Supporting Information

A series of 4,5,9,10-tetrahydropyrene-based tetraarylethenes: synthesis, structures and solid-state emission behaviors

Zhaoming Zhang a,b, Baoxi Miao a, Xinxue Tang a, Zhonghai Ni a,*

a School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou 221116, People’s Republic of China

b Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo 001-0021, Japan

* Corresponding author E-mail: nizhonghai@cumt.edu.cn; Tel: +86-516-83883927

Table S1

Crystal data and structure refinement parameters for compounds 1 and 4

|                      | Compound 1 | Compound 4 |
|----------------------|------------|------------|
| Formula              | C_{35}H_{33} | C_{56}H_{44} |
| Formula weight       | 460.58     | 716.91     |
| Temperature (K)      | 293(2)     | 293(2)     |
| Crystal system       | monoclinic | triclinic  |
| Space group          | P 2_1/c    | P -1       |
| a (Å)                | 8.5141(17) | 8.1823(16) |
| b (Å)                | 17.426(4)  | 12.694(3)  |
| c (Å)                | 17.000(3)  | 19.994(4)  |
| α(°)                 | 90.0000(0) | 90.14(3)   |
| β(°)                 | 97.44(3)   | 93.52(3)   |
| γ(°)                 | 90.0000(0) | 101.80(3)  |
| Volume (Å³)          | 2500.9(9)  | 2028.7(7)  |
| Z                    | 4          | 2          |
| ρ calc (g cm⁻³)      | 1.223      | 1.174      |
| μ(Mo – Kα) (mm⁻¹)    | 0.069      | 0.066      |
| F(000)               | 976        | 760        |
| Crystal size (mm)    | 0.10×0.08×0.06 | 0.08×0.08×0.06 |
| Independent reflections | 4387      | 7079       |
| Reflections [I > 2σ(I)] | 3540      | 4032       |
| θ range (°)          | 3.19-25.00 | 3.16-25.00 |
| Goodness-of-fit on F² | 1.091      | 1.051      |
| R₁[I > 2σ(I)]        | 0.0832     | 0.0816     |
| wR₂(all data)        | 0.2169     | 0.2150     |