

0(mod 4). On the other hand:

$$\begin{aligned}\Sigma^* &= 3\mu m^2 + dn^2 \\ &= 3\mu(8p+1) + d(8p+1) \\ &= 4[\pi + \mu(2p+1)] \equiv 0(\text{mod } 4)\end{aligned}$$

[where  $(8p+1)$  means 'a multiple of  $p$  plus one', which implies  $\alpha_i = 4$ .

Finally when the condition (A2) is fulfilled,  $\alpha_i$  may be 1 or 4.

Let us now consider the case where the numbers  $3\mu m^2$  and  $dn^2$  are not relatively prime. The existence of a common factor may be obtained from one or more of the following cases (a last case is excluded according to the relation A1):

$$\begin{array}{ll}(i) (3, d) \div 3 & (iv) (3, n) \div 3 \\ (ii) (\mu, d) \div q & (v) (\mu, n) \div p \\ (iii) (m, d) \div t & q, p, t \neq t.\end{array} \quad (A7)$$

We shall examine every condition (31) as an independent one.

(i)  $(3, d) \div 3$ . Since  $3|d$  and 3 should divide  $r_{33}^*$  we have  $3|2w^2\mu n^2$  which means  $3|w$ , then we have

$$3|u^2 + v^2 - uv \quad (A8)$$

or  $3|v$ . The last condition leads to the fact  $k = 3$  and in particular this  $k$  value is a factor of  $v$ . The condition (A8) implies  $3|(u+v)^2 - 3uv$  from which we have  $u+v \equiv 0(\text{mod } 3)$ . On the other hand,  $2u - v + v + u = 3u \equiv 0(\text{mod } 3)$  which implies  $2u - v \equiv 0(\text{mod } 3)$  and also  $2v - u \equiv 0(\text{mod } 3)$ , thus the  $r_{ij}^*$  elements are of the form  $0(\text{mod } 3)$  which implies  $\alpha_i = 3$ . Taking into account the case  $\alpha_i = 4$  which is fulfilled for the conditions  $u$  and  $v \equiv 0(\text{mod } 2)$  and  $m$  and  $n \equiv 1(\text{mod } 2)$  we have that  $\alpha_i$  may have the value 12.

(ii)  $(\mu, d) = q$ . We shall prove that  $k$  may have the value  $q$  which in particular is a factor of  $\mu$ . Since  $d \equiv 0(\text{mod } q)$  and since  $\mu w^2 \equiv 0(\text{mod } q)$  from (14) we have

$$u^2 + v^2 - uv \equiv 0(\text{mod } q), \quad (A9)$$

taking into account the condition (13b). For (A9), if  $(u, v) \div 1$  then  $q$  may be only 3, and  $k = 3$ ; in particular 3 is a factor of  $\mu$ . If  $u$  and  $v$  are not relatively prime then  $k = q$  if  $(u, v) = q$ .

(iii)  $(m, d) \div t$ . From the  $r_{33}^*$  element we may see that  $t|2w$ . The case  $t = 2$  implies  $u$  and  $v \equiv 0(\text{mod } 2)$  (from  $r_{12}^*$  and  $r_{21}^*$ ) but since  $d \equiv 0(\text{mod } t)$  we have  $w \equiv 0(\text{mod } 2)$  which is improper, or  $\mu \equiv 0(\text{mod } 2)$ . The last condition implies  $k = 2$ . The condition  $t|w$  together with the condition  $d \equiv 0(\text{mod } t)$  implies  $t|u^2 + v^2 - uv$  or  $t|v$ . The first of these two conditions may be fulfilled if  $t = 3$  and  $(u, v) \div 1$  a known value of  $\alpha_i$ . Any other condition implies the improper relation  $(u, v, w) \div t$ . The case  $t|v$  implies  $k = t$  as may be easily seen from (25).

(iv) The condition  $(3, n) \div 3$  implies  $\alpha_i = 3$  since all the matrix elements become of the form  $0(\text{mod } 3)$ .

(v) The condition  $(\mu, n) \div p$  implies  $k = p$  since all the  $r_{ij}^*$  elements become of the form  $0(\text{mod } p)$ .

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*Acta Cryst.* (1982). **A38**, 557–558

**Intermolecular energy, structure and stability of regular stacks of tetrathiafulvalene (TTF) and tetracyanoquinodimethane (TCNQ): erratum.** By H. A. J. GOVERS, *General Chemistry Laboratory, Chemical Thermodynamics Group, State University of Utrecht, Padualaan 8, 3508 TB Utrecht, The Netherlands*

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#### Abstract

Previous calculations of the stack structure of TTF and TCNQ by Govers [*Acta Cryst.* (1981), **A37**, 529–535] are corrected for a program error.

#### New results

During our calculation of the three-dimensional crystalline structure of TTF–TCNQ (Govers, 1982) we met a venomous program error. This error proved important only

Table 2. *Intermolecular van der Waals plus repulsive stack energies and structures of regular TTF and TCNQ stacks (corrected)*

Stack	Atom-atom potentials*	$E$ (kJ mol <sup>-1</sup> )†	$R$ (Å)	$\varepsilon$ (Å)	$\delta$ (Å)	$\chi$ (°)	$b$ (Å)‡
TTF lsl	Set 1	$-55.73 \pm 0.08$ <u><math>-55.3</math></u>	$3.55 \pm 0.02$ <u><math>3.51 \pm 0.11</math></u>	$0.05 \pm 0.05$ <u><math>0.12 \pm 0.12</math></u>	$1.1 \pm 0.3$ <u><math>1.60 \pm 0.2</math></u>	0.0 0.0	$3.72 \pm 0.12$ <u><math>3.90 \pm 0.15</math></u>
ecl		$-54.39 \pm 0.04$ § <u><math>-54.5</math></u>	<u><math>3.62 \pm 0.01</math></u> § <u><math>3.59 \pm 0.04</math></u>	0.0 <u><math>0.0 \pm 0.05</math></u>	0.0 <u><math>0.0 \pm 0.05</math></u>	0.0	<u><math>3.62 \pm 0.01</math></u> <u><math>3.59 \pm 0.04</math></u>
(ecl)		$-56.77 \pm 0.04$	$3.52 \pm 0.01$	0.0	0.0	36 ± 1	<u><math>3.52 \pm 0.01</math></u>
TCNQ lsl	Set 1	$-57.80 \pm 0.04$ <u><math>-55.3</math></u>	$3.46 \pm 0.01$ <u><math>3.30 \pm 0.13</math></u>	$0.1 \pm 0.1$ <u><math>0.04 \pm 0.04</math></u>	$1.21 \pm 0.01$ <u><math>2.02 \pm 0.20</math></u>	0.0 0.0	$3.67 \pm 0.02$ <u><math>3.84 \pm 0.06</math></u>
tsl		<u><math>-53.3</math></u>	<u><math>3.44 \pm 0.05</math></u>	<u><math>1.01 \pm 0.15</math></u>	<u><math>0.16 \pm 0.12</math></u>	0.0	<u><math>3.57 \pm 0.05</math></u>
(ecl)		$-57.65 \pm 0.4$	$3.46 \pm 0.01$	0.0	$0.4 \pm 0.1$	22 ± 1	<u><math>3.48 \pm 0.01</math></u>
TTF-TCNQ lsl	Set 1	<u><math>-46.5</math></u> ¶	<u><math>3.55</math></u> ¶	<u><math>0.24</math></u> ¶	<u><math>2.82</math></u> ¶	0.0¶	<u><math>4.54</math></u> ¶
ecl		$-59.04 \pm 0.04$	$3.50 \pm 0.01$	0.0	0.0	0.0	$3.50 \pm 0.01$

\* Set 1 from Table 1 (Govers, 1978).

† Results obtained *via* kcal mol<sup>-1</sup>  $\equiv$  4.19 kJ mol<sup>-1</sup> using set 1 (Govers, 1978).‡ Calculated *via* (5), except for the experimental values (underlined).§ No true minimum;  $E(R)$  minimized for an eclipse stack ( $\delta = \varepsilon = \chi = 0.0$ ).¶ Value for DMDBTTF-TCNQ.

for the calculations applying set 1 by Govers (1978) with its short summation limits. Therefore all calculations by Govers (1981) which apply set 1 were performed again after correction of the program error.

The new results for set 1 are given in a new Table 2. We remark that also the old Figs. 2(a)-(e) are partly incorrect.

From Table 2 we infer the following corrections for our previous conclusions concerning set 1. The absolute minimum for the TTF segregated stack now is accompanied with the pseudo-eclipsed stack ( $\chi = 36^\circ$ ). The mixed stack now only shows an eclipsed minimum. However, the local minima, TTF slipped longitudinally and pseudo-eclipsed TCNQ (a new result), are less stable only up to 1 kJ mol<sup>-1</sup>.

The mixed stack now is 1.7 kJ mol<sup>-1</sup> more stable than the mean segregated one.

A comparison of the structural parameters calculated *via* set 1 with their observed values shows serious deviations of  $-0.5$  to  $-0.8$  Å for the longitudinal slip,  $\delta$ .

A comparison of the results obtained *via* set 1 with those *via* set 2 now shows a growing consistency. Only the local and absolute minima for TCNQ are interchanged.

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## International Union of Crystallography

*Acta Cryst.* (1982). A **38**, 558-559

### Bibliography of Mathematical Crystallography

For many years Professor W. Nowacki of the University of Bern has kept, for his own purposes, a bibliography of mathematical crystallography. In the late 1970's he agreed to make this generally available to interested crystallographers and it had been hoped that it would have been made available on demand as a booklet. However, in view of the high cost of publication, it has instead been decided to make available photocopies of specific sections of Professor Nowacki's typescript on request. In total there are about 4750 references on 286 pages. The sections are as follows:

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2. *Space groups of  $E^1$  ( $E = \text{Euclidean space}$ )* (2 pages; 25 references)
3. *Space groups of  $E^2$*  (5 pages; 90 references)
4. *Space groups of  $E^3$*  (12 pages; 190 references)

5. *Nomenclature, Tables* (3 pages; 46 references)
6. *Space groups of  $E^4$*  (4 pages; 60 references)
7. *Space groups of  $E^n$  ( $n \geq 5$ )* (6 pages; 94 references)
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17. *Packings of circles (and of other polygons)* (2 pages; 25 references)
18. *Packings of spheres (and of other polyhedra)* (14 pages; 233 references)