Supporting Information for Infrared-Driven Dynamics and Scattering Mechanisms of NO Radicals with Propane and Butane: Impacts of Pseudo Jahn-Teller Effects

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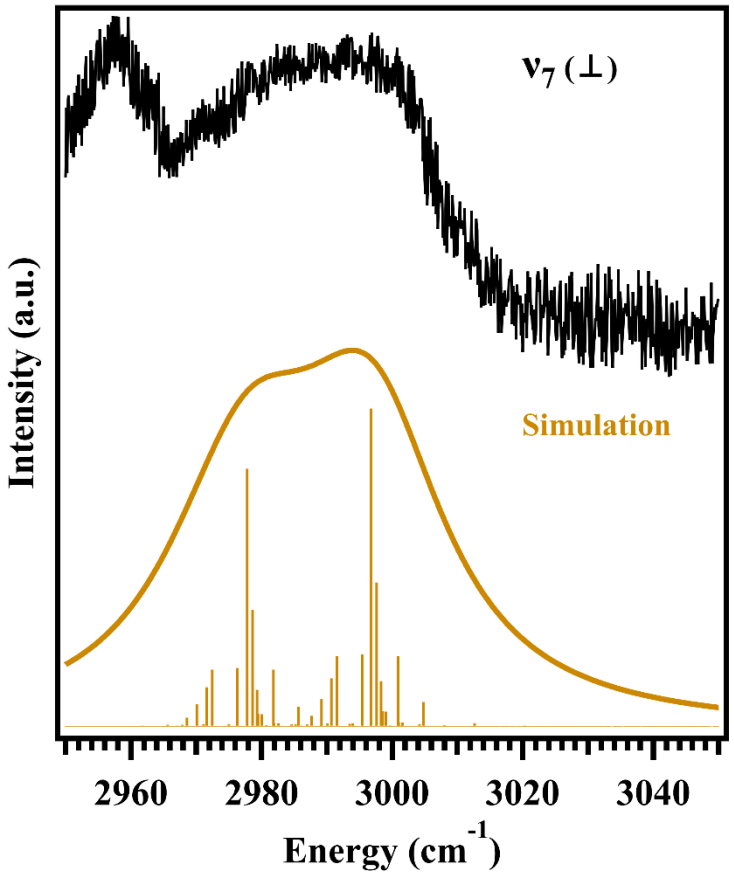

Figure S1: Experimental IR action spectrum for the NO-ethane collision complex compared with rovibrational simulations. The rovibrational simulations were obtained using the fitting procedure described in the main text and the spectroscopic constants listed in Table S1. The gold trace represents the fitted spectrum by convoluting each stick with a Lorentzian line shape function.

Table S1. Spectral Fitting Parameters Obtained for the NO-Ethane Rovibrational Simulations[a]

	ν_{18} (e_u)	ν_{17} (e_u)
Parameter[b]	Value	Value
ν_0	2994.1(3)	2975.3(3)
A'' / A'	2.67(1) / 2.34(1)[c]	0.7742(1) / 0.7736(1)[c]
B'' / B'	0.663(1) / 0.645(1)[c]	0.1199(1) / 0.1199(1)[c]
$D_{J''}$	1.03×10^{-6}(1)	1.03×10^{-6}(1)
$D_{J''K''}$	2.66×10^{-6}(1)	2.66×10^{-6}(1)
$D_{K''}$	1.09×10^{-5}(1)	1.09×10^{-5}(1)
$\Delta\nu_{Lor}$	25(1)	25(1)
T_{rot} (K)	4(1)	4(1)

[a] Standard deviations (2σ) for each parameter are given in parentheses.

[b] Otherwise indicated, all values are given in wavenumbers (cm^{-1}).

[c] Obtained from M. Hepp and M. Herman, Weak Combination Bands in the 3-mm Region of Ethane, *J. Mol. Spectrosc.*, **1999**, *197*, 56–63.

NO-Ethane Cartesian Coordinates

Atom	x	y	z
C	-1.600425	0.062307	0.000000
C	-1.088980	1.497929	0.000000
H	-2.689253	0.033222	0.000000
H	0.000000	1.531972	0.000000
H	-1.435771	2.038494	0.879619
H	-1.257661	-0.480460	-0.880475
H	-1.435771	2.038494	-0.879619
H	-1.257661	-0.480460	0.880475
N	1.333322	-1.474057	0.000000
O	1.859912	-0.465536	0.000000

NO-Propane Cartesian Coordinates

Atom	x	y	z
C	0.000000	0.958782	0.000000
C	1.466037	0.544460	0.000000
N	-1.334721	-2.069093	0.000000
O	-0.302558	-2.547793	0.000000
C	-0.162332	2.473937	0.000000
H	1.582822	-0.539192	0.000000
H	1.976570	0.936101	0.880704
H	-0.500537	0.539792	-0.875704
H	1.976570	0.936101	-0.880704
H	-0.500537	0.539792	0.875704
H	-1.211869	2.766267	0.000000
H	0.309133	2.912030	-0.880611
H	0.309133	2.912030	0.880611

NO-(n-Butane) Cartesian Coordinates

Atom	x	y	Z
C	1.450369	1.035223	0.000000
C	0.000000	0.569982	0.000000
C	-0.986924	1.730762	0.000000
N	0.516836	-2.687074	0.000000
O	1.644241	-2.533439	0.000000
H	2.145365	0.195557	0.000000
H	1.660240	1.642958	0.880918
H	-0.189316	-0.056035	-0.876745
H	1.660240	1.642958	-0.880918
H	-0.189316	-0.056035	0.876745
C	-2.436357	1.261467	0.000000
H	-0.800103	2.358338	-0.875521
H	-0.800103	2.358338	-0.875521
H	-3.131186	2.100769	0.000000
H	-2.645065	0.652790	0.880602
H	-2.645065	0.652790	-0.880602