Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Information

The supplemental information contains additional figures and tables documenting the experimental and modeling results presented in the main document. Specifically included are:

Figure S1: Interfragment distance dependence of the energetics of all of the entrance and exit channels for the Xe^{2+} + O_2 collision system for a perpendicular approach.

Figure S2: Cartoon schematic of a 2-exit, entrance channel multi-channel Landau-Zener model (MCLZ). The example equations for calculating the populations after each crossing are employed in every crossing shown in Figure S1.

Figure S3: Multi-channel LZ model results for the parameter set best found to reproduce the O_2^+ (*A*) and (*b*) vibrational populations and fall-within a factor of 2 of the experimental values at low collision energies.

Figure S4: Example schematic for MCLZ model including selected calculations for the best fit parameters as described in the main report.

Table S1: Reactant channels and their asymptotic energies used for the LZ modeling.

Table S2: Product channels and their asymptotic energies used for the LZ modeling.

Tables S3-S6: Franck-Condon factors used in the MCLZ

Table S7: Best fit experimental vibrational populations for the O_2^+ (*b*) state derived from fitting of the O_2^+ (*b-a*) emissions.

Table S8: O_2^+ (*b*) populations expected from charge-transfer as determined from the MCLZ model

Table S9: Experimental and simulated results for the O_2^+ (*A*) state.

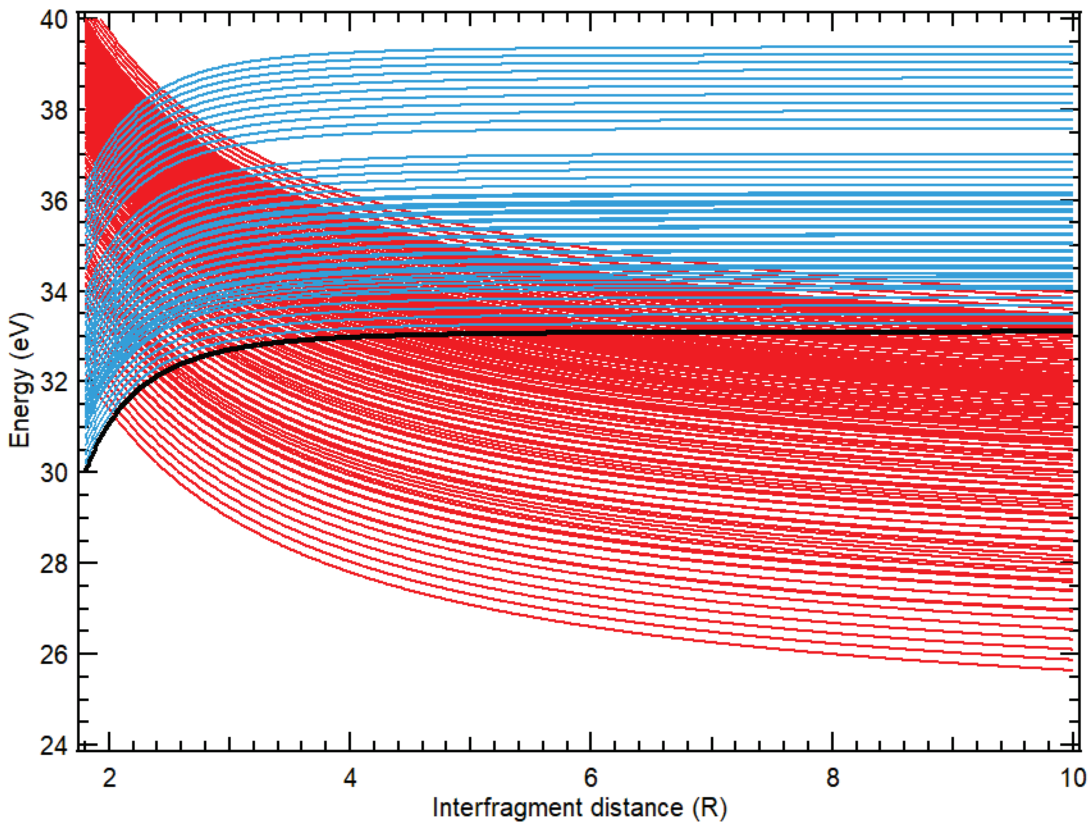


Figure S1: Example entrance (blue) and exit (red) channels for an O_2 polarizability of 7.57 au. Ground state entrance channel is shown in black.

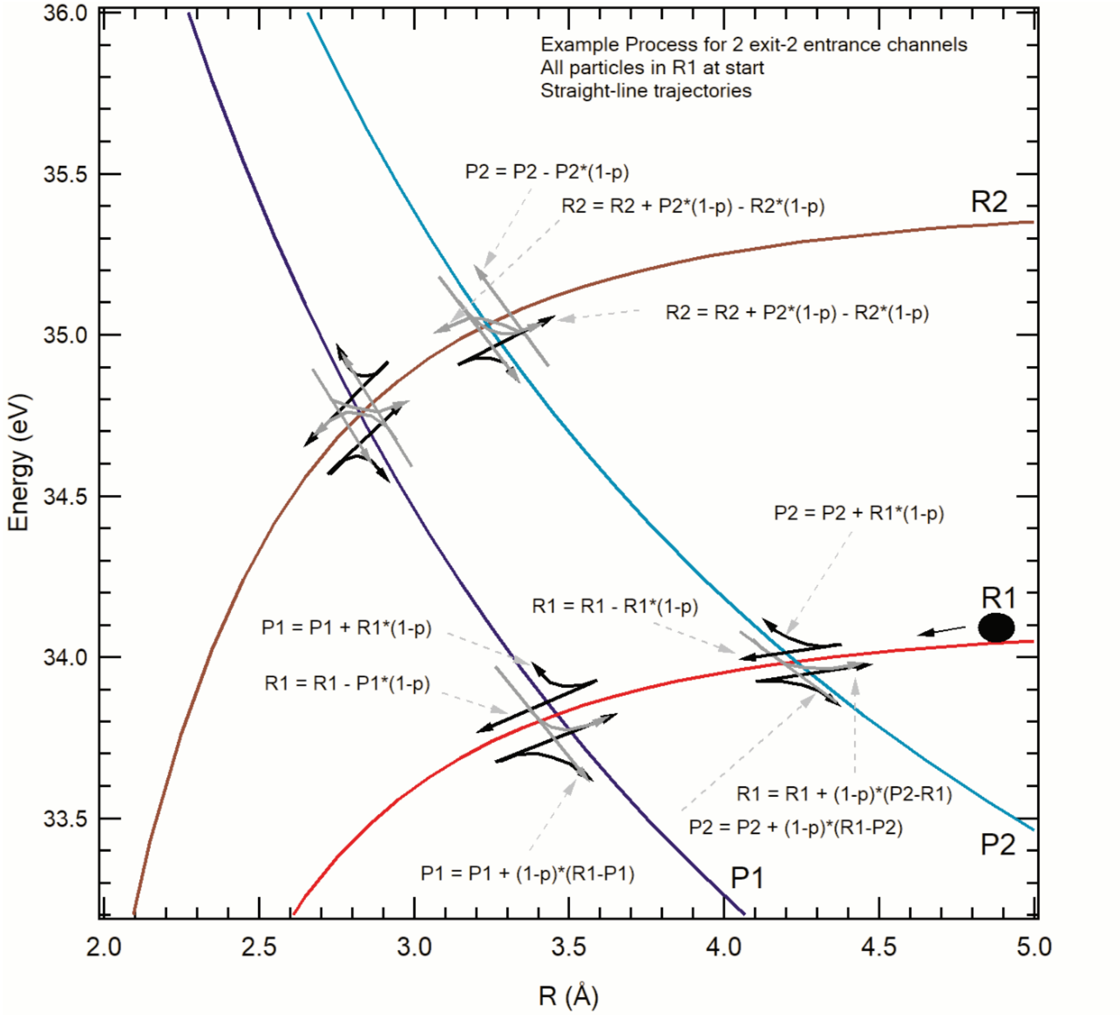


Figure S2: Cartoon depiction of a multi-channel LZ model for calculating resulting populations in two entrance, R1 and R2, and two exit, P1 and P2, channels. Only selected hops have their respective equations shown.

Table S1: Reactant Channels and Asymptotic Energies Used in Multi-Channel Landau-Zener Model

Reactant Channel	Asymptotic Energy (eV)	Reactant Channel	Asymptotic Energy (eV)
Xe^{2+} ($^3P_2$) + O_2 (X, v = 0)	33.1048	Xe^{2+} (^1D) + O_2 (X, v = 9)	36.8536
Xe^{2+} ($^3P_2$) + O_2 (X, v = 1)	33.2978	Xe^{2+} (^1D) + O_2 (X, v = 10)	37.0196
Xe^{2+} ($^3P_2$) + O_2 (X, v = 2)	33.4877	Xe^{2+} (^1S) + O_2 (X, v = 0)	37.5810
Xe^{2+} ($^3P_2$) + O_2 (X, v = 3)	33.6747	Xe^{2+} (^1S) + O_2 (X, v = 1)	37.7740
Xe^{2+} ($^3P_2$) + O_2 (X, v = 4)	33.8587	Xe^{2+} (^1S) + O_2 (X, v = 2)	37.9639
Xe^{2+} ($^3P_2$) + O_2 (X, v = 5)	34.0396	Xe^{2+} (^1S) + O_2 (X, v = 3)	38.1509
Xe^{2+} ($^3P_2$) + O_2 (X, v = 6)	34.2176	Xe^{2+} (^1S) + O_2 (X, v = 4)	38.3349
Xe^{2+} ($^3P_2$) + O_2 (X, v = 7)	34.3926	Xe^{2+} (^1S) + O_2 (X, v = 5)	38.5158
Xe^{2+} ($^3P_2$) + O_2 (X, v = 8)	34.5646	Xe^{2+} (^1S) + O_2 (X, v = 6)	38.6938
Xe^{2+} ($^3P_2$) + O_2 (X, v = 9)	34.7336	Xe^{2+} (^1S) + O_2 (X, v = 7)	38.8688
Xe^{2+} ($^3P_2$) + O_2 (X, v = 10)	34.8996	Xe^{2+} (^1S) + O_2 (X, v = 8)	39.0408
Xe^{2+} ($^3P_0$) + O_2 (X, v = 0)	34.1129	Xe^{2+} (^1S) + O_2 (X, v = 9)	39.2098
Xe^{2+} ($^3P_0$) + O_2 (X, v = 1)	34.3058	Xe^{2+} (^1S) + O_2 (X, v = 10)	39.3758
Xe^{2+} ($^3P_0$) + O_2 (X, v = 2)	34.4957		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 3)	34.6827		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 4)	34.8667		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 5)	35.0476		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 6)	35.2256		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 7)	35.4006		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 8)	35.5726		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 9)	35.7416		
Xe^{2+} ($^3P_0$) + O_2 (X, v = 10)	35.9076		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 0)	34.3192		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 1)	34.5121		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 2)	34.7021		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 3)	34.8891		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 4)	35.0730		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 5)	35.2540		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 6)	35.4320		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 7)	35.6070		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 8)	35.7789		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 9)	35.9479		
Xe^{2+} ($^3P_1$) + O_2 (X, v = 10)	36.1139		
Xe^{2+} (^1D) + O_2 (X, v = 0)	35.2248		
Xe^{2+} (^1D) + O_2 (X, v = 1)	35.4178		
Xe^{2+} (^1D) + O_2 (X, v = 2)	35.6077		
Xe^{2+} (^1D) + O_2 (X, v = 3)	35.7947		
Xe^{2+} (^1D) + O_2 (X, v = 4)	35.9787		
Xe^{2+} (^1D) + O_2 (X, v = 5)	36.1596		
Xe^{2+} (^1D) + O_2 (X, v = 6)	36.3376		
Xe^{2+} (^1D) + O_2 (X, v = 7)	36.5126		
Xe^{2+} (^1D) + O_2 (X, v = 8)	36.6846		

Table S2: Product Channels and Asymptotic Energies Used in Multi-Channel Landau-Zener Model

Channel #	Reactant Channel	Asymptotic Energy (eV)	Channel #	Reactant Channel	Asymptotic Energy (eV)
1	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 0)	31.6058	43	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 5)	29.6859
2	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 1)	31.7499	44	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 6)	29.7771
3	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 2)	31.8898	45	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 7)	29.8649
4	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 3)	32.0255	46	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 8)	29.9493
5	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 4)	32.1569	47	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 9)	30.0304
6	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 5)	32.2841	48	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 10)	30.1081
7	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 6)	32.4071	49	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 11)	30.1824
8	Xe^+ ($^2P_{1/2}$) + O_2^+ (b, v = 7)	32.5258	50	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 12)	30.2534
9	Xe^+ ($^2P_{3/2}$) + O_2^+ (b, v = 0)	30.2993	51	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 13)	30.3210
10	Xe^+ ($^2P_{3/2}$)+ O_2^+ (b, v = 1)	30.4435	52	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 14)	30.3853
11	Xe^+ ($^2P_{3/2}$)+ O_2^+ (b, v = 2)	30.5834	53	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 15)	30.4461
12	Xe^+ ($^2P_{3/2}$) + O_2^+ (b, v = 3)	30.7190	54	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 16)	30.5036
13	Xe^+ ($^2P_{3/2}$)+ O_2^+ (b, v = 4)	30.8505	55	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 17)	30.5578
14	Xe^+ ($^2P_{3/2}$)+ O_2^+ (b, v = 5)	30.9777	56	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 18)	30.6086
15	Xe^+ ($^2P_{3/2}$) + O_2^+ (b, v = 6)	31.1006	57	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 19)	30.6560
16	Xe^+ ($^2P_{3/2}$)+ O_2^+ (b, v = 7)	31.2193	58	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 20)	30.7000
17	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 0)	30.4860	59	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 0)	25.5060
18	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 1)	30.5940	60	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 1)	25.7381
19	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 2)	30.6986	61	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 2)	25.9662
20	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 3)	30.7999	62	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 3)	26.1902
21	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 4)	30.8978	63	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 4)	26.4103
22	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 5)	30.9923	64	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 5)	26.6263
23	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 6)	31.0835	65	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 6)	26.8382
24	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 7)	31.1713	66	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 7)	27.0462
25	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 8)	31.2557	67	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 8)	27.2501
26	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 9)	31.3368	68	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 9)	27.4499
27	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 10)	31.4145	69	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 10)	27.6458
28	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 11)	31.4889	70	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 11)	27.8376
29	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 12)	31.5598	71	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 12)	28.0253
30	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 13)	31.6274	72	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 13)	28.2091
31	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 14)	31.6917	73	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 14)	28.3888
32	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 15)	31.7526	74	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 15)	28.5645
33	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 16)	31.8101	75	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 16)	28.7361
34	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 17)	31.8642	76	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 17)	28.9037
35	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 18)	31.9150	77	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 18)	29.0673
36	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 19)	31.9624	78	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 19)	29.2269
37	Xe^+ ($^2P_{1/2}$) + O_2^+ (A, v = 20)	32.0065	79	Xe^+ ($^2P_{1/2}$) + O_2^+ (X, v = 20)	29.3824
38	Xe^+ ($^2P_{3/2}$) + O_2^+ (A, v = 0)	29.1796	80	Xe^+ ($^2P_{3/2}$)+ O_2^+ (X, v = 0)	24.1995
39	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 1)	29.2876	81	Xe^+ ($^2P_{3/2}$)+ O_2^+ (X, v = 1)	24.4317
40	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 2)	29.3922	82	Xe^+ ($^2P_{3/2}$)+ O_2^+ (X, v = 2)	24.6598
41	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 3)	29.4935	83	Xe^+ ($^2P_{3/2}$)+ O_2^+ (X, v = 3)	24.8838
42	Xe^+ ($^2P_{3/2}$)+ O_2^+ (A, v = 4)	29.5914	84	Xe^+ ($^2P_{3/2}$)+ O_2^+ (X, v = 4)	25.1038

Table S2-Cont.

Channel #	Reactant Channel	Asymptotic Energy (eV)	Channel #	Reactant Channel	Asymptotic Energy (eV)
85	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 5)	25.3198	127	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 5)	28.8363
86	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 6)	25.5318	128	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 6)	28.9492
87	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 7)	25.7397	129	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 7)	29.0596
88	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 8)	25.9436	130	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 8)	29.1674
89	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 9)	26.1435	131	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 9)	29.2726
90	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 10)	26.3393	132	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 10)	29.3753
91	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 11)	26.5311	133	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 11)	29.4754
92	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 12)	26.7189	134	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 12)	29.5728
93	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 13)	26.9027	135	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 13)	29.6678
94	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 14)	27.0824	136	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 14)	29.7601
95	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 15)	27.2580	137	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 15)	29.8499
96	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 16)	27.4297	138	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 16)	29.9371
97	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 17)	27.5973	139	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 17)	30.0217
98	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 18)	27.7609	140	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 18)	30.1037
99	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 19)	27.9204	141	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 19)	30.1832
100	Xe^+ ($^2P_{3/2}$) + O_2^+ (X, v = 20)	28.0760	142	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 20)	30.2600
101	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 0)	29.5393			
102	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 1)	29.6652			
103	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 2)	29.7884			
104	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 3)	29.9091			
105	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 4)	30.0272			
106	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 5)	30.1427			
107	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 6)	30.2557			
108	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 7)	30.3661			
109	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 8)	30.4738			
110	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 9)	30.5791			
111	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 10)	30.6817			
112	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 11)	30.7818			
113	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 12)	30.8793			
114	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 13)	30.9742			
115	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 14)	31.0665			
116	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 15)	31.1563			
117	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 16)	31.2435			
118	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 17)	31.3281			
119	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 18)	31.4101			
120	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 19)	31.4896			
121	Xe^+ ($^2P_{1/2}$) + O_2^+ (a, v = 20)	31.5665			
122	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 0)	28.2329			
123	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 1)	28.3587			
124	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 2)	28.4820			
125	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 3)	28.6027			
126	Xe^+ ($^2P_{3/2}$) + O_2^+ (a, v = 4)	28.7208			

Table S3: Franck-Condon Factors for O_2^+ (X) – O_2 (X). Taken from ref. 1.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	0.186	0.271	0.23	0.15	0.084	0.0424	0.02	0.00902	0.00394	0.00169	0.000715
1	0.362	0.0832	0.00496	0.0833	0.134	0.125	0.0898	0.0553	0.0309	0.0161	0.00802
2	0.291	0.0427	0.165	0.0534	0.000555	0.0441	0.0895	0.0982	0.0808	0.0561	0.0349
3	0.125	0.257	0.0165	0.0724	0.109	0.031	0.000616	0.0316	0.0673	0.0791	0.0703
4	0.0307	0.236	0.11	0.0965	0.00415	0.0821	0.0744	0.0164	0.00138	0.0265	0.0545
5	0.00433	0.091	0.267	0.0157	0.128	0.0132	0.0282	0.0766	0.0489	0.0076	0.00261
6	0.000326	0.0173	0.161	0.225	0.00347	0.0976	0.0542	0.000873	0.0467	0.0633	0.0307
7	1.07e-5	0.0016	0.0406	0.22	0.151	0.0389	0.0465	0.0808	0.00867	0.0148	0.0528
8	7.14e-8	5.94e-05	0.00453	0.0729	0.257	0.0787	0.0809	0.01	0.0783	0.0331	0.00036
9	7.16e-10	3.47e-07	0.000185	0.00965	0.111	0.267	0.028	0.106	0.000133	0.0554	0.0537
10	4.25e-11	8.65e-09	8.54e-07	0.000422	0.0172	0.151	0.257	0.00357	0.107	0.0114	0.028
11	2.46e-13	3.23e-10	5.21e-8	1.32e-06	0.000791	0.027	0.191	0.231	0.00123	0.0915	0.0318
12	2.1e-14	6.1e-12	1.19e-9	2.13e-07	1.21e-06	0.00128	0.0389	0.226	0.198	0.013	0.0671
13	7.65e-16	2.04e-13	5.31e-11	2.68e-09	6.66e-07	3.72e-07	0.00184	0.0521	0.258	0.162	0.031
14	8.53e-16	1.66e-14	7.48e-13	3.02e-10	3.67e-09	1.7e-06	2.56e-07	0.0024	0.0662	0.284	0.13
15	6.53e-16	4.35e-17	1.35e-13	8.8e-13	1.23e-09	1.96e-09	3.7e-06	5.83e-06	0.00286	0.0803	0.307
16	2.09e-15	1.28e-17	6.77e-17	8.09e-13	4.23e-17	3.9e-09	4.34e-10	6.94e-06	2.76e-05	0.00312	0.0938
17	3.66e-16	1.93e-18	5.85e-16	1.34e-14	3.46e-12	1.32e-11	9.97e-09	2.74e-08	1.14e-05	8.32e-05	0.00307
18	4.26e-16	4.23e-17	7.54e-17	6.24e-17	1.28e-13	9.64e-12	1.55e-10	2.07e-08	1.8e-07	1.62e-05	0.000197
19	1.44e-15	8.81e-17	4.29e-16	9.12e-19	2.47e-15	7.26e-13	1.94e-11	8.78e-10	3.4e-08	6.92e-07	1.97e-05
20	5.52e-16	1.88e-17	1.82e-16	1.13e-18	3.38e-15	5.89e-16	3.52e-12	2.3e-11	3.47e-09	4.17e-08	1.99e-06
21	3.76e-17	1.38e-17	3.02e-18	5.37e-17	3.47e-16	6.02e-15	2.49e-14	1.22e-11	5.3e-12	1.06e-08	3.01e-08

Table S4: Franck-Condon Factors for O_2^+ (a) – O_2 (X). Taken from ref. 1.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	0.00987	0.0544	0.138	0.215	0.23	0.178	0.105	0.0472	0.0167	0.00464	0.00102
1	0.036	0.124	0.158	0.0732	5.34e-4	0.053	0.152	0.179	0.129	0.0644	0.0236
2	0.072	0.142	0.0601	0.00233	0.0829	0.0951	0.0132	0.0237	0.123	0.168	0.126
3	0.105	0.102	0.00125	0.063	0.0698	2.02e-4	0.0616	0.0879	0.0121	0.0259	0.125
4	0.124	0.0461	0.0198	0.0767	0.00327	0.051	0.0584	1.05e-4	0.0665	0.0739	0.00335
5	0.128	0.00865	0.0579	0.0311	0.0203	0.0608	8.72e-05	0.0584	0.0389	0.00608	0.0794
6	0.118	4.45e-4	0.0688	8.06e-4	0.0557	0.0117	0.0351	0.0408	0.00533	0.0658	0.0144
7	0.101	0.013	0.0505	0.0108	0.0468	0.00405	0.0521	1.12e-4	0.0515	0.0148	0.0272
8	0.0817	0.0327	0.0234	0.0357	0.0154	0.0324	0.019	0.0244	0.0315	0.0105	0.0502
9	0.0629	0.0494	0.00483	0.0486	0.00909	0.0446	6.92e-06	0.044	3.33e-4	0.0443	0.00512
10	0.0467	0.0587	1.05e-4	0.043	0.00832	0.0292	0.0147	0.0243	0.0161	0.0268	0.0125
11	0.0338	0.0605	0.00599	0.0272	0.0253	0.00821	0.0333	0.00222	0.036	0.00103	0.0379
12	0.024	0.0567	0.0164	0.0116	0.0361	5.45e-07	0.0338	0.00393	0.0277	0.00912	0.0248
13	0.0168	0.0497	0.0265	0.00228	0.0359	0.00595	0.0199	0.0194	0.00779	0.0275	0.00263
14	0.0116	0.0416	0.0334	5.7e-05	0.0276	0.0175	0.00573	0.0292	2.88e-05	0.0284	0.00365
15	0.00805	0.0336	0.0366	0.0029	0.0168	0.0264	3.9e-05	0.0265	0.00724	0.0145	0.0184
16	0.00558	0.0266	0.0366	0.00805	0.00776	0.029	0.00299	0.0162	0.0185	0.00236	0.0257
17	0.00388	0.0207	0.0344	0.0133	0.00219	0.0261	0.0101	0.00604	0.0243	5.91e-4	0.0199
18	0.00272	0.016	0.031	0.0175	9.01e-05	0.0202	0.017	6.51e-4	0.0224	0.0069	0.0089
19	0.00193	0.0122	0.0271	0.0201	4.92e-4	0.0136	0.021	4.82e-4	0.0157	0.0147	0.00136
20	0.00138	0.00941	0.0231	0.0212	0.00227	0.00789	0.0217	0.00368	0.00832	0.0193	0.000343
21	0.001	0.00724	0.0195	0.0211	0.00451	0.00382	0.0199	0.00794	0.00292	0.0193	0.00409

Table S5: Franck-Condon Factors for O_2^+ (A) – O_2 (X). Taken from ref. 1.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	0.00284	0.0195	0.0634	0.129	0.186	0.202	0.171	0.116	0.0643	0.0296	0.0114
1	0.0123	0.06	0.123	0.131	0.0634	0.003	0.0249	0.101	0.153	0.144	0.0988
2	0.0291	0.0971	0.112	0.0373	0.00221	0.0622	0.0925	0.0375	1.83e-4	0.0474	0.12
3	0.05	0.109	0.055	0.00024	0.055	0.0671	0.00689	0.0234	0.0804	0.0552	0.00258
4	0.0697	0.0923	0.00974	0.0292	0.0644	0.00734	0.0256	0.0655	0.0165	0.0111	0.0695
5	0.0843	0.0611	0.00101	0.057	0.0239	0.0105	0.0565	0.013	0.0164	0.0605	0.019
6	0.0918	0.0304	0.0175	0.0514	2.3e-4	0.0423	0.0251	0.00696	0.051	0.0126	0.0154
7	0.0925	0.00951	0.0375	0.0265	0.011	0.043	1.92e-4	0.0382	0.021	0.00824	0.0478
8	0.0878	6.28e-4	0.0474	0.00582	0.0312	0.0189	0.0127	0.036	7.87e-05	0.0383	0.0145
9	0.0797	0.00143	0.0449	8.8e-05	0.0387	0.00154	0.0319	0.0108	0.0177	0.0284	0.00183
10	0.0698	0.00788	0.0344	0.00646	0.0309	0.00285	0.0326	3.67e-05	0.0327	0.00384	0.0241
11	0.0596	0.0163	0.0215	0.017	0.0167	0.0146	0.0185	0.00944	0.0243	0.0029	0.0306
12	0.0499	0.0242	0.0106	0.0254	0.0051	0.0246	0.00477	0.0223	0.00755	0.0176	0.0143
13	0.0412	0.0303	0.00348	0.0288	0.00019	0.0268	6.14e-07	0.0258	3.1e-05	0.0254	0.000947
14	0.0336	0.034	3.24e-4	0.0273	0.00135	0.0221	0.00362	0.0196	0.00421	0.0198	0.00289
15	0.0272	0.0357	0.00033	0.0226	0.00586	0.0142	0.0105	0.00997	0.0127	0.00877	0.0125
16	0.0219	0.0356	0.00237	0.0167	0.011	0.00691	0.0161	0.0027	0.0182	0.0013	0.0188
17	0.0176	0.0342	0.0054	0.0109	0.0149	0.00207	0.0182	2.64e-05	0.0183	3.51e-4	0.0177
18	0.0141	0.0319	0.00862	0.00618	0.0168	1.07e-4	0.0169	0.00123	0.0142	0.00392	0.0117
19	0.0113	0.0292	0.0115	0.00287	0.0169	4.03e-4	0.0136	0.00435	0.0088	0.00851	0.00534
20	0.00907	0.0262	0.0137	9.25e-4	0.0155	0.002	0.00953	0.00756	0.00412	0.0116	0.00123
21	0.00724	0.0231	0.0151	9.62e-05	0.0132	0.00398	0.00581	0.00972	0.00119	0.0124	3.85e-08

Table S6: Franck-Condon Factors for O_2^+ (b) – O_2 (X). Taken from ref. 1.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	0.411	0.376	0.161	0.0431	0.00821	0.00119	1.36e-4	1.25e-05	9.81e-07	6.34e-08	3.54e-09
1	0.336	0.00278	0.234	0.261	0.123	0.0349	0.00696	0.00105	1.24e-4	1.2e-05	9.46e-07
2	0.162	0.169	0.0818	0.0485	0.231	0.196	0.0831	0.0225	0.00443	6.62e-4	7.88e-05
3	0.0613	0.209	0.0169	0.162	0.00255	0.12	0.218	0.141	0.0528	0.0134	0.00252
4	0.0204	0.135	0.128	0.0165	0.119	0.0644	0.0225	0.172	0.185	0.0965	0.032
5	0.00636	0.0653	0.154	0.029	0.0859	0.032	0.122	0.00327	0.0854	0.187	0.143
6	0.00193	0.0272	0.111	0.105	0.0143	0.112	6.48e-4	0.106	0.051	0.015	0.14
7	5.83e-4	0.0104	0.0615	0.122	0.0339	0.0424	0.0672	0.0397	0.0417	0.1	0.00359
8	1.79e-4	0.00383	0.0297	0.0934	0.088	1.07e-4	0.084	0.0109	0.0846	8.29e-4	0.0949
9	5.6e-05	0.00138	0.0132	0.0574	0.1	0.0329	0.0221	0.0733	0.00535	0.076	0.0203
10	1.8e-05	5.01e-4	0.00563	0.0311	0.0812	0.0729	9.22e-4	0.0611	0.0259	0.0448	0.0271
11	5.96e-06	1.83e-4	0.00235	0.0156	0.0544	0.0841	0.0282	0.0136	0.0661	2.73e-06	0.0694
12	2e-06	6.74e-05	9.68e-4	0.00752	0.0325	0.0721	0.0591	9.75e-4	0.047	0.0311	0.0221
13	6.79e-07	2.51e-05	3.99e-4	0.00352	0.0181	0.0523	0.0706	0.0214	0.011	0.0561	0.00118
14	2.27e-07	9.39e-06	1.65e-4	0.00162	0.00966	0.0342	0.0646	0.046	0.00033	0.0393	0.0286
15	7.2e-08	3.47e-06	6.78e-05	7.42e-4	0.005	0.0209	0.0507	0.0583	0.0138	0.0115	0.0466
16	0.411	0.376	0.161	0.0431	0.00821	0.00119	1.36e-4	1.25e-05	9.81e-07	6.34e-08	3.54e-09

Table S7: Averaged Best Fit Populations Derived from O_2^+ (*b*-*a*) fitting. Energy in eV.

E_{CM}	$v' = 0$	$v' = 1$	$v' = 2$	$v' = 3$	$v' = 4$
9.8	0.434	0.263	0.191	0.068	0.043
19.6	0.433	0.277	0.186	0.072	0.032
39.2	0.426	0.294	0.176	0.077	0.027
58.9	0.457	0.283	0.163	0.074	0.022
118	0.482	0.276	0.153	0.063	0.026
235.5	0.506	0.278	0.137	0.069	0.009
471.1	0.502	0.302	0.119	0.076	0.001
942.3	0.498	0.289	0.138	0.062	0.014

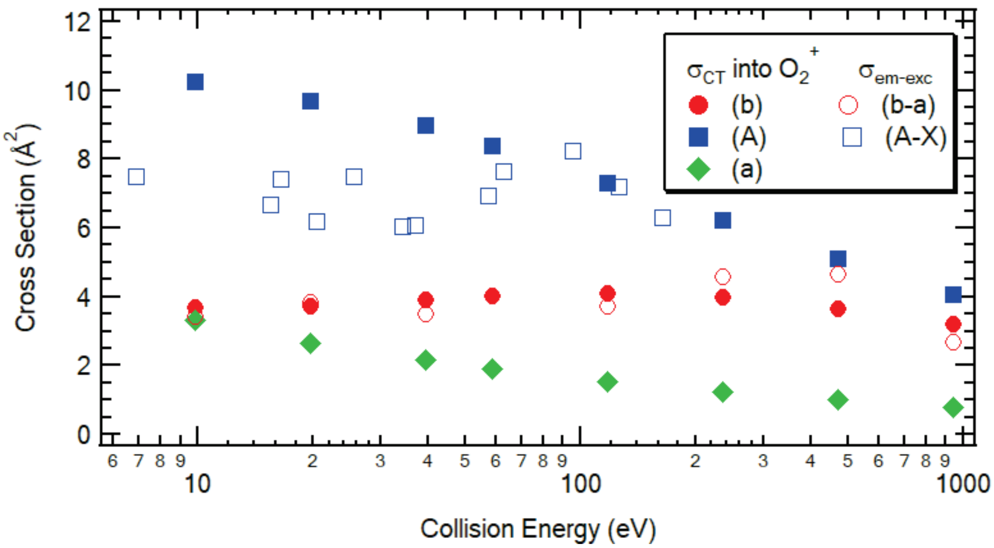
Table S8: Simulated populations for the O_2^+ (*b*) state using the best-fit MCLZ model

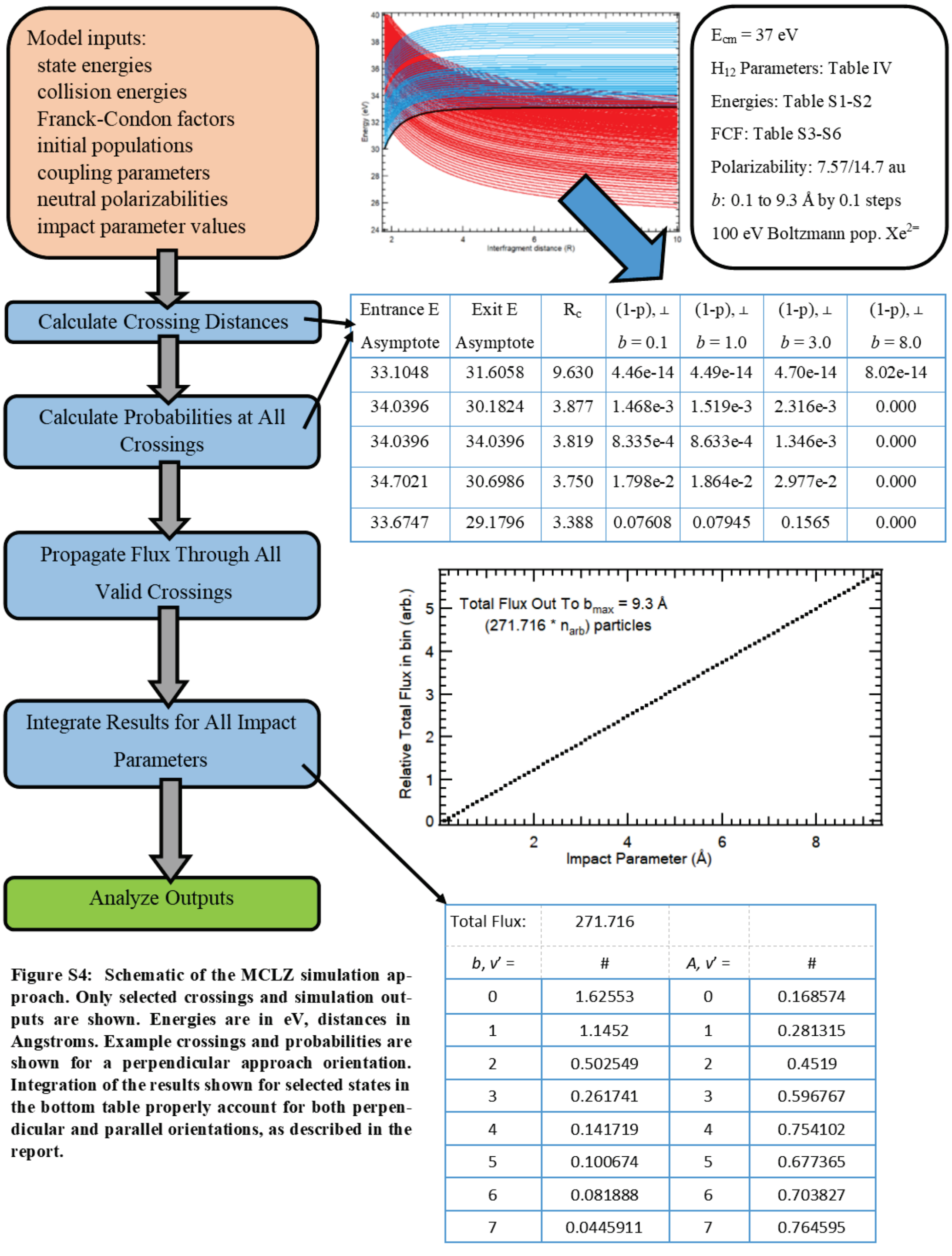
E_{CM}	$v' = 0$	$v' = 1$	$v' = 2$	$v' = 3$	$v' = 4$
9.8	0.392	0.270	0.155	0.107	0.076
19.6	0.419	0.299	0.146	0.085	0.051
39.3	0.442	0.311	0.137	0.071	0.039
58.9	0.461	0.319	0.130	0.061	0.029
117.8	0.485	0.325	0.121	0.049	0.020
235.6	0.500	0.329	0.115	0.041	0.014
471.2	0.509	0.333	0.111	0.037	0.011
942.3	0.513	0.336	0.108	0.034	0.009

Table S9: Averaged Best Fit Experimental Populations, Standard Deviations and Modeled Pop. derived from O_2^+ (*A*-*X*) fitting.

v'	E_{cm} = 37 eV	σ	Model	E_{cm} = 58 eV	σ	Model	E_{cm} = 233 eV	σ	Model
0	0.013	0.0000	0.019	0.013	0.0000	0.016	0.014	0.0005	0.011
1	0.024	0.0004	0.031	0.025	0.0000	0.030	0.039	0.0003	0.026
2	0.038	0.0005	0.050	0.046	0.0000	0.050	0.063	0.0017	0.049
3	0.039	0.0004	0.066	0.049	0.0000	0.067	0.066	0.0009	0.069
4	0.043	0.0005	0.084	0.057	0.0005	0.088	0.062	0.0019	0.097
5	0.055	0.0005	0.075	0.071	0.0005	0.077	0.062	0.0016	0.082
6	0.068	0.0005	0.078	0.081	0.0008	0.078	0.071	0.0022	0.076
7	0.074	0.0005	0.085	0.078	0.0010	0.084	0.072	0.0022	0.079
8	0.087	0.0008	0.059	0.093	0.0010	0.057	0.094	0.0040	0.054
9	0.086	0.0011	0.069	0.083	0.0013	0.071	0.071	0.0030	0.077
10	0.078	0.0018	0.057	0.072	0.0017	0.058	0.076	0.0071	0.060
11	0.063	0.0013	0.041	0.062	0.0018	0.041	0.060	0.0020	0.044
12	0.067	0.0008	0.032	0.051	0.0020	0.031	0.057	0.0057	0.031
13	0.054	0.0024	0.053	0.050	0.0049	0.056	0.022	0.0067	0.062
14	0.046	0.0012	0.043	0.047	0.0060	0.044	0.045	0.0087	0.048
15	0.057	0.0023	0.042	0.024	0.0080	0.042	0.022	0.0117	0.041
16	0.023	0.0058	0.032	0.050	0.0086	0.031	0.048	0.0166	0.028
17	0.034	0.0117	0.026	0.0003	0.0008	0.024	0.023	0.0233	0.021
18	0.023	0.0121	0.024	0.011	0.0045	0.023	0.005	0.0039	0.020
19	0.006	0.0088	0.017	0.002	0.0039	0.016	0.000	0.0000	0.013
20	0.005	0.0084	0.015	0.013	0.0039	0.014	0.002	0.0154	0.011
21	0.012	0.0089		0.019	0.0027		0.022	0.0102	

Figure S3: Simulated charge-transfer cross sections into three electronic states of O_2^+ (solid symbols) and the experimental emission excitation cross sections measured for O_2^+ (A-X) and (b-a) (open symbols). Simulated values are the result from the MCLZ parameters that best reproduce the vibrational populations and have the cross sections at low collision energy within a factor of 2.





Entrance E Asymptote	Exit E Asymptote	R_c	(1-p), ⊥ b = 0.1	(1-p), ⊥ b = 1.0	(1-p), ⊥ b = 3.0	(1-p), ⊥ b = 8.0
33.1048	31.6058	9.630	4.46e-14	4.49e-14	4.70e-14	8.02e-14
34.0396	30.1824	3.877	1.468e-3	1.519e-3	2.316e-3	0.000
34.0396	34.0396	3.819	8.335e-4	8.633e-4	1.346e-3	0.000
34.7021	30.6986	3.750	1.798e-2	1.864e-2	2.977e-2	0.000
33.6747	29.1796	3.388	0.07608	0.07945	0.1565	0.000

Total Flux:	271.716		
b, v′ =	#	*A, v′* =	#
0	1.62553	0	0.168574
1	1.1452	1	0.281315
2	0.502549	2	0.4519
3	0.261741	3	0.596767
4	0.141719	4	0.754102
5	0.100674	5	0.677365
6	0.081888	6	0.703827
7	0.0445911	7	0.764595

Figure S4: Schematic of the MCLZ simulation approach. Only selected crossings and simulation outputs are shown. Energies are in eV, distances in Angstroms. Example crossings and probabilities are shown for a perpendicular approach orientation. Integration of the results shown for selected states in the bottom table properly account for both perpendicular and parallel orientations, as described in the report.

References:

[1] Gilmore, F. R., Laher, R. R. and Espy, P. J., "Frank-Condon Factors, R-Centroids, Electronic Transition Moments, and Einstein Coefficients for Many Nitrogen and Oxygen Band Systems," *J. Phys. Chem. Ref. Data*, Vol. 21, No. 1992, pp. 1005.