Title

CRYSTAL STRUCTURE OF VANADYL BISACETYL-ACETONATE. GEOMETRY OF VANADIUM IN FIVE-FOLD COORDINATION

Authors

Dodge, Richard P.
Templeton, David H.
Zalkin, Allan.

Publication Date

1960-11-01

UCRL -8225 Rev.

UNIVERSITY OF CALIFORNIA

Ernest O. Lawrence Radiation Laboratory

BERKELEY, CALIFORNIA

DISCLAIMER

UCRL-8225 Rev.

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

CRYSTAL STRUCTURE OF VANADYL BISACETYLACETONATE. GEOMETRY OF VANADIUM IN FIVE-FOLD COORDINATION

Richard P. Dodge, David H. Templeton, and Allan Zalkin

CRYSTAL STRUCTURE OF VANADYL BISACETYLACETONATE. GEOMETRY OF VANADIUM IN FIVE-FOLD COORDINATION

Richard P. Dodge, David H. Templeton, and Allan Zalkin

Department of Chemistry and Lawrence Radiation Laboratory
University of California, Berkeley, California

November, 1960

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 $a = 7.53 \pm 0.02$ Å, $b = 8.23 \pm 0.03$ Å, $c = 11.24 \pm 0.04$ Å, $\alpha = 73.0^\circ$, $\beta = 71.3^\circ$, $\gamma = 66.6^\circ$, $Z = 2$. The structure consists of discrete molecules of $VO(C_5H_7O_2)_2$. 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 Å to the apex atom (vanadyl oxygen) and 1.96, 1.96, 1.97, and 1.98 Å to the others. Other bond distances average 1.28 Å for C--O, 1.40 Å for C--C (ring), and 1.52 Å for C--C (methyl). Standard deviations are 0.01 Å for V--O bonds and 0.02 Å. for C--O and C--C bonds. Each acetylacetone skeleton is planar, and this plane makes an angle of 163° with the plane of the other acetylacetone skeleton of the same molecule.

CRYSTAL STRUCTURE OF VANADYL BISACETYLACETONATE. GEOMETRY OF VANADIUM IN FIVE-FOLD COORDINATION*

Richard P. Dodge, David H. Templeton, and Allan Zalkin

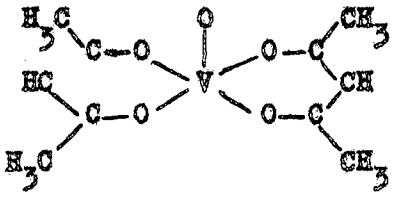
Department of Chemistry and Lawrence Radiation Laboratory

University of California, Berkeley, California

November, 1960

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, Jones[1] 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 Feltham[2] 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-calibrated[4] 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 CuKα radiation.

UNIT CELL AND SPACE GROUP

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

$a^* = 0.1459$	$b^* = 0.1349$	$c^* = 0.0957$
$\alpha^* = 101.0^\circ$	$\beta^* = 103.5^\circ$	$\gamma^* = 109.5^\circ$

By the transformation formulas, the direct cell parameters are:

$a = 7.53 \pm 0.02$ Å	$\alpha = 73.0^\circ$
$b = 8.23 \pm 0.03$ Å	$\beta = 71.3^\circ$
$c = 11.24 \pm 0.04$ Å	$\gamma = 66.6^\circ$.

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, $\pm$ (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 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" $R = \Sigma \| F_o | - | F_c \| / \Sigma | F_o |$ 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 Freeman[5] 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 Templeton[7] modified for space group $P\bar{1}$. The weighting and treatment of undetected reflections was done as described elsewhere.[8] Five cycles of refinement reduced 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 F_c exceeded 7.3, a value about

1.5 times the average limit of detection; in the latter case $\underline{F}_o$ 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 $3\bar{4}\bar{4}$ 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 $\underline{R}$ is 0.092 (observed reflections only).

The final atomic parameters are listed in Table I. The results confirm that the earlier refinement[9] 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 $V\text{--}O_6$ bond which was 1.59 Å after the diagonal refinement and 1.56 Å 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 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 goemetry 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 acetylacetone skeleton is accurately planar as expected, but not quite coplanar with the other acetylacetone 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. 9, 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	x	y	z	σ(x)	σ(y)	σ(z)	B, $Å^2$
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--C_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	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	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	7	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	l	F_o	F_c
0	2	516	-542
0	3	553	529
0	-3	371	-399
0	4	168	145
0	5	97	-63
0	-5	350	327
0	6	123	-115
0	7	77	-63
0	-7	212	-194
0	9	122	109
0	-9	92	81
0	8	153	157
0	-8	115	100
0	10	223	-235
0	-10	164	140
0	11	64	-49
0	-12	114	-89
0	13	78	72
1	2	452	456
1	-2	663	593
1	3	380	332
1	-3	*	-27
1	4	141	-164
1	-4	43	10
1	5	348	-336
1	-5	108	68
1	6	*	-1
1	-6	242	234
1	7	224	240
1	-7	218	205
1	-9	66	-59
1	8	184	188
1	-8	91	-82
1	11	233	215
1	-11	109	93
1	12	81	74
-1	0	257	225
-1	1	763	827
-1	-1	373	-291
-1	2	558	-476
-1	-2	427	-398
-1	3	71	-46
-1	-3	66	87
-1	-4	563	519
-1	5	87	82
-1	6	107	-94
-1	-6	419	-444
-1	7	233	-223
-1	-7	130	-114
-1	-9	188	-176
-1	8	160	-162
-1	10	106	104
-1	-10	104	-90
-1	-11	151	-127
-1	12	72	-51
-1	-13	43	41
2	0	162	-119
2	1	425	371
2	-1	243	-283
2	2	215	-167
2	-2	92	27
2	3	246	-220
2	-3	248	230
2	4	*	-75
2	-4	223	-171
2	5	132	136
2	-5	189	-180
2	6	473	497
2	-6	323	-263
2	7	186	-175
2	-7	*	81
2	9	145	-130
2	8	226	-224
2	-8	212	211
2	-10	77	-61
2	12	101	-88
2	-12	78	74
2	13	110	-88
-2	0	99	67
-2	1	138	126
-2	-1	350	-307
-2	2	197	192
-2	-2	*	84
-2	3	110	-86
-2	-3	405	368
-2	4	168	-146
-2	-4	476	-444
-2	-5	263	-282
-2	7	135	115
-2	-7	391	393
-2	9	160	-167
-2	-9	107	-106
-2	11	96	95
-2	-11	95	94
-2	-13	30	-32
3	0	655	603
3	1	137	107
3	-1	182	136
3	2	114	-56
3	-2	413	-373
3	3	*	12
3	-3	227	-199
3	4	111	137
3	-4	193	180
3	5	287	257
3	-5	146	130
3	6	213	-215
3	-6	*	-14
3	7	127	-146
3	-7	186	-186
3	9	104	111
3	-9	87	95
3	8	*	67
3	-8	92	-90
3	-10	64	-57
3	11	132	-108
3	-11	77	-60
3	12	120	-102
-3	0	331	-315
-3	1	219	-210
-3	-1	123	-92
-3	2	266	-263
-3	-2	370	339
-3	3	180	184
-3	-3	269	-235
-3	4	216	199
-3	-4	240	-229
-3	5	119	-95
-3	6	141	-154
-3	-6	211	210
-3	8	125	130
-3	-8	167	-172
-3	10	66	-58
-3	-10	228	204
-3	-11	65	72
-3	12	92	102
-3	-12	90	-64
4	0	433	-372
4	1	309	-283
4	-1	374	349
4	2	150	-106
4	-2	111	71
4	3	149	150
4	-3	197	-171
4	4	106	94
4	-4	184	-169
4	5	332	-341
4	-5	*	52
4	6	*	-64
4	7	143	136
4	9	106	-109
4	8	*	42
4	-8	153	-133
4	10	113	-100
4	-10	106	88
4	12	149	116
4	13	106	74
-4	0	228	216
-4	1	134	103
-4	-1	134	126
-4	2	89	58
-4	-2	115	-109
-4	3	228	-227
-4	-3	62	-46
-4	4	138	124
-4	-4	111	97
-4	5	199	207
-4	-5	169	162
-4	7	107	-121
-4	-7	91	-95
-4	9	127	113
-4	-9	203	195
-4	11	86	-88
-4	-11	176	-159
5	0	222	-213
5	1	116	103
5	-1	110	-100
5	2	300	299
5	-2	176	172
5	3	*	-30
5	4	443	-454
5	-4	73	61
5	5	92	-93
5	-5	76	-85
5	6	60	71
5	-6	150	129
5	7	103	93
5	-7	122	98
5	9	*	24
5	8	106	-115
5	10	65	86
5	-10	55	-57
5	11	96	84
5	13	77	-57
-5	0	114	-99
-5	1	85	81
-5	-1	152	-150
-5	-2	170	159
-5	3	103	-89
-5	-3	219	225
-5	4	205	-236
-5	-4	160	153
-5	8	167	-158
-5	-8	91	91
-5	10	56	62
6	0	*	0
6	1	167	153
6	-1	72	-71
6	2	*	42
6	-2	98	-96
6	3	224	-225
6	-3	*	
6	4	254	
6	-4	131	144
6	5	332	344
6	-5	116	-112
6	6	74	64
6	-6	104	-95
6	7	107	-85
6	9	133	136
6	8	92	-93
6	10	103	81
6	11	61	-60
6	12	61	-46
-6	0	145	-145
-6	1	135	-130
-6	-1	111	115
-6	2	107	131
-6	-2	*	-26
-6	3	125	130
-6	-3	205	-201
-6	4	65	-68
-6	-4	181	-174
-6	-6	84	88
-6	7	163	180
-6	-9	87	-84
-6	-8	77	-59
-6	-11	45	42
7	0	99	77
7	-1	76	74
7	2	140	-131
7	-2	*	-34
7	3	76	-60
7	-3	137	-122
7	4	168	184
7	5	107	-93
7	-5	65	81
7	9	76	65
7	8	130	128
7	11	84	-80
-7	0	127	120
-7	1	103	-102
-7	-1	174	177
-7	2	101	-113
-7	-2	118	-139
-7	4	106	109
-7	-5	72	94
-7	6	59	-57
-7	-7	110	-115
-7	-9	48	63
8	0	87	-98
8	-1	61	57
8	2	65	67
8	-2	57	62
8	3	74	80
8	-3	62	79
8	-5	64	-66
8	9	175	-155
-8	0	54	64
-8	-1	109	-109
-8	-2	78	-84
-8	3	95	-115
-8	-3	55	57
-8	-4	80	91
-8	-7	67	62
-8	-8	78	84
9	1	95	82
9	-1	65	-80
9	3	107	-96
9	4	68	-61
9	8	79	-79
-9	-2	66	71
-9	-3	95	109
10	2	43	-59
10	3	55	52
10	4	78	66

h = 2

k	l	F_o	F_c
0	0	617	-681
0	1	424	-511
0	-1	64	35
0	-2	184	187
0	3	248	219
0	-3	182	-199
0	4	*	9
0	-4	275	-268
0	5	221	-236
0	-5	*	45
0	6	163	-154
0	-6	211	203
0	7	80	69
0	-7	*	-1
0	9	*	1
0	-9	*	-42
0	8	184	186
0	-8	48	-23
0	10	171	-162
0	-10	186	155
0	11	*	55
0	11	*	55
0	-11	*	20
0	12	178	172
0	-12	73	-64
1	-1	161	-182
1	-2	101	107
1	3	53	70
1	-3	62	60
1	4	77	-92
1	-4	*	-23
1	5	134	-124
1	-5	323	-330
1	6	135	137
1	-6	*	33
1	7	309	335
1	-7	239	235
1	9	126	-117
1	-9	150	-133
1	8	116	-119
1	-8	*	-7
1	10	*	-4
1	-10	123	-85
1	11	200	205
1	-11	80	63
1	12	*	-43
1	-12	89	81
1	13	100	-85
-1	0	141	130
-1	1	457	422
-1	-1	60	62
-1	2	135	-119
-1	-2	275	-264
-1	3	247	-218
-1	-3	183	-187
-1	4	412	408
-1	-4	245	242
-1	5	42	16
-1	-5	228	231
-1	6	173	-215
-1	-6	225	-228
-1	7	262	-274
-1	-7	*	-19
-1	9	181	188
-1	-9	152	127
-1	8	*	34
-1	-8	*	-76
-1	10	*	19
-1	-10	*	22
-1	11	147	-132
-1	-11	126	-111
2	0	316	319
2	1	373	364
2	-1	108	-144
2	2	242	-258
2	-2	286	-269
2	3	87	62
2	-3	*	-1
2	4	322	318
2	-4	328	340
2	5	192	200
2	-5	*	6
2	6	369	378
2	-6	329	-330
2	7	84	-70
2	-7	134	-137
2	9	*	59
2	-9	*	16
2	8	157	-163
2	-8	113	113
2	10	118	114
2	-10	76	-64
2	11	*	-51
2	-11	60	-42
2	12	122	-101
2	13	*	-17
2	14	73	75
-2	0	85	76
-2	1	332	342
-2	-1	157	-159
-2	2	250	206
-2	-2	236	226
-2	3	228	-207
-2	-3	404	409
-2	4	197	-203
-2	-4	214	215
-2	5	*	56
-2	-5	161	-161
-2	6	253	274
-2	-6	124	-137
-2	7	102	-112
-2	-7	93	107
-2	9	*	-59
-2	-9	*	-8
-2	8	176	-162
-2	-8	102	96
-2	10	*	-1
-2	-10	131	-104
-2	11	*	9
-2	-11	*	1
-2	12	63	-74
-2	-12	41	39
3	0	399	379
3	1	433	-430
3	-1	506	489
3	2	254	124
3	-2	132	-123
3	3	193	208
3	-3	224	-214
3	4	111	-71
3	-4	*	27
3	5	318	-277
3	-5	272	294
3	6	274	-285
3	-6	132	147
3	7	124	-108
3	-7	136	-134
3	9	65	64
3	-9	155	118
3	8	129	131
3	-8	*	-18
3	10	102	-105
3	11	116	-121
3	12	*	-31
3	13	106	90
-3	0	239	-232
-3	1	50	46
-3	-1	62	-69
-3	2	219	222
-3	-2	216	233
-3	3	270	263
-3	-3	254	-225
-3	4	*	13
-3	-4	145	-147
-3	5	184	-192
-3	-5	87	-84
-3	6	*	27
-3	-6	122	116
-3	7	170	202
-3	-7	118	115
-3	9	*	-23
-3	-9	146	-147
-3	8	*	14
-3	-8	153	-162
-3	-10	72	72
-3	11	41	52
-3	-11	105	76
4	0	691	-652
4	1	456	-395
4	-1	109	97
4	2	285	270
4	-2	355	367
4	3	*	33
4	-3	75	74
4	4	205	-211
4	-4	123	-118
4	5	183	-195
4	-5	*	-5
4	6	*	34
4	6	76	34
4	-6	118	131
4	7	102	114
4	-7	67	66
4	9	94	-99
4	-8	54	-69
4	10	*	64
4	11	58	64
4	12	130	109
4	14	75	-71
-4	0	93	95
-4	1	211	-202
-4	-1	213	205
-4	-2	141	-134
-4	3	70	-67
-4	-3	144	-176
-4	4	163	170
-4	-4	63	-63
-4	5	82	106
-4	-5	73	86
-4	6	*	-43
-4	-6	95	105
-4	7	*	10
-4	-7	76	-61
-4	9	70	59
-4	-9	131	123
-4	8	135	147
-4	-8	*	-47
-4	-10	114	98
-4	-11	72	-57
5	0	102	-81
5	1	274	282
5	-1	231	-204
5	2	145	134
5	-2	184	-165
5	3	329	-333
5	-3	160	164
5	4	264	-264
5	-4	192	-195
5	5	241	253
5	-5	160	-159
5	6	184	198
5	-6	*	-67
5	7	141	-146
5	-7	*	-6
5	9	*	2
5	8	93	-104
5	-8	96	79
5	10	90	90
5	11	*	-21
5	12	100	-67
5	13	58	-53
-5	0	*	32
-5	1	129	122
-5	-1	203	-222
-5	2	*	-55
-5	-2	*	-49
-5	3	108	-103
-5	-3	*	43
-5	4	83	-96
-5	-4	102	103
-5	5	95	101
-5	-5	*	-17
-5	6	*	-47
-5	-6	108	-115
-5	7	139	-143
-5	-7	73	-83
-5	-9	*	27
-5	8	125	-131
-5	-8	87	72
-5	-10	87	-66
6	0	141	140
6	1	75	67
6	-1	*	14
6	2	101	-110
6	-2	156	-161
6	3	74	-69
6	-3	59	-56
6	4	261	279
6	-4	153	148
6	5	375	407
6	-5	*	10
6	6	178	-205
6	-6	82	64
6	7	*	21
6	-7	98	-96
6	9	132	139
6	8	83	93
6	10	*	26
6	11	95	-85
6	12	*	6
6	13	66	57
-6	0	119	-146
-6	1	*	14
-6	-1	67	84
-6	2	116	138
-6	-2	108	120
-6	3	*	3
-6	-3	152	163
-6	4	150	-155
-6	-4	*	-58
-6	-5	*	-31
-6	-6	*	42
-6	-7	93	89
-6	-9	58	-54
-6	-8	*	33
7	0	96	96
7	1	75	-83
7	-1	128	122
7	2	*	32
7	-2	108	103
7	3	66	53
7	-3	*	-16
7	4	75	74
7	-4	77	-77
7	5	223	-241
7	-5	*	5
7	6	119	-130
7	-6	83	70
7	7	96	105
7	9	*	-77
7	8	82	81
7	10	164	-142
7	11	*	11
7	12	81	78
-7	0	*	50
-7	1	125	-141
-7	-1	*	61
-7	2	*	40
-7	-2	*	-4
-7	3	130	152
-7	-3	*	-78
-7	-4	79	-82
-7	-5	89	98
-7	-6	*	30
-7	-7	64	-64
-7	-8	63	-53
8	0	93	-86
8	1	*	-4
8	-1	72	-73
8	2	122	129
8	-2	*	5
8	3	*	3
8	-3	149	137
8	4	95	-100
8	-4	51	51
8	5	*	-48
8	-5	54	-54
8	6	*	24
8	7	*	30
8	9	119	-117
8	8	61	-68
8	10	73	70
8	11	48	42
-8	0	109	130
-8	-2	74	-92
-8	-3	51	-82
-8	-4	48	58
9	2	106	-99
9	-2	89	-84
9	3	112	-94
9	-3	42	-40
9	4	*	36
9	5	87	70
9	9	71	70
10	2	49	-53
10	3	62	63
10	6	55	-51

h = 3

k	l	F_o	F_c
0	0	228	-271
0	1	61	-83
0	2	147	-165
0	-2	126	106
0	3	326	331
0	-3	73	74
0	4	86	30
0	-4	163	-154
0	5	435	-405
0	-5	138	-125
0	7	223	237
0	9	171	-194
0	11	96	92
0	-11	120	102
0	12	168	160
0	13	89	-87
1	-1	80	-89
1	-2	449	-417
1	-3	82	75
1	4	232	-258
1	-4	149	126
1	5	69	51
1	-5	267	-267
1	6	208	207
1	-6	185	-186
1	7	139	129
1	-7	46	38
1	9	109	-118
1	-9	49	-42
1	8	234	-226
1	-8	158	148
1	10	60	55
1	-10	116	-101
1	11	53	-41
1	12	168	-181
1	13	109	-111
1	14	50	43
-1	0	194	178
-1	1	129	-96
-1	-1	222	225
-1	2	238	-233
-1	-2	243	-231
-1	3	333	-332
-1	-3	200	-210
-1	4	516	537
-1	-4	62	73
-1	5	87	-80
-1	-5	185	178
-1	6	192	-206
-1	-6	173	192
-1	7	65	66
-1	-7	163	150
-1	9	93	109
-1	-9	163	148
-1	8	212	244
-1	-8	75	-73
-1	10	69	-64
-1	-10	118	98
-1	11	64	-65
-1	12	67	52
-1	13	48	58
2	0	206	218
2	1	138	-136
2	-1	180	147
2	2	157	-179
2	-2	65	19
2	3	70	85
2	-3	173	-161
2	4	217	273
2	-4	366	316
2	5	59	62
2	-5	275	281
2	6	136	-147
2	-6	164	-173
2	7	178	-178
2	-7	190	-192
2	9	279	290
2	-9	101	77
2	8	109	-108
2	-8	*	23
2	10	99	104
2	11	70	-57
2	-11	67	-70
2	12	*	2
2	13	100	96
2	14	66	62
-2	0	114	114
-2	1	227	234
-2	-1	241	-219
-2	2	117	-125
-2	-2	62	56
-2	3	283	-307
-2	-3	180	183
-2	4	*	15
-2	-4	211	232
-2	5	268	313
-2	-5	177	-174
-2	6	*	-35
-2	-6	79	-79
-2	7	169	-209
-2	-7	120	-102
-2	9	98	109
-2	-9	83	77
-2	8	132	-143
-2	-8	82	62
-2	-10	80	-62
-2	-11	44	-48
3	0	114	-109
3	1	481	-478
3	-1	382	347
3	2	64	-53
3	-2	207	217
3	3	190	188
3	-3	116	-115
3	4	245	-232
3	-4	296	-296
3	5	150	-153
3	-5	126	134
3	6	*	-47
3	-6	266	272
3	7	*	15
3	-7	*	-33
3	9	84	-67
3	8	183	199
3	-8	*	17
3	10	131	-133
3	-10	66	58
3	11	*	8
3	12	106	87
3	13	72	62
-3	0	280	-308
-3	1	246	261
-3	-1	*	-14
-3	2	355	398
-3	-2	185	194
-3	3	*	9
-3	-3	117	101
-3	4	121	-109
-3	-4	80	-82
-3	5	63	-78
-3	-5	102	-132
-3	6	99	108
-3	-6	*	35
-3	7	85	90
-3	-7	113	105
-3	8	69	-86
4	0	173	-158
4	1	115	99
4	-1	292	-267
4	2	516	506
4	-2	246	248
4	3	107	-98
4	-3	165	160
4	4	180	-167
4	-4	61	-58
4	5	102	108
4	-5	109	-107
4	6	143	157
4	-6	*	45
4	7	124	129
4	-7	103	95
4	9	90	-85
4	-9	66	-52
4	8	133	-138
4	-8	*	-13
4	10	92	97
4	11	130	131
4	13	103	-70
4	14	73	-69
-4	0	98	-101
-4	1	249	-260
-4	-1	197	200
-4	2	*	-20
-4	-2	*	45
-4	3	90	117
-4	-3	131	-141
-4	4	*	-33
-4	-4	102	-102
-4	5	85	-71
-4	-5	*	20
-4	6	84	-87
-4	-6	102	103
-4	-7	98	-92
-4	-8	109	-115
-4	10	58	-70
-4	-10	70	65
5	0	205	190
5	1	153	169
5	-1	250	-242
5	2	181	-174
5	-2	316	-308
5	3	231	-234
5	-3	*	57
5	4	*	4
5	-4	109	-81
5	5	267	279
5	-5	*	-15
5	6	210	204
5	-6	142	-136
5	7	188	-199
5	-7	82	-63
5	9	*	21
5	-9	54	47
5	8	63	62
5	-8	77	69
5	10	*	42
5	11	113	-110
5	14	66	57
-5	0	93	87
-5	1	*	27
-5	-1	*	-64
-5	2	125	-137
-5	-2	182	-223
-5	3	*	-24
-5	-3	133	-143
-5	4	*	63
-5	-4	46	55
-5	5	81	73
-5	-5	109	123
-5	-6	54	-56
-5	-7	45	-57
-5	-9	60	63
-5	-8	55	46
6	0	96	100
6	1	152	-137
6	-1	181	188
6	2	74	-70
6	-2	65	-66
6	3	122	123
6	-3	*	3
6	4	47	38
6	-4	*	37
6	5	59	-54
6	-5	125	117
6	6	370	-404
6	-6	90	73
6	7	90	-87
6	-7	97	-81
6	9	*	0
6	8	131	134
6	-8	76	-75
6	10	*	-46
6	11	91	-81
6	13	81	74
-6	1	88	88
-6	-3	179	169
-6	-5	67	-61
-6	6	60	82
-6	-7	76	78
-6	-8	57	63
7	0	92	-92
7	1	46	-51
7	-1	*	22
7	2	82	90
7	-2	168	188
7	3	138	154
7	-3	*	35
7	4	64	-72
7	-4	84	-77
7	5	*	-41
7	-5	85	-84
7	6	*	50
7	-6	52	47
7	7	161	160
7	9	97	-92
7	8	*	-15
7	11	82	78
7	12	69	60
-7	1	88	-101
-7	-2	96	107
-7	3	55	87
-7	-4	64	-68
-7	-6	49	59
8	0	*	12
8	1	46	40
8	-1	127	-139
8	2	46	57
8	-2	83	-79
8	3	139	-157
8	-3	77	76
8	4	80	-80
8	-4	47	40
8	5	88	83
8	-5	26	-34
8	6	70	72
8	10	126	109
8	11	83	69
9	0	76	74
9	-1	40	47
9	2	119	-124
9	-2	54	-48
9	-3	62	-70
9	4	139	137
9	5	75	81
10	3	76	78
10	5	137	-143

h = 4

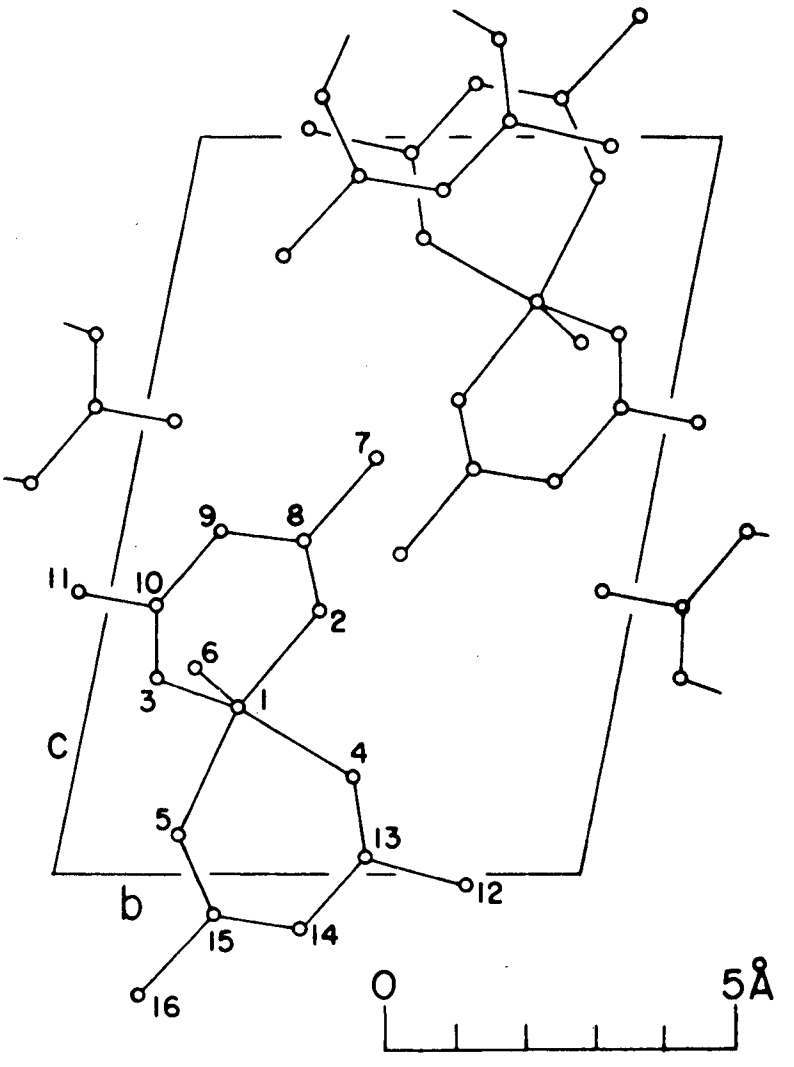
k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c	k	l	F_o	F_c
0	0	104	-98	1	-8	165	137	2	-9	36	32	3	-9	110	-96	4	-8	101	89	-5	-1	129	129	7	4	124	-134
0	1	168	148	1	10	123	133	2	8	60	35	3	8	119	127	4	10	123	133	-5	2	56	-51	7	-4	*	-26
0	-1	120	-119	1	-10	77	-73	2	-8	84	-66	3	-8	35	-30	4	11	*	25	-5	-2	*	-31	7	5	106	108
0	2	503	577	1	11	93	-86	2	10	96	-84	3	10	59	-61	4	12	175	-173	-5	3	54	51	7	-5	91	-88
0	-2	157	135	1	12	66	-73	2	-10	76	71	3	11	144	135	4	13	57	-51	-5	-3	104	-110	7	6	147	145
0	3	231	262	-1	0	71	55	2	11	47	-45	3	12	89	80	-4	0	108	-130	-5	4	78	80	7	7	123	121
0	-3	196	196	-1	1	282	-273	2	12	87	69	3	13	47	-34	-4	1	122	-132	-5	-4	*	3	7	9	*	-39
0	4	151	129	-1	-1	272	269	2	13	81	78	-3	0	84	-90	-4	-1	*	55	-5	-5	147	151	7	8	*	-48
0	-4	83	-58	-1	2	*	16	-2	0	155	153	-3	1	206	249	-4	2	146	186	-5	-7	70	-70	7	11	127	110
0	5	113	-128	-1	-2	39	15	-2	1	33	-22	-3	-1	55	-55	-4	-2	163	180	6	0	112	-94	7	12	62	46
0	-5	102	-106	-1	3	54	51	-2	-1	160	-151	-3	2	81	79	-4	3	110	124	6	1	139	-137	7	13	86	-80
0	6	209	229	-1	-3	161	-148	-2	2	259	-276	-3	-2	*	-5	-4	-3	*	49	6	-1	138	142	-7	-2	42	60
0	-6	142	-131	-1	4	103	97	-2	-2	287	-310	-3	3	236	-278	-4	4	63	-57	6	2	48	53	8	0	155	144
0	7	98	104	-1	-4	*	9	-2	3	104	-120	-3	-3	200	206	-4	-4	140	-156	6	-2	*	41	8	1	119	113
0	-7	119	99	-1	5	149	-150	-2	-3	54	-26	-3	4	120	-132	-4	5	*	-37	6	3	94	94	8	-1	95	-84
0	9	109	-117	-1	-5	*	-44	-2	4	130	133	-3	-4	*	-2	-4	-5	64	-61	6	-3	*	-34	8	2	53	-53
0	-9	91	-82	-1	6	198	-199	-2	-4	104	100	-3	5	63	64	-4	-6	100	90	6	4	95	-68	8	-2	162	-159
0	8	118	-130	-1	-6	186	185	-2	5	178	212	-3	-5	107	-120	-4	9	72	-88	6	-4	222	-191	8	3	92	-100
0	-8	*	-6	-1	7	211	258	-2	-5	*	32	-3	6	68	70	-4	-8	97	-92	6	5	196	-193	8	4	48	32
0	10	67	50	-1	-7	*	14	-2	6	130	-152	-3	-6	*	3	5	0	283	289	6	6	161	-163	8	-4	54	50
0	-10	56	-50	-1	9	48	-48	-2	-6	*	2	-3	7	*	-22	5	1	95	-82	6	-6	96	85	8	5	107	106
0	11	44	57	-1	8	122	170	-2	7	63	-81	-3	-7	118	101	5	-1	*	26	6	7	141	-132	8	6	*	-9
0	13	82	-98	-1	-8	102	-87	-2	-7	126	-123	-3	9	44	-23	5	2	239	-219	6	9	123	-132	8	7	74	-70
1	0	64	75	-1	10	91	-91	-2	9	109	130	-3	8	81	-84	5	-2	133	105	6	8	154	148	8	9	*	76
1	1	59	46	-1	-10	54	50	-2	-9	74	59	-3	10	60	71	5	3	*	-13	6	10	108	-120	8	8	81	49
1	-1	40	36	-1	12	60	52	-2	8	*	31	4	0	*	2	5	-3	*	-19	6	11	*	-24	8	12	80	-73
1	2	233	-319	2	0	91	98	-2	10	46	33	4	1	297	307	5	4	123	116	6	12	71	56	9	1	54	-63
1	-2	237	-214	2	1	120	-155	3	0	178	-179	4	-1	265	-275	5	-4	93	98	-6	0	39	33	9	-1	119	117
1	3	314	-375	2	-1	160	182	3	1	166	-189	4	2	311	333	5	5	137	131	-6	-1	83	-85	9	2	60	-48
1	-3	120	103	2	-2	*	-4	3	2	48	-23	4	-2	70	-79	5	-5	195	165	-6	-2	89	-92	9	3	99	92
1	4	186	-223	2	3	41	36	3	-2	194	182	4	3	57	12	5	6	*	9	-6	3	59	-63	9	4	166	151
1	-4	177	165	2	-3	246	-245	3	3	244	310	4	-3	62	56	5	-6	76	-61	-6	-4	65	82	9	5	43	-45
1	5	224	251	2	4	183	259	3	-3	*	-4	4	4	152	-126	5	7	243	-270	-6	6	32	64	9	6	133	-126
1	-5	*	-34	2	-4	*	16	3	4	232	-283	4	-4	105	99	5	-7	105	-83	-6	-6	67	-90	9	9	72	-20
1	6	30	-13	2	5	167	-192	3	-4	261	-265	4	5	125	135	5	9	154	180	7	0	152	-159	9	10	75	-62
1	-6	107	-114	2	-5	275	281	3	5	91	-99	4	-5	83	-77	5	8	*	33	7	1	82	77	10	2	68	73
1	7	171	-204	2	6	289	-340	3	-5	91	-83	4	6	189	201	5	10	41	-37	7	-1	170	-169	10	3	59	68
1	-7	58	-45	2	-6	63	54	3	6	215	249	4	-6	105	-92	5	11	107	-82	7	2	40	-12	10	4	49	-47
1	9	*	5	2	7	69	-81	3	-6	93	65	4	7	*	-2	5	13	101	104	7	-2	81	85	10	5	105	-103
1	-9	81	70	2	-7	40	-38	3	7	259	290	4	9	*	36	-5	0	65	45	7	3	57	-51	10	6	42	43
1	8	88	-86	2	9	92	96	3	9	140	-153	4	8	158	-164	-5	1	39	-25	7	-3	106	89	10	7	70	77

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.

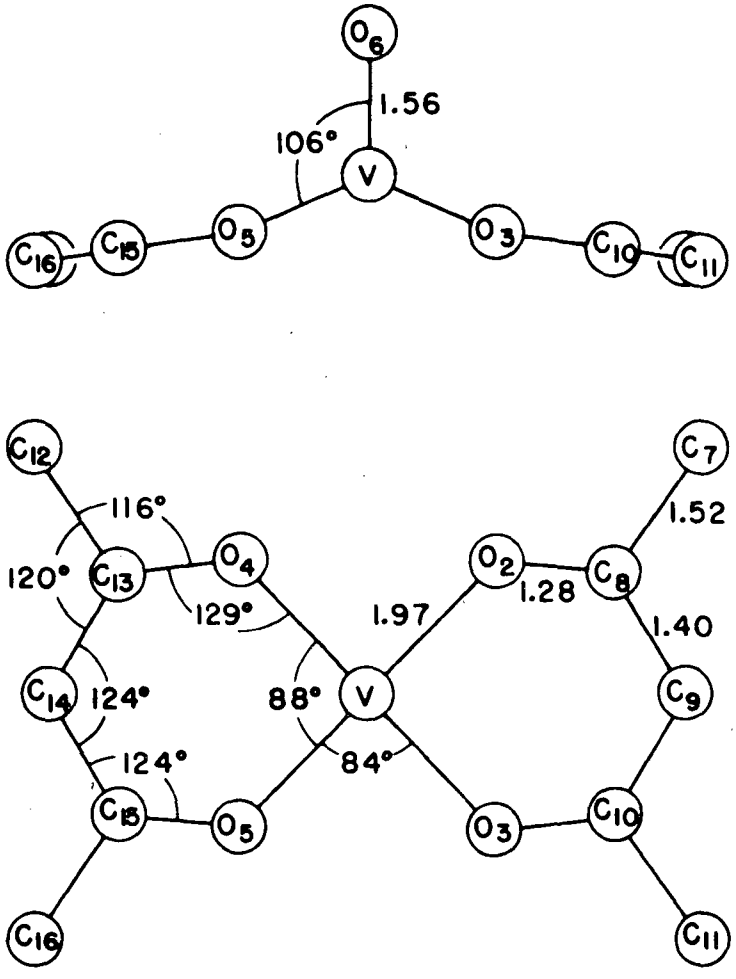
Fig. 2. Average bond distances and bond angles.

Fig. 3. Individual isotropic temperature parameters.



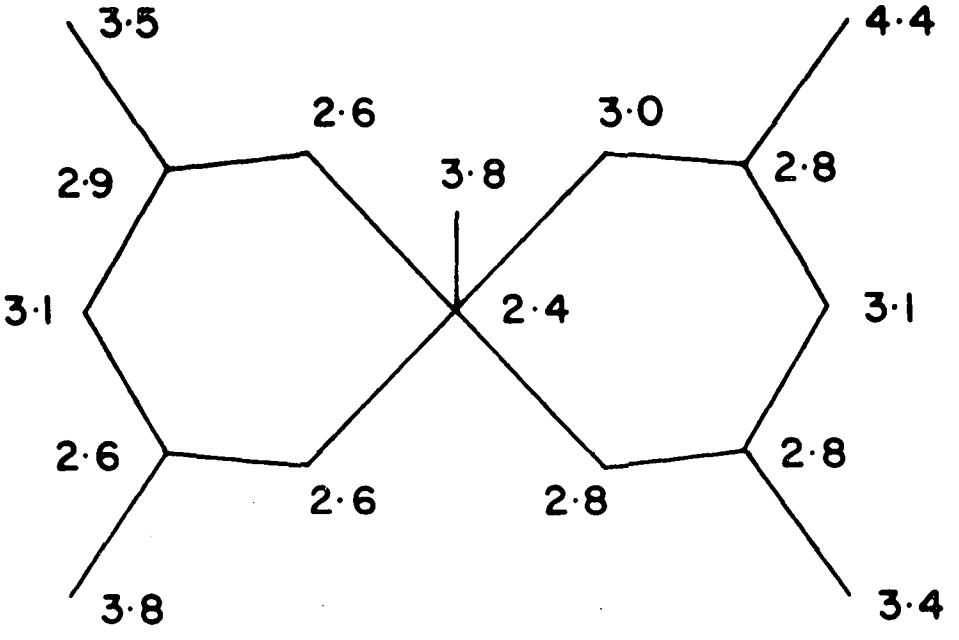
MU-22078

Fig. 1.


O6
1.56
106°
V
O5
O3
C16
C15
C10
C11
C12
116°
120°
C13
O4
129°
O2
C8
C7
1.52
1.28
1.97
1.40
C14
124°
88°
V
C9
124°
84°
C15
O5
O3
C10
C16
C11

MU-22079

Fig. ..



MU-22080

Fig. 3.