

mean plane. It makes dihedral angles of 17.4 (2), 85.22 (17) and 65.39 (16)°, respectively, with the phenyl, xanthen and anthracene ring systems. In the crystal structure, there are intramolecular C—H...O and C—H...N contacts and molecules are also linked by C—H... π interactions.

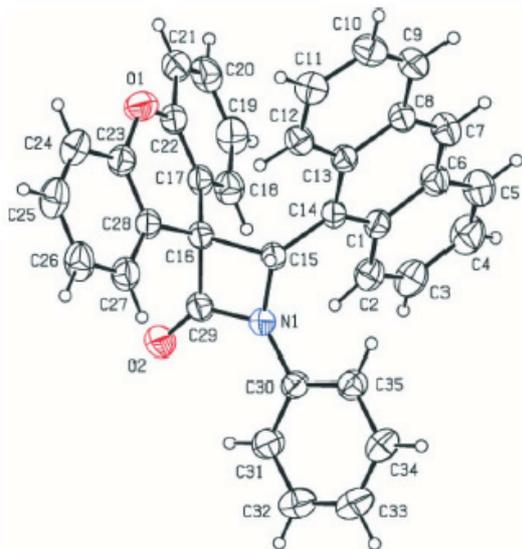


Fig 1: The molecular structure of title compound

The title compound, $C_{35}H_{23}NO_2$, crystallizes in the monoclinic $P2_1/c$ space group with $a = 13.6906$ (8) Å, $b = 13.3085$ (7) Å, $c = 17.3527$ (10) Å, $\beta = 127.548$ (4)°, $V = 2506.7$ (3) Å³, $Z = 4$, $\mu = 0.08\text{mm}^{-1}$, $R = 0.051$, $wR = 0.110$, $S = 0.90$.

Keyword: crystal structure; 4-(9-Anthryl)-1-phenylspiro[azetidine-3,90-xanthen]-2-one; the β -lactam ring

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Concentration Modulations and Short-Range vs. Long-Range Order in Layered Tellurides. Oliver Oeckler^a, Matthias N. Schneider^a. ^aDepartment of Chemistry and Biochemistry, LMU Munich.

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Multinary tellurides have received much attention both as phase-change alloys for data storage and as promising thermoelectrics.[1,2] In the systems $M\text{-Y-Te}$ ($M = \text{Ge, Sn, Pb, Ag, In, ...}$; $Y = \text{Sb, Bi}$) thermodynamically stable phases are found on pseudobinary lines $(M\text{Te})_n(\text{Y}_2\text{Te}_3)_m$ and $(\text{Y}_2\text{Te}_3)_m(\text{Y}_2)_k$, they exhibit rocksalt-type as well as $A7$ -type building blocks and can exhibit extremely long translation periods.

Quenching and subsequent annealing yields series of trigonal metastable phases $(M\text{Te})_n(\text{Y}_2\text{Te}_3)_m(\text{Y}_2)_k$ with building blocks from both types of stable compounds. [3] Although long-periodic order is evidenced by sharp superstructure reflections, pronounced positional disorder is present. Single-crystal X-ray analysis as well as TEM show that the element concentrations vary continuously along the stacking direction of hexagonal atom layers.

Typical examples include $(\text{Ge}_x\text{Sb}_{1-x/2})_2\text{Te}_3\text{:}[(\text{GeTe})_y\text{Sb}_{1-2y}]_8$ ($x = 0.31$, $y = 0.0325$; $R\text{-}3m$, $a = 4.266$, $c = 75.02$ Å, $R1 = 0.051$) and $\text{Ge}_{2-x}\text{Sb}_{2+x}\text{Te}_2\text{Sb}_8$ ($x = 0.43$; $R\text{-}3m$, $a = 4.258$, $c = 97.23$ Å, $R1 = 0.044$). This variation can be described as a long-range ordered occupational modulation which blurs the boundaries between “building blocks”. Quenching obviously leads to partial spinodal decomposition involving wavy concentration fluctuations. These “waves” are perfected by short-range diffusion during annealing, whereas decomposition is impossible as it requires long-range diffusion. Incommensurate concentration modulations have also been observed.

If the basic structure is close to cubic, e. g. in $(\text{GeTe})_x(\text{Sb}_2\text{Te}_3)$ ($x \gg 3$), high-temperature phases with disordered rocksalt-type structures are sometimes observed. Superstructure formation (i. e. either concentration waves or block formation) upon cooling consequently involves multiple twinning. Strain can impede this ordering, resulting in pseudocubic crystals with remarkable diffuse scattering; the maxima coincide with the positions of the strongest superstructure reflections of the corresponding long-range ordered (meta-)stable phases.

Concerning metastable crystalline phases of phase-change alloys, disordered cubic rocksalt-type structures are often assumed.[1] Investigations on comparable bulk samples (e. g. with compositions $\text{Ge}_{0.73}\text{Sb}_{0.20}\text{Te}$ or $\text{Ge}_{0.57}\text{Sb}_{0.34}\text{Te}$) evidence that pronounced short-range ordering matches with small (distorted) cutouts of the corresponding stable phases. This leads to the hypothesis that metastable crystalline samples may contain twinned and strained nanoscale domains of stable compounds and long-range order is impeded by the stress associated with volume change resulting from partial superstructure formation.

[1] Wuttig, M., Yamada N., *Nat. Mater.* **2007**, 6, 824. [2] Snyder G. J., Toberer E. S., *Nat. Mater.* **2008**, 7, 105. [3] Schneider M. N., Seibald M., Oeckler O., *Dalton Trans.* **2009**, 2004.

Keywords: phase-change technology; modulated structures; tellurium compounds

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The Modulated Structure of Λ -Co(Sepulchrates)-Trinitrate at $T = 100$ K. Andreas Schönleber^a, Sander van Smaalen^a, Wolfgang Morgenroth^b, Finn Krebs Larsen^c. ^aLaboratory of Crystallography, University of Bayreuth, Bayreuth, Germany. ^bInstitute of Geosciences, University of Frankfurt, Frankfurt am Main, Germany. ^cDepartment of Chemistry, University of Aarhus, Aarhus, Denmark.

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Λ -Co(sepulchrates)-trinitrate, $C_{12}H_{18}N_8Co^{3+} \cdot 3(NO_3)^-$ crystal-lizes at room temperature in symmetry $P6_322$ [1]. Sepulchrates is (*S*)-(1,3,6,8,10,13,16,19-octa-azabicyclo-[6.6.6]eicosane). The cation and two of the nitrate anions are centred on three fold rotation axes, linked to each other by $N\text{-H}\cdots\text{O}$ hydrogen bonds. The third nitrate anion is centred on the intersection of the two fold rotation axes and shows orientational disorder.