Structural analysis and IR-spectroscopy of a new anilinium hydrogenselenite hybrid compound: A subtle structural phase transition

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Description
An interesting structural behavior has been detected and characterized in a new anilinium based compound by single crystal X-ray diffraction measurements and infrared spectroscopy. The temperature dependent structural investigation reveals that the studied compound undergoes a subtle non-centrosymmetric to centrosymmetric structural phase transition. At room temperature the crystal structure is non-centrosymmetric and is characterized by an important disorder in the organic part where the independent aromatic rings are rotated around the C1—C4 and C7—C10 molecular axis by 52.06(6)° and 56.25(4)° respectively. By decreasing the temperature to 100 K the organic cation is less disordered and the rotation angle of the aromatic rings changes to 54.73(2)°. As a consequence, the low temperature structure becomes centrosymmetric. The infrared spectra recorded on cooling and heating the sample in the …