The observed intensities for each zone were scaled together and processed by means of a least-squares program (Milledge & Walley, to be published) which proved very efficient in eliminating gross errors of indexing, intensity estimation and punching, as well as providing experimental weights. These weights were in fact used in the refinement, but are not likely to have had a very large effect on the final result since there was already a fairly even distribution of ΔF values among the observed reflexions. The results appear to indicate that *molecular orientations* derived from inertia calculations on coordinates obtained by refining relatively inaccurate data do have a much greater significance than the coordinates themselves. All estimates of errors derived from these diagonal SFLS refinements are certainly lower limits.

One of us (K. El S.) wishes to acknowledge with thanks the award of a research scholarship by the Ein-Shams University, Cairo, U.A.R. A grant from the Department of Scientific and Industrial Research has helped to provide computing facilities and apparatus; we are also indebted to Ferranti Ltd and to International Computers and Tabulators for the gift and servicing of the computer PEGASUS on which the greater part of the computing was carried out. Dr B. V. R. Murty very kindly sent us his lists of uncorrected intensities at room temperatures for comparison with our own.

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Methods of Testing for Independent Vibrations of Atoms in a Molecule, Illustrated by Anthraquinone

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(*Received* 29 *March* 1965)

Thermal coefficients have been measured for anthraquinone at five different temperatures. These indicated that the oxygen atom possessed a large independent out-of-plane libration. This was confirmed by treating first the whole molecule and then the anthracene nucleus alone as if they were rigid bodies, and noting the *differences* in the $\mathbf{T}$, $\boldsymbol{\omega}$ values thus determined. These were particularly large for ω_{11}. This method of using successively smaller parts of the molecule as a basis for a rigid-body thermal analysis seems capable of extension to more complicated molecules. A critical consideration of the individual values of $(U\text{ obs} - U\text{ calc})_{ii}$ may also reveal large discrepancies which are consistent at different temperatures, even when the *average* value is similar to the e.s.d. for the experimental data. Such an inspection has revealed a translatory vibration of the anthracene nucleus along the inertia axis L, relative to the oxygen atom. This may be a consequence of the strong intermolecular C(6)(000) --- O(8)$(\frac{1}{2}\frac{1}{2}0)$ bond, combined with the large out-of-plane O(8) libration. There is no sign of any accompanying out-of-plane libration of the outer carbon atoms, such as would be expected for a 'butterfly' motion.

During an investigation of the crystal structure, thermal vibrations and thermal expansion of anthraquinone, for which measurements were made at five temperatures (Lonsdale, Milledge & El Sayed, 1966) it was noticed that the thermal vibration of the oxygen atoms normal to the molecular plane (Fig. 1) was rather larger at all temperatures than would have been expected by comparison with the remainder of the molecule. In order to test whether this could conceivably be due to a particularly large libration about the L axis the values of the U_{ij} were computed and hence the $\mathbf{T}$, $\boldsymbol{\omega}$ matrices (Cruickshank's notation), with a program written for Pegasus by one of us (D.W.).

The calculations were carried out:

(1) For the whole molecule, which is centrosymmetrical.
(2) For the anthracene nucleus alone, omitting oxygen atoms.

If the rigid-body hypothesis were adequate, then the $\mathbf{T}$, $\boldsymbol{\omega}$ matrices obtained for (1) and (2) should be effectively identical. In fact they were very different, the main difference being that the presence of the oxygen

Table 1. *Anthraquinone: Comparison of T_{ij}, ω_{ij} calculated on the assumption that (a) all atoms (b) all carbon atoms only vibrate as a rigid body: all at five temperatures*

(1) All atoms

T	T_{11}	T_{22}	T_{33}	T_{23}	T_{31}	T_{12}	
+20·5 °C	4·30	2·98	2·64	0·07	0·46	−0·81	10^{-2} Å^2
−12·5	3·47	2·70	2·40	0·07	0·08	−0·24	
−72	2·89	2·39	0·86	0·57	0·09	−0·21	
−112	2·62	2·04	1·08	0·28	0·05	−0·13	
−170	1·94	1·35	1·00	0·17	−0·16	−0·25	

ω_{ij} T	ω_{11}	ω_{22}	ω_{33}	ω_{23}	ω_{31}	ω_{12}	
+20·5 °C	29·26	1·35	10·14	−0·20	4·04	−0·20	deg.^{2}
−12·5	20·45	0·72	7·16	−0·69	−1·31	−1·18	
−72	17·90	2·56	4·73	0·56	0·56	−1·25	
−112	16·29	0·95	3·94	0·66	0·66	−0·53	
−170	8·99	−0·03	1·58	−0·03	−0·85	−0·79	

(2) Molecule less oxygen atoms

T	T_{11}	T_{22}	T_{33}	T_{23}	T_{31}	T_{12}	
+20·5 °C	4·46	2·88	3·37	0·19	0·47	−0·86	10^{-2} Å^2
−12·5	3·54	2·56	3·48	0·03	0·08	−0·28	
−72	3·00	2·30	1·65	0·52	0·09	−0·29	
−112	2·70	1·87	1·47	0·26	0·06	−0·16	
−170	2·02	1·17	1·43	0·18	−0·16	−0·26	

T	ω_{11}	ω_{22}	ω_{33}	ω_{23}	ω_{31}	ω_{12}	
+20·5 °C	10·11	0·69	10·96	0·13	5·88	−0·20	deg^2
−12·5	−7·78	−0·26	7·81	−0·82	−1·05	−1·18	
−72	−2·76	1·84	5·32	0·39	−0·03	−1·25	
−112	6·23	0·59	4·73	0·59	0·89	−0·52	
−170	−2·30	−0·43	2·40	0	0·10	−0·79	

Note: The presence of negative values of ω_{11}, ω_{22}, in the (2) data indicates that no real solution was capable of accounting for the measured (unsmoothed) results, for which high accuracy was not claimed.

Table 2. *Comparison of* **T**, **ω** *for anthraquinone* (1)(2), *anthracene and two methyl-*1,2*-benzanthraquinones, all at room temperature*

Anthraquinone

(1) All atoms

$$\mathbf{T}\begin{bmatrix} 4{\cdot}30 & 0{\cdot}07 & 0{\cdot}46 \\ & 2{\cdot}98 & -0{\cdot}81 \\ & & 2{\cdot}65 \end{bmatrix} \text{Å}^2 \qquad \boldsymbol{\omega}\begin{bmatrix} 29{\cdot}15 & -0{\cdot}20 & 4{\cdot}04 \\ & 1{\cdot}35 & -0{\cdot}20 \\ & & 14{\cdot}14 \end{bmatrix} \text{deg.}^2$$

(2) Molecule less oxygen atoms

$$\mathbf{T}\begin{bmatrix} 4{\cdot}46 & 0{\cdot}19 & 0{\cdot}47 \\ & 2{\cdot}88 & -0{\cdot}86 \\ & & 3{\cdot}37 \end{bmatrix} \text{Å}^2 \qquad \boldsymbol{\omega}\begin{bmatrix} 10{\cdot}11 & 0{\cdot}13 & 5{\cdot}88 \\ & 0{\cdot}69 & -0{\cdot}20 \\ & & 10{\cdot}96 \end{bmatrix} \text{deg.}^2$$

Anthracene (Cruickshank, 1956, 1957)

$$\mathbf{T}\begin{bmatrix} 3{\cdot}87 & -0{\cdot}12 & 0{\cdot}01 \\ & 2{\cdot}70 & 0{\cdot}06 \\ & & 2{\cdot}66 \end{bmatrix} \text{Å}^2 \qquad \boldsymbol{\omega}\begin{bmatrix} 14{\cdot}56 & 1{\cdot}57 & 0{\cdot}87 \\ & 5{\cdot}03 & -0{\cdot}57 \\ & & 9{\cdot}64 \end{bmatrix} \text{deg.}^2$$

$$\sigma(\mathbf{T})\begin{bmatrix} 0{\cdot}12 & 0{\cdot}11 & 0{\cdot}12 \\ & 0{\cdot}16 & 0{\cdot}17 \\ & & 0{\cdot}29 \end{bmatrix} \text{Å}^2 \qquad \sigma(\boldsymbol{\omega})\begin{bmatrix} 5{\cdot}45 & 0{\cdot}79 & 1{\cdot}51 \\ & 0{\cdot}77 & 0{\cdot}66 \\ & & 0{\cdot}66 \end{bmatrix} \text{deg.}^2$$

5-Methyl-1,2-benzanthraquinone (Ferrier & Iball, 1963*a*)

$$\mathbf{T}\begin{bmatrix} 5{\cdot}86 & 0 & -0{\cdot}70 \\ & 4{\cdot}49 & 0{\cdot}02 \\ & & 3{\cdot}74 \end{bmatrix} \text{Å}^2 \qquad \boldsymbol{\omega}\begin{bmatrix} 37{\cdot}92 & 4{\cdot}95 & 4{\cdot}27 \\ & 1{\cdot}59 & 1{\cdot}34 \\ & & 6{\cdot}20 \end{bmatrix} \text{deg.}^2$$

2′-Methyl-1,2-benzanthraquinone (Ferrier & Iball, 1963*b*)

$$\mathbf{T}\begin{bmatrix} 5{\cdot}82 & 0{\cdot}55 & -0{\cdot}63 \\ & 3{\cdot}59 & -0{\cdot}20 \\ & & 4{\cdot}34 \end{bmatrix} \text{Å}^2 \qquad \boldsymbol{\omega}\begin{bmatrix} 20{\cdot}35 & 0{\cdot}46 & -3{\cdot}07 \\ & 5{\cdot}76 & -0{\cdot}40 \\ & & 3{\cdot}25 \end{bmatrix} \text{deg.}^2$$

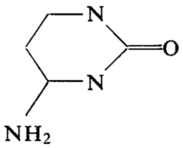
raised the value of the rigid-body libration about the long axis from a real semi-amplitude of 3·2° to an apparent 5·4° (at room temperature). The results for all temperatures are given in Table 1.

It was thought to be of interest to compare the matrices obtained (on the assumption of rigid-body vibrations) for anthraquinone (1) and for anthraquinone minus oxygen atoms (2) with anthracene (Cruickshank, 1956, 1957) and with two methyl-1,2-benzanthraquinones studied by Ferrier & Iball (1963 *a, b*). (See Table 2).

The value of ω_{11} is high for both the methyl-1,2-benzanthraquinones. Moreover, Ferrier & Iball commented on the large discrepancy between their calculated and observed U_{33} ($\overline{u^2}$ normal to molecular plane) for the O(2) atom in particular; and ascribed this to a probable independent libration of the oxygen atom. The disadvantage of including in the calculation atoms which, by inspection of the observed U_{ij} can be seen to have values obviously inconsistent with a rigid-body hypothesis is that by doing so all the other $\mathbf{T}$, $\boldsymbol{\omega}$ values are falsified to a greater or less extent. The average discrepancy $[U_{ii}(\text{calc}) - U_{ii}(\text{obs})]$ for the 5-methyl compound [less U_{33} for O(2)] is 0.89 [as compared with 6·96 for U_{33} of O(2)] which is high relative to the standard deviation that might be expected in work of this accuracy ($R=0{\cdot}082$). The average for the 2′-methyl compound [less U_{33} for O(2)] is 0·60 [as compared with 5.01 for U_{33} of O(2)] which is still rather high.

This means also that by including the oxygen atoms in the calculation a value of ω_{11} is obtained which is much too high and the values of carbon atomic coordinates adjusted for rotational oscillations are correspondingly over-corrected. In contrast the value of the 'corrected' ketonic bond is under-corrected, for the independent libration of the oxygen atom normal to the molecular plane is not properly allowed for.

Barker & Marsh (1964), who have recently studied the structure of cytosine, realized that there are almost certainly large out-of-plane, non-rigid-body librations of the ketonic oxygen and of the NH_2 group about the carbon atoms to which they are attached and that a special allowance must be made for these in correcting those particular bond lengths.



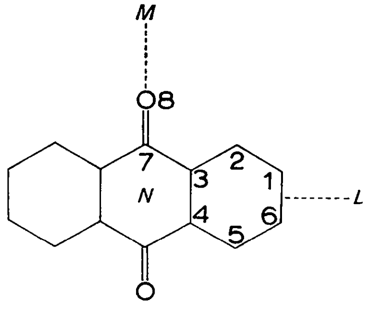


Fig. 1. Numbering of atoms and directions of inertia axes in molecule of anthraquinone (*cf.* Lonsdale, Milledge & El Sayed, 1965).

In the case of anthraquinone, even the moderate accuracy of the experimental data could not hide the outstanding magnitude of the oxygen libration relative to the anthracene nucleus. The values of the out-of-plane semi-amplitude of libration of the oxygen atom relative to the carbon to which it is attached (which is superimposed on the rigid-body librations and translations) are approximately

T	+20·5	−12·5	−72	−112	−170°C
φ	8·8	8·4	7·5	6·9	5·8 degrees

as deduced from b_{ij} values smoothed in respect of temperature. These values may be compared with the rigid-body libration $(\omega_{11})^{\frac{1}{2}}$ which is about 3·2 degrees at room temperature. It may be noted that this independent normal libration of the oxygen atom is *not* accompanied by any corresponding normal libration of C(1), C(6) *etc.* such as would be implied by a butterfly distortion.

A second possible form of independent vibration associated with the oxygen atoms of anthraquinone is revealed by comparing U(calc) and U(obs) in detail for both sets of $\mathbf{T}$, $\boldsymbol{\omega}$. Considering the 'errors' $\varepsilon = U(\text{obs}) - U(\text{calc})$, as given by a Cruickshank analysis, then for rigid-body vibrations $|\varepsilon|$ should be of the order of the average e.s.d. on the U_{ij} (that is, on the $\overline{u^2}$) values, and $\Sigma\varepsilon^2$ is minimized by the calculation itself. This is in fact the case for anthraquinone, when the calculation is carried out for the whole molecule, even though (as already demonstrated) the results are not physically correct. The values of ε (for all atoms, for all five temperatures) corresponding to U_{11}, U_{22}, U_{33} (that is to the molecular inertia axes L, M, N, which are the pseudo-symmetry axes of the molecule) are shown in Table 3, together with $|\varepsilon|$ and $\Sigma|\varepsilon|$. The 'average error', 0.466. 10^{-2} Å^2 at +20·5°C, is very similar to the average e.s.d. in $\overline{u^2}$, which is of the order of 0·5. 10^{-2} Å^2.

It is not sufficient, however, to use this value as a criterion. The individual values should be studied, and if any particular value is large, it should be looked at more critically. Measurements made at several temperatures are particularly useful in this connection, because they may help to eliminate odd discrepancies which are due to inaccuracies of measurement or of data processing. In Table 3, for example, the values of ε for −12.5° in particular show some odd large values; but these are not repeated at the other temperatures. At *all* the temperatures, however, the values of $\varepsilon(L)$ [that is of $U_{11}(\text{obs}) - U_{11}(\text{calc})$] for oxygen are large and *negative.*

Table 4 shows similar data, but based now on the rigid-body theory as applied only to the carbon atoms

C(1) − C(7). When the $|\varepsilon|$ are *averaged*, the mean value is still similar to the average e.s.u. of u (obs), but for the O(8) atom $\varepsilon(L)$ is still large and negative, and $\varepsilon(N)$ is even larger and positive, at all temperatures. The *positive* $\varepsilon(N)$ values have been explained in terms of the independent out-of-plane libration of the oxygen atom about the C(7) atom to which it is bonded. But the explanation of the *negative* $\varepsilon(L)$ values must be more subtle. They cannot be explained in terms of any positive $\overline{u^2}(L)$ for the oxygen atom. They can *only* mean either (1) that the oxygen atoms are not scattering spherically (bonding anisotropy) or (2) that the whole

Table 3. *Errors* ε_i Å^2 (*where* $i=$C(1) · · · C(7)O) *for the five temperatures, with* $\Sigma/\varepsilon_i|$, *and* $(\Sigma|\varepsilon_i|)/24$ (*based on the 'whole molecule' analysis*)

These values are (U_{ii}obs − U_{ii}calc), in Cruickshank's notation.

		−170	−112	−72	−12·5	+20·5 °C	
C(1)	*L*	+0·593	−0·008	+0·101	+0·094	+0·519	10^{-2} Å^2
	M	+0·921	+0·589	+0·189	+1·464	+0·871	
	N	−0·094	+0·166	+0·070	+0·358	+0·246	
C(2)	*L*	+0·132	+0·270	+0·189	+0·748	+0·115	
	M	−0·308	−0·101	−0·046	+0·221	+0·131	
	N	−0·158	−0·429	−0·619	−1·058	−0·639	
C(3)	*L*	−0·458	−0·253	+0·093	−0·616	−0·407	
	M	+0·248	+0·376	−0·144	+0·258	−0·703	
	N	+0·237	+0·308	+0·382	+0·709	−0·148	
C(4)	*L*	+0·668	−0·094	−0·390	−0·297	+0·211	
	M	−0·186	−0·339	+0·128	−0·273	+0·666	
	N	+0·235	+0·044	+0·320	+0·281	+0·730	
C(5)	*L*	+0·329	+0·298	+0·147	+0·493	−0·002	
	M	−0·496	−0·818	−0·293	−1·079	+0·444	
	N	−0·469	−0·331	−0·978	−1·030	−0·993	
C(6)	*L*	−0·203	+0·439	+0·697	+0·374	+0·818	
	M	−0·351	+0·046	+0·153	−0·624	−0·369	
	N	+0·323	+0·137	−0·571	+0·472	+0·427	
C(7)	*L*	−0·261	+0·091	+0·025	−0·084	+0·036	
	M	−0·002	+0·081	+0·173	−0·045	−0·683	
	N	−0·268	−0·069	−0·103	−0·219	+0·047	
O(8)	*L*	−0·800	−0·742	−0·860	−0·712	−1·290	
	M	+0·173	+0·165	−0·160	+0·078	−0·355	
	N	+0·193	+0·174	+0·356	+0·488	+0·329	
Sum of $-^{\mathrm{ve}}$ values		−4·054	−3·184	−3·593	−6·037	−5·589	
Sum of $+^{\mathrm{ve}}$ values		+4·052	+3·184	+3·594	+6·038	+5·590	
$\Sigma\lvert\varepsilon_i\rvert$		8·106	6·368	7·187	12·075	11·179	
$\overline{\lvert\varepsilon\rvert}=\frac{\Sigma\lvert\varepsilon_i\rvert}{24}$		0·338	0·265	0·299	0·503	0·466	

Table 4. *Errors* $\varepsilon_i=(U_{ii}\text{obs}-U_{ii}\text{calc})$ *for* C(1) - - - C(7), *and for oxygen* (*based on the '7-atom' analysis*)

		−170	−112	−72	−12·5	+20·5 °C	
C(1)	*L*	+0·495	−0·099	−0·011	+0·005	+0·351	10^{-2} Å^2
	M	+0·754	+0·433	+0·029	+1·319	+0·351	
	N	−0·197	+0·074	−0·124	+0·095	+0·067	
C(2)	*L*	−0·002	+0·146	+0·052	+0·630	−0·088	
	M	−0·284	−0·079	−0·069	+0·231	+0·078	
	N	+0·138	−0·161	−0·076	−0·315	−0·129	
C(3)	*L*	−0·556	−0·344	−0·019	−0·705	−0·576	
	M	+0·388	+0·507	−0·085	+0·363	−0·643	
	N	−0·006	+0·092	−0·062	+0·102	−0·557	
C(4)	*L*	+0·569	−0·185	−0·502	−0·385	+0·042	
	M	−0·045	−0·207	+0·188	−0·169	+0·726	
	N	−0·006	−0·174	−0·124	−0·327	+0·325	
C(5)	*L*	+0·195	+0·173	+0·010	+0·375	−0·205	
	M	−0·473	−0·796	−0·317	−1·069	+0·392	
	N	−0·177	−0·071	−0·440	−0·292	−0·498	
C(6)	*L*	−0·301	+0·348	+0·586	+0·285	+0·649	
	M	−0·519	−0·109	−0·007	−0·768	−0·602	
	N	+0·216	+0·042	+0·381	+0·209	+0·246	
C(7)	*L*	−0·401	−0·039	−0·116	−0·206	−0·172	
	M	+0·180	+0·251	+0·263	+0·094	−0·582	
	N	+0·031	+0·199	+0·445	+0·528	+0·545	
O(8)	*L*	−1·071	−0·994	−1·095	−0·940	−1·625	
	M	+0·355	+0·336	−0·070	+0·217	−0·254	
	N	+2·270	+2·037	+4·154	+5·683	+3·831	

anthracene nucleus is moving with a lateral translation (along L) relative to the oxygen atoms. (1) seems to be ruled out as the main explanation because of the magnitude of the negative $\varepsilon(L)$ value. It is much larger than any bonding-anisotropy effect could be expected to be. This leaves us with the possibility of an L-translation of the whole anthracene nucleus relative to the oxygen atoms, which seem to be partially immobilized along L by 'bonds' to neighbouring molecules. This movement could possibly be phase-related to the oxygen out-of-plane libration; in which case the assumption that we are justified in using u_{ij} values for purposes of calculation would be invalid. There is some evidence that where an outer and otherwise 'mobile' atom takes part in an 'intermolecular bond', that atom *is* to a certain extent immobilized (the hydrogen atoms in urea, for example). The shortest intermolecular bond in anthraquinone (Lonsdale *et al.*, 1966) is that linking C(6) of (000) with an oxygen atom of ($\frac{1}{2}\frac{1}{2}0$), which is 3·33 Å at +20·5°C and 3.25 Å at −170°C (all other C $\cdots$ O and C $\cdots$ C intermolecular distances at room temperatures are over 3·5 Å). It is not unreasonable to suppose that a large out-of-plane movement of the oxygen atom would exert some translatory pull on the anthracene nucleus of the neighbouring molecules to which it is attached by such a relatively strong van der Waals force.

Conclusion

The results for anthraquinone indicate two methods of testing for non-rigid-body vibrations in any given molecule for which the axes of libration are known with a good degree of certainty.

(1) First the whole molecule and then limited parts of the molecule should be treated as if they were vibrating as rigid bodies about the molecular axes of inertia. If there are no independent vibrations then the values of translatory and libratory amplitudes should be invariant with respect to the number of atoms taken to determine them. If they are not invariant then the differences can be used to determine the nature of the independent vibrations.

(2) The values of $U_{ii}(\text{calc}) - U_{ii}(\text{obs})$ should be examined critically, preferably using data for more than one temperature, to determine whether any individual values are consistently too high to be accounted for by experimental error or as artefacts of the calculation, even when the *average* value is well within the expected e.s.d. If there are such anomalies, these may provide a guide as to which atoms to omit from a 'difference' rigid-body analysis of the thermal data.

One of us (K. El S.) is indebted to the authorities of Ein-Shams University, Cairo, for the award of a research scholarship. D. W. is indebted to International Computers and Tabulators for a research grant.

We acknowledge with thanks the help we have had from Ferranti Ltd. and International Computers and Tabulators for the gift and servicing of the computer PEGASUS, without which this work would not have been possible.

Financial help from the Department of Scientific and Industrial Research has also been given to enable many of the computer calculations to be carried out, and we have been grateful to Mrs Maureen Walley for assistance with the computing involved, and to our colleagues for useful discussions.

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The Electrostatic Interaction Energy of Ionic Lattices with Statistical Distribution of Charges

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(*Received* 26 *April* 1965)

The method due to Bertaut (1952) for calculating interaction energies is extended to include statistical distribution of charges on geometric lattices. Explicit expressions are developed for statistically random charge distributions and implicit expressions for statistical charge distributions with correlation between occurrences of charges.

Introduction

Ewald (1921) has developed methods to calculate the electrostatic potential of ionic lattices by the use of theta functions. The rapid convergence of his series makes possible the evaluation of the electrostatic interaction energy and the Madelung constant for ideal ionic crystals. Bertaut (1952) by use of faltung theory has developed general expressions for the electrostatic energy of ideal ionic crystals, which, as a special case,

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