**X-ray, Hirshfeld surface analysis, spectroscopic and DFT studies of PAHs: fluoranthene and acenaphthene**

WIOLETA ŚMISZEK-LINDERT1\*, ANNA MICHTA2, ALEKSANDRA TYL2, GRZEGORZ MAŁECKI2, ELŻBIETA CHEŁMECKA3 and SŁAWOMIR MAŚLANKA2

*1*\**Institute of Mechanised Construction & Rock Mininig, W. Korfantego 193A Street, 40-157 Katowice,2Institute of Chemistry, University of Silesia, 9 Szkolna Street, 40-006 Katowice and*

*3Division of Statistics, Department of Instrumental Analysis, Medical University of Silesia, 30 Ostrogórska Street, 41-200 Sosnowiec*

Corresponding author: E-mail: w.lindert@imbigs.pl

Phone: (+4832) 258-13-73

Fax: (+4832) 258-35-53

*Abstract*: The X-ray structure, theoretical calculation, Hirshfeld surfaces analysis, IR and Raman spectra of fluorantheneand acenaphthene were reported.The acenaphthene crystallizes in the [orthorhombic](file:///C%3A%5CUsers%5CWiola%5CDesktop%5CIMBiGS%5CPRACA%20NAUKOWA%20-%20%20POSTERY%2C%20ARTYKU%C5%81Y%2C%20KONFERENCJE%5C2014%20-%2056%20KONWERSATORIUM%20KRYSTALOGRAFICZNE%202014%5CABSTRAKTY%5Cwl3%20_symmetry_cell_setting) crystal system and space group [*P*21*ma*](file:///C%3A%5CUsers%5CWiola%5CDesktop%5CIMBiGS%5CPRACA%20NAUKOWA%20-%20%20POSTERY%2C%20ARTYKU%C5%81Y%2C%20KONFERENCJE%5C2014%20-%2056%20KONWERSATORIUM%20KRYSTALOGRAFICZNE%202014%5CABSTRAKTY%5Cwl3%20_symmetry_space_group_name_H-M), with crystal parameters *a* = [7.2053 (9)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl3%20_cell_length_a) Å, *b* = [13.9800 (15)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl3%20_cell_length_b) Å, *c* = [8.2638 (8)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl3%20_cell_length_c) Å, *Z* = 4 and *V* = [2135.5 (4)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl4%20_cell_volume) Å3. In turn, the grown crystals of fluoranthene are in monoclinic system with space group P21/n. The unit cell parameters are *a* = [18.349 (2)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl4%20_cell_length_a) Å, *b* = [6.2273 (5)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl4%20_cell_length_b) Å, *c* = [19.861 (2)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl4%20_cell_length_c) Å, β = [109.787 (13)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl4%20_cell_angle_beta)°, Z = 8 and unit cell volume is [832.41 (16)](file:///I%3A%5CIMBIGS%5CIMBIGS%20-%20WWA%20I%20WELNA%20XRF%20XPS%5CWWA%5CW%C5%81ASNE%20ARTYKU%C5%81Y%20DO%20CZASOPISM%20ANGLOJ%C4%98ZYCZNYCH%5Cwl3%20_cell_volume) Å3. The structure was solved by direct methods and refined by full-matrix least squares based on F2 with weight w=1/[σ2(F02)+(0.0702P)2+0.5131P] where P=(F02+2Fc2)/3 and w=1/[σ2(F02)+(0.0589P)2] where P = (F02 +2Fc2)/3 for fluorantheneand acenaphthene respectively. Theoretical calculations of the title compounds isolated molecule have been carried out using DFT at the B3LYP level. The intermolecular interactions in the crystal structure, for both the title PAHs, were analyzed using Hirshfeld surfaces computational method.

*Keywords*: crystal structure; IR spectroscopy; Raman; density functional theory (DFT) calculation; Hirshfeld surfaces.

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