**TABLE CAPTIONS**

TABLE I. Crystal data and structure refinement details of fluoranthene (**I**) and acenaphthene (**II**)

TABLE II. Comparison of selected calculated geometry parameters of fluoranthene with experiment

TABLE III. Comparison of selected calculated geometry parameters of acenaphthene with experiment

TABLE I.

|  |  |  |
| --- | --- | --- |
|  | **I** | **II** |
| Empirical formula | C16H10 | C12H10 |
| Compound weight | 202.24 | 154.20 |
| Temperature, K | 295.0(2) | 295.0(2) |
| Crystal system | Monoclinic | Orthorhombic |
| Space group | *P21/n* | *P21ma* |
| Crystal dimension, mm3 | 0.39 x 0.32 x 0.09 | 0.41 x 0.22 x 0.12 |
| Crystal form, colour | Plate, colourless | Plate, colourless |
| Unit cell dimensions | | |
| *a* / Å | 18.3490 (2) | 7.2053 (9) |
| *b* / Å | 6.2273 (5) | 13.9800 (15) |
| *c* / Å | 19.8610 (2) | 8.2638 (8) |
| *β* / ° | 109.787 (13) | 90.00 |
| *V* / Å3 | 2135.50 (4) | 832.41 (16) |
| *Z* | 8 | 4 |
| *Dc* /g cm-3 | 1.258 | 1.230 |
| *F*(000) | 848 | 328 |
| *Θ* range for data collection, ° | 4.0-29.2 | 4.8-27.5 |
| Data collection method | *ω* scan | *ω* scan |
| Absorption coefficient, mm-1 | 0.071 | 0.069 |
| Final *R* indices (*I* > 2*σ*(*I*)) | *R*1 =0.0696 , w*R*2 = 0.1711 | *R*1 = 0.0442, w*R*2 = 0.0964 |
| R indices (all data) | *R*1 = 0.1043, w*R*2 = 0.1936 | *R*1= 0.0550, w*R*2 = 0.1022 |
| Reflections collected/unique | 2527 [*R*int = 0.089] | 1075 [*R*int = 0.020] |
| Limiting indices | -21 ≤ h ≤ 20, -7 ≤ k ≤ 7,  -23 ≤ l ≤ 23 | -8 ≤ h ≤ 6, -16 ≤ k ≤ 16,  -7 ≤ l ≤ 9 |
| Refinement method | Full-matrix least-squares on *F2* | Full-matrix least-squares on *F2* |
| *S* | 1.10 | 1.05 |
| Parameters refined | 289 | 105 |
| *Δρ*max, *Δρ*min / e Å-3 | 0.22-0.21 | 0.25-0.28 |

TABLE II.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Experimental (XRD) | | | | | | Theoretical | |
| Bond lengths, Å | | | | | | 6-31+G (d, p) | 6-311++G(3df,2pd) |
| C1-C2 | 1.396 | C17-C18 | | 1.365 | | 1.381 | 1.374 |
| C2-C3 | 1.406 | C18-C19 | | 1.401 | | 1.425 | 1.419 |
| C3-C4 | 1.358 | C19-C20 | | 1.361 | | 1.386 | 1.379 |
| C4-C5 | 1.410 | C20-C21 | | 1.410 | | 1.426 | 1.420 |
| C5-C6 | 1.416 | C21-C22 | | 1.410 | | 1.419 | 1.416 |
| C6-C7 | 1.356 | C22-C23 | | 1.357 | | 1.386 | 1.379 |
| C7-C8 | 1.399 | C23-C24 | | 1.401 | | 1.425 | 1.418 |
| C8-C9 | 1.368 | C24-C25 | | 1.356 | | 1.381 | 1.374 |
| C9-C10 | 1.403 | C25-C26 | | 1.405 | | 1.404 | 1.398 |
| C10-C5 | 1.396 | C26-C21 | | 1.396 | | 1.419 | 1.413 |
| C10-C1 | 1.407 | C26-C17 | | 1.405 | | 1.393 | 1.386 |
| C9-C11 | 1.477 | C25-C27 | | 1.472 | | 1.477 | 1.473 |
| C11-C12 | 1.381 | C27-C28 | | 1.376 | | 1.402 | 1.395 |
| C12-C13 | 1.394 | C28-C29 | | 1.362 | | 1.400 | 1.392 |
| C13-C14 | 1.370 | C29-C30 | | 1.372 | | 1.380 | 1.379 |
| C14-C15 | 1.383 | C30-C31 | | 1.393 | | 1.402 | 1.395 |
| C15-C16 | 1.380 | C31-C32 | | 1.383 | | 1.393 | 1.386 |
| C16-C11 | 1.410 | C32-C27 | | 1.416 | | 1.428 | 1.422 |
| C16-C1 | 1.473 | C32-C17 | | 1.475 | | 1.477 | 1.472 |
| Angles, ° | | | | | |  |  |
| C10-C1-C2 | 118.00 | | C26-C17-C18 | | 117.16 | 118.34 | 118.31 |
| C1-C2-C3 | 119.00 | | C17-C18-C19 | | 119.00 | 118.71 | 118.74 |
| C2-C3-C4 | 122.60 | | C18-C19-C20 | | 122.50 | 122.48 | 122.48 |
| C3-C4-C5 | 120.50 | | C19-C20-C21 | | 120.40 | 120.07 | 120.08 |
| C4-C5-C10 | 115.60 | | C20-C21-C26 | | 115.70 | 116.13 | 116.12 |
| C5-C10-C1 | 124.20 | | C21-C26-C17 | | 124.40 | 124.27 | 124.26 |
| C10-C5-C6 | 115.50 | | C26-C21-C22 | | 115.40 | 116.13 | 116.12 |
| C5-C6-C7 | 120.70 | | C21-C22-C23 | | 120.50 | 120.07 | 120.08 |
| C6-C7-C8 | 122.40 | | C22-C23-C24 | | 122.90 | 122.48 | 122.48 |
| C7-C8-C9 | 119.30 | | C23-C24-C25 | | 118.70 | 118.71 | 118.75 |
| C8-C9-C10 | 118.00 | | C24-C25-C26 | | 118.50 | 118.34 | 118.31 |
| C9-C10-C5 | 124.10 | | C25-C26-C21 | | 124.00 | 124.27 | 124.26 |
| C9-C10-C1 | 111.60 | | C25-C26-C17 | | 111.60 | 111.45 | 111.48 |
| C10-C9-C11 | 106.20 | | C26-C25-C27 | | 106.30 | 106.20 | 106.18 |
| C9-C11-C16 | 107.90 | | C25-C27-C32 | | 107.90 | 108.08 | 108.07 |
| C11-C16-C1 | 108.30 | | C27-C32-C17 | | 108.00 | 108.08 | 108.08 |
| C16-C1-C10 | 106.00 | | C32-C17-C26 | | 106.20 | 106.20 | 106.19 |
| C9-C11-C12 | 131.90 | | C25-C27-C28 | | 131.80 | 131.66 | 131.71 |
| C11-C12-C13 | 118.10 | | C27-C28-C29 | | 119.50 | 119.02 | 119.04 |
| C12-C13-C14 | 121.30 | | C28-C29-C30 | | 120.90 | 120.72 | 120.73 |
| C13-C14-C15 | 121.20 | | C29-C30-C31 | | 121.50 | 120.72 | 120.73 |
| C14-C15-C16 | 118.30 | | C30-C31-C32 | | 118.10 | 119.02 | 119.03 |
| C15-C16-C11 | 120.80 | | C31-C32-C27 | | 119.80 | 120.26 | 120.26 |
| Dihedral angles, ° | | | | | | |  |
| C15–C16–C1–C2 | -0.006 | | C31-C32-C-17-C18 | | -4.1(6) | 0.002 | 0.023 |
| C15–C16–C1–C10 | 179.4(3) | | C31-C32-C17-C26 | | 179.0(3) | 179.99 | -179.99 |
| C12–C11–C9–C8 | -2.4(6) | | C28-C27-C25-C24 | | -0.3(6) | 0.01 | -0.01 |
| C12–C11–C9–C10 | 179.3(3) | | C28-C27-C25-C26 | | 179.5(3) | 179.98 | 179.98 |
| C8–C9–C10–C1 | -178.5(3) | | C24-C25-C26-C17 | | -179.3(3) | 179.99 | 179.99 |
| C2–C1–C10–C9 | -179.5(2) | | C18-C17-C26-C25 | | -178.1(3) | 179.99 | 179.99 |
| C16–C1–C10–C5 | -177.6(2) | | C32-C17-C26-C21 | | 179.1(3) | -179.99 | 179.98 |
| C11–C9–C10–C5 | 178.7(2) | | C27-C25-C26-C21 | | -178.7(3) | 180.00 | -180.00 |

TABLE III.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Experimental (XRD) | | | | | Theoretical | |
| Bond lengths, Å | | | | | 6-31G (d, p) | 6-31G\* (d, p) |
| C1i-C6i | 1.358 | | C8ii-C9ii | 1.358 | 1.370 | 1.377 |
| C6-C5 | 1.403 | | C9ii-C10ii | 1.397 | 1.426 | 1.423 |
| C5-C4 | 1.359 | | C10ii-C11ii | 1.354 | 1.384 | 1.383 |
| C4i-C3 | 1.410 | | C11ii-C12 | 1.414 | 1.425 | 1.422 |
| C3-C4 | 1.410 | | C12-C11 | 1.414 | 1.425 | 1.422 |
| C4-C5 | 1.359 | | C11-C10 | 1.354 | 1.384 | 1.383 |
| C5-C6 | 1.403 | | C10-C9 | 1.397 | 1.426 | 1.423 |
| C6-C1 | 1.358 | | C9-C8 | 1.358 | 1.378 | 1.377 |
| C1-C2 | 1.400 | | C8-C13 | 1.400 | 1.414 | 1.412 |
| C2-C3 | 1.398 | | C13-C12 | 1.393 | 1.414 | 1.414 |
| C2-C1i | 1.400 | | C13-C8ii | 1.400 | 1.414 | 1.412 |
| C1-C7 | 1.506 | | C8-C14 | 1.503 | 1.523 | 1.520 |
| C7-C7i | 1.547 | | C14-C14ii | 1.534 | 1.575 | 1.570 |
| C7i-C1i | 1.506 | | C14ii-C8ii | 1.503 | 1.523 | 1.520 |
| Angles, ° | | | | |  |  |
| C7i-C1i-C6i | 132.93 | | C14ii-C8ii-C9ii | 133.14 | 132.40 | 132.40 |
| C7i-C1i-C2 | 108.41 | | C14ii-C8ii-C13 | 108.21 | 108.70 | 108.70 |
| C1i-C6i-C5i | 119.14 | | C8ii-C9ii-C10ii | 118.90 | 118.80 | 118.80 |
| C6i-C5i-C4i | 122.20 | | C9ii-C10ii-C11ii | 122.80 | 122.30 | 122.30 |
| C5i-C4i-C3 | 120.60 | | C10ii-C11ii-C12 | 120.20 | 120.30 | 120.20 |
| C4i-C3-C2 | 115.87 | | C11ii-C12-C13 | 115.86 | 116.30 | 116.30 |
| C4i-C3-C4 | 128.30 | | C11ii-C12-C11 | 128.30 | 127.40 | 127.40 |
| C3-C4-C5 | 120.60 | | C12-C11-C10 | 120.20 | 120.20 | 120.20 |
| C4-C5-C6 | 122.20 | | C11-C10-C9 | 122.80 | 122.30 | 122.30 |
| C5-C6-C1 | 119.14 | | C10-C9-C8 | 118.30 | 118.90 | 118.80 |
| C6-C1-C2 | 118.66 | | C9-C8-C13 | 118.60 | 118.90 | 118.90 |
| C6-C1-C7 | 132.93 | | C9-C8-C14 | 133.14 | 132.40 | 132.40 |
| C1-C7-C7i | 105.13 | | C8-C14-C14ii | 105.40 | 104.80 | 104.80 |
| C7-C7i-C1i | 105.13 | | C14-C14ii-C8ii | 105.40 | 104.80 | 104.80 |
| C1-C2-C1i | 112.90 | | C8-C13-C8ii | 112.80 | 112.80 | 112.80 |
| Dihedral angles, ° | | | | |  |  |
| C7i-C1i-C6i-C5i | | 179.3(2) | C14ii-C8ii-C9ii-C10ii | 179.4(2) | 180.00 | 180.00 |
| C7-C1-C6-C5 | | -179.3(2) | C14-C8-C9-C10 | -179.4(2) | -180.00 | -180.00 |
| C1-C2-C1i-C6i | | 179.2(2) | C8-C13-C8ii-C9ii | 179.9(2) | 180.00 | 180.00 |
| C4i-C3-C4-C5 | | -179.6(3) | C11ii-C12-C11-C10 | -179.6(3) | -180.00 | -180.00 |