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BIS(PENTAMETHYLCYCLOPENTADIENYL)CARBOXYLATO AND DITHIOCARBAMATO DERIVATIVES OF NEODYMIUM(III) AND YTTERBIUM(III) . CRYSTAL STRUCTURE OF BIS (PENTAMETHYL-CYCLOPENTADIENYL) DIETHYLDITHIOCARBAMATOYTTERBIUM(III)

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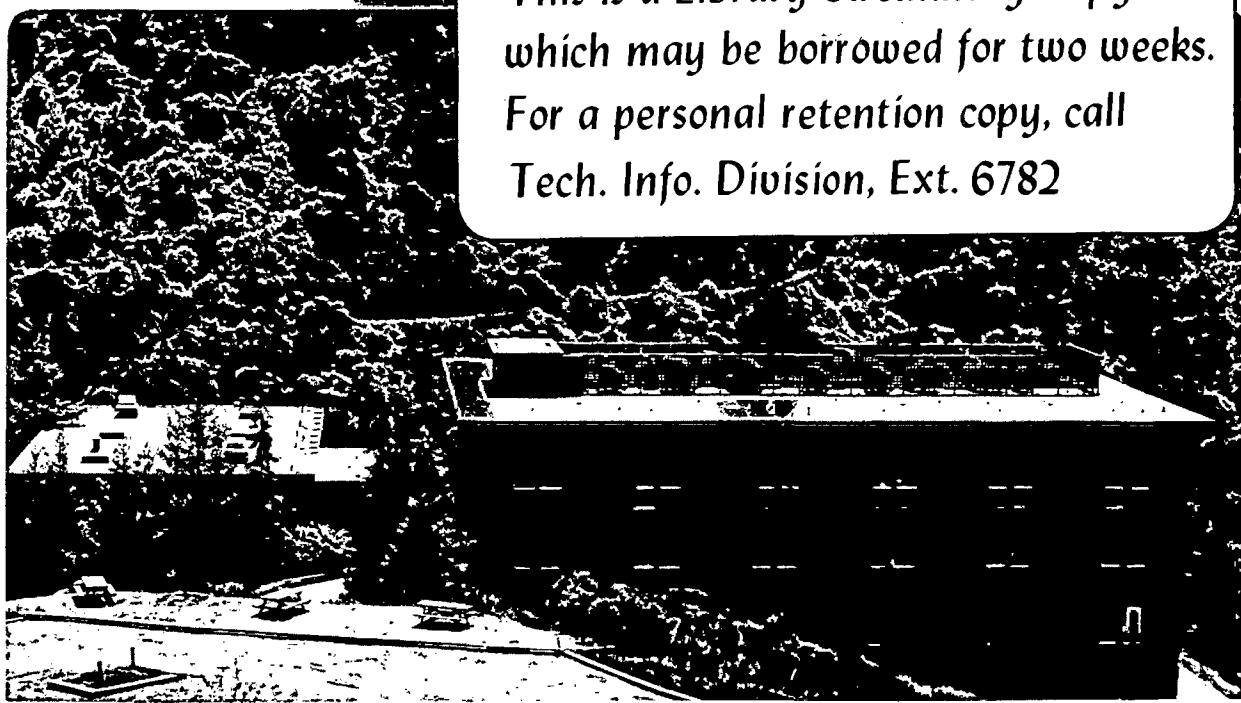
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July 1981

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ABSTRACT

The pentamethylcyclopentadienyl derivatives,  $(Me_5C_5)_2Yb(O_2CR)$  where R is  $Me_3C$  or  $CF_3$ ,  $(Me_5C_5)_2Yb(S_2CNET_2)$  and  $(Me_5C_5)_2Nd(S_2CNET_2)$  have been prepared by metathetical exchange reactions on the anionic species,  $[(Me_5C_5)_2MCl_2]^-$ . The crystal structure of  $(Me_5C_5)_2Yb(S_2CNET_2)$  has been determined by single crystal X-ray diffraction methods. The crystals are monoclinic, C2/c, with cell dimensions  $a = 12.268(4) \text{ \AA}$ ,  $b = 15.536(6) \text{ \AA}$ ,  $c = 14.269(5) \text{ \AA}$ ,  $\beta = 105.23(3)^\circ$  and  $V = 2624 \text{ \AA}^3$ . For  $Z = 4$  the calculated density is  $1.14 \text{ g/cm}^3$ . The structure was refined to a conventional R factor of 0.039 using 2179 data where  $F^2 > 3\sigma(F^2)$ . The Yb(III) atom is bonded to two sulfur atoms and to two pentamethylcyclopentadienyl

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groups. The Yb atom lies on a crystallographic two-fold axis. The dithiocarbamato ligand is disordered in the structure. The Yb-S distance is 2.70(1) Å, and the average of 5 Yb-C distances is 2.63(3) Å.

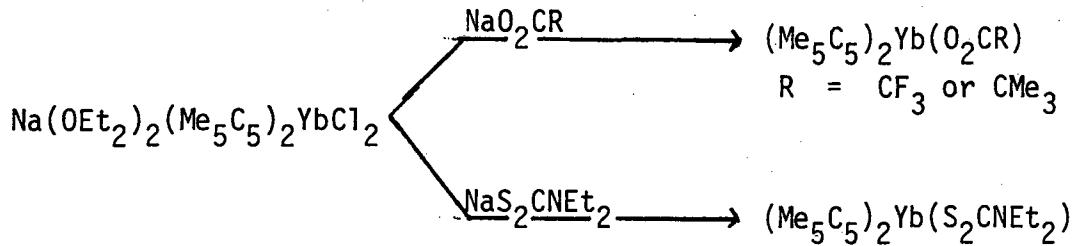
## INTRODUCTION

In attempting to develop the chemistry of reactive organometallic lanthanide systems, we have had an interest in preparing neutral, base-free pentamethylcyclopentadienyl derivatives of the di- and trivalent metals. The strong Lewis-acidic nature of these metals has led to isolation of trivalent species such as  $(C_5Me_5)_2YbCl_2Na(OEt_2)_2$  and  $(C_5Me_5)_2YbCl(\text{thf})$ ,<sup>1,2</sup> as well as the divalent species  $Yb(C_5Me_5)_2(\text{thf})$  and  $Eu(C_5Me_5)_2(\text{thf})$ .<sup>3</sup> The neutral base-free systems are of interest since these coordinatively unsaturated species are expected to exhibit a rich chemistry and, perhaps, to lead to compounds of unusual structural types.

Isolation of  $(C_5Me_5)_2YbCl_2Na(OEt_2)_2$  and  $(C_5Me_5)_2YbCl(\text{thf})$  suggests that a chelating ligand that can donate four electrons to the metal could yield neutral, base-free trivalent compounds. Such compounds might then be useful for preparation of the base-free ytterbium(II) metallocenes, if reduction in a non-coordinating solvent can be effected. Since carboxylate  $(RCO_2^-)$  ligands have been effectively utilized as leaving groups in transition metal chemistry, they seemed to be ideally suited for this task. Another chelating ligand, diethyldithiocarbamate ( $Et_2NCS_2^-$ ), is electronically similar, but contains the softer sulfur atoms as donors. Because little is known about the properties of sulfur-based ligands in molecular lanthanide systems, we have conducted a low-temperature magnetic susceptibility study, as well as an X-ray crystal structure determination of  $(C_5Me_5)_2Yb(S_2CNET_2)$ .

## RESULTS AND DISCUSSION

Preparation of the carboxylate and dithiocarbamate derivatives of ytterbium is straightforward. The analogous neodymium dithio-



carbamate, (Me<sub>5</sub>C<sub>5</sub>)<sub>2</sub>Nd(S<sub>2</sub>CNET<sub>2</sub>), was prepared similarly. The physical properties are described in the experimental section. Because two donor atoms are present, R<sub>2</sub>CO<sub>2</sub><sup>-</sup> and the softer Et<sub>2</sub>NCS<sub>2</sub><sup>-</sup> allow isolation of ether-free complexes. Unfortunately the ytterbium(III) species could not be reduced with sodium amalgam in refluxing toluene. Further, (Me<sub>5</sub>C<sub>5</sub>)<sub>2</sub>YbN(SiMe<sub>3</sub>)<sub>2</sub><sup>1</sup> could not be reduced under similar conditions.

The similarity in the magnetic behavior of (C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>Yb(O<sub>2</sub>CCMe<sub>3</sub>) and (C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>Yb(S<sub>2</sub>CNET<sub>2</sub>) at low temperature (see experimental section) suggests that the magnetic properties of the ytterbium ions in these complexes are not effected by the change from carboxylate to dithiocarbamate ligand. The magnetic moments (5-45K), 3.29 and 3.39 B.M., respectively, are close in value to those observed for other ytterbium(III) complexes over this temperature range.<sup>1,4,5</sup>

The ytterbium dithiocarbamate complex crystallizes as well-formed, purple prisms that are monoclinic, space group C2/c, with cell dimensions  $a = 12.268(4)$  Å,  $b = 15.536(6)$  Å,  $c = 14.269(5)$  Å, and  $\beta = 105.23(3)^\circ$ . For  $Z = 4$  and a molecular weight of 652.98, the calculated density is 1.14 g/cm<sup>3</sup>. A few structures containing lanthanide to sulfur bonds have been determined,<sup>6,7,8</sup> but the present structure is the first example of an Yb-S bond.

Positional parameters, with labelling as shown in Fig. 1, are given in Table I. A list of selected distances and angles are given in Tables II and III.

The molecule consists of the Yb atom bonded to two pentamethylcyclopentadienyl rings and to two sulfur atoms of the diethyldithiocarbamate ligand, Fig. 1. The average of five Yb-C distances is  $2.63 \pm 0.03$  Å and the Yb-S distance is 2.70 Å. The pentamethylcyclopentadienyl rings are in a staggered configuration with respect to each other, see Fig. 2. The diethyldithiocarbamate ligand is disordered; atoms N, C(12A), C(13A), C(12B) and C(13B) are in general positions with half of the molecules in the given conformation (Fig. 1) and half in the conformation that would result from a  $180^\circ$  rotation about the two-fold axis. The sulfur atoms are most probably disordered as well, as seen by their elliptical shape in Fig. 1, but the separation of the two positions was too small to be treated in the least-squares as separate half-atoms and instead was refined as a large thermally anisotropic atom. Because of this disorder the molecule as a whole has low symmetry  $C_1$ , however the

$(Me_5C_5)_2Yb$  part of the molecule has perfect  $C_2$  symmetry. Attempts to define the structure in a lower symmetry space group were unsuccessful.

The Yb-C distances (to the  $C_5$  ring) average  $2.63 \pm 0.03 \text{ \AA}$ . The Yb atom is  $2.33 \text{ \AA}$  from the mean plane of atoms C(1) though C(5). These ring atoms are all within  $0.006 \text{ \AA}$  of this plane. The five methyl carbon atoms of the pnetamethylcyclopentadienyl group are all bent out of the mean plane away from the Yb atom; the distances from the plane are 0.18, 0.19, 0.12, 0.07 and  $0.34 \text{ \AA}$  for atoms C(6) through C(10), respectively.

The ytterbium-carbon bond length of  $2.63 \pm 0.03 \text{ \AA}$  in the trivalent, dithiocarbamate complex is identical within experimental error to that found for this bond length ( $2.66 \pm 0.01 \text{ \AA}$ ) in the divalent species,  $(Me_5C_5)_2Yb(\text{thf})$ .<sup>3</sup> Since the oxidation state and coordination number of the latter are one less than the former, both quantities are important in determining average metal to ligand bond lengths.<sup>9</sup>

## EXPERIMENTAL

All operations were carried out under nitrogen. Microanalyses were performed by the microanalytical laboratory of this department. Infrared spectra were recorded on a Perkin-Elmer instrument as Nujol mulls between cesium iodide windows. The  $^1\text{H}$  NMR spectra were recorded on a JEOL-FX90Q instrument on toluene-d<sub>6</sub> solutions and are reported in  $\delta$ -units (positive values to high field of Me<sub>4</sub>Si). Solid state magnetic susceptibilities were obtained as previously described.<sup>10</sup>

Bis(pentamethylcyclopentadienyl)(2,2-dimethylpropionato)ytterbium (III). Sodium bis(pentamethylcyclopentadienyl)dichloroytterbium bis(diethylether)<sup>5</sup> (1.7 g, 0.0025 mol) in diethyl ether (30 mL) was added to a suspension of sodium 2,2-dimethylpropionate [prepared by stirring sodium hydride with pivalic acid in diethyl ether for 12 h] (0.31 g, 0.0025 mol) in diethyl ether (20 mL). After stirring for 6 h the red solution was evaporated to dryness and the residue was extracted with pentane (35 mL). The extract was filtered and cooled (-70°C). The red prisms (0.65 g, 48%) were collected and dried under reduced pressure, mp 154-155°C. Anal. Calcd for C<sub>25</sub>H<sub>39</sub>O<sub>2</sub>Yb: C, 55.1; H, 7.22. Found: C, 55.2; H, 7.19. The mass spectrum gave a monomeric molecular ion (545) as well as peaks due to higher oligomers at 924, 889, 820, 802, 749, 612, and 571.  $^1\text{H}$  NMR (+35°C):  $\delta$  10.95 ( $\nu_{1/2} = 107$  Hz), 30 H;  $\delta$  - 26.45 ( $\nu_{1/2} = 21$  Hz), 9 H. IR: 2713 w, 1503 m, 1489 m, 1430 m, 1225 s, 1169 w, 1064 w, 1026 m, 940 w, 896 s, 810 m, 793 m, 617 m,

474 w, 408 m, 388 m, 319 s,  $\text{cm}^{-1}$ . The magnetic susceptibility followed Curie behavior from 5-35 K, with  $\mu_B = 3.29$  B.M.

Bis(pentamethylcyclopentadienyl)(trifluoroacetato)ytterbium(III).

The salt,  $\text{Na(OEt}_2)_2(\text{Me}_5\text{C}_5)_2\text{YbCl}_2$  (1.1 g, 0.0016 mol) in tetrahydrofuran (30 mL) was added to  $\text{NaO}_2\text{CCF}_3$  (0.22 g, 0.0016 mol) in tetrahydrofuran (10 mL) and the red solution was stirred for 12 h. The tetrahydrofuran was removed under reduced pressure and the residue was extracted with diethyl ether (2 x 40 mL). The extract was filtered, and cooling (-10°C) yielded violet prisms in 57% (0.50 g) yield, mp 262-263°C. Anal. Calcd for  $\text{C}_{22}\text{H}_{30}\text{F}_3\text{O}_2\text{Yb}$ : C, 47.5; H, 5.43. Found: C, 47.7; H, 5.49. The mass spectrum afforded a monomeric molecular ion at 557. IR: 3140 w, 3092 w, 2726 w, 1680 s, 1204 s, 1158 s, 1023 w, 847 m, 785 m, 718 m, 614 w, 592 w, 523 w, 468 w, 385 m, 312 s,  $\text{cm}^{-1}$ .

Bis(pentamethylcyclopentadienyl)(diethyldithiocarbamato)ytterbium(III).

The anionic complex,  $\text{Na(OEt}_2)_2(\text{Me}_5\text{C}_5)_2\text{YbCl}_2$  (1.4 g, 0.0020 mol) in diethyl ether (40 mL) was added to sodium diethyldithiocarbamate (0.35 g, 0.0020 mol) in diethyl ether (20 mL). After stirring for 8 h the diethyl ether was removed under reduced pressure. The residue was extracted with pentane (40 mL), and filtered. Concentration of the filtrate to ca. 10 mL and cooling (-10°C) yielded purple prisms in 81% (0.97 g) yield, mp 226-227°C. Anal. Calcd for  $\text{C}_{25}\text{H}_{40}\text{NS}_2\text{Yb}$ : C, 50.7; H, 6.81; N, 2.37; S, 10.8. Found: C, 50.7; H, 6.76; N, 2.29; S, 10.7. The mass spectrum

gave a monomeric molecular ion at 592.  $^1\text{H}$  NMR (+35°C):  $\delta$  7.45 ( $\nu_{1/2} = 61$  Hz), 30 H;  $\delta$  - 5.76 ( $\nu_{1/2} = 18$  Hz), 4 H;  $\delta$  - 9.00 ( $\nu_{1/2} = 13$  Hz), 6 H. All of the resonances were singlets. IR: 2723 w, 1487 s, 1424 s, 1360 m, 1306 w, 1277 s, 1209 m, 1241 m, 1089 m, 1023 w, 987 m, 911 m, 841 m, 800 w, 779 w, 608 w, 593 w, 564 m, 473 w, 392 m, 360 m, 311 s,  $\text{cm}^{-1}$ . The magnetic susceptibility followed Curie behavior (5-55 K), giving  $\mu_B = 3.39$  B.M.

Bis(pentamethylcyclopentadienyl)(diethyldithiocarbamato)neodymium (III). The anionic complex,  $\text{Li(OEt}_2)_2(\text{Me}_5\text{C}_5)_2\text{NdCl}_2$ , (2.2 g, 0.034 mol) in diethyl ether (40 mL) was added to  $\text{NaS}_2\text{CNET}_2$  (0.58 g, 0.0034 mol) in diethyl ether (20 mL). After stirring for 8 h the green solution was filtered and the filtrate was concentrated to ca. 30 mL. Cooling (-10°C) yielded green prisms in 72% (1.4 g) yield, mp 229-231°C. Anal. Calcd for  $\text{C}_{25}\text{H}_{40}\text{NNdS}_2$ : C, 53.3; H, 7.16; N, 2.49. Found: C, 53.5; H, 7.03; N, 2.47. The mass spectrum gave a monomeric molecular ion at 562.  $^1\text{H}$  NMR (+70°C):  $\delta$  7.00 ( $\nu_{1/2} = 23$  Hz), 30 H;  $\delta$  - 0.10 ( $\nu_{1/2} = 17$  Hz), 4 H;  $\delta$  - 0.94 ( $\nu_{1/2} = 16$  Hz), 6 H. The resonances were singlets. IR: 2722 w, 1482 s, 1420 s, 1357 m, 1402 w, 1273 s, 1203 s, 1138 m, 1087 m, 1063 w, 1021 w, 979 m, 905 m, 836 m, 798 w, 773 w, 607 w, 560 m, 470 w, 430 w, 382 m, 348 m, 310 s,  $\text{cm}^{-1}$ . The magnetic susceptibility followed Curie behavior (5-50 K) giving  $\mu_B = 2.75$  B.M.

Some of the air sensitive purple crystals were inserted into thin walled quartz capillaries in an argon filled dry box. A crystal was examined with a Picker FACS-I automated diffractometer equipped with a graphite monochromator and a Mo X-ray tube ( $\lambda(K\alpha_1)$  0.70930 Å). Omega scans of several low angle reflections showed peaks with half-widths of 0.13° to 0.20°. The space group is C2/c. The setting angles of twelve manually centered reflections ( $4 < 2\theta < 49^\circ$ ) were used to determine cell parameters by least-squares.

Intensity data were collected using a  $\theta$ - $2\theta$  scan technique with a scan speed of 2°/min on  $2\theta$ . Each peak was scanned 0.9° before the  $K\alpha_1$  peak to 0.9° after the  $K\alpha_2$  peak, and backgrounds were counted for 10 s at each end of the scan range. The temperature during the data collection was  $24 \pm 1^\circ\text{C}$ . Three standard reflections were measured every 250th scan. A total of 4748 scans ( $4^\circ < 2\theta < 45^\circ$ ) yielded 2327 unique data of which 2175 had  $F^2 > 3\sigma$ . Absorption correction ( $\mu = 37.0 \text{ cm}^{-1}$ ) was applied<sup>11</sup> which ranged from 1.53 to 1.98. The intensities of the three standard reflections decayed about 4% during the data collection period and the data were corrected for this effect.

A three dimensional Patterson calculation showed the Yb and S atom positions, and a subsequent least-squares refinement and Fourier calculation revealed all the non-hydrogen atoms in the structure. After a few cycles of least-squares refinements of the structure in which only the Yb and S atoms were assigned anisotropic thermal parameters the R factor,  $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ , was 0.055.

The ethyl carbon atoms of the diethyldithiocarbamate ligand were ill behaved in the refinements as indicated by large thermal parameters and chemically unsatisfactory bond distances to adjacent atoms. A difference Fourier map showed additional electron density in the region of the ethyl carbon atoms as well as the nitrogen atom, indicating disorder. The two ethyl carbon atoms were subsequently described as four half-atoms and the nitrogen atom was allowed to wander from the special position on the two-fold axis. With further refinements the structural parameters converged to their final and satisfactory results. Several attempts were made to refine the structure in the non-centric space group Cc, but the resulting structure would not converge to a reasonable chemical model, and the resulting R factors, despite the increased number of parameters, were not significantly different from the centric refinements. The least-squares function used minimizes the function  $\Sigma w(|F_o| - |F_c|)^2 / \Sigma w F_o^2$ . The expressions used in processing the data and estimating weights are given in the supplementary material; the "ignorance factor" was set to 0.05. Scattering factors from International Tables<sup>12</sup> and anomalous dispersion corrections<sup>13</sup> were applied. In the final refinement all of the atoms with the exception of the carbon atoms in the dithiocarbamate ligand were assigned anisotropic thermal parameters. Hydrogen atoms were not included.

The discrepancy indices for 2175 data were  $F^2 > 3\sigma$  are

$$R = \Sigma ||R_o| - |F_c|| / \Sigma |F_o| = 0.039$$

$$R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2} = 0.052$$

R for all 2327 data is 0.041. The error in an observation of unit weight is 1.84. In the last cycle, no parameter changed more than 0.1  $\sigma$ . In the final difference Fourier the largest electron density peak was  $\sim 0.5 \text{ e}/\text{\AA}^3$  and was near the Yb atom.

#### ACKNOWLEDGMENT

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#### SUPPLEMENTARY MATERIAL AVAILABLE

Data processing formulas, the table of thermal parameters and the listing of structure factor amplitudes (10 pages). Ordering information is given on any current masthead page.

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Table I. Positional Parameters<sup>a</sup>

Atom	X	y	z
YB	0	.20517(2)	.250
S	.0541(2)	.3539(1)	.3565(1)
N	.0376(8)	.4957(6)	.2433(9)
C(1)	.1806(5)	.1109(4)	.3012(4)
C(2)	.2238(5)	.1953(4)	.2979(5)
C(3)	.1918(6)	.2255(4)	.2007(5)
C(4)	.1295(5)	.1593(4)	.1426(4)
C(5)	.1228(5)	.0883(4)	.2039(4)
C(6)	.2873(6)	.0528(6)	.3897(6)
C(7)	.3844(7)	.2424(7)	.3808(6)
C(8)	.2298(8)	.3101(6)	.1665(8)
C(9)	.0840(8)	.1608(6)	.0334(5)
C(10)	.0880(7)	-.0017(5)	.1665(7)
C(11)	0	.4078(8)	.250
C(12A)	.108(2)	.544(1)	.330(2)
C(13A)	.031(3)	.580(2)	.384(3)
C(12B)	.005(1)	.541(1)	.151(1)
C(13B)	-.116(2)	.577(2)	.125(2)

<sup>a</sup>Here and in the following tables the number in parentheses is the estimated standard deviation in the least significant digit.

Table II. Interatomic Distances ( $\text{\AA}$ )

Yb	- 2 C(1)	2.63(1)	C(1) - C(2)	1.42(1)
Yb	- 2 C(2)	2.66(1)	C(2) - C(3)	1.42(1)
Yb	- 2 C(3)	2.64(1)	C(3) - C(4)	1.41(1)
Yb	- 2 C(4)	2.60(1)	C(4) - C(5)	1.42(1)
Yb	- 2 C(5)	2.60(1)	C(5) - C(1)	1.43(1)
Yb	- 2 S	2.70(1)	C(1) - C(6)	1.52(1)
S	- C(11)	1.71(1)	C(2) - C(7)	1.52(1)
C(11)	- N	1.45(2)	C(3) - C(8)	1.52(1)
N	- C(12A)	1.50(2)	C(4) - C(9)	1.51(1)
N	- C(12B)	1.46(2)	C(5) - C(10)	1.52(1)
C(12A)	- C(13A)	1.49(4)		
C(12B)	- C(13B)	1.53(3)		

Table III. Selected angles (deg.)<sup>a</sup>

S	- Yb	- S'	67.1(3)	C(5) - C(1) - C(2)	107(1)
C(1)	- Yb	- S	105.2(3)	C(1) - C(2) - C(3)	109(1)
C(2)	- Yb	- S	80.7(2)	C(2) - C(3) - C(4)	108(1)
C(3)	- Yb	- S	88.0(2)	C(3) - C(4) - C(5)	108(1)
C(4)	- Yb	- S	118.9(2)	C(4) - C(5) - C(1)	108(6)
C(5)	- Yb	- S	132.2(2)	C(6) - C(1) - C(2)	125(1)
C(1)	- Yb	- S'	134.8(2)	C(6) - C(1) - C(5)	127(1)
C(2)	- Yb	- S'	107.3(2)	C(7) - C(2) - C(1)	126(1)
C(3)	- Yb	- S'	82.8(2)	C(7) - C(2) - C(3)	124(1)
C(4)	- Yb	- S'	90.8(3)	C(8) - C(3) - C(2)	125(1)
C(5)	- Yb	- S'	122.2(3)	C(8) - C(3) - C(4)	127(1)
S	- C(11) - S'		121.4(8)	C(9) - C(4) - C(3)	126(1)
S	- C(11) - N		117.6(6)	C(9) - C(4) - C(5)	125(1)
S'	- C(11) - N		117.2(6)	C(10) - C(5) - C(1)	126(1)
C(11)	- N	- C(12A)	122(1)	C(10) - C(5) - C(4)	124(1)
C(11)	- N	- C(12B)	120(1)		
N	- C(12A)- C(13A)		108(2)		
N	- C(12B)- C(13B)		114(2)		

<sup>a</sup>Primed atoms are at positions -x, y, 1/2-z.

FIGURE CAPTIONS

Fig. 1. ORTEP drawing of the molecule.

Fig. 2. ORTEP view of the molecule parallel to a line through the  
ring centers.

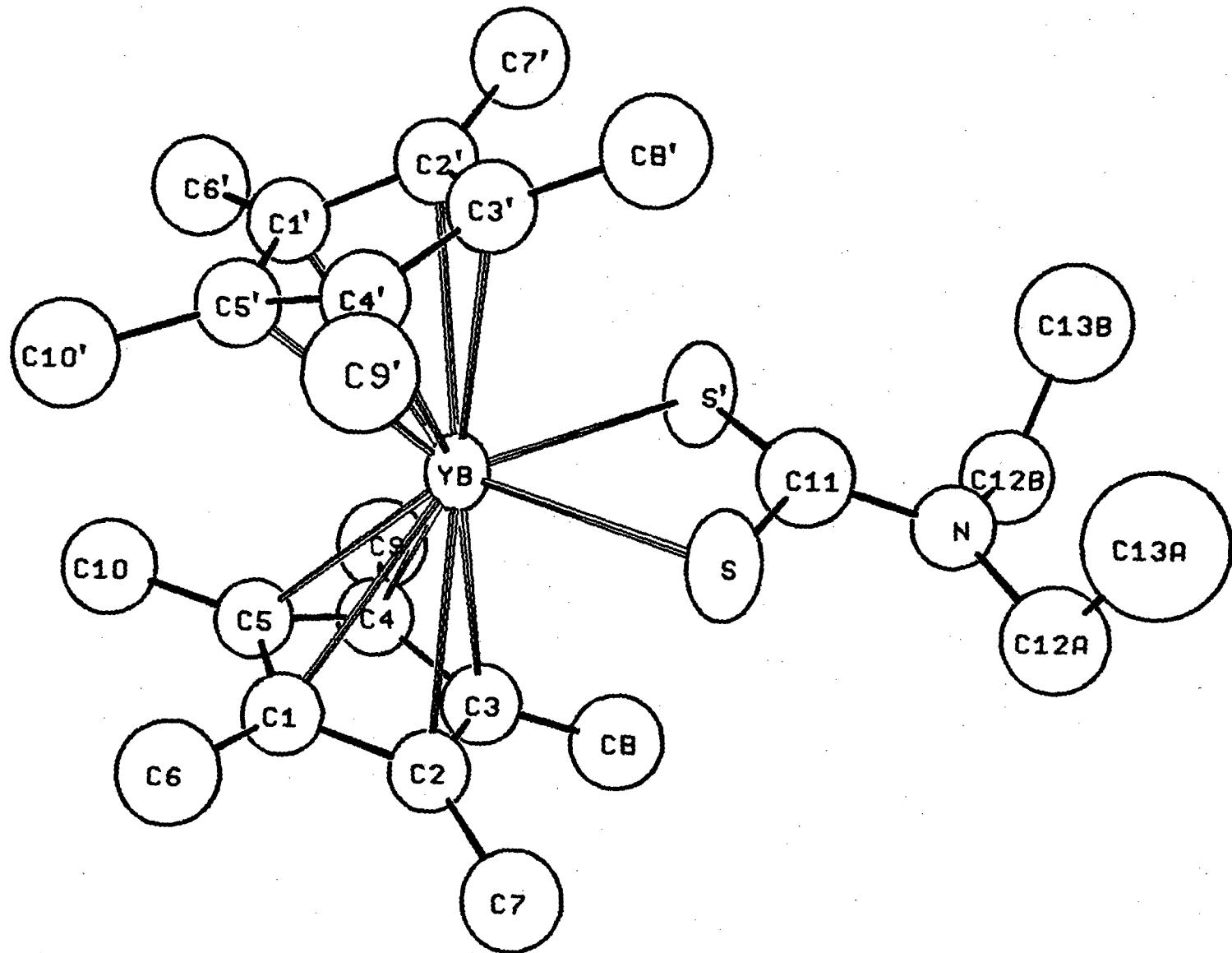


Fig. 1

XBL 812-8216

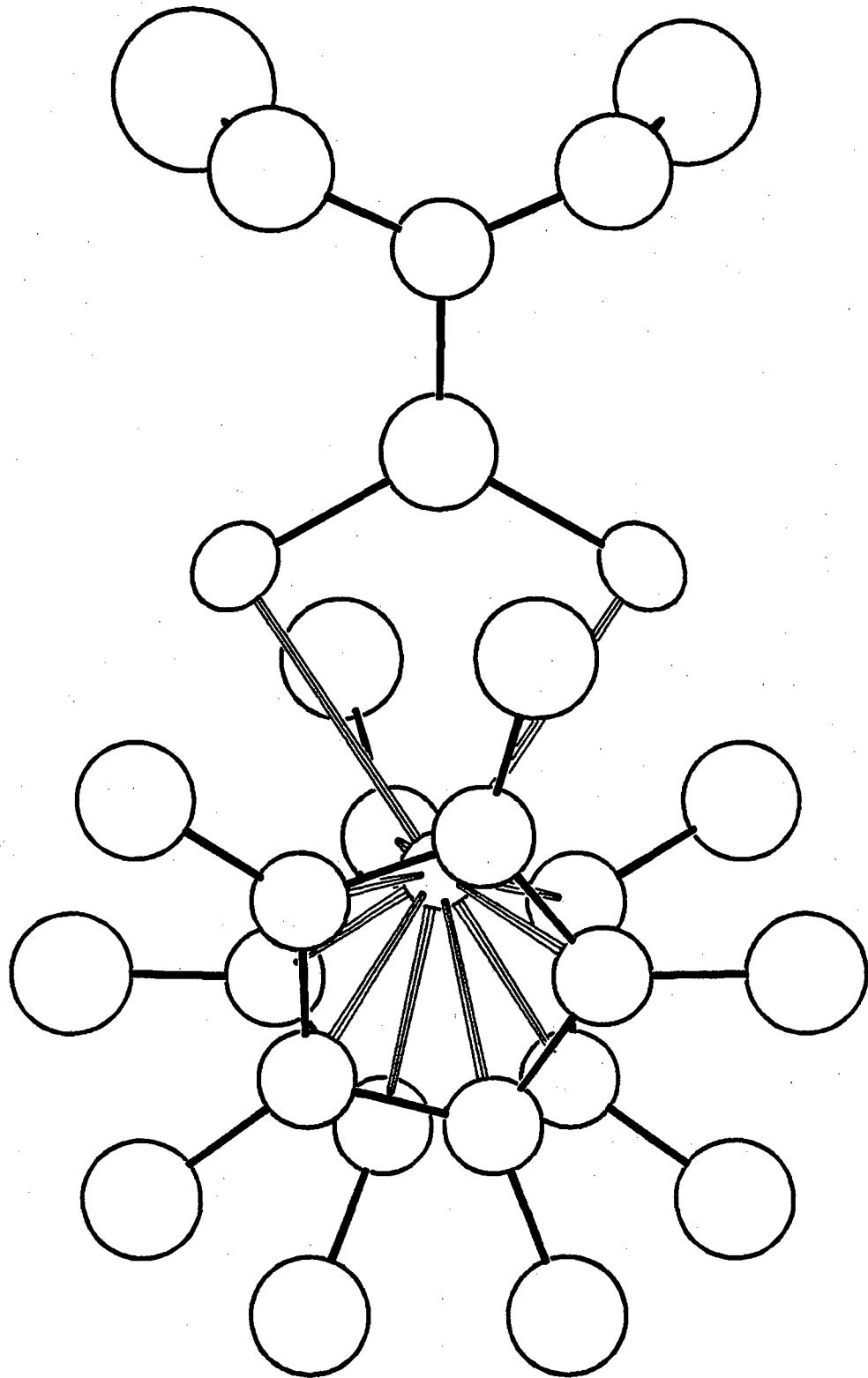


Fig. 2

XBL 816-10260

SUPPLEMENTARY MATERIALS FOR

BIS(PENTAMETHYLCYCLOPENTADIENYL)CARBOXYLATO  
AND DITHIOCARBAMATO DERIVATIVES OF NEODYMIUM(III)  
AND YTTERBIUM(III). CRYSTAL STRUCTURE OF  
BIS(PENTAMETHYLCYCLOPENTADIENYL)DIETHYLDITHIOCARBAMATO-  
YTTERBIUM (III)

T. Don Tilley, Richard A. Andersen, Allan Zalkin\*,  
and David H. Templeton

Thermal Parameters for  $(C_5Me_5)_2Yb(S_2CNET_2)$ .<sup>a</sup>

ATOM	811	822	833	812	813	823
YB	3.89(2)	2.55(2)	2.58(2)	0	-0.00(1)	0
S	7.49(9)	3.33(6)	3.68(6)	.17(6)	-0.85(6)	-0.73(5)
N	3.9(4)	3.4(4)	5.6(5)	.1(3)	.5(4)	-0.4(4)
C(1)	4.0(2)	4.1(3)	3.8(2)	1.2(2)	.4(2)	.6(2)
C(2)	3.3(2)	4.9(3)	3.7(3)	-0.3(2)	.1(2)	-0.6(2)
C(3)	4.0(2)	5.0(3)	4.0(3)	-0.3(2)	1.0(2)	-0.0(2)
C(4)	4.6(3)	4.7(3)	2.9(2)	.3(2)	.9(2)	-0.8(2)
C(5)	4.0(2)	3.4(2)	4.4(3)	.5(2)	.2(2)	-1.0(2)
C(6)	5.9(3)	7.0(4)	5.6(4)	1.2(3)	.3(3)	2.6(3)
C(7)	5.4(3)	7.8(4)	4.8(4)	-0.3(3)	-0.9(3)	-2.3(4)
C(8)	7.0(5)	5.9(4)	7.5(5)	-1.7(3)	2.8(4)	.6(4)
C(9)	7.9(4)	7.9(5)	3.1(3)	.3(4)	.2(3)	-0.5(3)
C(10)	6.6(4)	3.5(3)	8.7(5)	-0.1(3)	.9(3)	-2.4(3)
C(11)	5.8(2)					
C(12A)	6.8(4)					
C(13A)	11.6(8)					
C(12B)	5.5(3)					
C(13B)	9.3(6)					

<sup>a</sup>The anisotropic temperature factor has the form  $\exp[-0.25(B_{11}h^2a^*{}^2 + 2B_{12}hka^*b^* + \dots)]$ . The isotropic thermal parameter has the form  $\exp(-B\sin^2\theta/\lambda^2)$ .

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 5.0)  
 YTTERBIUM BIS(C5ME5)DITHIOOETHYLVARBAMATE  
 $F(0,0,0) = 2585$

F0B AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.  
 SG = ESTIMATED STANDARD DEVIATION OF F0B. DEL = |F0B| - |FCA|.

\* INDICATES ZERO WEIGHTED DATA.

L	F0B	SG	DEL	L	F0B	SG	DEL	L	F0B	SG	DEL	L	F0B	SG	DEL
H, K= 0, 0	6 156	4	2	10 169	4	-1	5 580	15	73	-10	324	8	27		
21226 31	-6	7 430	11	5	11 0	14	-1*	6 85	2	-10	-9	18	5	-9*	
4 173 5	-44	8 41	2	-8	12 161	4	-2	7 377	10	-8	383	10	-2		
6 232 6	-19	9 369	10	18	H, K= 0, 0	14	8 90	3	9	-7	126	3	3		
8 503 13	9	10 123	3	-5	0 296	8	-9	9 417	11	15	-6	358	9	-17	
10 396 10	12	11 257	7	-1	1 117	3	4	10 16	17	7*	-5	236	6	-4	
12 190 5	15	12 3	19	-4*	2 235	6	-11	11 289	8	29	-4	431	11	-11	
14 152 4	-1	13 171	4	-1	3 110	3	4	12 74	3	-8	-3	287	7	16	
16 139 4	-2	14 38	3	3	4 158	4	-4	13 185	5	3	-2	552	14	17	
H, K= 0, 2		15 129	4	-2	5 97	3	2	14 81	5	-2	-1	14	6	-12*	
0 579 15	-44	H, K= 0, 0	8	6 162	4	1	15 143	4	-3	0 630	16	16			
1 526 13	12	0 146	4	-15	7 106	3	-2	16 22	8	-4*	1 205	5	53		
2 495 13	-14	1 562	14	-3	8 195	5	-1	H, K= 1, 0	3	2 456	12	2			
3 295 7	-21	2 158	4	-2	9 83	3	4	-16 118	3	3 378	10	4			
4 519 14	49	3 425	11	6	10 181	5	-5	-15 134	4	-1 4 381	10	-4			
5 420 11	26	4 220	6	2	H, K= 0, 0	16	-14	183	5	5 473	12	29			
6 356 9	-8	5 280	7	5	0 142	4	1	-13 176	5	6 376	10	-9			
7 141 4	-20	6 202	5	-3	1 97	3	-7	-12 133	4	7 191	5	5			
8 348 9	3	7 287	8	2	2 119	3	6	-11 218	6	22 8 370	10	8			
9 51 2	-2	8 112	3	7	3 172	4	-5	-10 113	3	3 9 68	3	-9			
10 284 7	20	9 231	6	31	4 90	3	3	-9 243	6	-3 10 322	8	38			
11 19 6	2*	10 68	3	-1	5 195	5	-1	-8 298	8	18 11 41	6	6			
12 178 5	9	11 173	4	-4	6 82	3	-3	-7 279	7	-11 12 230	6	1			
13 121 3	-1	12 91	3	4	7 137	4	-1	-6 534	14	15 13 115	3	-1			
14 150 4	0	13 111	3	-3	8 99	3	-2	-5 313	8	-11 14 172	5	1			
15 111 3	1	14 93	3	3	H, K= 0, 0	18	-4	770 20	39	15 54	4	-6			
16 128 4	-2	H, K= 0, 0	10	0 0	18	-2*	-3 340	9	5 H, K= 1, 0	7					
H, K= 0, 4		0 264	7	2	1 146	4	1	-2 340	9	-26 15 18	9	-6*			
0 205 5	34	1 196	5	-2	2 16	8	7*	-1 342	9	19 -14 127	3	-6			
1 297 8	-35	2 392	10	-14	3 164	4	-3	0 387	10	-15 -13 23	5	-1*			
2 320 8	-8	3 224	6	-4	H, K= 1, 0	1	1	1 349	9	19 -12 220	6	0			
3 656 17	36	4 458	12	-8	-16 46	4	-3	2 365	9	-46 -11 43	3	4			
4 299 8	-53	5 189	5	7	-15 115	3	-9	3 414	10	13 -10 311	8	19			
5 670 17	27	6 312	8	24	-14 61	3	-3	4 502	13	17 -9 151	4	8			
6 357 9	24	7 152	4	10	-13 172	4	-1	5 394	10	-8 -8 303	8	0			
7 343 9	6	8 129	3	14	-12 0	19	-9*	6 309	8	-6 -7 150	4	-9			
8 182 5	10	9 101	3	-1	-11 314	8	40	7 309	8	-4 -6 274	7	-13			
9 277 7	6	10 104	3	0	-10 17	6	1*	8 180	5	6 -5 86	2	1			
10 82 3	9	11 99	3	3	-9 515	13	3	9 205	6	1 -4 376	10	-17			
11 215 6	21	12 167	4	-1	-8 77	3	6	10 222	6	20 -3 28	2	9			
12 150 4	-2	13 88	3	-3	-7 389	10	6	11 186	5	15 -2 667	17	-9			
13 200 5	-2	H, K= 0, 0	12	-6	118	3	-13	12 209	5	4 -1 32	2	-8			
14 152 4	1	0 258	7	33	-5 332	8	-15	13 180	5	1 0 553	14	-20			
15 153 5	-0	1 28	4	-5	-4 221	6	4	14 188	5	6 1 112	3	-9			
16 89 3	-5	2 295	8	32	-3 609	15	-4	15 127	4	-2 2 405	10	-24			
H, K= 0, 6		3 35	2	4	-2 25	2	3	H, K= 1, 0	5	3 34	2	-1			
0 137 4	12	4 280	7	19	-1 944	24	-38	-16 129	4	-1 4 389	10	9			
1 681 17	-38	5 91	3	1	0 47	2	14	-15 107	4	6 5 59	2	-10			
2 32 2	0	6 240	6	-5	1 986	28	23	-14 176	5	-2 6 425	11	1			
3 406 10	-21	7 34	3	2	2 138	4	-8	-13 91	3	3 7 61	2	-6			
4 131 3	23	8 189	5	-5	3 585	15	42	-12 241	6	-3 8 423	11	31			
5 340 9	7	9 28	4	3	4 360	9	61	-11 46	3	6 9 97	3	8			

**STRUCTURE FACTORS CONTINUED FOR  
YTTERBIUM BIS(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub>DITHIODIETHYLVARBAMATE**

PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	292	7	15	8	57	2	4	0	114	3	-4	15	88	3	-0	6	28	3	-1
11	54	3	-0	9	145	4	-12	1	66	3	-1	H,K=	2,	4	7	420	11	8	
12	168	4	-6	10	23	5	0*	2	170	4	-7	-16	96	3	3	8	4	13	-5*
13	42	4	4	11	158	4	-8	3	63	2	1	-15	163	4	-1	9	391	10	26
14	94	3	-9	12	68	3	-4	4	199	5	-9	-14	132	4	1	10	5	16	-4*
	H,K=	1,	9	H,K=	1,	13	5	67	3	2	-13	227	6	-4	11	266	7	-5	
-14	88	3	-2	-11	169	5	-5	6	156	4	-6	-12	139	4	0	12	47	4	2
-13	138	4	3	-10	62	3	-0	H,K=	2,	0	-11	202	5	21	13	160	5	6	
-12	153	4	1	-9	198	5	-2	-16	120	3	-7	-10	115	3	4	14	13	18	9*
-11	97	3	2	-8	74	3	5	-14	172	5	-6	-9	304	8	4	H,K=	2,	8	
-10	189	5	-7	-7	196	5	-1	-12	336	9	28	-8	141	4	-5	-15	98	3	-4
-9	101	3	10	-6	74	3	6	-10	496	13	-4	-7	480	12	7	-14	81	3	3
-8	169	4	21	-5	177	5	-15	-8	551	14	-5	-6	336	9	-3	-13	163	4	-2
-7	257	7	14	-4	88	3	2	-6	309	8	-35	-5	551	14	-18	-12	58	2	1
-6	165	4	-2	-3	237	6	-4	-4	533	14	8	-4	300	8	3	-11	293	8	-2
-5	353	9	-15	-2	138	4	-5	-2	494	13	-59	-3	343	9	-20	-10	78	4	1
-4	204	5	3	-1	294	8	6	0	635	16	-30	-2	129	3	-10	-9	283	7	21
-3	274	7	-13	0	87	3	1	2	592	15	42	-1	227	6	-0	-8	157	4	11
-2	349	9	-11	1	257	7	9	4	566	14	52	0	92	3	-11	-7	217	6	1
-1	186	5	6	2	13	21	-8*	6	567	15	15	1	637	16	46	-6	186	5	-4
0	359	9	-12	3	206	5	-1	8	554	14	36	2	493	13	29	-5	181	5	-10
1	275	7	-1	4	48	3	-9	10	505	13	50	3	539	14	-2	-4	214	6	3
2	324	8	-11	5	188	5	-10	12	259	7	6	4	532	14	29	-3	310	8	-21
3	402	10	-14	6	30	3	-2	14	158	4	-0	5	445	11	20	-2	156	4	-3
4	213	6	-1	7	211	5	-7	H,K=	2,	2	6	235	6	23	-1	445	11	-32	
5	305	8	-9	8	90	3	-3	-16	116	3	-4	7	278	7	11	0	75	2	-17
6	193	5	15	9	200	5	-8	-15	117	3	0	8	103	3	-1	1	320	8	-3
7	153	4	24	10	38	4	-4	-14	173	5	-7	9	273	7	29	2	131	3	3
8	214	6	18	11	153	4	-8	-13	128	4	1	10	110	3	7	3	256	7	1
9	94	3	4	H,K=	1,	15	-12	239	6	9	11	273	7	7	4	228	6	3	
10	149	4	-2	-9	141	4	-2	-11	65	4	15	12	173	5	-3	5	263	7	-10
11	126	3	0	-8	109	3	-2	-10	275	7	1	13	225	6	5	6	195	5	2
12	114	3	-1	-7	111	3	-1	-9	180	5	-2	14	116	4	0	7	399	10	20
13	148	4	5	-6	146	4	-2	-8	381	10	0	15	154	4	3	8	105	3	13
	H,K=	1,	11	-5	91	3	2	-7	295	8	5	H,K=	2,	6	9	337	9	12	
-13	151	4	-1	-4	148	4	2	-6	488	12	-9	-15	129	4	-3	10	87	3	-4
-12	44	3	1	-3	136	4	-1	-5	289	7	-35	-14	41	3	0	11	162	4	-5
-11	155	4	-9	-2	143	4	5	-4	538	14	26	-13	214	6	-1	12	101	3	4
-10	45	2	2	-1	229	5	3	-3	189	5	23	-12	20	6	-2*	13	98	3	-5
-9	165	4	-0	8	119	3	2	-2	138	4	-39	-11	345	9	7	14	89	3	4
-8	96	3	-1	1	242	6	5	-1	82	3	-26	-10	36	4	4	H,K=	2,	10	
-7	298	8	14	2	129	3	2	0	185	5	-42	-9	357	9	15	-14	143	4	-1
-6	159	4	9	3	157	4	5	1	226	6	29	-8	74	2	-7	-13	83	3	3
-5	389	10	31	4	127	3	-3	2	421	11	25	-7	255	7	-7	-12	144	4	-4
-4	150	4	14	5	121	4	2	3	305	8	-24	-6	48	2	2	-11	123	4	3
-3	355	9	10	6	110	3	-5	4	396	10	-1	-5	268	7	-25	-10	164	4	1
-2	68	2	7	7	157	4	-4	5	350	9	4	-4	43	2	-5	-9	136	4	-4
-1	267	7	-5	8	92	3	2	6	387	10	-11	-3	520	13	-26	-8	265	7	17
0	14	6	2*	9	175	5	-0	7	69	2	-8	-2	35	2	11	-7	183	5	7
1	276	7	1	H,K=	1,	17	8	388	10	17	-1	631	16	-32	-6	374	10	18	
2	106	3	8	-6	179	5	2	9	105	3	2	0	156	4	-1	-5	220	6	3
3	350	9	21	-5	54	3	6	10	329	9	51	1	465	12	-21	-4	293	8	-0
4	234	6	13	-4	184	5	-6	11	212	6	5	2	5	12	0*	-3	177	5	-1
5	290	7	39	-3	40	3	-6	12	194	5	2	3	346	9	-16	-2	206	5	-5
6	192	5	7	-2	127	3	-5	13	188	5	10	4	147	4	10	-1	140	4	-6
7	221	6	3	-1	50	3	-5	14	144	4	-6	5	343	9	9	0	212	E	-10

STRUCTURE FACTORS CONTINUED FOR  
YTTERBIUM BIS(C5ME5)DITHIODIETHYLVARBAMATE

PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	146	4	0	6	190	5	0	11	274	7	5	2	537	14	1
2	334	9	-12	7	89	3	-7	12	96	3	-3	3	324	8	-7
3	184	5	-7	8	198	5	-6	13	152	4	0	4	461	12	8
4	377	10	8	9	79	3	2	14	58	3	-4	5	82	3	-8
5	161	4	11	H,K=	2,	16	15	161	4	-2	6	384	10	9	2
6	289	7	26	-8	78	3	-1	H,K=	3,	3	7	6	15	-6*	3
7	149	4	-1	-7	151	4	3	-16	134	4	1	8	270	7	27
8	195	5	3	-6	58	3	-8	-15	126	3	-2	9	76	2	12
9	124	3	5	-5	157	4	-5	-14	174	5	-1	10	234	6	2
10	142	4	-2	-4	77	2	2	-13	127	4	-3	11	103	3	2
11	106	3	4	-3	120	3	-8	-12	154	4	6	12	198	5	-8
12	173	5	-8	-2	118	3	-8	-11	134	4	24	13	102	3	1
13	93	3	-3	-1	113	3	-4	-10	145	4	8	14	165	4	5
	H,K=	2,	12	0	140	4	-1	-9	224	6	-12	H,K=	3,	7	10
-12	155	4	-6	1	142	4	-8	-8	369	9	-2	-15	26	6	2*
-11	39	3	7	2	102	3	3	-7	363	9	-12	-14	142	4	-6
-10	194	5	-3	3	184	5	-5	-6	412	10	-13	-13	32	4	-6
-9	18	19	0*	4	76	3	1	-5	336	9	-18	-12	264	8	-3
-8	196	5	-6	5	165	4	-2	-4	333	8	-22	-11	23	5	0*-12
-7	45	3	2	6	107	3	2	-3	329	8	-24	-10	338	9	17
-6	252	6	-1	7	115	3	3	-2	85	3	-16	-9	17	12	9*-10
-5	85	3	8	H,K=	2,	18	-1	513	13	12	-8	248	6	10	-9
-4	295	8	14	-3	129	4	-3	0	246	6	-0	-7	30	3	2
-3	7	13	2*	-2	0	16	-11*	1	400	10	6	-6	246	6	-7
-2	320	8	27	-1	119	3	0	2	497	13	-13	-5	121	3	2
-1	80	2	-9	0	0	21	-2*	3	242	6	-19	-4	350	9	-9
0	245	6	29	1	146	4	-3	4	481	12	15	-3	198	5	-4
1	25	3	10	2	31	11	-2*	5	258	7	-8	-2	503	13	-24
2	196	5	24	H,K=	3,	1	6	371	10	24	-1	87	2	6	-2
3	157	4	9	-16	55	3	-8	7	251	6	3	0	461	12	-24
4	201	5	5	-15	156	4	-4	8	153	4	-1	1	103	3	-8
5	115	3	4	-14	76	3	1	9	196	5	30	2	290	7	-16
6	214	6	-7	-13	269	7	-7	10	228	6	8	3	131	3	7
7	29	4	1	-12	68	3	2	11	171	4	-1	4	256	7	-5
8	215	6	-8	-11	332	9	25	12	242	6	8	5	118	3	-9
9	47	3	5	-10	40	4	-6	13	162	4	1	6	365	9	6
10	174	5	-6	-9	385	10	-5	14	164	4	4	7	42	2	11
11	22	6	3*	-8	140	4	0	H,K=	3,	5	8	448	12	18	7
	H,K=	2,	14	-7	407	10	-15	-16	121	4	1	9	17	14	4*
-11	92	3	6	-6	165	4	-14	-15	70	3	-3	10	281	7	-6
-10	176	5	-8	-5	415	10	-31	-14	166	5	-5	11	37	10	1*
-9	103	3	2	-4	12	13	-4*	-13	49	6	3	12	133	4	-12
-8	160	4	1	-3	495	13	-22	-12	230	7	-1	13	16	20	-14*
-7	86	3	-2	-2	501	13	27	-11	43	3	6	H,K=	3,	9	-12
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1	93	3	6	6	98	3	12	-3	30	2	-2	-7	215	6	18
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3	58	3	0	8	16	18	3*	-1	16	4	2*	-5	248	6	-5
4	165	4	0	9	478	13	58	0	531	14	-9	-4	145	4	-12
5	67	3	-1	10	90	3	8	1	197	5	13	-3	184	5	6
												0	88	3	-3

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L	F08	SG	DEL	L	F08	SG	DEL	L	FCB	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
1	226	6	-8	12	154	4	-1	5	443	11	8	-1	417	11	-20	2	274	7	-4
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4	36	2	11	-16	114	3	-1	8	66	2	10	2	244	6	-8	5	15	10	-4*
5	183	5	-8	-15	105	3	-1	9	156	4	19	3	191	5	-6	6	168	4	-4
6	80	2	4	-14	137	4	-6	10	124	3	-1	4	135	4	3	7	53	2	0
7	199	5	-7	-13	111	3	0	11	207	5	-3	5	286	7	15	8	190	5	-4
8	90	3	-6	-12	198	5	6	12	157	4	-1	6	68	2	12	9	27	4	4
9	174	5	-8	-11	61	2	11	13	169	5	3	7	316	8	5	10	164	4	-5
10	31	6	-8*	-10	235	6	4	14	103	3	-2	8	77	3	-5	H,K=	4,	14	0
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-8	106	3	-2	-7	301	8	-8	-15	116	3	-1	11	126	3	-7	-8	136	4	1
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10	263	7	19	4	277	7	-1	-2	142	4	-1	1	51	4	3	-6	151	4	-16

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	
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-2	49	2	3	-8	264	7	-9	-10	150	4	-9	1	201	6	-5	-9	154	4	4	
-1	599	15	-20	-7	195	5	1	-9	206	5	-6	2	9	15	-7*	-8	203	5	-14	
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1	447	11	-5	-5	160	4	-8	-7	263	7	14	4	28	4	-1	-6	280	7	-21	
2	135	3	-7	-4	489	13	-25	-6	175	5	20	5	192	5	2	-5	146	4	7	
3	400	10	4	-3	14	7	-12*	-5	199	5	15	6	65	3	1	-4	322	8	-5	
4	67	2	-6	-2	481	12	-22	-4	241	6	7	7	195	5	0	-3	204	5	-3	
5	416	11	9	-1	85	2	-5	-3	118	3	8	8	54	3	-3	-2	330	9	-3	
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8	23	15	10*	2	385	10	6	0	247	6	2	-8	119	3	4	1	264	7	-3	
9	203	5	12	3	208	5	2	1	298	8	9	-7	92	3	-1	2	384	10	1	
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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-13	184	7	-1	-12	71	2	0	0	123	3	1	-8	247	6	2	-9	26	7	3*
-12	41	3	3	-11	66	2	-3	1	59	3	-3	-7	199	5	-2	-8	165	4	5
-11	220	6	-10	-10	135	4	1	2	104	3	-1	-6	162	4	-8	-7	29	4	14
-10	15	18	0*	-9	91	3	-3	3	59	3	-2	-5	97	3	-2	-6	212	6	20
-9	232	6	14	-8	230	6	-1	4	157	4	-2	-4	38	2	3	-5	53	3	12
-8	51	3	-3	-7	102	3	-0	5	83	3	-2	-3	68	2	-4	-4	301	8	7
-7	237	6	5	-6	277	7	5	6	180	5	-4	-2	194	5	2	-3	66	3	6
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-12	72	3	1	-6	171	5	-8	-4	116	3	-1	-7	79	2	2	-5	165	4	7
-11	141	4	-1	-5	29	4	2	-3	397	10	-35	-6	228	6	-9	-4	202	5	7
-10	145	4	-3	-4	192	5	-5	-2	138	4	-3	-5	65	3	5	-3	130	3	13
-9	149	4	1	-3	60	2	-1	-1	351	9	-15	-4	208	5	-13	-2	169	4	18
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-5	289	7	-1	1	72	3	3	3	248	6	-10	0	257	7	-15	2	131	4	3
-4	85	2	7	2	210	5	-7	4	28	4	-0	1	159	4	1	3	187	5	3
-3	317	8	-1	3	69	3	-1	5	334	9	22	2	285	7	6	4	158	4	-7
-2	121	3	6	4	200	5	-3	6	11	16	2*	3	118	3	5	5	99	3	1
-1	284	7	-8	5	11	14	-1*	7	350	9	7	4	310	8	29	6	174	5	-3
0	126	3	3	6	171	4	-8	8	44	4	-2	5	68	2	5	7	82	3	1
1	234	6	14	7	8	15	6*	9	203	5	-4	6	314	8	-2	8	127	3	3
2	129	3	9	8	140	4	-5	10	75	3	1	7	6	19	-12*	9	131	4	-8
3	213	6	26	H, K=	6,	14	11	139	4	-2	8	260	7	-5	H, K=	7,	11		
4	119	3	9	-10	97	3	-2	12	58	4	0	9	68	3	-2	-12	29	4	-7
5	246	6	8	-9	75	3	1	H, K=	7,	3	10	180	5	-4	-11	101	3	-1	
6	88	3	0	-8	94	3	1	-16	76	3	4	11	80	3	3	-10	58	3	1
7	199	5	-5	-7	62	3	-3	-15	110	3	2	H, K=	7,	7	-9	150	4	2	
8	64	2	-1	-6	127	4	-3	-14	68	3	-1	-15	23	6	-4*	-8	66	3	-4
9	146	4	-7	-5	71	3	-2	-13	127	3	-2	-14	135	4	-5	-7	194	5	-1
10	94	3	1	-4	188	5	-2	-12	125	3	-1	-13	39	7	-8	-6	39	3	-2

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-5	202	5	-5	6	274	7	-1	8	94	3	-1	-12	79	3	-1	-13	117	3	-1
-4	25	7	6*	8	220	6	-1	9	176	5	-5	-11	83	3	-7	-12	29	3	6
-3	167	4	-4	10	149	4	-4	10	119	4	-5	-10	103	3	2	-11	133	3	-5
-2	34	3	-2	H,K=	8,	2	H,K=	8,	6	-9	100	3	-3	-10	34	3	0		
-1	175	5	-5	-16	90	3	-8	-15	105	4	1	-8	141	4	-8	-9	139	4	-7
0	83	3	2	-15	43	3	7	-14	21	10	15*	-7	95	3	-3	-8	48	2	7
1	214	6	-4	-14	121	3	0	-13	141	4	-3	-6	137	4	-2	-7	210	5	8
2	100	3	2	-13	35	3	7	-12	0	15	-8*	-5	101	3	0	-6	69	2	2
3	186	5	-6	-12	156	4	-1	-11	160	4	-3	-4	147	4	-8	-5	274	7	0
4	75	2	-8	-11	107	3	0	-10	30	3	-2	-3	106	4	-2	-4	45	2	8
5	149	4	-9	-10	189	5	5	-9	166	4	-5	-2	178	5	-3	-3	240	6	5
6	42	3	-4	-9	153	4	2	-8	51	4	-6	-1	86	3	-2	-2	56	2	4
7	129	3	-3	-8	187	5	13	-7	193	5	13	0	215	6	-3	-1	232	6	2
8	49	3	-1	-7	147	4	3	-6	22	6	-3*	1	79	3	-2	0	109	3	8
H,K=	7,	13	-6	205	5	-9	-5	255	7	18	2	179	5	4	1	253	6	14	
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-9	111	3	1	-4	235	6	-11	-3	260	7	12	4	117	3	-6	3	288	7	12
-8	13	14	4*	-3	45	2	-1	-2	19	5	12*	5	93	3	-2	4	35	5	-3
-7	125	3	-0	-2	267	7	-5	-1	220	6	20	6	121	3	-6	5	224	6	0
-6	34	3	4	-1	181	5	-1	0	29	4	-4	7	76	3	-4	6	24	8	-10*
-5	166	4	-1	0	212	6	-6	1	237	6	27	8	135	4	-1	7	161	4	-5
-4	68	2	6	1	220	6	-4	2	49	2	8	H,K=	8,	12	8	76	3	0	
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-2	41	3	6	3	161	4	12	4	0	21	-3*	-10	128	4	5	10	55	3	1
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1	129	4	-3	6	240	6	-4	7	206	5	-2	-7	17	11	-5*	-14	47	2	-2
2	15	10	8*	7	79	3	-3	8	14	15	2*	-6	149	4	3	-13	69	2	2
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4	47	3	0	9	138	4	0	10	25	5	-3*	-4	146	4	-1	-11	109	3	4
5	174	5	-7	10	130	4	-7	H,K=	8,	8	-3	14	10	8*	-10	139	4	3	
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-6	85	3	1	-14	57	3	0	-11	107	3	-1	1	39	5	-3	-6	139	4	13
-5	100	3	-1	-13	96	3	-3	-10	72	2	-1	2	175	5	5	-5	172	4	17
-4	87	3	4	-12	80	3	-1	-9	116	4	-3	3	8	16	4*	-4	89	2	5
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H,K=	8,	0	-4	107	3	-9	-1	151	4	7	-5	66	3	3	4	133	3	-1	
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0	234	6	-16	5	195	5	-5	8	82	3	3	H,K=	9,	1	-12	96	3	-3	
2	245	6	-11	6	88	3	1	9	97	3	-4	-15	101	3	2	-11	37	5	2
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	46	2	-5	0	116	3	-5	-11	59	2	6	-2	34	3	-7	0	130	4	-1
-8	184	5	-4	1	191	5	4	-10	118	3	2	-1	212	5	-3	1	27	4	1
-7	69	2	-5	2	113	3	-2	-9	81	2	4	0	55	2	-3	2	125	3	3
-6	253	6	9	3	123	3	3	-8	171	4	-2	1	177	5	-3	H, K=	11,	1	
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-4	281	7	12	5	90	3	-8	-6	227	6	5	3	152	4	-1	-13	88	3	-4
-3	66	2	3	6	129	4	0	-5	52	2	10	4	20	9	14*-12	32	3	3	0
-2	275	7	15	7	93	3	0	-4	217	6	7	5	149	4	-1	-11	89	3	3
-1	69	2	2	H, K=	9,	11	-3	73	2	9	6	39	3	-0	-18	39	3	4	
0	242	6	17	-11	109	3	6	-2	177	5	6	7	125	3	-2	-9	113	3	1
1	107	3	3	-10	48	3	-6	-1	162	4	8	H, K=	10,	8	-8	31	3	4	
2	205	5	4	-9	132	4	6	0	176	5	6	-12	45	2	-3	-7	142	4	-6
3	33	3	-8	-8	68	3	2	1	145	4	6	-11	80	3	-3	-6	22	5	4*
4	181	5	-2	-7	118	3	1	2	179	5	-6	-10	73	2	3	-5	180	5	-10
5	11	14	2*	-6	55	2	2	3	84	3	-4	-9	81	2	2	-4	35	3	5
6	151	4	-4	-5	107	3	-4	4	171	4	-3	-8	88	3	-0	-3	159	4	-10
7	49	2	-2	-4	30	3	-3	5	64	2	-1	-7	104	3	1	-2	68	2	2
8	138	4	-5	-3	152	4	5	6	129	3	-2	-6	80	2	-6	-1	137	4	-4
9	80	3	2	-2	35	4	-6	7	81	3	0	-5	140	4	1	0	68	2	4
	H, K=	9,	7	-1	168	4	4	8	104	3	-1	-4	72	3	-5	1	139	4	-6
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-13	13	16	2*	1	160	4	-6	-14	25	4	4	-2	87	3	3	3	189	5	-6
-12	109	3	1	2	50	3	0	-13	69	3	-2	-1	133	4	-3	4	45	3	0
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-10	88	3	-1	4	10	13	-3*	-11	91	3	-3	1	134	4	-4	6	42	6	-2
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-8	125	3	-2	H, K=	9,	13	-9	127	3	-3	3	3	154	4	-3	H, K=	11,	3	
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-6	208	5	-3	-7	127	3	6	-7	167	4	-7	5	158	4	-2	-12	69	2	1
-5	54	4	6	-6	32	3	9	-6	74	3	2	6	53	3	-1	-11	84	3	1
-4	251	6	-2	-5	147	4	3	-5	216	6	-1	H, K=	10,	10	-10	89	3	5	
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-1	72	3	3	-2	14	15	2*	-2	151	4	-1	-9	59	2	-5	-7	96	3	1
0	164	4	1	-1	123	4	1	-1	191	5	-3	-8	88	3	-2	-6	91	3	0
1	51	2	-2	0	22	5	11*	0	157	4	2	-7	60	3	-3	-5	113	3	1
2	198	5	4	1	121	4	6	1	168	4	-7	-6	85	2	4	-4	102	3	0
3	44	3	-0	2	13	14	-3*	2	71	2	2	-5	64	2	-0	-3	137	4	-0
4	213	5	1	3	117	3	-0	3	143	4	-1	-4	110	3	2	-2	111	3	-2
5	29	5	1	H, K=	10,	0	4	18	5	6*	-3	88	3	0	-1	138	4	2	
6	191	5	-2	-14	104	3	0	5	99	3	-4	-2	136	4	1	0	128	3	-0
7	22	6	1*	-12	85	3	-2	6	49	3	0	-1	104	3	1	1	115	3	1
8	114	3	-4	-10	110	3	-5	7	97	3	-2	0	138	4	2	2	102	3	1
	H, K=	9,	9	-8	150	4	-14	8	89	3	1	1	102	3	-0	3	93	3	-1
-12	100	3	-0	-6	202	6	5	H, K=	10,	6	2	125	3	3	4	89	3	-0	
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-10	92	3	-5	-2	200	5	4	-12	0	13	-13*	4	97	3	1	6	84	3	-1
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-8	89	3	-5	2	228	6	-1	-10	17	7	4*	-8	110	3	1	H, K=	11,	5	
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-6	103	3	-5	6	172	5	-7	-8	14	10	5*	-6	120	3	1	-12	99	3	-2
-5	77	3	-3	8	116	3	-5	-7	172	4	-8	-5	16	7	13*-11	42	3	-3	
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-3	128	3	-4	-14	71	3	0	-5	201	5	-12	-3	12	13	6*	-9	41	3	-4
-2	160	4	0	-13	43	3	2	-4	36	7	13*	-2	134	4	-0	-8	132	4	-6
-1	192	5	-0	-12	79	2	-8	-3	219	6	-10	-1	34	3	-3	-7	22	5	10*

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-6	142	4	-7	0	39	4	-7	-6	9	14	5*	-2	92	3	3
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-4	157	4	-7	H,K=	12,	0	-4	8	17	-4*	0	74	3	1	
-3	58	2	-0	-12	94	3	-1	-3	98	3	1	1	91	3	-2
-2	162	4	-6	-10	93	3	-1	-2	13	15	-1*	2	47	4	1
-1	74	3	-8	-8	90	3	-4	-1	99	4	0	3	78	3	-2
0	161	4	-2	-6	119	3	-5	0	8	15	-0*	H,K=	13,	5	
1	42	2	-6	-4	149	4	1	1	128	4	0	-10	69	3	3
2	147	4	-1	-2	110	3	2	2	14	15	5*	-9	21	8	-9*
3	15	7	-6*	0	100	3	-6	3	148	4	-2	-8	80	3	5
4	136	4	-3	2	144	4	-2	4	8	17	3*	-7	36	5	2
5	33	3	-6	4	162	5	-2	H,K=	12,	8	-6	73	3	-9	
6	118	3	-4	H,K=	12,	2	-9	78	3	3	-5	18	11	-5*	
H,K=	11,	7	-12	80	3	-2	-8	45	3	9	-4	96	3	1	
-12	84	3	3	-11	58	3	3	-7	99	3	7	-3	17	17	-3*
-11	27	4	9	-10	77	3	-0	-6	40	6	6	-2	107	3	-0
-10	95	3	2	-9	61	4	5	-5	92	3	6	-1	29	4	1
-9	37	3	2	-8	92	3	3	-4	58	3	6	0	117	4	-4
-8	117	3	6	-7	36	3	-1	-3	75	3	-0	1	29	5	0
-7	55	3	2	-6	118	3	2	-2	61	3	2	2	121	3	-4
-6	129	3	11	-5	62	2	5	-1	71	3	-4	H,K=	13,	7	
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-4	124	3	5	-3	79	3	6	1	97	4	-0	-7	18	9	5*
-3	23	4	1*	-2	100	3	-3	2	38	6	-5	-6	105	3	9
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-1	0	15	-5*	0	113	3	-3	-6	60	3	2	-4	86	3	4
0	102	3	-5	1	52	3	3	-5	45	18	-10*	-3	31	4	3
1	11	14	6*	2	129	4	-5	-4	59	4	-4	-2	74	3	3
2	137	4	-3	3	44	4	-1	-3	60	3	-2	-1	25	5	-4*
3	24	7	9*	4	133	4	-4	-2	96	3	3	0	83	3	1
4	152	4	-3	5	55	3	-6	-1	62	3	-3	H,K=	14,	0	
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H,K=	11,	9	-12	55	3	4	-11	76	3	-1	-6	94	3	-5	
-10	61	3	-1	-11	75	3	-5	-10	34	4	5	-4	89	3	-5
-9	79	3	-1	-10	58	3	1	-9	91	3	1	-2	87	3	-2
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-5	72	3	4	-6	33	3	10	-5	112	3	0	-7	42	3	3
-4	92	3	2	-5	93	3	-2	-4	44	3	2	-6	74	3	0
-3	80	3	3	-4	36	5	5	-3	98	3	-5	-5	52	3	3
-2	111	3	1	-3	92	5	-5	-2	31	4	-2	-4	90	3	-2
-1	90	3	-1	-2	68	3	5	-1	100	3	-4	-3	64	3	4
0	116	3	-2	-1	113	4	-3	0	22	6	-3*	-2	98	3	-1
1	87	3	-1	0	78	3	2	1	110	3	-4	-1	54	4	3
2	122	3	2	1	122	3	-1	2	23	8	8*	0	87	3	2
3	65	3	-1	2	72	3	-2	3	100	4	-3	H,K=	14,	4	
H,K=	11,	11	3	111	3	-3	H,K=	13,	3	-7	51	6	-2		
-8	28	4	2	4	57	3	1	-10	57	3	3	-6	38	3	-1
-7	90	3	-0	5	114	3	-4	-9	56	3	1	-5	74	3	1
-6	25	4	-1	H,K=	12,	6	-8	59	3	5	-4	44	3	2	
-5	89	3	-0	-11	90	3	-1	-7	58	3	5	-3	93	3	-6
-4	36	3	-3	-10	19	7	-2*	-6	58	3	-0	-2	51	4	1
-3	106	3	-2	-9	99	3	-2	-5	53	3	3				
-2	56	3	-0	-8	8	15	-9*	-4	88	3	4				
-1	125	3	3	-7	100	3	-2	-3	72	3	3				

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