

Fig. S-1. o-TDB and HMB in ORTHO. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The views are normal to the (001) plane. Only one of the two sets of the disordered H atom positions are shown.

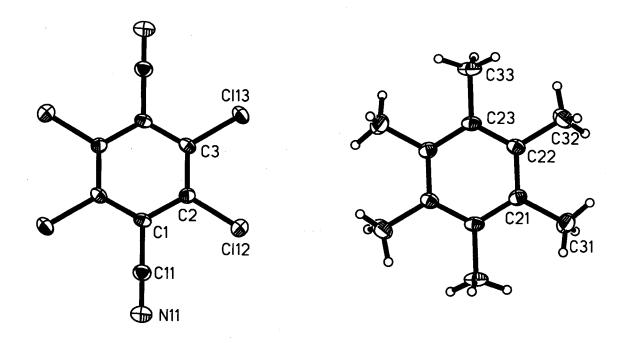


Fig. S-2. p-TDB and HMB in PARA-I. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The views are normal to the (2,-1,0) plane. Only one of the two sets of the disordered H atom positions are shown.

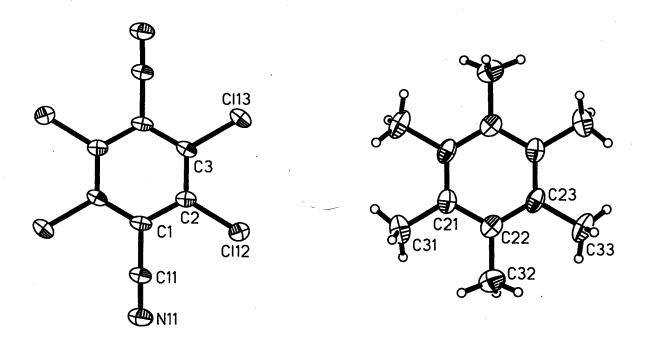


Fig. S-3. p-TDB and HMB in PARA-II. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The views are normal to the (100) plane. Only one of the two sets of the disordered H atom positions are shown.

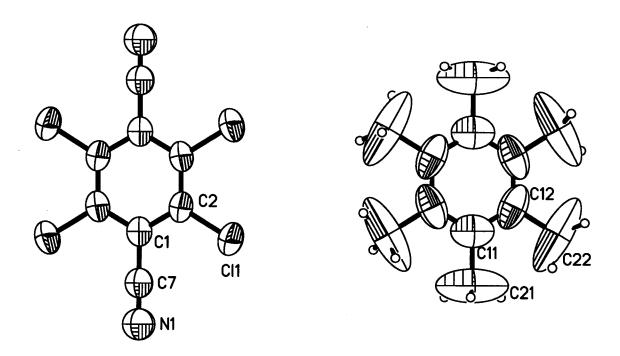


Fig. S-4. p-TDB and HMB in PARA-III. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The views are normal to the (001) plane. Only one of the two sets of the disordered H atom positions are shown.

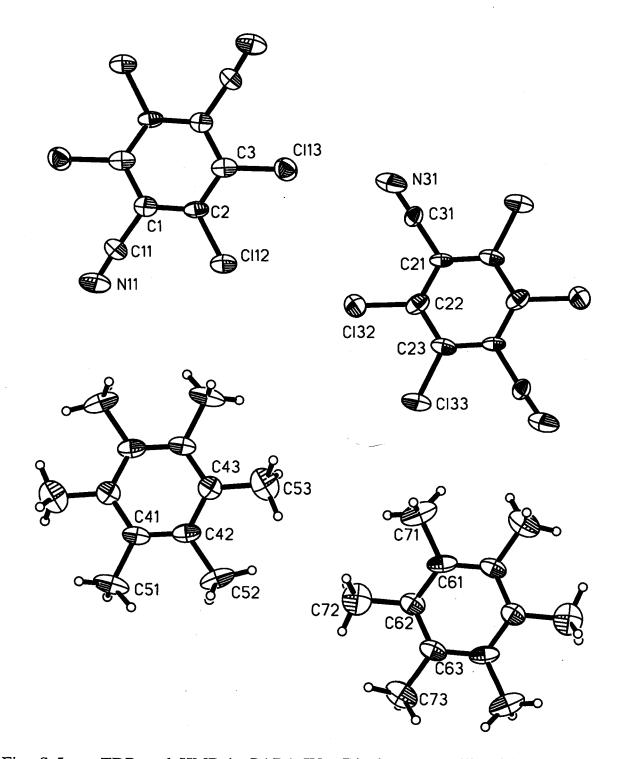


Fig. S-5. p-TDB and HMB in PARA-IV. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The top pair of molecules are shown in the correct orientation with respect to each other as are the bottom pair. The views are normal to the (101) plane. Only one of the two sets of the disordered H atom positions are shown.

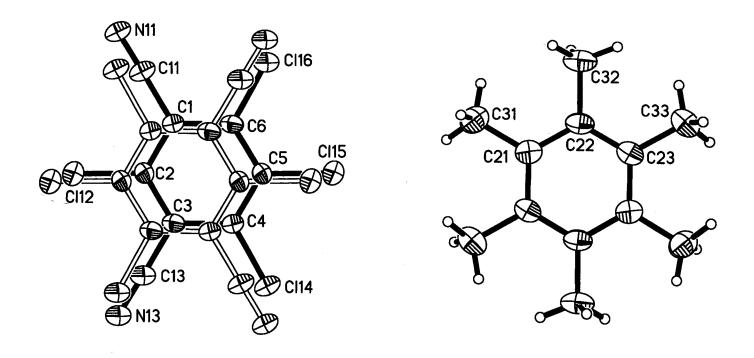


Fig. S-6. m-TDB and HMB in META-I. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. Both orientations of the disordered TDB are shown. The views are normal to the (100) plane. Only one of the two sets of the disordered H atom positions are shown.

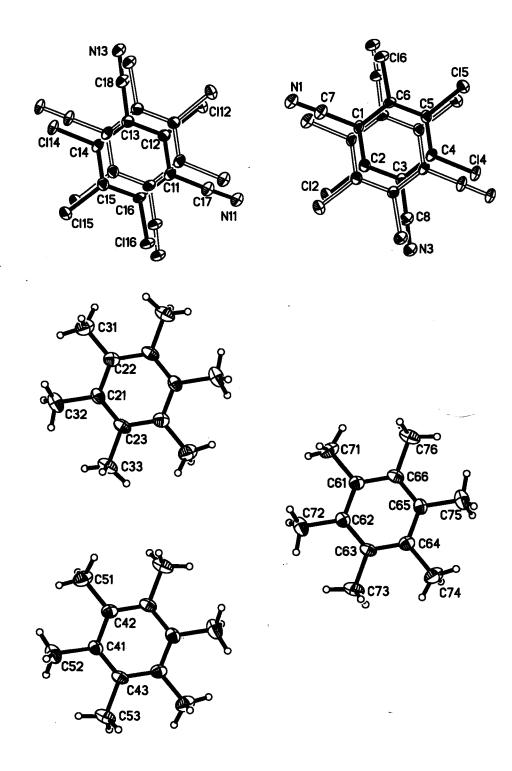


Fig. S-7. m-TBD and HMB in META-II. Displacement ellipsoids are shown at the 50% probability level. Only the crystallographically independent atoms are labelled. The major components of the disordered TDB's are shown with solid bonds. The views are normal to the (100) plane. Only one of the two sets of disordered H atoms are is shown.

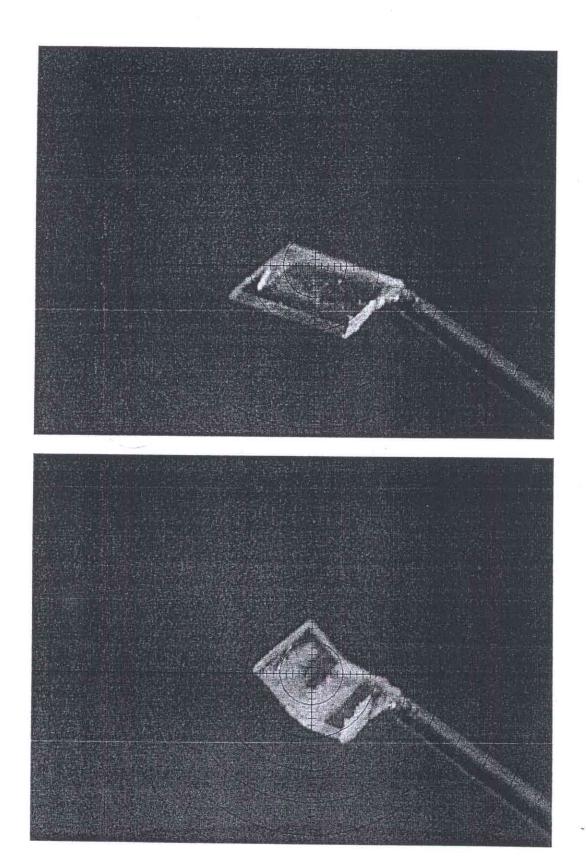


Fig. S-8. Above: A crystal of PARA-III at 297 K. Below: the same crystal at 173 K after conversion to PARA-II.

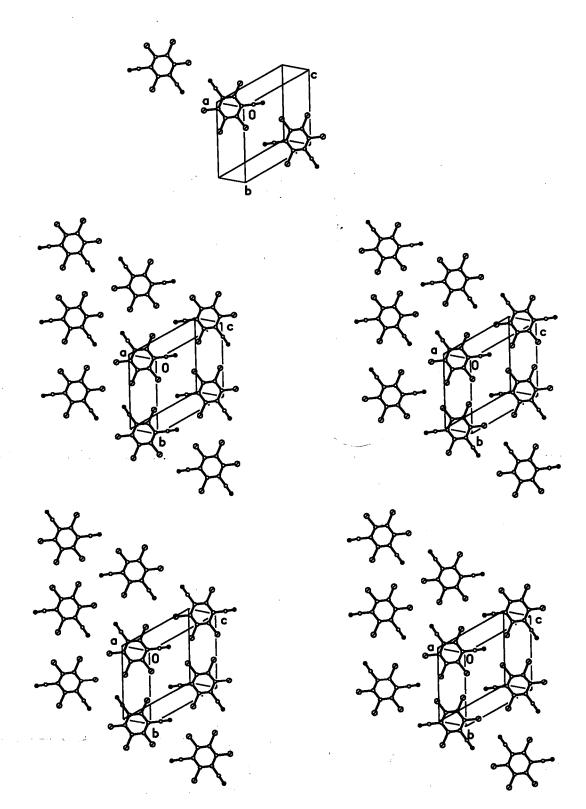


Fig. S-9. Determination of the ordered layers in META-I. Top: the starting point; alternating orientations along [011]. Middle-left: adjacent rows arranged so that there is translation along the b diraction. This is the structure shown in Fig. 13. Middle-right: adjacent rows arranged so that there is translation along the c direction. Bottom: arrangements with no translation along b or c. These are equivalent but both are shown for completeness. A two-fold rotation around the center of the unit cell brings them into coincidence.

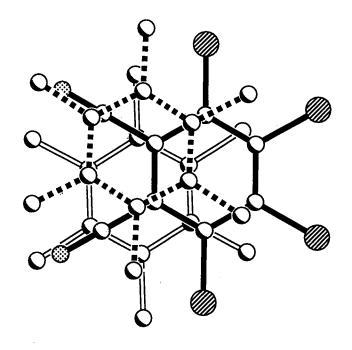


Fig. S-10. Overlap diagram for ORTHO

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds. HMB above: average distance 3.43(5) Å; tilt away from parallel  $2.7^{\circ}$ 

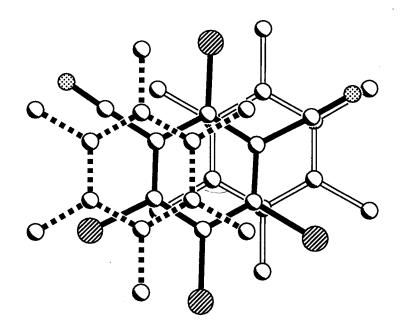


Fig. S-11. Overlap diagram for META-I

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds. HMB above: average distance 3.46(3) Å; tilt away from parallel 1.7°. HMB below: average distance 3.46(3) Å; tilt away from parallel 1.7°.

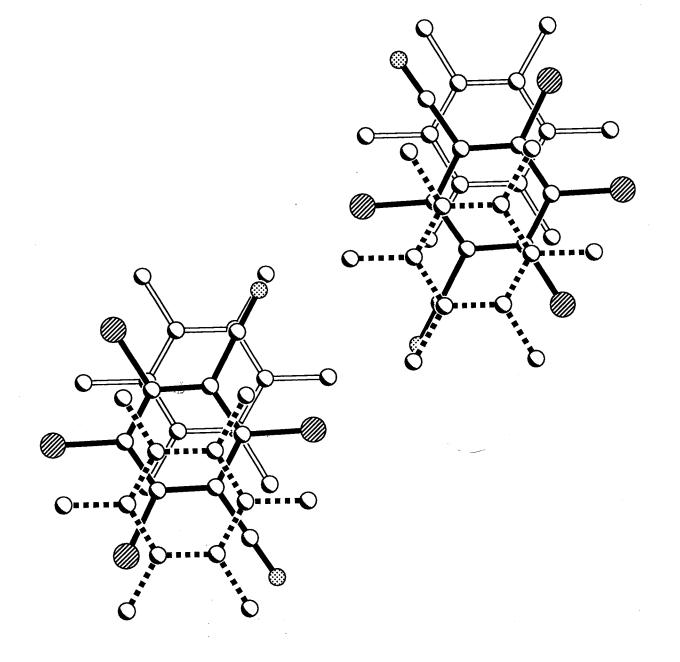


Fig. S-12. Overlap diagram for META-II

The TDB molecules are shown with solid bonds, the HMB molecules above with dashed bonds, the HMB molecules below with open bonds. Left:

HMB above: average distance 3.47(4) Å; tilt away from parallel 2.3°

HMB below: average distance 3.46(3) Å; tilt away from parallel 1.7°

Right:

HMB above: average distance 3.47(3) Å; tilt away from parallel 1.7°

HMB below: average distance 3.46(3) Å; tilt away from parallel 1.1°

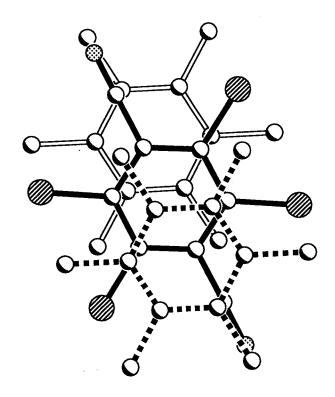


Fig. S-13. Overlap diagram for PARA-I

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds. HMB above: average distance 3.45(4) Å; tilt away from parallel 2.1°

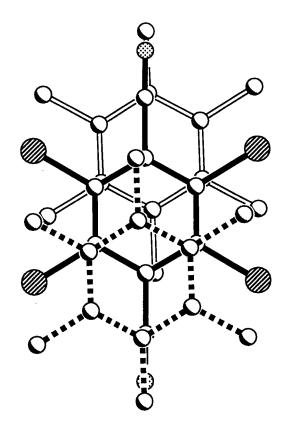


Fig. S-14. Overlap diagram for PARA-II

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds.

HMB above: average distance  $3.45(4)\mbox{\normalfont\AA}$ ; tilt away from parallel  $2.2^{\circ}$ 

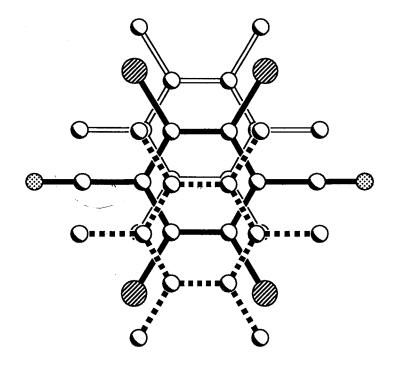


Fig. S-15. Overlap diagram for PARA-III

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds. HMB above: average distance 3.56(1) Å; tilt away from parallel  $0.7^{\circ}$ 

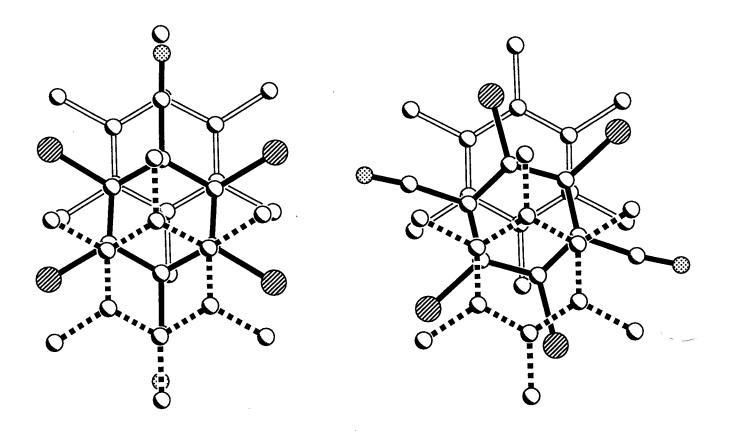


Fig. S-16. Overlap diagram for PARA-IV

The TDB molecule is shown with solid bonds, the HMB molecule above with dashed bonds, the HMB molecule below with open bonds.

## Left:

HMB above: average distance 3.43(4) Å; tilt away from parallel 2.1°

HMB below: same

## Right:

HMB above: average distance 3.51(5) Å; tilt away from parallel 4.5°