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Pressure-induced local lattice distortions in Co(dca)$_2$[1] J.L. MUSFELDT, University of Tennessee, Z. LIU, Carnegie Institute of Washington, A. LITVINCHUK, University of Houston, T.V. BRINZARI, University of Tennessee, G.L. CARR, Brookhaven National Laboratory, J.A. SCHLUETER, Argonne National Laboratory, J.L. MANSON, Eastern Washington University, M.-H. WHANGBO, North Carolina State University — We employed vibrational spectroscopy along with complementary lattice dynamics and spin density calculations to investigate local structure and magnetism through the series of pressure-induced transitions in Co(dca)$_2$. Analysis of several ligand bending modes reveals compression and distortion of molecular linkages and a major change in the crystal lattice through the 1 GPa transition, whereas a modified local structure (due to a change in molecular symmetry) but similar crystal lattice is anticipated above 3 GPa. We discuss our findings in terms of the competition between antiferromagnetic and ferromagnetic exchange interactions.

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