

*Charge density study of bis(clonixato)bis(ethanol)bis(imidazole)copper(II) complex*Peter Herich¹, Jan Moncol², Julia Koziskova¹, Jozef Kožíšek¹¹Institute Of Physical Chemistry And Chemical Physics, Faculty Of Chemical And Fo, Bratislava, Slovak Republic, ²Institute of Inorganic Chemistry, Technology and Materials, Faculty of Chemical and Food Technology, Slovak University of Technology, SK-812 37 Bratislava, Slovakia, Bratislava, Slovak Republic

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Clonixin or chlonixic acid is a novel member of fenamate family drugs that show non-steroidal anti-inflammatory, antipyretic, analgesic and platelet-inhibitory actions when administered intravenously or intramuscularly. It is used primarily in the treatment of chronic arthritic conditions and certain soft tissue disorders associated with pain and inflammation. The complex was prepared by standard procedure. The solution of $\text{Cu}(\text{CO}_2\text{CH}_3)_2 \cdot \text{H}_2\text{O}$ (1.0 mmol) in EtOH (50 cm³) was added to imidazole (2.0 mmol) resulting in the blue-coloured solution. Clonixin (2.0 mmol) was added to the mixture afterwards, changing the colour of the solution to green. The final solution was stirred at room temperature for 24 hours. The crystals, suitable for X-ray diffraction, were formed by slow evaporation of the solution. Experiments were performed by means of Stoe STADIVARI diffractometer with a Dectris Pilatus 300K detector and with an Incoatec I μ S Ag microfocus source (Ag-K α , $\lambda = 0.56083 \text{ \AA}$) at 100 K using a nitrogen gas open-flow cooler Cobra Oxford Cryosystems. Data reduction was processed using X-Area (Stoe, 2016), where the value of average redundancy was 13.1 and Rint of 4.71%. Direction cosines were applied for anisotropic secondary extinction correction. The results of multipole refinement and the topological analysis were performed via XD2006.

[1] J.S. Finch, T.J. De Kornfeld, (1971) J. Clin. Pharmacol. 11, 371-377.

[2] J.E. Weder, C.T. Dillon, T.W. Hambley, B.J. Kennedy, P.A. Lay, J.R. Biffin, H.L. Regtop, N.M. Davies, (2002) Coordination Chemistry Reviews. 232, 95-126.

[3] STOE & Cie GmbH (2016). X-Area 1.76, software package for collecting single-crystal data on STOE area-detector diffractometers, for image processing, scaling reflection intensities and for outlier rejection; Darmstadt, Germany.

Keywords: [charge density](#), [copper\(II\) complex](#), [clonixin](#)