

PACKING EFFECTS IN THE SOLID STATE STRUCTURE OF MOLECULAR CRYSTALS

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We examined packing effects in the solid state structure of donor–acceptor complexes. All acceptor molecules (\mathcal{A}) considered here contained a boron atom whereas the donor molecules (\mathcal{D}) contained oxygen, nitrogen or phosphor atoms. We focused on the length of the dative $\mathcal{A}-\mathcal{D}$ bond both in the free molecule and in the solid state at various pressures. In one of the complexes investigated (\mathcal{C}_4), a biphenyl unit is present. Its torsion angle in the solid state structure depends on the pressure. Thus, the packing effect on the value of the torsion angle in some biphenyl compounds was investigated, too.

We considered the complexes (\mathcal{C}_i) of BF_3 with acetonitrile (\mathcal{C}_1), with pyridine (\mathcal{C}_2) and (E)–3–diethylamino–3–phenyl–2–propenal (\mathcal{C}_3) as well as the complex dicyclohexyl(2', 4', 6'–triisopropylbiphenyl–2–yl)phosphine-dichlorophenylborane (\mathcal{C}_4).

The calculations were carried out using the plane wave DFT code VASP [1] for the solid state and for a single molecule in a large box. The results obtained for the free molecules were checked using molecular codes. The van der Waals interactions necessary for an accurate description of molecular crystals can be included in a semiempirical way [2,3].

The length ℓ of the dative $\mathcal{A}-\mathcal{D}$ bond in a complex was found to be influenced substantially by interactions with the surrounding molecules. In the solid state, ℓ is considerably shorter than in the free molecule and it rapidly shortens with a decreasing volume of the unit cell.

The torsion angles calculated for the biphenyls in both the solid state at various pressures and for the free molecule show a good agreement with the experimental values.

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