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Structural Characterization of a Chloride-Bridged Lanthanide Cyclopentadienyl Dimer, $[Yb(C_5H_4CH_3)_2Cl]_2$

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The structure of $[Yb(C_5H_4CH_3)_2Cl]_2$ has been determined from three-dimensional X-ray diffraction data collected by counter methods. The molecular unit is a dimer which is located about a crystallographic inversion center with a Yb–Yb distance of 3.979 (1) Å. The five cyclopentadienyl carbon atoms of each ring form a plane equidistant from the Yb atom with an average Yb–C distance of 2.585 (7) Å. The coordination about the ytterbium ions is distorted tetrahedral; the bridging unit is symmetrical and approximately square with an average Yb–Cl distance of 2.64 Å and a Yb–Cl–Yb angle of 97.95 (5)°. Orange-red platelets crystallized from benzene conform to space group $C2/c$ with $a = 20.377$ (6) Å, $b = 9.185$ (2) Å, $c = 13.235$ (4) Å, $\beta = 108.97$ (2)°, $Z = 4$, and $\rho_{\text{calcd}} = 2.08$. A total of 7786 reflections were collected of which 2751 independent reflections with $F^2 > 3\sigma(F^2)$ were used in the final refinement by full-matrix least-squares methods to give weighted and unweighted R factors of 3.69 and 3.46%, respectively.

Introduction

Interest in the organometallic compounds of the lanthanides and actinides has expanded rapidly in recent years.[2] Possible applications as chemical shift reagents[3] or homogeneous catalysts in organic reactions have contributed to this interest.[4] Although the chemistry of π-carbocyclic complexes of f transition metals is now extensive, the nature of the bonding in these compounds and the extent of involvement of the f electrons are still in question. The synthesis of lanthanide dicyclopentadienyl chlorides and related phenoxy and carboxylate derivatives by Maginn, Manastyrskyj, and Dubeck[5] stands out both because of the fact that these compounds appear to be somewhat more stable than the parent tricyclopentadienides and because of the suggestion by Dubeck that these complexes may be dimeric in noncoordinating solvents. This latter supposition was particularly intriguing because, if true, it would allow a unique opportunity to study the magnetic interaction between two isolated f-series paramagnetic ions in close proximity. Furthermore, as a dimeric cerium complex containing the cyclooctatetraene ligand is already known,[6,7] the effect of changing the bridging group and/or carbocyclic ligand could be examined. The only other previous study of relevance has been of a scandium dimer[8] which, while structurally similar, contains no f electrons. Thus a single-crystal X-ray diffraction study of the ytterbium member of the lanthanide bis(methylcyclopentadienyl) chloride series was undertaken. The ytterbium member of the series was chosen because of its f^{13} configuration. The methyl-substituted cyclopentadienyl complex was used because of its greater solubility in benzene and because of the fact that we wanted to reduce rotation of the cyclopentadienyl rings in the solid.

Experimental Section

Crystals of $[Yb(C_5H_4CH_3)_2Cl]_2$ suitable for diffraction analysis were grown using a modification[9] of the literature preparation[5] of the monomer followed by slow, controlled evaporation from benzene. Several crystals were sealed in thin-walled glass capillaries under a nitrogen atmosphere. A series of precession photographs exhibited

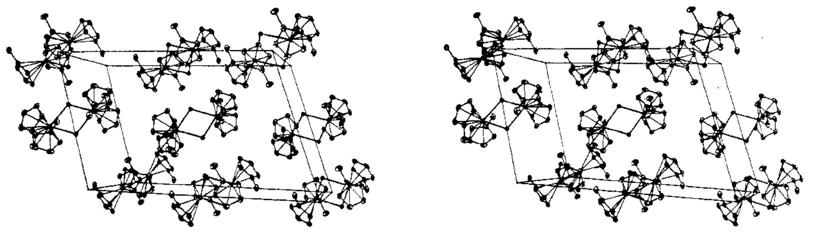

Figure 1. A stereoscopic view of the unit cell for $[Yb(C_5H_4CH_3)_2Cl]_2$. The origin is at the lower back left corner, the horizontal axis is *a*, and the vertical is *c*.

Table I. Summary of Crystal Data

Molecular formula	$[Yb(C_6H_7)_2Cl]_2$	Cell constants[a]	
Mol wt	733.48	*a*	20.377 (6) Å
Linear absorption coeff, μ	85.42 cm^{-1}	*b*	9.185 (2) Å
Calcd density	2.08 g cm^{-3}	*c*	13.235 (4) Å
Crystal dimensions	0.28 × 0.15 × 0.08 mm	β	108.97 (2)°
Space group	*C*2/*c*, monoclinic	Cell vol	2343 Å^3
Formula units/cell	4 dimers		

[a] Ambient temperature of 22°; Mo Kα_1 radiation, λ 0.70926 Å.

Laue symmetry 2/*m* and the absences *hkl*, $h + k \neq 2n$, and *h*0*l*, $l \neq 2n$. These absences are consistent with either of the space groups *Cc* (C_s^4, No. 9) or *C*2/*c* (C_{2h}^6, No. 15). Subsequent structure determination has shown the latter to be the correct choice.

Crystal unit cell and diffraction data were collected following procedures previously described, with minor modifications,[10,11] and are summarized in Table I. After processing and correction for absorption,[12] the 7786 intensity data sampled were averaged to give the 2751 independent reflections with $F^2 > 3\sigma(F^2)$ used in the subsequent structure analysis. The *R* factor for averaging was 1.6%.

Solution and Refinement of the Structure

The structure was solved by the application of Patterson, Fourier, and least-squares techniques.[13] Full-matrix least-squares refinements on *F* were used in which the function minimized was $\sum w(|F_o| - |F_c|)^2$, where F_o and F_c are the observed and calculated structure factors and the weighting factor, *w*, is $4F_o^2/\sigma^2(F_o^2)$. The atomic scattering factors for neutral Yb, Cl, and C were taken from the values tabulated by Cromer and Mann[14] and those for neutral hydrogen were from Stewart, Davidson, and Simpson.[15] Corrections for anomalous dispersion effects[16] of ytterbium using both $\Delta f'$ and $\Delta f''$ were included in the calculation.

The position of the ytterbium atom was determined from a three-dimensional Patterson map. Isotropic least-squares refinement assuming the centric space group followed by a difference Fourier enabled the chlorine and several of the carbons to be located. Further refinement and a second difference Fourier yielded the location of all nonhydrogen atoms. The hydrogen atom positions for the two cyclopentadienyl rings and their respective methyl groups were calculated by assuming planar and tetrahedral geometry, respectively, and C–H bond lengths of 1.0 Å. The ring hydrogens were included as a fixed contribution and not refined, but the methyl hydrogens were allowed to rotate about a threefold axis passing through the methyl carbon and the ring carbon bonded to it. One methyl group failed to refine in this fashion and so was not included in the final least-squares cycle. In the final refinement all nonhydrogen atoms were treated anisotropically, the ring hydrogens were included as a fixed contribution with a fixed isotropic thermal parameter of 6.0 Å, and the one set of methyl hydrogens was treated as a rigid, triangular group whose threefold axis lay along the ring carbon–methyl carbon vector. The degree of rotation about that axis and the isotropic group thermal parameter were refined. The model converged to give final weighted and unweighted *R* factors of 3.69 and 3.46%, respectively. On the final cycle no parameter shifted more than 0.05 times its standard deviation. The final error in an observation of unit weight was 1.14 and did not vary systematically with either $(\sin \theta)/\lambda$ or $|F_o|$. Examination of the final difference Fourier showed no peak greater than 1.7 e/Å^3 (approximately 25% of a carbon atom). The several highest peaks in the difference Fourier are very close to the Yb atom and to C_{2M} (the methyl carbon whose hydrogen atoms did not refine). Table II gives the positional and thermal parameters for the nonhydrogen atoms. Positional parameters for the hydrogens included in the refinement are listed in Table III. Table IV lists the root-mean-square (rms) amplitudes of vibration of the nonhydrogen atoms derived from the anisotropic thermal motion.[17]

Description and Discussion of the Structure

The crystal structure consists of discrete dimers which are located about inversion centers in the unit cell, the monomeric units being inversion related. There are four dimers per unit cell and their centers occupy the symmetry-related positions 0, 0, 0; 0, 0, $^1/_2$; $^1/_2$, $^1/_2$, 0; and $^1/_2$, $^1/_2$, $^1/_2$. A stereoscopic view of the packing in the unit cell, looking along the *b* axis, is shown in Figure 1.

A perspective drawing of the dimer is shown in Figure 2. The molecular structure consists of two ytterbium atoms, each with two η^5-bound methylcyclopentadienyl rings, which are nearly symmetrically bridged by the two chlorine atoms. The ytterbium–chlorine distances are 2.628 (2) and 2.647 (2) Å, respectively. The bridging unit, required by symmetry to be planar, is nearly square, with a Yb–Cl–Yb angle of 97.96 (5)°. These and other important bond distances and angles are listed in Table V.

The coordination of the ytterbium atom in this structure

Table II. Positional and Thermal[a] Parameters (×10^4) for Nonhydrogen Atoms

	x	*y*	*z*	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Yb	0.094742 (10)[b]	0.083992 (26)	0.060548 (17)	13.44 (5)	71.25 (28)	42.35 (15)	−0.02 (12)	5.13 (6)	1.76 (20)
Cl	0.47891 (7)	0.56234 (17)	0.10897 (11)	19.3 (3)	118.0 (21)	41.7 (8)	−7.1 (7)	10.9 (4)	−14.5 (10)
C_1M[c]	0.3383 (4)	0.2253 (8)	0.4803 (7)	30.3 (21)	118 (11)	119 (7)	−13 (4)	19 (3)	8 (7)
C_2M	0.0891 (5)	0.4120 (8)	0.1994 (7)	63 (4)	122 (11)	85 (6)	3 (5)	31 (4)	−34 (7)
C_{11}	0.3317 (3)	0.3414 (7)	0.3991 (5)	19.9 (17)	105 (9)	72 (5)	−16 (3)	8.3 (24)	−9 (5)
C_{12}	0.28524 (28)	0.4594 (7)	0.3766 (6)	14.4 (14)	116 (8)	95 (6)	−9.6 (27)	11.3 (23)	−10 (6)
C_{13}	0.2922 (4)	0.5368 (8)	0.2864 (6)	23.8 (19)	138 (10)	76 (6)	−7 (4)	−11.5 (27)	−4 (6)
C_{14}	0.1555 (4)	−0.0325 (9)	0.2436 (6)	33.9 (24)	177 (12)	53 (5)	31 (5)	6.8 (27)	20 (6)
C_{15}	0.3684 (3)	0.3475 (7)	0.3259 (6)	25.7 (18)	93 (8)	75 (5)	−9 (3)	14.9 (25)	−28 (5)
C_{21}	0.0986 (3)	0.3614 (7)	0.0965 (6)	27.7 (21)	69 (7)	73 (5)	−1 (3)	12.8 (26)	4 (5)
C_{22}	0.1612 (3)	0.3258 (7)	0.0771 (6)	22.0 (17)	101 (9)	92 (6)	−9 (3)	9.0 (26)	2 (6)
C_{23}	0.3534 (3)	0.2184 (7)	0.0283 (6)	31.5 (22)	109 (10)	91 (6)	−5 (4)	30 (3)	15 (6)
C_{24}	0.5743 (4)	0.2096 (7)	0.4219 (5)	34.1 (21)	87 (8)	65 (5)	6 (3)	13.5 (27)	−18 (5)
C_{25}	0.4543 (3)	0.1609 (6)	0.0026 (5)	22.7 (17)	73 (7)	72 (5)	1.8 (27)	11.2 (24)	12 (5)

[a] The form of the anisotropic thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. [b] Standard deviations of the least significant figures are given here and in subsequent tables in parentheses. [c] The subscripts on carbon atoms specify first the ring number and then the atom number. The M represents the methyl carbon which is attached to C_1.

Table III. Calculated Positions for Cyclopentadienide and Methyl Hydrogen Atoms

Atom	*x*	*y*	*z*
H_{12}[a]	0.2520	0.4881	0.4172
H_{13}	0.2633	0.6227	0.2508
H_{14}	0.3626	0.5003	0.1961
H_{15}	0.4063	0.2769	0.3229
H_{22}	0.2087	0.3290	0.1320
H_{23}	0.1824	0.2504	0.0618
H_{24}	0.0486	0.2664	0.1558
H_{25}	0.0054	0.3569	0.0156
H_{M_1}[b]	0.3004	0.1492	0.4531
H_{M_2}	0.3840	0.1775	0.4974
H_{M_3}	0.3330	0.2690	0.5472

[a] The subscripts specify first the ring number and then the atom number. Trigonal geometry is assumed with C–H bond lengths of 1.0 Å and an isotropic thermal parameter of 6.0 $Å^2$. [b] H_{M_1}–H_{M_3} are the hydrogens of the methyl group attached to ring 1. The group thermal parameter refined to 9.4 $Å^2$.

Table IV. Root-Mean-Square Amplitude of Vibration along Principal Axes (Å × 10^3)

Atom	Axis 1	Axis 2	Axis 3
Yb	157.8 (3)	174.0 (4)	191.3 (4)
Cl	172 (2)	185 (2)	234 (2)
C_{1M}	200 (10)	256 (9)	312 (10)
C_{2M}	185 (10)	282 (11)	345 (11)
C_{11}	161 (9)	236 (9)	247 (9)
C_{12}	155 (8)	228 (8)	281 (9)
C_{13}	165 (8)	245 (9)	316 (11)
C_{14}	179 (9)	238 (10)	315 (10)
C_{15}	173 (9)	220 (8)	261 (9)
C_{21}	171 (8)	228 (8)	245 (9)
C_{22}	184 (9)	223 (8)	282 (10)
C_{23}	181 (10)	235 (9)	281 (9)
C_{24}	172 (9)	236 (8)	264 (9)
C_{25}	172 (9)	207 (8)	247 (9)

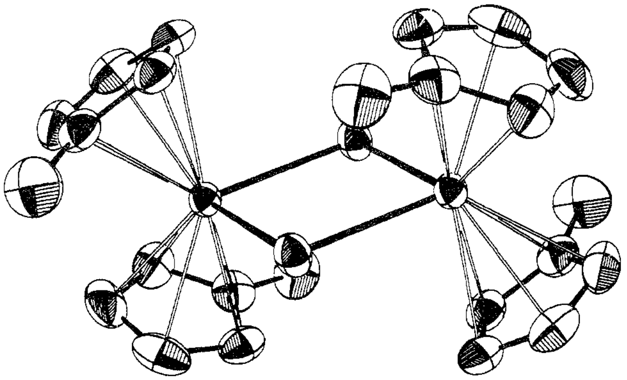

Figure 2. A perspective drawing of $[Yb(C_5H_4CH_3)_2Cl]_2$. The thermal ellipsoids enclose 50% of the electron probability distribution. Hydrogen atoms are not shown.

Table V. Bond Distances and Angles in $[Yb(C_5H_4CH_3)_2Cl]_2$

Bond Distances, Å			
Yb–Yb (nonbonded)	3.979 (1)	Yb–C_{21}	2.589 (6)
Yb–Cl	2.628 (2)	Yb–C_{22}	2.573 (6)
Yb–Cl′	2.647 (2)	Yb–C_{23}	2.569 (6)
Cl–Cl′ (nonbonded)	3.462 (3)	Yb–C_{24}	2.577 (6)
Yb–C_{11}	2.641 (6)	Yb–C_{25}	2.578 (6)
Yb–C_{12}	2.581 (5)	Yb–C(av)[a]	2.585 (7)
Yb–C_{13}	2.563 (6)	C_i–C_{i+1}(av)[b]	1.408 (5)
Yb–C_{14}	2.569 (6)	C_{11}–C_{1M}	1.489 (10)
Yb–C_{15}	2.609 (6)	C_{21}–C_{2M}	1.509 (11)
Bond Angles, Deg			
Yb–Cl–Yb	97.95 (5)	Cp_1–Yb–Cl′	112.4
Cl–Yb–Cl′	82.05 (5)	Cp_2–Yb–Cl	108.0
Cp_1–Yb–Cp_2[c]	126.7	Cp_2–Yb–Cl′	109.1
Cp_1–Yb–Cl	109.4	C_i–C_{i+1}–C_{i+2}(av)[b]	108.0 (5)

[a] The average in this and other quantities reported is calculated as $\bar{x} = (\Sigma x_i)/n$ and the standard deviation as $\sigma(\bar{x}) = [\Sigma(x_i - \bar{x})^2/n(n-1)]^{1/2}$. [b] C_i–C_{i+1} refers to adjacent carbons on the cyclopentadienyl ring. [c] Cp represents the centroid of the cyclopentadienyl ring.

Table VI

Weighted Least-Squares Planes[a] of Cyclopentadienyl Rings

Atom	Ring 1	Ring 2
C_1	−0.006 (5)[b]	−0.005 (6)
C_2	0.009 (6)	0.006 (7)
C_3	−0.009 (6)	−0.003 (6)
C_4	0.003 (6)	−0.0007 (60)
C_5	0.002 (6)	0.004 (6)
C_M[c]	−0.103	−0.023

Parameters of the Planes[a]

Parameter	Ring 1	Ring 2
A	10.546	3.853
B	5.358	8.692
C	5.609	−4.096
D	7.572	3.131

[a] The equation of the plane in monoclinic coordinates is $Ax + By + Cz - D = 0$. See W. C. Hamilton, *Acta Crystallogr.*, **14**, 185 (1961). [b] Displacement of atom from plane (Å). [c] The methyl carbon was not used in calculating the least-squares plane.

Table VII. Comparison of Molecular Parameters for Three Dimers

	$[Sc(C_5H_5)_2Cl]_2$[a]	$[Yb(C_6H_7)_2Cl]_2$[b]	$[Ce(C_8H_8)Cl\cdot 2THF]_2$[c]
M–M, Å	3.90	3.98	4.64
M–Cl, Å	2.57	2.64	2.85 2.93
M–C, Å	2.46	2.58	2.71
Cl–Cl′, Å		3.46	3.46
Cl–M–Cl, deg	81.5	82.0	73.4
M^{3+} radius,[d] Å	0.87	0.98	1.15

[a] Reference 8. [b] Present work. [c] Reference 7. [d] Reference 18.

can be described as slightly distorted tetrahedral, with the centers of the two cyclopentadienyl rings and the two chlorine atoms forming the apices of the tetrahedron. The vectors from the center of either ring to the ytterbium and from either chlorine to the ytterbium form angles ranging from 108 to 113°. The two cyclopentadienyl rings, due to their size and the fact that they occupy more than one coordination site, are at an angle somewhat greater than the tetrahedral; the vectors from the center of either ring to the ytterbium form an angle of 126.7°. Due to the requirement of bridge formation, the Cl–Yb–Cl angle is reduced to 82° and the Cl–Cl nonbonded distance is 3.462 (3) Å, somewhat shorter than the van der Waals contact distance of 3.6 Å. The corresponding Yb–Yb nonbonded distance is 3.979 (1) Å.

The five cyclopentadienyl carbons of each ring form very good planes, as shown in Table VI, with the maximum deviation from the weighted least-squares plane being 0.009 Å. Although exhibiting much greater thermal motion, the methyl carbon of each ring also lies essentially in this same plane. The rings are very well defined with carbon–carbon distances for adjacent carbon atoms ranging from 1.386 to 1.419 Å and averaging 1.408 (5) Å and C–C–C angles within a ring ranging from 104.9 to 110.1° and averaging 108.0 (5)°. The rings are symmetrically bound to the ytterbium with an average Yb–C distance of 2.585 (8) Å.

This is the first structure determination of a lanthanide dimer with a cyclopentadienyl ligand, but its molecular parameters can be compared with the cerium cyclooctatetraene chloride dimer[7] and the scandium cyclopentadienyl chloride dimer[8] (Table VII). The most significant comparison is the symmetry of the bridge. In the compound described here and in the scandium dimer the bridge is essentially symmetric, but in the

Table VIII. Comparison of Metal Radius and Metal–Carbon Distance (All Å)

Compd	M^{3+} radius[a]	Δ radius	M–C distance	Δ distance
$[Yb(C_6H_7)_2Cl]_2$[b]	0.98	0.0	2.58	0.0
$Sm(C_9H_7)_3$[c]	1.15	0.17	2.75	0.17
$Sc(C_5H_5)_3$[d]	0.87	−0.11	2.48	−0.10
$[Sc(C_5H_5)_2Cl]_2$[e]	0.87	−0.11	2.46	−0.12
$[Ce(C_8H_8)Cl\cdot 2THF]_2$[f]	1.15	0.17	2.71	0.13
$[Ce(C_8H_8)_2]^{2-}$[g]	1.19	0.21	2.74	0.16

[a] From ref 18 assuming an η^5 ring to occupy three coordination sites and an η^8 ring to occupy five coordination sites. Where the required coordination number was not given, linearity of CN with radius was assumed. [b] Present work. [c] J. L. Atwood, J. H. Burns, and P. G. Laubereau, *J. Am. Chem. Soc.*, 95, 1830 (1973). [d] J. L. Atwood and K. D. Smith, *ibid.*, 95, 1488 (1973). [e] Reference 8. [f] Reference 7. [g] K. O. Hodgson and K. N. Raymond, *Inorg. Chem.*, 11, 3030 (1972).

cerium compound it is definitely asymmetric. This can be attributed to the increasing radius of the metal ion and the corresponding increase in metal–metal distance. For the small scandium(III) ion the metal–metal contact distance is short enough to allow a symmetric bridge. As the metals move further apart, the chloride ion can no longer span the gap and is pulled preferentially toward one metal atom. The extreme of this process is asymmetric fission to two monomers.

The effect of the change in metal radius is apparent in other structural parameters of these compounds as well, in particular the metal–carbon distances. If the effect of ligand charge and different effective coordination numbers is taken into account, then the metal to carbocyclic carbon bond lengths can be predicted quite accurately from knowledge of one bond length and the metal radii. Table VIII shows how the change in metal–carbon bond length parallels the change in ionic radius, adjusted for coordination number.[18] Note that for the cyclooctatetraene compounds at the bottom of the table, an adjustment of 0.04 Å must be made for the shortening due to a 2− charge on the ligand. This is reasonable in view of the observed variation of bond length with charge on the actinides[19] and the transition metals.[20] It should be recognized that in some structures steric factors may lengthen the bond from what one might predict by this method.

In summary, this structure provides proof of the dimeric nature of the lanthanide dicyclopentadienyl halides. A series of dimeric complexes can now be prepared in which the bridging chloride is replaced by other ligands. The investigation of their properties is in progress.

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Supplementary Material Available. A listing of structure factor amplitudes will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the supplementary material from this paper only or microfiche (105 × 148 mm, 24× reduction, negatives) containing all of the supplementary material for the papers in this issue may be obtained from the Journals Department, American Chemical Society, 1155 16th St., N.W., Washington, D.C. 20036. Remit check or money order for $4.50 for photocopy or $2.50 for microfiche, referring to code number AIC40695R.

References and Notes

(1) (a) National Science Foundation Predoctoral Fellow, 1972–present. (b) NDEA IV Fellow, 1970–1973.

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(9) Details of the experimental procedure will appear in a future paper.

(10) The data crystal was a small orange-red plate, cleaved from a larger plate, and bounded by the following nine planes: 100, $0\bar{1}0$, $\bar{1}01$, $\bar{1}00$, 010, $10\bar{1}$, 410, $1\bar{1}\bar{1}$, and $\bar{1}11$. The perpendicular distance to each of these planes from the intersection of the first three, defined as the crystal origin, was 0.0, 0.0, 0.0, 0.147, 0.283, 0.081, 0.080, 0.030, and 0.220 mm, respectively. The crystal in its capillary was mounted on a eucentric goniometer head such that the 010 axis was nearly parallel to the ϕ axis of a Picker FACS-1 four-circle diffractometer. The lattice constants and orientation angles were determined from a least-squares refinement of the setting and 2θ angles of 16 carefully centered reflections whose 2θ values ranged from 37 to 45°. The crystal gave ω-scan widths at half-height of 0.10, 0.10, and 0.08° for the 400, 002, and 020 reflections, respectively. The programs used by the PDP-8/E computer were those written by Busing and Levy as modified by the Picker Corp. and further modified locally. Intensity data were collected in the θ–2θ scan mode using monochromatic Mo Kα radiation and a scintillation counter. The Bragg 2θ angle for the highly oriented graphite monochromator crystal was 12.02°, and the X-ray tube takeoff angle was 2.0°. The pulse height analyzer was centered on the Mo Kα peak and set to admit approximately 90% of the maximum intensity at full window width. The detector was located 33 cm from the source with a 7 × 7 mm receiving aperature. The 2θ scans were from 0.75° below the Kα_1 peak to 0.75° above the Kα_2 with a scan rate of 1.0°/min. Copper foil attenuators were automatically inserted in the path of the diffracted beam to keep the count rate for a given reflection below 10^4 counts/sec. Stationary 10-sec background counts were taken at the start and finish of each scan. Throughout the data collection the intensities of the three standard reflections 400, 040 and 006 were measured every 80 reflections as a check on the stability of the crystal and the instrument. A maximum variation in intensities of less than 4% was noted and no decay correction was applied to the data. A total of 7786 reflections were collected including one unique form ($\pm h,+k,+l$) out to $2\theta = 70°$ and two equivalent forms ($\pm h,+k,-l$ and $\pm h,-k,+l$) out to $2\theta = 40°$ and $2\theta = 30°$, respectively. The data reduction and processing were carried out by our program UCFACS as previously described,[11] except that standard deviations in the measured intensity were assigned according to the formula, $\sigma(I) = [\mathrm{CT} + 18 + {}^1/_4(t_c/t_b)^2(B_1 + B_2 + 36) + (pI)^2]^{1/2}$, where CT is the total integrated peak count obtained in time t_c, B_1 and B_2 are the background counts each obtained in time t_b, and $I = \mathrm{CT} - 0.5(t_c/t_b)(B_1 + B_2)$. The appearance of the constants 18 and 36 is due to the statistical effect of integer truncation. The parameter p is introduced to avoid overweighting strong reflections and represents the standard deviation as a percentage error when counting statistics are negligible. It was assigned a value of 0.04 for this data set. The intensities were corrected for Lorentz and polarization effects and converted to values of F^2. The calculated absorption coefficient, μ, is 85.42 cm^{-1} and the maximum and minimum thickness gave a range of μt from 0.70 to 1.25, so an absorption correction was applied using an analytical integration method.[12] The correction factors ranged from 1.8 to 3.3 with an average value of 2.25.

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