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Polymorphism and phase transformations in cobaltacarborane molecular crystals: Evidence for very weak intermolecular C–H···H–B interactions

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Table S1. Comparison of Bond Lengths (Å) for both polymorphs of **1**

	Form I	Form II
C1–C2	1.637(6)	1.630(3)
C1–B5	1.698(6)	1.692(3)
C1–B4	1.697(6)	1.719(3)
C1–B6	1.724(6)	1.721(3)
C1–Co1	1.991(4)	2.0092(18)
C2–B11	1.692(6)	1.691(3)
C2–B6	1.717(6)	1.718(3)
C2–B7	1.709(6)	1.723(3)
C2–Co1	2.005(4)	2.0047(18)
C3–C7	1.417(6)	1.402(4)
C3–C4	1.421(6)	1.409(3)
C3–Co1	2.059(4)	2.056(2)
C4–C5	1.415(7)	1.406(3)
C4–Co1	2.030(5)	2.036(2)
C5–C6	1.404(7)	1.422(4)
C5–Co1	2.028(5)	2.035(2)
C6–C7	1.384(6)	1.418(4)
C6–Co1	2.044(5)	2.046(2)
C7–Co1	2.055(4)	2.069(2)
B4–B9	1.792(6)	1.786(3)
B4–B5	1.800(6)	1.789(3)
B4–B8	1.803(6)	1.808(3)
B4–Co1	2.054(5)	2.076(2)
B5–B6	1.758(6)	1.771(3)
B5–B10	1.770(6)	1.779(3)
B5–B9	1.768(6)	1.784(3)
B6–B11	1.768(6)	1.763(3)
B6–B10	1.768(5)	1.769(3)
B7–B12	1.772(7)	1.778(3)
B7–B11	1.778(7)	1.793(3)
B7–B8	1.812(6)	1.817(3)
B7–Co1	2.065(5)	2.069(2)
B8–B9	1.784(6)	1.791(3)
B8–B12	1.783(6)	1.794(3)
B8–Co1	2.106(4)	2.106(2)
B9–B12	1.777(6)	1.786(3)
B9–B10	1.768(6)	1.790(3)
B10–B11	1.766(6)	1.773(3)
B10–B12	1.766(6)	1.786(3)
B11–B12	1.761(7)	1.781(3)

Figure S1. IR spectrum of form **I**.

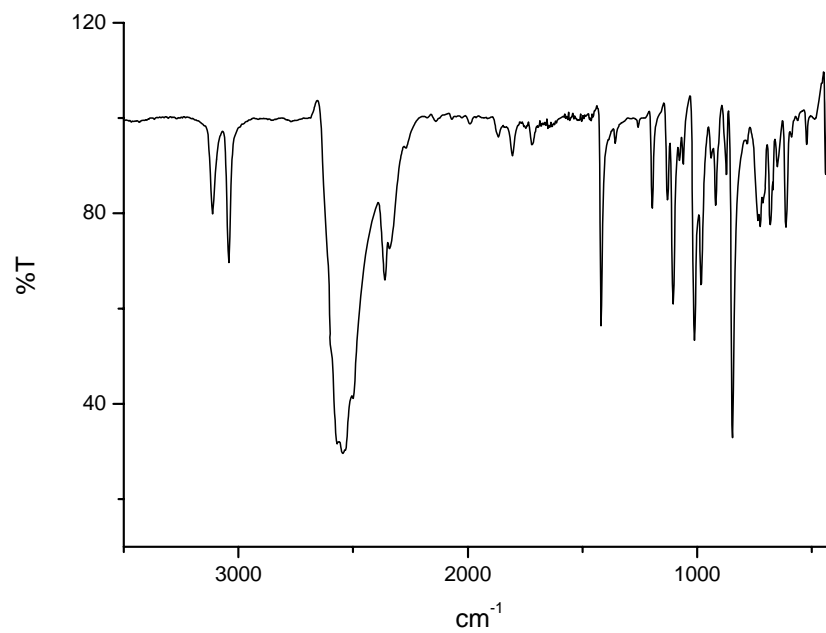


Figure S2. IR spectrum of form **II**.

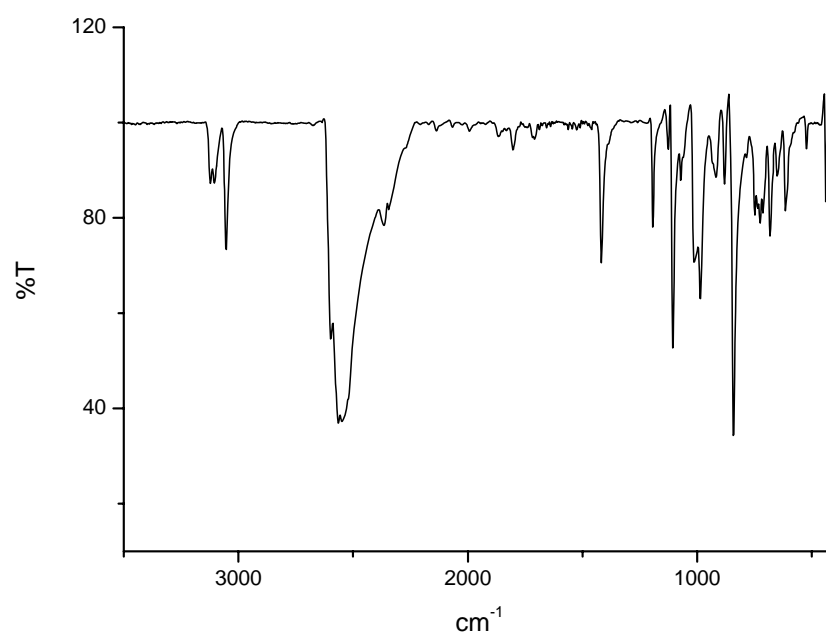


Figure S3. Phase transformation by IR.

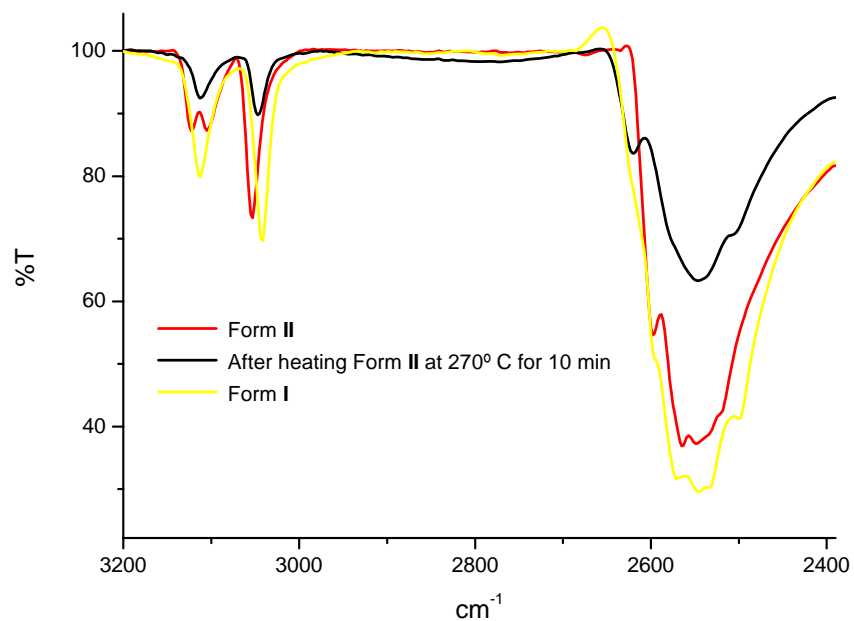


Figure S4. Comparison between experimental (Bottom: 0.047M solution in CH₂Cl₂) and calculated in the gas phase (top) IR Spectra of *closo*-[3-Co(η^5 -C₅H₅)-1,2-C₂B₉H₁₁] (1). Only the relevant section with the C-H and B-H stretching bands are shown.

