Supporting Information for

Improved direct diabatization and coupled potential energy surfaces for the photodissociation of ammonia

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Table 1 Nonlinear parameters

Parameter	Value
$\gamma^{(1)}$ (Å^{-1})	1.872
$r_0^{(1)}$ (Å)	0.428
$\delta^{(1)}$ (Å^{-2})	0.101
$\hat{a}_{NH1}^{(1)}$ (Å^{-2})	4.067
$\hat{a}_{HH}^{(1)}$ (Å^{-2})	4.174
$\eta_1^{(1)}$ (Å^{-1})	3.000
$r_e^{(1)}$ (Å)	1.024
$\beta_{NH2}^{(1)}$ (Å^{-2})	11.00
$\gamma^{(2)}$ (Å^{-1})	1.634
$r_0^{(2)}$ (Å)	0.199
$\delta^{(2)}$ (Å^{-2})	0.304
$\alpha^{(2)}$ (Å^{-2})	4.547
$r_{02}^{(2)}$ (Å)	0.715
$k^{(2)}$	-0.262
$C^{(2)}$ (rad^2)	0.050
$\beta_{NH2}^{(2)}$ (Å^{-2})	11.00
$r_0^{(3)}$ (Å)	1.501

Table 2 Linear coefficients (in eV) for the U_{11} potential energy surface.

i j k l m n p	Value	*i j k l m n p*	Value
000 001 1	-1.6983	000 001 2	1.1754
000 002 1	-3.1170	000 002 2	3.8887
000 011 1	49.8932	000 011 2	-36.5117
001 000 1	61.4054	001 000 2	-35.2209
001 001 1	-91.3790	001 001 2	87.2284
001 002 1	-41.7031	001 002 2	73.9830
001 011 1	-282.2911	001 011 2	187.2948
002 000 1	-132.4725	002 000 2	121.7029
002 001 1	45.5429	002 001 2	-38.6531
002 002 1	64.8251	002 002 2	-91.1205
002 011 1	162.2981	002 011 2	-89.0617
011 000 1	-141.8440	011 000 2	51.3039
011 001 1	312.8762	011 001 2	-293.5045
011 002 1	229.1158	011 002 2	-304.5399
011 011 1	421.2982	011 011 2	-245.6763
012 000 1	590.4053	012 000 2	-482.7739
012 001 1	-201.1576	012 001 2	166.5285
012 002 1	-284.7075	012 002 2	347.8381
012 011 1	-420.7882	012 011 2	182.6086
022 000 1	-340.1129	022 000 2	302.7131
022 001 1	-101.7601	022 001 2	121.9770
022 002 1	-31.3577	022 002 2	41.7123
022 011 1	77.6688	022 011 2	-9.6474
111 000 1	-186.3623	111 000 2	203.5053
111 001 1	-245.4113	111 001 2	229.7924
111 002 1	-231.1745	111 002 2	273.1855
111 011 1	-78.1083	111 011 2	37.4602
112 000 1	147.6582	112 000 2	-157.4955
112 001 1	280.9941	112 001 2	-270.8242
112 002 1	303.3039	112 002 2	-348.6652
112 011 1	61.6306	112 011 2	-19.2778
$\Delta E_1^{(1)}$ (eV)	0.0019	$B_{\mathrm{NH1}}^{(1)}$ (eV Å)	32.3630
$\Delta E_2^{(1)}$ (eV)	0.2197	$B_{\mathrm{HH}}^{(1)}$ (eV Å)	12.7430
$B_{\mathrm{NH2}}^{(1)}$ (eV Å)	209.8300		

Table 3 Linear coefficients (in eV) for the U_{22} potential energy surface.

$i\ j\ k\ l\ m\ n\ p$	Value	$i\ j\ k\ l\ m\ n\ p$	Value
000 000 0	-5.8393	000 001 2	-175.0594
000 001 1	194.8308	000 002 2	-134.3885
000 002 1	147.6399	000 011 2	199.7872
000 011 1	-195.2771	001 000 2	491.9735
001 000 1	-495.6220	001 001 2	-1486.2088
001 001 1	1455.0349	001 002 2	648.2491
001 002 1	-685.2363	001 011 2	789.5413
001 011 1	-798.0708	002 000 2	33.9129
002 000 1	-71.5031	002 001 2	1900.2894
002 001 1	-1898.8850	002 002 2	-672.4669
002 002 1	694.4385	002 011 2	-1274.9089
002 011 1	1278.0738	003 000 2	-256.3702
003 000 1	249.6162	003 001 2	667.3492
003 001 1	-660.5420	003 002 2	222.6065
003 002 1	-225.9061	003 011 2	-317.8753
003 011 1	320.8342	011 000 2	-1352.9041
011 000 1	1438.8807	011 001 2	2450.8155
011 001 1	-2462.1171	011 002 2	-126.9877
011 002 1	126.5000	011 011 2	-1626.5266
011 011 1	1618.8084	012 000 2	419.1477
012 000 1	-427.7636	012 001 2	-2837.7980
012 001 1	2889.2055	012 002 2	459.8348
012 002 1	-452.5183	012 011 2	2208.8717
012 011 1	-2216.7826	013 000 2	549.6795
013 000 1	-547.4397	013 001 2	-976.5929
013 001 1	952.3772	013 002 2	-763.8624
013 002 1	800.1805	013 011 2	237.8198
013 011 1	-241.3673	111 000 2	435.9354
111 000 1	-468.9797	111 001 2	91.5700
111 001 1	-122.6083	111 002 2	-202.8118
111 002 1	201.3096	111 011 2	-230.4178
111 011 1	249.7300	113 000 2	-232.5038
113 000 1	235.4985	113 001 2	179.7589
113 001 1	-160.9356	113 002 2	554.7260
113 002 1	-593.3048	113 011 2	231.6886
113 011 1	-230.1960		
$\Delta E_1^{(2)}$ (eV)	0.0473	$B_{\mathrm{NH2}}^{(2)}$ (eV Å)	419.6600
$\Delta E_2^{(2)}$ (eV)	0.1970		

Table 4 Linear coefficients (in eV Å$^{-(i+j+k)}$ rad$^{-(l+m+n)}$ for the U_{12} potential energy surface.

i j k l m n p	Value	*i j k l m n p*	Value
000 001 3	-1.3708	002 001 4	1.0585
000 002 3	0.6837	002 002 4	-0.8694
000 011 3	0.6332	002 011 4	0.1169
001 000 3	1.0484	011 000 4	0.9741
001 001 3	1.4509	011 001 4	-0.5185
001 002 3	-0.6762	011 002 4	0.4463
001 011 3	-1.7635	011 011 4	-0.8328
002 000 3	-0.2758	000 001 5	-0.4614
002 001 3	-0.1771	000 002 5	0.3513
002 002 3	0.1521	000 011 5	-0.0631
002 011 3	0.3338	001 000 5	0.6509
011 000 3	-0.7012	001 001 5	0.3788
011 001 3	0.1057	001 002 5	-0.6678
011 002 3	-0.1500	001 011 5	0.1524
011 011 3	0.8059	002 000 5	0.1114
000 001 4	1.1005	002 001 5	-0.3191
000 002 4	-0.9055	002 002 5	0.5041
000 011 4	-0.1502	002 011 5	-0.2955
001 000 4	-0.5756	011 000 5	-0.7789
001 001 4	-1.8595	011 001 5	0.5061
001 002 4	1.3764	011 002 5	-0.2055
001 011 4	0.8781	011 011 5	0.1836
002 000 4	-0.3399		