

## Generation and structural characterization of aluminum cyanoacetylide

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## Supplementary Material

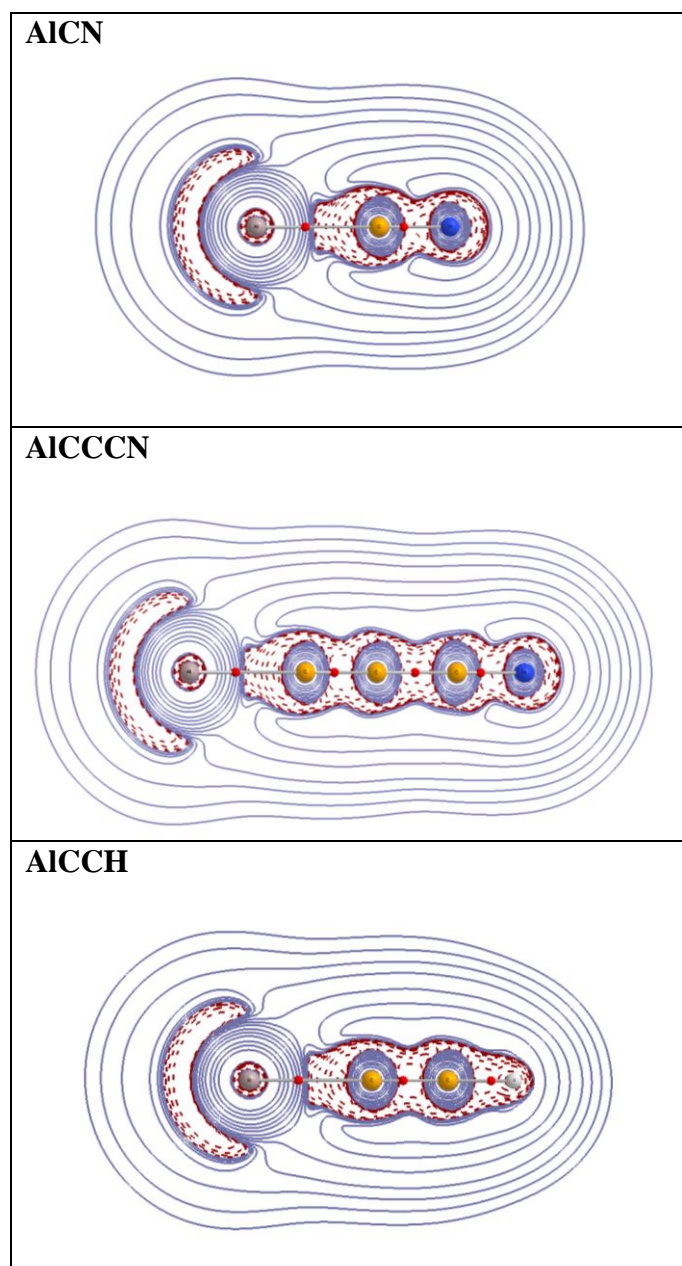
**Page 2:** Table S1, with the anharmonic vibrational frequencies ( $\omega$ ,  $\text{cm}^{-1}$ ) and IR intensities (I,  $\text{km/mol}$ ) for AlCCCN evaluated at the MP2/aug-cc-pVTZ level.

**Page 3:** Figure S1, with the contour maps of the Laplacian distribution of the electron density for the AlCN, AlCCCN and AlCCH species.

**Table S1.** Anharmonic vibrational frequencies ( $\omega$ ,  $\text{cm}^{-1}$ ) and IR intensities ( $I$ ,  $\text{km/mol}$ ) for AlCCCN evaluated at the MP2/aug-cc-pVTZ level.

Symmetry / Mode	$\omega$	$I$
1 $\pi$ AlC <sub>1</sub> C <sub>2</sub> bend	69	0.77
2 $\pi$ C <sub>1</sub> C <sub>2</sub> C <sub>3</sub> bend	247	3.25
3 $\sigma$ Al-C <sub>1</sub> stretch	386	120.08
4 $\pi$ C <sub>2</sub> C <sub>3</sub> N bend	511	2.64
5 $\sigma$ C <sub>2</sub> -C <sub>3</sub> stretch	918	107.86
6 $\sigma$ C <sub>1</sub> -C <sub>2</sub> stretch	1966	53.49
7 $\sigma$ C <sub>3</sub> -N stretch	2132	11.40

**Figure S1.** Contour maps of the Laplacian distribution of the electron density for the AICN, AICCCN and AICCH species.



Red dashed lines indicate regions of electronic charge concentration ( $\nabla^2\rho(r) < 0$ ), and blue continuous lines denote regions of electronic charge depletion ( $\nabla^2\rho(r) > 0$ ). Also molecular graphs of electron density are shown. Small red spheres are bond critical points (BCPs)