

becomes significant in describing the vibrational properties of the atoms of lithium.

(c) *The parameter α*

The agreement between all subsets of data analysed for the isotropic harmonic parameters α_0 and α_{293} is excellent. The mean values from all subsets are

$$\alpha_0 = 45.3 \pm 0.4 \text{ eV nm}^{-2}$$

and

$$\alpha_{293} = 42.2 \pm 0.3 \text{ eV nm}^{-2}.$$

Hence, the corresponding values of $u_{\text{r.m.s.}}$ and Debye temperature calculated from them must be considered to be very reliable. The root-mean-square displacement $u_{\text{r.m.s.}} = 0.0424 \pm 0.0001 \text{ nm}$. The Debye temperature θ_D is given by

$$\langle u^2 \rangle = \frac{9\hbar^2 T}{Mk_B \theta_D^2} \left[1 + \frac{1}{36} \left(\frac{\theta_D}{T} \right)^2 \right].$$

where M is the atomic mass. The value obtained was $\theta_D =$

$326 \pm 1 \text{ K}$. This may be compared with the value of $352 \pm 12 \text{ K}$ obtained by Pankow (1936).

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Six regular polygons at a four-connected vertex. By A. L. MACKAY, *Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HC, England*

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Abstract

Six angles are formed between four straight lines meeting at a point in space. Since there is one relationship between them, only certain combinations of six regular polygons will fit together at such a point. Some of these are enumerated.

When four straight lines meet at a tetrahedral vertex in space they make six angles, any one of which is determined by the other five as the solution to a quadratic equation. The relationship between them was known to Carnot (1803) and was stated by Fedorov (1886) in the modern determinantal form:

$$\begin{vmatrix} 1 & \cos \theta_{12} & \cos \theta_{13} & \cos \theta_{14} \\ \cos \theta_{12} & 1 & \cos \theta_{23} & \cos \theta_{24} \\ \cos \theta_{13} & \cos \theta_{23} & 1 & \cos \theta_{34} \\ \cos \theta_{14} & \cos \theta_{24} & \cos \theta_{34} & 1 \end{vmatrix} = 0.$$

In dealing, for example, with network silicates, we can ask what combinations of six regular polygons may meet at such a tetrahedral vertex. The corresponding solutions for a vertex in a plane at which three regular polygons meet are quoted in Table 1 (from Holiday & Philpot, 1977).

The formula quoted derives from the metric matrix of a unit cell with four axes of unit length, the terms of the matrix being the scalar products $\mathbf{a}_i \cdot \mathbf{a}_j$ of all pairs of axes. The determinant of the metric matrix gives the square of the four-dimensional content of the unit cell. If the metric matrix

Table 1. *The possible combinations of three regular polygons at a common vertex in the plane*

(1–2)	(1–3)	(2–3)
3	7	42
3	8	24
3	9	18
3	10	15
3	12	12
4	5	20
4	6	12
4	8	8
5	5	10
6	6	6
3	3	–6
4	3	–12
5	3	–30

If the number of sides of the polygon is given as negative it indicates that the corresponding polygon contains the other two.

Table 2. *Regular polygons meeting at a tetrahedral vertex*

Numbers of sides of the polygon between axes 1, 2, 3, 4.

	(1-2)	(1-3)	(1-4)	(2-3)	(2-4)	(3-4)	Symmetry	Notes
1	4	3	3	3	3	4	$\bar{4}2m$	
2	5	5	3	3	5	3	2	
3	5	5	4	5	3	3	<i>m</i>	(a)
4	6	4	3	4	3	4	<i>m</i>	
5	6	6	4	4	3	3	<i>m</i>	
6	6	6	4	5	5	5	<i>m</i>	(b)
7	6	6	4	4	6	6	$\bar{4}2m$	(c)
8	8	4	4	3	3	4	<i>m</i>	
9	8	6	3	4	4	4	1	
10	8	6	6	4	4	4	<i>m</i>	
11	8	8	4	3	3	3	<i>m</i>	
12	8	4	4	4	3	8	2	
13	8	6	4	4	4	8	2	
14	8	8	4	3	6	6	<i>m</i>	(d)
15	10	5	3	4	4	4	1	
16	10	5	4	3	5	3	1	
17	10	6	4	3	3	5	1	
18	10	6	4	4	3	5	1	
19	10	6	5	4	4	4	1	
20	10	5	4	4	5	6	2	
21	10	6	6	4	3	5	1	
22	10	10	3	3	5	4	1	
23	10	5	4	4	3	10	2	
24	10	5	3	3	5	10	222	
25	10	10	4	3	5	5	<i>m</i>	
26	10	6	4	3	5	10	1	
27	10	10	3	3	10	6	2	
28	30	7	5	3	3	5		(e)
29	30	7	3	3	5	9		(e)

Notes: (a) includes vertex of dodecahedron; (b) includes vertex of dodecahedron; (c) vertex in space filling by Thomson cubes; (d) vertex in packing of alternating truncated cubes and cuboctahedra with inserted truncated tetrahedra (Wells, 1977, p. 170); (e) approximate solutions; determinant $\approx 10^{-7}$.

is of rank less than four and its determinant thus zero, then the four vectors can be embedded in ordinary three-dimensional space, where any one of them can be expressed as a linear combination of the other three. If any three vectors are co-planar, the rank of the metric matrix will be further lowered. Extension to higher dimensionality is obvious.

Table 2 shows the results of computer enumeration (systematically examined for polygons with up to 20 sides and sporadically searching thereafter). Configurations in which three lines are co-planar have been excluded.

In the computer program* it was necessary to consider how many different tetrahedral vertices (counting enantiomorphs as identical) may be constructed, given six different angles. The number found is 30 so that this number of combinations had to be checked for each set of six different angles. The question is very similar to that of indexing a powder photograph where the six elements of the metric matrix may be chosen in 30 ways from six different observed spacings.

Not only must the determinant be zero but no triplet of angles between three axes must add to 360° or more. Examples, such as (3, 4, 14, 14, 4, 7), can be found where the determinant is zero but which are impossible because here the angle (1-4) is greater than the angles (1-2) and (2-4) combined.

No case of six different regular polygons meeting at a point was found. Two cases were found where the solution was not exact but was nevertheless closely approximated. In these two cases regular polygons with 30.7 and 3 sides give a vertex total of 356.57° so that three edges are nearly co-planar.

A number of the types of vertices listed in Table 2 occur in the networks described by Wells (1977) in terms of their topology, rather than of actual bond angles. One case (12, 6, 4, 4, 4, 6) which occurs in faujasite, is topologically possible, but, if the polygons are to be regular, would require the triplet of polygons with 12, 4 and 6 sides to be co-planar.

* A listing of the *ANGLES* computer program has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36245 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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