Crystal structure of pimolin, C₂₆H₂₀O₈

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Abstract

C₂₆H₂₀O₈, triclinic, $P\bar{1}$ (No. 2), $a = 9.002(2)$ Å, $b = 9.140(2)$ Å, $c = 14.501(3)$ Å, $\alpha = 104.90(3)^\circ$, $\beta = 95.34(3)^\circ$, $\gamma = 113.83(3)^\circ$, $V = 1028.2$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.074$, $wR_{\text{ref}}(F^2) = 0.250$, $T = 293$ K.

Source of material

Pimolin has been isolated from the chloroform extracts of the seeds of the plant *Pimpinella monoica* Dalz using column chromatography (SiO₂) and purified according to [1]. The compound was crystallized from its solution in methanol by slow evaporation.

Discussion

In order to understand the stereochemical features of pimolin, the crystal structure of the title compound was determined. The structure shows a *cis* arrangement for the two pyranobenzofuran moieties. The presence of eight oxygen atoms in the structure indicate that the molecule can function as a host molecule.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.1 × 0.2 × 0.2 mm
Wavelength:	Cu K α radiation (1.54180 Å)
μ :	9.30 cm ⁻¹
Diffractometer, scan mode:	Enraf Nonius CAD4, $\omega/2\theta$
$2\theta_{\text{max}}$:	149.86°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4179, 3991
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2608
$N(\text{param})_{\text{refined}}$:	308
Programs:	SHELXS-97 [2], SHELXL-97 [3], PLUTON [4]

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(6A)	2i	0.3119	0.8523	0.2548	0.08
H(12A)	2i	-0.1642	0.3682	0.3693	0.08
H(19A)	2i	0.0275	0.3665	-0.0286	0.08
H(1A)	2i	0.7574	0.9118	0.5340	0.08
H(16A)	2i	-0.2255	0.1426	0.2285	0.08
H(2A)	2i	0.8598	1.1082	0.4442	0.08
H(14A)	2i	-0.0861	0.7245	0.3812	0.08
H(14B)	2i	-0.2659	0.5742	0.3480	0.08
H(14C)	2i	-0.1979	0.6812	0.2792	0.08
H(15A)	2i	-0.3279	0.3231	0.1860	0.08
H(25A)	2i	0.5014	0.1363	0.0117	0.08
H(27A)	2i	0.0681	-0.0343	0.3050	0.08
H(27B)	2i	0.0247	-0.1002	0.1903	0.08
H(27C)	2i	-0.0802	-0.0225	0.2469	0.08
H(10A)	2i	0.5331	0.6385	0.6509	0.08
H(10B)	2i	0.5676	0.8121	0.6357	0.08
H(10C)	2i	0.6365	0.6953	0.5746	0.08
H(24A)	2i	0.5641	0.2508	-0.1203	0.08
H(24B)	2i	0.5229	0.4049	-0.1080	0.08
H(24C)	2i	0.4003	0.2278	-0.1835	0.08

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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
O(3)	2i	0.0535(3)	0.6084(3)	0.2521(2)	0.033(1)	0.052(2)	0.038(1)	0.016(1)	0.006(1)	0.017(1)
O(2)	2i	0.3956(3)	0.6159(3)	0.5295(2)	0.035(1)	0.049(2)	0.041(1)	0.012(1)	−0.003(1)	0.015(1)
O(1)	2i	0.6204(3)	0.9999(3)	0.3594(2)	0.041(1)	0.047(2)	0.051(2)	0.012(1)	0.017(1)	0.014(1)
O(7)	2i	0.1367(4)	0.1429(4)	0.2464(2)	0.056(2)	0.064(2)	0.049(2)	0.026(2)	−0.004(1)	0.022(1)
C(13)	2i	0.0874(4)	0.4500(4)	0.3962(2)	0.033(2)	0.037(2)	0.031(2)	0.012(1)	0.007(1)	0.011(1)
O(8)	2i	0.0978(3)	0.3663(4)	0.4469(2)	0.045(2)	0.055(2)	0.047(2)	0.013(1)	0.002(1)	0.024(1)
C(9)	2i	0.3844(4)	0.6773(4)	0.4559(2)	0.032(2)	0.034(2)	0.035(2)	0.015(1)	0.009(1)	0.008(1)
C(5)	2i	0.5163(4)	0.8105(5)	0.4399(3)	0.035(2)	0.039(2)	0.038(2)	0.018(2)	0.014(1)	0.009(1)
C(7)	2i	0.2024(4)	0.6717(4)	0.3178(2)	0.032(2)	0.040(2)	0.032(2)	0.019(1)	0.010(1)	0.010(1)
C(8)	2i	0.2260(4)	0.6017(4)	0.3910(2)	0.032(2)	0.039(2)	0.032(2)	0.015(1)	0.010(1)	0.009(1)
C(6)	2i	0.3284(5)	0.8065(5)	0.3028(3)	0.048(2)	0.041(2)	0.036(2)	0.023(2)	0.018(2)	0.016(2)
O(5)	2i	0.2596(4)	0.2890(5)	−0.0433(2)	0.059(2)	0.091(2)	0.041(2)	0.038(2)	0.022(1)	0.017(2)
C(12)	2i	−0.0782(4)	0.3967(5)	0.3313(2)	0.027(2)	0.046(2)	0.032(2)	0.013(1)	0.009(1)	0.013(1)
C(4)	2i	0.4807(4)	0.8673(4)	0.3651(3)	0.038(2)	0.034(2)	0.039(2)	0.011(1)	0.015(1)	0.007(1)
C(18)	2i	−0.0199(4)	0.2475(5)	0.1662(3)	0.030(2)	0.043(2)	0.032(2)	0.013(1)	0.005(1)	0.007(1)
C(17)	2i	−0.0450(4)	0.3090(5)	0.0909(3)	0.036(2)	0.054(2)	0.035(2)	0.022(2)	0.006(1)	0.013(2)
C(19)	2i	0.0454(5)	0.3224(6)	0.0201(3)	0.048(2)	0.068(3)	0.037(2)	0.033(2)	0.013(2)	0.018(2)
C(22)	2i	0.1019(4)	0.1914(5)	0.1698(3)	0.038(2)	0.042(2)	0.038(2)	0.017(2)	−0.001(2)	0.007(2)
C(21)	2i	0.1976(5)	0.1980(5)	0.0967(3)	0.037(2)	0.048(2)	0.039(2)	0.019(2)	0.002(2)	0.002(2)
C(1)	2i	0.6936(4)	0.9174(5)	0.4820(3)	0.030(2)	0.052(2)	0.045(2)	0.013(2)	0.008(2)	0.005(2)
C(11)	2i	−0.0995(4)	0.5155(5)	0.2795(3)	0.032(2)	0.052(2)	0.036(2)	0.020(2)	0.010(1)	0.017(2)
C(16)	2i	−0.1411(4)	0.2529(5)	0.2301(3)	0.027(2)	0.049(2)	0.035(2)	0.011(1)	0.004(1)	0.011(2)
C(2)	2i	0.7467(5)	1.0242(5)	0.4319(3)	0.032(2)	0.047(2)	0.053(2)	0.009(2)	0.011(2)	0.008(2)
C(14)	2i	−0.1686(5)	0.6347(6)	0.3262(3)	0.055(2)	0.060(3)	0.052(2)	0.036(2)	0.017(2)	0.019(2)
O(6)	2i	0.3533(5)	0.0596(5)	0.1467(3)	0.082(3)	0.104(3)	0.089(3)	0.067(2)	0.016(2)	0.034(2)
C(23)	2i	0.3867(5)	0.2409(7)	−0.0444(3)	0.040(2)	0.083(3)	0.042(2)	0.024(2)	0.008(2)	−0.008(2)
C(20)	2i	0.1661(5)	0.2648(5)	0.0267(3)	0.040(2)	0.059(2)	0.036(2)	0.024(2)	0.011(2)	0.007(2)
C(15)	2i	−0.2085(4)	0.3604(5)	0.1891(3)	0.032(2)	0.061(2)	0.035(2)	0.022(2)	0.009(1)	0.017(2)
C(26)	2i	0.3253(5)	0.1340(6)	0.0926(3)	0.045(2)	0.067(3)	0.052(2)	0.033(2)	0.001(2)	0.004(2)
C(25)	2i	0.4160(5)	0.1684(6)	0.0169(4)	0.039(2)	0.076(3)	0.060(3)	0.028(2)	0.002(2)	−0.005(2)
C(27)	2i	0.0291(7)	−0.0157(7)	0.2472(4)	0.069(3)	0.066(3)	0.085(4)	0.021(3)	−0.002(3)	0.041(3)
C(10)	2i	0.5455(5)	0.6971(6)	0.6038(3)	0.039(2)	0.054(2)	0.046(2)	0.013(2)	−0.006(2)	0.016(2)
C(24)	2i	0.4763(7)	0.2849(9)	−0.1207(4)	0.061(3)	0.119(5)	0.057(3)	0.033(3)	0.023(2)	−0.004(3)
O(4)	2i	−0.1673(3)	0.3627(4)	0.0967(2)	0.044(1)	0.077(2)	0.034(1)	0.036(1)	0.010(1)	0.021(1)

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