Isolated $[SiO_4]^{4-}$ Tetrahedra in the Chloride-Poor Oxosilicate $Ce_3Cl[SiO_4]_2$

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In an attempt to synthesize $CeSb_2O_4Cl$, colorless rod-shaped single crystals with the composition $Ce_3Cl[SiO_4]_2$ were obtained as a by-product from silica ampoules. $Ce_3Cl[SiO_4]_2$ crystallizes isotypically to the A-type $Ln_3Cl[SiO_4]_2$ series with *Ln* = La, Pr and Nd[1–4] in the monoclinic space group *C*2/*c* with *a* = 1439.13(9) pm, *b* = 646.24(4) pm, *c* = 877.96(6) pm and *β* = 98.341(3)° for *Z* = 4 (CSD-2124078).

The crystal structure of $Ce_3Cl[SiO_4]_2$ contains isolated $[SiO_4]^{4-}$ tetrahedra (Figure 1) as the defining building blocks, showing a slight distortion with angles O–Si–O in the range from 105.9(2) to 118.4(2)°. The Si–O distances reside between 160.6(5) and 164.2(4) pm, which are quite typical values. Furthermore, two crystallographically distinct Ce^{3+} cations are present with $(Ce1)^{3+}$ being surrounded by one Cl^- anion *plus* another more distant Cl^- one as well as eight oxygen atoms forming a 9+1-fold coordination sphere. The $(Ce2)^{3+}$ cations show a tricapped trigonal prismatic coordinative environment, built up by one Cl^- anion and eight oxygen atoms. The distances *d*(Ce–O) = 243.2(4) – 290.8(4) pm and *d*(Ce–Cl) = 287.6(1) – 295.4(2) pm *plus* 350.8(1) pm range in common intervals, when compared with PbFCl-type CeOCl[5] (*d*(Ce–O) = 237 pm (4×) and *d*(Ce–Cl) = 312 pm (1×) and 319 pm (4×)) for example.

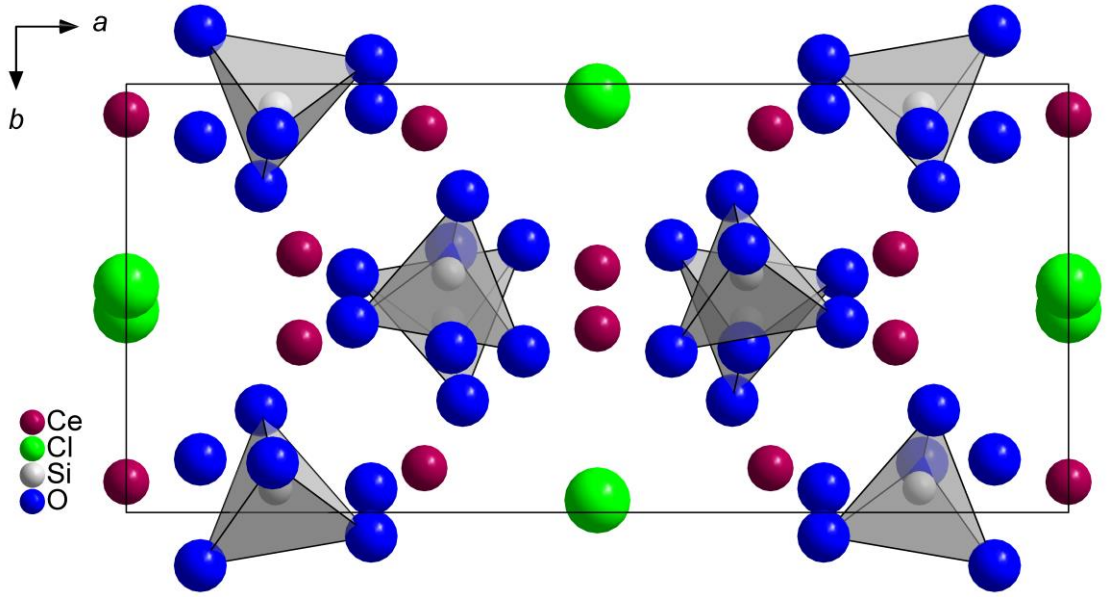

Figure 1. Projection of the monoclinic crystal structure of $Ce_3Cl[SiO_4]_2$ onto (001) emphasizing the isolated $[SiO_4]^{4-}$ tetrahedra.

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