

Structures of 7,10-Diphenylfluoranthene and 7,14-Diphenylacenaphtho[1,2-*k*]fluoranthene

BY WILLIAM H. WATSON* AND RAM P. KASHYAP

Department of Chemistry, Texas Christian University, Fort Worth, Texas 76129, USA

AND BENJAMIN F. PLUMMER AND WILLIAM GREGORY REESE

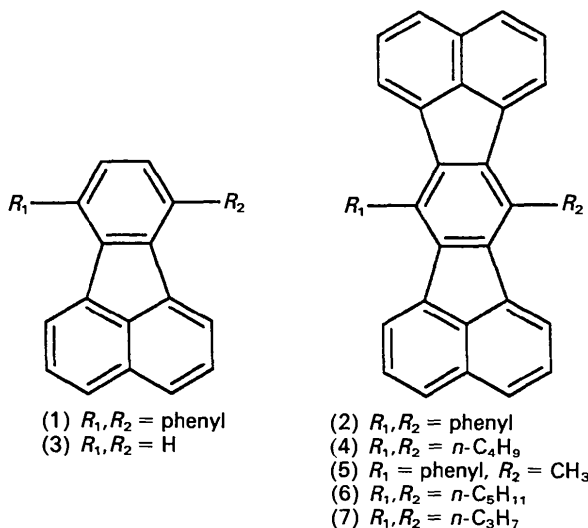
Department of Chemistry, Trinity University, San Antonio, Texas 78212, USA

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Abstract. 7,10-Diphenylfluoranthene (1), $C_{28}H_{18}$, $M_r = 354.45$, triclinic, $P\bar{1}$, $a = 10.657$ (2), $b = 13.019$ (2), $c = 14.535$ (2) Å, $\alpha = 101.01$ (1), $\beta = 90.90$ (1), $\gamma = 108.01$ (1)°, $V = 1876.4$ (4) Å³, $Z = 4$, $D_x = 1.254$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.66$ cm⁻¹, $F(000) = 744$, $T = 298$ K, $R = 0.0663$ for 5106 reflections. 7,14-Diphenylacenaphtho[1,2-*k*]fluoranthene (2), $C_{38}H_{22}$, $M_r = 478.60$, orthorhombic, $Abam$ ($Cmca$), $a = 13.752$ (8), $b = 7.877$ (5), $c = 22.907$ (16) Å, $V = 2481$ (2) Å³, $Z = 4$, $D_x = 1.281$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.68$ cm⁻¹, $F(000) = 1000$, $T = 298$ K, $R = 0.0552$ for 1287 reflections. The fluoranthene moieties in the two independent molecules of (1) are significantly nonplanar (0.07 and 0.09 Å r.m.s.d.) with the phenyl rings containing the diphenyl substituents slightly folded [7.9 (6) and 9.0 (6)°] to minimize steric interactions and strain energies. Molecular mechanics reproduces the observed deviations from planarity. The acenaphtho[1,2-*k*]fluoranthene moiety in (2) is planar (0.009 Å r.m.s.d.) and the phenyl substituents are twisted out of the plane by 77.3 (4)°. Molecular-mechanics calculations indicate that the molecule should distort from planarity more than (1); however, the thermal parameters are consistent with a rigidly planar molecule.

Introduction. As part of a program to investigate the effects of strain in π -electron systems, we have examined the diphenyl derivatives of fluoranthene (1) and acenaphtho[1,2-*k*]fluoranthene (2). The structures of fluoranthene (3) (Hazell, Jones & Sowden, 1977) and acenaphtho[1,2-*k*]fluoranthene derivatives (4)–(7) (Seth & Chakraborty, 1981, 1982, 1983; Seth, Sur & Chakraborty, 1988) have been reported. These authors report alternation of bond lengths around the naphthalene rings, small but significant deviations from planarity of the fluoranthene moieties, and expansion and contraction of specific bond

angles due to transmission of strain related to the mode of fusion of the five-membered ring.



Experimental. All data were collected on a Nicolet $R3m/\mu$ update of a $P2_1$ diffractometer. Unit-cell parameters were obtained by a least-squares refinement of 25 reflections. Intensity data were collected in the ω mode with a variable scan rate of 4 to 29.3° min⁻¹ using graphite-monochromated Mo $K\alpha$ radiation. Lorentz and polarization corrections were made, and ψ -scan-based empirical absorption corrections were applied. The intensities of standard reflections varied by a maximum of $\pm 1\%$. The structures were solved by direct methods and refined by a block-cascade least-squares technique. H atoms were located in difference maps, and were refined with isotropic thermal parameters; $\sum w(|F_o| - |F_c|)^2$ minimized with $w = [\sigma^2(F_o) + gF_o^2]^{-1}$. Crystal and refinement data are presented in Table 1. All computer programs supplied by Nicolet (Nicolet Instrument Corporation, 1986) for Desktop 30 Microclipse and NOVA 4/C configuration; atomic

* Author to whom correspondence should be addressed.

Table 1. *Crystal and refinement data*

	(1)	(2)
Color	Light yellow	Pale yellow
Crystal size (mm)	0.38 × 0.25 × 0.15	0.38 × 0.25 × 0.25
2θ range for data collection (°)	3–55	3–55
2θ range for lattice parameters (°)	23.05–28.78	22.88–27.92
Systematic extinctions	None	$hkl, k + l = 2n + 1$ $0kl, k, l = 2n + 1$ $h0l, h, l = 2n + 1$
Space group	$P\bar{1}$	$Abam (Cmca)$
Monitored reflections	$\bar{1}\bar{1}4, 1\bar{4}\bar{5}$	$\bar{3}20, 4\bar{1}\bar{1}$
hkl range	0,13; –16,16; –18,18	0,17;0,10; –6,29
Number of reflections measured	9069	2097
Number of unique reflections	8611	1882
R_{int}	0.004	0.007
Number with $I \geq 3\sigma(I)$	5106	1287
Transmission factors	0.848–0.897	0.845–0.876
Number of parameters	650	114
R	0.0663	0.0552
wR	0.0455	0.0493
R (all data)	0.1149	0.0803
wR (all data)	0.0493	0.0512
S	1.506	1.656
$(\Delta/\sigma)_{max}$	0.036	0.057
Max. electron density ($e \text{ \AA}^{-3}$)	0.24	0.25
Min. electron density ($e \text{ \AA}^{-3}$)	–0.23	–0.26
g (weight)	0.00007	0.00017
x (isotropic extinction parameter)*	0.0022 (1)	0.00026 (5)

$$*F = F_c/[1.0 + (x)0.002F_c^2/\sin(2\theta)]^{0.25}$$

scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV). Tables 2 and 3 give the atomic positional parameters for (1) and (2) while Tables 4 and 5 list selected interatomic distances and valence angles. Figs. 1 and 2 are drawings of the two compounds.* *PCMODEL* (1989) was used for all molecular-mechanics calculations.

Discussion. A least-squares plane fitted to the acenaphtho[1,2-*k*]fluoranthene moiety in (2) exhibits an r.m.s.d. of 0.009 Å while the fluoranthene moieties in the two independent molecules of (1) deviate considerably more from planarity (0.07 and 0.09 Å r.m.s.d.). In (1), C(27) and C(28) show the greatest deviations from the mean plane. Least-squares planes fitted to the fluoranthene molecule omitting these atoms give r.m.s.d.'s of 0.02 to 0.04 Å. The phenyl rings are folded along C(12)⋯C(20) with angles of 7.9 (6) and 9.0 (6)°, MM (molecular-mechanics) calculations reproduce reasonably well the deviations from planarity in (1a) and (1b) (see

* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors for (1) and (2) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53719 (71 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$) for (1)*

	x	y	z	U
Molecule (1a)				
C(1)	11497 (2)	4063 (2)	6220 (1)	39 (1)
C(2)	10538 (2)	4607 (2)	6395 (1)	39 (1)
C(3)	10917 (3)	5619 (2)	6982 (2)	51 (1)
C(4)	12219 (3)	6054 (2)	7413 (2)	58 (1)
C(5)	13119 (3)	5510 (2)	7273 (2)	56 (1)
C(6)	12782 (2)	4468 (2)	6652 (2)	46 (1)
C(7)	13597 (2)	3795 (2)	6402 (2)	54 (1)
C(8)	13115 (3)	2816 (2)	5776 (2)	54 (1)
C(9)	11812 (2)	2432 (2)	5338 (2)	48 (1)
C(10)	11004 (2)	3067 (2)	5550 (1)	39 (1)
C(11)	9628 (2)	2976 (2)	5259 (1)	38 (1)
C(12)	8719 (2)	2204 (2)	4573 (1)	41 (1)
C(13)	9083 (2)	1347 (2)	3905 (1)	43 (1)
C(14)	10118 (2)	1678 (2)	3347 (2)	51 (1)
C(15)	10491 (3)	923 (3)	2716 (2)	64 (1)
C(16)	9834 (3)	–180 (3)	2626 (2)	72 (1)
C(17)	8800 (3)	–522 (2)	3157 (2)	77 (1)
C(18)	8419 (3)	237 (2)	3803 (2)	59 (1)
C(19)	9317 (2)	3880 (2)	5815 (1)	39 (1)
C(20)	8048 (2)	3953 (2)	5747 (2)	42 (1)
C(21)	7621 (2)	4814 (2)	6366 (2)	42 (1)
C(22)	7010 (2)	5456 (2)	5992 (2)	49 (1)
C(23)	6610 (3)	6246 (2)	6571 (2)	61 (1)
C(24)	6798 (2)	6404 (2)	7529 (2)	60 (1)
C(25)	7382 (3)	5763 (2)	7913 (2)	61 (1)
C(26)	7792 (2)	4972 (2)	7338 (2)	54 (1)
C(27)	7120 (2)	3143 (2)	5075 (2)	52 (1)
C(28)	7459 (2)	2314 (2)	4487 (2)	51 (1)
Molecule (1b)				
C(1)	4300 (2)	2039 (2)	9998 (1)	41 (1)
C(2)	5634 (2)	2463 (2)	9806 (2)	41 (1)
C(3)	5935 (2)	3213 (2)	9233 (2)	53 (1)
C(4)	4901 (3)	3495 (2)	8839 (2)	65 (1)
C(5)	3610 (3)	2034 (2)	8987 (2)	66 (1)
C(6)	3257 (2)	2274 (2)	9589 (2)	48 (1)
C(7)	1975 (2)	1717 (2)	9820 (2)	54 (1)
C(8)	1812 (2)	998 (2)	10412 (2)	51 (1)
C(9)	2890 (2)	790 (2)	10836 (2)	44 (1)
C(10)	4146 (2)	1324 (2)	10636 (1)	38 (1)
C(11)	5493 (2)	1318 (2)	10898 (1)	36 (1)
C(12)	5957 (2)	838 (2)	11546 (1)	38 (1)
C(13)	5130 (2)	303 (2)	12248 (1)	42 (1)
C(14)	4367 (3)	827 (2)	12795 (2)	58 (1)
C(15)	3634 (3)	348 (3)	13468 (2)	79 (2)
C(16)	3677 (3)	–656 (3)	13608 (2)	87 (2)
C(17)	4439 (3)	–1174 (2)	13085 (2)	75 (1)
C(18)	5168 (2)	–699 (2)	12410 (2)	54 (1)
C(19)	6386 (2)	1957 (2)	10338 (1)	37 (1)
C(20)	7708 (2)	2023 (2)	10365 (1)	39 (1)
C(21)	8657 (2)	2611 (2)	9752 (2)	41 (1)
C(22)	9788 (2)	3455 (2)	10136 (2)	52 (1)
C(23)	10679 (3)	3992 (2)	9564 (2)	62 (1)
C(24)	10452 (3)	3678 (2)	8603 (2)	62 (1)
C(25)	9337 (3)	2830 (2)	8209 (2)	60 (1)
C(26)	8449 (2)	2298 (2)	8780 (2)	50 (1)
C(27)	8157 (2)	1501 (2)	10998 (2)	43 (1)
C(28)	7302 (3)	931 (2)	11570 (2)	44 (1)

Table 3. *Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$) for compound (2)*

U is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U
C(1)	6113 (2)	1178 (3)	0	44 (1)
C(2)	5857 (1)	2065 (2)	510 (1)	44 (1)
C(3)	6063 (1)	1351 (2)	1040 (1)	52 (1)
C(4)	6525 (1)	–261 (2)	1049 (1)	58 (1)
C(5)	6770 (1)	–1114 (3)	553 (1)	58 (1)
C(6)	6570 (2)	–414 (3)	0	50 (1)
C(19)	5403 (1)	3664 (2)	310 (1)	42 (1)
C(20)	5000	5000	631 (1)	43 (1)
C(21)	5000	5000	1275 (1)	45 (1)
C(22)	5830 (1)	5404 (2)	1587 (1)	59 (1)
C(23)	5831 (2)	5405 (3)	2188 (1)	74 (1)
C(24)	5000	5000	2587 (2)	83 (1)

Table 4. Bond distances (Å) for (1) and (2)

	(1a)	(1b)	(2)
C(1)—C(2)	1.413 (4)	1.410 (3)	1.407 (2)
C(1)—C(6)	1.396 (3)	1.394 (4)	1.403 (3)
C(1)—C(10)	1.410 (3)	1.411 (3)	—
C(2)—C(3)	1.362 (3)	1.369 (4)	1.367 (3)
C(2)—C(19)	1.483 (3)	1.475 (4)	1.479 (2)
C(3)—C(4)	1.411 (4)	1.409 (4)	1.420 (2)
C(4)—C(5)	1.355 (4)	1.359 (4)	1.361 (3)
C(5)—C(6)	1.415 (3)	1.413 (4)	1.410 (2)
C(6)—C(7)	1.419 (4)	1.414 (3)	—
C(7)—C(8)	1.362 (3)	1.364 (4)	—
C(8)—C(9)	1.415 (3)	1.415 (4)	—
C(9)—C(10)	1.367 (4)	1.370 (3)	—
C(10)—C(11)	1.483 (3)	1.481 (3)	—
C(11)—C(12)	1.389 (3)	1.388 (3)	—
C(11)—C(19)	1.425 (3)	1.433 (3)	1.421 (3)*
C(12)—C(13)	1.484 (3)	1.490 (3)	—
C(12)—C(28)	1.399 (4)	1.401 (3)	—
C(13)—C(14)	1.389 (3)	1.484 (4)	—
C(13)—C(18)	1.376 (3)	1.381 (4)	—
C(14)—C(15)	1.369 (4)	1.382 (4)	—
C(15)—C(16)	1.369 (4)	1.375 (5)	—
C(16)—C(17)	1.365 (4)	1.361 (5)	—
C(17)—C(18)	1.390 (4)	1.381 (4)	—
C(19)—C(20)	1.389 (3)	1.384 (3)	1.398 (2)
C(20)—C(21)	1.489 (3)	1.487 (3)	1.475 (3)
C(20)—C(27)	1.405 (3)	1.401 (4)	—
C(21)—C(22)	1.389 (4)	1.388 (3)	1.384 (4)
C(21)—C(26)	1.385 (4)	1.377 (3)	—
C(22)—C(23)	1.383 (4)	1.380 (4)	1.377 (3)
C(23)—C(24)	1.371 (5)	1.373 (3)	1.370 (3)
C(24)—C(25)	1.370 (4)	1.373 (4)	—
C(25)—C(26)	1.379 (4)	1.386 (4)	—
C(27)—C(28)	1.388 (4)	1.384 (3)	—

* C(11) = C(19B).

Table 5. Selected valence angles (°) for (1) and (2)

	(1a)	(1b)	(2)*
C(2)—C(1)—C(6)	124.1 (2)	124.1 (2)	123.8 (1)
C(2)—C(1)—C(10)	111.9 (2)	111.8 (2)	112.4 (2)
C(6)—C(1)—C(10)	124.0 (2)	124.1 (2)	—
C(1)—C(2)—C(3)	117.8 (2)	117.9 (2)	118.8 (2)
C(1)—C(2)—C(19)	106.1 (2)	106.2 (2)	105.7 (1)
C(2)—C(3)—C(4)	119.1 (3)	118.8 (2)	118.2 (2)
C(3)—C(4)—C(5)	122.9 (2)	122.7 (3)	122.7 (2)
C(4)—C(5)—C(6)	120.1 (2)	120.3 (3)	120.5 (2)
C(1)—C(6)—C(5)	116.0 (2)	115.9 (2)	115.9 (1)
C(1)—C(6)—C(7)	116.1 (2)	116.1 (2)	—
C(5)—C(6)—C(7)	127.9 (2)	127.9 (3)	128.2 (2)
C(6)—C(7)—C(8)	120.2 (2)	120.2 (2)	—
C(7)—C(8)—C(9)	122.6 (3)	122.7 (2)	—
C(8)—C(9)—C(10)	118.9 (2)	118.7 (2)	—
C(1)—C(10)—C(9)	118.3 (2)	118.1 (2)	—
C(1)—C(10)—C(11)	105.9 (2)	106.3 (2)	—
C(10)—C(11)—C(12)	130.5 (2)	132.0 (2)	—
C(10)—C(11)—C(19)	108.1 (2)	107.4 (2)	—
C(12)—C(11)—C(19)	121.4 (2)	120.7 (2)	—
C(11)—C(12)—C(13)	122.0 (2)	123.8 (2)	—
C(11)—C(12)—C(28)	117.2 (2)	117.1 (2)	—
C(13)—C(12)—C(28)	120.7 (2)	119.0 (2)	—
C(2)—C(19)—C(11)	107.6 (2)	108.0 (2)	108.1 (1)
C(2)—C(19)—C(20)	131.8 (2)	131.2 (2)	130.2 (2)
C(11)—C(19)—C(20)	120.6 (2)	120.9 (2)	121.7 (1)
C(19)—C(20)—C(21)	123.4 (2)	123.1 (2)	121.7 (1)
C(19)—C(20)—C(27)	117.4 (2)	117.8 (2)	116.6 (2)
C(27)—C(20)—C(21)	119.2 (2)	119.1 (2)	—

* Some atom labels are generated by symmetry operations, i.e. C(10) = C(12A).

fluoranthene moieties in compounds (3)–(7) (Hazell, Jones & Sowden, 1977; Seth & Chakraborty, 1981, 1982, 1983; Seth, Sur & Chakraborty, 1988). Expansion of the C(5)C(6)C(7) angles to 127.9 (3)° and the compression of the C(11)C(12)C(28) and C(19)C(20)C(27) angles to 117.1 (2)–117.8 (2)° in (1a) and (1b) are consistent with those observed in (3)–(7). This has been attributed to the transmission of strain from the fusion of the five-membered ring.

In (2), all chemically equivalent bonds are symmetry related and are identical. They are statistically equivalent to the bonds in (1a) and (1b). MM calculations (Table 6) indicate that strain and steric interactions should lead to greater deviations from planarity for the acenaphtho[1,2-*k*]fluoranthene. In fact, constraints must be placed upon the model to prevent twisting along the C(1)⋯C(1a) direction. The planar conformation is calculated to be about 47 kJ mol⁻¹ higher in energy than the twisted conformation.

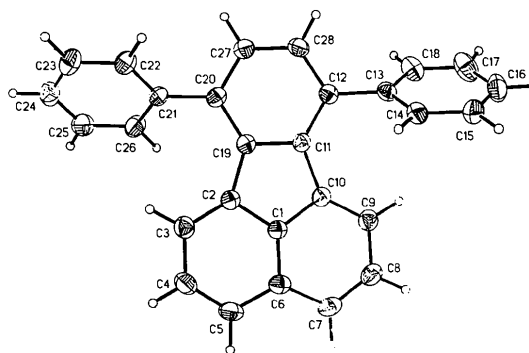


Fig. 1. Drawing of (1a) with thermal ellipsoids shown at the 30% probability level. H atoms are represented by spheres of arbitrary size.

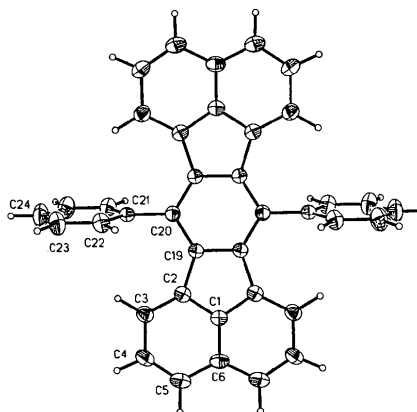


Fig. 2. Drawing of (2) with thermal ellipsoids shown at the 30% probability level. H atoms are represented by spheres of arbitrary size.

Table 6). The internal consistency of these deviations in (1a) and (1b) and the correlation with MM calculations indicate that the deviations are real and strain related. The bond lengths in the two independent molecules of (1) are internally consistent with excellent agreement between chemically equivalent bonds, and they are in very good agreement with the

Table 6. *Least-squares planes and interplanar angles for (1) and (2) and the results of molecular-mechanics calculations*

Plane	(1a) r.m.s.d. (Å)	(1b) r.m.s.d. (Å)	(2) r.m.s.d. (Å)
A = C(1)C(2)C(3)C(4)C(5)C(6)	0.012	0.016	0.000
B = C(1)C(6)C(7)C(8)C(9)C(10)	0.009	0.010	—
C = C(1)C(10)C(11)C(19)C(2)	0.022	0.025	0.002
D = C(1)C(12)C(19)C(20)C(27)C(28)	0.022	0.017	0.000
E = C(13)C(14)C(15)C(16)C(17)C(18)	0.005	0.006	—
F = C(21)C(22)C(23)C(24)C(25)C(26)	0.005	0.004	0.009

Angle	(1a) (°)*	(1b) (°)	MM (°)	(2) (°)	MM (°)
A,B	1.9	2.2	1.2	0.0	3.5
A,C	3.6	3.3	3.5	0.2	1.5
B,C	2.4	4.3	—	—	1.9
C,D	4.8	4.9	4.8	1.4	8.0
D,E	57.6	48.3	60	—	39†
D,F	52.9	58.0	—	77.3	39
E,F	70.1	74.9	60	0.0	0

* Standard deviations in angles 0.5–0.8°.

† The angle is 90° if the π system is forced to be planar.

The shortest intramolecular contacts involving the substituent phenyl rings are H(3)⋯C(26) = 2.70 (4) Å and 2.72 (4) Å and H(9)⋯C(14) = 2.68 (4) Å and

2.66 (4) Å for (1a) and (1b) and H(3)⋯C(22) = 2.76 (4) Å for (2).

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Structure of Di(*S*-methylthiuronium)–Tri(7,7,8,8-tetracyano-*p*-quinodimethane) Dihydrate, (MT)₂(TCNQ)₃·2H₂O*

BY O. A. USOV, I. A. BURSHEIN, N. F. KARTENKO, I. V. ROZHDESTVENSKAYA, R. M. VLASOVA, V. N. SEMKIN, G. G. ABASHEV AND V. S. RUSSKIKH

A. F. Ioffe Physico-Technical Institute, Academy of Sciences of the USSR, Polytechnic str. 26, Leningrad 194021, USSR

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Abstract. (C₂H₇N₂S)₂(C₁₂H₄N₄)₃·2H₂O, *M_r* = 831.0, triclinic, *P*1̄, *a* = 8.033 (2), *b* = 13.002 (3), *c* = 9.895 (3) Å, α = 94.32 (2), β = 108.12 (2), γ = 88.90 (3)°, *V* = 979.4 (6) Å³, *Z* = 1, *D_x* = 1.141 g cm⁻³, λ (Mo *K* α) = 0.71069 Å, μ = 2.0 cm⁻¹, *F*(000) = 430, room temperature, *R* = 0.039 for 1928 observed reflections. The structure contains stacks of planar TCNQ radical anions located as trimers with a distance of 3.17 Å between molecules in trimers and 3.33 Å between neighbouring trimers. The central molecule of a trimer is centrosymmetric and has a charge of about -0.9 e; the charge of the non-centrosymmetric molecules is about -0.4 e. Hydrogen bonds connect cations, water molecules and anions and have an unusual effect on the anion

packing. Among the known trimerized TCNQ salts (MT)₂(TCNQ)₃·2H₂O has the highest electrical conductivity.

Introduction. As part of our continuing study of conducting organic materials, a new TCNQ salt of *S*-methylthiuronium was grown. The simple MT–TCNQ salt, prepared and studied earlier, exhibits low electrical conductivity due to the presence of isolated TCNQ radical anion pairs. The structure and some physical properties of the new conducting salt, (MT)₂(TCNQ)₃·2H₂O, are reported below.

Experimental. Black plate-like crystals of (MT)₂(TCNQ)₃·2H₂O were grown from a mixture of 5 cm³ ethanolic thiuronium iodide solution (1.1 mmol) and 20 cm³ boiling solution of TCNQ in acetonitrile (1 mmol). This mixture was left exposed

* TCNQ = 2,2'-(2,5-cyclohexadiene-1,4-diyliidene)bispropane-dinitrile.