Supplementary Information

Low-energy electron scattering by cyanamide: anion spectra and dissociation pathways†

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We present in Tables 1 and 2 the cartesian coordinates for the optimized ground state geometry of cyanamide (C_s group) and cabodiimide (C_2 group) respectively. In Table 3 we present the exponents of the uncontracted Cartesian Gaussian functions used for the carbon and nitrogen atoms. Table 4 presents the energy and width of the shape resonances of cyanamide at the equilibrium and stretched geometries.

Table 1 Cartesian coordinates (in units of Bohr) for the cyanamide molecule at the equilibrium geometry in the C_s group.

Atom	x	y	z
C	2.4875595795	0.2125513205	0.0000000000
N	−0.0770430846	0.4561469040	0.0000000000
N	4.7040125887	−0.1430216492	0.0000000000
H	−0.7389272038	1.3192403094	−1.5856698779
H	−0.7389272038	1.3192403094	1.5856698779

Table 2 Cartesian coordinates (in units of Bohr) for the carbodiimide molecule at the equilibrium geometry in the C_2 group.

Atom	x	y	z
C	0.0000000000	0.0000000000	−0.0585618606
N	0.0127016232	−2.3379314386	0.1632777301
N	−0.0127016232	2.3379314386	0.1632777301
H	1.2085322614	−3.3341398604	−0.9725627068
H	−1.2085322614	3.3341398604	−0.9725627068

Table 3 Exponents of the uncontracted Cartesian Gaussian functions for C and N.

	Exponents	
Type	Carbon	Nitrogen
s	12.496280	17.567340
s	2.470286	3.423615
s	0.614028	0.884301
s	0.184028	0.259045
s	0.039982	0.055708
p	5.228869	7.050692
p	1.592058	1.910543
p	0.568612	0.579261
p	0.210326	0.165395
p	0.072250	0.037192
d	1.794795	0.975269
d	0.420257	0.253058
d	0.101114	0.078904

Table 4 Energy and widths (in parenthesis), in units of eV, for the anion states of cyanamide along the displacement $\Delta R_{\mathrm{C-N}}$ of the C−N stretching coordinate.

$\Delta R_{\mathrm{C-N}}$ (Å)	π_1^* (A'')	π_2^* (A')	σ_{CN}^* (A')
0.0	2.11 (0.16)	2.89 (0.25)	4.57 (0.95)
0.1	2.03 (0.09)	2.80*	2.80*
0.2	1.95 (0.06)	2.53 (0.17)	1.20 (0.33)
0.3	1.83 (0.06)	2.37 (0.18)	0.08 (0.07)
0.4	1.76 (0.07)	2.20 (0.11)	−0.91
0.5	1.70 (0.08)	2.13 (0.11)	−1.72
0.6	1.65 (0.10)	2.03 (0.08)	−2.49

* both π_2^* and σ_{CN}^* resonances overlap.