

# Supporting Information

## Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>2</sub>(C<sub>2</sub>): A Crystalline Acetylide with Bridging C<sub>2</sub> Units

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Table S1: Fractional atomic coordinates and isotropic displacement parameters of Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>2</sub>(C<sub>2</sub>).

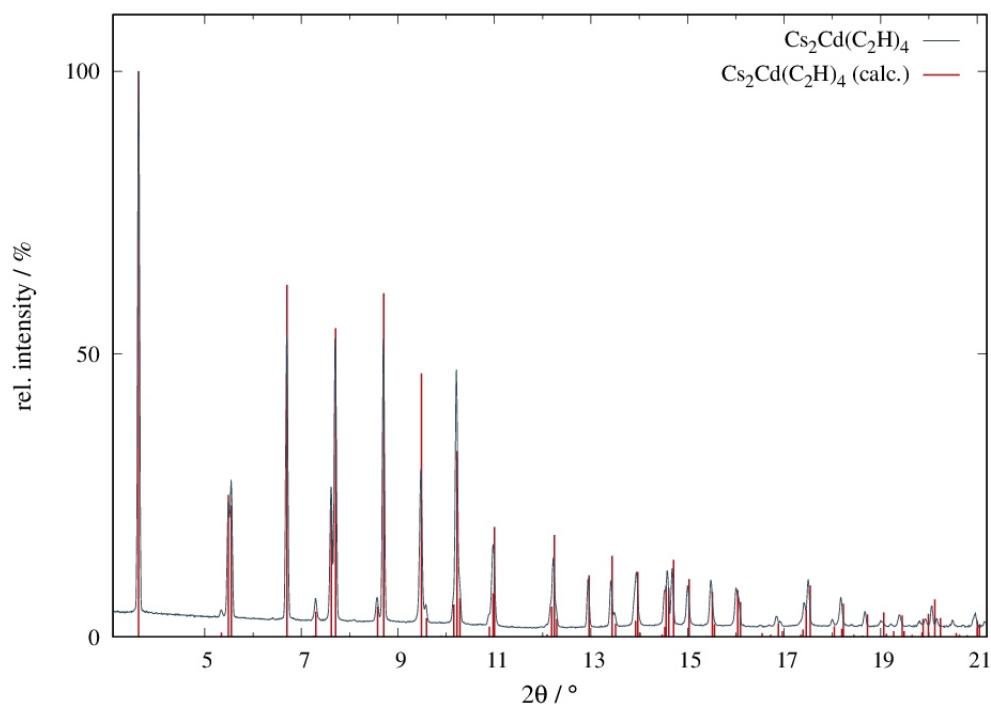
Figure S1: Synchrotron powder diffraction pattern of Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>4</sub>.

Figure S2: XRPD pattern of Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>2</sub>(C<sub>2</sub>) synthesized under ammonothermal conditions.

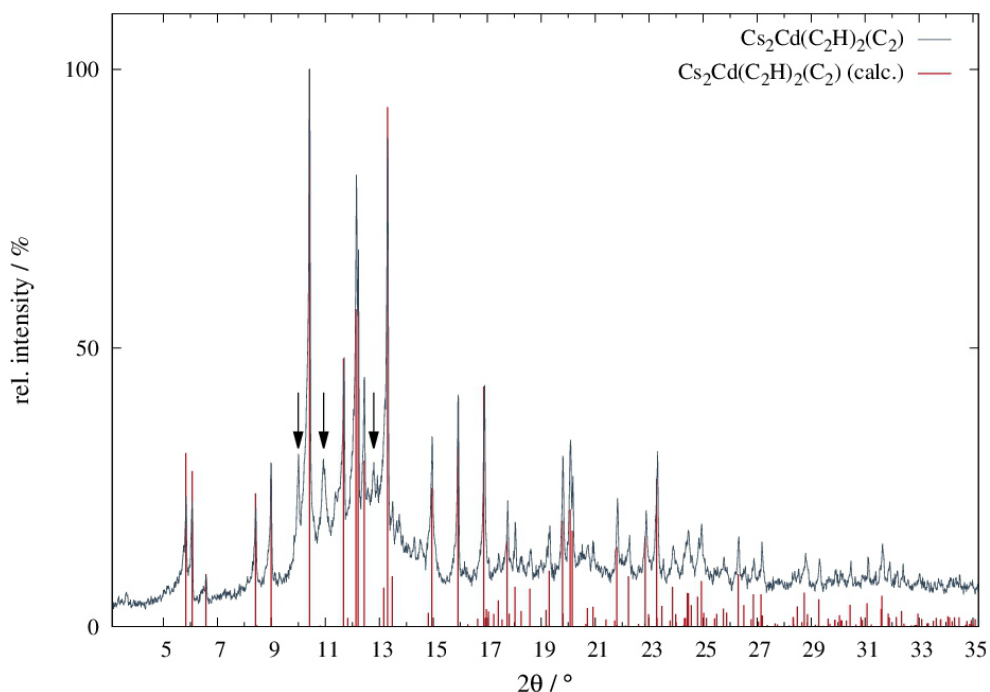
Figure S3: Synchrotron powder diffraction patterns of different samples of Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>2</sub>(C<sub>2</sub>).

**Table S1.** Fractional atomic coordinates and isotropic displacement parameters (Å<sup>2</sup>) of Cs<sub>2</sub>Cd(C<sub>2</sub>H)<sub>2</sub>(C<sub>2</sub>).

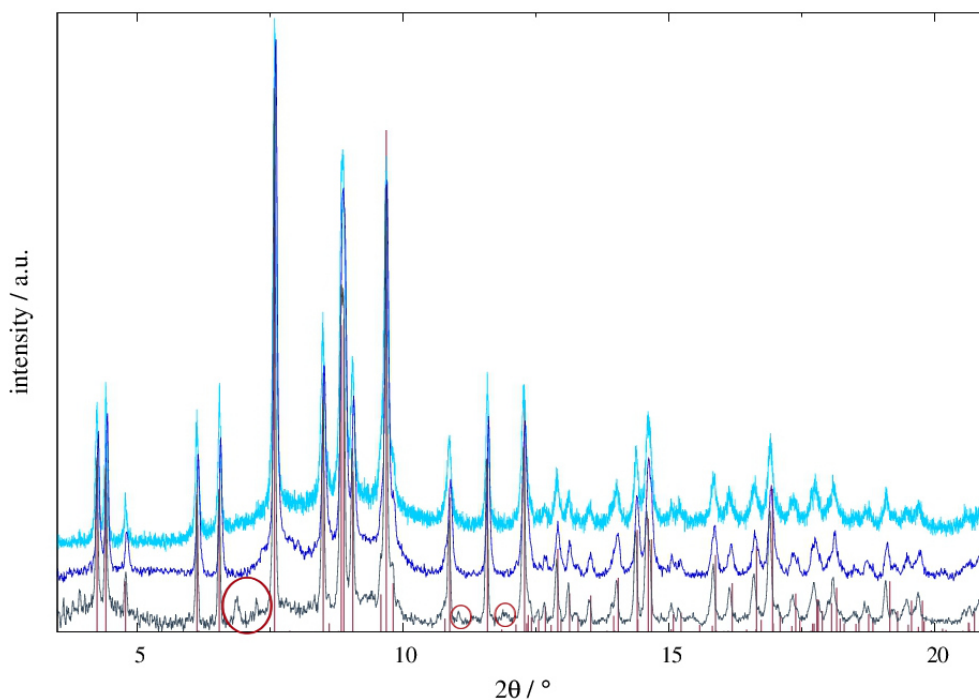
a)	Wyckoff letter	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub>
Cs1	4 <i>c</i>	0	0.2392(3)	¼	0.049(2)
Cs2	4 <i>a</i>	0	0	0	0.049(2)
Cd	4 <i>c</i>	0	0.5182(3)	¼	0.032(2)
C1	8 <i>f</i>	½	0.178(2)	0.058(2)	0.015(7)
C2	8 <i>f</i>	½	0.114(2)	0.117(2)	0.015(7)
C3	8 <i>g</i>	0.38287(4)	0.441(2)	¼	0.015(7)
H1	8 <i>f</i>	½	0.226(7)	0.012(8)	0.015(7)



**Figure S1.** Synchrotron powder diffraction pattern of  $\text{Cs}_2\text{Cd}(\text{C}_2\text{H})_4$  (dark blue curve; DELTA beamline BL9,  $\lambda = 0.47674 \text{ \AA}$ , capillary:  $\varnothing = 0.5 \text{ mm}$ ). For comparison the theoretical pattern calculated from the structure data given in the literature (*Z. Anorg. Allg. Chem.* **2004**, 630, 337) is shown (red line diagram).



**Figure S2.** XRPD pattern of  $\text{Cs}_2\text{Cd}(\text{C}_2\text{H})_2(\text{C}_2)$  synthesized under ammonothermal conditions (dark blue curve, Stoe Stadi P,  $\text{Mo-K}\alpha_1$ , capillary:  $\varnothing = 0.3 \text{ mm}$ ). For comparison the theoretical pattern calculated from its crystal structure is added as a red line diagram. The most intense impurity reflections are indicated with an arrow.



**Figure S3.** Comparison of different samples of  $\text{Cs}_2\text{Cd}(\text{C}_2\text{H})_2(\text{C}_2)$  measured with synchrotron radiation: ESRF, SNBL beamline (light blue curve); DELTA, BL9 beamline (grey and dark blue curve). All data were converted to the same wavelength ( $\lambda = 0.51655 \text{ \AA}$ ). A theoretical pattern calculated from the crystal structure of  $\text{Cs}_2\text{Cd}(\text{C}_2\text{H})_2(\text{C}_2)$  is added as a red line diagram. Some additional reflections in the “DELTA sample” are indicated with red circles.