RECEIVED
LAWRENCE
RADIATION LABORATORY

NOV 20 1972

LIBRARY AND
DOCUMENTS SECTION

Submitted to Acta Cryst

LBL-1268
Preprint

INVESTIGATIONS OF ALKALINE-EARTH β-DIKETONE COMPLEXES. III. THE CRYSTAL AND MOLECULAR STRUCTURE OF BIS(1, 3-DIPHENYL-1, 3-PROPANEDIONATO) STRONTIUM HEMIACETONATE

Frederick J. Hollander, David H. Templeton,
and Allan Zalkin

September 1972

AEC Contract No. W-7405-eng-48

For Reference

Not to be taken from this room

LBL-1268

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

0 0 0 0 3 8 0 7 1 9 3

LBL-1268

Investigations of Alkaline-earth β-diketone Complexes. III. The crystal and molecular structure of bis(1,3-diphenyl-1,3-propanedionato)strontium hemiacetonate*

By Frederick J. Hollander, David H. Templeton and Allan Zalkin
Lawrence Berkeley Laboratory and Department of Chemistry,
University of California, Berkeley, California 94720 U.S.A.

The crystals of bis(1,3-diphenyl-1,3-propanedionato) strontium hemiacetonate are triclinic, space group $\underline{P\bar{1}}$, with $\underline{a}$ = 13.759(50) Å, $\underline{b}$ = 14.182(10) Å, $\underline{c}$ = 16.031(20) Å, α = 107.57(3)°, β = 90.36(20)°, γ = 113.07(20)° at 23°C. The calculated density for two units of empirical formula $Sr_2C_{63}H_{50}O_9$ in the unit cell is 1.38 gm/cm^3. X-ray diffraction measurements were made of 2204 independent reflections from a single crystal by θ-2θ scans with a scintillation counter using monochromatized Mo$\underline{K}\alpha$ radiation. The non-hydrogen atoms were found by Fourier methods and refined by least-squares to $\underline{R}$ = 0.088 for 1561 reflections with $\underline{F}^2 > \sigma(\underline{F}^2)$. Hydrogen atoms were not located. The conformation of the complex is similar to that of the corresponding $Ca(DPP)_2$ hemiethanolate, consisting of

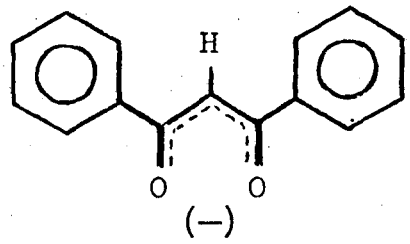
tetrameric polymers around a center of symmetry, but the packing is such that the two structures are not isomorphous. These two structures are compared with those of other polymeric β-diketone complexes.

---

*Work done under the auspices of the U.S. Atomic Energy Commission

Introduction

Alkaline-earth metal cations form complexes with the anion of 1,3-diphenyl-1,3-propanedione:



This paper reports the structure of $Sr(DPP)_2$ hemiacetonate. The complex forms tetrameric polymers of the same general configuration as those found for the DPP complex of calcium (Hollander, Templeton and Zalkin, 1973a). However, the solvent molecule included in the Sr complex is acetone, rather than the ethanol of the Ca complex and there are differences in the details of the polymer shape. Thus, despite the fact that the general forms of the complexes are similar and the space group ($\underline{P}\bar{1}$) the same, the structures are not isomorphous and the unit cells cannot be brought into congruence.

Experimental Procedure

The complex was synthesized using a modification of the method of Hammond, Nonhebel and Wu (1963). Strontium nitrate was dissolved in a small amount of water, and ethanol added until precipitation was just observed. This solution was added to an ethanolic solution of 1,3-diphenyl-

1,3-propanedione (HDPP), and a strong aqueous NH_3/NH_4Cl, pH 10, buffer was added to the mixture. A whitish precipitate (probably either $Sr(NO_3)_2$ or HDPP) immediately formed, and the mixture was heated to reflux for an hour and stirred continuously. Heating caused the precipitate to dissolve, and cooling yielded a very pale yellow crystalline precipitate which was filtered and dried in air.

Attempts to recrystallize the compound generally yielded a viscous oil, but finally a few crystals were obtained by very slow evaporation of an ethanol solution with a very small amount of acetone added to it. Of these few, only one was good enough for crystallographic study.

This crystal, a thin plate of approximate dimensions 0.03 mm x 0.17 mm x 0.32 mm was affixed to a glass fiber. Precession photographs indicated a triclinic unit cell. It was then mounted on a Picker/Nuclear four-circle diffractometer automated by a DEC PDP 8I computer and disc and equipped with a molybdenum x-ray tube.

Twelve reflections which were in the range 20° to 25° of 2θ were carefully centered in χ, ω and 2θ using Mo$K\alpha$ radiation (λ = 0.7107 Å). The cell dimensions and orientation matrix were determined from these angles using the FACS-1 least-squares program on the PDP 8I. The cell dimensions were determined again by the same method

after the data collection and were found to have changed by as much as five standard deviations. The second set of cell parameters, $\underline{a}$ = 13.759(10) Å, $\underline{b}$ = 14.182(9) Å, $\underline{c}$ = 16.031(9) Å, α = 107.57(3)°, β = 90.36(3)°, γ = 113.07(3)° at 23°C, where the standard deviations are those estimated by least squares, were used throughout the structure analysis. We estimate respectively 0.05 Å, 0.01 Å, 0.02 Å, 0.03°, 0.2°, and 0.2° as standard deviations which reflect the variation of parameters during the experiment. The calculated density for $\underline{Z}$ = 4 is 1.38 gm/cm^3. The density was not measured directly for lack of suitable material. Inspection of the intensities before data collection revealed a rapid fall-off of intensity with increasing 2θ, there being very few appreciable intensities beyond 2θ = 25° and none at all beyond 2θ = 30°.

Data were collected using a θ-2θ scan technique and graphite monochromatized ($2\theta_{\underline{m}}$ = 11.80°) Mo$\underline{K}\alpha$ radiation. Peaks were scanned 0.7° below the predicted $\underline{K}\alpha_1$ position to 0.7° above the predicted $\underline{K}\alpha_2$ position at a scan speed of 1°/min. Backgrounds were counted for 10 seconds at positions offset 0.3° from each end of the scan (all angles 2θ). Copper foil attenuators were automatically inserted in the diffracted beam any time the count rate exceeded 10000 cps and the peak was rescanned and the backgrounds measured with the attenuators in place. All reflections in the hemisphere of reciprocal space $+\underline{h},\pm\underline{k},\pm\ell$ were collected for $2\theta < 30°$ ($\sin\theta/\lambda < 0.370$). Two reflections, the (3 0 0) and the (1 $\bar{3}$ 0), were measured

after every 100 data to monitor crystal decay and alignment. The (1 $\bar{3}$ 0) showed a steady linear decline to 84% of its original intensity over the data collection period, while the (3 0 0) showed large (±10%) random variations around a similar drop. Not including repetitions of the standards, 2371 reflections were measured. Of these, 260 were measured with zero intensity, and in all 684 had $\underline{I} < \sigma(\underline{I})$. Intensities and their standard deviations were calculated as previously described (Hollander, Templeton and Zalkin, 1973b).

An absorption correction was applied to the intensities assuming that the crystal composition was $Sr(DPP)_2(C_2H_5OH)_{1/2}$ with $\underline{Z}$ = 4, in compositional isomorphism with the related Ca compound (Hollander, Templeton and Zalkin, 1973a). This yielded μ = 21.2 cm^{-1}. (The actual composition differs from this by one carbon atom, but the effect on μ is negligible.) The correction factors ranged from 1.07 to 1.41. The data were corrected for the linear crystal decay and Lorentz and polarization effects. Those reflections taken more than once were averaged to give 2204 unique reflections of which 1561 had $\underline{F}^2 > \sigma(\underline{F}^2)$.

The atomic scattering factors of Doyle and Turner (1968) were used for neutral strontium, carbon and oxygen, together with the real and imaginary dispersion corrections

of Cromer and Liberman (1970). Our least-squares program minimizes the function $\Sigma \underline{w}(\Delta \underline{F})^2 / \Sigma \underline{w}\underline{F}_o^2$. The weighting scheme used throughout gave zero weight when $\underline{F}^2 < \sigma(\underline{F}^2)$ and $\underline{w} = 1/\sigma^2(\underline{F})$ otherwise; $\sigma(F)$ was calculated as previously described (Hollander, Templeton and Zalkin, 1973b) using $\underline{p} = 0.05$.

Programs used in the structure analysis are listed in the paper referenced above.

Structure Determination and Refinement

Due to the low resolution of the data (few reflections with $\underline{d} < 1.6$ Å) the structure refinement did not proceed smoothly. Least-squares did not distinguish well between atoms and groups of atoms, allowing large excursions and producing some poor bond distances.

Two independent Sr atoms were located by the three-dimensional Patterson function and gave $\underline{R}_1 = \Sigma |\Delta \underline{F}| / \Sigma |\underline{F}_o| = 0.36$. A Fourier phased by these atoms revealed 38 additional atoms which refined to $\underline{R}_1 = 0.27$. Another Fourier revealed the other 30 atoms of the DPP ligands and another peak, designated O(9), which was assumed, in analogy to the Ca complex (Hollander, Templeton and Zalkin, 1973a), to be the oxygen of an ethanol molecule. Three cycles of least-squares on these atoms, all refined with isotropic thermal parameters brought $\underline{R}_1$ to 0.14. With Sr atoms given anisotropic thermal parameters, $\underline{R}_1$ was

reduced to 0.094, but attempts to refine an ordered or disordered ethanol in the vicinity of O(9) failed to converge satisfactorily.

A difference Fourier phased after removal of the "ethanol" atoms ($\underline{R}_1$ = 0.13) showed a large triangular area of electron density with a peak at each corner and high density in the center. Still assuming similarity to the Ca structure, a disordered ethanol model was hand-fitted to the peaks and the positions of the six atoms with occupancy factor of 0.5 were fixed in least-squares. Refinement of the rest of the structure and of four thermal parameters for the ethanol gave an $\underline{R}_1$ of 0.094 and $\underline{R}_2 = (\Sigma \underline{w}(\Delta \underline{F})^2 / \Sigma \underline{wF}_o^{\,2})^{1/2}$ of 0.080. However, the thermal parameters of the methyl carbons of the two half-ethanols refined to the lowest values of any in the structure. It was then realized that the triangular region of electron density could also be fitted by an acetone molecule. Inclusion of these atoms in the refinement brought $\underline{R}_1$ to 0.088, $\underline{R}_2$ to 0.072, standard deviation of observation of unit weights was 1.47, and all shifts to less than 10% of their standard deviations after four cycles. The thermal parameters of all of the acetone atoms were in keeping with those of the rest of the structure, and the refinement was considered complete.

A difference Fourier showed no peaks greater than 0.6 $\underline{e}^-/Å^3$. No attempt was made to refine hydrogen atoms.

The observed F's and their standard deviations are compared to the final differences in Table 1. The final positional and thermal parameters of the atoms are given in Table 2.

Results and Discussion

The complex consists of clusters of composition $(Sr_2(DPP)_4(CH_3)_2CO)_2$ around the center of symmetry at 0,0,0. The clusters are related only by unit cell translations, and the only inter-cluster contact of less than 3.50 Å is 3.42 Å between C(26) and C(26) across the center of symmetry at 0,1/2,0.

The Sr(1) and Sr(2) atoms are respectively seven- and six-coordinated by the oxygens of the DPP ligands and the acetone (Fig. 1). Each Sr atom shares two oxygen atoms with each of two neighboring Sr atoms, forming a cluster around the center of symmetry. The bridging oxygens, O(1) and O(2) of DPP(1) and O(3) and O(4) of DPP(2), occupy the corners of a slightly distorted parallelopiped, with four rectangular faces capped by Sr atoms and the two non-rectangular faces occupied by the DPP ligands (Fig. 2). The uncapped face, referred to here as core plane 1 (CP 1), forms almost right angles with the planes capped by Sr(1)

and Sr(2) (CP 2 and CP 3 respectively). The acute angle between CP 2 and CP 3 is 83°, significantly different from right angles. The core planes are planar to within less than a standard deviation of the coordinates of the four atoms that define them. The distance between symmetry-related planes is 3.04 Å for CP 1, 3.30 Å for CP 2 and 2.83 Å for CP 3. The mean plane of the Sr atoms lies halfway between CP 1 and the symmetry-related CP 1'. Sr(1) is 1.50 Å away from CP 2 and the three other oxygens coordinated to Sr(1) are 3.25 Å, 3.17 Å and 3.21 Å from the same plane for O(5), O(6) and O(9) respectively. Sr(2) is 1.14 Å and O(7) and O(8) of DPP(4) are 3.08 and 3.24 Å respectively from CP 3.

The distances from Sr to the bridging oxygens average 2.55 Å with no significant difference between the two differently coordinated Sr atoms. The distances from the Sr atoms to the unshared oxygens average to 2.44 Å, indicating the expected tighter bonding to the unshared ligands, and the Sr(1) to O(9) distance is 2.60 Å, in keeping with the fact that the acetone is uncharged and thus not as tightly bound as the negative DPP ligands.

The angles from the diketone planes of the bridging DPP molecules to CP 1 are 89° for DPP(1) and 108° for DPP(2) and the angle between the two is 17°.

The larger angle for DPP(2) reflects the less crowded environment it encounters (Fig. 2), whereas DPP(1) is forced to near perpendicularity with CP 1 by interaction with the acetone molecule. DPP(3) forms an angle of 71° with CP 2, and the acetone plane forms a right angle with the same plane, again reflecting this steric interaction. The diketone of DPP(4) forms an angle of 86° with CP 3, reflecting its nearly symmetrical environment with respect to CP 1 and CP 1'. DPP(4) is tilted within its plane as already noted.

Each DPP ligand can be described in terms of three planes; the two phenyl rings (phenyl(1), 1-6; phenyl(2), 10-15, Fig. 3) and the diketone residue (7-9, oxygen 1 and 2, Fig. 3). All such planes in this structure are planar to within two standard deviations of the coordinates of the atoms involved. The plane of the acetone molecule is also good to two standard deviations. The phenyl planes are twisted along the 6-7 and 9-10 axes with respect to the diketone residue planes by angles ranging from 10° to 45° (Table 4).

Due to the low resolution of the data noted above, the distances within the DPP ligands (Table 5) are not well defined. The average C-C distance in the phenyl groups of 1.41 Å is close to other phenyl C-C values where the hydrogens have been omitted, and the other average

distances, C-O = 1.28 Å, C-C(diketone) = 1.40 Å, C(phenyl)-C(diketone) = 1.53 Å, are in reasonable agreement with other values for this ligand (Williams, 1966; Hollander, Templeton and Zalkin, 1973a, 1973b).

Since Sr is larger than Ca, it is not unreasonable that a larger molecule, acetone, would replace the ethanol which is found in the Ca complex. However, it is not obvious why the preference should be so specific, as seems to be the case, nor why the packing is not more nearly isomorphous.

The primary difference in molecular conformation is the degree of distortion of the central parallelopiped of O atoms (Fig. 1). In the Ca complex it is strongly distorted from rectangularity while in the Sr complex the acute angle between the rectangular faces is much closer to 90° (69° for the Ca and 83° for the Sr complex). The planes that make up the central parallelopiped are closer together in the Ca compound than they are in the Sr complex (2.90, 2.87 and 2.60 Å vs. 3.04, 3.30 and 2.83 Å).

These effects can be explained by the differences between the Ca-O and Sr-O bond lengths, which are compatible with the difference in ionic radius between Ca and Sr ($Ca\text{-}O_{ave}$ = 2.37 Å, $Sr\text{-}O_{ave}$ = 2.55 Å; r_{Ca} = 0.99 Å, r_{Sr} = 1.13 Å) (Pauling, 1960). Given the coordination

geometry, shorter bonds between the metal and the bridging oxygens mean that the DPP ligands doing the bridging must move closer together (Fig. 2). In the Ca complex they are forced close enough together that they must slide parallel to one another to achieve a staggered configuration and increase the distances between the atoms, thus decreasing the acute angle of the parallelogram of core plane 1. In the case of the Sr complex, the distances from the Sr to the oxygen allow enough room between DPP ligands so that they are not forced into close proximity and can assume a more eclipsed configuration with respect to one another.

The reason that $Mg(DPP)_2$ (Hollander, Templeton and Zalkin, 1973b) does not polymerize in the same manner as the Ca and Sr complexes is thus apparent, since the Mg-O distances of around 2.05 Å would have required very close proximity of the DPP ligands even with full staggering of the diketone residues.

We now compare the polymerization observed for the Ca and Sr DPP complexes with the structures of other polymeric β-diketone complexes. Most of the known examples of such polymers involve acetylacetone anion (AA) as the ligand, and the cations share oxygen atoms to achieve octahedral coordination. $Ni(AA)_2$ forms linear trimers; each Ni atom is octahedrally coordinated and the octahedra share faces

(Bullen, Mason and Pauling, 1961). $Co(AA)_2$ forms a tetrameric chain with octahedra sharing faces between the two Co atoms at each end and sharing an edge between the two central Co atoms (Cotton and Elder, 1965). $Co(AA)_2(H_2O)$ dimerizes so that each cobalt can be octahedrally coordinated, and the octahedra share an edge (Cotton and Elder, 1966).

Gerlach and Holm (1969) note that β-diketones with bulky side groups act to suppress polymerization and force the complexes to become monomeric even though octahedral coordination may be lost. Thus the structures of bis(2,2,6,6-tetramethyl-3,5-heptanedionato)zinc and nickel, $Zn(DPM)_2$ and $Ni(DPM)_2$, have been determined by crystallographic means to be monomeric, and tetrahedral and planar respectively (Cotton and Wood, 1964; Cotton and Wise, 1966). Various evidence indicates that the structures of the DPM complexes of other divalent transition metals are monomeric and either tetrahedral or planar (Gerlach and Holm, 1969). The results of our studies indicate that bulky side groups cannot be counted on to reduce polymerization. The existence of the dimer in the study of $Pr(DPM)_3$ (Erasmus and Boeyens, 1970), which involves sharing bulky DPM ligands to achieve seven-fold coordination, indicates that this ability to polymerize is not specific to DPP. Further, a recent study of the DPM

complexes of the alkaline-earth metals by means of vapor-phase diffusion, mass spectroscopy and molecular weight measurements indicates that the Ca, Sr and Ba complexes are polymeric in solution and in the vapor phase, but that the Mg complex is monomeric (Schwarberg, Sievers and Moshier, 1970).

These results suggest that a combination of the bulk of the ligand and the length of the M-O bond is the criterion for whether or not polymerization is favorable. With a short M-O bond length, as with Mg or the divalent first-row transition metals, ligands with side groups as bulky as t-butyl (DPM) or phenyl (DPP) are forced too close to one another in the configurations necessary for polymerization. When the M-O distance increases, as for Ca, Sr or Pr(III), then neighboring ligands need not be so close together, and the advantage of sharing ligands to get greater coordination from the negative ions can be realized.

References

Bullen, G. J., Mason, R. and Pauling, P. (1961). Nature, 189, 291.

Cotton, F. A. and Elder, R. C. (1965). Inorg. Chem. 4(8), 1145.

Cotton, F. A. and Elder, R. C. (1966). Inorg. Chem. 5(3), 423.

Cotton, F. A. and Wise, J. J. (1966). Inorg. Chem. 5(7), 1201.

Cotton, F. A. and Wood, J. S. (1964). Inorg. Chem. 3(2), 245.

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53(5), 1891.

Doyle, P. A. and Turner, P. S. (1968). Acta Cryst. A24, 390.

Erasmus, C. S. and Boeyens, J. C. A. (1970). Acta Cryst. B26, 1843.

Gerlach, D. H. and Holm, R. H. (1969). Inorg. Chem. 8(11), 2292.

Hammond, G. S., Nonhebel, D. C. and Wu, C-H. S. (1963). Inorg. Chem. 2(1), 73.

Hollander, F. J., Templeton, D. H. and Zalkin, A. (1973a). In press: Ca paper

Hollander, F. J., Templeton, D. H. and Zalkin, A. (1973b). In press: Mg paper

Pauling, L. (1960). The Nature of the Chemical Bond, Third Ed., Cornell University Press, Ithaca, N. Y.

Schwarberg, J. E., Sievers, R. E. and Moshier, R. W. (1970). Anal. Chem. 42(14), 1828.

Williams, D. E. (1966). Acta Cryst. 21, 340.

Table 1. Observed structure factors, standard deviations and final differences. Reflections marked with an * were given zero weight in least-squares.

(Table to be reproduced photographically.)

Table 1.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES IN 1.01 FOR
SAIOPPIZ - 1/2 D-CILHSIZ FIO.0-01 - 2006
SG = ESTIMATED STANDARD DEVIATION OF FOB- DEL = /FOB/-/FCAL/. * INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	0,	0		H,K=	0,	3	1	99	3	-3	-4	19	4	1	-7	33	3	-4	-1	19	7	1	-10	27	6	19	3	24	24	24	-4	42	3	-3	9	17	8	11	2	9	13	-13	-7	10	14	-4	1	12	14	3		H,K=	1,	1
2	143	9	17	-7	8	15	-8	2	97	2	-1	-3	28	3	-24	-6	19	4	-1	0	28	4	1	-9	43	3	1	0	15	4	1	-5	19	4	1	-3	32	4	1	-4	23	7	-1	-3	27	3	2	1	18	14	-6	-4	8	10	-14
3	44	2	-7	1	15	3	-8	3	97	2	1	-2	13	14	9	-4	42	3	1	1	31	3	1	0	45	2	1	H,K=	5,	0,	0	-7	37	3	1	0	19	11	10	4	38	7	0	-3	68	2	1	2	11	14	-6	-1	8	14	-8
3	60	2	-1	-5	26	3	9	6	93	2	1	-3	15	14	-14	-4	37	3	-2	2	30	4	3	-7	4	37	-2	-2	27	3	3	-4	19	17	3	-3	9	19	-10	6	70	3	-3	-1	68	2	1	3	8	14	-4	-1	9	14	-8
4	41	2	-1	-4	43	3	0	7	19	11	-14	-2	38	4	3	-3	28	3	1	3	28	3	1	-8	28	3	1	1	29	4	1	-3	32	4	1	1	32	4	1	6	8	15	-3	-2	21	4	1	4	11	14	-4	-1	10	14	-10
4	4	12	-10	-3	44	3	-9	8	30	3	-1	-2	14	4	1	-7	8	10	-2	-3	15	4	1	-9	29	4	1	H,K=	5,	1,	1	-3	37	3	1	2	37	3	1	-3	37	3	1	-2	81	4	1	5	7	14	-7	-2	31	4	-1
5	16	3	-1	-2	34	4	1	9	44	2	1	0	34	3	-1	-5	57	2	-4	-4	42	3	1	-3	46	4	1	2	33	14	1	-3	57	3	1	-3	79	3	1	-2	9	12	1	-1	8	13	1	6	7	14	-7	-1	14	3	1
5	21	2	1	-1	12	15	13	10	42	2	1	1	63	3	1	-5	42	3	1	-4	21	20	-2	-2	91	3	1	3	24	3	1	-1	133	3	1	0	77	3	1	-3	23	4	1	-1	7	3	1	7	8	14	-7	-1	14	3	1
6	31	2	1	H,K=	1,	-1	11	14	16	2	1	1	47	2	1	-4	31	3	1	-3	31	3	1	-2	91	3	1	3	24	3	1	-1	133	3	1	0	77	3	1	-3	23	4	1	-1	7	3	1	7	8	14	-7	-1	14	3	1
6	36	2	1	-1	30	7	1	H,K=	1,	0,	0	-7	14	22	-9	2	37	3	1	3	19	21	1	-4	31	3	1	4	37	3	1	0	81	3	1	-1	8	13	-17	0	77	3	1	-3	32	3	1	-3	32	3	1	-2	10	7	1
10	25	2	-1	3	24	7	1	-1	25	7	1	-2	20	7	-1	-3	21	3	1	4	21	3	1	5	37	3	1	5	37	3	1	0	30	3	1	-1	32	3	1	-3	32	3	1	-2	16	7	1	3	8	13	1	-1	13	3	1
11	14	2	1	3	6	70	-1	-10	15	18	-3	3	21	23	-10	4	127	3	1	-4	29	3	-1	-3	1974	3	1	2	8	14	-2	-1	24	3	-1	3	16	17	10	-4	21	3	1	3	9	7	1	4	8	14	-4	1	14	3	1
	H,K=	0,	1	-7	11	70	-7	-1	62	3	1		H,K=	7,	-10	3	24	10	-1	2	24	10	-1	2	12	10	-1	2	41	4	1	-2	11	2	-2	1	8	13	-10	-2	40	2	-1	3	10	17	-1	-3	24	3	1	-1	24	3	1
-11	42	3	1	3	25	5	-1	-2	20	4	1	3	40	2	1	H,K=	6,	0,	0	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-10	42	2	0	4	81	6	-7	-1	55	2	-1	3	15	12	0	7	116	3	1	3	28	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-9	37	2	1	5	32	4	-3	-1	25	3	-1	4	17	14	-4	8	27	3	1	3	18	3	1	-3	45	3	1	4	31	14	-1	-3	57	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-8	14	2	1	6	37	3	-2	-1	25	3	-1	5	17	14	-4	9	27	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-7	19	2	1	7	15	12	-1	-1	32	2	1	-4	18	13	1	8	19	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-6	14	2	1	8	10	15	-7	-1	27	2	1	5	17	14	-4	10	19	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-5	15	2	1	H,K=	1,	-1	-2	24	3	1	6	24	3	1	-1	11	10	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-4	46	3	1	-2	41	3	-2	-1	16	21	1	2	21	3	1	-2	14	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-3	14	2	1	-3	21	3	-2	-1	16	21	1	2	21	3	1	-2	14	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-2	28	3	1	-3	41	3	-2	-1	16	21	1	2	21	3	1	-2	14	3	1	3	18	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
-1	140	3	1	-4	10	4	7	1	83	-10	3	1	24	4	1	3	37	3	1	-1	29	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
0	171	4	1	5	21	7	1	2	24	4	1	4	15	-1	10	12	24	4	1	-3	32	3	1	-3	45	3	1	4	31	3	1	-3	82	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
1	72	3	-1	3	47	2	1	4	79	3	1	4	90	4	1	-3	12	3	1	3	15	-4	-7	-3	45	3	1	4	22	10	-2	-3	78	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
2	14	2	1	6	34	3	1	5	34	3	1	5	34	3	1	-3	12	3	1	3	15	-4	-7	-3	45	3	1	4	22	10	-2	-3	78	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
3	12	12	1	7	11	-4	1	7	11	-4	1	3	15	3	1	-3	4	15	-7	-3	45	3	1	4	22	10	-2	-3	78	3	1	-3	46	2	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1	-3	19	3	1
4	46	3	3	8	11	17	-6	7	26	3	-1		H,K=	2,	-4	-2	15	3	1	5	8	14	-10	-3	15	3	1	5	36	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1
5	21	2	1	9	11	17	-6	7	26	3	-1	4	8	14	-10	-3	15	3	1	5	8	14	-10	-3	15	3	1	5	36	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1	-2	14	3	1
6	21	2	1	7	14	14	-4	1	31	2	1	7	14	14	-4	1	31	2	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1
7	22	2	-1	8	0	14	-4	10	25	3	-4	-2	22	3	1	1	8	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1
8	14	2	1	9	14	14	-4	H,K=	1,	1,	1	2	22	3	1	2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1	-2	22	3	1
9	43	2	1		H,K=	1,	-7	1	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1	3	19	3	1
10	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
11	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
12	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
13	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
14	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
15	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
16	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
17	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
18	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
19	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
20	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
21	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
22	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
23	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
24	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
25	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
26	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
27	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
28	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
29	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
30	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
31	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
32	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
33	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
34	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
35	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
36	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
37	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
38	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
39	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
40	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
41	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
42	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
43	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1
44	14	2	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3	1	1	14	3

Table 2. Final coordinates and thermal parameters. In this and following tables the standard deviation of the least significant digit(s) is given in parentheses. The form of the temperature factor (B in units of $Å^2$) is $T = \exp(-0.25(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}\ell^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}h\ell a^*c^* + 2B_{23}k\ell b^*c^*))$ for anisotropic and $T = \exp(-B \sin^2\theta/\lambda^2)$ for isotropic thermal parameters.

(Table to be reproduced photographically.)

Table 2.

ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23
SR(1)	.2003(3)	-.0410(2)	.0449(2)	7.4(3)	4.5(2)	4.4(2)	3.1(2)	.4(2)	.5(2)
SR(2)	.0158(3)	.1118(2)	.1623(2)	7.4(3)	4.2(2)	2.6(2)	2.5(2)	.6(2)	.0(1)
O(1)	.178(1)	.016(2)	-.088(1)	5.9(5)					
O(2)	.183(1)	.139(2)	.089(1)	6.3(5)					
C(01)	.241(3)	.003(3)	-.247(2)	8.7(10)					
C(02)	.263(3)	.005(3)	-.335(3)	12.3(12)					
C(03)	.286(3)	.101(4)	-.355(3)	12.8(13)					
C(04)	.326(3)	.205(4)	-.293(3)	13.3(13)					
C(05)	.298(3)	.203(3)	-.203(2)	10.1(11)					
C(06)	.265(3)	.110(3)	-.185(2)	8.4(10)					
C(07)	.234(2)	.113(3)	-.094(2)	7.2(9)					
C(08)	.274(2)	.211(2)	-.023(2)	5.0(7)					
C(09)	.240(2)	.218(2)	.062(2)	5.5(8)					
C(10)	.275(2)	.331(2)	.126(2)	5.8(8)					
C(11)	.293(2)	.416(2)	.094(2)	5.4(8)					
C(12)	.334(2)	.529(2)	.163(2)	6.7(8)					
C(13)	.342(2)	.537(3)	.250(2)	7.8(9)					
C(14)	.322(2)	.449(3)	.275(2)	7.0(9)					
C(15)	.289(2)	.341(2)	.215(2)	6.6(8)					
O(3)	-.035(1)	.066(1)	-.125(1)	5.0(5)					
O(4)	-.027(1)	.189(2)	.055(1)	6.4(5)					
C(16)	-.028(3)	.068(3)	-.293(2)	8.4(9)					
C(17)	-.013(3)	.070(3)	-.383(3)	11.6(12)					
C(18)	.043(3)	.165(4)	-.399(3)	12.5(13)					
C(19)	.098(3)	.261(3)	-.326(3)	11.9(12)					
C(20)	.082(3)	.256(3)	-.237(2)	9.7(11)					
C(21)	.020(3)	.163(3)	-.226(2)	7.2(9)					
C(22)	.002(2)	.159(3)	-.138(2)	6.7(9)					
C(23)	.017(2)	.256(2)	-.066(2)	4.2(7)					
C(24)	.004(2)	.265(2)	.022(2)	5.8(8)					
C(25)	.024(2)	.379(2)	.089(2)	5.4(8)					
C(26)	.079(2)	.472(3)	.061(2)	6.9(8)					
C(27)	.104(2)	.576(2)	.128(2)	7.3(9)					
C(28)	.070(3)	.583(3)	.212(2)	8.4(10)					
C(29)	.020(3)	.487(3)	.234(2)	9.0(10)					
C(30)	-.003(2)	.381(3)	.168(2)	7.4(9)					
O(5)	.260(1)	-.078(1)	.171(1)	6.5(5)					
O(6)	.259(1)	-.187(1)	-.010(1)	6.7(5)					
C(31)	.257(3)	-.113(3)	.325(2)	9.7(10)					
C(32)	.270(3)	-.112(3)	.420(3)	12.4(12)					
C(33)	.361(3)	-.126(3)	.443(2)	10.6(11)					
C(34)	.434(3)	-.139(3)	.392(3)	13.4(14)					
C(35)	.428(3)	-.135(3)	.300(2)	10.6(11)					
C(36)	.336(3)	-.125(2)	.281(2)	6.5(8)					
C(37)	.311(2)	-.129(2)	.185(2)	6.0(8)					
C(38)	.344(2)	-.199(2)	.118(2)	6.2(8)					
C(39)	.315(2)	-.221(2)	.026(2)	5.7(8)					
C(40)	.337(3)	-.318(2)	-.039(2)	6.1(8)					
C(41)	.425(3)	-.337(3)	-.015(2)	8.5(10)					
C(42)	.440(3)	-.423(3)	-.080(3)	10.7(11)					
C(43)	.376(3)	-.478(3)	-.157(2)	9.2(10)					
C(44)	.290(3)	-.461(3)	-.186(2)	8.8(9)					
C(45)	.271(3)	-.364(3)	-.118(3)	10.1(10)					
O(7)	.129(1)	.177(1)	.302(1)	5.6(5)					
O(8)	-.048(1)	.219(1)	.283(1)	5.0(5)					
C(46)	.301(3)	.199(3)	.409(2)	8.9(10)					
C(47)	.399(3)	.232(3)	.463(2)	9.6(10)					
C(48)	.442(3)	.329(3)	.537(2)	10.0(11)					
C(49)	.387(3)	.390(3)	.555(2)	10.7(11)					
C(50)	.285(3)	.369(3)	.511(2)	9.0(10)					
C(51)	.252(2)	.268(3)	.434(2)	5.6(8)					
C(52)	.148(3)	.251(2)	.387(2)	6.8(9)					
C(53)	.073(3)	.286(2)	.414(2)	5.8(8)					
C(54)	-.016(3)	.271(2)	.370(2)	6.0(8)					
C(55)	-.105(3)	.309(2)	.404(2)	7.9(10)					
C(56)	-.087(3)	.351(3)	.502(2)	9.7(10)					
C(57)	-.168(4)	.391(3)	.537(2)	11.0(12)					
C(58)	-.248(3)	.387(2)	.488(2)	8.3(9)					
C(59)	-.256(3)	.347(3)	.395(3)	12.2(12)					
C(60)	-.177(3)	.311(2)	.358(2)	8.2(10)					
O(9)	.404(2)	.082(2)	.075(2)	13.4(8)					
C(61)	.479(4)	.104(4)	.134(3)	13.7(14)					
C(62)	.565(4)	.075(4)	.141(3)	16.1(15)					
C(63)	.476(3)	.203(3)	.214(3)	14.7(13)					

Table 3. Distances (Å) in the coordination cluster. (See Fig. 1)

Atoms		Distance	Atoms		Distance
Sr(1)	O(1)	2.54(2)	O(2)	O(3)	3.05(3)[a]
Sr(1)	O(2)	2.54(2)	O(2)	O(4)	3.30(3)[a]
Sr(1)	O(3)	2.57(2)	O(3)	O(4)	2.86(2)[a,b]
Sr(1)	O(4)	2.58(2)	O(1)	O(8)	3.61(3)
Sr(1)	O(5)	2.46(2)	O(1)	O(9)	3.67(3)
Sr(1)	O(6)	2.43(2)	O(2)	O(7)	3.42(3)
Sr(1)	O(9)	2.60(3)	O(2)	O(9)	3.43(3)
Sr(2)	O(1)	2.59(2)	O(3)	O(5)	3.27(3)
Sr(2)	O(2)	2.53(2)	O(3)	O(7)	3.48(2)
Sr(2)	O(3)	2.53(2)	O(4)	O(6)	3.26(3)
Sr(2)	O(4)	2.47(2)	O(4)	O(8)	3.58(3)
Sr(2)	O(7)	2.42(2)	O(5)	O(6)	2.85(2)[b]
Sr(2)	O(8)	2.47(2)	O(5)	O(9)	3.18(3)
O(1)	O(2)	2.83(2)[a,b]	O(6)	O(9)	3.36(3)
O(1)	O(3)	3.37(2)[a]	O(7)	O(8)	2.76(2)[b]
O(1)	O(4)	3.04(3)[a]			

(a) Edge of the central oxygen parallelopiped.

(b) Bite of the ligand.

Table 4. Rotation of phenyl ring planes with respect to diketone planes and each other (deg)

DPP	Phenyl 1 to diketone.	Phenyl 2 to diketone.	Phenyl 1 to Phenyl 2.
1	16.0	27.2	14.6
2	19.6	10.4	18.4
3	32.8	25.3	45.0
4	22.8	14.8	37.1

Table 5. Intra-molecular distances (Å)

Atoms		Distance	Atoms		Distance
DPP(1)			DPP(2)		
C(01)	C(02)	1.45(4)	C(16)	C(17)	1.47(4)
C(02)	C(03)	1.41(4)	C(17)	C(18)	1.38(4)
C(03)	C(04)	1.39(5)	C(18)	C(19)	1.42(4)
C(04)	C(05)	1.51(4)	C(19)	C(20)	1.45(4)
C(05)	C(06)	1.34(4)	C(20)	C(21)	1.33(4)
C(06)	C(01)	1.44(4)	C(21)	C(16)	1.34(3)
C(06)	C(07)	1.51(3)	C(21)	C(22)	1.45(3)
C(07)	O(1)	1.32(3)	C(22)	O(3)	1.31(3)
C(07)	C(08)	1.41(3)	C(22)	C(23)	1.44(3)
C(08)	C(09)	1.43(3)	C(23)	C(24)	1.40(3)
C(09)	O(2)	1.29(3)	C(24)	O(4)	1.28(3)
C(09)	C(10)	1.50(3)	C(24)	C(25)	1.56(3)
C(10)	C(11)	1.38(3)	C(25)	C(26)	1.45(3)
C(11)	C(12)	1.53(3)	C(26)	C(27)	1.44(3)
C(12)	C(13)	1.36(3)	C(27)	C(28)	1.41(3)
C(13)	C(14)	1.35(3)	C(28)	C(29)	1.43(4)
C(14)	C(15)	1.43(3)	C(29)	C(30)	1.46(4)
C(15)	C(10)	1.40(3)	C(30)	C(25)	1.32(3)
DPP(3)			DPP(4)		
C(31)	C(32)	1.54(4)	C(46)	C(47)	1.43(4)
C(32)	C(33)	1.40(4)	C(47)	C(48)	1.42(4)
C(33)	C(34)	1.34(4)	C(48)	C(49)	1.33(4)
C(34)	C(35)	1.51(4)	C(49)	C(50)	1.44(4)
C(35)	C(36)	1.36(4)	C(50)	C(51)	1.48(3)
C(36)	C(31)	1.34(4)	C(51)	C(46)	1.36(3)
C(36)	C(37)	1.55(3)	C(51)	C(52)	1.51(3)
C(37)	O(5)	1.25(3)	C(52)	O(7)	1.39(3)
C(37)	C(38)	1.44(3)	C(52)	C(53)	1.34(3)
C(38)	C(39)	1.42(3)	C(53)	C(54)	1.32(3)

Table 5. (continued)

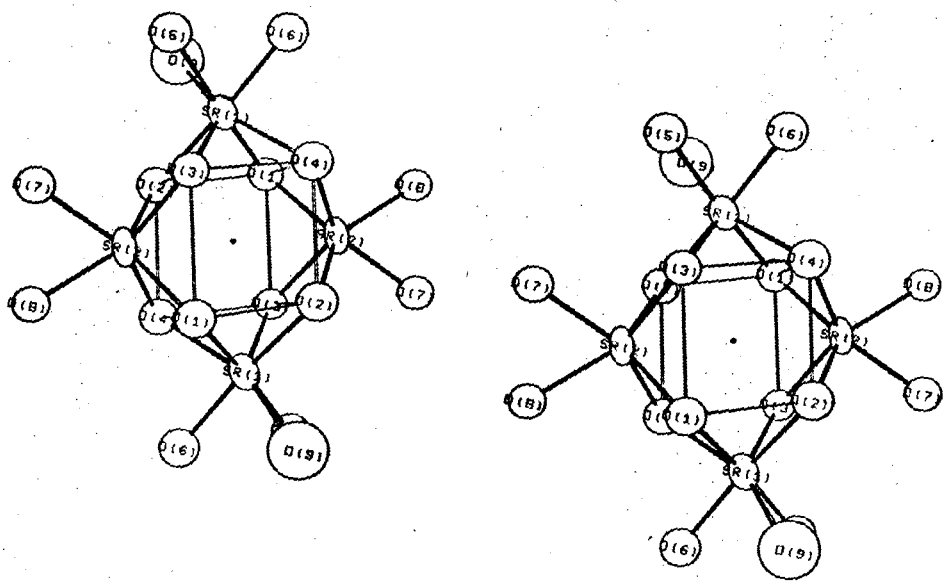
Atoms		Distance	Atoms		Distance
C(39)	O(6)	1.27(3)	C(54)	O(8)	1.33(3)
C(39)	C(40)	1.61(3)	C(54)	C(55)	1.57(4)
C(40)	C(41)	1.40(4)	C(55)	C(56)	1.48(4)
C(41)	C(42)	1.44(4)	C(56)	C(57)	1.47(4)
C(42)	C(43)	1.33(4)	C(57)	C(58)	1.32(4)
C(43)	C(44)	1.39(4)	C(58)	C(59)	1.41(4)
C(44)	C(45)	1.59(4)	C(59)	C(60)	1.46(4)
C(45)	C(40)	1.37(3)	C(60)	C(55)	1.26(4)
	Acetone				
O(9)	C(61)	1.28(4)			
C(61)	C(62)	1.42(5)			
C(61)	C(63)	1.60(5)			

Figure Captions

Fig. 1. Stereoscopic view of the coordination around the Sr atoms. The center of symmetry at 0,0,0 is indicated. Thermal ellipsoids have been scaled to include 50% probability.

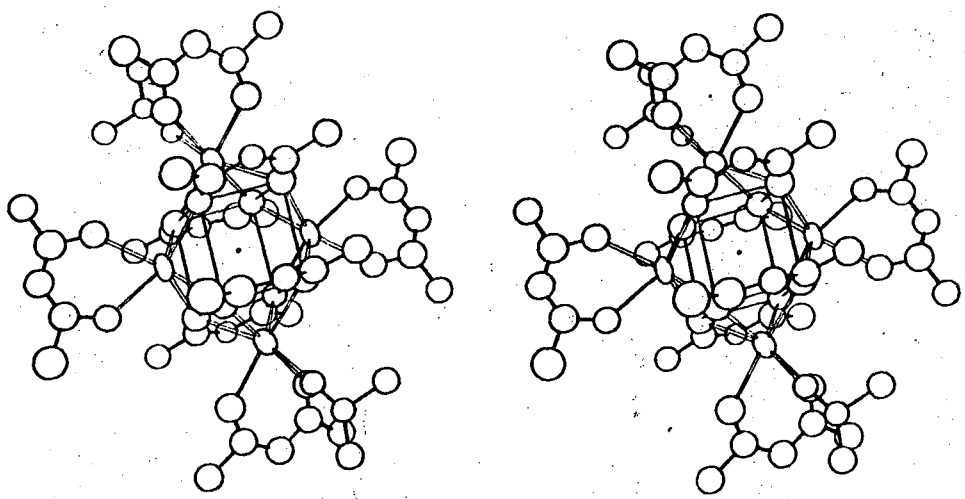
Fig. 2. Stereoscopic view of the complex cluster. Phenyl carbons except for those attached directly to the diketone have been omitted and the acetone atoms have been given artificial thermal parameters for clarity. View direction and scaling of the thermal ellipsoids are the same as in Fig. 1.

Fig. 3. Generalized labeling system for DPP ligands. Carbon atoms are single circles, oxygen atoms are double circles. Numbering shown is for DPP(1), for successive DPP molecules add 2 to the oxygen numbers and 15 to the carbon numbers.



XBL 724-793

Fig. 1.



XBL 724-792

Fig. 2.

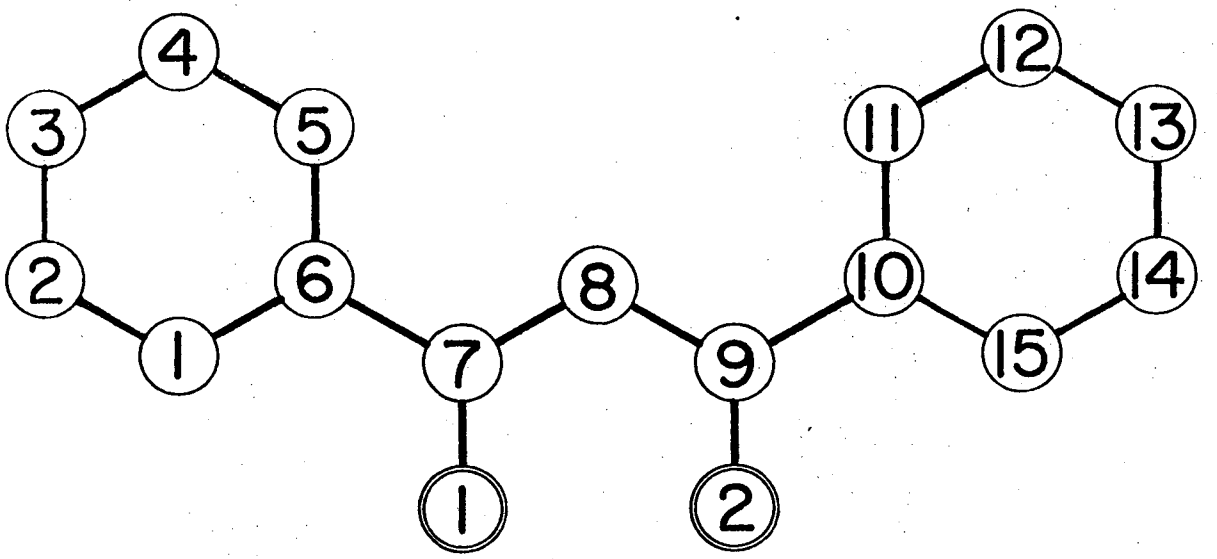


Fig. 3.

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720