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SUPPLEMENTARY MATERIAL TO

X-Ray, Hirshfeld surface analysis, spectroscopic and DFT studies of polycyclic aromatic hydrocarbons: fluoranthene and acenaphthene

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TABLE S-I. Comparison of selected calculated geometric parameters of fluoranthene with experiment values

Experimental (XRD)				Theoretical	
				6-31+G (d, p)	6-311++G(3df,2pd)
Bond length, Å					
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

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TABLE S-I. Continued

Experimental (XRD)				Theoretical	
				6-31+G (d, p)	6-311++G(3df,2pd)
Angle, °					
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 angle, °					
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–C1–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 S-II. Comparison of selected calculated geometric parameters of acenaphthene with experiment values

Experimental (XRD)				Theoretical	
				6-31G (d, p)	6-31G* (d, p)
Bond length, Å					
$C1^{i}$–$C6^{i}$	1.358	$C8^{ii}$–$C9^{ii}$	1.358	1.370	1.377
C6–C5	1.403	$C9^{ii}$–$C10^{ii}$	1.397	1.426	1.423
C5–C4	1.359	$C10^{ii}$–$C11^{ii}$	1.354	1.384	1.383
$C4^{i}$–C3	1.410	$C11^{ii}$–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
$C2–C1^{i}$	1.400	$C13–C8^{ii}$	1.400	1.414	1.412
C1–C7	1.506	C8–C14	1.503	1.523	1.520
$C7–C7^{i}$	1.547	$C14–C14^{ii}$	1.534	1.575	1.570
$C7^{i}$–$C1^{i}$	1.506	$C14^{ii}$–$C8^{ii}$	1.503	1.523	1.520
Angle, °					
$C7^{i}$–$C1^{i}$–$C6^{i}$	132.93	$C14^{ii}$–$C8^{ii}$–$C9^{ii}$	133.14	132.40	132.40
$C7^{i}$–$C1^{i}$–C2	108.41	$C14^{ii}$–$C8^{ii}$–C13	108.21	108.70	108.70
$C1^{i}$–$C6^{i}$–$C5^{i}$	119.14	$C8^{ii}$–$C9^{ii}$–$C10^{ii}$	118.90	118.80	118.80
$C6^{i}$–$C5^{i}$–$C4^{i}$	122.20	$C9^{ii}$–$C10^{ii}$–$C11^{ii}$	122.80	122.30	122.30
$C5^{i}$–$C4^{i}$–C3	120.60	$C10^{ii}$–$C11^{ii}$–12	120.20	120.30	120.20
$C4^{i}$–C3–C2	115.87	$C11^{ii}$–C12–C13	115.86	116.30	116.30
$C4^{i}$–C3–C4	128.30	$C11^{ii}$–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
$C1–C7–C7^{i}$	105.13	$C8–C14–C14^{ii}$	105.40	104.80	104.80
$C7–C7^{i}–C1^{i}$	105.13	$C14–C14^{ii}–C8^{ii}$	105.40	104.80	104.80
$C1–C2–C1^{i}$	112.90	C8–C13–$C8^{ii}$	112.80	112.80	112.80
Dihedral angle, °					
$C7^{i}$–$C1^{i}$–$C6^{i}$–$C5^{i}$	179.3(2)	$C14^{ii}$–$C8^{ii}$–$C9^{ii}$–$C10^{ii}$	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
$C1–C2–C1^{i}–C6^{i}$	179.2(2)	$C8–C13–C8^{ii}–C9^{ii}$	179.9(2)	180.00	180.00
$C4^{i}$–C3–C4–C5	–179.6(3)	$C11^{ii}$–C12–C11–C10	–179.6(3)	–180.00	–180.00

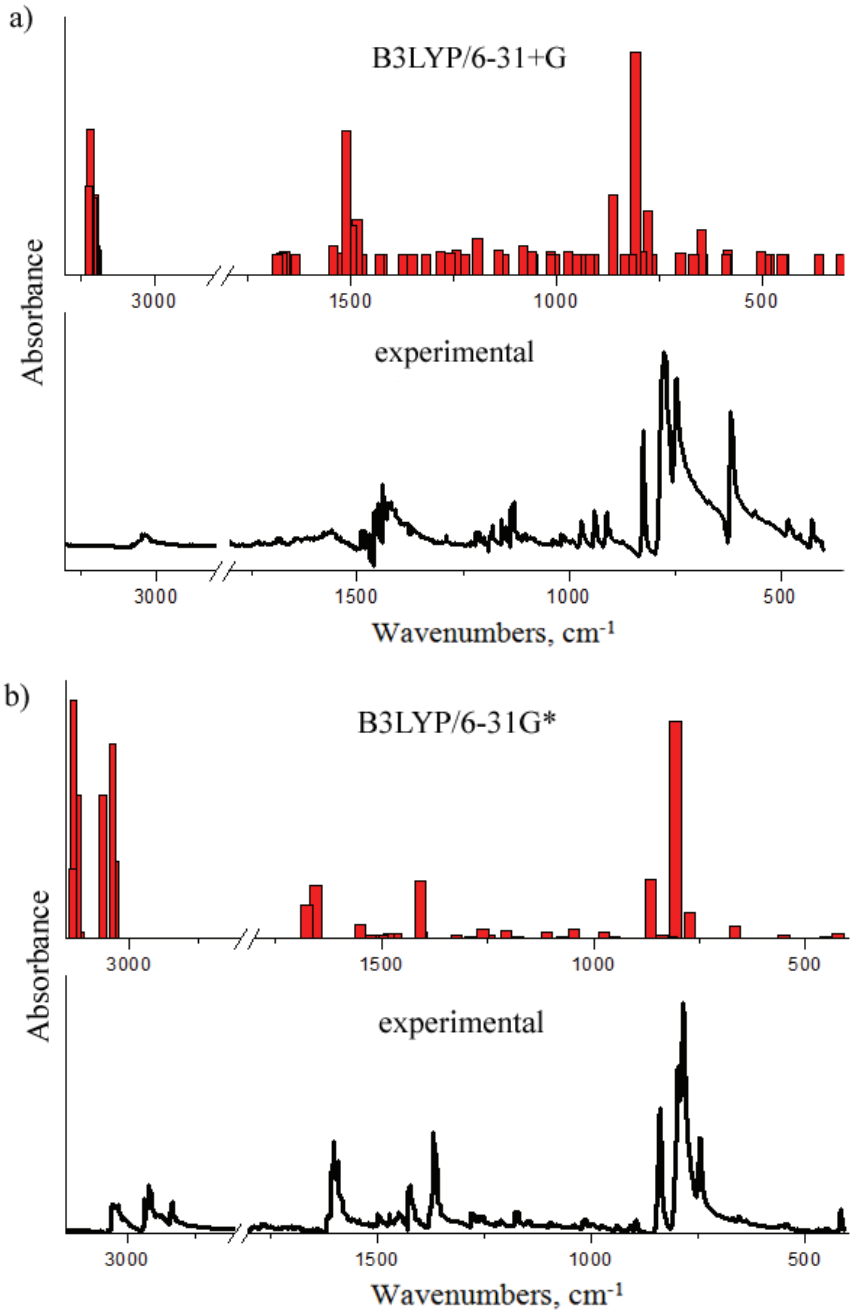

Fig. S-1. Comparison of B3LYP calculated IR spectra of: a) fluoranthene and b) acenaphthene with the corresponding experimental spectra.