**FIGURE CAPTIONS**

Fig. 1. The conformation of (a) fluoranthene and (b) acenaphthene molecules with the atom numbering scheme. Atomic displacement ellipsoids represent 50 % probability level. H atoms are shown as small spheres of arbitrary radius.

Fig. 2. Hirshfeld surfaces mapped with dnorm and part of the crystal structure of (a) fluoranthene and (b) acenaphthene showing the intermolecular interactions.

Fig. 3. Fingerprint plot of the fluoranthene; (a) C···H, (b) C···C and (c) H···H interactions showing the percentage of contacts created to the total Hirshfeld surface area of molecules. di is the closest internal distance from a given point on the Hirshfeld surface; de is the closest external contact.

Fig. 4. Fingerprint plot of the acenaphthene; (a) C···H, (b) C···C and (c) H···H interactions showing the percentage of contacts created to the total Hirshfeld surface area of molecules.

Fig. 5. IR spectra of polycrystalline samples of (a) fluoranthene and (b) acenaphthene measured at 293 K by the KBr pellet technique. The Raman spectra for identification of the C-H bond vibration lines.

Fig. 6.Polarized spectra of a single crystal of (a) fluoranthene and (b) acenaphthene measured at 77 K; and c) packing diagram of acenaphthene viewed along the *b* axis.

Fig. 7.Polarized spectra of a single crystal of (a) fluoranthene and (b) acenaphthene are illustrative of the temperature effect.

Fig. 8. Comparison of B3LYP calculated IR spectrum of (a) fluoranthene and (b) acenaphthene with the experiment.