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## A second triclinic modification of 2',6'-dimethoxyflavone

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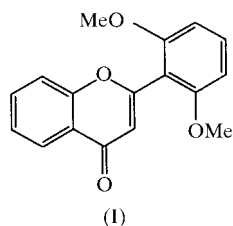
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Crystals of a second triclinic modification of the title compound, 2-(2,6-dimethoxyphenyl)-4*H*-1-benzopyran-4-one, C<sub>17</sub>H<sub>14</sub>O<sub>4</sub>, were grown from a hot cyclohexane solution. In the molecule, the O—C—C torsion angle at the junction between the benzopyran and phenyl rings is 67.6 (3)°.

### Comment

The triclinic modification of the title compound, (I), was described a few years ago (Tinant *et al.*, 1991). It contains altogether *Z* = 6 molecules of three geometries characterized by different torsion angles of the substituted phenyl ring [O1—C2—C1'—C6' = −65.9 (2), −83.9 (3) and −96.6 (3)°]. As part of our extensive study of the polymorphism of this compound, of its inclusion compounds (Wallet *et al.*, 1989, 1993, 1994, 1998, 2000; Espinosa *et al.*, 1999) and of its adducts (Manniukiewicz *et al.*, 1996), we report a second modification of (I), which was obtained from hot cyclohexane. This is an illustration of the comment of McCrone (1965) that the number of forms known for a given compound is proportional



to the time spent on that compound. There are no structural differences at the molecular level except for the torsion angle. The density difference at room temperature between both triclinic modifications is rather small (1%).

The calculation of energy *versus* torsion angle about the C2—C1' bond shows that the barrier of rotation in the region 20–90° is small (Vrielynck *et al.*, 2000). Any value of the torsion angle in this range is plausible, and other polymorphs remain to be found.

### Experimental

The synthesis of the title compound has been described previously (Wallet *et al.*, 1989). It was recrystallized from boiling cyclohexane. Slow cooling gave single crystals (m.p. 420–421 K).

#### Crystal data

C <sub>17</sub> H <sub>14</sub> O <sub>4</sub>	<i>Z</i> = 2
<i>M<sub>r</sub></i> = 282.28	<i>D<sub>x</sub></i> = 1.327 Mg m <sup>−3</sup>
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 7.721 (2) Å	Cell parameters from 25 reflections
<i>b</i> = 8.905 (5) Å	<i>θ</i> = 2.41–25.89°
<i>c</i> = 11.231 (4) Å	<i>μ</i> = 0.095 mm <sup>−1</sup>
<i>α</i> = 97.57 (4)°	<i>T</i> = 293 (2) K
<i>β</i> = 105.69 (3)°	Prism, colourless
<i>γ</i> = 103.60 (3)°	0.42 × 0.40 × 0.05 mm
<i>V</i> = 706.7 (5) Å <sup>3</sup>	

#### Data collection

Enraf–Nonius CAD-4 ( <i>κ</i> -geometry) diffractometer	<i>R</i> <sub>int</sub> = 0.05
Non-profiled <i>ω</i> scans	<i>θ</i> <sub>max</sub> = 29.99°
Absorption correction: <i>ψ</i> scan (North <i>et al.</i> , 1968)	<i>h</i> = −10 → 10
<i>T</i> <sub>min</sub> = 0.907, <i>T</i> <sub>max</sub> = 0.979	<i>k</i> = −12 → 12
4215 measured reflections	<i>l</i> = 0 → 15
4021 independent reflections	3 standard reflections every 76 reflections
1476 reflections with <i>I</i> > 2σ( <i>I</i> )	frequency: 60 min
	intensity decay: none

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	H-atom parameters constrained
<i>R</i> ( <i>F</i> ) = 0.055	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0566 <i>P</i> ) <sup>2</sup> ]
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.143	where <i>P</i> = [2 <i>F<sub>o</sub></i> <sup>2</sup> + max( <i>F<sub>o</sub></i> <sup>2</sup> , 0)]/3
<i>S</i> = 0.917	(Δ/σ) <sub>max</sub> = 0.004
4021 reflections	Δρ <sub>max</sub> = 0.133 e Å <sup>−3</sup>
192 parameters	Δρ <sub>min</sub> = −0.161 e Å <sup>−3</sup>

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1994); cell refinement: CAD-4 EXPRESS; data reduction: XCAD4 (Harms & Wocadlo, 1995); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); software used to prepare material for publication: WinGX (Farrugia, 1998).

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