

Table S2 Supplementary data: total BHandHLYP/6-311G** energies (E) and zero point energies (zpe), both in a.u., of transition state structures; also, molecular symmetries and (for radicals) electronic states, together with imaginary and 1st harmonic frequencies in cm^{-1}

		sym	E	zpe	ω_i	ω_1
1	$trans\text{-HONO} \rightarrow cis\text{-HONO}$	C_1	-205.6169	.0197	545i	633
2	$trans\text{-HONO} \rightarrow \text{H-NO}_2$	C_s	-205.5352	.0160	2337i	428
3	$\text{NO}_2 + \text{H}_2 \rightarrow trans\text{-HONO} + \text{H}$	$C_s/{}^2A'$	-206.1186	.0180	1860i	268
4	$\text{NO}_2 + \text{H}_2 \rightarrow cis\text{-HONO} + \text{H}$	$C_s/{}^2A'$	-206.1300	.0189	1960i	301
5	$\text{NO}_2 + \text{H}_2 \rightarrow \text{H-NO}_2 + \text{H}$	$C_{2v}/{}^2A_1$	-206.1252	.0210	1292i	295
6	$\text{NO}_2 + \text{HO}_2 \rightarrow trans\text{-HONO} + \text{O}_2$	$C_s/{}^3A''$	-355.8677	.0234	2336i	172
6b	$\text{NO}_2 + \text{HO}_2 \rightarrow trans\text{-HONO} + \text{O}_2$	$C_s/{}^3A''$	-355.8536	.0215	3789i	25
7	$\text{NO}_2 + \text{HO}_2 \rightarrow cis\text{-HONO} + \text{O}_2$	$C_1/{}^3A$	-355.8649	.0218	2947i	57
7b	$\text{NO}_2 + \text{HO}_2 \rightarrow cis\text{-HONO} + \text{O}_2$	$C_s/{}^3A''$	-355.8499	.0228	2895i	148
8	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{H-NO}_2 + \text{O}_2$	$C_s/{}^3A''$	-355.8654	.0223	2468i	75
9	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HO}_2\text{NO}_2$	$C_1/{}^1A$	-355.8830	.0281	273i	100
10	$\text{NO}_2 + \text{HCHO} \rightarrow trans\text{-HONO} + \text{HCO}$	$C_s/{}^2A'$	-319.4333	.0322	1507i	56
11	$\text{NO}_2 + \text{HCHO} \rightarrow cis\text{-HONO} + \text{HCO}$	$C_1/{}^2A$	-319.4467	.0335	1823i	66
12	$\text{NO}_2 + \text{HCHO} \rightarrow \text{H-NO}_2 + \text{HCO}$	$C_s/{}^2A'$	-319.4419	.0340	2082i	31
13	$\text{NO}_2 + \text{H}_2\text{O} \rightarrow trans\text{-HONO} + \text{OH}$	$C_1/{}^2A$	-281.3484	.0267	2630i	138
13b	$\text{NO}_2 + \text{H}_2\text{O} \rightarrow trans\text{-HONO} + \text{OH}$	$C_1/{}^2A$	-281.3482	.0264	2708i	140
14	$\text{NO}_2 + \text{H}_2\text{O} \rightarrow cis\text{-HONO} + \text{OH}$	$C_1/{}^2A$	-281.3643	.0302	2265i	189
15	$\text{NO}_2 + \text{H}_2\text{O} \rightarrow \text{H-NO}_2 + \text{OH}$	$C_1/{}^2A'$	-281.3532	.0292	1140i	110
16	$\text{NO}_2 + \text{H}_2\text{S} \rightarrow trans\text{-HONO} + \text{SH}$	$C_1/{}^2A$	-604.3507	.0207	2063i	90
16b	$\text{NO}_2 + \text{H}_2\text{S} \rightarrow trans\text{-HONO} + \text{SH}$	$C_1/{}^2A$	-604.3506	.0209	2083i	59
17	$\text{NO}_2 + \text{H}_2\text{S} \rightarrow cis\text{-HONO} + \text{SH}$	$C_1/{}^2A$	-604.3729	.0247	2030i	135
18	$\text{NO}_2 + \text{H}_2\text{S} \rightarrow \text{H-NO}_2 + \text{SH}$	$C_s/{}^2A'$	-604.3696	.0246	1892i	106
19	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow trans\text{-HONO} + \text{CH}_2\text{OH}$	$C_1/{}^2A$	-320.6514	.0586	1401i	105
19b	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow trans\text{-HONO} + \text{CH}_2\text{OH}$	$C_1/{}^2A$	-320.6491	.0579	1281i	22
20	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow cis\text{-HONO} + \text{CH}_2\text{OH}$	$C_1/{}^2A$	-320.6595	.0585	1777i	45
21	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow \text{H-NO}_2 + \text{CH}_2\text{OH}$	$C_1/{}^2A$	-320.6573	.0600	1895i	81
22	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow trans\text{-HONO} + \text{CH}_3\text{O}$	$C_1/{}^2A$	-320.6437	.0572	3358i	123
23	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow cis\text{-HONO} + \text{CH}_3\text{O}$	$C_1/{}^2A$	-320.6537	.0593	2491i	123
24	$\text{NO}_2 + \text{CH}_3\text{OH} \rightarrow \text{H-NO}_2 + \text{CH}_3\text{O}$	$C_1/{}^2A'$	-320.6501	.0581	2182i	10
25	$\text{NO}_2 + \text{HBr} \rightarrow trans\text{-HONO} + \text{Br}$	$C_s/{}^2A'$	-2779.6794	.0169	2290i	122
26	$\text{NO}_2 + \text{HBr} \rightarrow cis\text{-HONO} + \text{Br}$	$C_s/{}^2A'$	-2779.6938	.0160	1839i	121
27	$\text{NO}_2 + \text{HBr} \rightarrow \text{H-NO}_2 + \text{Br}$	$C_{2v}/{}^2A_1$	-2779.6875	.0167	1288i	122
28	$\text{NO}_2 + \text{HI} \rightarrow cis\text{-HONO} + \text{I}$	$C_s/{}^2A'$	-216.9402	.0148	1755i	74
29	$\text{NO}_2 + \text{HI} \rightarrow \text{H-NO}_2 + \text{I}$	$C_{2v}/{}^2A_1$	-216.9386	.0155	1722i	129
30	$\text{NO}_2 + trans\text{-HONO} \rightarrow trans\text{-HONO} + \text{NO}_2$	$C_{2v}/{}^2B_2$	-410.6171	.0293	2238i	68
30b	$\text{NO}_2 + trans\text{-HONO} \rightarrow trans\text{-HONO} + \text{NO}_2$	$C_{2h}/{}^2B_u$	-410.6007	.0280	4031i	24
31	$\text{NO}_2 + trans\text{-HONO} \rightarrow cis\text{-HONO} + \text{NO}_2$	$C_s/{}^2A'$	-410.6149	.0287	2319i	62
32	$\text{NO}_2 + trans\text{-HONO} \rightarrow \text{H-NO}_2 + \text{NO}_2$	$C_s/{}^2A'$	-410.6000	.0285	2763i	42
33	$\text{NO}_2 + cis\text{-HONO} \rightarrow cis\text{-HONO} + \text{NO}_2$	$C_{2h}/{}^2B_u$	-410.6170	.0275	2676i	9.9i
34	$\text{NO}_2 + cis\text{-HONO} \rightarrow \text{H-NO}_2 + \text{NO}_2$	$C_s/{}^2A'$	-410.6127	.0285	2625i	52

Note: See footnote to Table S1.