which should lead to a speed up by a factor of five. We expect this will bring the phase-extension capabilities of *MICE* up to those of *SAYTAN*; the superiority of likelihood over other figures of merit should then confer a definite advantage to the maximum-entropy approach over other direct methods. We will put these expectations to the test by attempting the direct structure determination of APP as soon as possible.

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Elastic-Tensor Atom–Atom Potential Calculations for Molecular Crystals: C_6H_6 and $CO(NH_2)_2$

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Abstract

The numerical method for calculating the elastic constants of molecular crystals, using the crystal packing program *PCK*83, developed and applied to the model case of CO_2 in previous work is here extended to benzene (C_6H_6) and urea [$(NH_2)_2CO$] crystals. Interatomic potential-energy functions coupled with rigid-molecule constraints are used, taking the entire angular dependence into account. Correlation with other calculations and experimental data is good.

Introduction

Various methodologies for modelling intermolecular and interatomic forces in crystals have been developed over the years, in crystal packing programs such as *PCK*83 (Williams, 1983) and *WMIN* (Busing, 1981), with a view to predicting their physicochemical properties (Catlow, Cox, Jackson, Parker, Price, Tomlinson & Vetrivet, 1989; Kitaigorodsky, 1973, 1978). Of particular interest, and the subject of this paper, are the elastic constants of crystals, which are related to the second derivatives of the energy hypersurface at the minimum. Knowledge of the elastic behaviour of solids is of importance in, for example, investigating the effects of strain on crystal growth.

The general theory of modelling the elastic properties of solids developed by Born & Huang (1968) has been applied to ionic systems by Catlow & Norgett (1976) and Catlow & Mackrodt (1982) and extended to the study of molecular crystals by Walmsley (1968*a*, *b*, 1987). An alternative approach is the numerical method developed by Busing & Matsui (1984), using *WMIN*, to simulate the application of external forces.

In the present paper, the numerical method of calculating the elastic constants of molecular crystals using the packing analysis program *PCK*83 (Williams, 1983), developed and applied to the model case of CO_2 in previous work (Pavlides, Pugh & Roberts 1991*a*), is extended to benzene and urea crystals. The elastic constants of CO_2 are also recalculated in an attempt to address the problem of symmetry relaxation, occurring upon distorting the lattice, in more detail. Within the numerical limitations

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of the method, inherent in any technique involving an optimization routine, its predictive ability was found to be satisfactory. Analytical equations for the elastic constants of molecular crystals have also been developed by the present authors within the pair-potential rigid-molecule approximation, taking interatomic rather than intermolecular interactions into account (Pavlides, Pugh & Roberts, 1991*b*). The results of the analytical method for the tensor components of CO_2 are in very good agreement with those of the present method obtained with the same set of atom–atom potentials.

Details of the method

In the pair potential approximation employed in the present paper, the intermolecular or non-bonded energy of the lattice is approximated by a sum of terms each referring to a pair of atoms in different molecules. Furthermore, in the rigid-molecule approximation, also used in the present calculations, no intramolecular effects are taken into account, which is valid to a first approximation, since in molecular crystals intramolecular forces are characteristically stronger than intermolecular forces. For larger molecules, however, this becomes less defensible.

The energy of the lattice may be considered as a hypersurface, *i.e.* a function of the elementary cell parameters and the variables describing the internal dispositions of the constituent molecules. The deepest minimum obtained on this surface by minimizing with respect to the above variables corresponds to the optimal atomic configuration, which will approach the experimental one as closely as possible if the interatomic potentials of a given class of compounds are fitted to their structural and physical properties. It can be shown that the elastic constants, which correlate crystal strain and applied stress through

$$\sigma_i = c_{ij}\varepsilon_j, \qquad (1)$$

can be related to the second derivatives of the lattice energy, *i.e.* of the energy hypersurface at the minimum, with respect to the strain parameters (Kitaigorodsky & Mirskaya, 1964):

$$c_{ij} = \left[\frac{\partial^2 E}{\partial\varepsilon_i\,\partial\varepsilon_j}\right]_0. \qquad (2)$$

In the above σ_i and ε_i $(i = 1, \ldots, 6)$ are the six independent components of the stress and strain matrices respectively and c_{ij} $(i, j = 1, \ldots, 6)$ are the elastic constants. In (1) the repeated index summation convention is assumed and the Voigt notation used. In the limits of linear elasticity, the strain energy per unit volume, E, as obtained from (2), is

$$E = \tfrac{1}{2}c_{ij}\varepsilon_i\varepsilon_j. \qquad (3)$$

The above is a bivariant quadratic holding only in the harmonic approximation, in which higher-order terms are neglected. The elastic constants of a crystal may be obtained by considering the strain energy per unit volume stored due to a homogeneous deformation. On the microscopic level, a homogeneous deformation is one in which a lattice structure is preserved and all cells are equivalent. It is entirely specified by the six independent external strain components, ε_i, describing the changes in the lattice parameters which displace the molecular centres of mass proportionally, three internal translations and three internal rotations per molecule describing the accompanying changes in the positions and orientations of the constituent molecules.

In accord with the above considerations the general method of calculation can be outlined as follows:

(i) The lattice energy is minimized with respect to the lattice parameters and the variables describing molecular positions and orientations relative to some general crystal-fixed Cartesian-axis system. In the initial set-up, for the systems under investigation, the symmetry of the lattice parameters was used and the positions of the molecules were generated by the symmetry operators of the appropriate space group. In subsequently minimizing the energy, all the lattice parameters and molecular variables were allowed to vary independently, in order to obtain the absolute minimum-energy configuration for the given set of potentials. For this purpose, the asymmetric unit was expanded to include all molecules in the unit cell thus eliminating the need for the symmetry operators of the space group.

(ii) The minimum-energy structure obtained in (i) is distorted by the application of axial or shear strains (bulk components). The changes in the lattice parameters are thus described in terms of the six independent components of ε, according to

$$\mathrm{d}p = \sum_{i=1}^{6} (\partial p/\partial\varepsilon_i)_0\,\mathrm{d}\varepsilon_i \qquad (4)$$

where p can be a, b, c, α, β or γ. The derivatives of p with respect to ε_i evaluated at zero strain are given by

$$(\partial r'/\partial\varepsilon_{ij})_0 = r_ir_j/r\,(2 - \delta_{ij}) \qquad (5)$$

for the cell dimensions $r = a$, b, c and

$$(\partial\theta'/\partial\varepsilon_{ij})_0 = (rs\sin\theta)^{-1}[r_is_j + r_js_i + (\cos\theta/rs)(r^2s_is_j + s^2r_ir_j)](2 - \delta_{ij}) \qquad (6)$$

for the cell angles $\theta = \alpha$, β, γ, where $\mathbf{r}$ and $\mathbf{s}$ are the vectors containing θ. The components of $\mathbf{r}$ and $\mathbf{s}$ appearing in the above refer to a general crystal-fixed Cartesian-axis frame. The energy of the distorted lattice is then minimized with respect to the molecular variables to allow for internal relaxation. Again, these are allowed to vary independently with no symmetry restrictions, as described in (i).

(iii) From (ii), strain energy curves were obtained with three pairs of points symmetrically disposed about the equilibrium position and fitted with quadratic functions using a least-squares technique, yielding values for the elastic constants, formally defined in (2). In the limit of linear elasticity, using the appropriate symmetry conditions for c_{ij}, (3) yields expressions of the form

$$\begin{aligned} E &= \tfrac{1}{2}c_{11}\varepsilon_1^2 \\ E &= 2c_{44}\varepsilon_4^2 \qquad (7) \\ E &= \tfrac{1}{2}c_{11}\varepsilon_1^2 + \tfrac{1}{2}c_{22}\varepsilon_2^2 + c_{12}\varepsilon_1\varepsilon_2. \end{aligned}$$

Similar expressions exist for the other non-zero components of the systems under investigation, *i.e.* c_{22}, c_{33}, c_{55}, c_{66}, c_{13} and c_{23}. The first and second equations (7) define strain-energy curves for the uniaxial- and shear-strain components, ε_1 and ε_4 respectively, from which c_{11} and c_{44} are obtained, whereas the third of these equations defines a strain-energy surface for ε_1 and ε_2 from which the biaxial component c_{12} may be obtained. This surface consists of strain ellipses rotated by 45° to the principal-axis system (Pavlides *et al.*, 1991*a*) in which the elastic constants matrix

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{12} & c_{22} \end{pmatrix} \qquad (8)$$

is diagonalized. The diagonal terms are $c_{\bar{1}1} = (c_{11} + c_{12})$ and $c_{\bar{2}2} = (c_{11} - c_{12})$, with similar expressions for the other biaxial components c_{13} and c_{23}. Univariant calculations were performed in the principal-axis system, one with $\varepsilon_2 = \varepsilon_1$ yielding $(c_{11} + c_{12})$ and the second with $\varepsilon_2 = -\varepsilon_1$ yielding $(c_{11} - c_{12})$, from which values for c_{11} and c_{12} were obtained. Again, similar calculations were performed for the other biaxial components. In all cases in the present work, two regions of strain were investigated for $-0{\cdot}03 < \varepsilon < +0{\cdot}03$ and $-0{\cdot}008 < \varepsilon < +0{\cdot}008$, the aim being to obtain as parabolic a curve as possible near the minimum. A major source of error is the numerical accuracy of the minimization procedure which affects the smoothness of the computed curve.

Results and discussion

The systems investigated in the present work are:

(*a*) CO_2 which solidifies in a cubic structure (space group *Pa*3) with a tetramolecular unit cell;

(*b*) C_6H_6 solidifying in orthorhombic form (space group *Pbca*) again with a tetramolecular unit cell;

(*c*) $(NH_2)_2CO$ with tetragonal symmetry (space group $P\bar{4}2_1m$) and a bimolecular unit cell.

Table 1. *Fractional coordinates* (*xyz*) *for the asymmetric units of carbon dioxide* (*Williams*, 1983), *benzene* (*Williams*, 1983) *and urea* (*Swaminathan, Craven & Mullan*, 1984)

Molecule	Atom	*x*	*y*	*z*
CO_2	C	0·0	0·0	0·0
	O1	0·6697	0·6697	0·6697
	O2	−0·6697	−0·6697	−0·6697
C_6H_6	C1	−0·4660	1·3160	−0·0560
	C2	0·4660	−1·3160	0·0560
	C3	−0·9960	0·4270	0·8810
	C4	0·9960	−0·4270	−0·8810
	C5	−0·5310	−0·8890	0·9380
	C6	0·5310	0·8890	−0·9380
	H7	−0·8080	2·2830	−0·0980
	H8	0·8080	−2·2830	0·0980
	H9	−1·7290	0·7410	1·5300
	H10	1·7290	−0·7410	−1·5300
	H11	−0·9210	−1·5430	1·6270
	H12	0·9210	1·5430	−1·6270
$CO(NH_2)_2$	C	0·00000	0·50000	0·32600
	O	0·00000	0·50000	0·59530
	N1	0·14590	0·64590	0·17660
	H1	0·25750	0·75750	0·28270
	H2	0·14410	0·64410	−0·03800
	N2	−0·14590	0·35410	0·17660
	H3	−0·25750	0·24250	0·28270
	H4	−0·14410	0·35590	−0·03800

The lattice parameters and fractional coordinates for the asymmetric unit are given in Table 1. The fractional coordinates for the other molecules in the unit cell are generated *prior* to calculations using the standard symmetry operators for the given space groups as detailed in *International Tables for Crystallography* (1983). For carbon dioxide (CO_2) and benzene (C_6H_6), interactions between atoms of types α and β, functionally dependent on their separation r_{jk}, are described by exp − 6 − 1 potential-energy functions of the form

$$\varphi_{\alpha\beta}(r_{jk}) = -\frac{A_{\alpha\beta}}{r_{jk}^6} + B_{\alpha\beta}\exp(-C_{\alpha\beta}r_{jk}) + \frac{q_\alpha q_\beta}{r_{jk}} \qquad (9)$$

whereas in the case of urea [$O{=}C(NH_2)_2$], 12 − 6 − 1 interatomic functions are used:

$$\varphi_{\alpha\beta}(r_{jk}) = -A_{\alpha\beta}/r_{jk}^6 + B_{\alpha\beta}/r_{jk}^{12} + q_\alpha q_\beta/r_{jk}. \qquad (10)$$

The terms in (9) and (10) represent the London dispersion, the repulsive energy and the Coulomb interactions respectively. The atom–atom parameters (*A*, *B*, *C* and *q*) for these two potentials are detailed in Table 2.

The elementary cell dimensions and angles of the minimum-energy structures obtained in the present calculations for the given set of potentials and no symmetry restrictions are compared with experimental data in Table 3. The elastic constants obtained in the two strain regions mentioned above are presented in Table 4, for all three systems. All calculations refer to the situation at 0 K and zero pressure.

In the case of CO_2 the deviation from cubic symmetry is marginal. The elastic-tensor components obtained herein are in very good agreement with those obtained using the analytical equations developed by Pavlides, Pugh & Roberts (1991*b*) with the same set

Table 2. *Details of the intermolecular potentials used in the calculations*

An exp-6-1 potential was used in calculations on carbon dioxide and benzene and a 12-6-1 potential used in the calculation on urea.

Molecule		*A*	*B*	*C*	*q*	Reference
CO_2	C-C	2439·8	$3\cdot7 \times 10^5$	3·60		(*a*)
	C-O	1656·0	$2\cdot9 \times 10^5$	3·78		(*b*)
	O-O	1129·0	$2\cdot3 \times 10^5$	3·96		(*c*)
	C				0·820	(*b*)
	O				−0·410	(*b*)
C_6H_6	C-C	2439·8	$3\cdot7 \times 10^5$	3·6		(*a*)
	C-H	576·82	$6\cdot63 \times 10^4$	3·67		(*d*)
	H-H	136·4	$1\cdot1 \times 10^4$	3·74		(*a*)
	C				−0·153	(*d*)
	H				0·153	(*d*)
$CO(NH_2)_2$	C-C	5601·0	$1\cdot26 \times 10^7$			(*a*)
	C-O	3428·0	$3\cdot81 \times 10^6$			(*a*)
	C-N	5366·0	$1\cdot10 \times 10^7$			(*a*)
	C-H	0·0	0			(*a*)
	O-O	2098·0	$1\cdot15 \times 10^6$			(*a*)
	O-N	3285·0	$3\cdot3 \times 10^6$			(*a*)
	O-H	0·0	0·0			(*a*)
	N-N	5141·0	$9\cdot49 \times 10^6$			(*a*)
	N-H	0·0	0·0			(*a*)
	H-H	0·0	0·0			(*a*)
	C				0·380	(*e*)
	O				−0·380	(*e*)
	N				−0·830	(*e*)
	H				0·415	(*e*)

References: (*a*) Williams & Cox (1984); (*b*) Williams (1983); (*c*) Cox, Hsu & Williams (1981); (*d*) Williams & Starr (1977); (*e*) Hagler, Huler & Lifson (1974).

Table 3. *Structural data for minimum-energy configuration*

	T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
Carbon dioxide							
Calc.	0	5·6818	5·6808	5·6807	90·00	90·00	90·00
Exp.[a]	83	5·575	5·575	5·575	90·00	90·00	90·00
Benzene							
Calc.	0	7·4206	9·2977	6·9899	90·00	90·00	90·00
Exp.[a]	270	7·460	9·666	7·034	90·00	90·00	90·00
	78	7·292	9·471	6·742	90·00	90·00	90·00
Urea							
Calc.	0	5·5461	5·5508	4·7903	90·04	89·93	89·97
Exp.[b]	Room temp.	5·662	5·5662	4·716	90·00	90·00	90·00
	133	5·582	5·582	4·686	90·00	90·00	90·00

References: (*a*) Williams (1983); (*b*) Swaminathan, Craven & Mullan (1984).

Table 4. *Elastic constants* (10^9 Nm^{-2})

Carbon dioxide

Region of strain	c_{11}	c_{12}	c_{44}
$-0\cdot03 < \varepsilon < +0\cdot03$	11·81	7·13	5·49
$-0\cdot008 < \varepsilon < +0\cdot008$	12·24	6·95	5·29
Other calculations	12·34	7·01	5·51[a]
	13·57	7·38	6·23[b]

Benzene

Region of strain	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
$-0\cdot03 < \varepsilon < +0\cdot03$	8·84	11·76	8·40	2·43	7·81	1·29	8·68	8·15	8·51
$-0\cdot008 < \varepsilon < +0\cdot008$	9·28	12·14	8·87	3·86	7·81	1·72	8·63	8·15	8·87
Other calculations	9·42	11·67	8·87	4·34	6·46	4·04	5·61	6·12	5·48[c]
Experiment (*T* = 138 K)	8·61	10·01	8·63	3·56	6·13	2·10	4·15	5·10	5·38[c]

Urea

Region of strain	c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}
$-0\cdot03 < \varepsilon < +0\cdot03$	18·19	63·90	5·15	23·61	17·71	12·87
$-0\cdot008 < \varepsilon < +0\cdot008$	18·42	61·65	5·12	23·65	17·52	12·58
Experiment	21·7	53·2	6·26	0·45	8·9	24[d]
At room temperature	11·2	-	5·9	8·44	10·2	-[e]

References: (*a*) Analytical method developed by Pavlides, Pugh & Roberts (1991*b*); (*b*) Walmsley (1968*a*); (*c*) Walmsley (1968*b*); (*d*) Fischer & Zarembowitch (1970); (*e*) Kretchetov, Svetlor, Teslenko & Kitaigorodsky (1971).

of potentials. As can be seen, these values are lower than those obtained by Walmsley's intermolecular potential calculations (Walmsley, 1968*a*) in which a Lennard-Jones function and a quadrupole term were used, both being functionally dependent on the intermolecular separation. The present calculations contain more angular dependence by considering interatomic interactions explicitly. All calculations predict the crystal to be elastically anisotropic with $(c_{11}-c_{12})/2c_{44}\simeq 0{\cdot}5$. The Cauchy relation $c_{12}=c_{44}$ is found not to hold, implying that the rigid-molecule approximation introduces an angular dependence of the intermolecular forces which are no longer central.

As in the present calculations, the results obtained by Walmsley (1968*b*) for the benzene crystal are also based on the interatomic potential functions developed by Williams (1966). The agreement between the two is good for all components except the biaxial elements c_{12}, c_{13} and c_{23}, for which univariant calculations in the principal-axis system were performed. Correlation with experiment is also good except for the aforementioned components. As mentioned in Walmsley (1968*b*), the experimental uncertainty for the shear constants is set to 10% as opposed to 2% for the other moduli.

The elastic constants calculated for urea using the potentials developed by Hagler, Huler & Lifson (1974) are in fairly good agreement with experiment. The data at room temperature suggest that there is a fair amount of uncertainty in the experimental values especially for c_{66}. The deviation from tetragonal symmetry in c_{ij} again is only marginal.

Concluding remarks

The elastic constants of molecular crystals may be obtained, using the crystal packing program *PCK*83, to compute strain-energy curves, for strains 10^{-3} to 10^{-2} and fitting them with quadratic unilinear functions. For the given set of atom-atom potentials the absolute minimum-energy configuration was sought and no symmetry restrictions were imposed.

The interatomic potential-energy functions employed, coupled with the rigid-body conditions, take the entire angular dependence into account. The analytical equations developed within the same approximations yield values for the elastic constants of CO_2 which are in very good agreement with those of the present method. Correlation with experiment in some cases is very good.

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