**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 |