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Key indicators

Single-crystal X-ray study

$T = 291$ K

Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å

R factor = 0.053

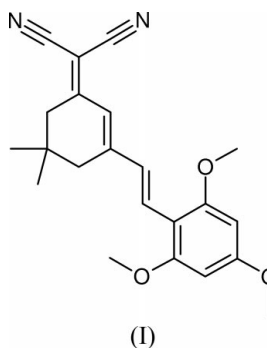
wR factor = 0.118

Data-to-parameter ratio = 17.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Triclinic form of 2-{5,5-dimethyl-3-[2-(2,4,6-trimethoxyphenyl)vinyl]cyclohex-2-enylidene}malononitrile

On slow evaporation of an ethylacetate solution, the title compound, $\text{C}_{22}\text{H}_{24}\text{N}_2\text{O}_3$, (I), crystallizes in two crystalline forms differing in colour, size and shape. For the structural data on the monoclinic violet form, as well as comment on the differences between the two structures and the details of preparation, see Kolev *et al.* [*Acta Cryst.* (2001). E57, o964–o965]. This paper reports the structural results of the red triclinic modification.



Experimental

The preparation of the title compound is described in Kolev *et al.* (2001).

Crystal data

$\text{C}_{22}\text{H}_{24}\text{N}_2\text{O}_3$
 $M_r = 364.43$
 Triclinic, $P\bar{1}$
 $a = 7.5983$ (3) Å
 $b = 11.4757$ (4) Å
 $c = 11.5774$ (4) Å
 $\alpha = 84.8457$ (15)°
 $\beta = 82.2149$ (16)°
 $\gamma = 79.0257$ (17)°
 $V = 979.77$ (6) Å³

$Z = 2$
 $D_x = 1.235$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8836 reflections
 $\theta = 3.4\text{--}27.4^\circ$
 $\mu = 0.08$ mm⁻¹
 $T = 291$ (1) K
 Block, red
 $0.25 \times 0.23 \times 0.23$ mm

Data collection

Nonius KappaCCD diffractometer
 303 frames via ω -rotation ($\Delta\omega = 1^\circ$)
 with 3 sets at different κ -angles
 and two times 30 s per frame
 8836 measured reflections
 4334 independent reflections

1655 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\text{max}} = 27.4^\circ$
 $h = -9 \rightarrow 9$
 $k = -14 \rightarrow 14$
 $l = -14 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.118$
 $S = 0.90$
 4334 reflections
 249 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0358P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.13$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.15$ e Å⁻³

H atoms were placed in calculated positions with U_{iso} constrained to be $1.5U_{\text{eq}}$ of the carrier atom for the methyl-H and $1.2U_{\text{eq}}$ for the remaining H atoms.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2001).

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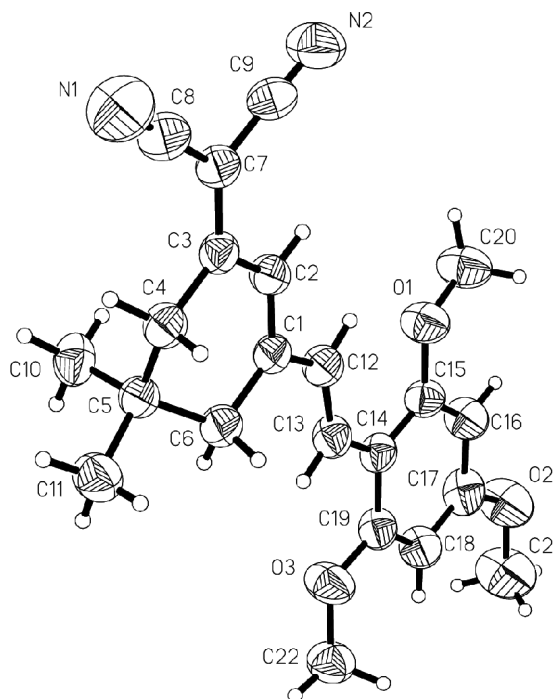


Figure 1

View of the title compound showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 50% probability level. H atoms are drawn as circles of arbitrary radii.