Acta Cryst. (1978). A**34**, 901–905

A Method, Based upon 'Bond-Strength' Calculations, for Finding Probable Lithium Sites in Crystal Structures

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(*Received* 3 *February* 1978; *accepted* 16 *May* 1978)

A method for finding probable Li positions in a given oxygen matrix in crystals is described. It is formally based upon bond strength–bond length discussions. The sums of bond strengths for simulated Li atoms are calculated and printed in three-dimensional maps. The method is tested on nine structures containing Li atoms. In five of these the Li sites are known from neutron diffraction studies, in two from X-ray powder diffraction data sets, and in the other two from X-ray single-crystal investigations. The calculated Li coordinates in all the tests are in fair agreement with the experimentally observed positions. The method is therefore likely to provide an auxiliary tool for determining Li sites in X-ray crystal structure studies.

Introduction

The bond-strength concept introduced by Pauling (1927, 1947, 1960) has been used for a number of practical purposes related to crystal structure determinations (Donnay, 1972; Brown & Shannon, 1973). Methods to predict the positions of hydrogen atoms, or rather to predict systems of hydrogen bonds in the presence of heavy atoms in inorganic crystals, have been given by Donnay & Allman (1970), Baur (1972) and Brown & Shannon (1973).

It is often difficult to obtain information about the positions of light atoms in the presence of heavy ones in crystal structures derived from X-ray diffraction data. The present paper describes a method, mainly based upon bond strength–bond length functions, useful for locating possible Li positions in a given oxygen matrix.

Procedure

The relation

$$s = s_0\left(\frac{d}{R_0}\right)^{-N} \qquad (1)$$

has been used by Brown & Shannon (1973) for the correlations between the bond lengths, d (in Å) and the bond strengths, s (in valence units, v.u.) for bonds between cations and oxygens in oxides. The empirical constants, s_0, R_0 and N were derived from least-squares refinements by requiring the sum of bond strengths around a cation to be equal to its valency. The authors found the following expression for Li–O bonds:

$$s = 0{\cdot}25\left(\frac{d}{1{\cdot}954}\right)^{-3{\cdot}9}. \qquad (2)$$

This function is shown in Fig. 1.

Consider a regular LiO_6 octahedron (or LiO_4 tetrahedron) with the Li atom at the centre, giving six (or four) Li—O bonds of equal length. The sum of bond strengths around the Li atom is assumed to be close to 1·0. An off-centre displacement of the Li atom in any direction will result in an increase in the $\sum s$ value calculated by (2) due to the shape of the $s = f(d_{\mathrm{Li-O}})$ curve (see Fig. 1). The increase in some of the s values caused by the shortening of Li—O bonds in the polyhedron is larger than the sum of decreases for the bonds being lengthened. The Li atom is therefore situated at a position corresponding to a minimum in the $\sum s$ value.

The Li atoms in distorted polyhedra are assumed to be located at similar but less clear-cut $\sum s$ minima.

However, it must be emphasized in this context that calculated $\sum s$ values $\gg 1{\cdot}0$ should not be regarded as true bond-strength sums. A sum larger than $\sim 1{\cdot}0$ indicates a less probable Li site because of too short Li—O separations and a value $\ll 1{\cdot}0$ (*e.g.* $<0{\cdot}8$) indicates a void in the structure too large for a Li atom.

Equation (2) may also be regarded as an expression for repulsion potentials between overlapping electron clouds as a function of the Li—O separations. The repulsion potentials are then on a scale resulting in

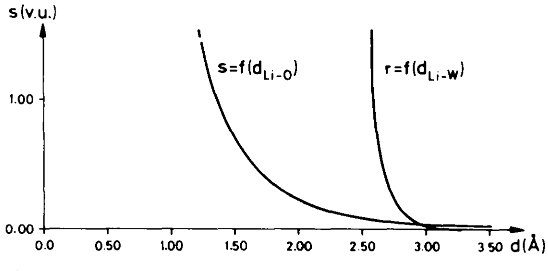

Fig. 1. The curves given by: $s_{\mathrm{Li-O}} = 0{\cdot}25\ (d_{\mathrm{Li-O}}/1{\cdot}954)^{-3{\cdot}9}$ and $r_{\mathrm{Li-W}} = 0{\cdot}15\ (d_{\mathrm{Li-W}}/2{\cdot}8)^{-25}$; v.u. = valence units.

repulsion minima with values close to 1·0 for Li positions.

The initial test calculations were performed on the structure of Li_2WO_4(iv) (Waltersson, Werner & Wilhelmi, 1977*a*). The result was printed in three-dimensional maps of $\sum s$ values for potential Li sites in the oxygen matrix. The hexagonally close-packed oxygen atoms form polyhedra which are either occupied by metal atoms or empty. An occupied octahedron or tetrahedron is nearly the same size as an unoccupied one. Therefore, when only the positions of the oxygens were introduced in the calculations, minima with reasonable $\sum s$ values close to 1·0 showed up in the maps indicating possible Li sites in all octahedral and tetrahedral voids, also including the oxygen octahedra occupied by W atoms.

In order to eliminate unavailable Li sites too close to the W atoms, 'repulsion' contributions due to too short Li—W separations were added to the map values. For simplicity it was assumed that the metal–metal repulsion, *r*, follows a relation similar to (1):

$$r = 0{\cdot}15\left(\frac{d_{\text{Li}-M}}{R_{\text{Li}-M}}\right)^{-25}. \quad (3)$$

When (3) with $R_{\text{Li-W}} = 2{\cdot}8$ Å was included in the test calculations only one minimum appeared in the asymmetric unit (see below). Fig. 1 shows a graphical representation of this equation for $R_{\text{Li-W}} = 2{\cdot}8$ Å.

The $R_{\text{Li}-M}$ value must be chosen small enough to make the Li—*M* repulsion terms negligible at the actual Li positions. The $R_{\text{Li}-M}$ value can be estimated from geometrical considerations. If face-sharings are possible between LiO_6 and MO_6 octahedra, the $R_{\text{Li}-M}$ value is estimated by $R_{\text{Li}-M} \sim (r_{\text{Li}} + r_M + 2r_{\text{O}})/\sqrt{3}$, and if edge-sharings are allowed: $R_{\text{Li}-M} \sim (r_{\text{Li}} + r_M + 2r_{\text{O}})/\sqrt{2}$. For a common vertex between the Li and *M* polyhedra, the $R_{\text{Li}-M}$ value can be estimated by $R_{\text{Li}-M} \sim 0{\cdot}75(r_{\text{Li}} + r_M + 2r_{\text{O}})$. The r_{Li}, r_M and r_{O} values are the effective ionic radii given by Shannon (1976). The empirical constant $R_{\text{Li}-M}$ can be regarded as the radius of a forbidden volume around the *M* atoms. Therefore the value of $R_{\text{Li}-M}$ can also be chosen for the structure being examined somewhat shorter (5–10%) than a reasonably short Li—*M* separation expected from previously determined Li—*M* distances.

Changes in minimum positions caused by the repulsion from symmetry-related minima were investigated by means of a new function, which generates Li atoms at positions symmetry-related to the particular map point being computed. The repulsion contribution was calculated by (3) with $R_{\text{Li-Li}} = 2{\cdot}45$ Å. The constant $R_{\text{Li-Li}}$ was estimated by the formula: $R_{\text{Li-Li}} \sim (0{\cdot}76 + 0{\cdot}76 + 2 \cdot 1{\cdot}35)/\sqrt{3} = 2{\cdot}44$ Å, valid for two octahedra with a shared face.

The procedure usually adopted was to calculate a first set of maps without using the 'symmetry' function, because it is easy to miss information in maps with the symmetry function included.

Before a minimum was accepted as a potential Li site, the Li—O and Li—Li distances were calculated. The Li—O distances must be within reasonable ranges, with mean values close to 1·97 and 2·14 Å for tetrahedral and octahedral coordination respectively. These values are estimated from the effective ionic radii given by Shannon (1976). Only when the distance between symmetry-related minima was shorter than 2·7 Å a further set of maps was calculated using the symmetry function.

The values printed in the maps are as follows:

$$p = \sum s_{\text{Li-O}} + \sum r_{\text{Li}-M} + \sum r_{\text{Li-Li}}. \quad (4)$$

The two first terms arise from (2) and (3), while the third results from the symmetry function described above. Expression (4) can be regarded as a probability function for Li positions, where the most probable sites must have *p* values close to ~1·0.

When atomic coordinates are derived from geometrical considerations, useful auxiliaries are maps with the forbidden volumes of already known atoms marked. In these maps one may also indicate the excluded volumes around the symmetry elements resulting in too short separations between symmetry-related atoms. The construction of these maps is often tedious and the result generally gives rough coordinate values only.

The plotting of maps with *p* values given by expression (4) is a method comparable to that of deriving atomic positions geometrically. The two latter terms in formula (4) can be regarded as expressions for radii of forbidden volumes around the atoms and the symmetry elements present. The use of 'bond strength' gives a more accurate method for determining Li positions than one directly based upon bond lengths.

Results

The method outlined above has been tested on a number of crystal structures. The results, partly summarized in Table 1, are in fair agreement with the reported Li positions derived from experimental (neutron or X-ray diffraction) data. The grid intervals along each axis used in the map calculations generally were in the range 0·15–0·20 Å, *i.e.* of the order of the accuracy in the minimum positions. The differences between the predicted and observed positions are expressed as deviations (in Å) and are less than 0·2 Å except in two examples: Li_2WO_4(iv) and Li_2WO_4(ii) (Waltersson, Werner & Wilhelmi, 1977*a*,*b*). The Li coordinates in these two structures were derived and refined together with the W and O atoms by the use of data obtained from X-ray powder photographs. Keeping this in mind, one may consider the agreement good.

Table 1. *The results of the test calculations*

The experimental data based upon: neutron diffraction N, X-ray diffraction X, powder p and single crystal sx. Minima listed under: (*a*) positions obtained from the first set of maps without using the Li–Li symmetry function, (*b*) positions obtained from the second set of maps with the Li–Li symmetry function included in the calculations. The minimum positions marked with an asterisk are the predicted Li sites to be compared with the experimentally observed sites.

Compound	$LiIO_3$		$Li(H_2O)_3ClO_4$		$LiH_3(SeO_3)_2$	$Ba_4Sb_3LiO_{12}$	$LiNb_3O_8$	Li_2WO_4 (iv)
Reference	1		2		3	4	5	6
Space group	$P6_3$		$P6_3mc$		Pn	$Im3m$	$P2_1/a$	$C2/c$
Data	N, p		N, sx		N, sx	N, p	X, sx	X, p
Z	2		2		2	2	4	4
$R_{\mathrm{Li}-M}$ (Å)	$R_{\mathrm{Li-I}}$ = 2·80 $R_{\mathrm{Li-Li}}$ = 2·45		$R_{\mathrm{Li-Cl}}$ = 2·80 $R_{\mathrm{Li-H}}$ = 2·00 $R_{\mathrm{Li-Li}}$ = 2·45		$R_{\mathrm{Li-Se}}$ = 2·80 $R_{\mathrm{Li-H}}$ = 2·00	$R_{\mathrm{Li-Ba}}$ = 3·00 $R_{\mathrm{Li-Sb}}$ = 2·50	$R_{\mathrm{Li-Nb}}$ = 2·90	$R_{\mathrm{Li-W}}$ = 2·80
	a	*b*	*a*	*b*	*a*	*a*	*a*	*a*
Minima	*A*	*A**	*A*	*A**	*A**	*A**	*A**	*A**
Point set	2(*a*)	2(*a*)	2(*a*)	2(*a*)	2(*a*)	2(*a*)	4(*e*)	8(*f*)
x	0	0	0	0	0·000	0	0·421	0·183
y	0	0	0	0	0·250	0	0·257	0·344
z	0·417	0·410	0·219	0·226	0·469	0	0·264	0·250
p	1·09	1·17	1·06	1·07	1·01	0·94	0·98	1·15
Polyhedra	AO_6	AO_6	AO_6	AO_6	AO_6	AO_6	AO_6	AO_4 AO_6
Mean distance (Å)	2·13	2·13	2·14	2·14	2·16	2·20	2·19	1·99 2·20
Distances (Å) between minima <3·0 Å	2·59 2·59	2·59 2·59	2·73 2·73	2·73 2·73	>3·0	>3·0	>3·0	>3·0
Observed sites x	0		0		0·0024 (15)	0	0·4201 (14)	0·174 (4)
y	0		0		0·2487 (15)	0	0·2673 (80)	0·362 (7)
z	0·4461		0·2254 (24)		0·4807 (16)	0	0·2597 (29)	0·305 (9)
Deviations (Å)	0·19		0·003		0·062	0	0·060	0·31

Table 1 (*cont.*)

Compound	$LiHCOO\cdot H_2O$				Li_2WO_4 (i)					Li_2WO_4 (ii)					
Reference	7				8					9					
Space group	$Pna2_1$				$R\bar{3}$ (hexagonal axes)					$I4_1/amd$					
Data	N, sx				X, sx					X, p					
Z	4				18					16					
$R_{\mathrm{Li}-M}$ (Å)	$R_{\mathrm{Li-C}}$ = 2·50 $R_{\mathrm{Li-H}}$ = 2·00				$R_{\mathrm{Li-W}}$ = 2·80					$R_{\mathrm{Li-W}}$ = 2·80 $R_{\mathrm{Li-Li}}$ = 2·45					
	a				*a*					*a*					*b*
Minima	*A*	*B*	*C**	*D*	*A*	*B**	*C*	*D*	*E**	*A**	*B*	*C*	*D*	*E*	*E**
Point set	4(*a*)	4(*a*)	4(*a*)	4(*a*)	18(*f*)	18(*f*)	18(*f*)	18(*f*)	18(*f*)	16(*g*)	4(*a*)	16(*h*)	16(*f*)	16(*f*)	16(*f*)
x	0·400	0·440	0·050	0·150	0·190	0·188	0·333	0·250	0·181	0·144	0	0·112	0·162	0·388	0·385
y	0·425	0·338	0·117	0·275	0·298	0·222	0·217	0·264	0·208	0·106	$\frac{1}{4}$	$\frac{1}{4}$	0	0	0
z	0·250	0·485	0·750	0·750	0·083	0·083	0·486	0·250	0·417	$-\frac{1}{8}$	$-\frac{1}{8}$	−0·05	0	0	0
p	0·76	1·06	1·04	0·90	0·93	0·97	0·96	1·03	0·98	0·88	1·14	0·99	0·93	1·20	1·21
Polyhedra	AO_3	BO_4	CO_4	DO_3	AO_4	BO_4	CO_3	DO_3	EO_4	AO_4	BO_4	CO_6	DO_6	EO_6	EO_6
Mean distance (Å)	2·01	2·16	1·96	2·01	2·00	1·98	1·87	1·89	1·97	2·03	1·89	2·29	2·24	2·07	2·07
Distances (Å) between minima <3·0	>3·0				*A–C* 0·81 *A–B* 1·08 *A–D* 1·99 *A–E* 2·58 *B–C* 1·59		*B–D* 1·79 *C–D* 1·60 *C–E* 2·22 *D–E* 1·85			*A–D* 1·66 *C–C* 2·28 *C–C* 2·28 *D–D* 2·57		*D–D* 2·57 *C–C* 2·69 *D–E* 2·69 *E–E* 2·69			2·75
Observed sites x	0·0493 (4)					0·187 (4)			0·191 (4)	0·134 (4)				0·351 (5)	
y	0·1165 (6)					0·214 (4)			0·205 (4)	0·116 (4)				0	
z	0·7702 (11)					0·089 (5)			0·408 (5)	$-\frac{1}{8}$				0	
Deviations (Å)	0·098					0·072			0·19	0·17				0·41	

Table 1 (*cont.*)

Compound	$Li_2WO_4\cdot\frac{4}{7}H_2O$				Li_2WO_4,(iii)					
Reference	10				11					
Space group	*P*$\bar{4}$3*m*				*Pnnm*					
Data	X, sx				X, sx					
Z	7				*8*					
R_{Li-Me} (Å)	$R_{Li-W} = 2.80$				$R_{Li-W} = 2.80$ $R_{Li-Li} = 2.45$					
	a				*a*			*b*		
Minima	*A*	*B*	*C**	*D**	*A*	*B*	*C*	*A**	*B**	*C**
Point set	1(*a*)	3(*c*)	12(*i*)	4(*e*)	4(*e*)	4(*f*)	8(*h*)	4(*e*)	4(*f*)	8(*h*)
x	0	$\frac{1}{2}$	0·375	0·875	0	0	0·000	0	0	0·000
y	0	$\frac{1}{2}$	0·375	0·875	0	$\frac{1}{2}$	0·233	0	$\frac{1}{2}$	0·240
z	0	0	0·896	0·875	0·167	0·408	0·275	0·168	0·390	0·292
p	1·18	1·11	1·11	1·13	1·08	1·09	1·00	1·18	1·27	1·04
Polyhedra	AO_4	BO_4	CO_6	DO_6	AO_4	BO_6	CO_6	AO_4	BO_6	CO_6
Mean distance (Å)	1·87	1·90	2·13	2·10	2·01	2·18	2·19	2·01	2·16	2·21
Distances (Å) between minima <3·0	*A–D* 1·80 *B–C* 1·71 *C–C* 2·71 *C–C* 2·94 *C–C* 2·95				*B–B* 2·15 *C–C* 2·62 *C–C* 2·62 *A–C* 2·67 *A–C* 2·67 *A–B* 2·68 *A–B* 2·68			*B–B* 2·57 *A–B* 2·62 *A–B* 2·62 *C–C* 2·73 *C–C* 2·73 *A–C* 2·83 *A–C* 2·83		

References: (1) Emiraliev, Kocharov, Yamzin & Lyubimtsev (1973). (2) Sequeira, Bernal, Brown & Faggiani (1975). (3) Tellgren & Liminga (1972). (4) Jacobson, Collins & Fender (1974). (5) Lundberg (1971). (6) Waltersson, Werner & Wilhelmi (1977*a*). (7) Thomas, Tellgren & Almlöf (1975). (8) Zachariasen & Plettinger (1961). (9) Waltersson *et al.* (1977*b*). (10) Hüllen (1966). (11) Wilhelmi, Walterson & Löfgren (1977).

For each of six tested structures only one minimum was obtained, closely corresponding to the true Li site. In three other test calculations given in Table 1 the number of minima exceeded that of the Li atoms present.

There are 36 Li atoms in the unit cell of Li_2WO_4(i) (Zachariasen & Plettinger, 1961). Thus two of the five minima ought to represent true Li positions. The *C* and *D* minima both yield improbable Li coordinations (see Table 1), while the other three minima result in acceptable LiO_4 tetrahedra. The very short *A*—*B* separation of 1·08 Å shows that only one of the two minima *A* and *B* is possible as a Li site. Therefore the *E* position must be occupied by Li atoms. The short *A*—*E* distance of 2·58 Å indicates that the *B* rather than the *A* position represents the remaining Li site. This conclusion is also supported by the R_{Li-Li} value estimated for LiO_4 tetrahedra sharing corners: $R_{Li-Li} \sim 0.75\ (2 \times 0.59 + 2 \times 1.35) = 2.91$ Å.

The maps for Li_2WO_4(ii) gave five minima, all with reasonable *p* values. Two of the minima giving 16 positions in the unit cell should represent the Li sites. The number of Li atoms in LiHCOO.H_2O (Thomas, Tellgren & Almlöf, 1975) shows that only one of the four minimum positions is occupied by Li atoms. The true minima in these two tests were obtained in a similar manner to those in Li_2WO_4(i) (see Table 1).

The structure of $Li_2WO_4.\frac{4}{7}H_2O$ was reported by Hüllen (1966). He concluded that all the Li atoms would be situated in tetrahedral coordination with the Li—O mean bond lengths: Li(1)O_4: 1·83; Li(2)O_4: 1·84; Li(3)O_4: 1·90 and Li(4)O_4: 1·73 Å. All these mean distances are unreasonably short for LiO_4 tetrahedra as judged by the bond lengths estimated from effective ionic radii given by Shannon (1976). Moreover, he suggested a tetrahedral interstice of a tetramer complex, $W_4O_{16}^{8-}$ as a likely site for Li(4) resulting in a LiO_4 tetrahedron sharing all the four faces with WO_6 octahedra. This result seems to be unrealistic. Therefore it was of interest to predict the Li positions in this structure.

The map calculations resulted in four minima (see Table 1). There are 14 Li atoms in the unit cell, which indicates that the *C* position in point set 12(*i*) must be occupied by Li atoms, and from the Li—O distances the *D* site in point set 4(*e*) (with half occupancy) seems to be a likely Li position. Therefore the 14 Li atoms in the unit cell are assumed to be situated in:

		x	*y*	*z*
C	12(*i*)	0·375	0·375	0·896
D	0·5 × 4(*e*)	0·875	0·875	0·875.

These positions are completely different from those that have been published. A redetermination of this structure by use of a neutron powder diffraction data set is in progress.

The structure of Li_2WO_4(iii) (Wilhelmi, Waltersson & Löfgren, 1977) was derived from single-crystal X-ray diffraction data. The Li positions (16 in the unit cell) were not determined. There are three minima in the maps giving altogether 16 locations in the unit cell (see Table 1).

The three minima result in short Li—Li separations (*e.g.* *B*–*B* 2·15 Å). Therefore, the influence on the minimum positions of the symmetry function described above was examined. The new positions thus obtained all result in acceptable Li—O coordinations and Li—Li distances (*e.g.* *B*–*B* 2·57 Å) (see also Table 1). Therefore, the 16 atoms in the unit cell are assumed to be situated in:

		x	*y*	*z*
A	4(*e*)	0	0	0·17
B	4(*f*)	0	$\frac{1}{2}$	0·39
C	8(*h*)	0·00	0·24	0·29.

This method gives information about all the potential LiO_4 and LiO_6 polyhedra in a given oxygen matrix. The most probable Li sites may be indicated by the Li—O and Li—Li separations among alternative suggestions. No other types of Li coordinations than LiO_4 and LiO_6 polyhedra have been tested.

The conclusion is that this method may be useful as a tool for determining Li positions in the presence of heavy atoms in crystal structures derived from X-ray diffraction data sets. The accuracy in the Li coordinates is comparable to that obtained by locating atomic positions from Fourier maps.

I am grateful to Professor Arne Magnéli and Dr Karl-Axel Wilhelmi for stimulating interest and discussions and to Dr Sven Westman for revising the English text.

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Acta Cryst. (1978). A**34**, 905–908

Dynamic Density and Structure Factors for Rigid Molecules with Large Librations

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(*Received* 17 *March* 1978; *accepted* 22 *May* 1978)

For rigid molecules which undergo large librations, the dynamic density and the dynamic molecular scattering factor are derived. The general case is treated where translations and librations of the molecule are coupled (no site symmetry). The dynamic molecular scattering factor is an integral which cannot generally be solved, and temperature factors generally do not appear. For the special case of statistically independent translations and librations, a temperature factor for the translations of the molecule is obtained. Moreover, temperature factors are obtained for density units which are spherically symmetric, since the motions of these density units can be described by translations only. The possible cases for which spherically symmetric density units can be assumed and, hence, temperature factors can be applied, are discussed.