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Molecular-Packing Analysis of Molecular Complexes Containing Hexafluorobenzene or Fluoranil

By Tor Dahl

Institute of Mathematical and Physical Sciences, University of Tromsø, N-9000 Tromsø, Norway

Abstract

Molecular-packing analyses of nine molecular complexes between hexafluorobenzene or fluoranil and methylated benzenes or aromatic amines have been performed using lattice-energy calculations in the atom-to-atom approach. Energy minimization with molecular orientations and positions and cell parameters as variables gave, for most of the complexes, structures somewhat different from the experimental structures. Minimization of energy was also performed with only the crystallographic axes as variables. For the experimental structures and the structures obtained after the energy minimizations the contributions to the lattice energy from dispersion, repulsion and Coulombic interactions within one single stack and between different stacks were calculated. The results indicate that for some complexes there are stacking interactions in addition to those predicted by the analytical potentials, which have a substantial effect on the molecular packing. For other complexes, where the interactions in the stacks are weak, the molecular packing seems to be influenced by additional interactions between different stacks, probably directional F···H interactions.

Introduction

Lattice-energy calculations based on analytical atom-to-atom potentials show that for many compounds the molecular packing giving the lowest calculated energy agrees fairly well with that of the experimental structure (Williams & Cox, 1984). In molecular complexes, however, there are usually special kinds of interactions, not included in the analytical potentials, in addition to the traditional van der Waals interactions. These additional interactions may cause differences between the experimental and lowest-energy structures. The purpose of the present work was to analyse such differences in complexes containing hexafluorobenzene (HFB) or tetrafluoro-p-benzoquinone (fluoranil) and from the observed trends try to draw conclusions concerning special kinds of interactions in these complexes.

The nature of the molecular complexes containing HFB has been a matter of dispute (Swinton, 1974). In the crystalline state the partner molecules are stacked alternately in infinite columns as in ordinary charge-transfer complexes, but the importance of charge-transfer interactions is doubtful because of the low electron affinity of HFB (Wentworth,

Limero & Chen, 1987) and the absence of charge-transfer bands in the spectra of many of these complexes. Crystal structures of complexes between HFB and methylated benzenes or aromatic amines show clear trends regarding intermolecular distance and molecular overlap in the stacks (Dahl, 1988). These trends demand an explanation.

Clear trends are also observed when the structures of the HFB complexes are compared with those of the fluoranil complexes with the same partner molecules. Fluoranil has approximately the same molecular shape as HFB, but has a much higher electron affinity and forms relatively strong charge-transfer complexes (Foster, 1969). The differences in structure may thus possibly be effects of charge-transfer interactions. It would be of interest to have this confirmed.

The complexes included in the present analysis are the HFB complexes with p-xylene, mesitylene, durene, hexamethylbenzene (HMB), N,N-dimethyl-aniline (DMA), $N,N,3,5$-tetramethylaniline (TMA) and N,N,N',N'-tetramethyl-p-phenylenediamine (TMPDA), and the fluoranil complexes with durene and HMB. References to the crystal structures are given in Table 1 and, except for the TMA–HFB (Dahl, 1989a) and HMB–fluoranil (Dahl, 1989b) structures, also in a review article (Dahl, 1988). Some results of the lattice-energy calculations on complexes between HFB and aromatic amines were reported in connection with the TMA–HFB structure. The structure of the complex between HFB and N,N-dimethyl-p-toluidine has also been published (Dahl, 1981b), but is regarded as uncertain because of disorder. In the complex between fluoranil and DMA (Dahl, 1981a) the effect of charge-transfer interactions seems unquestionable and cannot be further elucidated by this kind of analysis. The two latter complexes have therefore not been included in this series of calculations.

Description of the calculations

Using the computer program $PCK83$ (Williams, 1983) the lattice energy was calculated from the expression

$$E = \sum\sum - A_{jk} r_{jk}^{-6} + B_{jk} \exp(- C_{jk} r_{jk}) + q_j q_j r_{jk}^{-1}.$$

All intermolecular distances r_{jk} up to 9 Å were included in the sums and convergence acceleration was used. The non-bonded potential parameters A_{jk}, B_{jk} and C_{jk} were those given by Williams & Houpt (1986), Williams & Cox (1984) and Cox, Hsu & Williams (1981). The net atomic charges, q, were calculated by the $AM1$ method (Dewar, Zoebish, Healy & Stewart, 1985), using the computer program $GAUSSIAN86$ (Frisch et $al.$, 1984), except for the HFB molecule, where potential-derived charges

reported by Williams & Houpt (1986) were used. The calculations of atomic charges and lattice energies were based on the molecular geometries of the X-ray structures for complexes where these geometries are relatively accurately determined. For those where they are less accurately determined and where the H positions have not been found, adjustments were made and H positions calculated in agreement with known molecular structures of the pure compounds or with reasonable assumptions. For all complexes, however, the C—H distances were adjusted to be 1·08 Å in the charge calculations and 1·00 Å in the lattice-energy calculations, as the calculation of potential parameters for H was based on a slight foreshortening of the bond distance (Williams & Cox, 1984).

Lattice-energy calculations were performed for the experimental structures and for the structures giving the lowest calculated energy after varying molecular orientations and positions and cell parameters (the minimum-energy structures). In these energy minimizations centres of symmetry in all complexes and one twofold screw axis in each of the complexes mesitylene–HFB and TMA–HFB were kept. All other crystallographic symmetry elements were removed. As the minimizations may give local minima, they were also performed with the HFB or fluoranil molecules in starting orientations different from those of the experimental structures. For the HFB complexes with durene and TMA the lowest minima were obtained from such alternative starting orientations. For some of the complexes energy minimizations were also made with the torsion angles of the methyl groups included in the variable parameters. This increased the computing time considerably, but had little effect on the minimum-energy structures.

Minimum-energy structures should ideally be compared with low-temperature experimental structures. If they are compared with room-temperature structures the differences in calculated energy are largely results of differences in packing density. The structures giving the lowest lattice energy after varying only the length of the crystallographic axes (the optimum-density structures) were therefore calculated. By comparing the energy of the minimum-energy structures with that of the optimum-density structures the importance of molecular orientations and positions for the lattice energy may be estimated. In addition, the shifts in the axes in the packing-density optimizations give indications of the strength of the intermolecular interactions in different directions.

By increasing the crystallographic axes except the stack axis the stacks may be removed from each other so that only distances within one single stack are included in the energy calculations. In this way

Table 1. *Mean interplanar distances* (Å) *in the stacks*

Compound	Exp. structure	Optimum-density structure	Minimum-energy structure	Reference*
p-Xylene–HFB	3·547	3·416	3·420	ACAPCT 29 170
Mesitylene–HFB	3·557	3·409	3·411	ACSAA4 25 1031
Durene HFB	3·507	3·424	3·410	ACAPCT 29 699
HMB–HFB	3·433	3·424	3·485	ACSAA4 27 995
DMA–HFB	3·386	3·402	3·393	ACSCEE 41 931
TMA–HFB	3·514	3·432	3·434	ACSAA4 43 172
TMPDA–HFB†	3·438	3·354	3·371	ACAPCT 33 665
TMPDA HFB‡	3·426	3·407	3·371	ACAPCT 33 665
Durene–fluoranil	3·383	3·445	3·426	ACBOCV 39 423
HMB–fluoranil	3·317	3·429	3·511	ACSAA4 In press

* See *Notes for Authors* (1983) for a description of journal Codens.
† HFB in major orientation.
‡ HFB in minor orientation.

the contributions to the energy from such intrastack contacts and, by subtraction, also from interstack contacts were obtained.

The experimental structures are room-temperature structures except for mesitylene–HFB, HMB–HFB, DMA–HFB and HMB–fluoranil, where the data were collected at 238, 233, 120 and 223 K, respectively. Some of the structures are disordered with the HMB or the fluoranil molecule in two or more orientations. For complexes where these orientations are crystallographically equivalent or the minor orientations have low occupancy factors only one of the orientations was included in the experimental structure. Two orientations were therefore included only for the TMPDA–HFB complex.

Results and discussion

Interplanar distances in the experimental structures, the optimum-density structures and the minimum-energy structures are given in Table 1. Shifts in the crystallographic axes in the packing-density optimizations are given in Table 2. Lattice energies and their components for the experimental structures, the optimum-density structures, and the minimum-energy structures are given in Table 3. The molecular overlaps in the experimental structures and the minimum-energy structures are shown in Fig. 1.

Attempts at varying the potential parameters in order to obtain a better agreement between the experimental and minimum-energy structures were unsuccessful. Moderate variations in the net atomic charges have some effect on the interplanar distance, but little effect on the molecular overlap in the minimum-energy structures. As different methods have been used for the calculation of charges in the HFB and fluoranil molecules, the Coulombic energy for their complexes are not directly comparable. AM1 calculations on HFB give charges which are only 44% of those found by the potential-derived charge method. However, all arguments below concerning the fluoranil complexes hold even when the

charges in fluoranil used in the energy calculations are more than doubled.

The interpretation of the results is based on the assumption that the relatively simple analytical potentials describe the ordinary van der Waals interactions correctly. This very rough approximation is to some degree justified by the results of calculations on other compounds (Williams & Cox, 1984). Furthermore, the temperature has been assumed to affect only the packing densities. This is not correct if the entropy is sensitive to changes in other features of the molecular packing, so that $T\Delta S$ becomes significant for such changes at room temperature. However, comparisons of the low-temperature and room-temperature stuctures of the DMA–HFB and
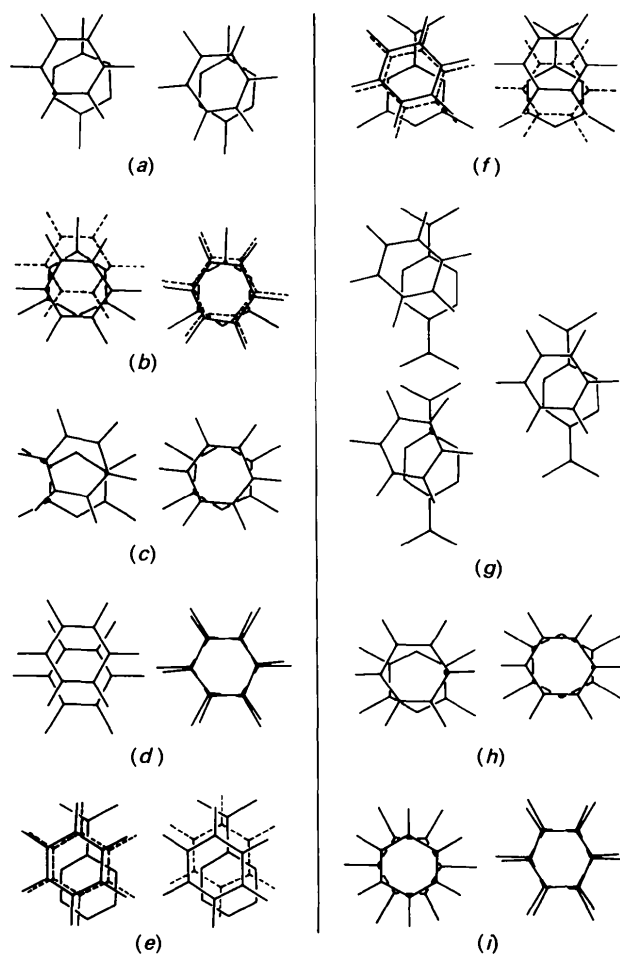

Fig. 1. The overlap of the molecules viewed perpendicular to their average plane for the experimental structures (left) and the minimum-energy structures (right). The complexes are (a) p-xylene–HFB, (b) mesitylene–HFB, (c) durene–HFB, (d) HMB–HFB, (e) DMA–HFB, (f) TMA–HFB, (g) TMPDA–HFB with HFB in the major orientation (top) and in the minor orientation (bottom), (h) durene–fluoranil, and (i) HMB–fluoranil.

HMB–fluoranil complexes show that the assumption is approximately correct for at least some of these complexes. Thus, although disagreements between experimental and minimum-energy structures may be due to shortcomings in the potentials or to entropy effects, it is believed that if clear trends in these disagreements are observed, the possibility of additional interactions may be worth considering.

A striking feature of complexes between HFB and methylated benzenes is the decrease in interplanar distance as the number of methyl groups increases. It appears from Table 1 that this trend is found neither in the minimum-energy structures nor in the optimum-density structures, where the molecular overlap is the same as in the experimental stuctures. For similar reasons the observation that the inter-planar distances in the fluoranil complexes are much shorter than those in the HFB complexes with the same partner molecules cannot be explained from the analytical potentials. This indicates additional stacking interactions in some of the HFB complexes and stronger such interactions in the fluoranil complexes.

As expected most of the crystallographic axes decrease considerably in the optimizations of the packing density, except those of the DMA–HFB complex, which were measured at low temperature. Table 2 shows, however, that for some complexes the stack axis decreases considerably less than the other axes, or even increases. The effect is most pronounced for the two fluoranil complexes and the HMB–HFB complex. This may be interpreted as an indication of stronger stacking interactions than those predicted by the energy calculations. For similar reasons Table 2 indicates that in some other complexes there are particularly strong interactions along one of the other axes. In the HFB complexes with mesitylene (Dahl, 1971) and durene (Dahl, 1975) strikingly short contacts along the b axis between an F atom and a methyl group have been called attention to. The results of these calculations thus seem to confirm the importance of these contacts. No particularly short contacts along the a axis to the major orientation of the HFB molecule are observed in the TMPDA–HFB complex. To the minor orientation, however, there is an F$\cdots$H contact of 2·18 Å in this direction, which may explain the short a axis in this complex. These results therefore indicate that the importance of F$\cdots$H contacts between different stacks has been underestimated in the energy calculations for these complexes.

Another striking feature of complexes between HFB and methylated benzenes is that an increasing number of methyl groups result in a more parallel orientation of the benzene rings of the overlapping molecules. The same trend is also observed for the minimum-energy structures (Fig. 1) and it may thus

Table 2. *Shifts in crystallographic axes* (%) *in the packing-density optimizations*

For each compound the stack axis is marked with an asterisk.

Compound	Δa	Δb	Δc
p-Xylene–HFB	−2·3	−2·9	−3·7*
Mesitylene–HFB	−2·4	−0·8	−4·2*
Durene–HFB	−3·4	−0·5	−2·4*
HMB–HFB	−2·0	−2·3	−0·3*
DMA–HFB	+0·5*	−0·3	+0·1
TMA–HFB	−2·3*	−3·3	−2·6
TMPDA–HFB†	+2·4	−2·5*	−2·4
TMPDA–HFB‡	+0·6	−0·5*	0·0
Durene–fluoranil	+1·8*	−4·0	−0·9
HMB–fluoranil	−1·5	−0·5	+3·4*

† HFB in major orientation.
‡ HFB in minor orientation.

be explained without considering interactions other than those included in the analytical potentials. For some of the other complexes, however, especially the HMB–fluoranil complex, there are substantial differences between the relative orientations of the overlapping molecules in the experimental structures and in the minimum-energy structures. It also appears from Fig. 1 that in the complexes of HFB the relative displacement of the centres of the overlapping molecules is larger in the experimental structures than in the minimum-energy structures, where in some cases the molecules have a direct face-to-face overlap. The largest disagreement in this respect is observed for the HMB–HFB complex. Only for the DMA–HFB structure is the molecular overlap in the minimum-energy structure very close to that in the experimental structure.

Partition of the total energy into dispersion, repulsion and Coulombic energy is quite usual in calculations of this kind (Williams & Cox, 1984), but may be regarded with some scepticism as especially the first two terms are strongly correlated (Mason, 1970). Table 3 indicates, however, some clear trends. The interactions within the stacks account for nearly half of the total lattice energy. In all complexes the contribution from intrastack contacts to the repulsion energy is larger, to the Coulombic energy considerably larger and, with exception of the experimental structure of HMB–fluoranil, to the dispersion energy smaller than that from interstack contacts.

The various contributions to the lattice energy may elucidate the disagreements between the experimental and optimum-density structures, and the minimum-energy structures. For the HFB complexes with p-xylene, mesitylene, durene and TMPDA, and the durene–fluoranil complex, the contribution of interstack Coulombic energy is larger for the optimum-density structure and, with one exception, also for the experimental structure than for the minimum-energy structure. As F$\cdots$H contacts contri-

Table 3. *Lattice energy and its components* (kJ mol⁻¹) *for the experimental structures* (first line), *the optimum-density structures* (second line) *and the minimum-energy structures* (third line)

The components Disp., Rep. and Coul. are the dispersion, repulsion and Coulombic energies and Sum is the total energy for only intrastack and only interstack interactions.

Compound	Intrastack				Interstack				Lattice energy
	Disp.	Rep.	Coul.	Sum	Disp.	Rep.	Coul.	Sum	
p-Xylene–HFB	-67·0	33·6	-36·8	-70·2	-102·6	19·4	-6·7	-89·9	-160·1
	-84·2	52·9	-40·5	-71·7	-127·8	40·7	-8·1	-95·2	-167·0
	-86·8	54·5	-44·2	-76·5	-132·9	43·2	-5·9	-95·6	-172·1
Mesitylene–HFB	-72·2	35·9	-42·0	-78·4	-104·0	20·9	-3·6	-86·7	-165·1
	-93·1	59·4	-46·5	-80·3	-122·0	35·5	-3·8	-90·3	-170·7
	-95·2	61·3	-48·8	-82·7	-122·7	35·3	-2·7	-90·1	-172·8
Durene–HFB	-85·1	47·3	-43·6	-81·4	-109·6	21·3	-6·3	-94·5	-175·9
	-98·4	63·0	-46·2	-81·5	-129·4	38·4	-7·9	-98·9	-180·5
	-105·3	67·1	-51·2	-89·3	-131·7	38·4	-4·1	-97·4	-186·7
HMB–HFB	-109·2	69·4	-48·9	-88·7	-126·8	22·8	-3·1	-107·1	-195·8
	-111·0	71·7	-49·2	-88·6	-148·2	41·4	-3·7	-110·5	-199·1
	-108·2	68·6	-54·8	-94·4	-157·1	46·5	-4·3	-114·8	-209·2
DMA-HFB	-95·9	63·2	-48·0	-80·7	-131·3	40·8	-9·8	-100·4	-181·1
	-93·4	60·0	-47·5	-80·9	-131·6	41·3	-9·9	-100·2	-181·1
	-94·7	61·0	-48·6	-82·3	-130·9	41·4	-10·2	-99·8	-182·1
TMA–HFB	-87·7	46·7	-47·8	-88·9	-115·2	20·4	-4·0	-98·8	-187·6
	-101·0	61·8	-50·3	-89·5	-145·0	45·4	-5·6	-105·2	-194·7
	-99·4	61·4	-49·9	-87·9	-150·7	48·3	-7·0	-109·5	-197·4
TMPDA–HFB (HFB in major orientation)	-83·7	45·9	-44·9	-82·7	-139·5	42·4	-8·9	-106·0	-188·7
	-97·1	61·5	-47·1	-82·7	-144·0	44·3	-9·9	-109·6	-192·3
	-98·3	61·9	-50·2	-86·6	-150·2	48·2	-9·5	-111·5	-198·1
TMPDA–HFB (HFB in minor orientation)	-86·0	50·1	-44·4	-80·3	-141·3	47·9	-10·4	-103·8	-184·1
	-88·9	53·5	-44·9	-80·3	-139·5	45·8	-10·3	-104·0	-184·3
	-98·3	61·9	-50·2	-86·6	-150·2	48·2	-9·5	-111·5	-198·1
Durene–fluoranil	-109·3	71·3	-36·0	-74·0	-117·0	24·3	-1·6	-94·4	-168·4
	-98·4	57·7	-34·5	-75·2	-137·4	43·1	-2·5	-96·8	-172·0
	-102·7	62·0	-35·8	-76·5	-136·2	40·4	-1·1	-96·8	-173·4
HMB–fluoranil	-141·8	102·7	-41·7	-80·8	-134·7	31·2	+1·5	-102·0	-182·8
	-117·2	70·5	-39·1	-85·8	-139·6	38·1	+0·9	-100·6	-186·4
	-105·2	63·6	-38·0	-79·6	-158·4	46·3	0·0	-112·1	-191·7

bute much more to the Coulombic energy than to the dispersion and repulsion energy, this indicates that the shifts in molecular positions and orientations in the energy minimizations result in a decreasing number of short interstack contacts of this kind. This interpretation is confirmed by the finding that the observed effect increases considerably when the charges are increased only for the F and H atoms. For these complexes a better agreement between experimental and minimum-energy structures would thus have been obtained if more weight had been given to attractive F···H interactions between different stacks, i.e. directional F···H interactions. With the exception of the durene–fluoranil complex, these are the complexes where the negative shifts in Table 2 are large for the stack axis relative to those for the other axes. The interactions in the stacks are thus relatively weak and probably dominated by ordinary van der Waals interactions. The reason why such F···H interactions seem to be less important in the remaining complexes may be that there are additional stacking interactions with greater influence on the molecular packing.

It seems reasonable to conclude from this analysis that for some of the complexes, in particular the two fluoranil complexes and the HMB–HFB complex, there are stacking interactions in addition to those predicted by the energy calculations with a substantial effect on the interplanar distance and probably also on the molecular overlap. Charge-transfer interactions may be among these additional interactions, at least for the fluoranil complexes. For other complexes where the interactions in the stacks are weak, the structures seem to be influenced by interstack interactions, probably directional F···H interactions, in addition to those included in the analytical potentials.

It is surprising that the TMPDA–HFB complex seems to be among those with weak interactions in the stacks. From the ionization potential of the donor (Laidlaw *et al.*, 1987) and the wavelength of the charge-transfer band (Beaumont & Davis, 1967) this would be expected to be the HFB complex with the strongest charge-transfer interactions. It should be mentioned, however, that the crystal used for the structure determination of this complex was very poor. A redetermination from better experimental data would be of interest.

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SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Structural studies on the biosides of *Digitalis lanata*: bisdigitoxosides of digitoxigenin, gitoxigenin and digoxigenin. Erratum.

By KUANTEE GO, *Biophysics Department, Roswell Park Memorial Institute, 666 Elm Street, Buffalo, New York* 14263, *USA* and KRISHNA K. BHANDARY, *Oral Biology Department, State University of New York at Buffalo, New York* 14214, *USA*

Abstract

A printer's error in the article by Go & Bhandary [*Acta Cryst.* (1989), B45, 306–312] is corrected. The space group of compound (III), given in the fourth line of page 307, should read $P2_12_12$ and not $P2_12_12_1$.

All relevant information is given in the *Abstract*.