Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Tsonko Kolev,[a] Zornitza Glavcheva,[b] Denitsa Yancheva,[b] Markus Schürmann,[a] Dirk-Christian Kleb,[a] Hans Preut[a]* and Paul Bleckmann[a]

[a]Fachbereich Chemie, Universität Dortmund, Otto-Hahn-Straße 6, 44221 Dortmund, Germany, and [b]Bulgarian Academy of Sciences, Institute of Organic Chemistry, 1113 Sofia, Bulgaria

Correspondence e-mail: uch002@uxp1.hrz.uni-dortmund.de

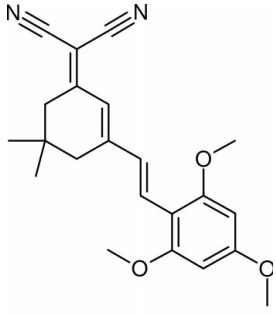
Received 15 August 2001
Accepted 17 September 2001
Online 29 September 2001

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–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.

On slow evaporation of an ethylacetate solution, the title compound, $C_{22}H_{24}N_2O_3$, (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). E**57**, o964–o965]. This paper reports the structural results of the red triclinic modification.



(I)

Experimental

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

Crystal data

$C_{22}H_{24}N_2O_3$
M_r = 364.43
Triclinic, $P\overline{1}$
a = 7.5983 (3) Å
b = 11.4757 (4) Å
c = 11.5774 (4) Å
α = 84.8457 (15)°
β = 82.2149 (16)°
γ = 79.0257 (17)°
V = 979.77 (6) Å^3
Z = 2
D_x = 1.235 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8836 reflections
θ = 3.4–27.4°
μ = 0.08 mm^{-1}
T = 291 (1) K
Block, red
0.25 × 0.23 × 0.23 mm

Data collection

Nonius KappaCCD diffractometer
303 frames *via* ω-rotation ($\Delta\omega$ = 1°) 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_{int} = 0.028
θ_{max} = 27.4°
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 15$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

H atoms were placed in calculated positions with U_{iso} constrained to be $1.5U_{eq}$ of the carrier atom for the methyl–H and $1.2U_{eq}$ 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: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97, *PARST*95 (Nardelli, 1995) and *PLATON* (Spek, 2001).

We thank the 'Internationales Büro bei der DLR' (Germany) for the support of our project BUL-006-99. One of us (TK) thanks the Alexander von Humboldt–Stiftung for financial support.

References

Kolev, T., Glavcheva, Z., Yancheva, D., Schürmann, M., Kleb, D.-C., Preut, H. & Bleckmann, P. (2001). *Acta Cryst.* E**57**, o964–o965.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter & R. M. Sweet, pp. 307–326. London: Academic Press.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus.* Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2001). *PLATON.* University of Utrecht, The Netherlands.

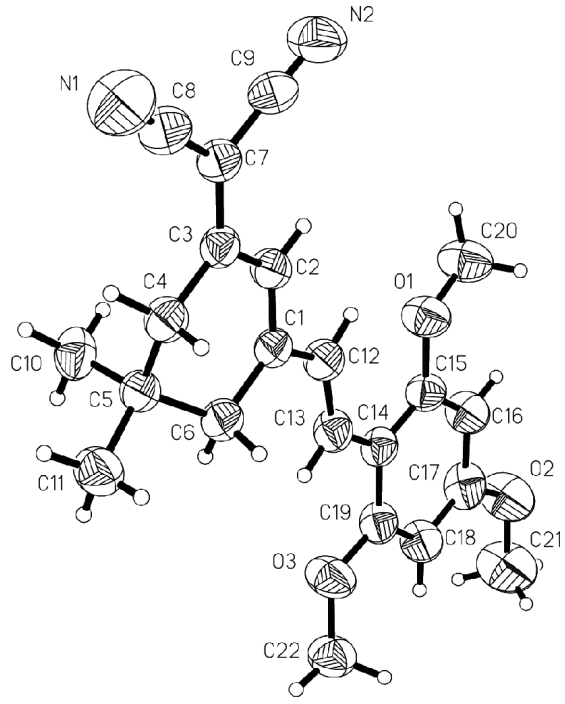


Figure 1
View of the title compound showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 50% probability level. H atoms are drawn as circles of arbitrary radii.