Crystal Structure of 2-Aminobenzoic Acid

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2-Aminobenzoic acid (anthranilic acid) is known to be a specific precursor of the alkaloids skimmianine and acronidine.¹ There have been many reports on the metal-anthranilate complexes along with the structures of many of these compounds. Some transition metal anthranilates have capability for arene hydrogenation.² However the structure of anthranilic acid has not yet been reported.

The title compound was obtained from ACROS, a Japanese chemical company. Single crystals for X-ray structure determination were obtained from MeOH/CHCl₃ by slow evaporation.

All hydrogen atoms were located from the difference Fourier map. Five of them H1-H5 were refined anisotropically, and the other two HN1 and HN2 fixed during refinement. There is no indication of a third atom near N atom in the final difference Fourier map. Therefore, migration of hydrogen atom from carboxyl group to amino group does not occur.

The six membered ring is coplanar within 0.004(2) Å. The torsional angle of C(5)-C(6)-C(7)-O(1) is 0.3(3)°, and that of C(1)-C(6)-C(7)-O(2) is 1.0(3)°. Thus the whole molecule is almost coplanar. The average C-C bond distance for the ring is 1.390(5) Å. The intermolecular hydrogen bond O2-H5...O1 (1-x, 1-y, -z) (O2...O1 2.660 Å, ∠O2-H5-O1 164.0°), and the intramolecular hydrogen bond N-HN1...O2 (N...O2 2.619 Å, ∠N-HN1-O2 145.2°) help stabilize the crystal structure.

Fig. 1 An ORTEP diagram drawn at the 30% probability level.

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Table 1 Crystal data and structure refinement

Empirical formula	C ₇ H ₇ NO ₂
Formula weight	137.14
Temperature	295(2)K
Radiation = Mo Kα	0.71073 Å
Crystal system, space group	monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 4.9301(7) Å <i>b</i> = 11.2252(15) Å <i>c</i> = 11.5587(16) Å <i>β</i> = 90.743(3)°
Volume of the unit cell	639.62(15) Å ³
Z, Calculated density	4.1424 Mg/m ³
<i>μ</i> (Mo Kα)	0.106 mm ⁻¹
<i>F</i> (0 0 0)	288
Crystal size	0.3 × 0.2 × 0.2 mm
Range for data collection	2.53 ≤ <i>θ</i> ≤ 28.04°
Limiting indices	-6 ≤ <i>h</i> ≤ 6, -14 ≤ <i>k</i> ≤ 13, -15 ≤ <i>l</i> ≤ 10
Reflections collected/unique	3646/1398 [<i>R</i> (int) = 0.0462]
Refinement method	full-matrix least-squares on <i>F</i> ²
Goodness-of-fit on <i>F</i> ²	1.716
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> = 0.0586 (on <i>F</i>) <i>wR</i> = 0.1878 (on <i>F</i> ²)
Extinction coefficient	0.09(3)
Largest diff. peak and hole	0.525 and -0.532 e Å ⁻³
Measurement	Siemens SMART CCD
Program system	SHELX-97 ³
Molecular graphics	NRCVAX ⁴

Table 2 Final coordinates (×10⁴) and equivalent temperature factors (Å² × 10³)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
O(1)	2702(3)	4832(1)	990(1)	51(1)
O(2)	3380(3)	3626(1)	-504(1)	54(1)
N	-1022(3)	4290(2)	2498(1)	49(1)
C(1)	-492(5)	2032(2)	206(2)	52(1)
C(2)	-2425(5)	1237(2)	573(2)	61(1)
C(3)	-3854(5)	1473(2)	1576(2)	61(1)
C(4)	-3379(5)	2496(2)	2210(2)	59(1)
C(5)	-1405(4)	3304(2)	1844(2)	46(1)
C(6)	58(4)	3075(2)	837(2)	42(1)
C(7)	2139(4)	3909(2)	453(2)	40(1)

$$U_{eq} = (1/3) \sum \sum U_{ij} a_i^* a_j^* (a_i a_j).$$

Table 3 Selected bond lengths (Å) and angles (deg)

O(1)-C(7)	1.237(2)
O(2)-C(7)	1.310(2)
N-C(5)	1.353(3)
C(1)-C(2)	1.377(3)
C(1)-C(6)	1.404(3)
C(2)-C(3)	1.391(4)
C(3)-C(4)	1.381(4)
C(4)-C(5)	1.400(3)
C(5)-C(6)	1.401(3)
C(6)-C(7)	1.462(2)
C(2)-C(1)-C(6)	120.7(2)
C(1)-C(2)-C(3)	119.6(2)
C(4)-C(3)-C(2)	121.1(2)
C(3)-C(4)-C(5)	119.5(2)
N-C(5)-C(4)	116.98(19)
N-C(5)-C(6)	123.03(17)
C(4)-C(5)-C(6)	119.99(19)
C(5)-C(6)-C(1)	119.09(18)
C(5)-C(6)-C(7)	120.37(17)
C(1)-C(6)-C(7)	120.54(18)
O(1)-C(7)-O(2)	121.51(16)
O(1)-C(7)-C(6)	122.51(16)
O(2)-C(7)-C(6)	115.98(16)

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