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Publication Date

1960-11-01

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UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

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ABSTRACT

The structure of vanadyl bisacetylacetonate has been determined from three-dimensional x-ray diffraction data. The crystals are triclinic, space group $P\bar{1}$, with $a = 7.53 \pm 0.02 \text{ \AA}$, $b = 8.23 \pm 0.03 \text{ \AA}$, $c = 11.24 \pm 0.04 \text{ \AA}$, $\alpha = 73.0^\circ$, $\beta = 71.3^\circ$, $\gamma = 66.6^\circ$, $Z = 2$. The structure consists of discrete molecules of $\text{VO}(\text{C}_5\text{H}_7\text{O}_2)_2$. Each vanadium atom has five oxygen neighbors at the corners of a rectangular (nearly square) pyramid, with vanadium near its center of gravity. The vanadium-oxygen distances are 1.56 \AA to the apex atom (vanadyl oxygen) and 1.96, 1.96, 1.97, and 1.98 \AA to the others. Other bond distances average 1.28 \AA for C--O, 1.40 \AA for C--C (ring), and 1.52 \AA for C--C (methyl). Standard deviations are 0.01 \AA for V--O bonds and 0.02 \AA for C--O and C--C bonds. Each acetylacetonate skeleton is planar, and this plane makes an angle of 163° with the plane of the other acetylacetonate skeleton of the same molecule.

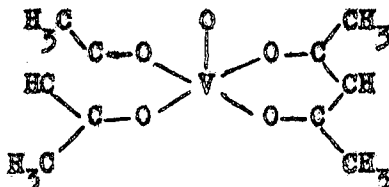
CRYSTAL STRUCTURE OF VANADYL BISACETYLACETONATE.
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INTRODUCTION

The crystal structure of vanadyl bisacetylacetonate,



has been determined to establish the geometry of the bonds about five-coordinated vanadium (IV). In his discussion of this compound and its reactions, Jones¹ assumed a square planar arrangement of four oxygen atoms about the vanadium atom, with the bond of the fifth oxygen presumably perpendicular to the plane of the other four. From the chemical evidence, it was impossible to rule out the trigonal bipyramidal arrangement of the five bonds. The work of Feltham² on the electron spin-resonance spectra of the compound indicates that the bipyramidal structure is improbable. The geometry of these five bonds can be expected to be similar in such compounds as vanadyl tetraphenylporphine.³ The present work shows that the five oxygen atoms are at the corners of an approximately square pyramid, but that vanadium is near the center of gravity of this pyramid rather than at the center of its base.

* This work was supported by the U.S. Atomic Energy Commission.

EXPERIMENTAL

Single crystals of vanadyl bisacetylacetonate were provided by Dr. Rue L. Belford. The crystals were blue-green in color, and those selected for study averaged 0.1 mm in thickness. Their shape corresponded to class $\bar{1}$ with only three forms appearing. These forms correspond to (100), (010), and (001) as we have chosen the axes.

The parameters of the reciprocal cell were obtained from quartz-calibrated⁴ zero-level Weissenberg photographs (rotation about a and b) and zero-level precession photographs (precession about a, b, and c). Intensities were evaluated by visual comparison with a set of standard intensities for 1165 independent reflections on multiple-film Weissenberg photographs with rotation about a. About 230 other reflections were recorded as too weak to be observed. Similar observations made with rotation about b were used to scale the intensities of the first set. All these photographs were made with $\text{CuK}\alpha$ radiation.

UNIT CELL AND SPACE GROUP

The diffraction symmetry confirms that the crystals are triclinic. The parameters found for the reciprocal cell are:

$$\begin{array}{lll} \underline{a}^* = 0.1459 & \underline{b}^* = 0.1349 & \underline{c}^* = 0.0957 \\ \alpha^* = 101.0^\circ & \beta^* = 103.5^\circ & \gamma^* = 109.5^\circ \end{array}$$

By the transformation formulas, the direct cell parameters are:

$$\begin{array}{ll} \underline{a} = 7.53 \pm 0.02 \text{ \AA} & \alpha = 73.0^\circ \\ \underline{b} = 8.23 \pm 0.03 \text{ \AA} & \beta = 71.3^\circ \\ \underline{c} = 11.24 \pm 0.04 \text{ \AA} & \gamma = 66.6^\circ \end{array}$$

The density found by suspension in a liquid of equal density is 1.49, which corresponds to 2.01 molecules in the unit cell. This value suggests that the space group is $P\bar{1}$, and the agreement with the intensity data which was achieved confirms this choice. All atoms occur in the general two-fold positions, $\pm (\underline{xyz})$.

DETERMINATION OF THE STRUCTURE

Preliminary attempts to solve the structure by projections failed because of lack of resolution and certain blunders. A three-dimensional Patterson function located the vanadium atom unambiguously. Starting with signs based on vanadium only, the [100] projection quickly refined to a point where six carbon atoms and one oxygen atom were shown as resolved peaks and the other carbon and oxygen atoms were shown as four unresolved double peaks. The [010] projection still failed to resolve atoms, but indicated that the chelate rings were nearly coplanar and approximately parallel with \underline{b} . This knowledge and assumptions of reasonable bond distances led to a trial structure in three dimensions. An electron density calculation in three dimensions then revealed all the carbon and oxygen atoms. In the meantime, about half of the oxygen and carbon atoms had been located independently by a study of the smaller peaks of the three-dimensional Patterson function. For this structure the "unreliability factor" $\underline{R} = \frac{\sum ||\underline{F}_O| - |\underline{F}_C||}{\sum |\underline{F}_O|}$ was 0.207.

REFINEMENT OF THE STRUCTURE

The structure was refined by the method of least squares, neglecting hydrogen atoms. Atomic scattering factors were taken from Freeman⁵ for V^{+2} and neutral C and from Berghuis, *et al.*,⁶ for neutral O. Individual isotropic temperature factors were used throughout. First we used the IBM-650 computer and the largely diagonal "LS-II" program of Senko and Templeton⁷ modified for space group $\overline{P1}$. The weighting and treatment of undetected reflections was done as described elsewhere.⁸ Five cycles of refinement reduced \underline{R} to 0.114 (observed reflections only). The resulting structure is described by Dodge.⁹

Examination of the records of these refinement cycles suggested that the best fit had not been achieved. Four additional cycles of refinement were carried out with the IBM-704 computer and the full-matrix program of Busing and Levy.¹⁰ Observed reflections were given unit weight. Unobserved reflections were given zero weight unless \underline{F}_C exceeded 7.3, a value about

1.5 times the average limit of detection; in the latter case F_{-2} was taken as zero and given unit weight. Before the final two cycles, six reflections with especially large discrepancies were removed from the data; these consisted of $15\bar{3}$, $1\bar{5}2$, and $2\bar{4}2$ which were erroneously recorded as absent when actually they fell off the films and 011 , 202 , and 212 which were observed very strong, but not as strong as calculated. After the last cycle, further checking revealed that 157 , $22\bar{8}$, and $3\bar{4}4$ had been recorded as absent by errors of transcription, that $22\bar{9}$ actually was absent but had been assigned the intensity of $22\bar{8}$, and that $36\bar{8}$ had been assigned an incorrect intensity. After correction, these five reflections were in excellent agreement with calculation. There remain eight absent reflections with structure factors calculated greater than 7.3, but none exceeding 8.4. This is considered to be satisfactory agreement, since hydrogen atoms are excluded from the calculation. The observed and calculated structure factors from the final cycle are listed in Table V (with the five corrections mentioned before); the corresponding R is 0.092 (observed reflections only).

The final atomic parameters are listed in Table I. The results confirm that the earlier refinement⁹ had not adequately converged and that one full-matrix cycle achieved results that would have required several diagonal cycles. Of 48 atomic coordinates, 29 changed by more than one standard deviation; two changed by more than 5 standard deviations. The largest change in a bond distance was that of the $V-O_6$ bond which was 1.59 \AA after the diagonal refinement and 1.56 \AA in the final structure. These differences are attributed more to lack of convergence than to the presence of the defective data in the earlier cycles.

DISCUSSION OF THE STRUCTURE

The structure consists of discrete molecules, arranged in the unit cell as indicated in Fig. 1. There are just two orientations of molecules, and one is the inverse of the other. This crystal may have application, because of this alignment, in the observation of directionally-dependent spectroscopic properties.

The bond distances and angles are listed in Tables II and III. The molecule has no crystallographic symmetry, but chemically equivalent bond distances are equal to the experimental accuracy. Chemically equivalent angles are nearly equal. If these quantities were exactly equal, the molecule (with the possible exception of the hydrogen atoms) would have symmetry $\underline{mm2}$ (C_{2v}). The molecular shape is shown in Fig. 2 with average values of equivalent distances and angles. The bond distance of the vanadyl ion, 1.56 Å, is of special interest because we know of no other measurement of this bond. The C--C and C--O bond distances are in accord with values for analogous structures.¹¹⁻¹⁶

The five neighbors of vanadium are at the corners of a rectangular (nearly square) pyramid, with vanadium approximately at its center of gravity. This geometry can be considered to be derived from the square planar configuration discussed in the Introduction by bending the two chelate rings away from the fifth oxygen. This bending lengthens four oxygen-oxygen distances, which otherwise would have been the shortest, and at the same time makes two others shorter. The distances in the actual structure are listed in Table IV. It is plausible that the distances O_2--O_4 and O_3--O_5 would be shorter than the distances to O_6 , but we find the difference unexpectedly large.

The structure of V_2O_5 also has vanadium in five-fold coordination, though in a different valence state.¹⁷ In that case there is one close neighbor, at 1.54 Å, and four others at 1.77, 1.88, 1.88, and 2.02 Å. The coordination geometry is said to consist of "distorted trigonal bipyramids."¹⁷ However, the distortion is so great that the coordination also can be described as a distortion of a square pyramid, with the close neighbor again at the apex. The fact that the distances are mostly slightly shorter than in our structure is consistent with the higher formal valence state.

Each acetylacetonone skeleton is accurately planar as expected, but not quite coplanar with the other acetylacetonone skeleton of the same molecule. The planes of these two parts of the molecule meet an angle of 163° . It is interesting that these planes are a compromise between those that would contain the vanadium atom and those that would be coplanar, assuming no change in the oxygen and vanadium positions. We interpret this fact as evidence for conjugation effects between the two rings.

The individual temperature parameters of the atoms are superimposed on an outline of the molecule in Fig. 3. There is a definite trend for the terminal atoms of the skeleton to have greater thermal motion than the atoms of the rings.

ACKNOWLEDGMENTS

We thank Dr. R.L. Belford for providing the crystals and Mrs. Helena W. Ruben, Dr. M.E. Senko, and Dr. R.E. Jones for their help.

REFERENCES

1. M.M. Jones, *J. Amer. Chem. Soc.* 76, 5995 (1954).
2. R.D. Feltham, Ph D Dissertation, University of California, Berkeley, 1957.
3. K. Ueno and A. Martell, *J. Phys. Chem.* 60, 934 (1956).
4. A. Pabst, *Am. Mineral.* 42, 664 (1957).
5. A.J. Freeman, *Acta Cryst.* 12, 261 (1959).
6. J. Berghuis, IJ.M. Haanappel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A.L. Veenendaal, *Acta Cryst.* 8, 478 (1955).
7. M.E. Senko, *Acta Cryst.* 10, 385 (1957).
8. G.L. Hardgrove and D.H. Templeton, *Acta Cryst.* 12, 29 (1959).
9. R.P. Dodge, Ph D Dissertation, University of California, Berkeley, 1958.
10. W.R. Busing and H.A. Levy, ORNL Central Files Memorandum 59-4-37 (April 1959).

11. H. Koyama, Y. Saito, and H. Kuroya, J. Inst. Polytech. Osaka City Univ., Ser. C. 4, 43 (1953).
12. R.B. Roof, Acta Cryst. 2, 781 (1956).
13. S. Shibata, Bull. Chem. Soc. Japan 30, 753 (1957).
14. V.M. Padmanabhan, Proc. Indian Acad. Sci. 47, 329 (1958).
15. L.M. Shkolnikova and E.A. Shugam, Kristallografiya 5, 32 (1960).
16. V. Amirthalingam, V.M. Padmanabhan, and J. Shankar, Acta Cryst. 13, 201 (1960).
17. A. Byström, K.A. Wilhelmi, O. Brotzen; Acta Chem. Scand., 4, 1119 (1950).

TABLE I

Final parameters

Atom	\bar{x}	\bar{y}	\bar{z}	$\sigma(\bar{x})$	$\sigma(\bar{y})$	$\sigma(\bar{z})$	$B, \text{\AA}^2$
Vanadium 1	0.1436	0.2902	0.2231	0.0004	0.0003	0.0002	2.4
Oxygen 2	0.9404	0.4142	0.3592	0.0014	0.0011	0.0008	3.0
Oxygen 3	0.9978	0.1214	0.2689	0.0014	0.0011	0.0008	2.8
Oxygen 4	0.1472	0.5359	0.1367	0.0014	0.0010	0.0007	2.6
Oxygen 5	0.2200	0.2302	0.0532	0.0014	0.0010	0.0007	2.6
Oxygen 6	0.3316	0.1887	0.2793	0.0016	0.0012	0.0009	3.8
Carbon 7	0.2753	0.5372	0.4396	0.0026	0.0020	0.0014	4.4
Carbon 8	0.8224	0.3521	0.4561	0.0022	0.0016	0.0012	2.8
Carbon 9	0.7836	0.1965	0.4661	0.0022	0.0017	0.0012	3.1
Carbon 10	0.8672	0.0924	0.3700	0.0022	0.0016	0.0011	2.8
Carbon 11	0.7900	0.9408	0.3825	0.0023	0.0017	0.0012	3.4
Carbon 12	0.7765	0.2166	0.0125	0.0024	0.0017	0.0013	3.5
Carbon 13	0.2215	0.5917	0.0195	0.0022	0.0016	0.0011	2.9
Carbon 14	0.7039	0.5090	0.0751	0.0022	0.0017	0.0012	3.1
Carbon 15	0.7070	0.6861	0.0565	0.0021	0.0015	0.0011	2.6
Carbon 16	0.6307	0.7855	0.1659	0.0024	0.0018	0.0013	3.8

TABLE II

Bond distances in vanadyl bisacetylacetonate.

Atoms	Distance, ^a Å	Atoms	Distance, ^a Å
V--O ₆	1.56	C ₇ --C ₈	1.51
		C ₁₀ --C ₁₁	1.53
V--O ₂	1.97	C ₁₂ --C ₁₃	1.52
V--O ₃	1.96	C ₁₅ --C ₁₆	1.51
V--O ₄	1.98		
V--O ₅	1.96	C ₈ --O ₉	1.39
		C ₉ --C ₁₀	1.40
O ₂ --C ₈	1.29	C ₁₃ --C ₁₄	1.38
O ₃ --C ₁₀	1.28	C ₁₅ --C ₁₆	1.42
O ₄ --C ₁₃	1.28		
O ₅ --C ₁₅	1.29		

^a Standard deviations are 0.01 Å for V--O bonds and 0.02 Å for C--O and C--C bonds. Chemically equivalent bonds are grouped together.

TABLE III

Bond angles in vanadyl bisacetylacetonate.

Atoms	Angle ^a	Atoms	Angle ^a
O ₂ --V--O ₃	87.2°	O ₂ --C ₈ --C ₇	114.9°
O ₄ --V--O ₅	87.9°	O ₃ --C ₁₀ --C ₁₁	117.2°
		O ₄ --C ₁₃ --C ₁₂	115.4°
O ₂ --V--O ₄	83.8°	O ₅ --C ₁₅ --C ₁₆	115.9°
O ₃ --V--O ₅	83.5°		
		O ₂ --C ₈ --C ₉	123.6°
O ₂ --V--O ₅	149.8°	O ₃ --C ₁₀ --C ₉	124.2°
O ₃ --V--O ₄	145.5°	O ₄ --C ₁₃ --C ₁₄	124.6°
		O ₅ --C ₁₅ --C ₁₄	122.5°
O ₂ --V--O ₆	104.5°		
O ₃ --V--O ₆	106.3°	C ₇ --C ₈ --C ₉	121.5°
O ₄ --V--O ₆	108.2°	C ₉ --C ₁₀ --C ₁₁	118.5°
O ₅ --V--O ₆	105.6°	C ₁₂ --C ₁₃ --C ₁₄	119.9°
		C ₁₄ --C ₁₅ --C ₁₆	121.5°
V--O ₂ --C ₈	128.6°		
V--O ₃ --C ₁₀	129.4°	C ₈ --C ₉ --C ₁₀	123.3°
V--O ₄ --C ₁₃	128.7°	C ₁₃ --C ₁₄ --C ₁₅	124.4°
V--O ₅ --C ₁₅	129.5°		

^a Standard deviations are about 1° or less. Chemically equivalent angles are grouped together.

TABLE IV

Oxygen-oxygen distances.

Atoms	Distance, Å	Atoms	Distance, Å
O ₂ --O ₃	2.71	O ₂ --O ₆	2.80
O ₄ --O ₅	2.73	O ₃ --O ₆	2.82
		O ₄ --O ₆	2.87
O ₂ --O ₄	2.64	O ₅ --O ₆	2.81
O ₃ --O ₅	2.61		

TABLE V.

Observed and calculated structure factors, \underline{F}_O and \underline{F}_C , each multiplied by 10. An asterisk (*) denotes that the reflection was too weak to be detected.

h=0

k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c
0	2	52	-41	1	9	200	-198	2	-8	210	207	3	10	164	177	4	11	120	-114	6	0	*	-48	7	-3	121	-104
0	3	93	90	1	-9	*	-45	2	10	74	67	3	-10	117	-101	4	-11	66	-63	6	1	140	145	7	4	128	142
0	4	269	273	1	8	247	229	2	-10	*	-54	3	-11	120	-109	4	13	65	67	6	-1	144	-141	7	-4	*	38
0	5	200	205	1	-8	141	-138	2	11	114	92	3	12	153	-121	5	0	140	-136	6	2	*	11	7	5	*	49
0	6	161	-149	1	-10	110	100	2	-11	99	73	4	0	93	175	5	1	*	5	6	-2	*	-1	7	-5	78	83
0	7	161	-151	1	-11	120	92	2	-12	91	69	4	1	105	59	5	-1	75	-62	6	3	328	-350	7	6	*	-33
0	-9	*	51	1	-12	*	-37	3	0	234	-135	4	-1	363	370	5	2	212	196	6	-3	121	123	7	7	113	-105
0	8	70	78	1	-13	83	-73	3	1	111	118	4	2	194	-197	5	-2	243	244	6	4	83	-67	7	9	132	119
0	10	120	-98	2	0	383	-370	3	-1	237	-207	4	-2	157	159	5	3	215	192	6	-4	134	117	7	8	*	74
0	-11	*	-26	2	1	315	-266	3	2	128	144	4	3	*	20	5	-3	*	67	6	5	85	-76	7	10	*	-13
0	12	108	-93	2	-1	251	-196	3	-2	335	-319	4	-3	275	-285	5	4	145	-138	6	-5	73	-90	7	11	111	-106
0	13	86	72	2	2	171	152	3	3	55	-97	4	4	315	328	5	-4	*	-2	6	6	105	110	8	0	*	-68
1	0	313	-329	2	-2	278	279	3	-3	*	-16	4	-4	169	-181	5	5	124	-123	6	-6	149	-148	8	1	79	-86
1	-1	375	388	2	3	62	39	3	4	*	1	4	5	*	37	5	-5	*	-38	6	7	*	-70	8	-1	106	110
1	2	67	-54	2	-3	167	164	3	-4	168	171	4	-5	106	89	5	6	*	14	6	-7	109	99	8	2	*	-21
1	-2	371	-387	2	4	785	-808	3	5	472	513	4	6	106	-118	5	-6	266	258	6	9	*	-11	8	-2	71	73
1	3	468	515	2	-4	228	-217	3	-5	*	-35	4	-6	*	5	5	7	133	158	6	8	132	-155	8	3	111	104
1	-3	168	-178	2	5	278	-280	3	6	*	58	4	7	*	-33	5	-7	140	125	6	10	*	62	8	4	67	67
1	4	109	118	2	-5	*	-30	3	-6	153	-147	4	-7	134	-112	5	9	85	-62	6	11	*	22	8	5	*	-36
1	-4	46	5	2	6	207	259	3	7	207	-221	4	9	*	53	5	-9	75	-66	6	0	*	45	8	6	*	-40
1	5	417	-430	2	-6	*	-55	3	-7	177	-177	4	-9	*	42	5	8	*	42	7	1	*	58	8	7	75	85
1	-5	329	333	2	7	140	124	3	9	140	137	4	8	*	61	5	-8	*	-53	7	-1	*	-26	9	1	67	75
1	6	159	-159	2	-7	153	160	3	-9	109	96	4	-8	130	-121	5	10	*	-44	7	2	164	-173	9	2	*	54
1	-6	132	120	2	9	103	-104	3	8	*	-56	4	10	144	-146	5	11	105	101	7	-2	156	-160	9	3	*	-13
1	7	138	115	2	-9	*	-41	3	-8	*	44	4	-10	108	104	5	12	79	58	7	3	*	55	9	4	59	-70
1	-7	*	-14	2	8	153	-139																				

h=1

k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c	k	I	F ₀	F _c
0	2	516	-542	-1	3	71	-46	-2	-2	*	84	-3	3	180	184	-4	4	138	124	6	0	*	0	7	5	107	-93				
0	3	553	529	-1	-3	66	87	-2	3	110	-86	-3	-3	269	-235	-4	-4	111	97	6	1	167	153	7	-5	65	81				
0	-3	371	-399	-1	-4	563	519	-2	-3	405	368	-3	4	216	199	-4	5	199	207	6	-1	72	-71	7	9	76	65				
0	4	168	145	-1	5	87	82	-2	4	168	-146	-3	-4	240	-229	-4	-5	169	162	6	2	*	42	7	8	130	128				
0	5	97	-63	-1	6	107	-94	-2	-4	476	-444	-3	5	119	-95	-4	7	107	-121	6	-2	98	-96	7	11	84	-80				
0	-5	350	327	-1	-6	419	-444	-2	-5	263	-282	-3	6	141	-154	-4	-7	91	-95	6	3	224	-225	-7	0	127	120				
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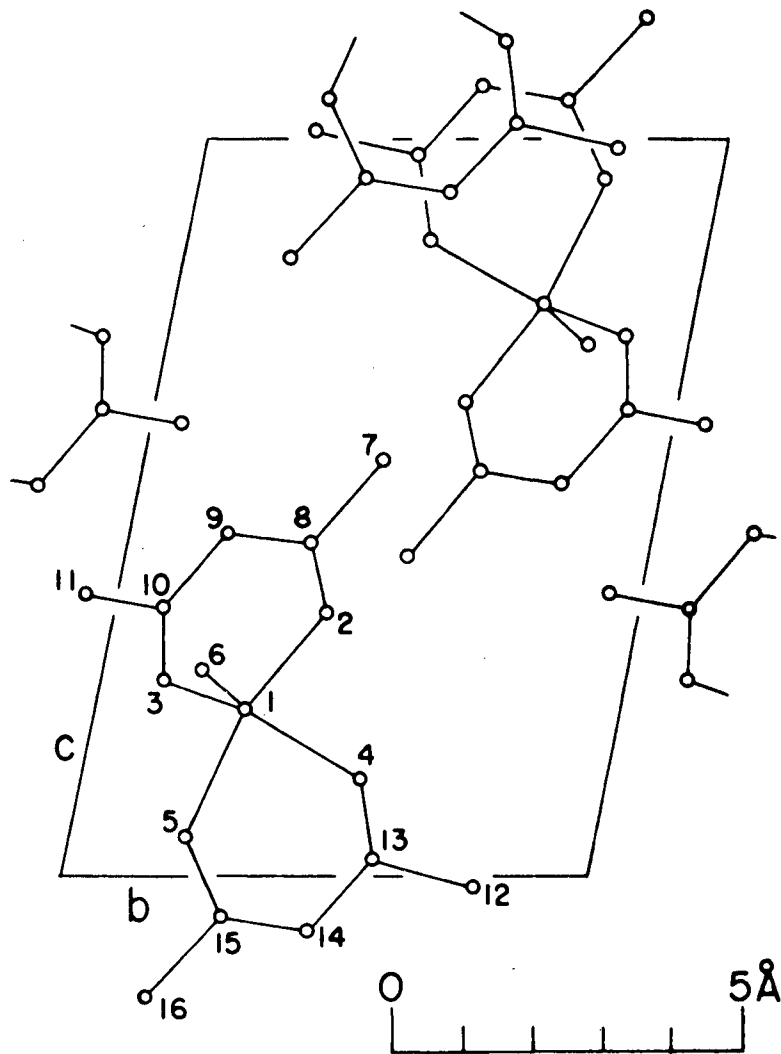
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LEGENDS

Fig. 1. The crystal structure of vanadyl bisacetylacetonate, projected along [100]. One unit cell is outlined. The numbering of the atoms corresponds to the identification in the text and tables.

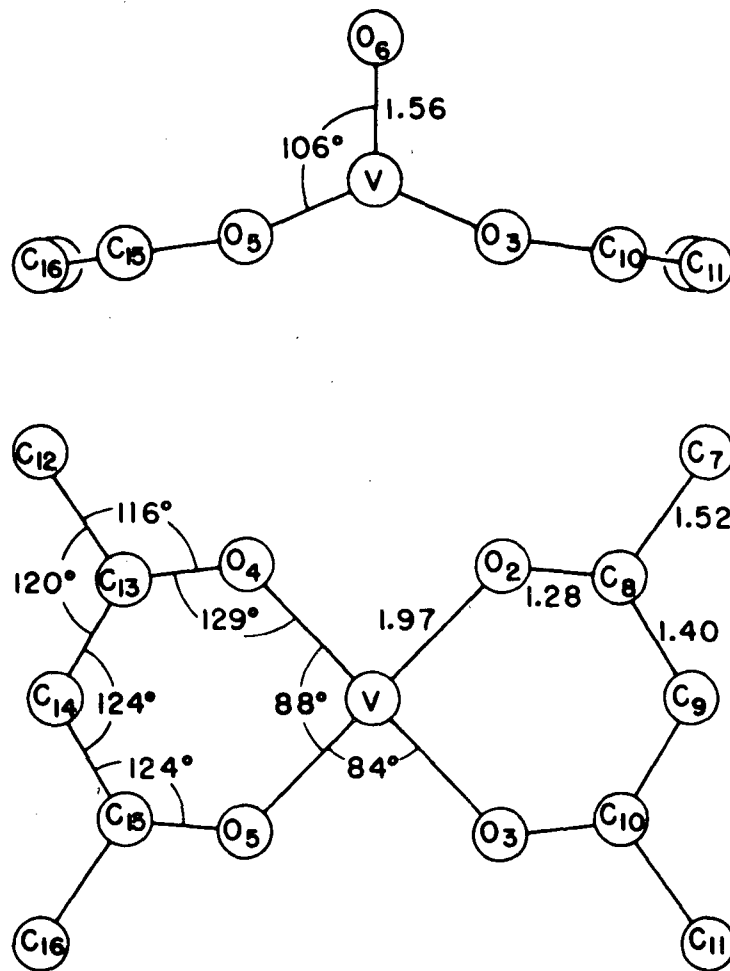
Fig. 2. Average bond distances and bond angles.

Fig. 3. Individual isotropic temperature parameters.



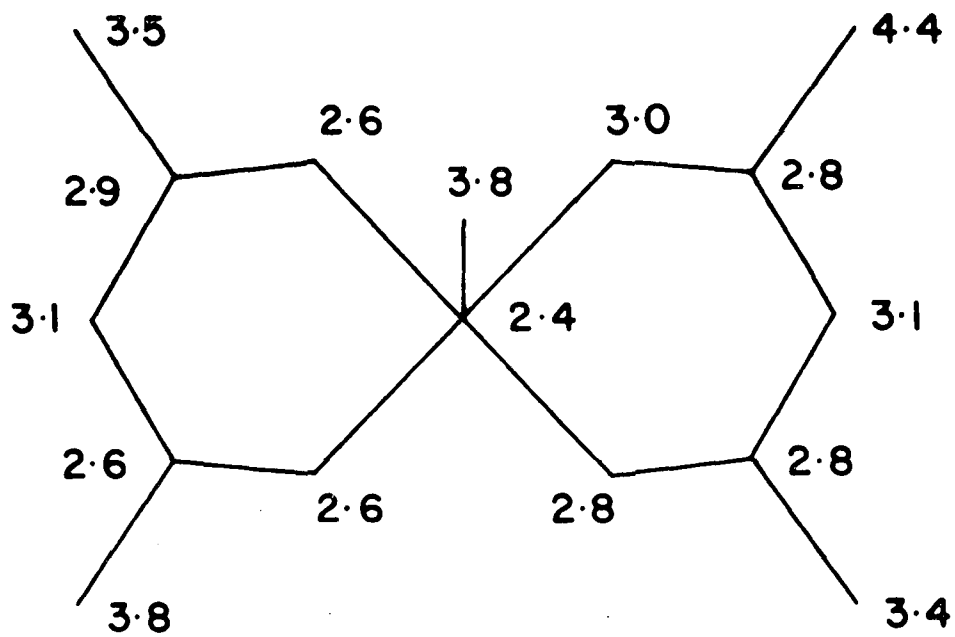
MU-22078

Fig. 1.



MU - 22079

Fig. . .



MU-22080

Fig. 3.

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