

α -amino-acid conjugates the amphipatic character is more pronounced than in an ω -amino acid.

Crystal packing is predominantly determined by intermolecular hydrogen bonds (Table 5, Figs. 5, 6 and 7). Three different types of hydrogen bonds were observed. In the crystal structures of *N*-(IAA)- β -Ala (1) (Fig. 5), *N*-(IAA)- γ -Abu (2) (Fig. 6) and *N*-(IAA)- ε -Ahx (3) (Fig. 7) the indole N atom acts as a donor to the carboxylic O atom. This type of interaction was not detected in the structure of *N*-(IAA)- δ -Ava (Kojić-Prodić, Nigović, Horvatić *et al.*, 1991). The hydroxyl group of the carboxylic moiety is a proton donor to the peptide O atom; hydrogen bonds of the type O—H...O were observed in all structures of the ω -amino-acid conjugates. Hydrogen bonds between the peptide groups were detected in the structures of *N*-(IAA)- γ -Abu (2) and *N*-(IAA)- δ -Ava (Kojić-Prodić, Nigović, Horvatić *et al.*, 1991). This type of hydrogen bond affects the relative orientation of peptide group towards the indole moiety (Fig. 2). The crystal structure of *N*-(IAA)- γ -Abu (2) is the only one exhibiting all three types of hydrogen bonds.

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A Test of Chlorine and Fluorine Nonbonded Potential Functions with Lattice-Dynamical Calculations

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Abstract

A lattice-dynamical calculation of vibrational frequencies and thermal parameters has been carried out in the harmonic approximation for chloro- and fluorohydrocarbons using the Born–von Kármán formalism in terms of molecular rotations and translations. Several empirical atom–atom potential functions from the literature were considered with or without explicit Coulombic terms. Their performance is analyzed by a comparison between the results of the calculations and experimental data.

Introduction

The atomic displacement parameters which are routinely obtained from a crystal structure determination by diffraction methods may be considered simply as adjustable parameters in the least-squares process. They, however, carry information about the mean atomic displacements which may be useful for correcting bond distances using a rigid-body model (Schomaker & Trueblood, 1968), or to detect the directions of preferred molecular displacements. A review of the meaning and use of displacement

parameters has been given recently by Dunitz, Schomaker & Trueblood (1988).

A precise determination of these parameters is also needed in careful charge-density determinations. Usually, however, they suffer from systematic errors arising mainly from thermal diffuse scattering. An independent determination of the displacement parameters is allowed by lattice-dynamical calculations. So far the best results have been obtained for molecular crystals, especially for hydrocarbons (Filippini, Gramaccioli, Simonetta & Suffritti, 1973; Filippini & Gramaccioli, 1989). Empirical 6-exp atom-atom potential-energy models proved to be very reliable (Pertsin & Kitaigorodsky, 1987). The method has recently been applied to silicates (Pilati, Bianchi & Gramaccioli, 1990), and the effects of molecular non-rigidity have also been considered (Gramaccioli, Filippini & Simonetta, 1982; Gramaccioli & Filippini, 1983; Filippini, 1990).

In the case of heteroatom-containing molecules, the potential model must be expanded to include Coulombic interactions. In an earlier paper (Criado, 1990) we presented calculations for azahydrocarbons, using a 6-exp-1 potential model; in this paper, we consider chloro- and fluorohydrocarbons. In the latter case, there is a previous study (Filippini, Gramaccioli, Simonetta & Suffritti, 1976) where 'reasonable' results were obtained for the displacement parameters using approximate potentials. The method of calculation has been thoroughly described in previous papers (Criado, Conde & Marquez, 1984; Criado, 1989); we have considered rigid molecular units, and molecular translations and rotations. The rigid-body librational tensors and individual atomic displacement parameters were easily obtained by standard procedures. Prior to the lattice-dynamical calculation, an energy minimization process with respect to molecular translations and rotations was carried out.

Potential parameters

Empirical $V(r) = -A/r^6 + B\exp(-Cr)$ potential functions with parameters taken from the literature have been used. For interactions involving carbon and hydrogen atoms the so-called Williams set IVa (Williams, 1967) was adopted (see Criado & Marquez, 1988). For interactions involving chlorine several parameter sets are available (Table 1). Another parameter set (Bonadeo & D'Alessio, 1973) was neglected because the Cl—C mixed interaction curve has no minimum, pointing to a non-physical adjustment. Sets RKW74 (Reynolds, Kjems & White, 1974) and MC78 (Mirsky & Cohen, 1978) are of the 6-exp type whereas BB74 (Bates & Busing, 1974) and LW80 (Hsu & Williams, 1980) 6-exp-1 sets use an atomic point-charge model ($q_C = 0.106$ and

Table 1. Potential parameter sets used in this work

		$V(r) = -A/r^6 + B\exp(-Cr)$			
		Reference	A (kJ mol ⁻¹ Å ⁶)	B (kJ mol ⁻¹)	C (Å ⁻¹)
C—C		(a)	2378.0	350142.0	3.60
C—H		(a)	521.3	36701.0	3.67
H—H		(a)	144.0	11112.0	3.74
Cl—Cl	LW80	(b)	7939.0	950430.0	3.51
	BB74	(c)	7302.0	889410.0	3.52
	RKW74	(d)	9630.0	1783577.0	3.65
	MC78	(e)	12477.0	19176.0	2.26
F—F	WH86	(f)	908.7	403832.0	4.16
	KMKK74	(g)	619.6	175846.0	4.15

References: (a) Williams (1967); (b) Hsu & Williams (1980) (includes 1/r terms with point charges $q_C = 0.106$ e); (c) Bates & Busing (1974) (includes 1/r terms with point charges $q_C = 0.102$ e); (d) Reynolds, Kjems & White (1974); (e) Mirsky & Cohen (1978); (f) Williams & Houpt (1986) [includes 1/r terms with point charges $q = \pm 0.174$ (C—F groups) and $q_C = 0.734$, $q_F = -0.367$ e (CF₂ groups)]; (g) Konshina, Mirskaya, Kozhin & Kozlava (1974).

0.102 e respectively). A detailed explanation of the derivation method of these potential sets can be found in Pertsin & Kitaigorodsky (1987).

For fluorine, set KMKK74 (Konshina, Mirskaya, Kozhin & Kozlava, 1974; Mirsky, 1978) is a 6-exp potential model whereas set WH86 (Williams & Houpt, 1986) is represented by a 6-exp-1 function; in this case, the properties of a series of perfluorohydrocarbon crystals were used in the fit. Point charges were obtained from *ab initio* quantum-mechanical calculations. For the C—F group, a charge of ± 0.174 e was obtained, and for CF₂ groups the charge was 0.734 for C and -0.367 e for F atoms. More sophisticated charge models were considered by these authors, using extra charges, but they gave essentially the same lattice-dynamical results, so we report here results for the simplest model.

Results

A series of halogenated hydrocarbons whose crystal structures have been fully determined have been taken from the literature for this study. Some of the chosen compounds are those considered by Williams and co-workers (Hsu & Williams, 1980; Williams & Houpt, 1986) in the derivation of their potential parameters, for which they obtained an atomic point-charge model; we selected those with reliable experimental displacement parameters. Besides these, some other compounds with similar point-charge distributions have been considered in this work. The chlorohydrocarbon compounds are: α , β and γ phases of *p*-dichlorobenzene (Wheeler & Colson, 1976), 1,2,3-trichlorobenzene (Hazell, Lehmann & Pawley, 1972), pentachlorobenzene (Marsh & Williams, 1981), hexachlorobenzene (Brown & Strydom, 1974), hexachloroethane (Hohlwein, Nägele & Prandl, 1979), octachloronaphthalene (Herbstein, 1979), decachloropyrene (Hazell & Jagner, 1976) and

the complex decachloropyrene-benzene (Hazell, 1978). The chosen fluorohydrocarbons are: the complex naphthalene-octafluoronaphthalene (Potenza & Mastropaolo, 1975), hexafluorobenzene (Boden, Davis, Stam & Wesselinck, 1973), perfluoro-1,2;3,4;5,6-triethanobenzene (1), $C_{12}F_{15}$ (Cobbledick & Einstein, 1976), and perfluorododecahydrotetracyclopentacyclooctene (2), $C_{20}F_{24}$ (Cobbledick & Einstein, 1977).

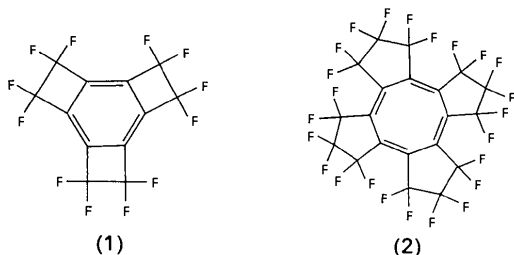


Table 2. Calculated and experimental lattice energies (kJ mol^{-1}) for the different chlorohydrocarbon compounds using the four potential sets, and the corresponding R disagreement factors

	Experimental (reference)	Calculated			
		LW80	BB74	RKW74	MC78
α - p -Dichlorobenzene	64.8 (a)	75.1	73.5	78.0	71.2
β - p -Dichlorobenzene	63.0 (a)	74.2	72.8	77.0	71.9
γ - p -Dichlorobenzene	-	79.3	77.5	79.2	71.8
1,2,3-Trichlorobenzene	65.7 (b)	81.2	79.9	85.3	77.1
Pentachlorobenzene	-	95.2	91.3	110.9	97.8
Hexachlorobenzene	91.7 (c)	97.2	91.9	126.0	109.2
Hexachloroethane	69.1 (e)	-	-	89.3	74.6
Octachloronaphthalene	-	38.9	132.5	171.8	152.7
Decachloropyrene	-	184.9	177.1	226.4	207.6
Decachloropyrene-benzene	-	267.7	261.6	271.0	252.2
R disagreement factor		0.111	0.072	0.288	0.137

References: (a) Walsh & Smith (1961); (b) Weast (1970); (c) Sears & Hopke (1949); (d) Stull, Westrum & Sinke (1969); (e) Chao, Rodgers, Wilhoit & Zwolinski (1974).

energy minimization process are similar, but, surprisingly, the lattice-dynamical calculations with the WH86 potential set produced imaginary frequencies for three compounds and a large disagreement in displacement parameters for the fourth. In Table 5 we show the calculated lattice energies and R discrepancy factors. The observed and calculated (KMKK74 set) displacement parameters have been deposited.*

Discussion

Considering the chlorohydrocarbon calculation, we note that both 6-exp-1 and 6-exp models give acceptable lattice-dynamical results indicating that $1/r$ Coulombic terms are not so important as in the case of azahydrocarbons (Criado, 1990). Besides, test calculations for hexachloroethane show that the omission of atomic point charges does not preclude the attainment of good agreement factors for the calculated quantities.

Looking at the R disagreement factors (Table 4) we observe that the values for the three phases of p -dichlorobenzene are somewhat high, with the calculated parameters lower than the experimental ones. This fact may be ascribed to the probable existence of static disorder (Wheeler & Colson, 1976) which leads to an overestimation of the experimental thermal parameters. On the other hand, octachloronaphthalene, decachloropyrene and the complex decachloropyrene-benzene also show a large disagreement. This may be a result of molecular flexibility caused by the large atomic mass of the peripheral Cl atoms, which gives rise to a relaxation of the lattice modes and consequently an increase of the experimental U_{ij} values with respect to a rigid-

For chlorohydrocarbons a Newton-Raphson minimization of the lattice energy was carried out for all the compounds and for the four potential sets. In the case of hexachloroethane we could not use the 6-exp-1 potentials because a point-charge model for the $C-Cl_3$ group is lacking. Table 2 shows the calculated lattice energy after minimization for the different compounds and potentials, together with the experimental data where available. The lattice vibration frequencies have been measured for most of these compounds and they provide useful information for assessing the reliability of the different potential sets. Table 3 shows the calculated and experimental frequencies.

The individual atomic displacement parameters U_{ij} have also been calculated using the four different potential sets; disagreement factors between experimental and calculated parameters are displayed in Table 4. The potential models LW80 and BB74 give the best results (in fact, the two sets are almost coincident). Nevertheless, in the case of pentachlorobenzene the Coulombic models gave rise to an unstable frequency pattern and, therefore, a test calculation of the displacement parameters was made using only the 6-exp part, which yielded a stable configuration. Some selected calculated and observed atomic displacement parameters (LW80 potential) have been deposited as supplementary material.*

Regarding the fluorohydrocarbons, a similar process has been carried out for the four chosen compounds using two potential sets. The results of the

* Lists of selected calculated and experimental thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54844 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* See deposition footnote.

Table 3. Observed and calculated lattice frequencies (THz) of the chlorohydrocarbon compounds with the four potential sets together with the corresponding disagreement factors

$$R = \sum_i |\nu_i(\text{exp.}) - \nu_i(\text{calc.})| / \sum_i \nu_i(\text{exp.})$$

	LW80	BB74	RKW74	MC78	
<i>α-p</i> -Dichlorobenzene: observed ^{a,b} at 77 K, calculated at 100 K					
<i>A_g</i>	3.208	3.157	3.125	3.275	3.105
	1.949	1.638	1.605	1.732	1.470
	–	1.524	1.489	1.614	1.336
<i>B_g</i>	3.418	3.347	3.306	3.479	3.249
	1.739	1.715	1.680	1.719	1.370
	0.960	0.869	0.864	0.825	0.723
<i>A_u</i>	1.918	1.641	1.581	1.798	1.497
	1.319	1.154	1.117	1.312	1.104
<i>B_u</i>	0.810	0.995	0.949	1.055	0.640
<i>R</i>		0.077	0.090	0.057	0.141
<i>β-p</i> -Dichlorobenzene: observed ^c at 300 K, calculated at 100 K					
	2.519	3.205	3.198	3.197	2.993
	1.679	1.512	1.471	1.511	1.441
	1.349	1.275	1.248	1.380	1.263
<i>R</i>		0.167	0.178	0.158	0.144
Hexachlorobenzene: observed ^d at 300 K, calculated at 293 K					
<i>A_g</i>	1.679	1.849	1.767	2.061	1.184
	1.349	1.335	1.279	1.442	0.974
	0.630	0.678	0.646	0.760	0.456
<i>B_g</i>	1.619	1.781	1.703	1.985	1.210
	1.139	1.225	1.171	1.343	0.873
	0.750	0.794	0.760	0.864	0.500
<i>A_u</i>	1.529	1.697	1.601	1.904	1.034
	–	1.261	1.196	1.411	0.749
<i>B_u</i>	–	0.724	0.690	0.804	0.481
<i>R</i>		0.080	0.043	0.191	0.283
Hexachloroethane: observed ^e at 300 K, calculated at 294 K					
<i>A_g</i>	1.019			1.279	0.825
	0.854			1.025	0.645
	0.630			0.805	0.500
<i>B_{1g}</i>	–			1.961	1.200
	–			1.835	1.094
	0.885			0.870	0.502
<i>B_{2g}</i>	1.649			1.664	1.087
	1.109			1.308	0.882
	–			0.931	0.632
<i>B_{3g}</i>	–			1.765	1.046
	1.379			1.464	0.908
	0.900			1.008	0.637
<i>A_u</i>	–			1.667	0.967
	–			1.471	0.923
	–			1.098	0.681
<i>B_{1u}</i>	1.649			1.685	1.096
	1.019			1.260	0.851
<i>B_{2u}</i>	–			1.852	1.127
	–			0.854	0.473
<i>B_{3u}</i>	–			1.429	0.915
	–			0.810	0.544
<i>R</i>				0.118	0.285

References: (a) Ito, Suzuki & Yokoyama (1968); (b) Wyncke, Hadni & Gerbaux (1970); (c) Burgos, Bonadeo & D'Alessio (1975); (d) Bates, Thomas, Bandy & Lippincott (1971); (e) Woost & Bougeard (1986).

body model, as in our case. This is in agreement with the fact that in the dodecachloropyrene–benzene crystal the calculated U_{ij} values for the 'rigid' benzene units show a good agreement with experimental ones, whereas those of the dodecachloropyrene unit do not.

A more realistic lattice-dynamical calculation should take into account the intramolecular degrees of freedom but this depends on the availability of intramolecular force fields, which are not usually available because they are difficult to model.

Table 4. *R* disagreement factors obtained for the thermal parameters of the chlorohydrocarbon compounds with the four potential sets

$$R = \sum_i \sum_j |U_{ij}(\text{exp.}) - U_{ij}(\text{calc.})| / \sum_i \sum_j |U_{ij}(\text{exp.})|$$

	LW80	BB74	RKW74	MC78
<i>α-p</i> -Dichlorobenzene	0.358	0.331	0.383	0.166
<i>β-p</i> -Dichlorobenzene	0.310	0.295	0.300	0.219
<i>γ-p</i> -Dichlorobenzene	0.282	0.249	0.296	0.120
1,2,3-Trichlorobenzene	0.146	0.195	0.107	0.444
Pentachlorobenzene	0.170	0.216	0.139	1.074
Hexachlorobenzene	0.135	0.145	0.227	1.056
Hexachloroethane	–	–	0.267	0.819
Octachloronaphthalene	0.392	0.346	0.477	0.385
Decachloropyrene	0.548	0.504	0.626	0.251
Decachloropyrene–benzene	0.305	0.268	0.366	0.367

Table 5. Calculated and experimental lattice energies (kJ mol⁻¹) of the fluorocarbon compounds, and *R* disagreement factors for the calculated displacement parameters U_{ij} values (RMKK74 set)

	E_{exp} (reference)	E_{calc}	<i>R</i>
Hexafluorobenzene	– 56.6 (a)	– 55.6	0.16
Naphthalene–octafluoronaphthalene	–	– 165.8	0.10
Perfluoro-1,2,3,4,5,6-triethanobenzene	–	– 94.6	0.12
Perfluorododecahydrotetracyclopentacyclooctene	–	– 113.3	0.26

Reference: (a) Counsell, Green, Hales & Martin (1981).

Regarding the fluorohydrocarbon results, the most surprising result is the fact that the parameters derived by Williams & Houpt (1986) give unstable lattice dynamics for the compounds considered here. In fact, the parameter sets developed by this research group over the last 25 years for different chemical species just from static considerations, proved to be extensible to lattice-dynamical calculations in a very satisfactory way. As a test, we have repeated the calculations omitting the Coulombic interactions; the results were similar, indicating that the 6-exp part may be the source of the problem. The closest F...F non-bonded contacts correspond to a highly repulsive force for this potential set, giving rise to the instability. This fact seems to be related with the comment made by Williams & Houpt (1986) that the van der Waals radii for fluorine atoms which would correspond to their potential (1.44 Å) are larger than the experimental ones (1.35 Å).

Similar negative results have been found by Dove, Powell, Pawley, Chaplot & Mierzejewski (1989) in a recent study of the phonon curves of 1,3,5-trichloro-2,4,6-trifluorobenzene using the potential sets developed by Williams and co-workers. (Hsu & Williams, 1980; Williams & Houpt, 1986). According to our work this may result from the fluorine contribution to the force field.

The KMKK74 6-exp potential set, on the contrary, gives a reasonable agreement between calculated and experimental displacement parameters and may be used for lattice-dynamical purposes until a

more reliable potential including Coulombic interactions is developed.

Concluding remarks

The comparison of experimental and calculated lattice energies, lattice frequencies and displacement parameters allows us to recommend the 6-exp-1 potentials BB73 and LW80 for modelling the statics and dynamics of molecular crystals containing chlorine atoms. In the case of fluorine, displacement parameters are the only experimental piece of information for comparison and the KMKK74 potential set turns out to be the best choice.

We must also point out that the test of the potentials made here is not complete since there are few Cl...H or F...H interactions for the crystal structures considered and these interactions usually play an important role in the packing.

A general remark concerning potentials for chlorine and fluorine atoms is that, although acceptable, the results are less satisfactory than in the hydrocarbon case. We think, however, that this must be ascribed to the fact that some potential-energy contributions are missing from the proposed potential model (such as polarizability), rather than to a failure of the 6-exp-1 potential parameters themselves.

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