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A detailed refinement of the crystal and molecular structure of anthracene: Corrigenda by

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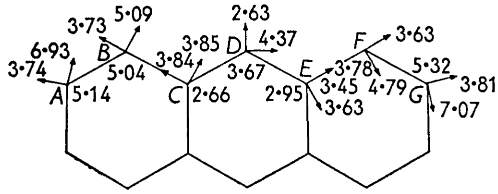
In the course of similar calculations on other structures, it has been found that incorrect transformations of the anisotropic thermal parameters b_{ij} were used in the analysis of anthracene (Cruickshank, 1956). The thermal parameters listed in the paper were intended to be the components of the mean square oscillation tensor **U** referred to the natural molecular axes. The transformation of the b_{ij}'s to the U_{ij}'s was carried out in two stages: the b_{ij}'s were first transformed to **U**′ tensors referred to orthogonal axes defined by the crystal, and these **U**′ tensors were then transformed to **U** tensors referred to the molecular axes. The mistake which has been found is that the **U**′ tensors were referred to the crystallographic axes a, b and c^*, whereas the transformations from **U**′ to **U** were made as if **U**′ had been referred to the axes a^*, b and c. The effect is that the $U_{ij}^{obs.}$ listed in Table 4 referred not to the molecular axes, but to another set of axes obtained by a rotation of $(\beta-\frac{1}{2}\pi) = 34° 42'$.

The general consequences are fortunately not very serious, and the general conclusions of the paper about the anisotropic thermal motion remain unaltered. The mistake resolves the discrepancy between the two estimates of $\sigma(U_{ij}^{obs.})$, obtained by comparison with the $U_{ij}^{calc.}$ and from the $|F_o-F_c|$. The molecular dimensions, etc. and the difference maps are entirely unaffected.

The corrected values of the $U_{ij}^{obs.}$ are shown in the new Table 4, together with the $U_{ij}^{calc.}$ obtained by the method of least squares on the hypothesis of rigid-body vibrations. The revised values of the mean square amplitudes in the directions radial and tangential to the centre, and perpendicular to the molecular plane are shown in the new Fig. 2(*b*). The revised values of the tensors **T** and **ω**, giving the translational vibrations of the mass centre and the angular oscillations, are shown in Table 5. The



r.m.s. amplitudes of translational oscillation in the directions of the molecular axes are now 0·20, 0·16 and 0·16 Å. The amplitudes of the angular oscillations are now 3·8, 2·2 and 3·1°. The e.s.d. of $U_{ij}^{obs.}$ is lowered to 0·0030 Å². The resulting e.s.d.'s of the elements of **T** and **ω** are shown in Table 6.

The former result that the greatest amplitude of translational vibration is along the long axis of the molecule is confirmed; nor is there any new evidence against supposing that the principal axes of **T** and **ω** coincide with the molecular axes. The amplitudes of angular oscillation correspond to mean frequencies of 83, 64 and 42 cm.⁻¹ for the rotational branches of the normal lattice vibrations, which are, as before, sufficiently close to the Raman frequencies.

Reference

CRUICKSHANK, D. W. J. (1956). *Acta Cryst.* 9, 915.

Table 4. *Observed and calculated* U_{ij}

(Values in 10^{-2} Å²)

	U_{11}		U_{12}		U_{13}		U_{22}		U_{23}		U_{33}	
Atom	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.
A	3·86	4·02	0·60	0·64	−0·20	0·04	6·81	6·59	0·58	0·22	5·14	5·17
G	4·14	4·02	−1·14	−0·88	0·20	−0·05	6·77	6·59	0·24	0·35	5·32	4·67
B	4·62	4·45	0·92	0·90	0·01	0·02	4·20	4·49	−0·24	0·07	5·04	4·81
F	4·58	4·45	−0·89	−1·14	−0·06	−0·10	3·84	4·49	0·32	0·25	3·78	4·14
C	3·90	4·02	0·04	0·14	0·01	0·01	3·79	3·13	0·03	0·06	2·66	3·20
E	3·95	4·02	−0·33	−0·37	0·03	−0·02	3·13	3·13	−0·10	0·10	2·95	3·03
D	4·37	4·45	−0·03	−0·12	−0·13	−0·04	2·63	2·70	0·28	0·06	3·67	3·54

Table 5. *Values of* T_{ij} *and* ω_{ij}

(Values of T_{ij} in 10^{-2} Å² and of ω_{ij} in deg.²)

$$\mathbf{T} = \begin{pmatrix} 3.87 & -0.12 & 0.01 \\ & 2.70 & 0.06 \\ & & 2.66 \end{pmatrix} \qquad \boldsymbol{\omega} = \begin{pmatrix} 14.56 & 1.57 & 0.87 \\ & 5.03 & -0.57 \\ & & 9.64 \end{pmatrix}$$

Table 6. *Values of* $\sigma(T_{ij})$ *and* $\sigma(\omega_{ij})$

(Values of $\sigma(T_{ij})$ in 10^{-2} Å² and of $\sigma(\omega_{ij})$ in deg.²)

$$\sigma(\mathbf{T}) = \begin{pmatrix} 0.12 & 0.11 & 0.12 \\ & 0.16 & 0.17 \\ & & 0.29 \end{pmatrix} \qquad \sigma(\boldsymbol{\omega}) = \begin{pmatrix} 5.45 & 0.79 & 1.51 \\ & 0.77 & 0.66 \\ & & 0.66 \end{pmatrix}$$