

A-7 17:40~17:55

Crystal Structure of 2-[11-(2-amino-2-oxoethyl)-7,14-dimethyl-4,11,diaza-1,8-diazonia-cyclo-tetradecanyl]acetamide diperchlorate dihydrate

Ki-Young Choi,^a Han-Hyoung Lee,^a Douglas R. Smyth,^b Il-Hwan Suh^c
and Edward R. T. Tienkink^b

^a*Department of Cultural Heritage Conservation Science, Kongju National University, Kougju 314-701, Korea*

^b*Department of Chemistry, The University of Adelaide, Adelaide 5005, Australia*

^c*Department of Physics, Chungnam National University, Taejon, 305-764 Korea*

The title compound has been prepared and characterized by X-ray crystallography. This compound crystallizes in the monoclinic space group $C2/c$, $a = 16.576(3)$ Å, $b = 10.877(6)$ Å, $c = 14.314(2)$ Å, $\beta = 90.25(1)^\circ$, $V = 2581(1)$ Å³, $Z = 4$. The cation is centrosymmetric so that the four N atoms within the macrocycle are co-planar. This compound features a doubly protonated macrocycle with the pendant arms disposed over the cavity, an arrangement that is facilitated by intramolecular hydrogen-bonding interactions. The crystal structure is stabilised by a variety of hydrogen-bonding contacts involving the dication, perchlorate anions and solvent water molecules