Supplementary Material (ESI) for *PCCP*

SUPPORTING INFORMATION

Electronic state dependence of the ion-molecule reaction $CH_3CN^+ + CH_3CN \rightarrow CH_4CN^+ + CH_2CN$: Threshold electron-secondary ion coincidence (TESICO) and direct ab-initio molecular dynamics Study

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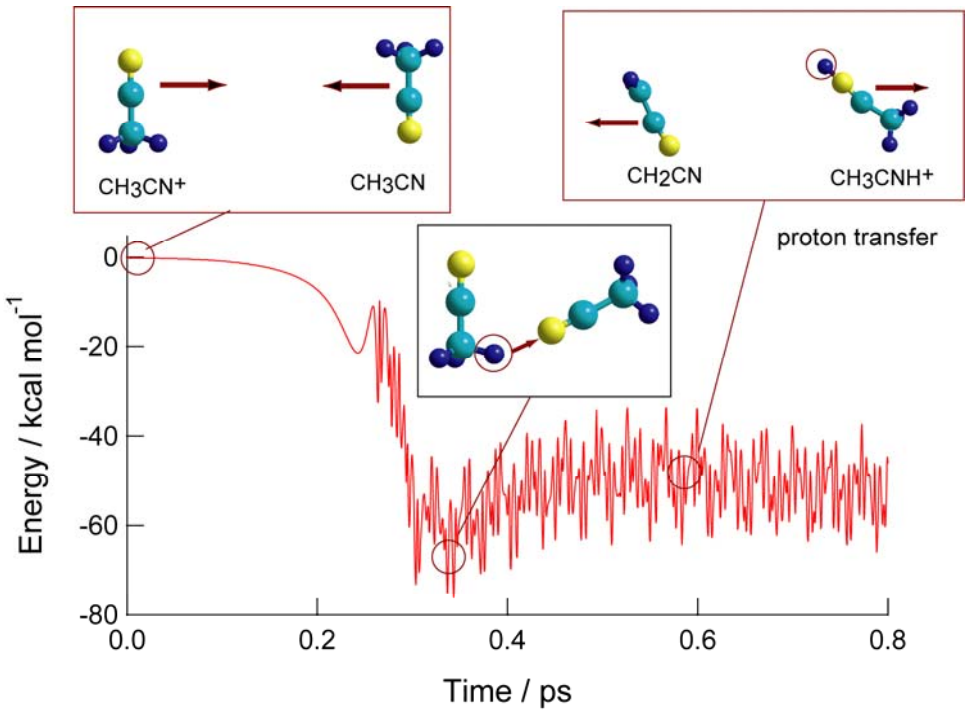
1. Graphical Abstract



2. Optimized structures of neutral and radical cation of CH_3CN

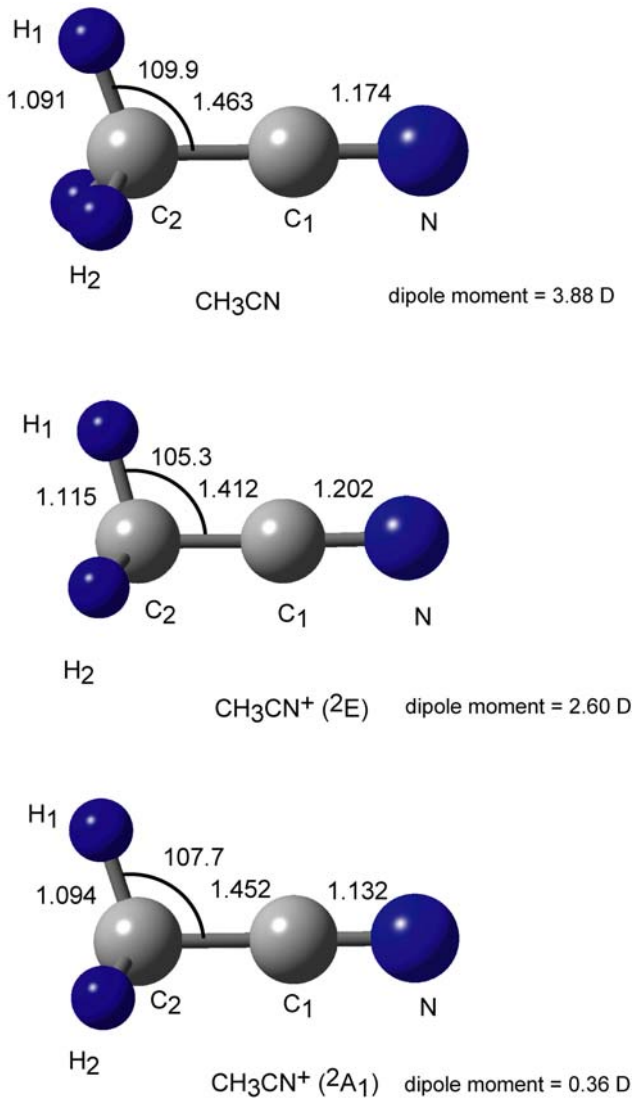


Figure S1. Optimized structures of (upper) neutral acetonitrile CH_3CN, (middle) $CH_3CN^+(^2E)$ and (lower) CH_3CN $(^2A_1)$ calculated at the MP2/6-311++G(d,p) level.

3. Spin densities

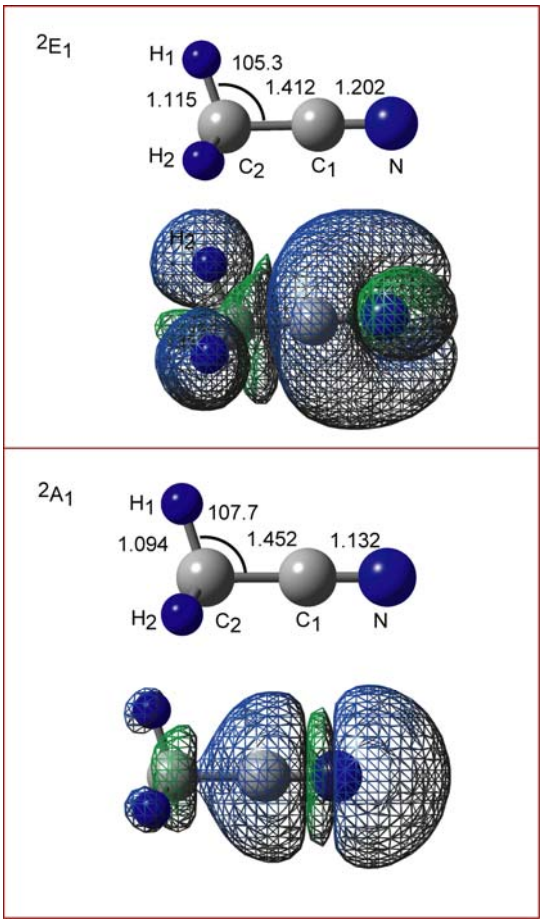


Figure S2. Special distributions of spin densities of $CH_3CN^+(^2E)$ and CH_3CN $(^2A_1)$ calculated at the MP2/6-311++G(d,p) level.