

SUPPLEMENT TO
**Electronic structures and spectra of
 conducting anthracene derivatives**

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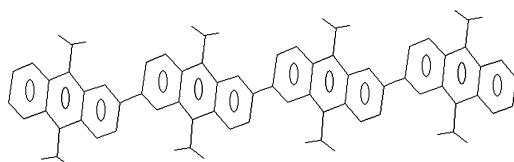


Fig. S1. The optimized geometry of compound **11** at the B3LYP/6-31G(d) level.

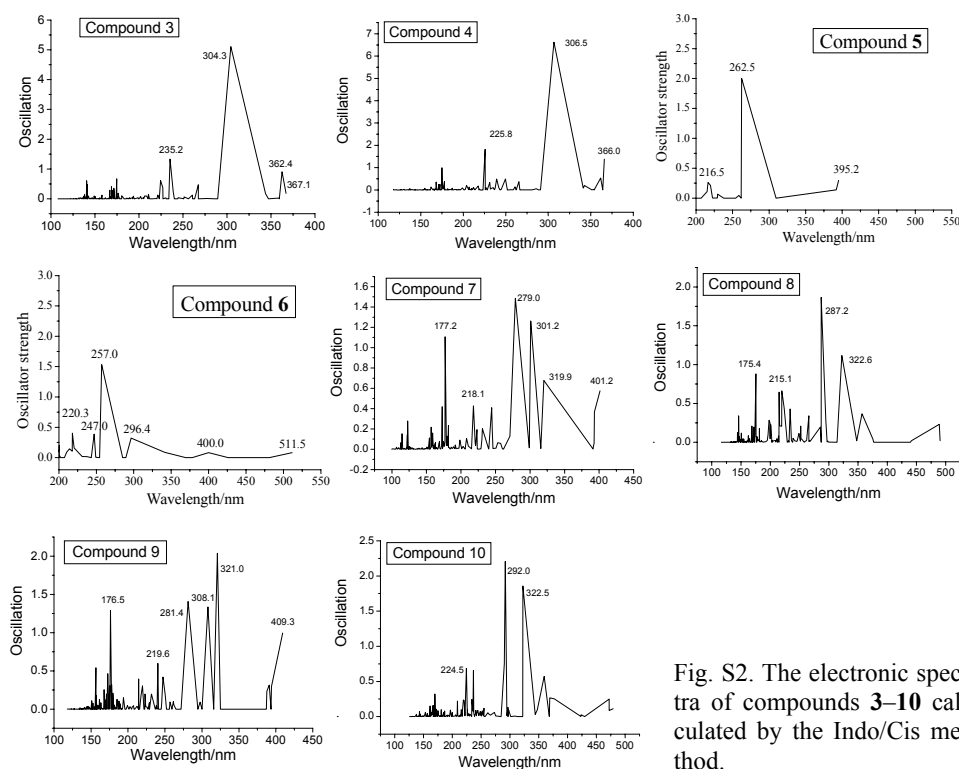


Fig. S2. The electronic spectra of compounds **3–10** calculated by the Indo/Cis method.

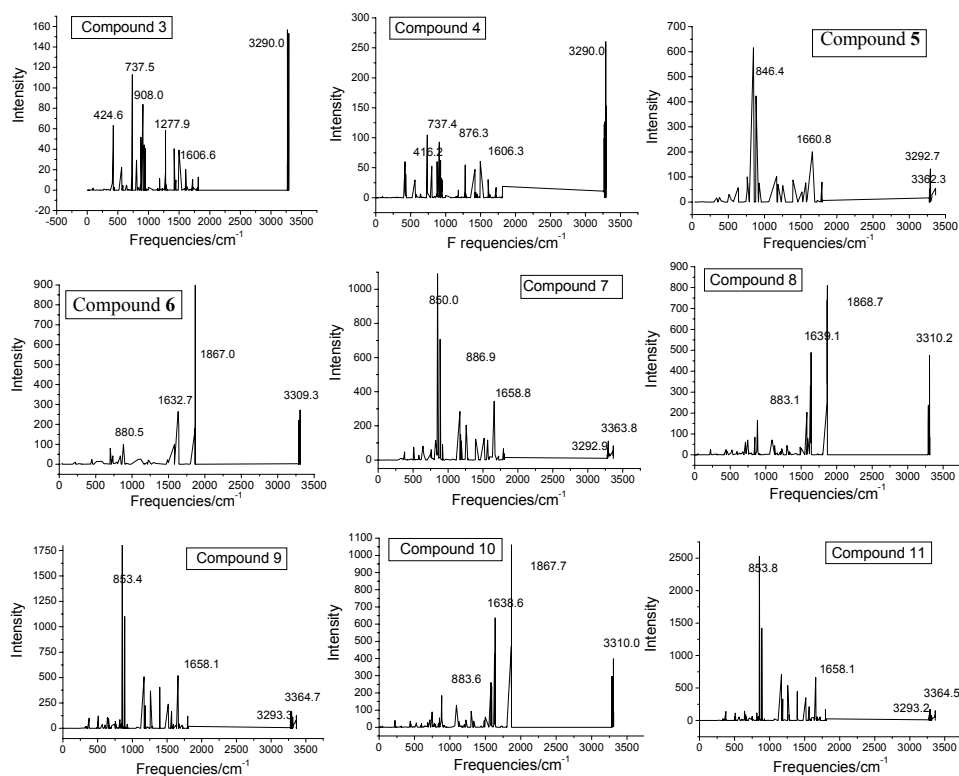
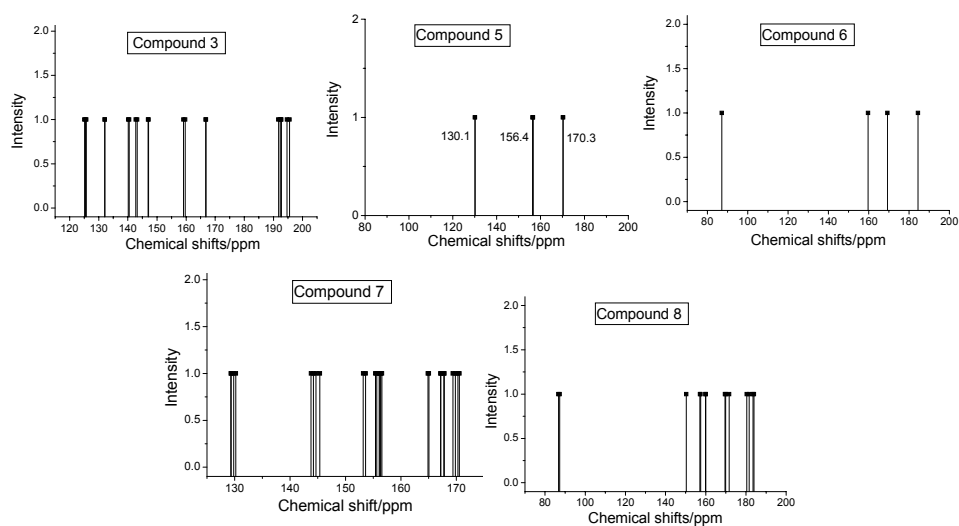


Fig. S3. The IR spectra of compounds 3–11 calculated by the AM1 method.

Fig. S4. ¹³C-NMR spectra of compounds 3 and 5–8 calculated at the B3LYP/6-31G(d) level.