CATIONS 
Institut undergo phase transitions to high temperature phases at 376 K and 415 K respectively. The cubic high temperature phases (CsCl-lattice) contain one formula unit in the unit cell. The lattice constants are 660 pm (393 K) in the perchlorate and 663 pm (420 K) in the tetrafluoroborate. 
The Cobaltocene cations Co(C₅H₅)₃ occupy 3 orientations statistically such a way that their fivefold axes lie parallel to the cubic crystal axes. 
The tetrahedral anions ClO₄⁻ or Br⁻ take 6 orientations statistically such that one of the threefold axes always points to a face centre of the cube. The 3 oxygen or fluorine atoms which do not lie on the preferentially oriented threefold axes, show additional disorder within their plane perpendicular to the threefold axis. 
Structure factor calculations have proved that the observed intensity data are best fitted by assuming the C, H and O or F atoms to be distributed on the surface of a sphere and describing their contributions to the structure factors by means of spherical Bessel functions and cubic harmonics. 

09. STRUCTURES OF ORGANIC, ORGANOMETALLIC AND COORDINATION COMPOUNDS

Cobaltocene perchlorate and tetrafluoroborate undergo phase transitions to high temperature phases at 376 K and 415 K respectively. The cubic high temperature phases (CsCl-lattice) contain one formula unit in the unit cell. The lattice constants are 660 pm (393 K) in the perchlorate and 663 pm (420 K) in the tetrafluoroborate. 
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Structure factor calculations have proved that the observed intensity data are best fitted by assuming the C, H and O or F atoms to be distributed on the surface of a sphere and describing their contributions to the structure factors by means of spherical Bessel functions and cubic harmonics.