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Full-dimensional Quantum State-to-state Non-adiabatic Dynamics for Photodissociation of Ammonia in its *A*-band

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Supporting Information

Table S-I. Single-coordinate functions used to expand diabatic potentials

Index	Function Type	Scaling Function	Scaling Parameter
1	Exponential [a]	$w = \exp\left[-C_1\left(r_{NH} - C_2\right)\right]$	C_1=1.0, C_2=1.5
2	Reciprocal [a]	$w = \exp\left[-C_1\left(r_{NH} - C_2\right)\right] / r_{NH}$	C_1=1.0, C_2=2.0
3	Exponential	$w = \exp\left[-C_1\left(r_{HH} - C_2\right)\right]$	C_1=1.0, C_2=1.5
4	Gaussian	$w = \exp\left[-C_1\left(r_{NH} - C_2\right)^2\right]$	C_1=1.0, C_2=2.0
5	Gaussian	$w = \exp\left[-C_1\left(r_{HH} - C_2\right)^2\right]$	C_1=0.6, C_2=1.4
6	Angular	$w = \dfrac{\cos\theta_{\angle HNH}}{1+\exp\left[C_1\left(r_1^2 + r_2^2 - C_2^2\right)\right]}$ [b]	C_1=0.15, C_2=3.0
7	Hyperbolic Tangent	$w = \tanh\left[\left(r_{NH} - C_2\right) / C_1\right]$	C_1=0.25, C_2=2.5
8	Out-of-Plane [c]	$w = \dfrac{\mathbf{r}_1}{r_1} \times \dfrac{\mathbf{r}_2}{r_2} \cdot \dfrac{\mathbf{r}_3}{r_3} / \sum_i \exp\left[C_1\left(r_i - C_2\right)\right]$ [d]	C_1=0.50, C_2=2.0

a. B. J. Braams and J. M. Bowman. Int. Rev. Phys. Chem. **28**, 577 (2009)

b. r_1 and r_2 are the length of the two side NH bonds of the H-N-H angle.

c. O. Godsi, C. R. Evenhuis, and M. A. Collins, J. Chem. Phys. **125**, 104105 (2006)

d. r_1, r_2 and r_3 are the three NH distances in the umbrella out-of-plane bending coordinate. The second term on the right is the harmonic mean of the exponentials of all the NH distances.

Table S-II. Numerical parameters (in a.u.) used in wave packet calculations.

Grid/basis ranges and sizes $r_3 \in [1.2,14.0]$, N_3=100 $r_1 \in [1.2,4.5]$, $r_2 \in [1.2,4.5]$, for $1 \le i_3 \le 21$, $N_1 = N_2$ =21; for $22 \le i_3 \le 100$, $N_1 = N_2$ =11 $j_{1\max} = j_{2\max} = m_{\max} = 30$
Damping functions $\exp[-0.006(r_3 - 10.6)^2]$, for $10.6 < r_3 < 14.0$ $\exp[-0.1(r_1 - 3.1)^2]$, for $3.1 < r_1 < 4.5$ $\exp[-0.1(r_2 - 3.1)^2]$, for $3.1 < r_2 < 4.5$
Propagation steps: 30000