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Inelastic rate coefficients based on an improved potential energy surface for N_2+N_2 collisions in a wide temperature range

Supporting Information

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Table S1: Rate coefficients for the transition (1, 0)$\longrightarrow$(0, 0).

	$k_{1,0\rightarrow0,0}$								
Source	100K	300K	500K	1000K	2000K	3000K	4000K	5000K	7000K
original PES	2.83E-20	3.73E-21	1.05E-20	1.54E-18	2.29E-16	3.14E-15	1.72E-14	5.88E-14	2.91E-13
modified PES	3.16E-20	5.23E-21	2.46E-20	3.90E-18	5.08E-16	6.52E-15	3.32E-14	1.07E-13	5.44E-13
Exp. [1]					6.89E-16		6.66E-14	3.33E-13	
Exp. [2]			5.17E-19						
Exp. [3]		6.33E-21							

Table S2: Rate coefficients for the transition (1, 0)$\longrightarrow$(0, 1).

	$k_{1,0\rightarrow0,1}$									
Source	77K	136K	226K	300K	500K	1000K	2000K	3000K	5000K	7000K
original PES	1.33E-13	4.11E-14	1.83E-14	1.39E-14	1.24E-14	1.93E-14	3.92E-14	6.31E-14	1.16E-13	1.62E-13
modified PES	9.56E-14	2.91E-14	1.42E-14	1.17E-14	1.22E-14	2.10E-14	4.37E-14	7.11E-14	1.32E-13	2.23E-13
Exp. [4]	2.26E-12	3.35E-13	9.21E-14	3.91E-14						
Exp. [5]				9.00E-15						
Exp. [6]				2.50E-14						
Exp. [7]				9.93E-14						

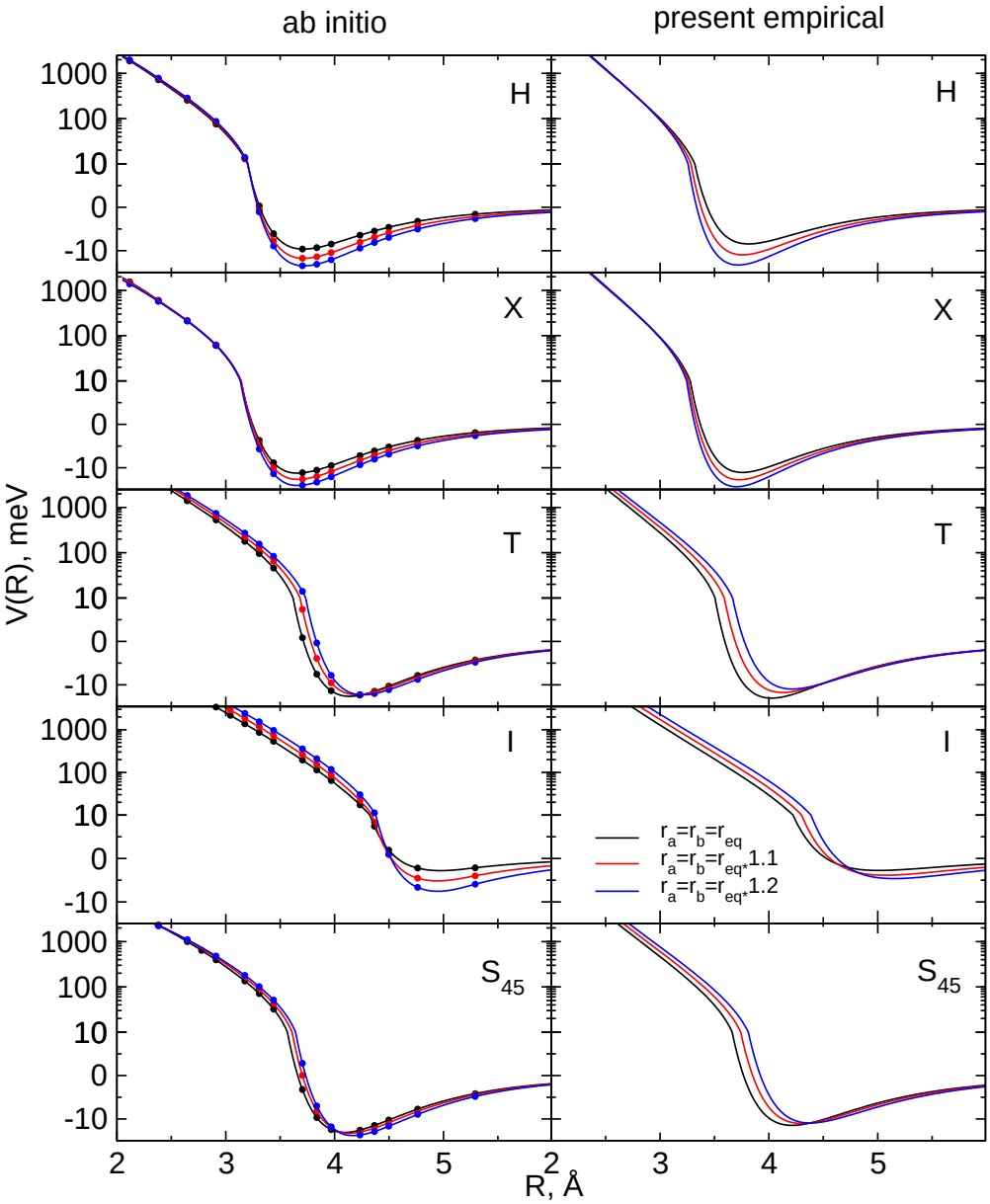

Figure S1: Dependence of the interaction energy on the internuclear distances r_a and r_b for five selected configurations of the N_2-N_2 complex

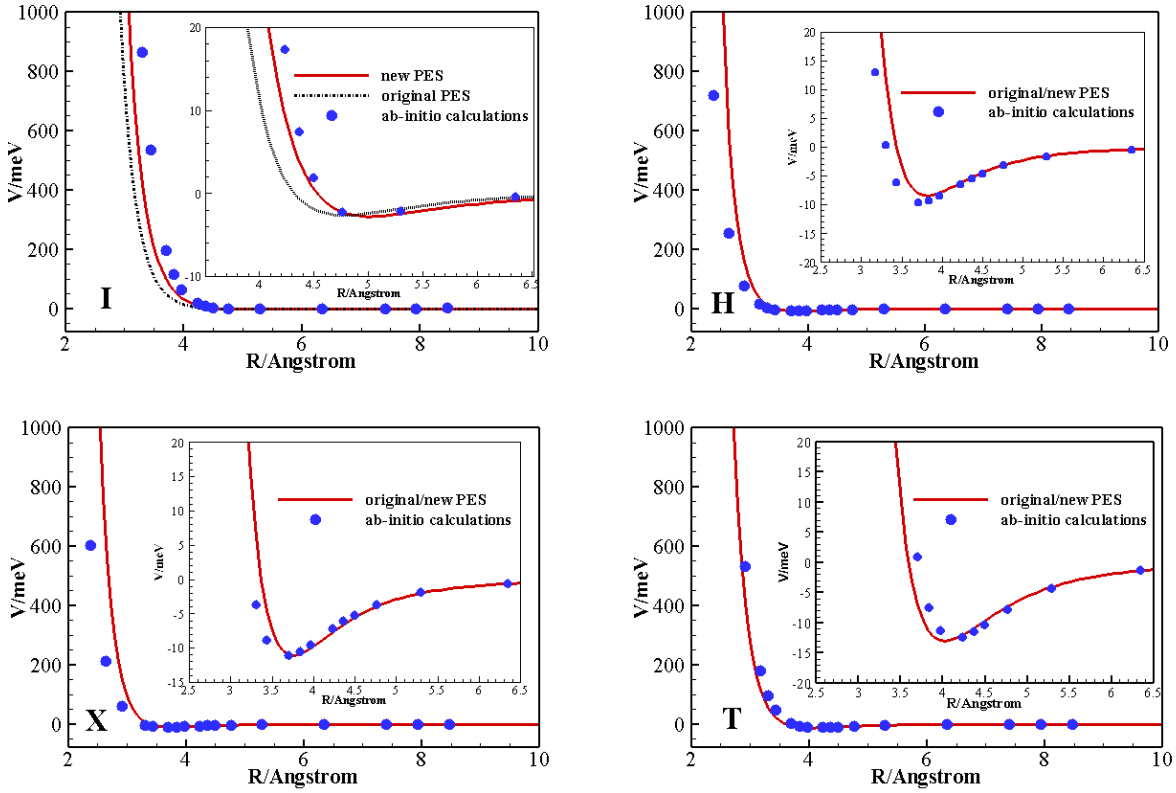

Figure S2: Behavior of the original and modified potential energy surfaces with respect to ab initio calculations as a function of the diatoms interaction distance for diatoms approaching in a collinear configuration, according to l ($D_{\infty h}$ symmetry, panel I), in a parallel fashion (H configuration, D_{2h} symmetry, panel H); in a crossed X fashion (D_{2d} symmetry, panel X) and perpendicularly, according to a T orientation (C_{2v} symmetry, panel T)

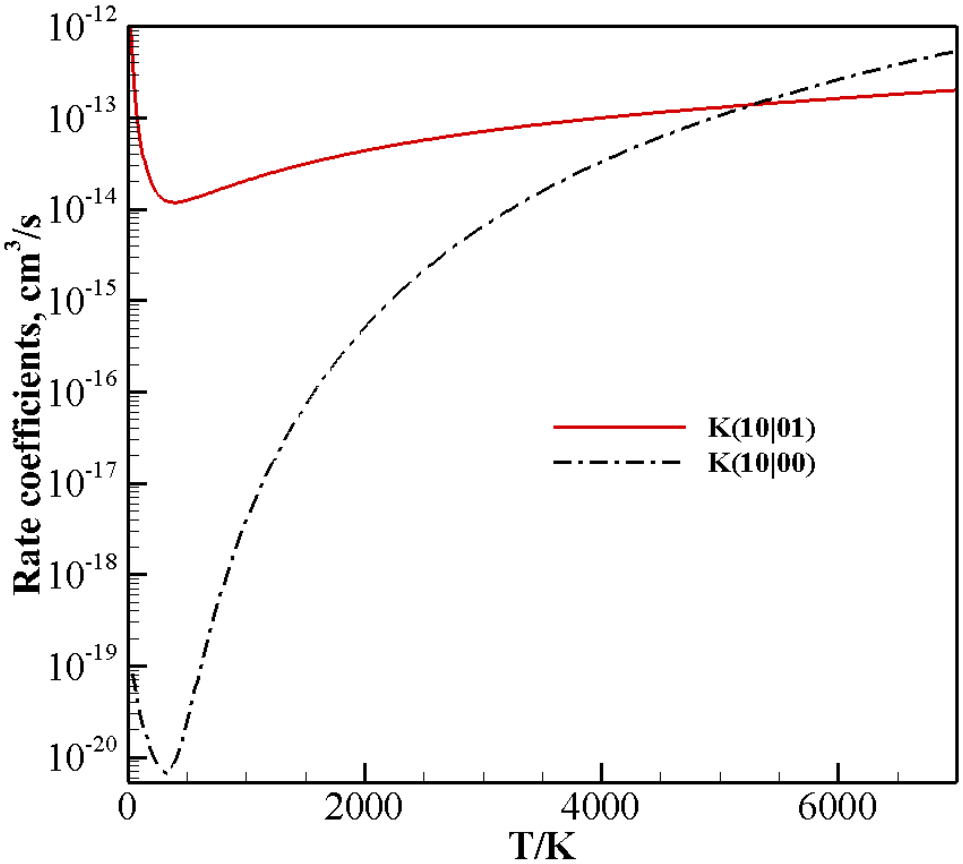

Figure S3: V-T/R and V-V rate coefficients for $N_2(1) + N_2(0) \rightarrow N_2(0) + N_2(0)$ and $N_2(1) + N_2(0) \rightarrow N_2(0) + N_2(1)$ processes, respectively, as a function of temperature

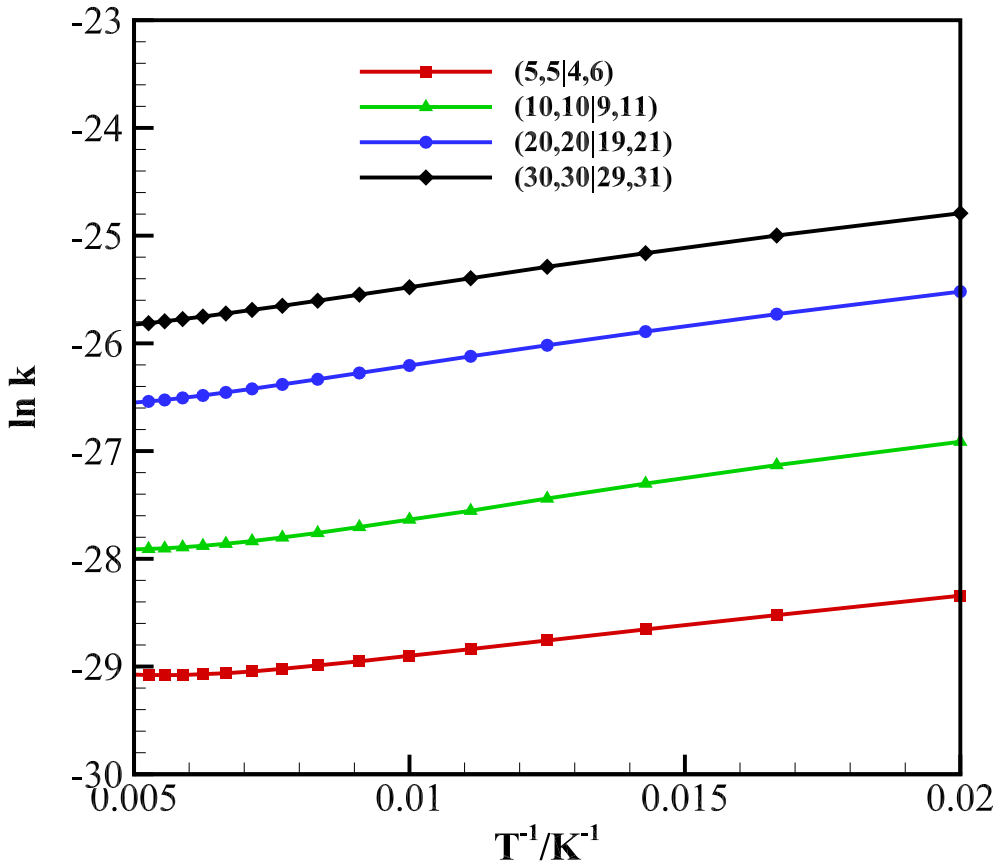

Figure S4: Arrhenius plot ($\ln k$ vs. $1/T$) for $N_2(v) + N_2(v) \rightarrow N_2(v-1) + N_2(v+1)$ processes at low temperature

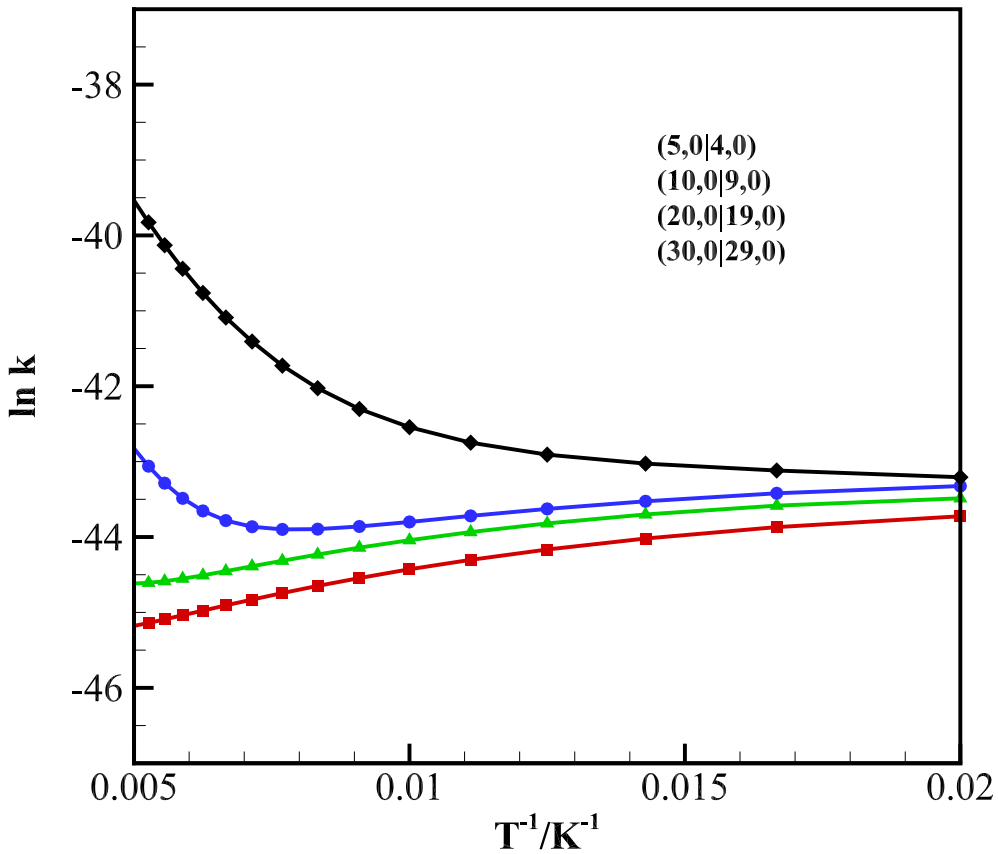

Figure S5: Arrhenius plot ($\ln k$ vs. $1/T$) for $N_2\,(v) + N_2\,(0) \rightarrow N_2\,(v-1) + N_2\,(0)$ processes at low temperature

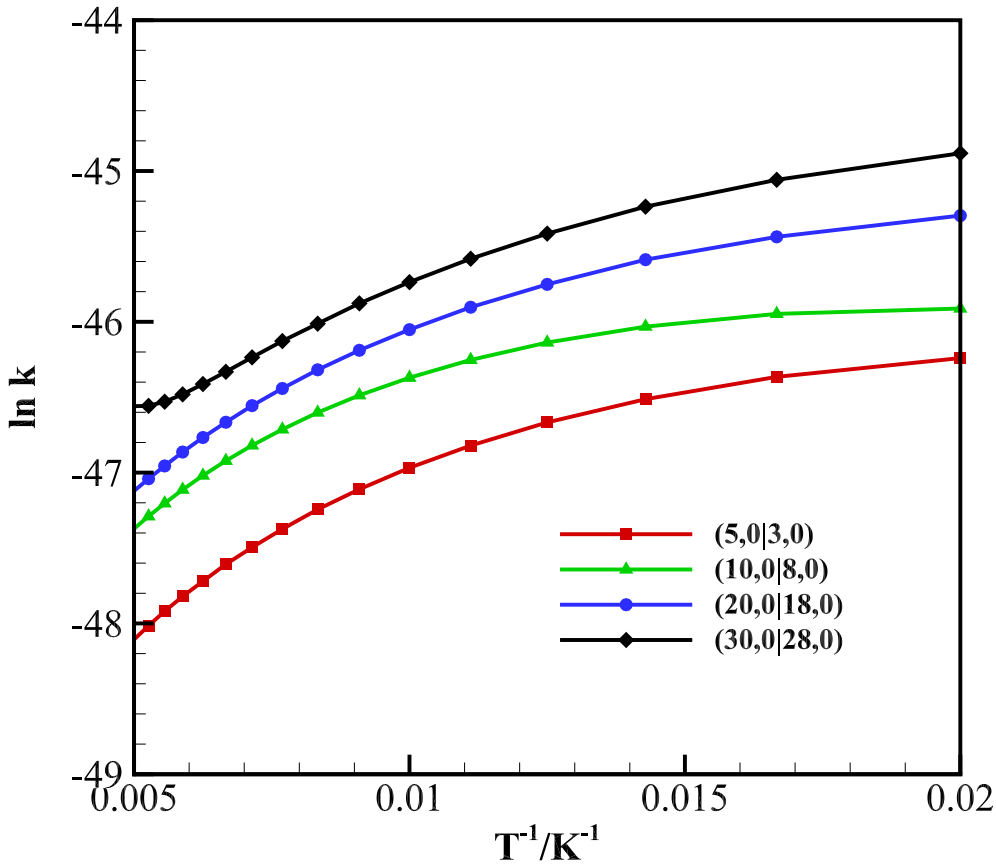

Figure S6: Arrhenius plot ($\ln k$ vs. $1/T$) for $N_2\,(v) + N_2\,(0) \rightarrow N_2\,(v-2) + N_2\,(0)$ processes at low temperature

Table S3: Single quantum V-V rate coefficients for the transition

$$N_2(v) + N_2(v) \rightarrow N_2(v+1) + N_2(v-1) + \Delta E.$$

		$k_{v,v\rightarrow v+1,v-1}$							
v	$\Delta E\left(\mathrm{cm}^{-1}\right)$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
4	28.69	1.81E-13	1.61E-13	2.17E-13	3.83E-13	7.92E-13	1.22E-12	2.14E-12	3.18E-12
5	28.66	2.81E-13	2.64E-13	3.46E-13	6.09E-13	1.21E-12	1.80E-12	3.12E-12	4.58E-12
6	28.61	3.76E-13	3.30E-13	4.40E-13	7.73E-13	1.59E-12	2.46E-12	4.25E-12	6.17E-12
7	28.57	5.06E-13	4.31E-13	5.76E-13	1.01E-12	2.08E-12	3.21E-12	5.51E-12	7.91E-12
8	28.53	6.89E-13	5.55E-13	7.30E-13	1.27E-12	2.61E-12	4.03E-12	6.89E-12	9.77E-12
9	28.48	8.40E-13	6.88E-13	8.99E-13	1.56E-12	3.19E-12	4.91E-12	8.35E-12	1.17E-11
10	28.43	1.03E-12	8.29E-13	1.08E-12	1.89E-12	3.81E-12	5.86E-12	9.89E-12	1.37E-11
12	28.34	1.38E-12	1.12E-12	1.47E-12	2.53E-12	5.15E-12	7.89E-12	1.31E-11	1.79E-11
14	28.25	1.88E-12	1.49E-12	1.92E-12	3.26E-12	6.59E-12	1.01E-11	1.65E-11	2.21E-11
16	28.16	2.59E-12	1.93E-12	2.41E-12	4.03E-12	8.10E-12	1.23E-11	1.99E-11	2.61E-11
18	28.07	3.31E-12	2.38E-12	2.94E-12	4.84E-12	9.66E-12	1.46E-11	2.33E-11	3.37E-11
20	27.98	4.20E-12	2.91E-12	3.53E-12	5.90E-12	1.15E-11	1.76E-11	2.88E-11	3.74E-11
22	27.89	4.80E-12	3.41E-12	4.03E-12	6.74E-12	1.32E-11	2.00E-11	3.19E-11	4.07E-11
24	27.80	5.71E-12	3.94E-12	4.61E-12	7.63E-12	1.48E-11	2.22E-11	3.46E-11	4.34E-11
26	27.71	6.85E-12	4.66E-12	5.28E-12	8.54E-12	1.63E-11	2.42E-11	3.69E-11	4.55E-11
28	27.62	7.74E-12	5.27E-12	5.92E-12	9.43E-12	1.78E-11	2.60E-11	3.87E-11	4.69E-11
30	27.53	9.10E-12	5.92E-12	6.54E-12	1.03E-11	1.92E-11	2.76E-11	3.99E-11	4.75E-11
35	27.30	1.23E-11	7.75E-12	8.26E-12	1.24E-11	2.21E-11	3.04E-11	4.09E-11	4.66E-11
40	27.08	1.66E-11	9.93E-12	1.01E-11	1.44E-11	2.41E-11	3.17E-11	4.11E-11	4.65E-11

Table S4: Symmetric multiquantum V-V rate coefficients for the transition

$$N_2\left(v_1\right) + N_2\left(v_2\right) \rightarrow N_2\left(v_1'\right) + N_2\left(v_2'\right) + \Delta E.$$

				$k_{v_1 v_2 \rightarrow v_1' v_2'}$							
$v_1 v_2$	$\rightarrow$	$v_1' v_2'$	$\Delta E\left(\mathrm{cm}^{-1}\right)$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
4 4	$\rightarrow$	6 2	114.8	7.99E-17	7.46E-17	1.24E-16	3.67E-16	1.24E-15	2.31E-15	6.39E-15	1.96E-14
5 5	$\rightarrow$	7 3	114.6	1.92E-16	1.71E-16	2.81E-16	8.22E-16	2.77E-15	5.16E-15	1.40E-14	3.97E-14
6 6	$\rightarrow$	8 4	114.5	3.96E-16	3.34E-16	5.41E-16	1.58E-15	5.30E-15	9.87E-15	2.62E-14	6.94E-14
7 7	$\rightarrow$	9 5	114.3	6.68E-16	5.69E-16	9.32E-16	2.72E-15	9.13E-15	1.69E-14	4.39E-14	1.09E-13
8 8	$\rightarrow$	10 6	114.1	1.79E-15	1.01E-15	1.53E-15	4.35E-15	1.45E-14	2.69E-14	6.82E-14	1.61E-13
9 9	$\rightarrow$	11 7	113.9	2.26E-15	1.52E-15	2.30E-15	6.55E-15	2.18E-14	4.03E-14	9.97E-14	2.24E-13
10 10	$\rightarrow$	12 8	113.7	3.44E-15	2.18E-15	3.32E-15	9.41E-15	3.12E-14	5.74E-14	1.39E-13	3.00E-13
12 12	$\rightarrow$	14 10	113.4	6.16E-15	3.99E-15	6.17E-15	1.74E-14	5.74E-14	1.05E-13	2.44E-13	4.93E-13
14 14	$\rightarrow$	16 12	113.0	1.07E-14	7.19E-15	1.07E-14	2.90E-14	9.44E-14	1.71E-13	3.85E-13	7.45E-13
16 16	$\rightarrow$	18 14	112.6	2.10E-14	1.18E-14	1.65E-14	4.43E-14	1.43E-13	2.57E-13	5.64E-13	1.05E-12
18 18	$\rightarrow$	20 16	112.3	2.54E-14	1.65E-14	2.41E-14	6.38E-14	2.04E-13	3.64E-13	7.78E-13	1.82E-12
18 18	$\rightarrow$	21 15	252.6	1.21E-16	9.77E-17	2.22E-16	8.75E-16	4.12E-15	1.21E-14	3.48E-14	7.21E-14
20 20	$\rightarrow$	22 18	111.9	4.99E-14	2.36E-14	3.64E-14	9.11E-14	2.81E-13	5.95E-13	1.39E-12	2.32E-12
20 20	$\rightarrow$	23 17	251.8	3.87E-16	1.87E-16	3.75E-16	1.32E-15	6.42E-15	1.81E-14	5.08E-14	1.06E-13
22 22	$\rightarrow$	24 20	111.6	6.39E-14	3.21E-14	4.65E-14	1.22E-13	3.68E-13	7.58E-13	1.73E-12	2.87E-12
22 22	$\rightarrow$	25 19	251.0	3.90E-16	2.44E-16	5.48E-16	2.18E-15	9.44E-15	2.53E-14	6.97E-14	1.49E-13
24 24	$\rightarrow$	26 22	111.2	8.23E-14	4.10E-14	5.96E-14	1.56E-13	4.62E-13	9.30E-13	2.09E-12	3.45E-12
24 24	$\rightarrow$	27 21	250.2	5.77E-16	3.86E-16	8.06E-16	3.17E-15	1.31E-14	3.34E-14	8.51E-14	2.05E-13
26 26	$\rightarrow$	28 24	110.8	1.35E-13	6.31E-14	7.92E-14	1.94E-13	5.64E-13	1.10E-12	2.44E-12	4.06E-12
26 26	$\rightarrow$	29 23	249.4	1.34E-15	7.93E-16	1.22E-15	4.43E-15	1.74E-14	4.20E-14	1.10E-13	2.81E-13
28 28	$\rightarrow$	30 26	110.5	1.73E-13	7.29E-14	9.46E-14	2.40E-13	6.80E-13	1.28E-12	2.79E-12	4.68E-12
28 28	$\rightarrow$	31 25	248.6	1.70E-15	8.52E-16	1.58E-15	6.13E-15	2.23E-14	5.09E-14	1.50E-13	3.87E-13
30 30	$\rightarrow$	32 28	110.1	2.67E-13	9.20E-14	1.15E-13	2.80E-13	7.76E-13	1.44E-12	3.12E-12	5.29E-12
30 30	$\rightarrow$	33 27	247.8	2.19E-15	1.14E-15	2.03E-15	7.72E-15	2.75E-14	6.00E-14	1.91E-13	5.28E-13
35 35	$\rightarrow$	37 33	109.2	3.87E-13	1.41E-13	1.70E-13	3.99E-13	1.03E-12	1.80E-12	3.96E-12	6.96E-12
35 35	$\rightarrow$	38 32	245.7	3.73E-15	2.04E-15	3.74E-15	1.33E-14	4.15E-14	8.69E-14	3.71E-13	1.07E-12
40 40	$\rightarrow$	42 38	108.3	7.25E-13	2.28E-13	2.43E-13	5.18E-13	1.25E-12	2.20E-12	5.11E-12	8.82E-12
40 40	$\rightarrow$	43 37	243.7	1.10E-14	4.24E-15	5.94E-15	1.95E-14	5.64E-14	1.39E-13	7.63E-13	2.09E-12

Table S5: Multiquantum V-V rate coefficients for the transition

$$N_2\,(0) + N_2\,(v) \rightarrow N_2\,(1) + N_2\,(v-2) + \Delta E.$$

		$k_{0,v\rightarrow 1,v-2}$							
v	$\Delta E\,(\mathrm{cm}^{-1})$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
38	284.0	4.63E-16	2.92E-15	6.39E-15	1.57E-14	3.62E-14	6.05E-14	1.47E-13	3.05E-13
39	229.6	2.03E-15	6.46E-15	1.06E-14	2.15E-14	4.31E-14	6.81E-14	1.55E-13	3.08E-13
40	175.3	6.71E-15	1.19E-14	1.63E-14	2.77E-14	5.51E-14	7.70E-14	1.65E-13	3.13E-13
41	121.1	1.60E-14	1.74E-14	2.11E-14	3.31E-14	5.95E-14	8.93E-14	1.77E-13	3.20E-13
42	67.0	3.33E-14	2.21E-14	2.47E-14	3.88E-14	7.03E-14	1.03E-13	1.90E-13	3.24E-13
43	13.0	3.43E-14	2.36E-14	2.62E-14	4.12E-14	7.59E-14	1.12E-13	1.96E-13	3.22E-13
44	-40.9	2.31E-14	2.14E-14	2.58E-14	4.37E-14	7.87E-14	1.08E-13	1.70E-13	2.86E-13
45	-94.8	8.54E-15	1.64E-14	2.28E-14	4.20E-14	7.99E-14	1.11E-13	1.73E-13	2.82E-13
46	-148.5	1.90E-15	1.06E-14	1.83E-14	3.78E-14	7.46E-14	1.05E-13	1.67E-13	2.72E-13
47	-202.2	3.59E-16	6.22E-15	1.36E-14	3.31E-14	6.84E-14	9.80E-14	1.56E-13	2.57E-13
48	-255.7	6.03E-17	2.90E-15	8.72E-15	2.73E-14	6.23E-14	9.02E-14	1.47E-13	2.44E-13

Table S6: Single quantum V-T/R rate coefficients for the transition

$$N_2(v) + N_2(0) \rightarrow N_2(v-1) + N_2(0) + \Delta E.$$

		$k_{v,0\rightarrow v-1,0}$							
v	$\Delta E\left(\mathrm{cm}^{-1}\right)$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
1	2330.7	1.57E-20	5.48E-21	2.41E-20	3.97E-18	5.19E-16	6.69E-15	1.09E-13	5.55E-13
2	2301.9	2.30E-20	9.76E-21	6.04E-20	1.02E-17	1.22E-15	1.53E-14	2.41E-13	1.18E-12
3	2273.1	3.82E-20	1.39E-20	1.11E-19	1.87E-17	2.14E-15	2.62E-14	3.97E-13	1.87E-12
4	2244.3	4.38E-20	1.91E-20	1.84E-19	3.04E-17	3.34E-15	4.01E-14	5.86E-13	2.66E-12
5	2215.6	4.84E-20	2.54E-20	2.94E-19	4.94E-17	4.87E-15	5.73E-14	8.06E-13	3.54E-12
6	2186.9	5.77E-20	3.24E-20	4.42E-19	6.84E-17	6.89E-15	7.86E-14	1.06E-12	4.51E-12
7	2158.3	6.35E-20	4.13E-20	6.82E-16	1.20E-16	9.43E-15	1.05E-13	1.36E-12	5.58E-12
8	2129.8	7.36E-20	5.28E-20	9.51E-19	1.37E-16	1.26E-14	1.37E-13	1.71E-12	6.77E-12
9	2101.2	7.96E-20	6.88E-20	1.37E-18	1.89E-16	1.67E-14	1.76E-13	2.21E-12	8.09E-12
10	2072.8	7.46E-20	8.73E-20	1.97E-18	2.57E-16	2.18E-14	2.23E-13	2.58E-12	9.57E-12
12	2015.9	8.64E-20	1.65E-19	4.04E-18	4.83E-16	3.72E-14	3.60E-13	3.81E-12	1.32E-11
15	1931.1	9.32E-20	4.17E-19	1.06E-17	1.08E-15	7.27E-14	6.45E-13	6.07E-12	1.92E-11
16	1902.8	8.01E-20	6.13E-19	1.55E-17	1.50E-15	9.60E-14	8.21E-13	7.25E-12	2.17E-11
20	1790.5	9.50E-20	2.46E-18	5.71E-17	4.41E-15	2.33E-13	1.74E-12	1.28E-11	3.39E-11
25	1651.0	1.26E-19	1.40E-17	2.83E-16	1.62E-14	6.55E-13	4.07E-12	2.36E-11	5.47E-11
30	1512.7	3.34E-19	6.92E-17	1.21E-15	5.23E-14	1.57E-12	8.06E-12	3.78E-11	7.81E-11
32	1457.7	6.99E-19	1.51E-16	2.52E-15	9.52E-14	2.47E-12	1.14E-11	4.75E-11	9.25E-11
35	1375.5	2.03E-18	3.72E-16	5.69E-15	1.82E-13	3.88E-12	1.59E-11	5.87E-11	1.09E-10
40	1239.5	1.68E-17	2.00E-15	2.61E-14	6.20E-13	9.00E-12	2.91E-11	8.36E-11	1.35E-10

Table S7: Multiquantum V-T/R rate coefficients for the transition

$$N_2(v) + N_2(0) \rightarrow N_2(v-2) + N_2(0) + \Delta E.$$

		$k_{v,0\rightarrow v',0}$							
v	$\Delta E\left(\mathrm{cm}^{-1}\right)$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
2	4632.6	1.12E-21	1.70E-22	7.29E-23	3.37E-22	4.26E-19	1.78E-17	1.19E-15	1.31E-14
3	4574.9	2.49E-21	3.89E-22	1.70E-22	1.19E-21	1.27E-18	4.89E-17	2.91E-15	3.00E-14
4	4517.4	2.87E-21	4.42E-22	1.91E-22	3.44E-21	4.08E-18	1.57E-16	8.94E-15	8.81E-14
5	4459.9	4.13E-21	6.54E-22	2.82E-22	7.65E-21	8.55E-18	3.14E-16	1.64E-14	1.53E-13
6	4402.6	5.13E-21	8.11E-22	3.45E-22	1.55E-20	1.61E-17	5.63E-16	2.70E-14	2.38E-13
7	4345.3	5.64E-21	9.29E-22	4.12E-22	2.92E-20	2.82E-17	9.40E-16	4.13E-14	3.44E-13
8	4288.1	6.20E-21	1.10E-21	5.12E-22	5.25E-20	4.70E-17	1.49E-15	5.99E-14	4.74E-13
9	4231.0	6.94E-21	1.27E-21	6.09E-22	9.10E-20	7.54E-17	2.27E-15	8.39E-14	6.29E-13
10	4174.0	7.27E-21	1.37E-21	7.04E-22	1.54E-19	1.18E-16	3.37E-15	1.14E-13	8.14E-13
12	4062.3	6.41E-21	1.38E-21	9.62E-22	4.38E-19	2.77E-16	7.07E-15	2.03E-13	1.30E-12
15	3890.3	1.60E-20	2.30E-21	2.45E-21	1.62E-18	8.18E-16	1.81E-14	4.20E-13	2.33E-12
16	3833.9	1.10E-20	1.69E-21	3.51E-21	2.83E-18	1.42E-15	3.19E-14	6.80E-13	3.34E-12
20	3608.9	1.00E-20	1.96E-21	2.12E-20	1.57E-17	5.63E-15	1.01E-13	1.62E-12	6.47E-12
25	3329.8	1.09E-20	4.38E-21	2.24E-19	1.18E-16	2.70E-14	3.58E-13	4.05E-12	1.30E-11
30	3052.9	1.37E-20	2.69E-20	1.92E-18	6.75E-16	1.00E-13	1.01E-12	8.27E-12	2.33E-11
32	2942.9	1.23E-20	8.94E-20	5.83E-18	1.66E-15	1.94E-13	1.67E-12	1.17E-11	2.89E-11
35	2778.4	1.10E-20	3.66E-19	1.95E-17	4.17E-15	3.66E-13	2.72E-12	1.64E-11	3.73E-11
40	2506.0	1.19E-20	5.38E-18	2.03E-16	2.45E-14	1.15E-12	6.30E-12	2.87E-11	5.56E-11

Table S8: Multiquantum V-T/R rate coefficients for the transition

$N_2(v) + N_2(0) \rightarrow N_2(v') + N_2(0) + \Delta E$.

			$k_{v,0\rightarrow v',0}$							
v	v'	$\Delta E\left(\mathrm{cm}^{-1}\right)$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
4	1	6819.3	5.01E-22	1.84E-22	7.78E-23	1.43E-23	7.10E-21	7.27E-19	1.33E-16	2.23E-15
5	2	6733.0	9.21E-22	1.92E-22	8.01E-23	2.83E-23	2.05E-20	1.86E-18	3.00E-16	4.62E-15
6	3	6646.9	1.41E-21	3.09E-22	1.30E-22	4.93E-23	4.95E-20	4.01E-18	5.70E-16	8.15E-15
7	4	6560.9	1.92E-21	4.34E-22	1.84E-22	7.77E-23	1.07E-19	7.80E-18	9.80E-16	1.31E-14
8	5	6475.1	2.30E-21	5.64E-22	2.42E-22	1.20E-22	2.15E-19	1.42E-17	1.58E-15	2.00E-14
9	6	6389.4	2.34E-21	6.18E-22	2.68E-22	1.78E-22	4.07E-19	2.45E-17	2.42E-15	2.92E-14
10	7	6303.8	2.15E-21	6.37E-22	2.89E-22	2.85E-22	7.40E-19	4.06E-17	3.58E-15	4.13E-14
12	9	6133.1	1.80E-21	6.30E-22	2.93E-22	8.71E-22	2.30E-18	1.05E-16	7.34E-15	7.78E-14
15	12	5877.9	1.27E-20	1.61E-21	6.03E-22	4.67E-21	9.57E-18	3.59E-16	1.83E-14	1.70E-13
16	13	5793.2	6.71E-21	9.09E-22	3.60E-22	1.44E-20	4.06E-17	1.67E-15	8.08E-14	6.53E-13
20	17	5455.5	6.50E-21	9.53E-22	4.28E-22	1.46E-19	2.44E-16	7.74E-15	2.41E-13	1.52E-12
25	22	5036.5	5.38E-21	1.03E-21	1.45E-20	2.19E-18	1.78E-15	4.03E-14	8.18E-13	3.82E-12
30	27	4620.8	1.23E-20	1.72E-21	1.57E-20	2.21E-17	9.54E-15	1.57E-13	2.21E-12	8.03E-12
30	26	6216.4	4.52E-21	1.42E-21	8.79E-22	4.97E-19	5.04E-16	1.20E-14	2.91E-13	1.57E-12
32	29	4455.5	1.56E-20	2.35E-21	6.22E-20	7.08E-17	2.14E-14	2.90E-13	3.34E-12	1.09E-11
32	28	5995.8	1.57E-20	1.97E-21	1.88E-21	2.06E-18	1.24E-15	2.42E-14	4.92E-13	2.39E-12
35	32	4208.6	8.74E-21	2.98E-21	2.65E-19	2.29E-16	5.08E-14	5.82E-13	5.43E-12	1.55E-11
35	31	5666.3	2.61E-20	3.27E-21	6.91E-21	8.65E-18	3.39E-15	5.59E-14	9.14E-13	3.85E-12
40	37	3799.8	1.39E-20	4.30E-20	4.54E-18	1.97E-15	2.29E-13	1.87E-12	1.22E-11	2.85E-11
40	36	5120.7	1.29E-20	2.83E-21	1.43E-19	1.21E-16	2.13E-14	2.43E-13	2.60E-12	8.50E-12

Table S9: V-T/R rate coefficients for the transition

$N_2\,(v) + N_2\,(v) \rightarrow N_2\,(v_1') + N_2\,(v_2') + \Delta E.$

				$k_{v_1 v_2 \rightarrow v_1' v_2'}$							
$v_1 v_2$	$\rightarrow$	$v_1' v_2'$	$\Delta E\,(\mathrm{cm}^{-1})$	100K	300K	500K	1000K	2000K	3000K	5000K	7000K
5 5	$\rightarrow$	5 4	2215.6	6.73E-20	3.83E-20	8.75E-19	1.20E-16	1.15E-14	1.24E-13	1.75E-12	7.34E-12
5 5	$\rightarrow$	4 4	4431.2	1.20E-20	1.69E-21	6.55E-22	3.87E-20	3.79E-17	1.41E-15	6.56E-14	4.51E-13
5 5	$\rightarrow$	5 3	4459.9	6.97E-21	1.02E-21	4.20E-22	1.80E-20	1.97E-17	7.15E-16	3.41E-14	2.30E-13
5 5	$\rightarrow$	3 3	8919.9	1.83E-23	1.33E-23	6.64E-24	2.57E-24	8.32E-21	1.66E-18	3.65E-16	6.34E-15
10 10	$\rightarrow$	10 9	2072.8	6.31E-20	1.18E-19	3.86E-18	5.35E-16	4.68E-14	4.51E-13	4.69E-12	1.55E-11
10 10	$\rightarrow$	9 9	4145.5	8.73E-21	1.68E-21	1.03E-21	7.05E-19	4.61E-16	1.15E-14	2.66E-13	1.33E-12
10 10	$\rightarrow$	10 8	4174.0	1.03E-20	2.01E-21	1.05E-21	3.69E-19	2.43E-16	6.31E-15	1.58E-13	8.85E-13
10 10	$\rightarrow$	8 8	8348.0	3.83E-23	6.08E-23	3.61E-23	4.61E-23	4.49E-19	3.54E-17	4.11E-15	4.48E-14
20 20	$\rightarrow$	20 19	1790.5	9.44E-20	3.11E-18	1.03E-17	9.57E-15	3.96E-13	2.51E-12	1.61E-11	3.90E-11
20 20	$\rightarrow$	19 19	3580.9	5.81E-21	1.59E-21	1.01E-19	5.39E-17	1.13E-14	1.41E-13	1.69E-12	5.64E-12
20 20	$\rightarrow$	20 18	3608.9	6.65E-21	1.74E-21	5.29E-20	3.15E-17	7.83E-15	1.07E-13	1.34E-12	4.77E-12
20 20	$\rightarrow$	18 18	7217.9	2.74E-21	4.18E-22	1.72E-22	5.91E-20	1.13E-16	4.33E-15	1.43E-13	7.50E-13
30 30	$\rightarrow$	30 29	1512.7	8.63E-19	1.74E-16	2.57E-15	1.07E-13	2.73E-12	1.17E-11	4.49E-11	8.22E-11
30 30	$\rightarrow$	29 29	3025.4	3.39E-21	1.12E-19	8.74E-18	2.28E-15	1.99E-13	1.40E-12	7.95E-12	1.73E-11
30 30	$\rightarrow$	30 28	3052.9	6.29E-21	5.48E-20	4.92E-18	1.46E-15	1.39E-13	1.06E-12	6.72E-12	1.56E-11
30 30	$\rightarrow$	28 28	6105.9	1.34E-21	5.17E-22	1.06E-20	2.14E-17	8.95E-15	1.15E-13	1.11E-12	3.19E-12
40 40	$\rightarrow$	40 39	1239.5	9.88E-17	4.80E-15	5.56E-14	1.21E-12	1.32E-11	2.63E-11	8.59E-11	1.12E-10
40 40	$\rightarrow$	39 39	2478.9	1.65E-18	3.09E-17	1.03E-15	7.87E-14	1.75E-12	6.25E-12	1.93E-11	3.12E-11
40 40	$\rightarrow$	40 38	2506.0	7.61E-19	1.40E-17	5.31E-16	4.54E-14	1.18E-12	4.80E-12	1.68E-11	2.96E-11
40 40	$\rightarrow$	38 38	5012.1	1.39E-20	6.74E-20	1.15E-17	4.53E-15	2.05E-13	9.63E-13	4.37E-12	8.90E-12

Listing 1: Subroutine of the modified PES for N_2+N_2 interaction.

```
      SUBROUTINE SUPN2N2(R,RRA,RRB,THETARADA,THETARADB,PHIRAD,POTTOT)
      IMPLICIT REAL*8 (A-H,O-Z)

c N2-N2 intermolecular PES
c
c R = intermolecular distance in angstrom (with respect to diatoms' centers of mass)
c rra = internuclear distance of monomer A in angstrom (equilibrium value =1.098 angstrom)
c rrb = internuclear distance of monomer B in angstrom (equilibrium value =1.098 angstrom)
c thetarada,thetaradb,phirad = diatom-diatom Jacobi angular coordinates ( in radiants)
c pottot = interaction energy in meV
c

      COMMON/PARAM/epsH,epsT,epsL,rmH,rmT,rmL,alfamedioA,alfamedioB,
     #deltalfaA,deltalfaB,c6medio

      real*8 nlj,mlj


      QA=-1.1d0+1.0165d0*(rra-1.098d0)/0.529177d0+0.1068d0
     #*((rra-1.098d0)/0.529177d0)**2+0.0463d0
     #*((rra-1.098d0)/0.529177d0)**3-0.2925d0
```

```
     #*((rra -1.098d0)/0.529177d0)**4

       QB=-1.1d0+1.0165d0*(rrb -1.098d0)/0.529177d0+0.1068d0
     #*((rrb -1.098d0)/0.529177d0)**2+0.0463d0
     #*((rrb -1.098d0)/0.529177d0)**3-0.2925d0
     #*((rrb -1.098d0)/0.529177d0)**4


       CALL EPSIRM(rra,rrb)

         epsX=epsH
         rmX=rmH


c-------------
         eps000=(2.d0*epsH+2.d0*epsX+4.d0*epsT+epsL)/9.d0

         eps202=(-epsH-epsX+epsT+epsL)*2.d0/(dsqrt(5.d0)*9.d0)

         eps220=(4.d0*epsH-2.d0*epsX-4.d0*epsT+2.d0*epsL)
     #/(dsqrt(5.d0)*9.d0)

         eps222=(epsH-2.d0*epsX+2.d0*epsT-epsL)*dsqrt(14.d0)/45.d0
c-------------

         rm000=(2.d0*rmH+2.d0*rmX+4.d0*rmT+rmL)/9.d0

         rm202=(-rmH-rmX+rmT+rmL)*2.d0/(dsqrt(5.d0)*9.d0)

         rm220=(4.d0*rmH-2.d0*rmX-4.d0*rmT+2.d0*rmL)
```

```
      #/(dsqrt(5.d0)*9.d0)

          rm222=(rmH-2.d0*rmX+2.d0*rmT-rmL)*dsqrt(14.d0)/45.d0



c========harmonic functions=========================

            ANG101=dsqrt(3.0d0)*p1(thetarada)

            ANG202=dsqrt(5.0d0)*p2(thetarada)

            ANG022=dsqrt(5.0d0)*p2(thetaradb)

            ANG123=-3.d0*(dsin(thetarada)*p1(thetaradb)*dsin(thetaradb)*
      #p1(phirad)-p1(thetarada)*p2(thetaradb))

            ANG220=dsqrt(5.0d0)*(3.d0/8.d0*(dsin(thetarada)**2)
      #*(dsin(thetaradb)**2)*2.d0*p1(2*phirad)+3.d0/2.d0*p1(thetarada)
      #*dsin(thetarada)*p1(thetaradb)*dsin(thetaradb)*2.d0*p1(phirad)
      #+p2(thetarada)*p2(thetaradb))

            ANG222=dsqrt(5.0d0**3)*3.d0/dsqrt(630.d0)*
      #(6.d0/8.d0*(dsin(thetarada)**2)
      #*(dsin(thetaradb)**2)*2.d0*p1(2*phirad)-3.d0/2.d0*p1(thetarada)
      #*dsin(thetarada)*p1(thetaradb)*dsin(thetaradb)*2.d0*p1(phirad)
      #-2*p2(thetarada)*p2(thetaradb))

            ANG224=15.d0/dsqrt(630.d0)*
```

```
      #(3.d0/8.d0*(dsin(thetarada)**2)
      #*(dsin(thetaradb)**2)*2.d0*p1(2*phirad)-6.d0*p1(thetarada)
      #*dsin(thetarada)*p1(thetaradb)*dsin(thetaradb)*2.d0*p1(phirad)
      #+6.d0*p2(thetarada)*p2(thetaradb))

            ANG303=dsqrt(7.0d0)*p3(thetarada)

c==========expression of the potential energy surface=======



              epsang=
      # eps000
      #+eps202*ANG202
      #+eps202*ANG022
      #+eps220*ANG220
      #+eps222*ANG222

              rmang=
      # rm000
      #+rm202*ANG202
      #+rm202*ANG022
      #+rm220*ANG220
      #+rm222*ANG222

              nlj=6


                mlj=10.0+4.0*(r/rmang)**2

```

```
      pes=epsang*(nlj/(mlj-nlj))*(rmang/r)**mlj-(mlj/(mlj-nlj))*
     * epsang*(rmang/r)**nlj


       VQUAD=QA*QB*dsqrt(14.d0/5.d0)*27212.d0*0.529177d0**5/R**5.d0

        pottot=pes+VQUAD*ANG224

      RETURN
      END



      SUBROUTINE EPSIRM(rra,rrb)

      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON/PARAM/epsiH,epsiT,epsiL,rmH,rmT,rmL,alfamedioA,alfamedioB,
     #deltalfaA,deltalfaB,c6medio


            c13=1.d0/3.d0


                  ELMOLA=7.6d0
                  ELMOLB=7.6d0

```

```
                    call   POLAR(rrA,aparA,aperA,amediaA,deltaA)

                    alfaperpA=aperA
                    alfaparA=aparA

                    alfamedioA=amediaA
                    deltalfaA=deltaA

                    call   POLAR(rrB,aparB,aperB,amediaB,deltaB)

                    alfaperpB=aperB
                    alfaparB=aparB

                    alfamedioB=amediaB
                    deltalfaB=deltaB


          pippoA=((rrA-0.74d0)/rrA)

          if(pippoA.lt.0.d0)then

          pippoA=-pippoA

          alfapareffA=alfaparA*(1.d0-deltalfaA/(deltalfaA+alfamedioA)*
     #pippoA**c13)

          alfaperpeffA=alfaperpA*(1.d0+0.5d0*deltalfaA/
     #(deltalfaA+alfamedioA)*pippoA**c13)

```

```
        else

        alfapareffA=alfaparA*(1.d0+deltalfaA/(deltalfaA+alfamedioA)*
    #pippoA**c13)

        alfaperpeffA=alfaperpA*(1.d0-0.5d0*deltalfaA/
    #(deltalfaA+alfamedioA)*pippoA**c13)

        endif

        pippoB=((rrB-0.74d0)/rrB)

        if(pippoB.lt.0.d0)then

        pippoB=-pippoB

        alfapareffB=alfaparB*(1.d0-deltalfaB/(deltalfaB+alfamedioB)*
    #pippoB**c13)

        alfaperpeffB=alfaperpB*(1.d0+0.5d0*deltalfaB/
    #(deltalfaB+alfamedioB)*pippoB**c13)

        else

        alfapareffB=alfaparB*(1.d0+deltalfaB/(deltalfaB+alfamedioB)*
    #pippoB**c13)

        alfaperpeffB=alfaperpB*(1.d0-0.5d0*deltalfaB/
    #(deltalfaB+alfamedioB)*pippoB**c13)

```

```
            endif
c Rm  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
c H c------------------------------------------------------------------
            rmH=(alfaperpeffA**(1.d0/3.d0)+alfaperpeffB**(1.d0/3.d0))/
       #((alfaperpA*alfaperpB)**0.095d0)

            rmH=rmH*1.767d0
c fit
           rmH=rmH*1.044d0
c------------------------------------------------------------------
c Ta c
            rmT=(alfaperpeffA**(1.d0/3.d0)+alfapareffB**(1.d0/3.d0))/
       #((alfaperpA*alfaparB)**0.095d0)

            rmT=rmT*1.767d0
c fit
           rmT=rmT*1.034d0
```

```
c-----------------------------------------------------------------
c L c
            rmL=(alfapareffA**(1.d0/3.d0)+alfapareffB**(1.d0/3.d0))/
        #((alfaparA*alfaparB)**0.095d0)


            rmL=rmL*1.767d0

c fit

           rmL=rmL*1.051d0


c=================================================================
c fit

           rmL=rmL*1.06d0

c=================================================================

c-----------------------------------------------------------------

c C6 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

           c6medio=(alfamedioA*alfamedioB)/
        #(dsqrt(alfamedioA/ELMOLA)+dsqrt(alfamedioB/ELMOLB))

           c6medio=c6medio*15700.d0

```

```
c fit

          c6medio=c6medio*1.1d0


        a2A= deltalfaA/(3.d0*alfamedioA)

        a2B= deltalfaB/(3.d0*alfamedioB)


c H c-------------------------------------------------------------

        c6H=c6medio*(1.d0-a2A/2.d0-a2B/2.d0)

c Ta c------------------------------------------------------------

        c6T=c6medio*(1.d0-a2A/2.d0+a2B)

c L  c------------------------------------------------------------

        c6L=c6medio*(1.d0+a2A+a2B)

c epsi ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


c H c-----------------------------------------------------------

           epsiH=0.72d0*c6H/rmH**6.d0

c Ta c----------------------------------------------------------
```

```
            epsiT=0.72d0*c6T/rmT**6.d0

c L   c-------------------------------------------------------------
            epsiL=0.72d0*c6L/rmL**6.d0



c=================================================================
c fit

            epsiL=epsiL*1.25d0

c=================================================================


             return
             end


c=========================


          REAL*8 FUNCTION P1(x)
          IMPLICIT REAL*8(A-H,O-Z)
             p1 = dcos(x)
          RETURN
          END

          REAL*8 FUNCTION P2(x)
          IMPLICIT REAL*8(A-H,O-Z)
```

```
            p2 = 0.5d0*(3.0d0*dcos(x)*dcos(x) - 1.0d0)
        RETURN
        END

        REAL*8 FUNCTION P3(x)
        IMPLICIT REAL*8(A-H,O-Z)
            p3 = 0.5d0*(5.d0*(dcos(x))**3-3.d0*dcos(x))
        RETURN
        END



      SUBROUTINE POLAR(rr,apar,aper,amedia,delta)
c-------------------------------
c  N2 polarizabilities
c-------------------------------

      implicit real*8(a-l,o-z)
      dimension abond(70,10)

c-----------------------------------------

      bo=3.0d0
      bl=1.098d0
      alf1=1.100d0
      alf2=1.100d0
      evt1=5.00d0
      evt2=5.00d0
      enb1=2.00d0
      enb2=2.00d0
```

```
c-----------------------------------------
C CONSTANTS
        c13=0.333333333d0
        c12=0.500000000d0
        c16=1.0d0/6.0d0
        c14=1.0d0/4.0d0
        c23=2.0d0/3.0d0
        c32=1.d0/c23
C PARAMETERS
        a1=alf1/evt1
        a2=alf2/evt2
        at=a1+a2
        alfa=alf1**c13+alf2**c13
        a13=a1**c13
        a23=a2**c13
c-----------------------------------------
c
            fc=rr/alfa
c
            fs=rr/bl
c
           fn=rr/(a13+a23)
c
           esp1=2.000d0*fc -1.000d0


           fe1=dexp(-1.000d0*(fs -1.d0)*2.d0*fc)


```

```
      esp2=0.7500d0*(fs -1.00d0)*(1.00d0-fc)*(fs**c12)*alfa**c12
      fe2=dexp(esp2)
      esp3=2.00d0*(1.00d0-fs)/bo
      fe3=dexp(esp3)


      esp4=esp1


      fe4=dexp(-0.75d0*esp4*(fs**c12)*alfa**c12)



      cex=(fs -1.0d0)*fe2/3.0d0
      camp=1.0d0+cex


      b2=4.d0*(fc**2)+1.00d0
      b2=(fs+2.00d0)/b2
      b1=((bo-2.d0)**2)-1.d0/8.d0
      b1=1.0d0*(bo**b1)/4.0d0


      bof=bo-b1*b2*fe1

c-----------------------------------------------

      alfnb=a1*enb1+a2*enb2
      alfv=at*bof
      amedia=(alfv+alfnb)*camp
```

```
c-----------------------------------------
c-----------------------------------------
          pre1=c32*alfa**c12*fn**2.d0
          pre21=fe3*(enb1+enb2)/2.0d0+(enb1*enb2)**c12
          pre21=(pre21/(evt1+evt2))
          pre24=bo**((bo-4.d0)/(bo+1.0d0))
          pre2=(1.0d0+pre24*pre21)**(3.d0)
          pre4=2.0d0*fc/(bo**c13)-dabs(alf1-alf2)/(alf1+alf2)
          delta=fe4*amedia*pre1*pre4/pre2
c-----------------------------------------
c-----------------------------------------
          apar=amedia+c23*delta
          aper=amedia-c13*delta
c-----------------------------------------
 1      continue
        return
        end
```

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