X-ray Structure Analysis Online

Multiple Molecules in the Crystallographic Asymmetric Unit of (*Z*)-3-(3-Chlorophenyl)-2-phenyl acrylic acid

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The ^{1}H-NMR spectrum of the compound displayed resonance signals at 7.90 (s, 1H) and 9.8 (br s, exch.D_2O, 1H) due to the protons of the propenoic acid, in addition to the expected resonance signals of the aryl groups. The ^{13}CNMR signals at δ173.9 (CO_2H), 106(C-2) and 154.1(C-3) confirmed the propenoic acid moiety in the compound. Normally, distinction between *cis* and *trans* isomers of stilbenes is done by comparing the extinction coefficients in the UV Spectra (*trans* showing~28000and *cis* ~11000-12000), or by the coupling constant of the vinylic protons, if the double bond contains no other substituent. However, X-ray studies are accurate and give the exact geometry of compounds.

X-ray intensity data of a well-defined rod-shaped light-yellow crystal (0.3 x 0.2 x 0.1 mm^3) were collected at room temperature (293K) by using a CCD area-detector diffractometer (*X'calibur system – Oxford diffraction make, U.K.*) equipped with graphite monochromated

MoKα radiation (λ=0.71073 Å). A total of 29559 reflections were collected, of which 8186 were treated as observed (I > 2σ(I)). Data were corrected for Lorentz, polarization and absorption factors. The structure was solved by direct methods using SHELXS-97, and refined by full-matrix least-squares procedures using SHELXL-97 software. All of the hydrogen atoms were geometrically fixed and allowed to ride on the corresponding non-H atoms with C-H = 0.93 Å, O-H = 0.82 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.5U_{eq}(O)$ for H atoms. The final refinement cycle yielded an R- factor of 0.0781 [wR (F^2) = 0.1813] for the observed data. The residual electron density ranged from -0.372 to 0.455 eÅ^{-3}. Atomic-scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4).

Table 2S Dihedral angles between the phenyl ring planes

	angle (e.s.d.)		angle (e.s.d.)
Molecule A	71.9(2)	Molecule B	77.9(2)
Molecule C	69.0(2)	Molecule D	72.1(2)
Molecule E	75.8(5)	Molecule F	70.9(3)
Molecule G	77.5(3)	Molecule H	73.9(3)
Molecule I	77.1(3)	Molecule J	70.5(4)

Table 3S O-H…O and C-H…π hydrogen–bonding geometry (e.s.d.`s in parentheses). Cg1-Cg10 represent the center of gravity of the phenyl ring of ten molecules (A-J) and Cg11- Cg19 represent the center of gravity of the chlorophenyl ring of ten molecules (A-J).

D–H…A	D–H(Å)	D…A(Å)	H…A(Å)	D–H…A(°)
C5B-H5B…Cg13	0.93	3.935(8)	3.0543	158.68
C5J-H5J…Cg14	0.93	3.818(10)	2.9241	161.79
C6A-H6A…Cg19^{i}	0.93	3.754(10)	3.0572	133.05
C6C-H6C…Cg14	0.93	3.615(7)	2.8038	146.39
C6D-H6D…Cg11^{ii}	0.93	3.663(10)	2.8465	147.25
C6F-H6F…Cg15 ^{iii}	0.93	3.636(1)	2.8445	143.73
C6G-H6G…Cg13^{iv}	0.93	3.745(11)	3.1009	127.92
C8B-H8B…Cg20	0.93	3.851(11)	3.2376	125.34
C8H-H8H…Cg16^{v}	0.93	3.577(12)	2.7409	150.09
C8J-H8J…Cg18^{ii}	0.93	3.641(13)	2.8949	138.21
C9C-H9C…Cg16^{vi}	0.93	3.959(8)	3.0810	158.11
C9G-H9G…Cg18	0.93	3.822(10)	2.9358	159.74
C11A-H11A…Cg1	0.93	3.694(8)	2.8636	149.31
C11B-H11B…Cg2	0.93	3.656(8)	2.8184	150.34
C11C-H11C…Cg3	0.93	3.656(6)	2.8198	150.26
C11D-H11D…Cg4	0.93	3.704(8)	2.8733	149.34
C11E-H11E…Cg5	0.93	3.693(7)	2.8410	152.99
C11F -H11F…Cg6	0.93	3.708(8)	2.8849	148.28
C11G-H11G…Cg7	0.93	3.637(10)	2.7831	153.15
C11H-H11H…Cg8	0.93	3.696(10)	2.8848	146.50
C11I-H11I…Cg9	0.93	3.674(11)	2.8255	152.19
C11J-H11J…Cg10	0.93	3.651(11)	2.8334	147.37
C14A-H14A…Cg10^{vii}	0.93	3.838(9)	2.9912	152.19
C14B-H14B…Cg4^{v}	0.93	3.814(8)	2.9807	149.95
C14C-H14C…Cg5^{v}	0.93	3.835(7)	3.0317	145.64
C14D-H14D…Cg2	0.93	3.839(9)	3.0220	147.54

C14E-H14E…Cg3	0.93	3.829(8)	2.9944	150.09
C14F-H14F… Cg7^{viii}	0.93	3.830(9)	3.0065	148.46
C14G-H14G…Cg6	0.93	3.829(10)	3.0188	146.55
C14H-H14H…Cg9^{vii}	0.93	3.875(11)	3.0811	144.36
C14I-H14I…Cg8^{ix}	0.93	3.845(12)	2.9993	151.88
C14J-H14J…Cg1 ^{ix}	0.93	3.811(11)	3.0040	145.97
O2A-H2A... O1H^{i}	0.82	2.597(8)	1.785	170.6
O2D-H2D...O2F	0.82	2.606(8)	1.799	167.7
O2J-H2J...O1I ^{ii}	0.82	2.611(10)	1.800	169.8
O2C-H2C... O1E^{iii}	0.82	2.578(7)	1.776	165.3
O2E-H2E...O1C^{vi}	0.82	2.608(7)	1.804	166.6
O2I-H2I ...O1J^{vii}	0.82	2.610(10)	1.801	168.8
O2B- H2B ...O1G^{x}	0.82	2.619(9)	1.815	166.4
O2G -H2G...O1B^{xi}	0.82	2.586(9)	1.783	166.1
O2H - H2H...O1A^{xii}	0.82	2.610(8)	1.799	169.8

Symmetry code : i) -*x*,1/2+*y*,1-*z* ii) 1-*x*,-1/2+*y*,1-*z* iii) 1-*x*,1/2+*y*,-*z*
iv) -*x*, 1/2+*y*, -*z* v) -1+*x*, *y*, *z* vi) 1-*x*, -1/2+*y*,-*z*
vii) 1-*x*,1/2+*y*,1-*z* viii) 1+*x*, *y*, *z* ix) -*x*,-1/2+*y*,1-*z*
x) *x*,- 1+*y*, *z* xi) *x*,1+*y*,*z* xii) -*x*,-1/2+*y*,1-*z*