RENNIE, M. J., BABIJ, P., TAYLOR, P. M., HUNDAL, H. S., MACLENNAN, P., WATT, P. M., JEPSON, M. M. & MILLWARD, D. J. (1986). *Lancet*, pp. 1008–1012.
ROBERTS, P. & SHELDRICK, G. M. (1975). *XANADU*. Program for torsion angle, mean plane and libration correction calculations. Univ. of Cambridge, England.
TAIRA, Z. & WATSON, W. H. (1977). *Acta Cryst.* B**33**, 3823–3827.
SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
SHELDRICK, G. M. (1986). *SHELXS86*. *Crystallographic Computing* 3, edited by G. M. SHELDRICK, C. KRUGER & R. GODDARD, pp. 175–189. Oxford Univ. Press.
WATKINS, J. C. & OLVERTON, H. J. (1987). *Top. Neurol. Sci.* **10**, 265–272.

Acta Cryst. (1988). C**44**, 1764–1767

Structure of the Cation Radical Salt 3,4;3′,4′-Bis(methylenedithio)tetrathiafulvalenium Triiodide

BY TADASHI SUGANO AND SHOICHI SATO

Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, *Japan*

MICHIKO KONNO

Department of Chemistry, Faculty of Science, Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo 112, *Japan*

AND MINORU KINOSHITA

Institute for Solid State Physics, University of Tokyo, Rippongi, Minato-ku, Tokyo 106, *Japan*

(*Received* 5 *March* 1988; *accepted* 18 *April* 1988)

Abstract. $C_8H_4S_8^+.I_3^-$, $M_r = 737{\cdot}31$, triclinic, $P\bar{1}$, $a = 13{\cdot}185\ (2)$, $b = 9{\cdot}433\ (1)$, $c = 7{\cdot}830\ (1)$ Å, $\alpha = 102{\cdot}99\ (1)$, $\beta = 104{\cdot}64\ (1)$, $\gamma = 67{\cdot}56\ (1)°$, $V = 861{\cdot}8\ (2)$ Å^3, $Z = 2$, $D_x = 2{\cdot}84$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 63{\cdot}0$ cm^{-1}, $F(000) = 678$, $T = 298$ K, $R = 0{\cdot}036$ for 4001 observed reflections. The cation radical and the anion form side-by-side molecular coordination pairs with short S···I contacts of 3·651–3·868 Å aligning their long molecular axes parallel. The cation radicals form face-to-face dimers with mean interplanar distance 3·41 Å. The adjacent dimers are connected to each other making one-dimensional arrays along the c axis by side-by-side S···S contacts of 3·395–3·772 Å between the cation radicals.

Introduction. Cation radical salts based on the π-electron-donor molecule 3,4;3′,4′-bis(ethylenedithio)-tetrathiafulvalene (BEDT-TTF) and quasi-linear anions exhibit superconductivity at ambient pressure and temperatures as high as 10 K (Urayama, Yamochi, Saito, Nozawa, Sugano, Kinoshita, Sato, Oshima, Kawamoto & Tanaka, 1988). Among the linear anions, triiodide gives four cation radical salts with BEDT-TTF exhibiting superconductivity at ambient pressure: β-(BEDT-TTF)$_2$I$_3$ (Yagubskii, Shchegolev, Laukhin, Kononovich, Kartsovnik, Zvarykina & Buravov, 1984), γ-(BEDT-TTF)$_6$(I$_3$)$_5$ (Yagubskii, Shchegolev, Pesotskii, Laukhin, Kononovich, Kartsovnik & Zvarykina, 1984), θ-(BEDT-TTF)$_2$I$_3$ (Kobayashi, Kato, Kobayashi, Nishio, Kajita & Sasaki, 1986), and κ-(BEDT-TTF)$_2$I$_3$ (Kato, Kobayashi, Kobayashi, Moriyama, Nishio, Kajita & Sasaki, 1987). Since the superconductivity of these salts is likely to be due to the quasi-two-dimensional character of the electrically conducting BEDT-TTF sheet, it is of great interest to investigate linear anion salts, in particular triiodide salts, of 3,4;3′,4′-bis(methylenedithio)tetrathiafulvalene (BMDT-TTF) in which the two-dimensional interaction is expected to be large compared with that of BEDT-TTF (Kato, Kobayashi, Kobayashi & Sasaki, 1985). In this paper, we report the crystal structure of the triiodide salt of BMDT-TTF.

Experimental. The crystals were prepared by electrochemical oxidation of BMDT-TTF in a benzonitrile solution of tetrabutylammonium triiodide at a platinum electrode (2 mm diameter). A constant current of 1 μA was passed through a fine fritted-glass separating anode and cathode of an electrochemical cell for a month to yield black rhombohedral crystals. A Rigaku automatic four-circle diffractometer with graphite-monochromatized Mo $K\alpha$ radiation was used for intensity data collection from a crystal of dimensions 0·5 × 0·5 × 0·4 mm at room temperature [298 (2) K]. θ–2θ scan employed within $2\theta = 60°$ [$(\sin\theta)/\lambda = 0{\cdot}704$ Å^{-1}]. Four standard reflections (200, 00$\bar{5}$, $\bar{1}\bar{1}\bar{1}$ and $\bar{1}\bar{2}$1) were monitored every 50 reflections and showed no evidence of crystal deterioration. 4001 observed reflections with

0108-2701/88/101764-04$03.00

Table 1. *Positional parameters and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$) *with e.s.d.'s in parentheses*

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} matrix.

	x	y	z	U_{eq}
I(1)	0·03969 (3)	0·11254 (5)	0·30732 (6)	341 (3)
I(2)	0·27289 (4)	−0·01887 (6)	0·26182 (9)	540 (4)
I(3)	−0·19216 (4)	0·24736 (6)	0·33219 (8)	447 (4)
S(1)	0·1741 (1)	0·4044 (2)	0·2792 (2)	331 (10)
S(2)	0·1538 (1)	0·6703 (2)	0·1212 (2)	346 (11)
S(3)	−0·0896 (1)	0·5405 (2)	0·2780 (2)	324 (10)
S(4)	−0·1109 (1)	0·8076 (2)	0·1196 (3)	372 (11)
S(5)	0·4301 (1)	0·2994 (2)	0·3354 (3)	580 (15)
S(6)	0·4093 (1)	0·5672 (2)	0·1734 (3)	525 (15)
S(7)	−0·3405 (1)	0·6700 (2)	0·2834 (3)	466 (13)
S(8)	−0·3632 (1)	0·9410 (2)	0·1223 (3)	513 (14)
C(1)	0·0886 (4)	0·5760 (6)	0·1998 (8)	249 (37)
C(2)	−0·0249 (5)	0·6358 (7)	0·1985 (8)	283 (40)
C(3)	0·2963 (5)	0·4202 (7)	0·2575 (9)	316 (42)
C(4)	0·2866 (4)	0·5447 (7)	0·1867 (9)	309 (42)
C(5)	−0·2200 (5)	0·6799 (7)	0·2407 (9)	335 (44)
C(6)	−0·2303 (5)	0·8044 (7)	0·1701 (9)	346 (43)
C(7)	0·4912 (6)	0·3686 (10)	0·2027 (15)	737 (74)
C(8)	−0·4159 (6)	0·8769 (10)	0·2729 (12)	618 (65)

$|F_o| > 3\sigma(|F_o|)$ ($-18 \le h \le 15$, $-13 \le k \le 0$, and $-10 \le l \le 10$) of 5038 independent reflections were used for the refinement. The data were corrected for Lp. No absorption correction was carried out. Unit-cell dimensions were determined by a least-squares fit for 20 reflections with $41·3 < 2\theta < 43·5°$.

The structure was solved by the heavy-atom method. The stoichiometry of the salt was found to be 1:1, (BMDT-TTF)I_3. The Fourier map showed the positions of S and C atoms. Positions of H atoms could not be determined from the difference Fourier map. Thus H atoms were not included in the refinement. Block-diagonal least-squares refinement, with anisotropic thermal parameters for non-H atoms only, gave residuals $R(F) = 0·036$ and $wR(F) = 0·039$ with $w = 0·5$ for weak reflections. $S = 3·50$, $(\Delta/\sigma)_{max} = 0·09$ for C(3), $\Delta\rho_{max} = 1·0$ e $Å^{-3}$ and $\Delta\rho_{min} = -1·2$ e $Å^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974) were used. All calculations were performed on a FACOM M-360 computer at the Institute for Solid State Physics with a local version of *UNICS* (Sakurai, 1967).

Discussion. Positional and equivalent isotropic thermal parameters are listed in Table 1.* Interatomic distances and angles for the BMDT-TTF molecule are summarized in Table 2. The atomic numbering schemes and the molecular geometries of BMDT-TTF and triiodide are shown in Fig. 1. The central C(1)—C(2) double

Table 2. *Interatomic distances* (Å) *and angles* (°) *for the* BMDT-TTF *cation radical and triiodide anion and selected intermolecular contact distances* (Å) *with e.s.d.'s in parentheses*

Distances within the molecule

C(1)—C(2)	1·382 (8)		
C(1)—S(1)	1·727 (6)	C(1)—S(2)	1·734 (8)
C(2)—S(3)	1·741 (8)	C(2)—S(4)	1·727 (6)
C(3)—S(1)	1·727 (7)	C(4)—S(2)	1·722 (5)
C(5)—S(3)	1·721 (5)	C(6)—S(4)	1·730 (8)
C(3)—C(4)	1·359 (11)	C(5)—C(6)	1·355 (11)
C(3)—S(5)	1·736 (5)	C(4)—S(6)	1·741 (7)
C(5)—S(7)	1·743 (8)	C(6)—S(8)	1·742 (5)
C(7)—S(5)	1·812 (12)	C(7)—S(6)	1·803 (9)
C(8)—S(7)	1·831 (8)	C(8)—S(8)	1·815 (11)
S(1)—S(2)	2·935 (3)	S(3)—S(4)	2·941 (3)
S(5)—S(6)	2·967 (4)	S(7)—S(8)	2·981 (3)
I(1)—I(2)	2·926 (1)	I(1)—I(3)	2·867 (1)

Bond angles within the molecule

C(1)—S(1)—C(3)	94·8 (3)	C(1)—S(2)—C(4)	94·5 (3)
C(2)—S(3)—C(5)	94·4 (3)	C(2)—S(4)—C(6)	94·8 (3)
C(3)—S(5)—C(7)	92·1 (4)	C(4)—S(6)—C(7)	92·4 (4)
C(5)—S(7)—C(8)	92·3 (4)	C(6)—S(8)—C(8)	92·3 (4)
S(1)—C(1)—S(2)	116·0 (3)	S(1)—C(1)—C(2)	122·5 (5)
S(2)—C(1)—C(2)	121·5 (5)	S(3)—C(2)—S(4)	116·0 (3)
S(1)—C(3)—C(4)	116·9 (5)	S(5)—C(3)—C(4)	117·6 (5)
S(2)—C(4)—S(6)	125·0 (5)	S(2)—C(4)—C(3)	117·4 (5)
S(6)—C(4)—C(3)	117·5 (5)	S(3)—C(5)—S(7)	124·4 (5)
S(3)—C(5)—C(6)	117·9 (6)	S(7)—C(5)—C(6)	117·7 (5)
S(4)—C(6)—S(8)	125·0 (5)	S(4)—C(6)—C(5)	116·9 (5)
S(8)—C(6)—C(5)	118·0 (6)	S(5)—C(7)—S(6)	110·3 (4)
S(7)—C(8)—S(8)	109·7 (4)	I(2)—I(1)—I(3)	176·7 (1)

Intermolecular contact distances within the dimer

S(1)—S(4^{i})	3·405 (2)	C(1)—C(2^{i})	3·403 (8)
S(2)—S(3^{i})	3·405 (2)	C(3)—C(6^{i})	3·633 (9)
S(5)—S(8^{i})	3·878 (3)	C(4)—C(5^{i})	3·634 (9)
S(6)—S(7^{i})	3·865 (3)	C(7)—C(8^{i})	4·028 (13)

Intermolecular contact distances between the dimers

S(1)—S(3^{ii})	3·772 (3)	S(3)—S(3^{ii})	3·731 (3)
S(1)—S(7^{ii})	3·625 (2)	S(5)—S(7^{ii})	3·395 (3)

Key to symmetry operations: none x, y, z; (i) $-x, 1-y, -z$; (ii) $-x, 1-y, 1-z$.

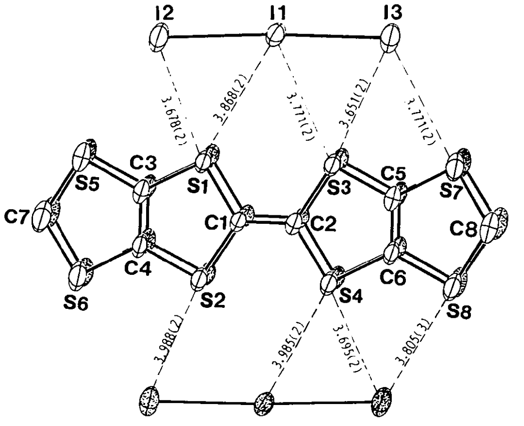

Fig. 1. Molecular arrangement in a coordination pair consisting of BMDT-TTF and I_3 with thermal-ellipsoid plot and numbering scheme. The adjacent coordination pair, which forms an eclipsed BMDT-TTF dimer with the pair, is shown by shaded ellipsoids. The S···I contacts shorter than 4·0 Å are represented by broken lines.

---

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51080 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

bond is 1·382 (8) Å. This bond distance is close to that observed for the +1-charged BMDT-TTF cation in (BMDT-TTF)AsF_6 [1·388 (4) Å (Nigrey, Duesler, Wang & Williams, 1987)] and somewhat larger than that in (BMDT-TTF)SbF_6 (1·361 Å; Kato, Kobayashi & Kobayashi, 1986). The C—S and C=C bond distances of the inner-ring atoms are also in good agreement with those reported by Nigrey *et al.* (1987) within the experimental errors.

Nigrey *et al.* (1987) demonstrated that there is another criterion to judge the charge of the BMDT-TTF cation. This criterion is based upon the ratio of the S···S distances of the outer(S_o)- and inner(S_i)-ring S atoms. The ratio S_o/S_i gives values of 1·014, 1·007, and 0·99 for the +1-, $+\frac{1}{2}$-, and zero-charged cations, respectively. The outer distance is 2·974 (7) and the inner distance 2·938 (4) Å in the present salt. The ratio 1·012 (3) is most close to that of the +1-charged BMDT-TTF cation radical.

Since the triiodide is not located at an inversion center, it is neither centrosymmetric nor linear. The distance I(1)—I(2) is 2·926 (1) Å and I(1)—I(3) is 2·867 (1) Å. The angle I(2)—I(1)—I(3) is 176·7 (1)°. These distances and angles are close to those observed in tetrabutylammonium triiodide (2·941, 2·910 Å, and 174·7°; Herbstein, Kaftory, Kapon & Saenger, 1981). The triiodide in (BMDT-TTF)I_3 would therefore be regarded as a −1-charged anion. This finding together with the fact that BMDT-TTF is a +1-charged cation radical suggests that almost complete one-electron oxidation of BMDT-TTF occurs.

The structure projection onto the (100) plane is shown in Fig. 2. The cation radical and the triiodide anion are aligned side-by-side and hence their long molecular axes are approximately parallel to each other. This side-by-side arrangement results in many S···I contacts of 3·651 (2)–3·868 (2) Å, shorter than the sum of the van der Waals radii (4·0 Å), and forms a coordination pair consisting of BMDT-TTF and triiodide as shown in Fig. 1. Similar short S···I contacts are reported for several iodine salts of BEDT-TTF: ε-(BEDT-TTF)$_4$(I_3)$_2$(I_8) (3·562–3·797 Å; Shibaeva, Lobkovskaya, Yagubskii & Kostyuchenko, 1986*a*), δ-(BEDT-TTF)I_3($C_2H_3Cl_3$)$_{0.333}$ (3·628–3·824 Å; Shibaeva, Lobkovskaya, Kaminskii, Lindemann & Yagubskii, 1986), ζ-(BEDT-TTF)$_2$(I_8)(I_2) (3·787–3·840 Å; Shibaeva, Lobkovskaya, Yagubskii & Kostyuchenko, 1986*b*), and η-(BEDT-TTF)I_3 (3·697–3·799 Å; Shibaeva, Lobkovskaya, Yagubskii & Laukhina, 1987). η-(BEDT-TTF)I_3 is not isostructural to (BMDT-TTF)I_3 employed here, though both salts have 1:1 stoichiometry. In these BEDT-TTF salts short S···I contacts are not found between the central I atom of triiodide and the S atoms of BEDT-TTF. In (BMDT-TTF)I_3, however, the central I atom makes short contacts with the inner-ring S atoms of BMDT-TTF. This discrepancy could be caused by the difference between the molecular geometries of BEDT-TTF and BMDT-TTF. The distance between the outer-ring S atoms is close to that of the inner-ring S atoms in BMDT-TTF ($S_o/S_i = 1{\cdot}012$), whereas the former is much longer than the latter in BEDT-TTF ($S_o/S_i = 1{\cdot}16$; Kato *et al.*, 1985). Therefore, the outer-ring S atoms are more prominent than the inner-ring S atoms for BEDT-TTF. This would be the reason why the inner-ring S atoms of BEDT-TTF do not make contact with the central I atom, while those of BMDT-TTF do.

The cation radicals in a pair form an almost eclipsed face-to-face dimer with mean interplanar distance 3·41 Å as shown in Fig. 1. The direction normal to the cation plane is oriented nearly along the [012] direction as shown in Fig. 2. The closest interplanar S···S contact of 3·405 (2) Å in the dimer [S(1)—S(4$^{\rm i}$) and S(2)—S(3$^{\rm i}$); see Table 2] is significantly shorter than the sum of the van der Waals radii (3·70 Å). This contact is very short compared to that observed in neutral BMDT-TTF (3·80 Å; Kato *et al.*, 1985) and even shorter than that observed in the eclipsed dimer of (BMDT-TTF)$_2$Au(CN)$_2$ (3·635 Å; Nigrey, Morosin, Kwak, Venturini & Baughman, 1986). The S···S contacts in the dimer of (BMDT-TTF)I_3 are rather close to those observed in the eclipsed dimer of tetrathiafulvalenium perchlorate (TTF)ClO_4 [3·347 (3)–3·555 (3) Å (Yakushi, Nishimura, Sugano & Kuroda, 1980)], which exhibits charge-transfer absorption between the TTF^+ cation radicals in the near infrared region (Sugano, Yakushi & Kuroda, 1978). The present compound (BMDT-TTF)I_3 also exhibits an intense absorption band in that region (Sugano & Kinoshita, 1988). Therefore, the short S···S contacts in the dimers of (BMDT-TTF)I_3 probably cause the charge-transfer interaction between the

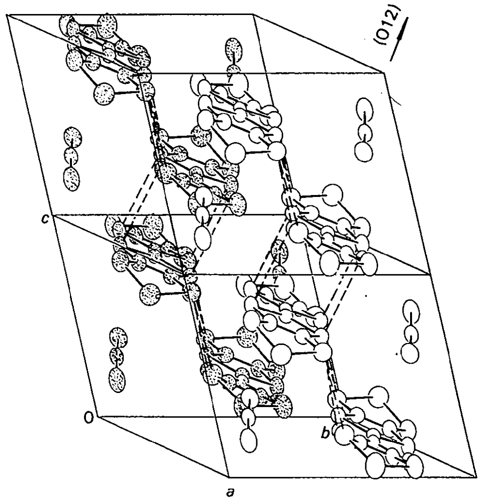

Fig. 2. Projection of the structure onto the (100) plane. The S···S contacts shorter than 3·70 Å are represented by broken lines. Molecules denoted by open ellipsoids lie on the glide plane at $x = 1$ with respect to the shaded molecules.

BMDT-TTF$^+$ cation radicals as in the case of (TTF)ClO$_4$.

The dimers are not isolated from each other but are connected by the side-by-side S···S contacts of 3·395 (3)–3·772 (3) Å. As summarized in Table 2, some side-by-side contacts between the cation radicals in the adjacent dimers are shorter than the sum of the van der Waals radii. The side-by-side contacts are nearly parallel to the direction along the *c* axis as shown in Fig. 2. Hence a one-dimensional array of the dimers extends along the *c* axis. This makes a marked contrast to the two-dimensional network of eclipsed dimers observed in (BMDT-TTF)$_2$Au(CN)$_2$ (Nigrey *et al.*, 1986). The side-by-side coordination of BMDT-TTF$^+$ with I$_3^-$ probably intercepts the extension of the dimer network along the *b* axis as seen in Fig. 2.

The authors are indebted to Professor Gunzi Saito of the Institute for Solid State Physics for kindly providing BMDT-TTF. This work was in part supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture, Japan.

References

HERBSTEIN, F. H., KAFTORY, M., KAPON, M. & SAENGER, W. (1981). *Z. Kristallogr.* **154**, 11–16.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KATO, R., KOBAYASHI, H. & KOBAYASHI, A. (1986). *Chem. Lett.* pp. 2013–2016.

KATO, R., KOBAYASHI, H., KOBAYASHI, A., MORIYAMA, S., NISHIO, Y., KAJITA, K. & SASAKI, W. (1987). *Chem. Lett.* pp. 507–510.

KATO, R., KOBAYASHI, H., KOBAYASHI, A. & SASAKI, Y. (1985). *Chem. Lett.* pp. 1231–1234.

KOBAYASHI, H., KATO, R., KOBAYASHI, A., NISHIO, Y., KAJITA, K. & SASAKI, Y. (1986). *Chem. Lett.* pp. 789–792.

NIGREY, P. J., DUESLER, E., WANG, H. H. & WILLIAMS, J. M. (1987). *Acta Cryst.* C**43**, 1073–1075.

NIGREY, P. J., MOROSIN, B., KWAK, J. F., VENTURINI, E. L. & BAUGHMAN, R. J. (1986). *Synth. Met.* **16**, 1–15.

SAKURAI, T. (1967). *UNICS – Universal Crystallographic Computation Program System.* The Crystallographic Society of Japan, Tokyo, Japan.

SHIBAEVA, R. P., LOBKOVSKAYA, R. M., KAMINSKII, V. F., LINDEMANN, S. V. & YAGUBSKII, E. B. (1986). *Kristallografiya,* **31**, 920–925.

SHIBAEVA, R. P., LOBKOVSKAYA, R. M., YAGUBSKII, E. B. & KOSTYUCHENKO, E. E. (1986*a*). *Kristallografiya,* **31**, 455–461.

SHIBAEVA, R. P., LOBKOVSKAYA, R. M., YAGUBSKII, E. B. & KOSTYUCHENKO, E. E. (1986*b*). *Kristallografiya,* **31**, 1110–1114.

SHIBAEVA, R. P., LOBKOVSKAYA, R. M., YAGUBSKII, E. B. & LAUKHINA, E. E. (1987). *Kristallografiya,* **32**, 901–904.

SUGANO, T. & KINOSHITA, M. (1988). In preparation.

SUGANO, T., YAKUSHI, K. & KURODA, H. (1978). *Bull. Chem. Soc. Jpn,* **51**, 1041–1046.

URAYAMA, H., YAMOCHI, H., SAITO, G., NOZAWA, K., SUGANO, T., KINOSHITA, M., SATO, S., OSHIMA, K., KAWAMOTO, A. & TANAKA, J. (1988). *Chem. Lett.* pp. 55–58.

YAGUBSKII, E. B., SHCHEGOLEV, I. F., LAUKHIN, V. N., KONONOVICH, P. A., KARTSOVNIK, M. V., ZVARYKINA, A. V. & BURAVOV, L. I. (1984). *Pis'ma Zh. Eksp. Teor. Fiz.* **39**, 12–15.

YAGUBSKII, E. B., SHCHEGOLEV, I. F., PESOTSKII, S. I., LAUKHIN, V. N., KONONOVISH, P. A., KARTSOVNIK, M. V. & ZVARYKINA, A. V. (1984). *Pis'ma Zh. Eksp. Teor. Fiz.* **39**, 275–277.

YAKUSHI, K., NISHIMURA, S., SUGANO, T. & KURODA, H. (1980). *Acta Cryst.* B**36**, 358–363.

Acta Cryst. (1988). C**44**, 1767–1770

CI Pigment Yellow 10, 4-[2′,5′-(Dichlorophenyl)hydrazono]-5-methyl-2-phenyl-3*H*-pyrazol-3-one

By A. WHITAKER

Department of Physics, Brunel University, Uxbridge, Middlesex, England

(*Received* 7 *March* 1988; *accepted* 3 *June* 1988)

Abstract. $C_{16}H_{12}Cl_2N_4O$, M_r = 347·2, triclinic, $P\bar{1}$, a = 8·879 (3), b = 9·073 (2), c = 10·021 (2) Å, α = 95·25 (2), β = 75·26 (2), γ = 94·09 (2)°, V = 776·5 (5) Å^3, Z = 2, D_m = 1·478 (5), D_x = 1·485 (1) Mg m^{-3}, $F(000)$ = 356, Cu $K\alpha$, λ = 1·54184 Å, μ = 3·70 mm^{-1}, room temperature. R = 6·5% for 2913 independent intensities. The molecule exists as the hydrazone tautomer and there are three intramolecular hydrogen bonds, one of which is very weak. These hydrogen bonds keep the molecule approximately planar. The molecules are linked by van der Waals forces into columns parallel to **a**.

Introduction. This paper is concerned with the crystal and molecular structure of an azo-pigment and with the long-term aim of relating colour and crystal structure in pigments.

The present compound, CI Pigment Yellow 10 (CI No. 12710), is a commercially available pigment used for printing inks of all types, emulsion paints and

0108-2701/88/101767-04$03.00