Supporting Information Ms-ID: BCREC-2025-20560-R1
DOI: https://doi.org/10.9767/bcrec.20560

Cold Plasma Modeling for Air Pollution Control: NOx Removal in Dielectric Barrier Discharge Reactors

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Tables S1 _S5 lists the significant reactions for Nitrogen, Oxygen, Argon and their mixtures with their rate coefficients in (m^6/s) and (m^3/s) for three-body and tow-body respectively

Table S1. Reaction set for Nitrogen with their Rate Coefficients

No	Reaction	Rate Coefficient (m^6/s), (m^3/s)	Ref
	Electron Impact Reactions with Nitrogen		
E1	$e+N_4 \Rightarrow N_2+0.38N_2(A3s)+0.38N_2(B3p)+0.24N2(C3p)$	2e-12*(0.026/Te) 0.5	[23]
E2	$e+N_3^+ \Rightarrow N_2+N$	2e-13*(0.026/Te) 0.5	[24]
E3	$e+N_2^+ \Rightarrow 1.143N+0.086N(p)+0.771N(d)$	1.6e-13*(0.026/Te) 0.37	[24]
E4	$e + N_2 \Rightarrow e+N_2$	Cross Section	[25]
E5	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E6	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E7	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E8	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E9	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E10	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E11	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E12	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E13	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E14	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E15	$e+ N_2 \Rightarrow e+N_2(A3s)$	Cross Section	[25]
E16	$e+ N_2(A3s) \Rightarrow e+N_2$	Cross Section	[25]
E17	$e+ N_2 \Rightarrow e+N_2(A3s)$	Cross Section	[25]
E18	$e+ N_2 \Rightarrow e+N_2(B3p)$	Cross Section	[25]
E19	$e+ N_2(B3p) \Rightarrow e+N_2$	Cross Section	[25]
E20	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E21	$e+ N_2 \Rightarrow e+N_2(A3s)$	Cross Section	[25]
E22	$e+ N_2 \Rightarrow e+N_2$	Cross Section	[25]
E23	$e+ N_2 \Rightarrow e+N_2(a1s)$	Cross Section	[25]

E24	e+ N_2(a1s) => e+N_2	Cross Section	[25]
E25	e+ N_2=> e+0.88N_2+0.12N+0.12N	Cross Section	[25]
E26	e+ N_2=> e+N_2	Cross Section	[25]
E27	e+ N_2=> e+N_2(C3p)	Cross Section	[25]
E28	e+ N_2(C3p) => e+N_2	Cross Section	[25]
E29	e+ N_2=> e+N_2	Cross Section	[25]
E30	e+ N_2=> e+N_2	Cross Section	[25]
E31	e+ N_2=> e+0.7N+0.7N(d)+0.3N_2	Cross Section	[25]
E32	e+ N_2=> e+e+N_2^+	Cross Section	[25]
E33	e+ N_2=> e+ e+ N+N^+	Cross Section	[25]
E34	e+ N_2(A3s) => e+e+N_2^+	Cross Section	[26]
E35	e+ N_2(B3p) => e+e+N_2^+	Cross Section	[26]
E36	e+ N_2(C3p) => e+e+N_2^+	Cross Section	[26]
E37	e+ N_2(a1s) => e+e+N_2^+	Cross Section	[26]
E38	e+ N=> e+N	Cross Section	[25]
E39	e+ N=> e+N(d)	Cross Section	[25]
E40	e+ N(d)=> e+N	Cross Section	[25]
E41	e+ N=> e+N(p)	Cross Section	[25]
E42	e+ N(p)=> e+N	Cross Section	[25]
E43	e+ N=> e+e+N^+	Cross Section	[25]
E44	e+ N(d)=> e+N(p)	Cross Section	[25]
E45	e+N(p)=>e+N(d)	Cross Section	[25]
E46	e+ N(d)=> e+e+N^+	Cross Section	[25]
E47	e+ N(p)=> e+e+N^+	Cross Section	[25]
	Nitrogen Reactions		
N1	N_2(A3s) + N_2(a1s) => e+N_4^+	5e-17	[23]
N2	N_2(a1s) + N_2(a1s) => e+N_4^+	2e-16	[23]
N3	N_2(a1s) + N(p) => e+N_3^+	1e-17	[23]
N4	N(d)+ N(p) => e+N_2^+	1.92e-21*(T0.98)/(1-exp(-3129/T))	[27]
N5	N(p)+ N(p) => e+N_2^+	3e-21*(T0.98)/(1-exp(-3129/T))	[28]
N6	N^++ N_2+ N_2=> N_3^++N_2	1.7e-41*(300/T)2.1	[24]
N7	N^++N+N_2=>N_2^++N_2	1e-41*(300/T)	[24]
N8	N_2^++N_2+N_2=>N_4^++N_2	5.2e-41*(300/T)2.2	[24]
N9	N_2^++N+N_2=>N_3^++N_2	1.7e-41*(300/T)2.1	[24]
N10	N_4^++N_2=>N_2^++N_2+N_2	2.1e-22*exp(T/121)	[24]
N11	N_4^++N=>N^++N_2+N_2	1e-17	[24]
N12	N_3^++N=>N_2^++N_2	6.6e-17	[24]
N13	N_2^++N=>N^++N_2	7.2e-19*(T/300)	[24]

N14	$N^+ + N => N_2^+$	3.71e-24*(T/300)0.24*exp(-26.12/T)	[24]
N15	$N_2^+ + N_2(A3s) => N_3^+ + N$	3e-16	[24]
N16	$N + N + N_2 => 0.31N_2(A3s) + 0.44N_2(B3p) + 1.25N_2$	8.26e-46*exp(490/T)	[23]
N17	$N_2(A3s) + N_2(A3s) => N_2(C3p) + N_2$	1.5e-16	[23]
N18	$N_2(A3s) + N_2(A3s) => N_2(B3p) + N_2$	7.7e-17	[23]
N19	$N_2(A3s) + N_2 => N_2 + N_2$	2e-24	[23]
N20	$N_2(B3p) + N_2 => 0.95N_2(A3s) + 1.05N_2$	3e-17	[23]
N21	$N_2(C3p) + N_2 => N_2(B3p) + N_2$	1.15e-17	[23]
N22	$N_2(C3p) + N_2 => N_2(a1s) + N_2$	1e-17	[29]
N23	$N_2(a1s) + N_2 => N_2(B3p) + N_2$	1.9e-19	[23]
N24	$N_2(A3s) + N => N_2 + N(p)$	4e-17*(300/T)0.66	[23]
N25	$N(p) + N_2 => N + N_2$	3e-22	[28]
N26	$N(p) + N => N(d) + N$	1.8e-18	[27]
N27	$N(d) + N_2 => N + N_2$	1e-19*exp(-510/T)	[28]
N28	$N + N + N => 0.31N_2(A3s) + 0.44N_2(B3p) + 0.25N_2 + N$	3.35e-43*T-0.5	[23]
N29	$N(p) + N + N_2 => 0.31N_2(A3s) + 0.44N_2(B3p) + 0.25N_2$	8.26e-46*exp(490/T)	[23]
N30	$Nd + N + N_2 => 0.31N_2(A3s) + 0.44N_2(B3p) + 0.25N_2$	8.26e-46*exp(490/T)	[23]
N31	$N_4^+ + N => N_3^+ + N_2$	1e-15	[24]
N32	$N(p) + N_2 => N(d) + N_2$	1.8e-24	[28]

Table S2. Reaction set for Oxygen with their Rate Coefficients.

No	Reaction	Rate Coefficient (m^6/s), (m^3/s)	Ref
	Electron Impact Reactions with Oxygen		
E1	$e + O_2 => e + O_2$	Cross Section	[30]
E2	$e + O_2 => O + O^-$	Cross Section	[30]
E3	$e + O_2 => e + O_2$	Cross Section	[30]
E4	$e + O_2 => e + O_2$	Cross Section	[30]
E5	$e + O_2 => e + O_2$	Cross Section	[30]
E6	$e + O_2 => e + O_2$	Cross Section	[30]
E7	$e + O_2 => e + O_2$	Cross Section	[30]
E8	$e + O_2 => e + O_2$	Cross Section	[30]
E9	$e + O_2 => e + O_2$	Cross Section	[30]
E10	$e + O_2 => e + O_2(a1d)$	Cross Section	[30]
E11	$e + O_2(a1d) => e + O_2$	Cross Section	[30]
E12	$e + O_2 => e + O_2(b1s)$	Cross Section	[30]
E13	$e + O_2(b1s) => e + O_2$	Cross Section	[30]
E14	$e + O_2 => e + O_2(45)$	Cross Section	[30]

E15	$e+O_2(45) \Rightarrow e+O_2$	Cross Section	[30]
E16	$e+O_2 \Rightarrow e+O+O$	Cross Section	[30]
E17	$e+O_2 \Rightarrow e+O+O(1d)$	Cross Section	[30]
E18	$e+O_2 \Rightarrow e+O+O(1s)$	Cross Section	[30]
E19	$e+O_2 \Rightarrow e+e+O_2^+$	Cross Section	[30]
E20	$e+O_2 \Rightarrow e+e+O+O^+$	Cross Section	[30]
E21	$e+O_2(a1d) \Rightarrow e+O+O$	Cross Section	[30]
E22	$e+O_2(a1d) \Rightarrow 2e+O_2^+$	Cross Section	[30]
E23	$e+O_2(b1s) \Rightarrow e+O+O$	Cross Section	[30]
E24	$e+O_2(b1s) \Rightarrow 2e+O_2^+$	Cross Section	[30]
E25	$e+O_2(45) \Rightarrow e+O+O$	Cross Section	[30]
E26	$e+O_2(45) \Rightarrow 2e+O_2^+$	Cross Section	[30]
E27	$e+O \Rightarrow e+ O(1d)$	Cross Section	[30]
E28	$e+O(1d) \Rightarrow e+O$	Cross Section	[30]
E29	$e+O \Rightarrow e+O(1s)$	Cross Section	[30]
E30	$e+O(1s) \Rightarrow e+O$	Cross Section	[30]
E31	$e+O \Rightarrow 2e+O^+$	Cross Section	[30]
E32	$e+O(1d) \Rightarrow e+O1s$	Cross Section	[30]
E33	$e+O(1d) \Rightarrow 2e+O^+$	Cross Section	[30]
E34	$e+O(1s) \Rightarrow 2e+O^+$	Cross Section	[30]
E35	$e+O_3 \Rightarrow e+O_3$	Cross Section	[30]
E36	$e+O_3 \Rightarrow O_2^- + O$	Cross Section	[30]
E37	$e+O_3 \Rightarrow O^- + O_2$	Cross Section	[30]
E38	$e+O_3 \Rightarrow 2e+O_3^+$	Cross Section	[30]
E39	$e+O^- \Rightarrow 2e+O$	Cross Section	[30]
E40	$e+O_2 \Rightarrow e+O_2$	Cross Section	[30]
E41	$e+O_2 \Rightarrow O+O^-$	Cross Section	[30]
E42	$e+O_2 \Rightarrow e+O_2$	Cross Section	[30]
	Oxygen Reactions		
O1	$O^- + O \Rightarrow O_2 + e$	1.9e-16	[31]
O2	$O^- + O_2 \Rightarrow O_3 + e$	5e-21	[31]
O3	$O^- + O_3 \Rightarrow O_3^- + O$	8e-16	[31]
O4	$O_2^- + O \Rightarrow O_3 + e$	1.5e-16	[31]
O5	$O_2^- + O \Rightarrow O^- + O_2$	1.5e-16	[31]
O6	$O_2^- + O_2 \Rightarrow O_2 + O_2 + e$	2.7e-16*(T/300)0.5*exp(-5590/T)	[31]
O7	$O_2^- + O_3 \Rightarrow O_3^- + O_2$	3.5e-16	[31]
O8	$O_3^- + O \Rightarrow O_2 + O_2 + e$	1e-16	[31]
O9	$O_3^- + O \Rightarrow O_2^- + O_2$	2.5e-16	[31]

O10	$O_3^-+O_3 \Rightarrow O_2+O_2+O_2+e$	1e-16	[31]
O11	$O_2^-+O_2+O_2 \Rightarrow O_4^-+O_2$	3.5e-42*(300/T)	[31]
O12	$O_4^-+O_2 \Rightarrow O_2^-+O_2+O_2$	1e-16*exp(-1044/T)	[31]
O13	$O_4^-+O \Rightarrow O_3^-+O_2$	4e-16	[31]
O14	$O_4^-+O \Rightarrow O^-+O_2+O_2$	3e-16	[31]
O15	$O^-+O_2+O_2 \Rightarrow O_3^-+O_2$	1.1e-42*(300/T)	[31]
O16	$O^++O_2 \Rightarrow O_2^++O$	2e-17*(300/T) 0.5	[31]
O17	$O^++O_3 \Rightarrow O_2^++O_2$	1e-16	[31]
O18	$O_2^++O_2+O_2 \Rightarrow O_4^++O_2$	2.4e-42*(300/T) 3.2	[31]
O19	$O_4^++O \Rightarrow O_2^++O_3$	3e-16	[31]
O20	$O_4^++O_2 \Rightarrow O_2^++O_2+O_2$	3.3e-12*((300/T)4)*exp(-5030/T)	[31]
O21	$O^++O+O_2 \Rightarrow O_2^++O_2$	1e-41	[31]
O22	$O_4^++O_2(a1d) \Rightarrow O_2^++O_2+O_2$	1e-16	[31]
O23	$O_4^++O_2(b1s) \Rightarrow O_2^++O_2+O_2$	1e-16	[31]
O24	$O_4^-+O_2(a1d) \Rightarrow O_2^-+O_2+O_2$	1e-16	[31]
O25	$O_4^-+O_2(b1s) \Rightarrow O_2^-+O_2+O_2$	1e-16	[31]
O26	$O_2^-+O_2(a1d) \Rightarrow O_2+O_2+e$	7e-16	[31]
O27	$O^-+O_2(a1d) \Rightarrow O_3+e$	6.1e-17	[31]
O28	$O^-+O_2(a1d) \Rightarrow O_2^-+O$	7.3e-16*exp(-890/T)	[31]
O29	$O_2^-+O_2(b1s) \Rightarrow O_2+O_2+e$	3.6e-16	[31]
O30	$O+O_3 \Rightarrow O_2+O_2$	1.43e-20*(T/300) 4.13	[31]
O31	$O+O+O_2 \Rightarrow O_2+O_2$	1.56e-45*(T/300) -3	[31]
O32	$O+O_2+O_2 \Rightarrow O_3+O_2$	6e-46*(T/300) -1.7	[31]
O33	$O_2(a1d) +O_3 \Rightarrow O_2+O_2+O$	3.5e-21*(T/300) 5.8	[31]
O34	$O_2(a1d) +O_2 \Rightarrow O_2+O_2$	2.2e-24*(T/300) 0.8	[31]
O35	$O_2(a1d) +O \Rightarrow O_2+O$	7e-22	[31]
O36	$O_2(b1s) +O_3 \Rightarrow O_2+O_2+O$	1.5e-17	[31]
O37	$O_2(b1s) +O_3 \Rightarrow O_2(a1d) +O_3$	3.3e-18	[31]
O38	$O_2(b1s) +O_2 \Rightarrow O_2(a1d) +O_2$	4.3e-28*T2.4*exp(-241/T)	[31]
O39	$O_2(b1s) +O \Rightarrow O_2(a1d) +O$	8.1e-20	[31]
O40	$O_2(b1s) +O \Rightarrow O_2+O(1d)$	8.1e-20	[31]
O41	$O_2(45) +O_2 \Rightarrow O_2(b1s) +O_2(b1s)$	2.9e-19	[31]
O42	$O_2(45) +O \Rightarrow O_2(b1s) +O(1d)$	9e-18	[31]
O43	$O(1d) +O_2 \Rightarrow O_2(a1d) +O$	0.25*6.4e-18*exp(67/T)	[32]
O44	$O(1d) +O_2 \Rightarrow O_2(b1s) +O$	2.56e-17*exp(67/T)	[32]
O45	$O(1d) +O_2 \Rightarrow O_2+O$	0.75*6.4e-18*exp(67/T)	[32]
O46	$O(1d) +O_3 \Rightarrow O_2+O+O$	1.2e-16	[32]
O47	$O(1d) +O_3 \Rightarrow O_2+O_2$	1.2e-16	[32]

O48	$O(1s) + O_2 => O + O_2(45)$	0.69*4.3e-18*exp(-850/T)	[32]
O49	$O(1s) + O_2 => O(1d) + O_2$	0.31*4.3e-18*exp(-850/T)	[32]
O50	$O(1s) + O_3 => O(1d) + O + O_2$	0.5*4.3e-16	[32]
O51	$O(1s) + O_3 => O_2 + O_2$	0.5*4.3e-16	[32]
O52	$O(1s) + O_2(a1d) => O_2(b1s) + O(1d)$	2.9e-17	[32]
O53	$O(1s) + O_2(a1d) => O_2(45) + O$	1.1e-16	[32]
O54	$O(1s) + O_2(a1d) => O + O + O$	3.2e-17	[32]
O55	$O(1s) + O => O(1d) + O$	5e-17*exp(-300/T)	[32]
O56	$O^- + O^+ => O + O$	7.51e-14*(300/T) 0.5	[31]
O57	$O^- + O_2^+ => O + O + O$	7.51e-14*(300/T) 0.5	[31]
O58	$O^- + O_4^+ => O + O_2 + O_2$	7.51e-14*(300/T) 0.5	[31]
O59	$O_2^- + O^+ => O_2 + O$	7.51e-14*(300/T) 0.5	[31]
O60	$O_2^- + O_2^+ => O_2 + O + O$	7.51e-14*(300/T) 0.5	[31]
O61	$O_2^- + O_4^+ => O_2 + O_2 + O_2$	7.51e-14*(300/T) 0.5	[31]
O62	$O_3^- + O^+ => O_3 + O$	7.51e-14*(300/T) 0.5	[31]
O63	$O_3^- + O_2^+ => O_3 + O + O$	7.51e-14*(300/T) 0.5	[31]
O64	$O_3^- + O_4^+ => O_3 + O_2 + O_2$	7.51e-14*(300/T) 0.5	[31]
O65	$O_4^- + O^+ => O_2 + O_2 + O$	7.51e-14*(300/T) 0.5	[31]
O66	$O_4^- + O_2^+ => O_2 + O_2 + O_2$	7.51e-14*(300/T) 0.5	[31]
O67	$O_4^- + O_4^+ => O_2 + O_2 + O_2 + O_2$	7.51e-14*(300/T) 0.5	[31]
O68	$O_2^- + O_2^+ + O_2 => O_2 + O_2 + O_2$	2e-37*(300/T) 2.5	[31]
O69	$O_2^- + O^+ + O_2 => O_2 + O + O_2$	2e-37*(300/T) 2.5	[31]
O70	$O^- + O^+ + O_2 => O + O + O_2$	2e-37*(300/T) 2.5	[31]
O71	$O_2^- + O^+ + O_2 => O_3 + O_2$	2e-37*(300/T) 2.5	[31]
O72	$O^- + O_2^+ + O_2 => O_3 + O_2$	2e-37*(300/T) 2.5	[31]
O73	$O^- + O^+ + O_2 => O_2 + O_2$	2e-37*(300/T) 2.5	[31]
O74	$O_3 + O_2 => O_2 + O + O_2$	7.3e-16*exp(-11400/T)	[31]
O75	$O_2(b1s) => O_2(a1s)$	1.5E-3	[33]
O76	$O_2(b1s) => O_2$	8.5E-2	[33]
O77	$O_2(a1s) => O_2$	2.6E-4	[33]
O78	$O_2(45) => O_2$	11	[33]

Table S3. Reactions Nitrogen-Oxygen with rate coefficient

No	Reaction	Rate Coefficient (m^6/s), (m^3/s)	Ref
	Electron Impact Reactions with NO		
E1	$e + NO => NO^-$	Cross Section	[34]
E2	$e + NO => e + NO$	Cross Section	[34]
E3	$e + NO => e + NO$	Cross Section	[34]

E4	e+NO=>e+NO	Cross Section	[34]
E5	e+NO=>e+NO	Cross Section	[34]
E6	e+NO=>e+NO	Cross Section	[34]
E7	e+NO=>e+NO	Cross Section	[34]
E8	e+NO=>e+NO	Cross Section	[34]
E9	e+NO=>e+e+NO^+	Cross Section	[34]
	Nitrogen-Oxygen Reactions		
R1	N^++O^-=>N+O	2.6e-13	[35]
R2	N^++O_2^-=>N+O_2	4e-13	[35]
R3	N_2^++O^-=>N_2+O	4e-13	[35]
R4	N_2^++O_2^-=>N_2+O_2	1.6e-13	[35]
R5	N_2+O_2^- =>O_2+N_2+e	1.9e-18*exp(-4990/T)	[35]
R6	N^++O=>O^++N	1e-18	[35]
R7	N^++O_2=>N+O_2^+	3e-16	[35]
R8	N_2^++N=>N^++N_2	1e-17	[35]
R9	N_2+O^+ =>N_2^++O	4.9e-15	[35]
R10	N_2+O+O =>O_2+N_2	2.76e-46*exp(720/T)	[35]
R11	N_2^++O=>O^++N_2	6e-18	[35]
R12	N_2^++O_2=>O_2^++N_2	4.7e-18	[35]
R13	N_2^++O_3=>O_2^++O+N_2	1e-16	[35]
R14	N_2+O+O_2 =>O_3+N_2	6.2e-46	[35]
R15	N+O^- =>NO+e	2.6e-16	[35]
R16	NO+O^- =>NO_2+e	2.6e-16	[35]
R17	N+O_2^- =>NO_2+e	5e-16	[35]
R18	N^++O_2=>NO^++O	2.6e-16	[35]
R19	N^++O_3=>NO^++O_2	5e-16	[35]
R20	N^++NO=>NO^++N	5.1e-16	[35]
R21	N^++NO=>N_2^++O	5e-17	[35]
R22	N^++NO_2=>NO+NO	5e-16	[35]
R23	NO^++O^-=>NO+O	4.9e-13	[35]
R24	NO^++O_2^-=>NO+O_2	4e-13	[35]
R25	N_2^++O=>NO^++N	1.4e-35	[35]
R26	N_2^++O_2=>NO^++NO	1e-23	[35]
R27	N_2+O^+ =>NO^++N	1.2e-18	[35]
R28	NO+O^+ =>NO^++O	1e-18	[35]
R29	NO_2+O^+ =>NO^++O_2	5e-16	[35]
R30	N+O_2^+ =>NO^++O	1.8e-16	[35]
R31	N_2+O_2^+ =>NO^++NO	1e-22	[35]

R32	$NO+O_2^+ \Rightarrow NO^+ + O_2$	3.5e-16	[35]
R33	$NO+O+O_2 \Rightarrow NO_2+O_2$	8.6e-44	[35]
R34	$NO+O+N_2 \Rightarrow NO_2+N_2$	1e-43	[35]
R35	$NO_2+O \Rightarrow NO+O_2$	1.3e-17*(T/1000)0.18	[35]
R36	$N+NO_2 \Rightarrow N_2+O+O$	9.1e-19	[35]
R37	$N+NO_2 \Rightarrow 2NO$	6e-19	[35]
R38	$NO_2+N \Rightarrow N_2+O_2$	7e-19	[35]
R39	$NO+NO+O_2 \Rightarrow 2NO_2$	1.4e-50	[35]
R40	$NO+O_3 \Rightarrow NO_2+O_2$	4.6e-20	[35]
R41	$N^+ + NO_2 \Rightarrow NO_2^+ + N$	3e-16	[35]
R42	$NO_2+O_2^+ \Rightarrow NO_2^+ + O_2$	6e-16	[35]
R43	$NO^+ + O_3 \Rightarrow NO_2^+ + O_2$	1e-20	[35]
R44	$NO_2^+ + NO \Rightarrow NO^+ + NO_2$	2.9e-16	[35]
R45	$N+NO_2 \Rightarrow N_2O+O$	3e-18	[35]
R46	$NO_2+O_3 \Rightarrow NO_3+O_2$	1.7e-22	[35]
R47	$NO_2^+ + O^- \Rightarrow NO+O_2$	4e-13	[35]
R48	$NO_2^+ + O_2^- \Rightarrow NO_2+O_2$	4e-13	[35]
R49	$NO_3+O \Rightarrow NO_2+O_2$	1e-17	[35]
R50	$NO+NO_3 \Rightarrow 2NO_2$	2e-17	[35]
R51	$NO+NO_3 \Rightarrow 2NO+O_2$	2.71e-17*(T)^ (-0.23) *exp(-947/T)	[35]
R52	$NO_2+NO_3 <=> N_2O_5$	1.1e-18	[35]
R53	$NO_3+NO_3 \Rightarrow 2NO_2+O_2$	1.2e-21	[35]
R54	$NO^+ + N_2O_5 \Rightarrow NO_2^+ + 2NO_2$	5.9e-16	[35]
R55	$N_2O_5+O_2^+ \Rightarrow NO_2^+ + NO_3 + O_2$	8.8e-16	[35]
R56	$N_2O_5+N_2 \Rightarrow NO_2+NO_3+N_2$	1.6e-25	[35]
R57	$N_2O_5+O_2 \Rightarrow NO_2+NO_3+O_2$	1.6e-25	[35]
R58	$e+NO^+ \Rightarrow N+O$	4e-13*(300/Te) 1.5	[35]
R59	$e+NO^+ \Rightarrow N(d)+O$	2e-13*(Te) -0.5	[36]
R60	$e+NO^+ \Rightarrow N+O(1d)$	2e-13*(Te) -0.5	[36]
R61	$e+NO_2^+ \Rightarrow NO+O$	2e-13*(Te) -0.5	[36]
R62	$e+NO_2^+ \Rightarrow NO+O(1d)$	2e-13*(Te) -0.5	[36]
R63	$N+O^- \Rightarrow NO+e$	0.26e-15	[36]
R64	$NO+O^- \Rightarrow NO_2+e$	0.26e-15	[36]
R65	$N_2+O^- \Rightarrow N_2O+e$	5e-19	[36]
R66	$e+NO \Rightarrow e+N+O$	6.4e-16	[36]
R67	$N_2(A)+O_2 \Rightarrow O+O+N_2$	1.5e-18	[37]
R68	$N_2(A)+NO_2 \Rightarrow NO+O+N_2$	1e-18	[37]
R69	$N_2(A)+N_2O \Rightarrow 2N_2+O$	0.8e-16	[37]

R70	$N_2(A) + O_2 \Rightarrow N_2O + O(1d)$	0.3e-19	[37]
R71	$N_2(A) + O_2 \Rightarrow N_2O + O$	2e-20*(T/300) 0.55	[37]
R72	$N_2(A) + O \Rightarrow NO + N(d)$	7e-18	[37]
R73	$N(d) + NO_2 \Rightarrow NO + NO$	1e-18	[37]
R74	$N(d) + O_2 \Rightarrow NO + O$	5.2e-18	[37]
R75	$N(d) + NO \Rightarrow N_2 + O$	1.8e-16	[37]
R76	$NO + O(1d) \Rightarrow O_2 + N$	1.7e-16	[37]
R77	$NO_2 + O(1d) \Rightarrow O_2 + NO$	2.5e-16	[37]
R78	$N_2O + O(1d) \Rightarrow 2NO$	7.2e-17	[37]
R79	$NO_2 + O(1d) \Rightarrow NO + O_2$	0.49e-16	[37]
R80	$N_2O + O(1d) \Rightarrow N_2 + O_2$	4.4e-17	[37]
R81	$N + O_3 \Rightarrow NO + O_2$	5e-22	[37]
R82	$N + NO \Rightarrow N_2 + O$	1.8e-17*(T/300) 0.5	[37]
R83	$N + O + N_2 \Rightarrow NO + N_2$	1e-44*(300/T) 0.5	[37]
R84	$N + O + O_2 \Rightarrow NO + O_2$	1e-44*(300/T) 0.5	[37]
R85	$NO_2 + O + O_2 \Rightarrow NO_3 + O_2$	8.9e-44*(T/300) -2	[37]
R86	$NO_2 + O + N_2 \Rightarrow NO_3 + N_2$	8.9e-44*(T/300) -2	[37]
R87	$N + NO_2 \Rightarrow N_2 + O + O$	0.9e-18	[37]
R88	$N + NO_2 \Rightarrow N_2O + O$	3e-18	[37]
R89	$N + O + O \Rightarrow O_2 + N$	3.2e-45*(300/T) 0.41	[37]
R90	$N + O \Rightarrow NO^+ + e$	2.33e-24*(T) 1.5*exp(-319000/T)	[37]
R91	$NO + O \Rightarrow O_2 + N$	7.5e-18*(T/300) -0.5	[37]
R92	$N + O_2 \Rightarrow NO + O$	3.2e-18*(T/300) *exp(-3150/T)	[37]
R93	$NO + O_3 \Rightarrow NO_2 + O_2$	2.5e-19*exp(-765/T)	[37]
R94	$NO + O_3 \Rightarrow NO_3 + O$	1.2e-19*exp(-2450/T)	[37]
R95	$N_2 + O + O \Rightarrow N_2 + O_2$	2.76e-46*exp(720/T)	[37]
R96	$NO + NO_3 \Rightarrow 2NO + O_2$	6.2e-11*(300/T) *exp(-25000/T)	[37]
R97	$N_2 + O \Rightarrow NO + N$	3e-16*exp(-38370/T)	[37]
R98	$NO + N_2 \Rightarrow N + O + N_2$	8.7e-15*exp(-75994/T)	[37]
R99	$NO + O \Rightarrow N + O + O$	17.4e-14*exp(-75994/T)	[37]
R100	$NO + NO \Rightarrow N + O + NO$	17.4e-14*exp(-75994/T)	[37]
R101	$NO_2 + O_2 \Rightarrow NO + O_3$	2.8e-18*exp(-25400/T)	[37]
R102	$NO_3 + O_2 \Rightarrow NO_2 + O_3$	1.5e-18*exp(-15020/T)	[37]
R103	$NO + O^+ \Rightarrow O_2^+ + N$	3e-16	[37]
R104	$NO_2 + O^+ \Rightarrow NO_2^+ + O$	1.6e-15	[37]
R105	$N_2^+ + NO \Rightarrow NO^+ + N_2$	3.3e-16	[37]
R106	$N_2^+ + NO_2 \Rightarrow NO_2^+ + N_2$	3.3e-16	[37]
R107	$N_2^+ + NO_2 \Rightarrow NO^+ + N_2O$	5e-17	[37]

R108	$N_2^+ + N_2O \Rightarrow NO^+ + N + N_2$	4e-16	[37]
R109	$N_2 + O_2^+ \Rightarrow NO^+ + NO$	1e-23	[37]
R110	$N + O_2^+ \Rightarrow NO^+ + O$	1.2e-16	[37]
R111	$N_2O + O^+ \Rightarrow NO^+ + NO$	2.3e-16	[37]
R112	$N_2^+ + O_2^- \Rightarrow N_2 + O_2$	2e-12*(T/300) -0.5	[37]
R113	$NO^+ + O_2^- \Rightarrow NO + O_2$	2e-12*(T/300) -0.5	[37]
R114	$NO_2^+ + O_2^- \Rightarrow NO_2 + O_2$	2e-12*(T/300) -0.5	[37]
R115	$NO^+ + O^- \Rightarrow NO + O$	3e-12*(T/300) -0.5	[37]
R116	$NO_2^+ + O^- \Rightarrow NO_2 + O$	3e-12*(T/300) -0.5	[37]
R117	$N_2^+ + O^- \Rightarrow N_2 + O$	3e-12*(T/300) -0.5	[37]
R118	$N + O_2 \Rightarrow NO + O$	8.9e-23	[38]
R119	$N(d) + O_2 \Rightarrow NO + O(1d)$	6e-18*exp(T/300) 0.5	[38]
R120	$NO + O_2(a1d) \Rightarrow NO + O_2$	2.5e-17	[35]
R121	$N + O_2(a1d) \Rightarrow NO + O$	2e-20*exp(-600/T)	[35]
R122	$N_2(A3s) + O_2 \Rightarrow N_2 + O + O$	2.54e-18	[35]
R123	$N_2(A3s) + O_2 \Rightarrow N_2O + O$	7.8e-20	[35]
R124	$N_2(A3s) + O_2^- \Rightarrow N_2 + O_2 + e$	2e-15	[35]
R125	$N_2(B3p) + O_2^- \Rightarrow N_2 + O_2 + e$	2.5e-16	[35]
R126	$N_2(B3p) + O^- \Rightarrow N_2 + O + e$	1.9e-15	[35]
R127	$N_2(A3s) + O^- \Rightarrow N_2 + O + e$	2.2e-15	[35]
R128	$NO + N_2(B3p) \Rightarrow NO + N_2(A3s)$	2.4e-16	[35]
R129	$N_2 + O_2(b1s) \Rightarrow N_2 + O_2(a1d)$	4.9e-21*exp(-253/T)	[35]
R130	$NO + O_2(b1s) \Rightarrow NO + O_2(a1d)$	4e-19	[35]
R131	$N(p) + NO \Rightarrow N_2(A3s) + O$	3.4e-17	[35]
R132	$N^+ + O_2 \Rightarrow NO^+ + O$	2.5e-17	[35]
R133	$N(d) + O^+ \Rightarrow N^+ + O$	1.3e-16	[37]
R134	$NO_2^+ + e \Rightarrow NO + O$	2e-13*(300/T) 0.5	[36]
R135	$N_2O^+ + e \Rightarrow N_2 + O$	2e-13*(300/T) 0.5	[36]
R136	$NO_2 + e \Rightarrow NO + O^-$	1e-17	[36]
R137	$N_2(A3s) + N_2O \Rightarrow N_2 + N + NO$	1e-17	[35]
R138	$N_2O + O(1d) \Rightarrow NO + NO$	7.2e-17	[36]
R139	$N^+ + NO \Rightarrow O^+ + N_2$	1e-18	[36]
R140	$N^+ + N_2O \Rightarrow NO^+ + N_2$	5.5e-16	[36]
R141	$N_2O + O^+ \Rightarrow N_2O^+ + O$	4e-15	[31]
R142	$N_2O + O^+ \Rightarrow O_2^+ + N_2$	2e-17	[31]
R143	$N_2^+ + N_2O \Rightarrow N_2O^+ + N_2$	5e-16	[31]
R144	$N + O_2^+ \Rightarrow NO^+ + O$	1.2e-16	[31]
R145	$NO + O_2^+ \Rightarrow NO^+ + O_2$	4.4e-16	[31]

R146	$NO_2+O_2^+ \Rightarrow NO^+ + O_3$	1e-17	[31]
R147	$NO_2+O_2^+ \Rightarrow NO_2^+ + O_2$	6.6e-16	[31]
R148	$N_3^+ + O_2 \Rightarrow O_2^+ + N + N_2$	2.3e-17	[31]
R149	$N_3^+ + O_2 \Rightarrow NO_2^+ + N_2$	4.4e-17	[31]
R150	$N_3^+ + NO \Rightarrow NO^+ + N_2 + N$	7e-17	[31]
R151	$N_3^+ + NO \Rightarrow N_2O^+ + N_2$	7e-17	[31]
R152	$N_2O^+ + NO \Rightarrow NO^+ + N_2O$	2.9e-16	[31]
R153	$N_4^+ + O_2 \Rightarrow O_2^+ + N_2 + N_2$	2.5e-16	[31]
R154	$NO + O_4^+ \Rightarrow NO^+ + O_2 + O_2$	1e-16	[36]
R155	$NO_2+O_2^- \Rightarrow NO_2^- + O_2$	8e-16	[31]
R156	$NO_2+O^- \Rightarrow NO_2^- + O$	1.2e-13	[31]
R157	$N_2O + O^- \Rightarrow NO^- + NO$	2e-16	[31]
R158	$NO_2+O_3^- \Rightarrow O_3 + NO_2^-$	7e-16	[31]
R159	$NO^- + O_2 \Rightarrow O_2^- + NO$	5e-16	[36]
R160	$NO_3+O_2^- \Rightarrow O_2 + NO_3^-$	5e-16	[37]
R161	$N_2O+O_2^- \Rightarrow O_3^- + N_2$	5e-16	[37]
R162	$NO_2+O^- \Rightarrow NO^- + NO$	1.2e-15	[37]
R163	$N_2O+O^- \Rightarrow N_2O^- + O$	2e-18	[37]
R164	$NO+O_3^- \Rightarrow NO_3^- + O$	1e-17	[37]
R165	$NO+O_3^- \Rightarrow NO_2^- + O_2$	2.6e-18	[37]
R166	$NO_2+O_3^- \Rightarrow NO_2^- + O_3$	7e-16	[37]
R167	$NO_2+O_3^- \Rightarrow NO_3^- + O_2$	2e-17	[37]
R168	$NO_3+O_3^- \Rightarrow NO_3^- + O_3$	5e-16	[37]
R169	$NO^- + O_2 \Rightarrow O_2^- + NO$	5e-16	[31]
R170	$NO^- + NO_2 \Rightarrow NO_2^- + NO$	7.4e-22	[31]
R171	$NO^- + N_2O \Rightarrow NO_2^- + N_2$	2.8e-20	[31]
R172	$NO_2^- + O_3 \Rightarrow NO_3^- + O_2$	1.8e-17	[31]
R173	$NO_2^- + NO_2 \Rightarrow NO_3^- + NO$	4e-18	[31]
R174	$NO_2^- + NO_3 \Rightarrow NO_3^- + NO_2$	5e-16	[31]
R175	$NO_2^- + N_2O_5 \Rightarrow NO_3^- + NO_3 + NO$	7e-16	[31]
R176	$NO_3^- + NO \Rightarrow NO_2^- + NO_2$	3e-21	[31]
R177	$NO + O_4^- \Rightarrow NO_3^- + O_2$	2.5e-16	[31]
R178	$N + O_2(a1d) \Rightarrow NO + O$	1e-22	[37]
R179	$N_2 + O(1d) \Rightarrow O + N_2$	2.6e-17	[37]
R180	$N_2(A3s) + O \Rightarrow NO + N$	7e-20	[35]
R181	$N_2(a1s) + O_2 \Rightarrow N_2 + O + O$	2.8e-17	[35]
R182	$N_2(a1s) + NO \Rightarrow N_2 + N + O$	3.6e-16	[35]
R183	$N_2(A3s) + N_2(a1s) \Rightarrow N_4^+ + e$	5e-17	[35]

R184	$N_2(a1s) + N_2(a1s) \Rightarrow N_4^+ + e$	2e-16	[35]
R185	$N_2 + O_2(a1d) \Rightarrow O_2 + N_2$	1.7e-16	[35]
R186	$N_2(A3s) + N_2 \Rightarrow 2N_2$	2.7e-17	[35]
R187	$N_2(A3s) + NO_2 \Rightarrow NO + O + N_2$	1e-18	[35]
R188	$N_2(A3s) + N_2O \Rightarrow 2N_2 + O$	8e-17	[35]
R189	$N_2(A3s) + N_2O \Rightarrow N_2 + N + NO$	8e-17	[35]

Table S4. Reaction set for Argon with Rate Coefficient

No	Reaction	$\Delta\varepsilon$ (eV)	Rate coefficient (m^6/s), (m^3/s)	Ref
	Electron Impact Reactions with Argon			
E1	$e + Ar \Rightarrow e + Ar$	0.136E-04	Cross section	[39]
E2	$e + Ar \Rightarrow e + Ar(s)$	11.50	Cross section	[39]
E3	$e + Ar(s) \Rightarrow e + Ar$	-11.50	Cross section	[39]
E4	$e + Ar \Rightarrow 2e + Ar^+$	15.80	Cross section	[39]
E5	$e + Ar(s) \Rightarrow 2e + Ar^+$	4.427	Cross section	[39]
	Argon Reactions			
A1	$Ar(s) + Ar \Rightarrow Ar + Ar$		1807	[38]
A2	$Ar^+ + Ar + Ar \Rightarrow Ar_2^+ + Ar$		2.5e-43*(300/T) 1.5	[38]
A3	$Ar(s) + Ar(s) \Rightarrow e + Ar + Ar^+$		3.3734e8	[38]
A4	$e + Ar_2^+ \Rightarrow Ar + Ar$		7.34e-14*(Te)-0.67*(T/300) -0.58	[38]

Table S5. Reaction set for Argon & Oxygen& Nitrogen with Rate Coefficient

No	Reaction	Rate Coefficient (m^6/s), (m^3/s)	Ref
R1	$Ar^+ + O^- \Rightarrow Ar + O$	7.51e-14*(300/T) 0.5	[40]
R2	$Ar^+ + O_2^- \Rightarrow Ar + O_2$	7.51e-14*(300/T) 0.5	[40]
R3	$Ar^+ + O_3^- \Rightarrow Ar + O_3$	7.51e-14*(300/T) 0.5	[40]
R4	$Ar^+ + O_4^- \Rightarrow Ar + 2O_2$	7.51e-14*(300/T) 0.5	[40]
R5	$Ar(s) + Ar \Rightarrow Ar + Ar$	1807	[40]
R6	$Ar(s) + O_2 \Rightarrow Ar + O + O$	0.46*2.2e-16	[40]
R7	$Ar(s) + O_2 \Rightarrow Ar + O + O(1d)$	0.52*2.2e-16	[40]
R8	$Ar(s) + O_2 \Rightarrow Ar + O + O(1s)$	0.02*2.2e-16	[40]
R9	$Ar(s) + O \Rightarrow Ar + O$	4.1e-17	[38]
R10	$Ar + O + O_2 \Rightarrow O_3 + Ar$	3.9e-46*(300/T) 1.9	[40]
R11	$Ar + O_2(b1s) \Rightarrow O_2 + Ar$	1.5e-23	[40]
R12	$Ar^+ + Ar + Ar \Rightarrow Ar_2^+ + Ar$	2.5e-43*(300/T) 1.5	[40]
R13	$Ar_2^+ + O^- \Rightarrow 2Ar + O$	7.51e-14*(300/T) 0.5	[40]
R14	$Ar_2^+ + O_2^- \Rightarrow 2Ar + O_2$	7.51e-14*(300/T) 0.5	[40]
R15	$Ar_2^+ + O_3^- \Rightarrow 2Ar + O_3$	7.51e-14*(300/T) 0.5	[40]

R16	$Ar_2^+ + O_4^- \Rightarrow 2Ar + 2O_2$	7.51e-14*(300/T) 0.5	[38]
R17	$Ar(s) + Ar(s) \Rightarrow e + Ar + Ar^+$	3.3734e8	[38]
R18	$Ar + O(1d) \Rightarrow Ar + O$	2.0947e-17*exp(-309.4467/T)	[40]
R19	$Ar^+ + O_2 \Rightarrow Ar + O_2^+$	6.3e-17*exp(T/300) -0.78	[40]
R20	$Ar^+ + O \Rightarrow Ar + O^+$	6.4e-18	[40]
R21	$Ar + O(1s) \Rightarrow Ar + O(1d)$	5e-23	[40]
R22	$Ar + 2O \Rightarrow Ar + O_2(A)$	9.85e-41	[40]
R23	$Ar + O_2(A) \Rightarrow Ar + O_2$	3e-24*exp(-200/T)	[40]
R24	$Ar + O_2(B) \Rightarrow Ar + O_2(A)$	1e-23	[40]
R25	$Ar + O_4^+ \Rightarrow Ar + O_2^+ + O_2$	3e-23	[40]
R26	$O_2 + Ar_2^+ \Rightarrow 2Ar + O_2^+$	1.2e-16	[40]
R27	$Ar + 2O \Rightarrow Ar + O_2$	4.5e-40*exp(630/T)	[38]
R28	$e + Ar_2^+ \Rightarrow 2Ar$	7.34e-14*(Te)-0.67*(T/300)-0.58	[40]
R29	$Ar + O_2(B) \Rightarrow O_2 + Ar$	1e-22	[40]
R30	$Ar + O \Rightarrow O + Ar$	3e-19	[40]
R31	$Ar^+ + O_2(A) \Rightarrow Ar + O_2^+$	5e-17	[40]
R32	$Ar^+ + O_2(B) \Rightarrow Ar + O_2^+$	5e-17	[40]
R33	$Ar + O^+ \Rightarrow Ar^+ + O$	2.1e-17	[40]
R34	$Ar + O_2^+ \Rightarrow Ar^+ + O_2$	2.1e-17	[40]
R35	$Ar + O(1d) \Rightarrow Ar + O$	5e-18	[40]
R36	$Ar + 2O \Rightarrow Ar + O_2$	2.45e-43*(T) -0.63	[40]
R37	$Ar + NO + O \Rightarrow Ar + NO_2$	1e-43*(T/300) -1.6	[38]
R38	$Ar + NO_2 + O \Rightarrow Ar + NO_3$	9e-44*(T/300) 2*exp(-0/T)	[38]
R39	$Ar + N_2 + N_2^+ \Rightarrow Ar + N_4^+$	1.8e6	[38]