The crystal structure of 4-(pyren-1-yl)butyl-3-nitrobenzoate, C_{27}H_{21}NO_{4}

Abstract

C_{27}H_{21}NO_{4}, triclinic, P1̅ (no. 2), a = 8.1182(5) Å, b = 9.0097(5) Å, c = 14.8013(10) Å, α = 72.603(2)°, β = 82.642(2)°, γ = 79.351(3)°, V = 1012.23(11) Å³, Z = 2, R_{gt}(F) = 0.0367, wR_{ref}(F²) = 0.1018, T = 150 K.

CCDC no.: 1939008

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

As proposed by Moscoso et al. [5], an equimolar quantity of 3,5-dinitrobenzoic chloride and 4-(pyren-1-yl)butanol is added in a flask with dry THF. The reaction was carried out for 24 h at room temperature forming an insoluble yellow precipitate, which was washed with a saturated solution of NaHCO₃, and finally washed with hot ethanol. 1.08 g of product was obtained with a 52.4% yield.

### Experimental details

Using Olex2 [2], the structure was solved, with the olex2.solve [3] using Charge Flipping and refined with the ShelXL [4] refinement package. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters, the constraint distances of C—H ranging from 0.95 Å to 1.00 Å. Due to the data collection strategy we only obtained a completeness of 98%.

### Comment

Nitro compounds are of interest due to the electrochemical properties they possess. This electrochemistry behavior was studied by many scientist [6–8]. The nitro compounds can be used as a mediator in NADH oxidation process due to oxidation mechanism, via two electrons and two protons [9–11]. The nitro compounds mediators can be used as a electrochemistry biosensor, using nanomaterials such as multiwalled carbon nanotubes under physisorption. The inclusion of pyrene rings major interaction with multiwalled...
carbon nanotubes as we previously reported [5]. The N–O bond lengths in the nitro group range from 1.226(17) to 1.2182(16) Å. The angle between O3–N1–O2 is 123.91(13)°, O2–C10–O11 is 126.91°, C13–O12–C10 is 116.38(12)°, O2–N1–C4 is 118.36(13)°, O3–N1–C4 is 117.72(13)°, C9–C4–N1 is 118.96(13)° and C5–C4–N1 is 117.99(13)°. These angles and distances are similar to those reported for 1,2-dimethyl-3,4-dinitrobenzene, C7H7N2O4. In the crystal structure of the title compound, coplanarity of the nitro group with the pyrene group is observed.

**Acknowledgements:** The authors thank FONDECYT Grant No. 1170054 and Thierry Roisnel for the DRX collection data.

**References**