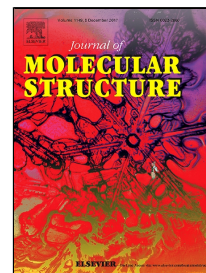


# Accepted Manuscript

Structural, vibrational, DFT and optical studies of a new non-centrosymmetric hybrid material (C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>)[CoBr<sub>4</sub>]



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**Highlights**

- A new hybrid compound (C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>)[CoBr<sub>4</sub>] was synthesized.
- The compound crystallizes in the non-centrosymmetric space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>.
- Anionic and cationic groups are linked thanks to N–H⋯Br hydrogen bonds.
- Raman and Infrared spectra were interpreted and assigned focused on the density functional theory (DFT) method.
- The optical energy gap determined by UV-Vis spectral analysis is 2.23 eV.

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