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CRYSTAL STRUCUTRE OF $NaBaCr_2F_9$ – STRUCTURAL CORRELATIONS WITH OTHER ENNEAFLUORIDES

G. Ferey*, M. Leblanc, A. de Kozak, M. Samouel and J. Pannetier

ERA 609, Faculté des Sciences, 72017 Le Mans Cedex (France)

$NaBaCr_2F_9$ was grown by hydrothermal synthesis. Its symmetry is monoclinic (SG $P2_1/n$) with parameters a = 7.318 (2), b = 17.311 (4), c = 5.398 (1) β = 91°14 (3). The structure was solved from 507 X ray reflections and refined to R_ω = 0.0252. The network is built from tilted double cis chains of octahedra $(Cr_2F_9)^{3n-}_n$ which insert Na^+ and Ba^{++} ions The structure is compared to previously described Ba_2CoFeF_9 [1], Ba_2ZnAlF_9 [2] and $KPbCr_2F_9$ [3] which have in common these double chains, but which different crystalline symmetry. The difference is analyzed in terms of tilting of octahedra, of active lone pair of Pb^{2+} ions and using the valence bond theory. A mechanism is proposed for the transition between the structures, which involves correlated rotations of the chains.

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