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Ferroelectric π-stacks of molecules with the energy gaps in the sunlight range

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1 Supplementary information

Table 1: Numerical data set for Fig. 2: the LUMO-HOMO energies (in eV) of the isolated molecules with variable number of benzene rings and three dipole groups: X=COOH, Y=CH_2CN, Z=CH_2CF_3.

$b2X_4$	$b2X_8$	$b5X_4$	$b5Z_6$	$b5X_8$	$b5Y_{10}$	$b5X_{10}$	$b5X_{14}$	$b9X_4$	$b9X_8$
4.384	4.099	1.783	1.745	1.770	1.766	1.748	1.677	0.820	0.814
$b9Z_{10}$	$b9Y_{14}$	$b9X_{14}$	$b9X_{22}$	$b17X_4$	$b17X_8$	$b17Z_{18}$	$b17X_{22}$	$b17Y_{22}$	$b17X_{38}$
0.808	0.821	0.810	0.778	0.568	0.568	0.547	0.556	0.544	0.549

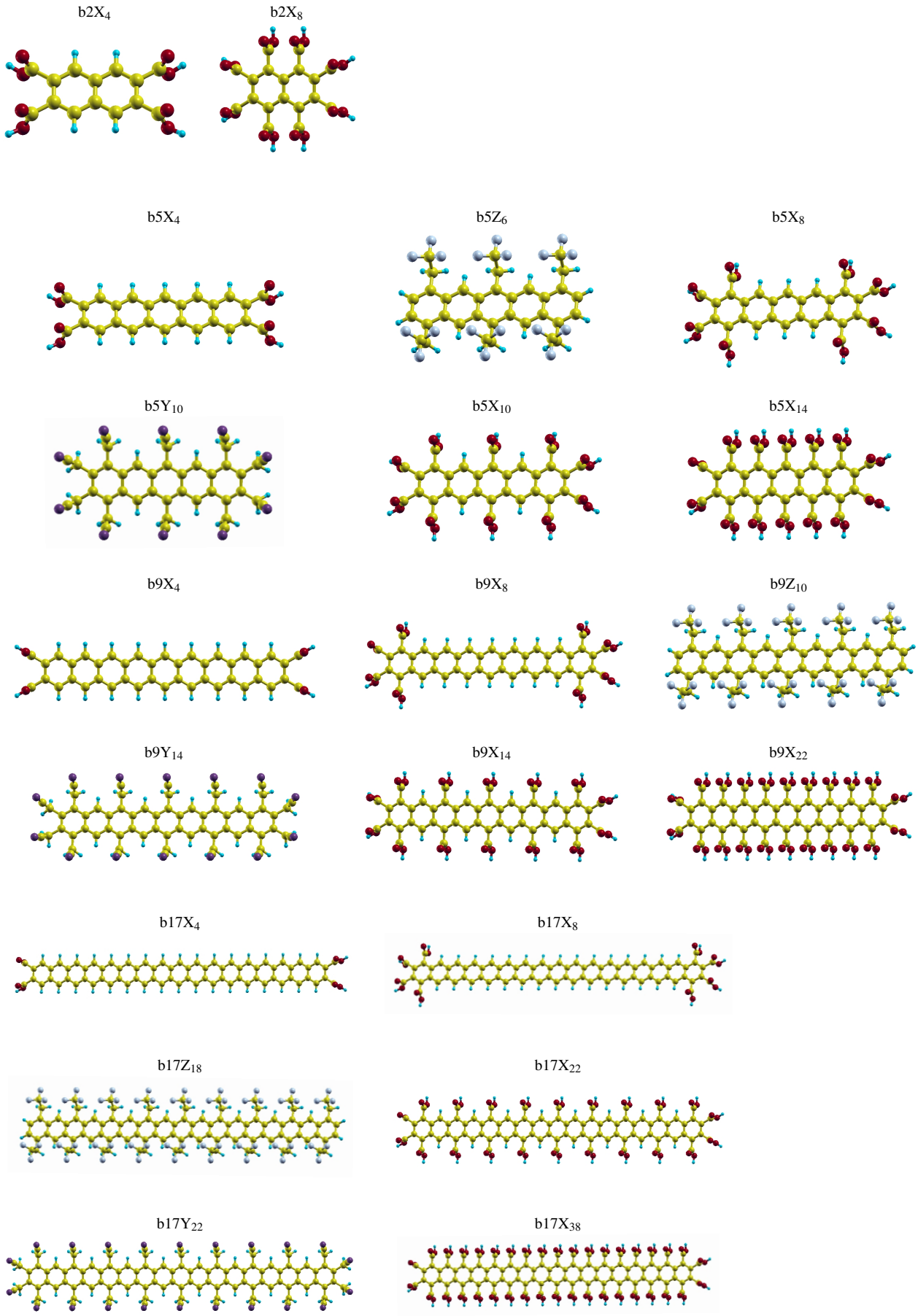

Fig. 1: Atomic structures of molecules for which the LUMO-HOMO gaps are presented in Figure 2.

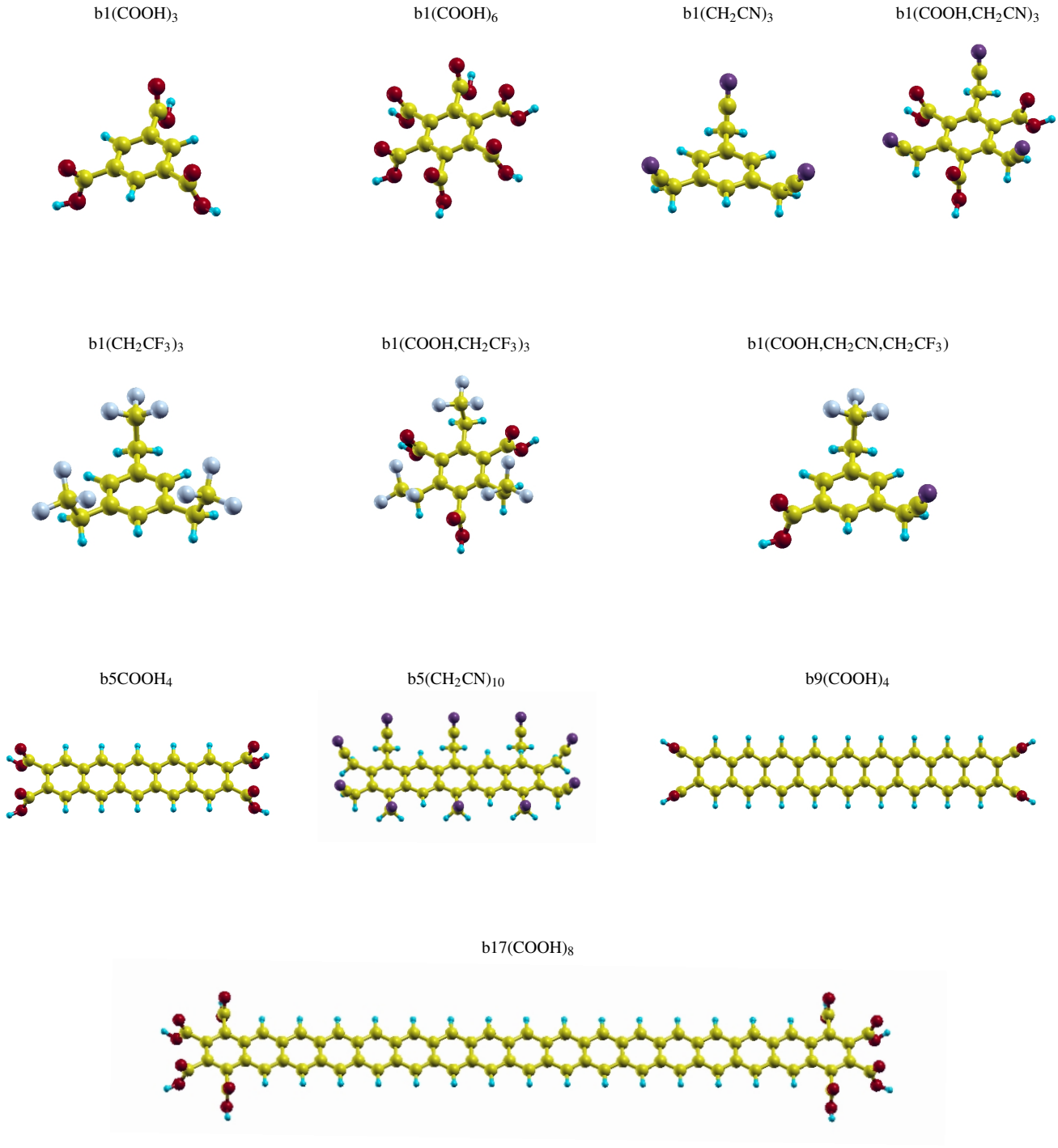

Fig. 2: Atomic structures of molecules mentioned in Table 2 of the paper.