and are invariably longer than the literature average. The bond angles which are known to be more sensitive to steric influences show a much larger scatter of up to 15°.

The bonds between tertiary and carbonyl carbon atoms have an average length of 1·56 Å which agrees fairly well with the values obtained in $Zn(thd)_2$ (Cotton & Wood, 1964) and $Ni(thd)_2$ (Cotton & Wise, 1966). Because of possible disorder, as indicated by exceptionally high thermal parameters, the positions of the methyl groups are poorly determined. The average bond length of 1·53 Å between methyl groups and the tertiary carbon atoms is, however, acceptable. The same applies to the bond angles within the tertiary butyl groups. Despite large deviations from the mean these groups are on the average tetrahedral. The intermolecular contacts are all between methyl groups, as shown in Fig. 5. Exceptionally loose packing is indicated by the fact that these approaches are all more than 4 Å.

Discussion of the structure

From first principles the chelate rings including the central metal ion are expected to be planar. In practice (Bennet, Cotton, Legzdins & Lippard, 1968; Cotton & Wood, 1964), however, it is found that although the acetylacetonato portions (O–C–C–C–O) are planar (Lingafelter, 1966; Cotton & Wise, 1966) the central ion is often displaced from this plane. To illustrate a similar effect in the present structure the best plane through each acetylacetonato portion and the deviations from this plane of all atoms associated with the chelate system concerned, were computed.

The numerical solutions obtained by a method of least-squares and displacements from these planes are given in Table 8. These results show the expected displacement of the Pr atoms from the planes although rings *C* and *D* should be considered as flat within experimental error. The deformations of the rings considered in pairs similarly disposed towards the Pr atoms are remarkably similar. The bending is particularly

Table 7. *Bond lengths and angles*

The subscripts *c*, *s*, *t* and *m* signify carbonyl, secondary, tertiary and methyl. Values marked by asterisks were not included in the averaging.

Bond	*A*	*B*	*C*	*D*	*E*	*F*	σ	Average	Literature
$O-C_c$	1·27 Å	1·32 Å	1·29 Å	1·26 Å	1·32 Å	1·40 Å*			
	1·33*	1·29	1·27	1·25	1·26	1·28	0·03 Å	1·28 Å	1·29 Å
C_c-C_s	1·51	1·41	1·39	1·41	1·43	1·40			
	1·36	1·34	1·44	1·46	1·42	1·46	0·04	1·42	
C_c-C_t	1·59	1·61	1·57	1·54	1·55	1·53			
	1·53	1·55	1·55	1·53	1·63	1·58	0·05	1·56	1·52
C_t-C_m	1·58	1·51	1·50	1·54	1·55	1·55			
	1·54	1·50	1·41	1·56	1·57	1·55			
	1·48	1·58	1·56	1·65	1·52	1·47			
	1·60	1·53	1·55	1·48	1·54	1·47			
	1·53	1·55	1·57	1·49	1·58	1·54			
	1·60	1·34	1·57	1·49	1·48	1·54	0·06	1·53	1·52
Angle									
$Pr-O-C_c$	131°	135°	138°	139°	130°	116°*			
	114*	133	138	139	134	130	2°	134·8°	136·8°
$O-C_c-C_s$	128	123	124	125	129	121			
	132	129	124	123	128	122	3°	125·6	125·3
$O-C_c-C_t$	115	112	113	113	112	115			
	111	112	112	118	111	113	3°	113·1	114·8
$C_c-C_s-C_c$	115*	124	125	122	121	129	3·5	124·1	124·0
$C_s-C_c-C_t$	117	125	123	122	119	124			
	117	119	124	119	121	125	3·5	121·1	124·1
$C-C_t-C$	108	108	111	111	115	108			
	107	111	109	110	112	112			
	115	106	111	110	109	112			
	107	114	123	110	105	107			
	112	107	108	107	109	104			
	108	110	95*	109	107	114			
	112	103	109	117	109	112			
	116	112	114	106	112	105			
	107	117	108	109	108	109			
	108	103	106	117	107	111			
	110	114	109	106	107	107			
	103	107	112	102	113	113	4		
Average	109·4	109·3	109·4	109·4	109·4	109·4		109·4	109·4

large for the chelate rings (*A* and *F*) involved in the bridging as has been observed previously for other polymeric acetylacetonato complexes (Lingafelter, 1966; Cotton & Wise, 1966; Bennet *et al.*, 1968). Specific explanations based on various kinds of intermolecular interactions have been proposed in individual cases. It seems more reasonable, however, to assume this folding of the rings to be a natural consequence of the essential ionic character of the β-diketonates. If the tris chelates are formulated at $M^{3+}[(RCO)_2CH^-]_3$, only the organic part of the ring is expected to be planar because of π-electron delocalization.

Furthermore the coordination geometry would not be fixed by orbital hybridization, but by electrostatic

Table 8. *Equations to the best planes through the six chelate rings not considering* Pr *positions but including tertiary carbon atoms, and the deviations* (*in* Å × 10^3) *of individual atoms from these planes*

The equations to the planes were obtained in the form $lu+mv+nw=d$, where u, v and w are orthogonal coordinates related to the fractional monoclinic coordinates by the equations

$$u=xa+zc\cos\beta$$
$$v=yb$$
$$w=zc\sin\beta$$

Ring	*l*	*m*	*n*	*d*
A	−0·01993	0·98959	−0·14250	0·44067
B	0·08596	−0·31166	0·94630	10·43785
C	0·86615	−0·34668	−0·36000	−1·99575
D	−0·12724	0·81101	0·57103	8·62294
E	−0·16593	−0·51614	0·84028	6·16325
F	0·77415	−0·47416	0·41936	4·44801

	A	*B*	*C*	*D*	*E*	*F*
Pr	−1240	471	54	61	−502	−1371
O	−220	−15	89	−111	55	204
C_c*	−34	17	19	8	2	15
C_t	144	−13	−88	27	−11	−122
C_s	0	32	53	60	−41	20
C_t	−116	−11	19	−81	49	127
C_c	−16	−26	13	−10	3	−36
O	240	16	−105	107	−56	−209

* Subscripts in as Table 7.

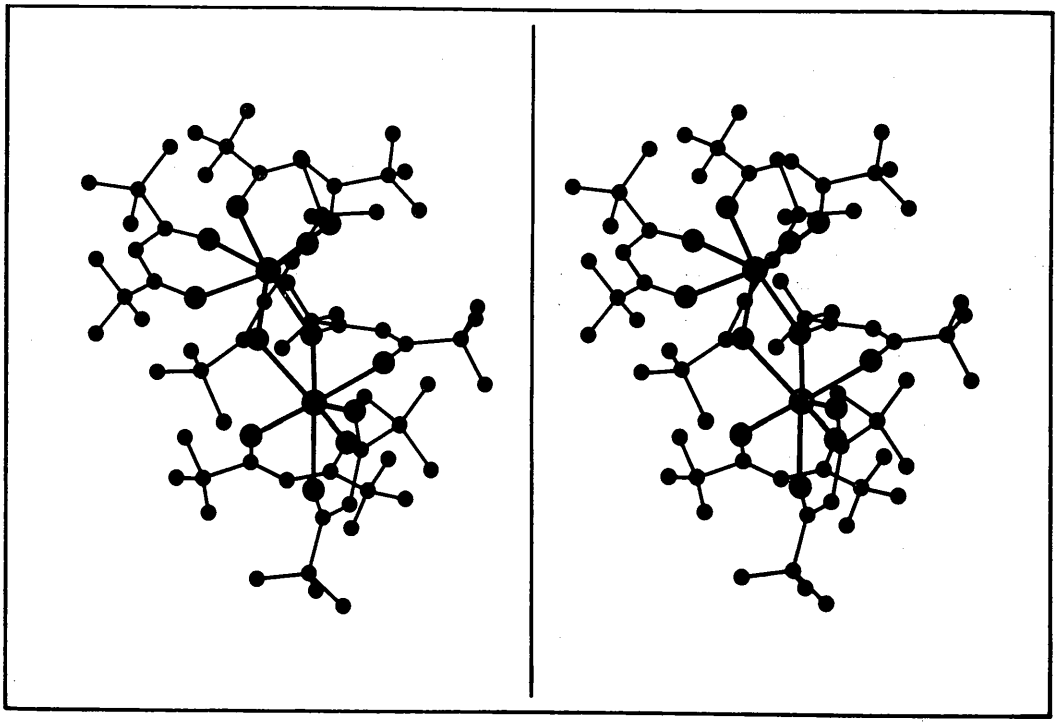

Fig. 4. Stereoscopic drawing showing the full three-dimensional structure of the dimer. This Figure should be viewed with a stereo viewer.

considerations. On this basis one expects the central ion to be surrounded by the maximum number of ligand atoms allowed by steric factors. These would arrange themselves according to the principle of maximum electrostatic repulsion (Dunitz & Orgel, 1960) allowing for deviations because of molecular constraints and secondary interactions. In this respect it would be instructive to study the structures of the dimethylformamide adducts formed by the thd lanthanide complexes (Schwarberg, Gere, Sievers & Eisentraut, 1967) to see whether an extra ligand atom is introduced between oxygen atoms 41 and 54 (28 and 68) to raise the coordination to eight.

The central ring defined by the bridging oxygen atoms and the Pr atoms was also investigated for planarity. The equation to the best plane is $0{\cdot}8018u+0{\cdot}5418v+0{\cdot}2521w=5{\cdot}664$. The displacements from this plane are: Pr(1) 0·097, Pr(41) 0·097, O(14) −0·096, O(68) −0·097 Å.

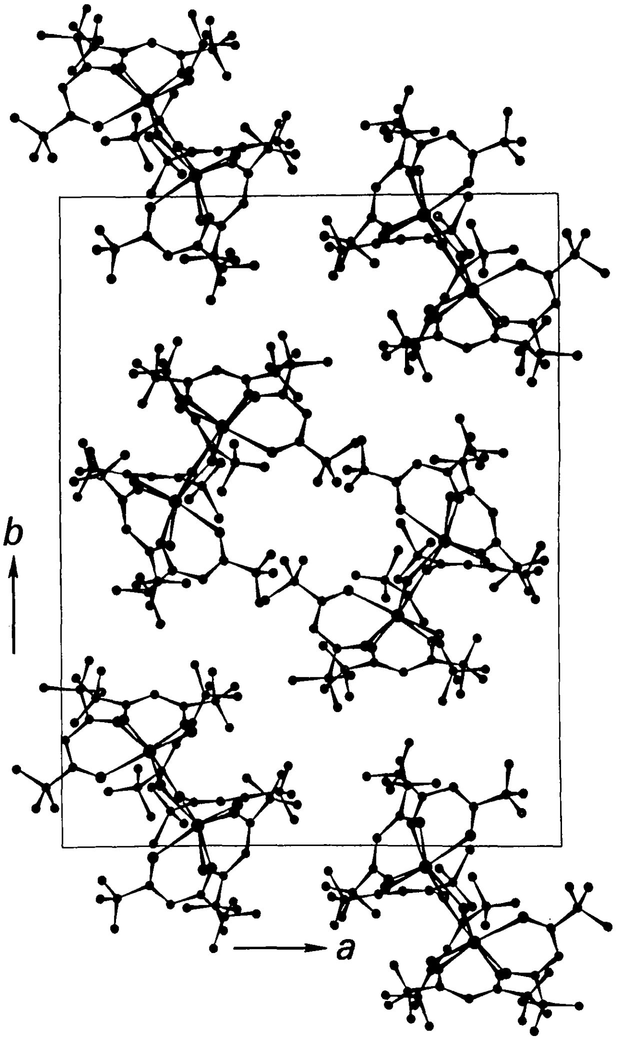

Fig. 5. Projection of the unit cell content down [001] to illustrate the packing.

The only structural feature that could throw some light on the volatility of the complex is the exceptionally high thermal parameters observed for the methyl groups. The average $B=9{\cdot}7$ Å^2 is interpreted as static disorder rather than thermal motion. This indicates rather weak and poorly directed intermolecular interactions since the dimeric molecule is almost completely enveloped by methyl groups. Intermolecular cohesion is therefore low and hence the vapour pressure is relatively high. Whether the dimers persist in the vapour phase is not known at this stage. If not, the relatively open shell of the monomer should drastically increase chromatographic retention times.

It is not yet known whether dimers also occur in the orthorhombic structure of the thd complexes of the heavy lanthanides. Assuming the bite of 2·83 Å observed in the present structure to be characteristic throughout the series, an upper limit for the occurrence of seven coordination can, however, be predicted since it seems unlikely that interligand O–O separations of less than this value can occur. The limiting Ln–O separation at which all thirteen nearest oxygen neighbours in the coordination polyhedron are 2·83 Å apart can be calculated from $2r\sin\theta/2=2{\cdot}83$ as $r=2{\cdot}27$ Å. This would occur for the lanthanide with an ionic radius of 0·14 Å smaller than Pr. It follows that seven coordination and hence dimerization becomes impossible towards the end of the lanthanide series.

APPENDIX

The most probable geometry for the coordination sphere was derived as follows:

Let ligands 6 and 7 in Fig. 3 each move down the sphere for a distance δ and let each of the equatorial ligands move down through a distance s. The equatorial ligands are now at a distance $a=(\pi r/2)-s$ from 5 and $(\pi r/2)+s=d$ from the original position of 6. Ligands 6 and 7 are a distance 2δ apart. Let the distance between 1, 2 and 7 or between 3, 4 and 6 be denoted by x. It follows that for $\delta=0$, $x=d$ and for $\delta=d$, $x=e/2$, where e is the distance between neighbouring equatorial ligands. This can be expressed as

$$x=\left(\frac{e}{2d}-1\right)\delta+d\,.$$

Let $x=e=2\delta=a$,

$$\text{then } a=\left(\frac{a}{2d}-1\right)\frac{a}{2}+d\,.$$

It follows that $a=(3-\sqrt{5})d\simeq\frac{3}{4}d$

$$\text{or } \left(\frac{\pi r}{2}-s\right)=\tfrac{3}{4}\left(\frac{\pi r}{2}+s\right)$$

$$s=\pi r/14\,.$$

$$\text{Therefore,}\qquad a=\pi r(\tfrac{1}{2}-\tfrac{1}{14})$$

$$=\tfrac{3}{7}\pi r\,.$$

Although this solution is geometrically impossible (compare Schütte & van der Waerden, 1951) it is a useful approximation in terms of which to describe the observed coordination.

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A Rotational Search Procedure for Detecting A Known Molecule In a Crystal*

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A computationally swift modification of the Rossmann–Blow rotation function has been developed. With the use of this function the single chains present in the D2 crystals of hemoglobin from the sea lamprey, *Petromyzon marinus*, have been shown to resemble the sperm-whale metmyoglobin molecule, and the orientation of the lamprey hemoglobin molecules in the unit cell of this crystal has been found. The results are confirmed by the crystal structure analysis of lamprey hemoglobin.

Introduction

The oxygen-carrying heme proteins from a variety of sources have similar tertiary structures, but occur in widely differing crystal forms. In particular, the α- and β-chains of horse and human hemoglobin (Cullis, Muirhead, Perutz, Rossmann & North, 1962; Muirhead, Cox, Mazzarella & Perutz, 1967), the single chains of the hemoglobins from the common bloodworm, *Glycera dibranchiata* (Padlan & Love, 1968) and from the larval form of the fly, *Chironomus thummi*, (Huber, Formanek & Epp, 1968), and the single chains of seal and sperm-whale myoglobin (Scouloudi, 1969; Bodo, Dintzis, Kendrew & Wyckoff, 1959) all appear to have essentially the same topology when viewed at low resolution, although the crystallographic arrangements in which they are found are quite diverse. The α- and β-chains of horse methemoglobin, for example, are nearly identical with those of human deoxyhemoglobin (Muirhead *et al.*, 1967), but the assembly into tetramers is somewhat different in the two cases, and the packing of these tetramers into their unit cells is very different indeed.

Situations like the above, in which a known molecular structure occurs in a variety of interesting crystallographic arrangements, are likely to arise for many large and important biological molecules. Much labor would be saved in these cases if the relevant crystal structures were determined starting from the known molecular structure, rather than *ab initio*. To piece together a structure in this way one must be able to find the orientation and location of each molecule in the unit cell. The problem of fixing the translations has been attacked by Nordman & Nakatsu (1963), Rossmann, Blow, Harding & Coller (1964), Tollin (1966) and Crowther & Blow (1967). The fundamental work on determining the orientations is that of Rossmann & Blow (1962). Tollin (1969) has combined these techniques to effect a complete protein structure determination.

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