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^{-1})†	R (Å)	ε (Å)	δ (Å)	χ (°)	b (Å)‡
TTF lsl	Set 1	−55·73 ± 0·08	3·55 ± 0·02	0·05 ± 0·05	1·1 ± 0·3	0·0	3·72 ± 0·12
		−55·3	3·51 ± 0·11	0·12 ± 0·12	1·60 ± 0·2	0·0	3·90 ± 0·15
ecl		−54·39 ± 0·04§	3·62 ± 0·01§	0·0	0·0	0·0	3·62 ± 0·01
		−54·5	3·59 ± 0·04	0·0 ± 0·05	0·0 ± 0·05	0·0	3·59 ± 0·04
(ecl)		−56·77 ± 0·04	3·52 ± 0·01	0·0	0·0	36 ± 1	3·52 ± 0·01
TCNQ lsl	Set 1	−57·80 ± 0·04	3·46 ± 0·01	0·1 ± 0·1	1·21 ± 0·01	0·0	3·67 ± 0·02
		−55·3	3·30 ± 0·13	0·04 ± 0·04	2·02 ± 0·20	0·0	3·84 ± 0·06
tsl		−53·3	3·44 ± 0·05	1·01 ± 0·15	0·16 ± 0·12	0·0	3·57 ± 0·05
(ecl)		−57·65 ± 0·4	3·46 ± 0·01	0·0	0·4 ± 0·1	22 ± 1	3·48 ± 0·01
TTF–TCNQ lsl	Set 1	−46·5¶	3·55¶	0·24¶	2·82¶	0·0¶	4·54¶
ecl		−59·04 ± 0·04	3·50 ± 0·01	0·0	0·0	0·0	3·50 ± 0·01

* Set 1 from Table 1 (Govers, 1978).
† Results obtained *via* kcal mol^{-1} ≡ 4·19 kJ mol^{-1} using set 1 (Govers, 1978).
‡ Calculated *via* (5), except for the experimental values (underlined).
§ No true minimum; $E(R)$ minimized for an eclipse stack ($\delta = \varepsilon = \chi = 0{\cdot}0$).
¶ 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 ($\chi = 36°$). 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^{-1}. The mixed stack now is 1·7 kJ mol^{-1} 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, δ.

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.

References

GOVERS, H. A. J. (1978). *Acta Cryst.* A**34**, 960–965.
GOVERS, H. A. J. (1981). *Acta Cryst.* A**37**, 529–535.
GOVERS, H. A. J. (1982). To be published in *Acta Cryst.*

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:

Introduction (4 pages – this will be sent with all sections)
1. *Point groups* (10 pages; 159 references)
2. *Space groups of* E^1 (*E = 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)
8. *Theory of representation (with application to physics)* (16 pages; 284 references)
9. *Subgroups and supergroups* (6 pages; 93 references)
10. *Lattice complexes and orbits in* E^2 (2 pages; 21 references)
11. *Lattice complexes and orbits in* E^3 (5 pages; 77 references)
12. *Hauptpunkte i.S. Weissenberg's* (1 page; 8 references)
13. *Space forms (differential geometry)* (2 pages; 31 references)
14. *Space partitionings of* E^2 (10 pages; 181 references)
15. *Space partitionings of* E^3 (12 pages; 193 references)
16. *Space partitionings of* E^n ($n \geq 4$) (4 pages; 61 references)
17. *Packings of circles (and of other polygons)* (2 pages; 25 references)
18. *Packings of spheres (and of other polyhedra)* (14 pages; 233 references)

19. *Groupoids*; *OD-structures*; *polytopes*; *enhancement of symmetry* (6 pages; 110 references)
20. *Characters* (1 page; 4 references)
21. *Homology, similarity* (3 pages; 33 references)
22. *Semicontinua, continua* (Lie groups) (1 page; 17 references)
23. *Coloured point and space groups in* E^n ($n = 0, 1, 2, \ldots$); *magnetic structures* (16 pages; 282 references)
24. *Generalised crystallography* (*modulated structures, space-time groups, non-Euclidean spaces*), *modulated structures* (10 pages; 178 references)
25. *Quadratic forms, theory of reduction, translation lattices, geometry of numbers, twins, relation: structure-morphology* (19 pages; 307 references)
26. *Polygons and polyhedra* (12 pages; 213 references)
27. *Polytopes* ($n \geq 4$) (8 pages; 129 references)
28. *Theory of graphs, topology* (5 pages; 78 references)
29. *Isomers, molecular structure* (2 pages; 24 references)
30. (*a*) *General chemistry, crystallography, mathematics and physics*; (*b*) *History*; (*c*) *Symmetry in philosophy, arts and biology* (72 pages; 1340 references).

Appendix. *Theory of Patterson syntheses and vector sets* (but mainly only when point 'atoms' are considered; otherwise it is part of diffraction theory) (12 pages; 159 references).

Within each topic the titles are basically arranged alphabetically and within each author chronologically, although there are a significant number of (non-alphabetical) addenda.

The original bibliography (but not the addenda) has been checked as far as possible by R. Allmann (Marburg/Lahn), L. N. Smirnova and L. A. Shuvalov (Moscow) and D. G. Watson (Cambridge). Requests, stating which sections are required, should be sent to The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. Photocopies will be sent at reduced size, *i.e.* two pages per A4 sheet of paper.

Notes and News

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

Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies

A letter from R. A. Young, E. Prince and R. A. Sparks to the Editor of *Journal of Applied Crystallography* has been published [*J. Appl. Cryst.* (1982), **15**, 357–359] with the above title. The first paragraphs read as follows:

At the request of the Commission on Journals, we drew up some draft guidelines for the publication of Rietveld analyses and of pattern decomposition studies with powder diffraction patterns. The draft was sent for comment to some 25 persons in Europe, Australia, Japan, and the USA. We are grateful for their responses, which both were generally supportive of the idea that there be guidelines and were most helpful in illuminating oversights and other deficiencies. Not all suggestions were incorporated in the revised draft, of course (in fact, a number were mutually contradictory), but all were carefully considered and many were incorporated in the version which follows.

In presenting these suggested guidelines, we emphasize that we offer them as guidelines, not rigid rules. They are intended primarily to be helpful to the co-editors; they are not intended to infringe on a co-editor's judgement of scientific worth of a submitted manuscript, nor should they be allowed to do so. For the most part, these suggested guidelines address matters of format and presentation of details, and not the fundamental question of scientific interest and worth of the submission. It is primarily for the making of such fundamental judgements that the co-editor system exists; for the health of our science it cannot and should not be replaced with a system of blind rules on a check-off sheet. It is against this background of more overreaching considerations that we offer the following suggestions for guidelines to assist, but not to control or coerce, the co-editors in their acceptance decisions.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1982). A**38**, 559–560

La structure de la matière – du ciel bleu à la matière plastique. By A. GUINIER. Pp. 288. Paris: Hachette, 1980. Price 140.18 FF.

This is the first of a series intended for science teachers in secondary schools in order to keep them informed of current developments in science. After a short discussion of atomic structure and chemical bonds, the author classifies matter in two states: the disordered (the perfect gas) and the ordered (the perfect crystal). A major part of the book is concerned with the field between these two extremes from liquids *via* colloids, liquid crystals, polymers, crystalline aggregates with their preferred orientations, to real crystals with their defects.

While the work covers the whole field of crystallography, there is little use of mathematics. The author's aim is not to give rigorous proofs of physical laws but to demonstrate the consequences of these laws in everyday life.

Many university teachers would do well to incorporate in