Low-enerngy electron scattering from cyanamide using R-matrix mehod

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Synopsis Low-energy electron collision with cyanamide is investigated in static-exchange (SE), static-exchange plus polarization (SEP) and close-coupling (CC) approximations. Two shape resonances, two core-excited resonances and two Feshbach resonances are detected in the CC approximation. The role of active space in the target and scattering problem including the resonances is discussed. The precise resonance parameters are found to be sensitive to the treatment of polarization effects employed. These resonances may be responsible for the fragments observed in a recent experiment of the dissociative electron attachments to cyanamide.

Cyanamide, NH_2CN, is an important astrophysical molecule observed in the gas clouds of the interstellar medium. It could serve as a model molecule for more complex species with biological relevance. Here, the low-energy electron scattering from cyanamide is studied using UK molecular R-matrix code [1].

Table 1. Parameters of identified *e*-cyanamide resonances (in eV). (AS means active space.)

State	Type	Parent state	AS	Position
^{2}A"	shape	X^{1}A'	(11,4)	4.25
			(10,6)	4.01
			(11,6)	4.25
^{2}A'	shape	X^{1}A'	(11,4)	6.04
			(11,6)	5.90
^{2}A'	Feshbach	2^{3}A'	(11,4)	7.22
			(10,6)	7.20
			(11,6)	8.24
^{2}A"	Feshbach	1^{1}A"	(11,4)	7.59
			(10,6)	8.21
			(11,6)	7.90
^{2}A'	Core-excited	2^{3}A'	(11,4)	7.93
			(11,6)	8.88
^{2}A'	Core-excited	3^{1}A'	(11,4)	9.06
			(11,6)	9.35

Elastic, momentum-transfer, and excitation cross sections have been presented. We predict a π^* resonance and an σ^* resonance at 5.06 eV and 6.51 eV in SE model, and at 3.34 eV and 4.99 eV in SEP model, respectively. In our 12-state CC model and the active space (11, 4), these two resonances are located at 4.25 eV and 6.04 eV. We also detected two core-excited resonances, and two Feshbach resonances in the CC model. The different active spaces are tested and the obtained resonance parameters are listed in Table 1. We find that the precise resonance parameters are sensitive to the treatment of polarization effects employed.

To explore the possible dissociative nature of two shape resonances, we have investigated their dependence on geometry by performing a series of R-matrix calculations by stretching the C-N single bond while fixing other bond length and bond angle at equilibrium in *Cs* symmetry. Figure 1 shows the position and the width of the resonances change with the C-N bond stretching. Our predicted π^* resonance was regarded as precursor of the observed CN fragment in the energy region around 5.3 eV in the recent dissociative electron attachment (DEA) experiment [2]. Our calculations show that an direct DEA pathway could take place for the C-N single bond, but the direct dissociations along the N-H bond can be ruled out [3].

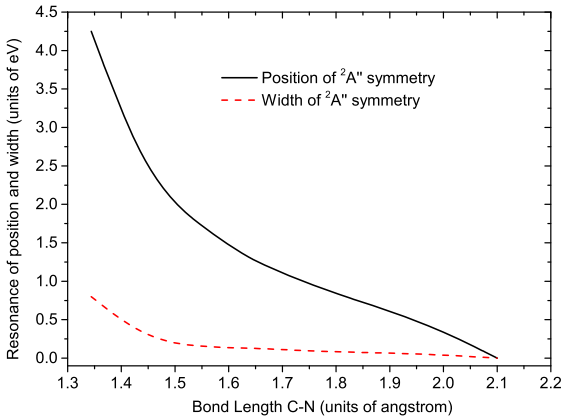

Figure 1. Variation of π^* shape resonance width and position with stretching length of C-N single bond.

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References

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