Crystal data for two enkephaline peptides. By M. Cotrait and S. Geoffre, Laboratoire de Cristallographie, Université de Bordeaux I, 351 Cours de la Libération, 33405 Talence, France

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The two enkephaline Tyr-Gly-Gly (I) and Phe-Met (II) peptides have been crystallized with the following crystal data:

(I) space group $P2_12_12_1$ or $P2_22_12_1$ ($Z=4$); $a=9.549(3)$, $b=8.073(2)$, $c=18.424(5)$ Å; (II) space group $I4_1$ ($Z=8$); $a=b=23.891(4)$, $c=5.589(3)$ Å.

Introduction

Enkephalines are endogenous pentapeptides isolated from mammalian brain with morphin-like activity. The amino acid sequence of the major component, Met-enkephalin is Tyr-Gly-Gly-Phe-Met. The conformation of the molecule has been proposed in solution by NMR spectroscopy (Roques, Garbay-Jauregui-Berry, Oberlin, Anteneus & Lala, 1976) and in vacuum by means of empirical energy calculations (Isogai, Nemethy & Scheraga, 1976). We intended to solve the crystal structures of the Tyr-Gly-Gly and Phe-Met peptides, as part of Met-enkephaline.

Crystal data

The two peptides were purchased from Bachem Biochemicals; Tyr-Gly-Gly was crystallized from water–methanol mixtures and Phe-Met from methanol solutions (thin needle-shaped crystals with square section).

Unit-cell dimensions and their associated standard deviations were derived from least-squares fits to the angular settings of about ten reflections on a Siemens four-circle diffractometer with Cu $K\alpha$ radiation ($\lambda=1.5418$ Å, $\theta=20^\circ$). Densities were determined by flotation. The crystal data for both compounds are given in Table 1.

Results

As far as Tyr-Gly-Gly is concerned there is a space-group ambiguity which has not been yet quite cleared. There is a clear systematic absence for the [00l] row. Along the [0k0] row, the 010 reflection only is present. On the [hk0] row, reflections with $h$ odd are present though they are all weak or very weak. So the space group could be $P2_22_1$ or $P2_12_12_1$ and we tried to solve the structure in both groups.

Diffracted intensities from Phe-Met crystals are very weak owing to the small dimensions of the crystals (0.1 x 0.1 x 1 mm) and the quite high thermal scattering ($B_M \approx 6.5$ Å² from a Wilson plot); the Bragg angle $\theta$ was then limited to 50°. On the other hand, the crystals were of too poor quality to permit a structure determination.

We plan to determine the Phe-Met crystal structure when better and bigger crystals are obtained.

* In which case $h$ and $k$ as well as $a$ and $b$ should be exchanged according to the international conventions.

References


Crystal data for an ilmenite variety of calcium stannate CaSnO$_3$. By B. Durand, Laboratoire de Chimie Minérale 3, Université Claude Bernard, 69621 Villeurbanne, France and H. Loiseleur, Laboratoire de Chimie Analytique 2, Université Claude Bernard, 69621 Villeurbanne, France

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An ordered ilmenite phase of the stannate CaSnO$_3$ is evidence from powder patterns. The hexagonal and rhombohedral unit-cell parameters are respectively: $a=5.487$ (1), $c=15.287$ (6) Å, $Z=6$ and $a=6.000$ (2) Å, $\alpha=54.42$ (3)°, $Z=2$; $D_n=5.16$, $D_x=5.17$ g cm$^{-3}$.

Origin of specimen

Calcium stannate CaSnO$_3$ was prepared by a double decomposition reaction between the lithium tin oxide Li$_2$SnO$_3$ and the eutectic (CaCl$_2$–1·13 NaCl):

$$\begin{align*}
\text{Li}_2\text{SnO}_3 + (\text{CaCl}_2 - 1\cdot13 \text{NaCl}) & \xrightarrow{600^\circ\text{C}} \text{CaSnO}_3 \\
\text{N}_2 & + 2 \text{LiCl} + 1\cdot13 \text{NaCl}.
\end{align*}$$


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