vely. Thus the copper salt appears to be rather tightly packed into the structure and the $H_2O(1)-O(4)$ bond length (2·54 Å) is exceptionally short. It is so short, that not only is it unlikely that a hydrogen bond will form but there is probably some repulsion between the two atoms. The authors suggest that this tighter packing and resultant strain is one of the reasons for the much poorer stability of the copper salt than that of the nickel salt to dehydration (Caven & Ferguson, 1922) even though the heats of hydration of the hexahydrated copper and nickel ions are practically identical (Griffith & Orgel, 1957). The close approach of $H_2O(1)$ and O(4) does not, in this case, lead to extra stability since it is imposed by the packing of sulphate group tetrahedra and $Cu(H_2O)_6$ octahedra and is not due to attractive forces between $H_2O(1)$ and O(4). Half of the hydrogen bonds lie across the $\bar{2}01$ plane and the average separation of the closest atoms across this plane in the copper salt is significantly smaller than in the nickel and magnesium salts (2·66 in comparison with 2·74 and 2·78 Å respectively). This may explain the poorer cleavage of the copper salt on this plane.

The bonding of the ammonium group to the sulphate oxygen atoms is very similar to that in the nickel and magnesium salts, so the cleavage parallel to (010) in the three salts is explained (Grimes, Kay & Webb 1963).

Paramagnetic resonance measurements on copper ammonium sulphate are given by Bleaney, Penrose & Plumpton (1949). They found that the angle between the projection of the tetragonal axis of the complex onto the *ac* plane and the *c* axis was 77°. The angle which the tetragonal axis makes with the *ac* plane was not measured at room temperature, but at 90 °K it was found to be 40° and in other copper Tutton salts at room temperature it was found to be approximately 40°. When these angles are calculated using the position of $H_2O(2)$, and assuming that the tetragonal axis of the complex passes through the oxygen atom of this water molecule, they are found to be $68° \pm 6°$ and $42° \pm 2°$ respectively. As with the nickel salt, the true symmetry of the copper complex must be less than orthorhombic owing to the non-symmetrical arrangement of the hydrogen atoms of the water molecules around the copper ion. However the orientation of the approximately tetragonally distorted octahedron confirms the paramagnetic resonance measurements.

Two of us, N.W.G. and M.W.W., would like to thank the Electrical Research Association and Department of Scientific and Industrial Research respectively for financial assistance.

References

BACON, G. E. & CURRY N. A. (1962). *Proc. Roy. Soc.* A, **266**, 95.

BHOWINK, G. (1961). *Indian J. Phys.* **35**, 499.

BLEANEY, B., PENROSE R. B. & PLUMPTON B. I. (1949). *Proc. Roy. Soc.* A, **198**, 406.

CAVEN, R. M. & FERGUSON J. (1922). *J. Chem. Soc.* **121**, 1407.

GRIFFITH, J. H. E. & ORGEL L. E. (1957). *Quart. Rev. Chem. Soc. Lond.* **11**, 381.

GRIMES, N. W., KAY H. F. & WEBB M. W. (1963). *Acta Cryst.* **16**, 823.

MARGULIS, T. N. & TEMPLETON D. M. (1962). *Z. Kristallogr.* **117**, 344.

TUTTON, A. E. H. (1916). *Phil. Trans.* **216**, 1.

Acta Cryst. (1965). **18**, 742

The Crystal Structure of the Centrosymmetric Photodimer of Cyclopentenone*

BY T. N. MARGULIS

Department of Chemistry, Brandeis University, Waltham, Massachusetts, U.S.A.

(*Received* 15 *June* 1964 *and in revised form* 10 *July* 1964)

The crystal structure of the centrosymmetric photodimer of cyclopentenone, $C_{10}H_{12}O_2$, has been determined from the three-dimensional X-ray diffraction data. The crystals are monoclinic, space group $P2_1/n$, with two molecules in the unit cell with dimensions

$$a=6.78,\ b=7.23,\ c=8.67\ \text{Å};\ \beta=98.9°.$$

The carbon–carbon bond lengths in the cyclobutane ring are 1·54 and 1·59 Å.

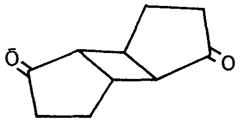
Introduction

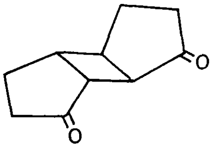
Many α,β-ethylenic carbonyl compounds dimerize in the presence of ultraviolet radiation to yield derivatives of cyclobutane (Yates & Jorgenson, 1963). These dimers have been investigated by a variety of physical and chemical techniques, but no crystal structure has been reported. Eaton (1962) found that cyclopentenone yields two dimers, $C_{10}H_{12}O_2$, upon ultraviolet irradiation, and assigned them structures (I) and (II) primarily on the basis of chemical evidence. The present paper describes the crystal structure determination of

---

* Work done in part at the Lawrence Radiation Laboratory, University of California, Berkeley, under the auspices of the U.S. Atomic Energy Commission, and supported in part by a grant (GP 1078) from the National Science Foundation.

the centrosymmetric photodimer (I), with results in agreement with those of Eaton.


(I)


(II)

Experimental

Single crystals, m.p. 125–126·5°, purified by sublimation, were provided by Professor Philip E. Eaton. X-ray diffraction photographs of numerous crystals were taken before an untwinned specimen was found. Weissenberg and rotation photographs using Cu $K\alpha$ X-rays ($\lambda=1{\cdot}5418$ Å) indicate a monoclinic unit cell with dimensions:

$$a=6{\cdot}78\pm0{\cdot}03,\ b=7{\cdot}23\pm0{\cdot}03,\ c=8{\cdot}67\pm0{\cdot}03\ \text{Å},$$
$$\beta=98{\cdot}9\pm0{\cdot}2°.$$

The space group suggested by systematic absences of reflections on the Weissenberg photographs is $P2_1/n$ (C_{2h}^5), and is confirmed by the successful structure determination. The calculated density is 1·30 g.cm^{-3} assuming two dimers per unit cell.

Intensity data were collected with a block-like single crystal with no dimension greater than 0·5 mm. Layers $h0l$ through $h4l$ were photographed with the use of the multiple-film, equi-inclination Weissenberg technique. The intensities of 354 reflections were estimated visually by comparison with a calibrated film strip and converted to structure factors in the usual way without correction for absorption. Exposure times were used to convert all reflections to a common relative scale.

Structure determination

The general position of space group $P2_1/n$ is $\pm(x,y,z;\ \frac{1}{2}+x,\ \frac{1}{2}-y,\ \frac{1}{2}+z)$. Since there are only two dimers per unit cell, the center of each molecule must coincide with a symmetry-center of the cell, so that each atom has a symmetry-related atom in the same molecule. The origin was chosen so that the molecular centers lie at 0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

Since the positions of the molecules and the approximate molecular geometry are known, only the orientation of the molecules with respect to the crystal axes must be determined to obtain a trial structure. Each atom was assigned Cartesian coordinates X, Y, Z (in Å) based on the assumed molecular structure. The orientation of the molecule with respect to the Cartesian system is specified by three Euler-like angles φ, θ, ϱ as defined by Scheringer (1963). Values of φ, θ, ϱ were assigned systematically, holding two angles constant and varying the third 10° at a time over a specified range. After each assignment of these angles, new Cartesian coordinates were calculated and transformed into fractional coordinates in crystal space (Patterson, 1959). Structure factors and the R index were calculated after each change in orientation for about 50 large-amplitude reflections. To save computer time a limited number of orientations were tested based on an examination of the Patterson function. About 1600 structures were tested which took two hours on the IBM 7094. The orientation which gave the lowest value of R (about 0·50) was used as a trial structure.

Refinement

Refinement of the trial structure was accomplished by full-matrix least-squares calculations on the IBM 7094 computer. The Busing, Martin & Levy (1962) program was used to refine the 5 scale factors, 18 positional pa-

Table 1. *Hydrogen atom coordinates*

Atom*	x	y	z
H(1)	0·028	−0·25	0·100
H(2)	0·265	0·08	0·040
H(3A)	−0·261	0·273	0·075
H(3B)	−0·361	0·081	0·176
H(4A)	0·031	0·282	0·250
H(4B)	−0·111	0·156	0·379

* Numerals refer to the carbon atom to which the hydrogen atom is bonded.

Tabel 2. *Observed* (OBS) *and calculated* (CALC) *structure factors each multiplied by* 10

H	K	L	OBS	CALC
0	0	2	183	-169
0	0	4	70	-56
0	0	6	57	-54
0	0	8	169	145
0	0	10	26	-10
1	0	1	145	141
1	0	3	132	145
1	0	5	34	-42
1	0	7	68	61
1	0	-3	194	138
1	0	-5	168	-128
2	0	0	41	-34
2	0	2	86	-93
2	0	4	167	159
2	0	6	147	-145
2	0	8	23	27
2	0	10	46	32
2	0	-4	258	198
2	0	-6	189	-145
2	0	-8	81	-69
3	0	3	155	-161
3	0	5	109	-115
3	0	7	34	30
3	0	-1	114	111
3	0	-3	171	-143
3	0	-5	171	-138
3	0	-7	64	-51
4	0	0	86	94
4	0	2	173	-188
4	0	4	98	-110
4	0	-2	166	178
4	0	-4	138	-129
4	0	-6	102	-88
4	0	-8	23	22
5	0	1	23	26
5	0	3	33	-37
5	0	-3	40	45
5	0	-5	49	51
6	0	2	77	93
6	0	4	22	-31
6	0	-2	60	64
6	0	-6	72	77
7	0	3	27	-30
7	0	5	34	47
7	0	-1	46	58
7	0	-3	56	67
8	0	0	17	-32
8	0	-2	47	67
8	0	-4	32	-31
2	1	0	205	206
3	1	0	111	-123
4	1	0	23	24
5	1	0	60	77
6	1	0	58	71
0	1	1	192	254
0	1	2	98	-92
0	1	3	220	226
0	1	4	39	29
0	1	6	73	63
0	1	7	28	31
0	1	8	64	-53
1	1	1	20	-20
1	1	2	170	190
1	1	3	159	157
1	1	5	82	-76
1	1	6	141	-118
1	1	8	121	105
1	1	10	47	33
1	1	-1	167	128
1	1	-3	242	-204
1	1	-4	147	104
1	1	-5	22	23
1	1	-8	29	25
1	1	-9	27	19
1	1	-10	54	-37
2	1	1	99	-107
2	1	2	174	191
2	1	3	72	-66
2	1	4	23	-22
2	1	5	63	-60
2	1	6	56	-62
2	1	7	65	53
2	1	-3	132	-106
2	1	-4	36	-28
2	1	-5	188	-156
2	1	-6	37	32
2	1	-7	63	-53
2	1	-8	71	44
2	1	-10	49	-27
3	1	1	48	-45
3	1	2	210	-223
3	1	3	84	94
3	1	4	26	16
3	1	5	20	-25
3	1	6	16	-25
3	1	8	35	-23
3	1	9	27	-16
3	1	-1	19	16
3	1	-2	67	55
3	1	-3	36	-36
3	1	-6	228	-178
3	1	-8	40	-35
4	1	2	43	-52
4	1	3	38	-42
4	1	4	53	50
4	1	5	91	-106
4	1	6	28	-19
4	1	-2	23	-9
4	1	-3	80	-79
4	1	-4	48	48
4	1	-6	81	-69
4	1	-7	29	-29
4	1	-8	19	19
5	1	1	47	55
5	1	4	81	-95
5	1	5	28	-31
5	1	-2	71	73
5	1	-3	39	-39
5	1	-4	56	-65
5	1	-5	54	-49
5	1	-6	54	52
5	1	-7	34	34
6	1	-1	50	57
6	1	-2	29	-30
6	1	-3	65	81
6	1	-4	20	-33
6	1	-5	28	31
6	1	-7	24	-26
7	1	-2	61	73
2	2	0	99	-74
3	2	0	31	16
4	2	0	44	-54
5	2	0	76	98
7	2	0	24	30
0	2	1	45	-56
0	2	2	58	51
0	2	3	171	166
0	2	4	49	49
0	2	5	57	-42
0	2	6	24	22
0	2	8	65	60
0	2	9	24	-27
1	2	1	104	-134
1	2	2	10	7
1	2	3	53	73
1	2	4	99	-116
1	2	5	60	62
1	2	6	44	24
1	2	7	71	57
1	2	-2	237	-189
1	2	-3	141	100
1	2	-4	230	-181
1	2	-5	43	-30
1	2	-7	59	-48
1	2	-8	119	105
1	2	-9	24	22
1	2	-10	27	-18
2	2	2	34	38
2	2	3	173	173
2	2	4	22	12
2	2	5	42	-51
2	2	6	37	-27
2	2	7	27	-20
2	2	-1	35	-26
2	2	-2	151	-148
2	2	-3	115	-79
2	2	-4	34	25
2	2	-6	99	-78
2	2	-8	27	-21
2	2	-10	38	-33
3	2	1	73	-77
3	2	2	108	110
3	2	4	77	91
3	2	5	117	-124
3	2	6	80	-89
3	2	7	26	23
3	2	-1	44	45
3	2	-2	246	-217
3	2	-3	328	-250
3	2	-4	126	108
3	2	-7	63	-49
4	2	1	28	35
4	2	2	53	-66
4	2	4	70	-67
4	2	5	27	-25
4	2	-1	49	50
4	2	-2	31	45
4	2	-3	46	-47
4	2	-4	35	-30
4	2	-5	84	-69
4	2	-6	42	-46
4	2	-7	27	28
4	2	-9	21	19
5	2	1	58	-66
5	2	2	53	-64
5	2	3	46	45
5	2	-1	50	51
5	2	-4	46	-47
5	2	-5	76	71
5	2	-6	62	-59
5	2	-7	35	-32
5	2	-8	49	50
5	2	-9	34	33
6	2	1	53	62
6	2	2	52	58
6	2	5	28	-35
6	2	6	15	24
6	2	-2	46	45
6	2	-3	27	-25
6	2	-6	34	41
6	2	-7	30	25
7	2	-1	35	44
7	2	-2	24	-36
8	2	-5	20	-31
1	3	0	17	35
2	3	0	143	147
3	3	0	99	-110
0	3	2	82	-112
0	3	3	151	170
0	3	4	70	69
0	3	5	110	109
0	3	6	59	42
0	3	8	61	-46
1	3	1	45	36
1	3	2	47	41
1	3	3	112	117
1	3	4	60	68
1	3	6	61	67
1	3	7	54	-44
1	3	-1	175	-162
1	3	-2	43	26
1	3	-3	48	-33
1	3	-4	57	46
1	3	-5	42	25
1	3	-6	21	-28
1	3	-7	22	20
1	3	-10	28	-18
2	3	1	109	-134
2	3	2	152	164
2	3	4	38	-39
2	3	5	51	-36
2	3	6	54	-65
2	3	7	69	66
2	3	-1	195	182
2	3	-2	263	-216
2	3	-3	262	-210
2	3	-4	55	-59
2	3	-6	67	61
2	3	-7	59	-43
2	3	-8	30	34
2	3	-9	26	16
2	3	-10	19	-17
3	3	1	24	21
3	3	3	27	5
3	3	4	51	-60
3	3	8	41	-30
3	3	-1	55	73
3	3	-2	138	-127
3	3	-4	27	-19
3	3	-5	90	-64
3	3	-6	31	-30
3	3	-7	31	20
3	3	-9	25	21
3	3	-10	59	-41
4	3	1	122	-131
4	3	3	81	90
4	3	4	44	57
4	3	5	67	-73
4	3	6	29	-25
4	3	7	24	-17
4	3	8	29	-21
4	3	-1	27	-13
4	3	-3	110	-108
4	3	-5	125	110
4	3	-6	50	-49
4	3	-7	74	-53
4	3	-8	27	11
4	3	-9	22	11
5	3	1	62	63
5	3	5	39	-40
5	3	-3	62	-62
5	3	-4	31	20
5	3	-5	31	-15
5	3	-7	34	23
5	3	-8	29	30
6	3	3	28	32
6	3	-1	82	84
6	3	-4	43	-50
6	3	-5	29	30
6	3	-8	23	26
7	3	2	33	44
1	4	0	72	83
2	4	0	15	-2
3	4	0	27	-24
4	4	0	85	-100
0	4	1	142	197
0	4	2	38	39
0	4	3	41	48
0	4	4	148	157
0	4	7	69	-52
0	4	9	36	21
1	4	1	72	-89
1	4	3	68	75
1	4	5	73	82
1	4	7	59	52
1	4	-1	108	92
1	4	-4	113	-98
1	4	-5	45	33
1	4	-6	34	30
2	4	2	45	-28
2	4	5	76	71
2	4	6	49	40
2	4	7	33	-35
2	4	-1	38	-18
2	4	-2	103	-83
2	4	-3	87	79
2	4	-4	29	-35
2	4	-5	72	-59
2	4	-6	34	-27
2	4	-8	32	20
2	4	-9	26	23
2	4	-10	61	-44
3	4	1	98	-110
3	4	2	85	92
3	4	3	56	53
3	4	5	69	-73
3	4	6	33	-32
3	4	-1	47	-30
3	4	-2	40	-47
3	4	-3	191	-166
3	4	-4	32	-18
3	4	-5	95	65
3	4	-6	35	36
3	4	-7	48	-30
4	4	1	65	80
4	4	3	34	-25
4	4	5	33	-28
4	4	-2	79	-66
4	4	-3	88	-86
4	4	-4	34	28
4	4	-7	32	26
5	4	1	60	-66
5	4	3	41	51
5	4	-1	34	40
5	4	-4	34	-25
5	4	-5	47	57
6	4	1	23	-10
6	4	2	31	33
6	4	3	20	26
6	4	-2	33	34
6	4	-6	37	28
6	4	-7	20	-22
7	4	1	42	30
7	4	-5	20	18

Table 3. *Final parameters*

Atom	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	B
C(1)	0·0285	−0·0986	0·0996	0·0013	0·0018	0·0010	3·39 Å^2
C(2)	−0·1582	0·0021	0·0151	0·0012	0·0019	0·0010	3·23
C(3)	−0·2303	0·1388	0·1327	0·0013	0·0018	0·0010	3·64
C(4)	−0·0563	0·1560	0·2676	0·0014	0·0020	0·0011	4·14
C(5)	0·0723	−0·0087	0·2584	0·0012	0·0018	0·0010	3·44
O	0·1957	−0·0638	0·3644	0·0010	0·0013	0·0008	4·74

rameters, and 6 individual atom, isotropic temperature factors. The function minimized was $\Sigma w(|F_o|-|F_c|)^2/\Sigma|F_o|^2$ where the weights, w, were assigned according to Hughes (1941). Hydrogen atom coordinates (Table 1) were estimated by examination of a difference Fourier map and by calculation of their expected positions. The hydrogen atom coordinates were not varied but were included in the last three cycles of refinement as fixed atoms with $B=4·5$ Å^2. The atomic scattering factors of *International Tables for X-ray Crystallography* (1962*a*) were used for all atoms. In the last cycle of refinement no fractional coordinate changed by more than 6×10^{-5}. The final value of R for the 354 observed reflections is 0·157. Observed and calculated structure factors are listed in Table 2. Table 3 gives the final atomic parameters and their standard deviations estimated from the least-squares results.

Discussion

The crystal structure, projected on (010), is shown in Fig. 1. As indicated in Fig. 1, the shortest intermolecular distances (excluding hydrogen atoms) are from oxygen to C(4) (3·53 and 3·50 Å) and to C(2) (3·51 Å). All other intermolecular distances are greater than 3·65 Å.

Two views of a single molecule are shown in Figs. 2 and 3. Bond distances and bond angles are given in Fig. 4. The standard deviations of the bond lengths are about 0·015 Å as estimated from the least-squares standard deviations of atomic coordinates. The bond distances given are uncorrected for thermal motion. This correction is estimated to be approximately 0·01 Å for the C(5)–O bond and negligible for all other bonds. The corrected value of 1·22 Å for the carbon–oxygen double bond is to be compared with the value of 1·23 Å reported in *International Tables for X-ray Crystallography* (1962*b*). The C(5)–C(4) and C(5)–C(1) bonds are 1·48 and 1·51 Å, respectively, somewhat shorter than the average value of 1·516 Å reported in *International Tables* (1962*b*) for C–C=O single bonds. The five-membered ring is non-planar, atoms C(2) and C(3) being 0·21 and 0·45 Å, respectively, above the plane formed by C(5) and its three substituents.

The cyclobutane ring is planar, a requirement of the center of symmetry. The C(1)–C(2) bond in the five-membered ring is of normal length but the C(1)–C(2) bond connecting the rings is 1·59 Å, about three standard deviations greater than 'normal' carbon–carbon single bonds. Long bonds in cyclobutane rings are not without precedent. The centrosymmetric isomer of 1,2,3,4-tetraphenylcyclobutane (Dunitz, 1949) has bonds of 1·585 ±0·02 and 1·555 ±0·02 Å in the four-membered ring, and octachlorocyclobutane (Owen & Hoard, 1951) has bond lengths of 1·58 and 1·60 Å.

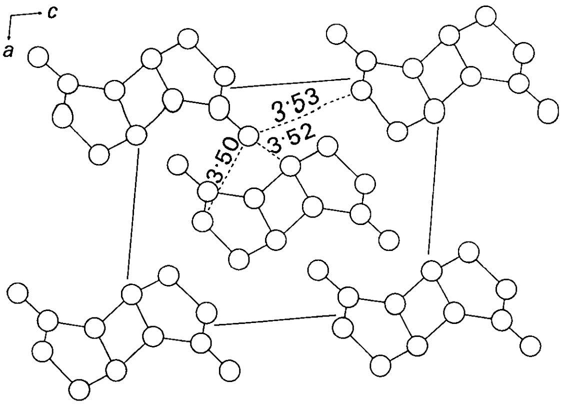


Fig. 1. The crystal structure projected on (010).

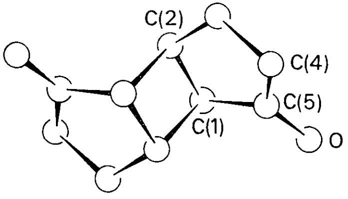


Fig. 2. One molecule viewed along [010].

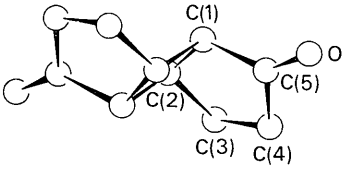


Fig. 3. One molecule viewed along [100].

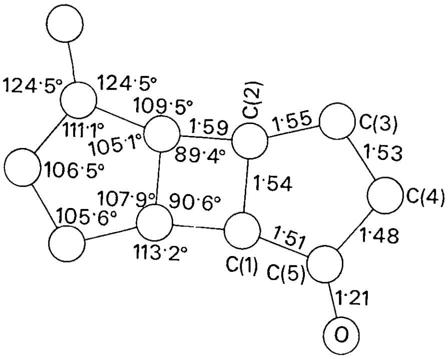


Fig. 4. Bond lengths and bond angles.

None of these structure determinations, including the present, are up to modern standards (counter data, anisotropic refinement, refinement of hydrogen atoms) but taken as a whole they suggest that bonds significantly longer than 1·54 Å occur in cyclobutane compounds. An explanation of long C–C bonds in cyclobutane rings has been given by Dunitz & Schomaker (1952) as arising from non-bonded carbon–carbon repulsion. In this compound only two of the four C–C bonds are lengthened; thus the non-bonded interaction is reduced without affecting the five-membered ring.

I am indebted to Professor David H. Templeton for permitting the use of his facilities and for his general encouragement of this work. I also thank Professor Philip E. Eaton for suggesting the problem and providing the crystals. The calculations were done at the Computation Center of the Massachusetts Institute of Technology, Cambridge, Massachusetts.

References

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). Oak Ridge National Laboratory Report ORNL-TM-305.
DUNITZ, J. D. (1949). *Acta Cryst.* **2**, 1.
DUNITZ, J. D. & SCHOMAKER, V. (1952). *J. Chem. Phys.* **20**, 1703.
EATON, P. E. (1962). *J. Amer. Chem. Soc.* **84**, 2344.
HUGHES, E. W. (1941). *J. Amer. Chem. Soc.* **63**, 1737.
International Tables for X-ray Crystallography (1962*a*). Vol. III, p. 202. Birmingham: Kynoch Press.
International Tables for X-ray Crystallography (1962*b*). Vol. III, p. 276. Birmingham: Kynoch Press.
OWEN, T. B. & HOARD, J. L. (1951). *Acta Cryst.* **4**, 172.
PATTERSON, A. L. (1959). In *International Tables for X-ray Crystallography.* Vol. II, p. 61. Birmingham: Kynoch Press.
SCHERINGER, C. (1963). *Acta Cryst.* **16**, 546.
YATES, P. & JORGENSON, M. J. (1963). *J. Amer. Chem. Soc* **85**, 2956.

Acta Cryst. (1965). **18**, 745

Combination of Multiple Isomorphous Replacement and Anomalous Dispersion Data for Protein Structure Determination
I. Determination of Heavy-Atom Positions in Protein Derivatives

BY G. KARTHA AND R. PARTHASARATHY

Roswell Park Memorial Institute, Buffalo, New York 14203, *U.S.A.*

(*Received* 8 *June* 1964 *and in revised form* 17 *July* 1964

In applying the multiple isomorphous replacement method to study the structure of proteins, it is necessary first to establish and correlate the positions occupied by the heavy atoms in the various derivatives. This paper discusses the advantages of systematic exploitation of the anomalous scattering information from the heavy atoms in these derivatives, in addition to the usual isomorphous crystal data, in establishing the heavy atom positions. It is shown that by proper combination of the isomorphous derivative and anomalous scattering information, one can remove many of the undesirable features that crop up when either of these alone is used to establish the heavy atom positions.

Introduction

As is well known, the problem of determining the phase angles of reflections for proteins is solved in the multiple isomorphous replacement method (Harker, 1956) by preparing a series of isomorphous derivatives of the protein, each one containing groups of heavy atoms attached to different, but definite, sites. The first main problem of the crystallographer is to locate the positions of these heavy atoms, and, in addition, in certain cases to correlate the positions of the heavy atom in the different derivatives. Once this stage has been successfully accomplished, the second problem is the refinement of heavy atom positions and occupancy parameters *etc.*, and the third is the use of this information to evaluate the phase angles of the protein reflections.

In our study of the protein ribonuclease, we have found that during all these stages of the structure determination, the additional information available as a result of the anomalous scattering of the heavy atom (besides the usual isomorphous data) was of great value, not only in confirming the results obtained by using isomorphous data in the usual way, but also complementing this information in a very elegant manner. Thus, for example, it has been found that by properly combining isomorphous and anomalous dispersion data, we are able to overcome many of the undesirable features that arise when either kind of data is used alone. Consequently, for all the heavy