Generation and structural characterization of aluminum cyanoacetylide

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Supplementary Material

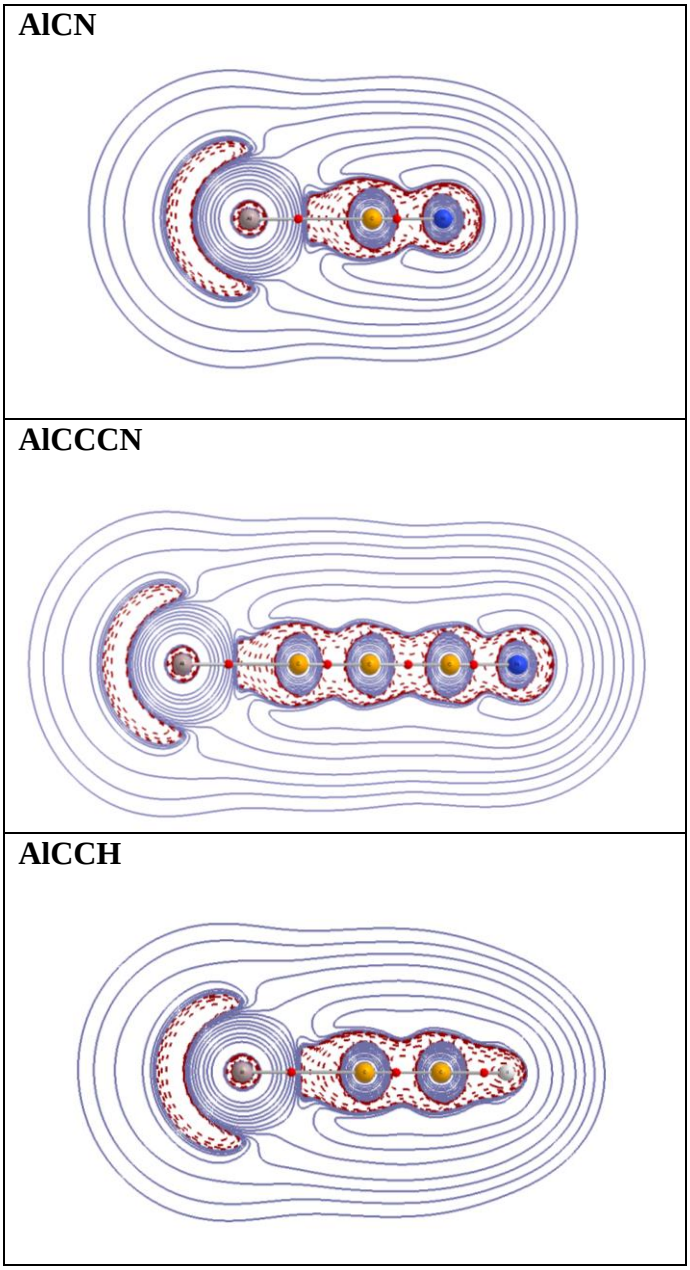
Page 2: Table S1, with the anharmonic vibrational frequencies (ω, cm^{-1}) and IR intensities (I, km/mol) for AlCCCN evaluated at the MP2/aug-cc-pVTZ level.

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 (ω, cm^{-1}) and IR intensities (I, km/mol) for AlCCCN evaluated at the MP2/aug-cc-pVTZ level.

	Symmetry / Mode	ω	I
1	π AlC_1C_2 bend	69	0.77
2	π $C_1C_2C_3$ bend	247	3.25
3	σ Al-C_1 stretch	386	120.08
4	π C_2C_3N bend	511	2.64
5	σ C_2-C_3 stretch	918	107.86
6	σ C_1-C_2 stretch	1966	53.49
7	σ C_3-N stretch	2132	11.40

Figure S1. Contour maps of the Laplacian distribution of the electron density for the AlCN, AlCCCN and AlCCH 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)