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Supplementary Information

Reversible Pressure Amorphization of a Piezochromic Metal-Organic Framework

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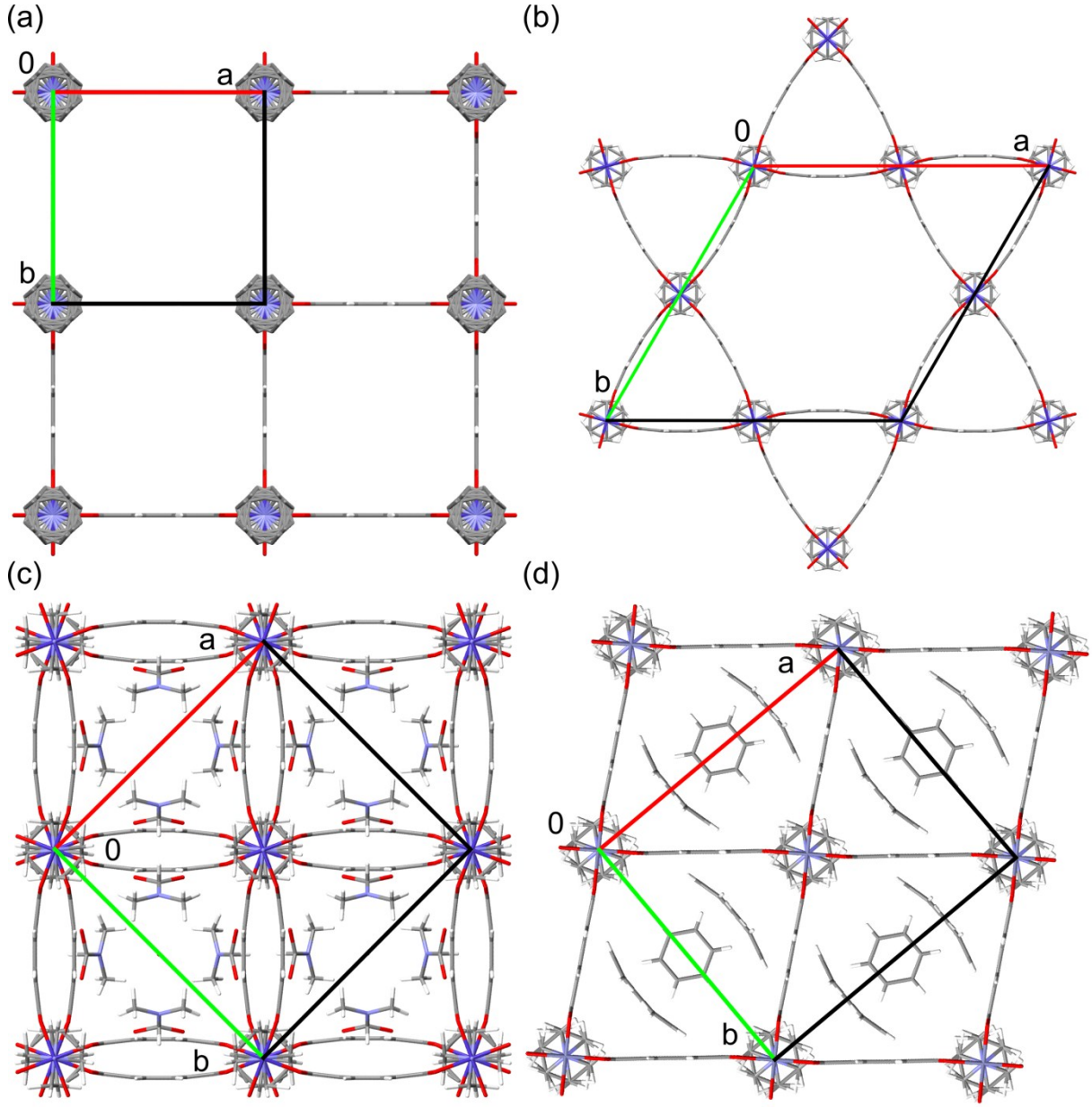

Figure S1. (a) The crystal structure of $Co_2(Bdc)_2Dabco$ polymorph I and (b) polymorph II with kagome-type lattice; and guest-dependent structural transformation of polymorph I host structure with (c) DMF and water and (d) benzene.

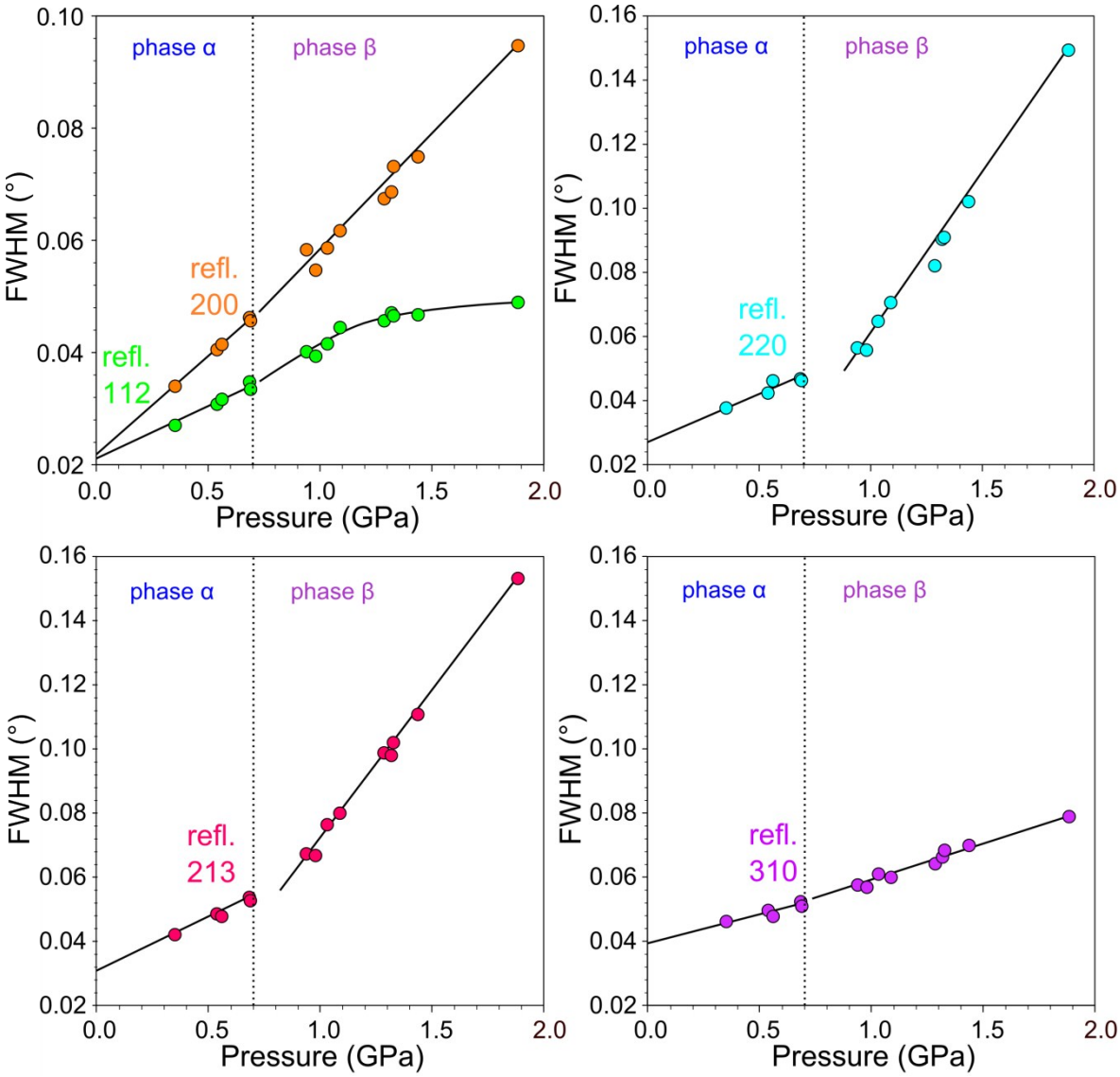

Figure S2. Full width at half maximum (FWHM) of main reflections for α and β phases plotted in a function of pressure.

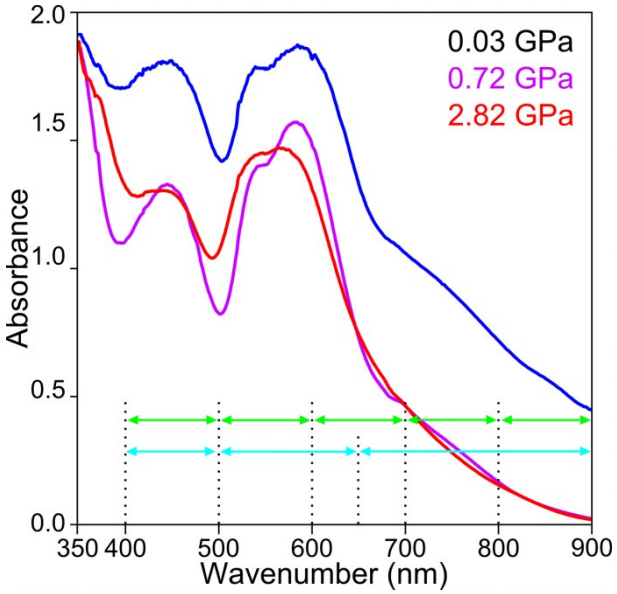

Figure S3. High-pressure VIS spectra of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ divided into main regions to integrate the signal ($\Delta\lambda$=100nm in green and $\Delta\lambda$=diverse in cyan arrows, *cf.* Table S1).

Table S1. Integrated areas of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ visible light absorption spectra. Area of three main peaks was highlighted in red (cyan arrows in Figure S3).

Phase	**400-500**	**500-600**	**600-700**	**700-800**	**800-900**	**500-650**	**650-900**
α at 0.03 GPa	218	222	187	137	102	323	317
β at 0.72 GPa	163	184	122	71	52	256	176
amorphous at 2.82 GPa	165	183	123	71	52	251	173
Change in %							
α to β	-25.3	-17.2	-34.8	-48.2	-49.0	-20.8	-44.5
α to amorphous	-24.3	-17.6	-34.3	-48.2	-49.0	-22.3	-45.4
β to amorphous	1.2	-0.6	0.9	0	0	-2.1	-1.7

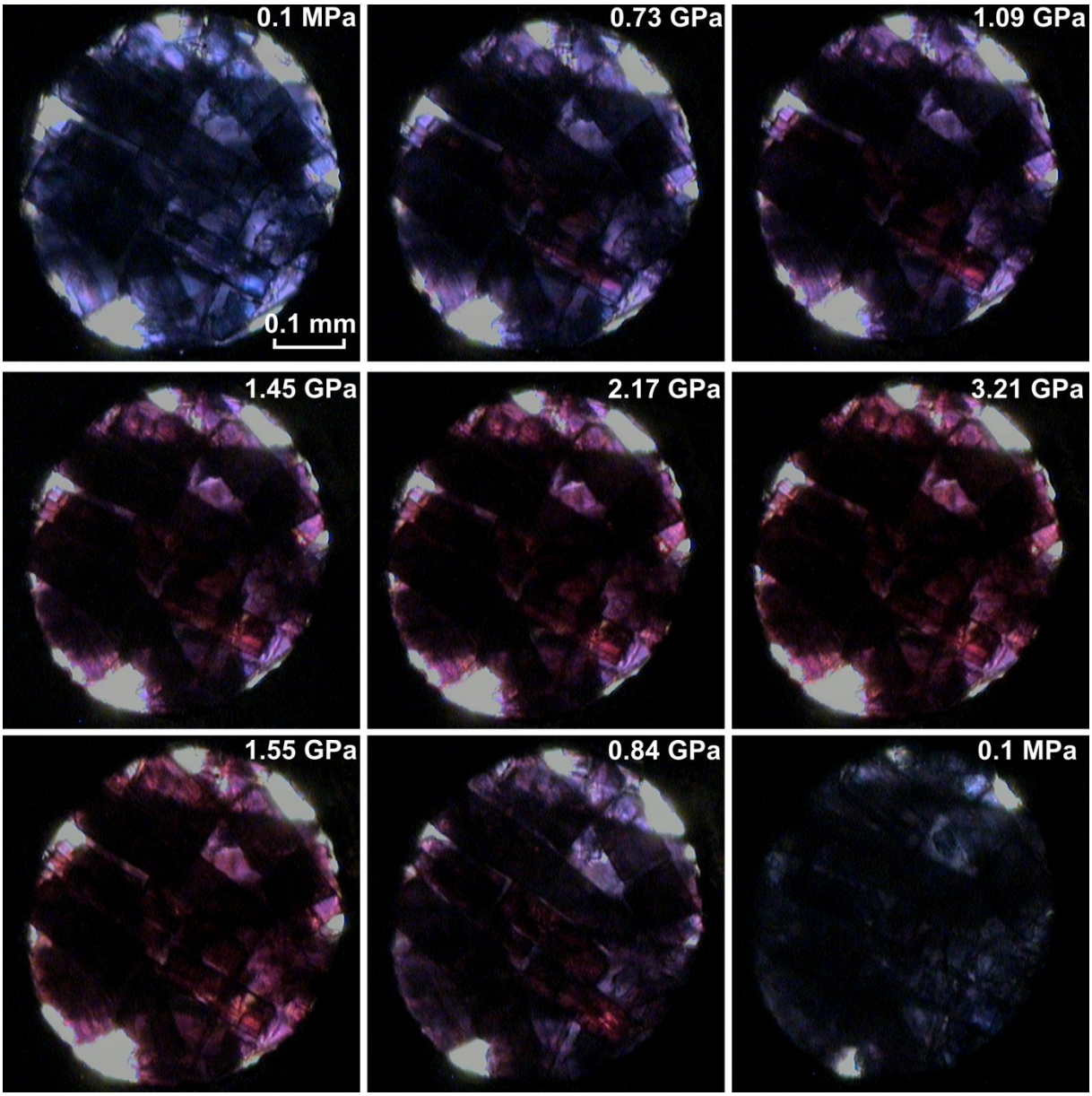

Figure S4. Single crystals of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ in a DAC during high-pressure spectroscopic measurements.

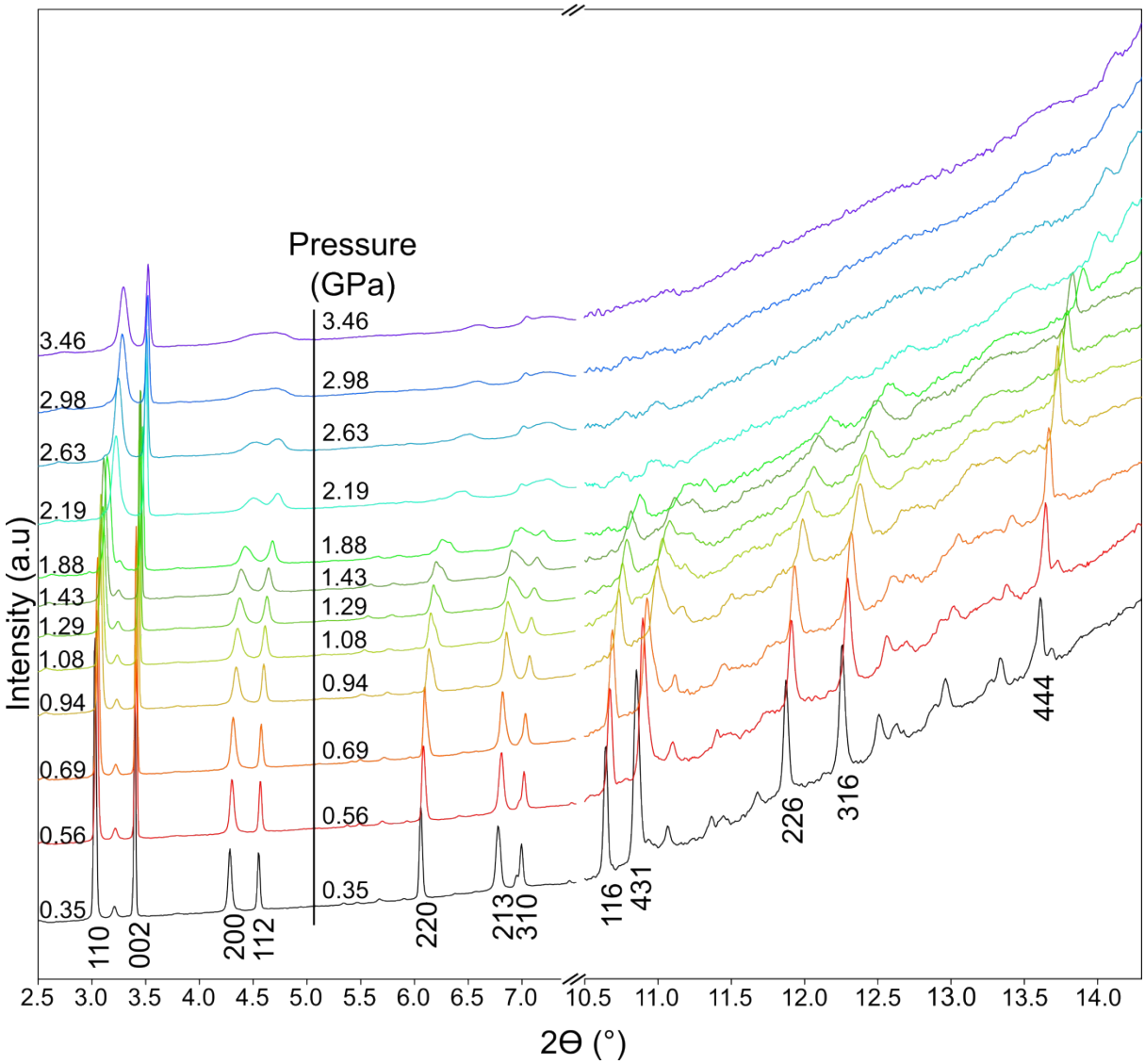

Figure S5. High-pressure powder XRD patterns of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$, measured with synchrotron radiation.

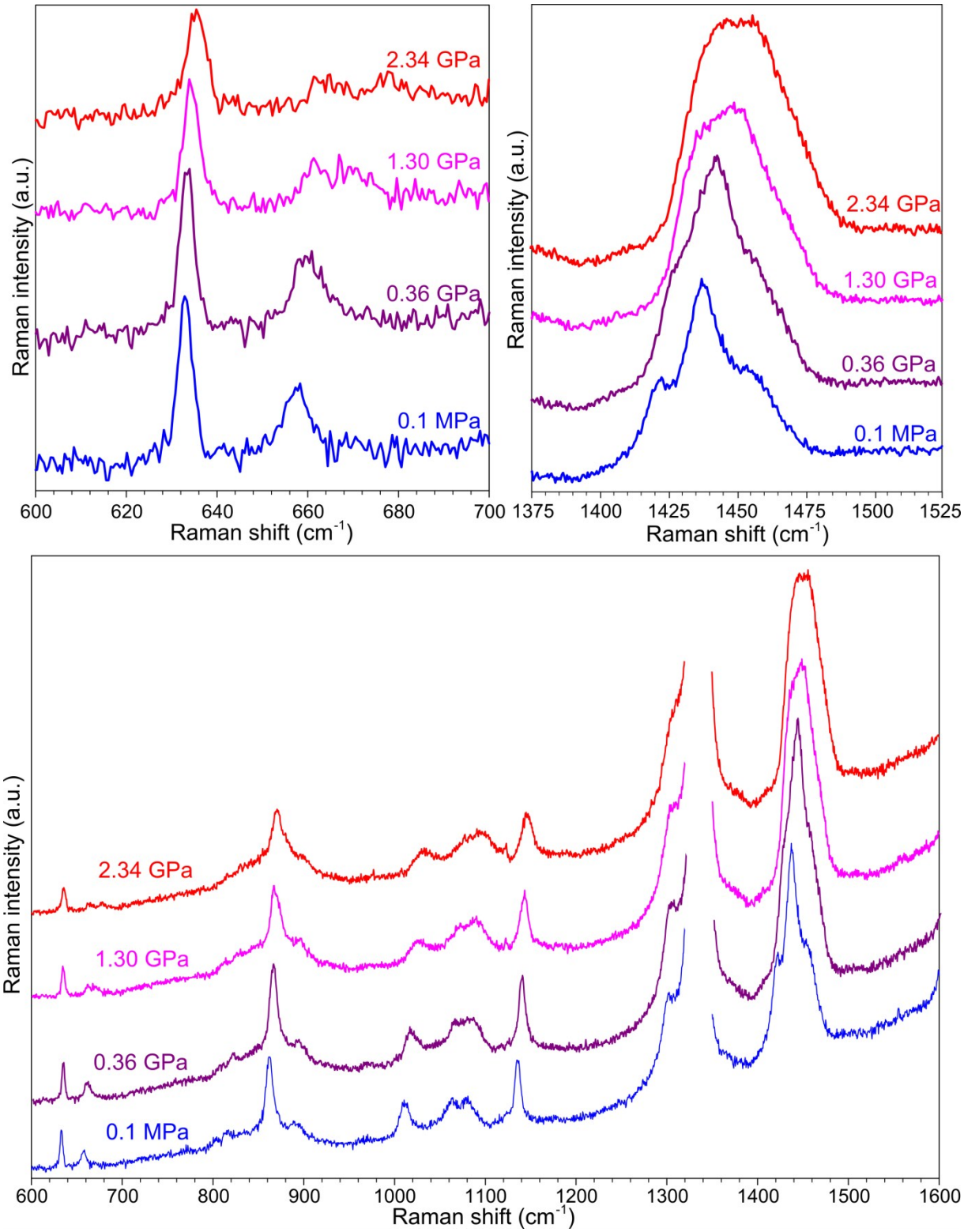

Figure S6. High-pressure Raman spectra of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ measured in Daphne oil.

Table S2. Detailed crystallographic data of $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ single crystal measured in a function of temperature.

Phase	**α**	**α**	**α**	**α**	**α**	**α**	**α**
p (GPa)	0.1 MPa	0.1 MPa	0.1 MPa	0.1 MPa	0.1 MPa	0.1 MPa	0.1 MPa
T (K)	296	273	250	220	180	150	100
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal
Space group	*I*4/*mcm*	*I*4/*mcm*	*I*4/*mcm*	*I*4/*mcm*	*I*4/*mcm*	*I*4/*mcm*	*I*4/*mcm*
a	15.2794(13)	15.2735(15)	15.2626(16)	15.2554(15)	15.2439(18)	15.2363(17)	15.2236(19)
b	15.2794(13)	15.2735(15)	15.2626(16)	15.2554(15)	15.2439(18)	15.2363(17)	15.2236(19)
c	18.9886(14)	18.9723(15)	18.9551(15)	18.9276(15)	18.9276(15)	18.8931(15)	18.8603(16)
Volume ($Å^3$)	4433.1(8)	4425.8(9)	4415.5(10)	4405.0(9)	4393.7(11)	4386.0(10)	4371.1(11)
Z/Z’	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125
Calculated density (g/cm^3)	1.095	1.096	1.099	1.102	1.104	1.109	1.113
Absorption coefficient (mm^{-1})	0.789	0.790	0.792	0.794	0.794	0.796	0.791
F(000)	1536	1536	1536	1536	1536	1536	1536
Crystal size (mm)	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5	0.2 x 0.2 x 0.5
θ-range for data collection (°)	5.712 – 57.78	5.716 – 58.828	5.72 – 57.884	6.86 – 57.962	6.352 – 58.026	6.356 – 58.072	5.744 – 53.964
Min/max indices:h, k, l	-20/19, -19/14, -23/25	-20/19, -19/14, -23/25	-14/19, -19/20, -25/23	-14/19, -19/20, -25/22	-19/20, -19/14, -25/22	-14/19, -20/19, -22/15	-14/18, -19/19, -22/24
Reflect. Collected/unique	11395/1507	11401/1505	11321/1500	11279/1490	11251	1116	10750
Rint	0.2246	0.2320	0.2291	0.2304	0.2426	0.2498	0.2553
Completeness (%)	94.96	94.83	94.52	94.14	93.18	93.83	99.69
Data/ parameters/restrains	1507/13/55	1505/18/55	1500/12/59	1490 / 0 / 52	1482 / 12 / 60	1488 / 19 / 62	1295 / 12 / 62
Goodness-of-fit on F2	1.059	1.006	1.079	1.081	1.065	1.037	1.027
Final R1/wR2 (I>2σ1)	0.0830 / 0.2008	0.1134 / 0.3037	0.0972 / 0.2151	0.1367 / 0.3149	0.0963 / 0.2076	0.1395 / 0.3433	0.0931 / 0.2088
R1/wR2 (all data)	0.1726 / 0.2375	0.2434 / 0.3818	0.1870 / 0.2540	0.2744 / 0.4026	0.1877 / 0.2444	0.2862 / 0.4481	0.1785 / 0.2296
Weighting parameters w_1,w_2	0.087 / 0	0.2 / 0	0.095 / 0	0.075 / 0	0.092 / 0	0.250 / 0	0.098 / 0
Largest diff. peak/hole (e.Å-3)	0.73 / -0.54	1.31 / -0.52	1.35 / -0.65	3.70 / -1.42	1.86 / -0.97	0.92 / -0.33	1.70 / -0.79

Table S3. Detailed crystallographic data of high-p1ressure $Co_2(Bdc)_2Dabco \cdot 4DMF \cdot H_2O$ phases extracted from powder XRD measurements. Unit-cell dimensions for β-phase were averaged to the orthorhombic system.

Phase	**α**	**α**	**α**	**α**	**α**	**α**	**β**	**β**	**β**	**β**
p (GPa)	0.1 MPa	0.3525	0.5399	0.5616	0.6853	0.6897	0.9399	0.9812	1.0899	1.2872
T (K)	296	296	296	296	296	296	296	296	296	296
Wavelength (Å)	0.71073	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338
Crystal system	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	-	-	-	-
Space group	I4/mcm	I4/mcm	I4/mcm	I4/mcm	I4/mcm	I4/mcm	-	-	-	-
a	15.2794(13)	15.0522	14.9815	14.9807	14.9302	14.9365	14.8148	14.8026	14.7538	14.6911
b	15.2794(13)	15.0522	14.9815	14.9807	14.9302	14.9365	14.8518	14.8322	14.7955	14.7289
c	18.9886(14)	18.9757	18.9208	18.9221	18.8968	18.9012	18.8207	18.8136	18.7771	18.7204
Volume ($Å^3$)	4433.1(8)	4299.3112	4246.6528	4246.5573	4212.3098	4216.8626	4141.4(8)	4130.6(3)	4098.8(3)	4050.7(5)
Z/Z’	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125	4 / 0.125

Table S3. Continued, for the amorphous phase volume and unit-cell parameters were calculated from 110 and 002 reflections, pA=pre-amorphous phase (*cf*. Figure S5).

Phase	**β**	**β**	**β**	**pA**	**pA**	**pA**	**pA**	**pA**	**pA**
p (GPa)	1.3194	1.4383	1.8858	2.1800	2.2900	2.6100	2.9500	3.0900	3.4300
T (K)	296	296	296	296	296	296	296	296	296
Wavelength (Å)	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338	0.56338
Crystal system	-	-	-	-	-	-	-	-	-
Space group	-	-	-	-	-	-	-	-	-
a	14.6733	14.6305	14.4604	14.1713	14.0733	13.9052	13.9003	13.8880	13.8691
b	14.7152	14.6703	14.5203	14.2318	14.1526	14.0257	13.9821	13.9617	13.9332
c	18.7182	18.6812	18.5827	18.4554	18.4177	18.3601	18.3569	18.3478	18.3400
Volume ($Å^3$)	4041.6(6)	4009.6(8)	3901.2(8)	3706.3481	3647.7500	3550.0289	3546.9105	3538.8924	3527.7621
Z/Z’	4 / 0.125	4 / 0.125	4 / 0.125	-	-	-	-	-	-