Poster

Crystallographic and quantum chemical studies of xanthene-1,8(2H)-dione derivatives

L. Radovanović[1], A. Lazić[1], I. Đorđević[2], N. Trišović[3], J. Rogan[3]

[1]Innovation Centre of the Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, [2]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, Belgrade, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

lradovanovic@tmf.bg.ac.rs

Xanthene derivatives are an important class of organic compounds due to wide usage as antimicrobial, anticancer, antiviral and anti-malarial agents [1]. They also found an application as dyes and fluorescent materials for imagining of bio-molecules because of their versatile spectroscopic properties [1]. In this work, two xanthene derivatives, 3,3,6,6-tetramethyl-9-(3-chloro-4-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**1**) and 3,3,6,6-tetramethyl-9-(3,4-dibromo-4-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H- xanthene-1,8(2H)-dione (**2**) (Fig.1), were synthesized through condensation of dimedone and the appropriate aromatic aldehyde. The single crystal X-ray analysis revealed that the main structural feature in **1** is the chains parallel to the *a*-axis formed by C–H···O interaction between neighbouring asymmetric units, which are further organised into zipper-like double chains via O–H ···O hydrogen bonds and Cl···π interactions. In **2**, alternating asymmetric units are linked by O–H···O hydrogen bonds, C–H···O and Br···Br interactions into supramolecular chain along the *a*-axis, while C–H···O and C–H···π interactions led to further networking. The Hirshfeld surface analysis was used to obtain a preliminary insight into the proportion and nature of the intermolecular interactions in the crystal structure, while the quantum-chemical calculations of interaction energies of dimeric motifs revealed which motifs have the most significant contribution to the overall energy of the crystal structure. Both molecules demonstrate a comparable distribution of predominant contacts H···H, O···H, C···H and H···X (X = Cl, Br), although the contributions from Br···H/H···Br and Br···C/H···C contacts are more pronounced in **2**. The primary distinction between these molecules arises from the lack of a Cl···Cl contacts in **1** and the presence of a Br···Br contacts in **2**. In **1**, there are four prominent motifs, of which two exhibit interaction energies of approximately 13 kcal mol^{-1}, while the other two motifs have energies of approximately 9 kcal mol^{-1}. In **2**, two pairs of motifs stand out significantly by interaction energies (approximately 10 kcal mol^{-1}) compared to the others.

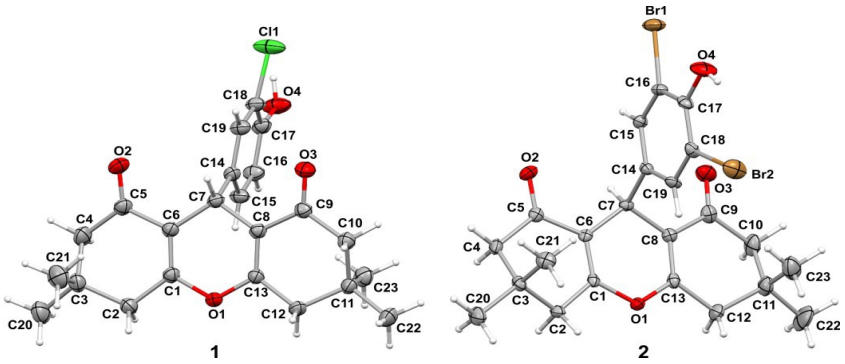

Figure 1. Asymmetric units of **1** and **2** showing 30% displacement ellipsoids (the H atoms are presented as small spheres of arbitrary radii).

Crystal data ***1***: $C_{23}H_{25}ClO_4$, M_r = 400.88, triclinic, *P*–1, *a* = 7.2040(14), *b* = 10.414(2), *c* = 14.235(3) Å, α = 95.57(3), β = 96.69(3), γ = 100.33(3) °, *V* = 1035.8(4) Å^3, *Z* = 2, *F*(000) = 424, ρ_x = 1.285 g cm^{-3}, μ(Mo*K*α) = 0.21 mm^{-1}. The refinement on F^2 (258 parameters) yielded R_1 = 0.0499, wR_2 = 0.1295, *S* = 1.026 for all data, and R_1 = 0.0444 for 3256 observed reflections with $I \geq 2\sigma(I)$.

Crystal data ***2***: $C_{23}H_{24}Br_2O_4$, M_r = 524.24, orthorhombic, $P2_12_12_1$, *a* = 11.250(2), *b* = 11.415(2), *c* = 17.193(3) Å, *V* = 2207.8(8) Å^3, *Z* = 4, *F*(000) = 1056, ρ_x = 1.577 g cm^{-3}, μ(Mo*K*α) = 3.698 mm^{-1}. The refinement on F^2 (267 parameters) yielded R_1 = 0.0447, wR_2 = 0.0651, *S* = 1.064, Flack *x* = –0.013(5) for all data, and R_1 = 0.0334 for 3507 observed reflections with $I \geq 2\sigma(I)$.

[1] Poly da Silva, I. E., Lopes da Silva, M., Dias, R. S., Santos, E. G., Brangioni de Paula, M. C., Silva de Oliveira, A., Costa da Silveira Oliveira, A. F., Marques de Oliveira, F., Canedo da Silva, C., Teixeira, R. R. & Oliviera de Paula, S. (2020). *Microbes Infect.* **22**, 489.

This work was supported financially by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contracts Nos. 451-03-66/2024-03/200287; 451-03-65/2024-03/200135 and 451-03-66/2024-03/200026).