Supplementary Information

Dissociation cross sections and rates in O_2 + N collisions: molecular dynamics simulations combined with machine learning

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Table S1. Re-optimized parameters of the short-range term V_{SR} (r) for the O_2 potential.[1,2]

Parameter	Value
α, Å^{-2}	9.439 784 362 354 936 × 10^{-1}
β	1.262 242 998 506 810
a_0, millihartree	-1.488 979 427 684 798 × 10^3
a_1, millihartree	1.881 435 846 488 955 × 10^4
a_2, millihartree	-1.053 475 425 838 226 × 10^5
a_3, millihartree	2.755 135 591 229 064 ×10^5
a_4, millihartree	-4.277 588 997 761 775 ×10^5
a_5, millihartree	4.404 104 009 614 092 ×10^5
a_6, millihartree	-2.946 204 062 950 765 ×10^5
a_7, millihartree	1.176 861 219 078 620 ×10^5

Table S2. Rovibrational energies (in eV) for the ground electronic state O_2, including 4572 bond states and 1540 quasi-bond states based on the WKB method.

v	$j_{max}(v)$	Energy range
0	248	0.098-8.703
1	242	0.292-8.477
2	237	0.483-8.303
3	233	0.671-8.177
4	228	0.855-8.013
5	224	1.037-7.895
6	216	1.215-7.617
7	215	1.391-7.631
8	210	1.564-7.488
9	206	1.733-7.386
10	202	1.9-7.288
11	197	2.064-7.159
12	193	2.226-7.069
13	188	2.384-6.949
14	184	2.54-6.866
15	179	2.693-6.756
16	175	2.843-6.681

17	170	2.99-6.579
18	165	3.134-6.483
19	160	3.276-6.392
20	155	3.414-6.305
21	150	3.55-6.224
22	145	3.682-6.146
23	140	3.811-6.074
24	134	3.936-5.984
25	129	4.058-5.921
26	123	4.177-5.843
27	117	4.291-5.772
28	111	4.401-5.706
29	105	4.507-5.646
30	98	4.608-5.577
31	91	4.704-5.516
32	84	4.795-5.463
33	76	4.879-5.406
34	68	4.956-5.358
35	59	5.026-5.31
36	49	5.086-5.267
37	40	5.135-5.239
38	36	5.169-5.232
39	30	5.187-5.224
40	25	5.197-5.219
41	19	5.205-5.215
42	13	5.209-5.213

Table S3. Progressive Nikitin factor in the dissociative reaction O_2 (v) + N→O + O + N [3]

vibrational levels	Nikitin factor
$v \leq 6$	1
$7 \leq v \leq 10$	5/3
$11 \leq v \leq 26$	2
$27 \leq v \leq 28$	7/3
$v = 29$	13/3
$30 \leq v$	16/3

References

1   Z. Varga, Y. Liu, J. Li, Y. Paukku, H. Guo and D. G. Truhlar, *J. Chem. Phys.*, 2021, **154**, 084304.

2   Y. Paukku, K. R. Yang, Z. Varga, G. Song, J. D. Bender and D. G. Truhlar, *J. Chem. Phys.*, 2017, **147**, 034301.

3   F. Esposito and I. Armenise, *J. Phys. Chem. A*, 2021, **125**, 3953–3964.