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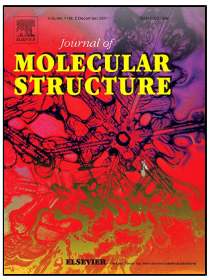

Structural, vibrational, DFT and optical studies of a new non-centrosymmetric hybrid material $(C_4H_{12}N_2)[CoBr_4]$

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Highlights

- A new hybrid compound $(C_4H_{12}N_2)[CoBr_4]$ was synthesized.
- The compound crystallizes in the non-centrosymmetric space group $P2_12_12_1$.
- 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.