

[3-(1, 4, 7, 10-Tetraazacyclododecan-1-yl)propane-1-amine]-Zinc(II)
Bis(perchlorate), [Zn^{II}L] (ClO₄)₂の結晶構造

市丸 嘉*、今井 幹典*、藤岡晴人、稗田雄三、小池 透**、黒崎博雅*、加藤 紘一*

X-Ray Structure Analysis Online, **36**, 43-44(2020)

Crystal Structure of [3-(1,4,7,10-Tetraazacyclododecan-1-yl)propane-1-amine]-Zinc(II) Bis(perchlorate),[Zn^{II}L](ClO₄)₂

Yoshimi Ichimaru,* Masanori Imai,* Haruto Fujioka, Tohru Koike,** Hiromasa Kurosaki,*
and Koichi Kato*

ABSTRACT The crystal structure of [3-(1,4,7,10-tetraazacyclododecan-1-yl)propan-1-amine = L]zinc(II) bis(perchlorate), [Zn^{II}L]·(ClO₄)₂, was determined by the single-crystal X-ray diffraction method at 93.15 K. The titled complex crystallized in the orthorhombic space group P212121 and Z = 4 with a = 9.09970(10), b = 14.0995(2), c = 14.9908(2) Å, and V = 1923.34(4) Å³. The R1 [I > 2σ(I)] and wR2 (all data) values were 0.0214 and 0.0538, respectively, for all 3079 independent reflections. In the crystal structure, the zinc center is coordinated with the three secondary amines and one tertiary amine of the macrocycle and with the primary amine from the N-propylamino pendant arm, forming a distorted square pyramidal geometry.

抄録 サイクレン(12aneN4)にプロピルアミン側鎖を持つ[3-(1,4,7,10-Tetraazacyclododecan-1-yl)propane-1-amine]-Zinc(II) Bis(perchlorate),[Zn^{II}L](ClO₄)₂の結晶構造をX線結晶構造解析により明らかにした。

*金城学院大学薬学部

**広島大学大学院医歯薬保健学研究院