Experimental Electron Density Distribution and QTAIM Topological Analysis for the Perovskite Mineral: Sulphohalite – $Na_6(SO_4)_2FCl$

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A quantitative experimental charge density study was undertaken for the double antiperovskite mineral – *sulphohalite* [$Na_6(SO_4)_2FCl$]. *High*-resolution X-ray diffraction data was collected employing Ag*K*α radiation (λ = 0.56087 Å) to a resolution of 0.3941 Å at 100K. *Electron density* (ED) distribution – $\rho(r)$ was modelled, in compliance with the Hansen-Coppens formalism [1], by consecutive least-square multipolar refinements. Based on such experimental distribution of charge, QTAIM *topological analysis* [2] was undertaken. Full-volume property integration over delineated *atomic basins* (AB's) yielded their appertaining charges [$Q_{AB\text{-}Cl}$ = -0.836e$^-$; $Q_{AB\text{-}S}$ = 03.168e$^-$; $Q_{AB\text{-}Na}$ = 0.910e$^-$; $Q_{AB\text{-}F}$ = -1.334e$^-$; and $Q_{AB\text{-}O}$ = -1.227e$^-$] and volumes [$V_{AB\text{-}Cl}$ = 38.920Å^3; $V_{AB\text{-}S}$ = 5.656Å^3; $V_{AB\text{-}Na}$ = 7.931Å^3; $V_{AB\text{-}F}$ = 14.178 Å^3 and $V_{AB\text{-}O}$ = 17.416 Å^3]. The percentage of unaccounted electrons and volume per unit cell was respectively 0.010% and 0.406%. Within the uncertainty range of performed numerical integration, such percentages can be unheeded. A total of 6·BCP's [$\nabla^2\rho(r_{Cl\cdots S})$ = 0.120e$^-$·Å^{-5}; $\nabla^2\rho(r_{Cl\cdots Na})$ = 0.575e$^-$·Å^{-5}; $\nabla^2\rho(r_{S\text{-}O})$ = -31.00e$^-$·Å^{-5}; $\nabla^2\rho(r_{Na\cdots O})$ = 1.931e$^-$·Å^{-5}; $\nabla^2\rho(r_{Na\cdots F})$ = 3.022e$^-$·Å^{-5} and $\nabla^2\rho(r_{F\cdots O})$ = 0.868e$^-$·Å^{-5}], 5·RCP's [$\nabla^2\rho(r_I)$ = 0.912e$^-$·Å^{-5}; $\nabla^2\rho(r_{II})$ = 0.332e$^-$·Å^{-5} and $\nabla^2\rho(r_{III,IV,V})$ = 0.201e$^-$·Å^{-5}] and 4·CCP's [$\nabla^2\rho(r_{I,II})$ = 0.514e$^-$·Å^{-5} and $\nabla^2\rho(r_{III,IV})$ = 0.401e$^-$·Å^{-5}] were identified (Figure 1). Hence, Morse's 'characteristic set' condition was met [3]. The study of primary bundles (PB's), as proposed by Pendás[4], revealed the interconnection between AB's and CP's onto basins of attraction or basins of repulsion. The nature of interatomic interactions was assessed through the dichotomous classification [3]. The S–O contact was acknowledged as a *covalent* with a *shared-shell.* The remaining contacts were characterized as *non-covalent closed-shell* (Cl···Na, Na···O and Na···F) or *weak van der Waals closed-shell* (Cl···S and F···O).

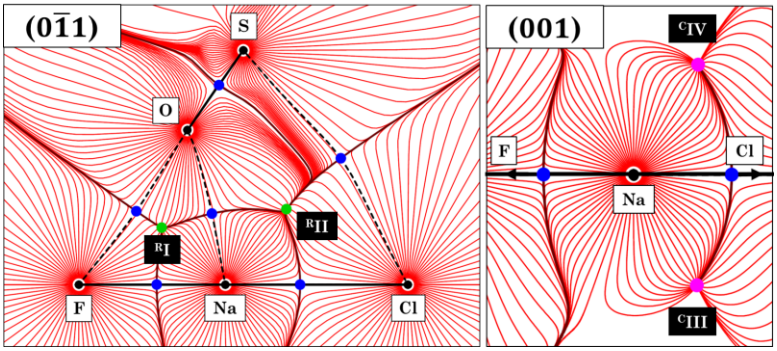

Figure 1. Gradient vector field of ED, drawn for two planes in the crystal of sulphohalite.
Bond CP's – (3, -1), Ring CP's – (3, +1) and Cage CP's – (3, -3) are respectively denoted by blue, green, and magenta circles.
Interatomic bonding is presented by black lines, whereas bonding paths are depicted by black dashed lines.

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Keywords: High-resolution X-ray Diffraction; Experimental Electron Density Distribution; Minerals; QTAIM; Perovskites.

This research was supported by the Polish National Science Centre (NCN) (grant agreement No. UMO-2019/33/B/ST10/02671) and was carried out at the Biological and Chemical Research Centre, University of Warsaw, established within the project co-financed by European Union from the European Regional Development Fund under the Operational Programme Innovative Economy, 2007 – 2013.

Acta Cryst. (2021), A**77**, C757