Crystal structure of 2-(2',4'-diphenylsulfonylbenzyl)pyridine, C₂₄H₁₉NO₄S₂

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Received November 28, 2003, accepted and available on-line December 19, 2003; CCDC no. 1267/1177

Abstract

C₂₄H₁₉NO₄S₂, triclinic, $P\bar{1}$ (no. 2), $a = 10.319(4)$ Å, $b = 10.275(7)$ Å, $c = 11.31(1)$ Å, $\alpha = 103.01(2)^\circ$, $\beta = 96.40(2)^\circ$, $\gamma = 64.37(3)^\circ$, $V = 1053.7$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.055$, $wR_{\text{ref}}(F) = 0.056$, $T = 296$ K.

Source of material

The title compound was prepared from 2-[2',4'-di-(phenylsulfonyl)benzyl]pyridine-1-oxide according to a published procedure [1] and purified by chromatography. Crystals of 2-(2',4'-diphenylsulfonylbenzyl)pyridine were grown by recrystallization from an ethanolic solution in the dark.

Discussion

In recent years, the photoinduced proton transfer (PIPT) reaction leading to crystals of 2-(2',4'-dinitrobenzyl)pyridine (α -DNBP) and some of its derivatives has drawn much attention due to the potential applications of these compounds in optical data storage and switching devices [2–4]. The proton transfer process from the methylene carbon atom towards the nitrogen atom of the pyridine

has been characterized for α -DNBP [4–6], and assumed to be assisted by the *o*-nitro group. To test this assumption, it was synthesized the 2-(2',4'-diphenylsulfonylbenzyl)-pyridine [1], a new α -DNBP derivative in which the electron withdrawing nitro groups have been replaced by sulfone groups, and shown that this derivative is photochromic in solution and in the crystal. We report here the crystal structure of this new compound determined by X-ray diffraction, in order to gain information on the reported PIPT process observed in such crystals.

The title compound crystallizes centrosymmetrically with a complete molecule in the asymmetric unit. In this molecule, the three phenyl rings and the pyridine one are all planar and despite the unfavorable donor-acceptor orientation in the reactant ($\angle \text{C6}–\text{H6} \cdots \text{N} = 31^\circ$), which is quite similar to the one measured in α -DNBP [7], the proton transfer reaction can proceed. The position of the H6 and its relatively short distance from nucleophilic N atom ($d(\text{H6} \cdots \text{N}) = 2.69$ Å) probably plays a role in the phototransformation of the molecule I into II (figure, bottom). In this atomic arrangement there is not any significant hydrogen bond.

Table 1. Data collection and handling.

Crystal:	colorless elongated prism, size $0.25 \times 0.40 \times 0.45$ mm
Wavelength:	Ag $K\alpha$ radiation (0.5608 Å)
μ :	1.54 cm^{-1}
Diffraction, scan mode:	MACH3, $\omega/2\theta$
$2\theta_{\text{max}}$:	49.92°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	7430, 7099
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4121
$N(\text{param})_{\text{refined}}$:	280
Programs:	teXsan [8], SIR92 [9]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	2i	1.1539	−0.7927	0.3466	0.037
H(2)	2i	1.2923	−0.9385	0.1770	0.037
H(3)	2i	1.2599	−0.8003	0.0227	0.037
H(4)	2i	1.1205	−0.5721	0.0833	0.037
H(5)	2i	0.9636	−0.3396	0.1521	0.037
H(6)	2i	0.9689	−0.3150	0.2966	0.037
H(7)	2i	0.8129	−0.5340	0.1122	0.037
H(8)	2i	0.5767	−0.4967	0.1032	0.037
H(9)	2i	0.4803	−0.1187	0.3416	0.037
H(10)	2i	0.5453	0.0916	0.1950	0.037
H(11)	2i	0.5818	0.1963	0.0580	0.037

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Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(12)	2i	0.8084	0.1771	0.0228	0.037
H(13)	2i	0.9995	0.0472	0.1349	0.037
H(14)	2i	0.9594	−0.0551	0.2839	0.037
H(15)	2i	0.4445	−0.5717	0.2695	0.037

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(16)	2i	0.4250	−0.6857	0.4223	0.037
H(17)	2i	0.2752	−0.5377	0.5910	0.037
H(18)	2i	0.1664	−0.2917	0.5967	0.037
H(19)	2i	0.1844	−0.1755	0.4454	0.037

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
S(1)	2i	0.71976(5)	−0.06314(5)	0.37186(4)	0.0490(3)	0.0351(2)	0.0345(2)	−0.0225(2)	0.0089(2)	0.0025(2)
S(2)	2i	0.32717(5)	−0.28710(5)	0.22585(4)	0.0351(2)	0.0426(3)	0.0406(3)	−0.0165(2)	−0.0040(2)	0.0158(2)
O(1)	2i	0.8485(2)	−0.1132(2)	0.4433(1)	0.070(1)	0.0577(9)	0.0399(8)	−0.0364(8)	−0.0111(7)	0.0144(7)
O(2)	2i	0.5894(2)	0.0434(2)	0.4303(1)	0.0649(9)	0.0432(8)	0.0558(9)	−0.0283(7)	0.0292(7)	−0.0096(7)
O(3)	2i	0.3053(2)	−0.3746(2)	0.1139(1)	0.0578(9)	0.079(1)	0.0394(8)	−0.0395(8)	−0.0107(7)	0.0137(7)
O(4)	2i	0.2364(1)	−0.1328(2)	0.2529(2)	0.0403(8)	0.0460(8)	0.078(1)	−0.0096(6)	−0.0001(7)	0.0310(8)
N	2i	1.0554(3)	−0.5991(3)	0.3080(2)	0.085(2)	0.110(2)	0.084(2)	−0.056(2)	−0.009(1)	0.046(2)
C(1)	2i	1.1494(4)	−0.7520(4)	0.2894(3)	0.099(2)	0.098(2)	0.103(2)	−0.063(2)	−0.038(2)	0.074(2)
C(2)	2i	1.2214(3)	−0.8251(3)	0.1864(3)	0.059(2)	0.055(2)	0.110(2)	−0.020(1)	−0.009(2)	0.027(2)
C(3)	2i	1.2064(3)	−0.7513(3)	0.0994(3)	0.084(2)	0.050(1)	0.092(2)	−0.011(1)	0.025(2)	−0.000(1)
C(4)	2i	1.1198(3)	−0.6083(2)	0.1115(2)	0.064(1)	0.037(1)	0.059(1)	−0.007(1)	0.018(1)	0.011(1)
C(5)	2i	1.0465(2)	−0.5336(2)	0.2131(2)	0.0344(9)	0.041(1)	0.053(1)	−0.0185(8)	−0.0013(9)	0.0123(9)
C(6)	2i	0.9479(2)	−0.3730(2)	0.2232(2)	0.041(1)	0.038(1)	0.075(2)	−0.0175(9)	0.011(1)	0.002(1)
C(7)	2i	0.7909(2)	−0.3434(2)	0.2246(2)	0.0364(9)	0.0326(9)	0.042(1)	−0.0137(8)	0.0077(8)	0.0049(7)
C(8)	2i	0.7460(2)	−0.4478(2)	0.1559(2)	0.042(1)	0.0340(9)	0.050(1)	−0.0123(8)	0.0108(9)	−0.0050(8)
C(9)	2i	0.6070(2)	−0.4312(2)	0.1553(2)	0.042(1)	0.040(1)	0.042(1)	−0.0206(9)	0.0026(8)	0.0001(8)
C(10)	2i	0.5065(2)	−0.3078(2)	0.2263(2)	0.0367(9)	0.0353(9)	0.0328(9)	−0.0153(8)	0.0022(7)	0.0096(7)
C(11)	2i	0.5445(2)	−0.1985(2)	0.2940(2)	0.040(1)	0.0292(9)	0.0358(9)	−0.0121(8)	0.0083(8)	0.0067(7)
C(12)	2i	0.6855(2)	−0.2162(2)	0.2912(2)	0.042(1)	0.0298(8)	0.0345(9)	−0.0182(7)	0.0035(8)	0.0058(7)
C(13)	2i	0.7487(2)	0.0107(2)	0.2560(2)	0.039(1)	0.0279(8)	0.0364(9)	−0.0134(7)	0.0081(8)	0.0038(7)
C(14)	2i	0.6328(2)	0.0870(2)	0.1872(2)	0.040(1)	0.046(1)	0.056(1)	−0.0131(9)	0.0025(9)	0.015(1)
C(15)	2i	0.6558(3)	0.1490(3)	0.0998(2)	0.069(2)	0.051(1)	0.061(1)	−0.011(1)	−0.008(1)	0.027(1)
C(16)	2i	0.7901(3)	0.1357(3)	0.0825(2)	0.092(2)	0.053(1)	0.057(1)	−0.032(1)	0.021(1)	0.018(1)
C(17)	2i	0.9040(3)	0.0597(3)	0.1505(2)	0.059(1)	0.060(1)	0.059(1)	−0.029(1)	0.016(1)	0.016(1)
C(18)	2i	0.8845(2)	−0.0041(2)	0.2380(2)	0.040(1)	0.045(1)	0.050(1)	−0.0189(9)	0.0049(9)	0.0128(9)
C(19)	2i	0.3163(2)	−0.3653(2)	0.3449(2)	0.0308(9)	0.0338(9)	0.0400(9)	−0.0156(7)	−0.0029(7)	0.0102(7)
C(20)	2i	0.3885(2)	−0.5174(2)	0.3361(2)	0.044(1)	0.034(1)	0.054(1)	−0.0123(8)	0.0054(9)	0.0080(9)
C(21)	2i	0.3756(2)	−0.5793(2)	0.4269(2)	0.057(1)	0.043(1)	0.070(2)	−0.023(1)	−0.007(1)	0.024(1)
C(22)	2i	0.2897(3)	−0.4919(3)	0.5245(2)	0.068(2)	0.067(2)	0.052(1)	−0.039(1)	−0.006(1)	0.028(1)
C(23)	2i	0.2182(3)	−0.3424(3)	0.5318(2)	0.066(2)	0.063(1)	0.044(1)	−0.030(1)	0.015(1)	0.004(1)
C(24)	2i	0.2319(2)	−0.2771(2)	0.4434(2)	0.044(1)	0.039(1)	0.046(1)	−0.0185(9)	0.0026(9)	0.0053(8)

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