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# Crystal structure of L-cysteine L-tartarte monohydrate, $C_7H_{15}NO_9S$

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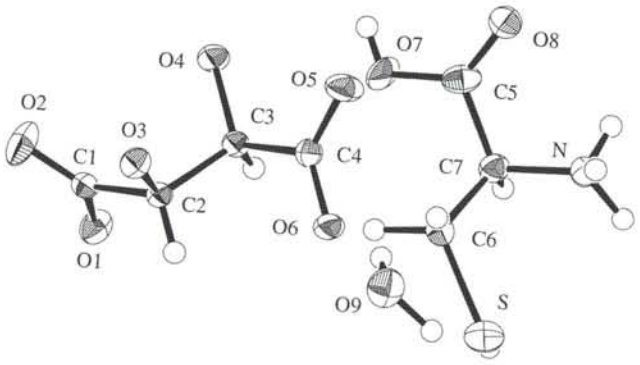


**Fig. 1.** Molecule plot.

**Abstract**

$C_7H_{15}NO_9S$, monoclinic, $P12_11$ (No. 4), $a = 7.9152(8)$ Å, $b = 7.7166(6)$ Å, $c = 10.4111(9)$ Å, $\beta = 111.0°$, $V = 593.7$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.035$, $R_w(F) = 0.059$, $T = 296$ K.

**Source of material**

The compound was prepared by the reaction of L-cysteine with L-tartaric acid in aqueous solution. Slow evaporation of the solution yielded colorless prism-shaped single crystals.

**Discussion**

The hydrogen atoms were either directly located from the difference Fourier electron density maps or calculated and included in the structural model, but not refined (fixed). Three H atoms could not be located. Because the Flack parameter was not well-defined in the structure refinement, the absolute configuration of the chiral centers was assigned based on the starting materials. This gives (*R*)-cysteine, and (2*R*,3*R*)-tartaric acid. The extensive intermolecular hydrogen bonds between the cycteine, tartaric and the crystallization water give rise to a three dimentional network.

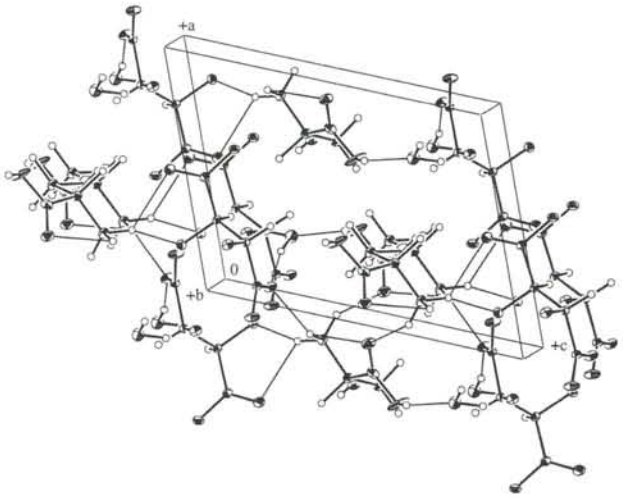


**Fig. 2.** Packing of the molecules, view along [010].

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colorless prism, size 0.20 x 0.20 x 0.30 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.7107 Å) |
| $\mu$: | 3.15 cm$^{-1}$ |
| Diffractometer, scan mode: | Quantum CCD, $\omega$ |
| $2\theta_{max}$: | 54.02° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 3215, 1282 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1223 |
| $N(param)_{refined}$: | 163 |
| Programs: | SIR92 [3], teXsan [1] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 2*a* | −0.6916 | −0.4402 | −0.9081 | 0.023 |
| H(2) | 2*a* | −0.6812 | −0.2077 | −0.7649 | 0.022 |
| H(3) | 2*a* | −0.6748 | 0.1647 | −0.5684 | 0.052 |
| H(4) | 2*a* | −0.6061 | −0.2519 | −0.5087 | 0.052 |
| H(5) | 2*a* | −0.8197 | −0.2925 | −0.5403 | 0.052 |
| H(6) | 2*a* | −0.5897 | −0.0880 | −0.2755 | 0.052 |
| H(7) | 2*a* | −0.9714 | −0.1788 | −0.3681 | 0.052 |
| H(8) | 2*a* | −0.8759 | −0.0312 | −0.2801 | 0.052 |
| H(9) | 2*a* | −0.8230 | −0.2068 | −0.2240 | 0.052 |
| H(10) | 2*a* | −0.6188 | −0.4624 | −0.3177 | 0.052 |
| H(11) | 2*a* | −0.1943 | −0.1212 | −0.2264 | 0.052 |
| H(12) | 2*a* | −0.2558 | −0.2867 | −0.1784 | 0.052 |

**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| S | 2*a* | −0.6830(1) | −0.4711 | −0.36770(9) | 0.0571(5) | 0.0227(4) | 0.0543(5) | 0.0044(3) | 0.0295(4) | 0.0041(3) |
| O(1) | 2*a* | −0.3908(2) | −0.2818(3) | −0.8458(2) | 0.0186(8) | 0.036(1) | 0.0318(9) | −0.0024(8) | 0.0087(6) | 0.0079(9) |
| O(2) | 2*a* | −0.5301(3) | −0.1963(4) | −1.0645(2) | 0.0291(9) | 0.057(2) | 0.0320(9) | −0.006(1) | 0.0133(8) | 0.016(1) |
| O(3) | 2*a* | −0.8497(2) | −0.3321(3) | −1.0797(2) | 0.0243(8) | 0.0221(9) | 0.0230(8) | −0.0044(7) | 0.0074(7) | −0.0011(7) |
| O(4) | 2*a* | −0.7855(3) | −0.0310(3) | −0.9046(2) | 0.0299(9) | 0.0152(9) | 0.037(1) | −0.0031(7) | 0.0164(8) | 0.0006(7) |
| O(5) | 2*a* | −1.0822(3) | −0.1708(3) | −0.8736(2) | 0.0238(9) | 0.023(1) | 0.061(1) | 0.0052(8) | 0.0205(9) | 0.009(1) |
| O(6) | 2*a* | −0.9548(3) | −0.4286(3) | −0.8149(2) | 0.0291(9) | 0.0199(9) | 0.046(1) | 0.0040(8) | 0.0225(9) | 0.0097(8) |
| O(7) | 2*a* | −0.6667(4) | 0.0720(5) | −0.5350(4) | 0.063(2) | 0.060(2) | 0.120(2) | 0.034(2) | 0.078(2) | 0.060(2) |
| O(8) | 2*a* | −0.9009(3) | 0.1388(4) | −0.4778(2) | 0.033(1) | 0.039(1) | 0.047(1) | 0.0143(9) | 0.0224(9) | 0.015(1) |
| O(9) | 2*a* | −0.2614(3) | −0.2169(4) | −0.2619(2) | 0.040(1) | 0.032(1) | 0.038(1) | −0.010(1) | 0.0152(9) | −0.0053(9) |
| N | 2*a* | −0.8569(3) | −0.1357(3) | −0.3118(2) | 0.029(1) | 0.022(1) | 0.026(1) | 0.0006(9) | 0.0146(9) | −0.0008(9) |
| C(1) | 2*a* | −0.5349(3) | −0.2613(4) | −0.9601(3) | 0.022(1) | 0.018(1) | 0.026(1) | 0.0017(9) | 0.0123(8) | 0.0004(9) |
| C(2) | 2*a* | −0.7106(3) | −0.3271(3) | −0.9470(2) | 0.019(1) | 0.017(1) | 0.022(1) | 0.0010(8) | 0.0095(8) | 0.0024(8) |
| C(3) | 2*a* | −0.7710(3) | −0.2048(3) | −0.8553(2) | 0.018(1) | 0.015(1) | 0.022(1) | −0.0022(9) | 0.0079(9) | −0.0012(9) |
| C(4) | 2*a* | −0.9514(3) | −0.2724(4) | −0.8476(2) | 0.0194(9) | 0.021(1) | 0.022(1) | −0.0004(8) | 0.0084(8) | 0.0005(9) |
| C(5) | 2*a* | −0.7734(4) | 0.0486(4) | −0.4690(3) | 0.025(1) | 0.021(1) | 0.032(1) | −0.0019(8) | 0.0030(9) | 0.002(1) |

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