

CO₂ 放电初始反应集合

表 1 CO₂ 放电初始反应集合中由 Bolsig+ 计算速率系数的电子碰撞反应及其参考文献

Tab. 1 The electron impact reactions with reaction rate coefficients calculated by Bolsig+ included in the initial reaction set of CO₂ discharge and the corresponding references

序号	反应	速率系数	参考文献	备注
X01	$e + \text{CO}_2 \rightarrow e + \text{CO}_2$	$f(\sigma)$	[1]	(a)
X02 _x	$e + \text{CO}_2 \rightarrow e + \text{CO}_2\text{v}_x$	$f(\sigma)$	[1]	
X03 _i	$e + \text{CO}_2 \rightarrow e + \text{CO}_2\text{v}_i$	$f(\sigma)$	[1]	(b)
X04 _{i,j}	$e + \text{CO}_2\text{v}_i \rightarrow e + \text{CO}_2\text{v}_j$	$f(\sigma)$	[1]	(b), $i < j$
X05 _i	$e + \text{CO}_2 \rightarrow e + \text{CO}_2\text{e}_i$	$f(\sigma)$	[1]	
X06	$e + \text{CO}_2 \rightarrow 2e + \text{CO}_2^+$	$f(\sigma)$	[1]	
X07 _x	$e + \text{CO}_2\text{v}_x \rightarrow 2e + \text{CO}_2^+$	$f(\sigma)$	[1]	(c)
X08 _i	$e + \text{CO}_2\text{v}_i \rightarrow 2e + \text{CO}_2^+$	$f(\sigma)$	[1]	(c)
X09 _i	$e + \text{CO}_2\text{e}_i \rightarrow 2e + \text{CO}_2^+$	$f(\sigma)$	[1]	(d)
X10	$e + \text{CO}_2 \rightarrow 2e + \text{O} + \text{CO}^+$	$f(\sigma)$	[1]	
X11 _x	$e + \text{CO}_2\text{v}_x \rightarrow 2e + \text{O} + \text{CO}^+$	$f(\sigma)$	[1]	(e)
X12 _i	$e + \text{CO}_2\text{v}_i \rightarrow 2e + \text{O} + \text{CO}^+$	$f(\sigma)$	[1]	(e)
X13 _i	$e + \text{CO}_2\text{e}_i \rightarrow 2e + \text{O} + \text{CO}^+$	$f(\sigma)$	[1]	(d)
X14	$e + \text{CO}_2 \rightarrow 2e + \text{CO} + \text{O}^+$	$f(\sigma)$	[1]	
X15 _x	$e + \text{CO}_2\text{v}_x \rightarrow 2e + \text{CO} + \text{O}^+$	$f(\sigma)$	[1]	(e)
X16 _i	$e + \text{CO}_2\text{v}_i \rightarrow 2e + \text{CO} + \text{O}^+$	$f(\sigma)$	[1]	(e)
X17 _i	$e + \text{CO}_2\text{e}_i \rightarrow 2e + \text{CO} + \text{O}^+$	$f(\sigma)$	[1]	(d)
X18	$e + \text{CO}_2 \rightarrow e + \text{CO} + \text{O}$	$f(\sigma)$	[1]	
X19 _x	$e + \text{CO}_2\text{v}_x \rightarrow e + \text{CO} + \text{O}$	$f(\sigma)$	[1]	(e)
X20 _i	$e + \text{CO}_2\text{v}_i \rightarrow e + \text{CO} + \text{O}$	$f(\sigma)$	[1]	(e)
X21 _i	$e + \text{CO}_2\text{e}_i \rightarrow e + \text{CO} + \text{O}$	$f(\sigma)$	[1]	(d)
X22	$e + \text{CO}_2 \rightarrow \text{CO} + \text{O}^-$	$f(\sigma)$	[1]	
X23 _x	$e + \text{CO}_2\text{v}_x \rightarrow \text{CO} + \text{O}^-$	$f(\sigma)$	[1]	(e)
X24 _i	$e + \text{CO}_2\text{v}_i \rightarrow \text{CO} + \text{O}^-$	$f(\sigma)$	[1]	(e)
X25 _i	$e + \text{CO}_2\text{e}_i \rightarrow \text{CO} + \text{O}^-$	$f(\sigma)$	[1]	(c)
X26	$e + \text{CO} \rightarrow 2e + \text{CO}^+$	$f(\sigma)$	[2]	
X27	$e + \text{CO} \rightarrow 2e + \text{C}^+ + \text{O}$	$f(\sigma)$	[2]	
X28	$e + \text{CO} \rightarrow \text{C} + \text{O}^-$	$f(\sigma)$	[2]	
X29	$e + \text{CO} \rightarrow e + \text{C} + \text{O}$	$f(\sigma)$	[2]	

续表 1 CO₂ 放电初始反应集合中由 Bolsig+ 计算速率系数的电子碰撞反应及其参考文献

Tab. 1 The electron impact reactions with reaction rate coefficients calculated by Bolsig+ included in the initial reaction set of CO₂ discharge and the corresponding references (continued)

序号	反应	速率系数	参考文献	备注
X30	$e + C \rightarrow 2e + C^+$	$f(\sigma)$	[3]	
X31	$e + O \rightarrow 2e + O^+$	$f(\sigma)$	[4]	
X32	$e + O_2 \rightarrow 2O + e$	$f(\sigma)$	[5]	
X33	$e + O_2 \rightarrow O + O^-$	$f(\sigma)$	[5]	
X34	$e + O_2 \rightarrow 2e + O_2^+$	$f(\sigma)$	[5]	
X35	$e + O_3 \rightarrow O_2 + O^-$	$f(\sigma)$	[6]	
X36	$e + O_3 \rightarrow O_2^- + O$	$f(\sigma)$	[6]	
X37	$e + O_3 \rightarrow O + O_2 + e$	$f(\sigma)$	[7]	
X38	$e + O_3 \rightarrow O_2^+ + O + 2e$	$f(\sigma)$	[7]	

- (a) 使用相同的碰撞截面计算电子和振动激发态 CO₂ 的弹性碰撞过程的速率系数。
- (b) 使用 Fridman 近似对碰撞横截面进行修改。
- (c) 使用与基态 CO₂ 分子相同的横截面。
- (d) 使用电子激发态 CO₂ 分子的能量阈值对横截面进行修正。
- (e) 使用振动激发态 CO₂ 分子的能量阈值对横截面进行修正。

表 2 CO₂ 放电初始反应集合中包含的电子-离子复合反应和电子吸附反应，以及相应的速率系数和参考文献

Tab. 2 The electron-ion recombination reactions and electron attachment reactions included in the initial reaction set of CO₂ discharge, as well as the corresponding rate coefficients and references

序号	反应	速率系数	参考文献	备注
E01	$e + O_2^+ \rightarrow O + O$	$6.0 \times 10^{-7} T_e^{-0.5} T_g^{-0.5}$	[8]	
E02	$e + CO_2^+ \rightarrow CO + O$	$2.0 \times 10^{-5} T_e^{-0.5} T_g^{-1}$	[9]	
E03	$e + CO_2^+ \rightarrow O_2 + C$	$3.94 \times 10^{-7} T_e^{-0.4}$	[8]	
E04	$e + O_2 + CO_2 \rightarrow O_2^- + CO_2$	$2.2 \times 10^{-29} (300/T_g)^{1.5} \exp(-600/T_g)$	[10]	
E05	$e + O_3 + O_2 \rightarrow O_3^- + O_2$	4.6×10^{-28}	[10]	
E06	$e + O_2^+ + CO_2 \rightarrow O_2 + CO_2$	1.0×10^{-26}	[11]	

表 3 CO₂ 放电初始反应集合中包含的离子-中性反应和离子-离子反应，以及相应的速率系数和参考文献

Tab. 3 The ion-neutral reactions and ion-ion reactions included in the initial reaction set of CO₂ discharge, as well as the corresponding rate coefficients and references

序号	反应	速率系数	参考文献	备注
I01	$O^- + O \rightarrow O_2 + e$	2.3×10^{-10}	[8]	
I02	$O^- + O_2 \rightarrow e + O + O_2$	6.9×10^{-10}	[10]	
I03	$O^- + O_3 \rightarrow 2O_2 + e$	3.0×10^{-10}	[12]	
I04	$O^- + O_3 \rightarrow O_3^- + O$	8.0×10^{-10}	[9]	
I05	$O^- + C \rightarrow CO + e$	5.0×10^{-10}	[11]	
I06	$O^- + CO_2 \rightarrow O + CO_2 + e$	4.0×10^{-12}	[13]	
I07	$O^- + CO \rightarrow CO_2 + e$	5.5×10^{-10}	[14]	
I08	$O^- + O_2^+ \rightarrow O_2 + O$	$2.6 \times 10^{-8} (300/T_g)^{0.44}$	[8]	
I09	$O^- + O_2^+ \rightarrow 3O$	$4.2 \times 10^{-7} (300/T_g)^{0.44}$	[8]	
I10 _x	$O^- + CO_2^+ \rightarrow O + CO_2$	1.0×10^{-7}	[15]	
I11 _i	$O^- + CO_2 + O_2 \rightarrow CO_3^- + O_2$	3.1×10^{-28}	[16]	
I12	$O^- + CO_2 + CO \rightarrow CO_3^- + CO$	1.5×10^{-28}	[16]	
I13	$O^- + CO_2 + CO_2 \rightarrow CO_3^- + CO_2$	9.0×10^{-29}	[10]	
I14	$O_2^- + O \rightarrow O_2 + O^-$	3.3×10^{-10}	[8]	
I15	$O_2^- + O \rightarrow O_3 + e$	3.3×10^{-10}	[9]	
I16 _x	$O_2^- + O_3 \rightarrow O_3^- + O_2$	4.0×10^{-10}	[9]	
I17 _i	$O_2^- + CO_2^+ \rightarrow CO + O_2 + O$	6.0×10^{-7}	[14]	
I18	$O_2^- + CO_2 + O_2 \rightarrow CO_4^- + O_2$	4.7×10^{-27}	[10]	
I19 _x	$O_2^- + CO_2 + CO_2 \rightarrow CO_4^- + CO_2$	1.0×10^{-29}	[10]	
I20 _i	$O_3^- + O \rightarrow O_2^- + O_2$	2.5×10^{-10}	[9]	
I21	$O_3^- + CO_2 \rightarrow CO_3^- + O_2$	5.5×10^{-10}	[9]	
I22	$O^+ + CO_2 \rightarrow O_2^+ + CO$	9.4×10^{-10}	[9]	
I23	$O^+ + CO_2 \rightarrow O + CO_2^+$	4.5×10^{-10}	[9]	(a)
I24 _i	$O^+ + CO_2 e_i \rightarrow O + CO_2^+$	$4.5 \times 10^{-10} (E_H^2/E_{Ei}^2)$	[9]	(b), $i = 1, 2$
I25	$O_2^+ + C \rightarrow CO^+ + O$	5.2×10^{-11}	[9]	
I26	$O_2^+ + C \rightarrow C^+ + O_2$	5.2×10^{-11}	[9]	
I27	$O_2^+ + O_2^- \rightarrow 2O_2$	$2.0 \times 10^{-7} (300/T_g)^{0.5}$	[8]	
I28	$O_2^+ + O_2^- \rightarrow O_2 + 2O$	4.2×10^{-7}	[8]	
I29	$O_2^+ + CO_4^- \rightarrow CO_2 + 2O_2$	3.0×10^{-7}	[9]	
I30	$C^+ + CO_2 \rightarrow CO + + CO$	1.1×10^{-9}	[9]	(a)
I31 _i	$C^+ + CO_2 e_i \rightarrow CO^+ + CO$	$1.1 \times 10^{-9} (E_H^2/E_{Ei}^2)$	[9]	(b), $i = 1, 2$

续表 3 CO₂ 放电初始反应集中包含的离子-中性反应和离子-离子反应，以及相应的速率系数和参考文献

Tab. 3 The ion-neutral reactions and ion-ion reactions included in the initial reaction set of CO₂ discharge, as well as the corresponding rate coefficients and references (continued)

序号	反应	速率系数	参考文献	备注
I32	$\text{CO}^+ + \text{CO}_2 \rightarrow \text{CO}_2^+ + \text{CO}$	1.0×10^{-9}	[17]	(a)
I33 _i	$\text{CO}^+ + \text{CO}_2\text{e}_i \rightarrow \text{CO}_2^+ + \text{CO}$	$1.1 \times 10^{-9}(\text{E}_{\text{H}}^2/\text{E}_{\text{Ei}}^2)$	[17]	(b), $i = 1, 2$
I34	$\text{CO}_2^+ + \text{O} \rightarrow \text{O}_2^+ + \text{CO}$	1.64×10^{-10}	[10]	
I35	$\text{CO}_2^+ + \text{O} \rightarrow \text{CO}_2 + \text{O}^+$	9.62×10^{-11}	[9]	
I36	$\text{CO}_2^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{CO}_2$	6.4×10^{-11}	[10]	
I37	$\text{CO}_3^- + \text{CO} \rightarrow 2\text{CO}_2 + \text{e}$	5.0×10^{-13}	[18]	
I38	$\text{CO}_3^- + \text{CO}_2^+ \rightarrow 2\text{CO}_2 + \text{O}$	5.0×10^{-7}	[18]	
I39	$\text{CO}_3^- + \text{O} \rightarrow \text{CO}_2 + \text{O}_2^-$	8.0×10^{-11}	[18]	
I40	$\text{CO}_3^- + \text{O}_2^+ \rightarrow \text{CO}_2 + \text{O}_2 + \text{O}$	3.0×10^{-7}	[9]	
I41	$\text{CO}_4^- + \text{CO}_2^+ \rightarrow 2\text{CO}_2 + \text{O}_2$	5.0×10^{-7}	[9]	
I42	$\text{CO}_4^- + \text{O} \rightarrow \text{O}_3^- + \text{CO}_2$	1.4×10^{-10}	[9]	
I43	$\text{CO}_4^- + \text{O} \rightarrow \text{CO}_3^- + \text{O}_2$	1.1×10^{-10}	[9]	
I44	$\text{CO}_4^- + \text{O} \rightarrow \text{CO}_2 + \text{O}_2 + \text{O}^-$	1.4×10^{-11}	[9]	

(a) 电子激发态 CO₂ 分子除外。

(b) 使用电子激发态 CO₂ 分子的能量阈值对横截面进行修正。

表 4 CO₂ 放电初始反应集中包含的中性粒子反应，以及相应的速率系数和参考文献

Tab. 4 The neutral reactions included in the initial reaction set of CO₂ discharge, as well as the corresponding rate coefficients and references

序号	反应	速率系数	参考文献	备注
N01	$\text{O}_2 + \text{C} \rightarrow \text{O} + \text{CO}$	3.0×10^{-11}	[8]	
N02	$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	$2.8 \times 10^{-11} \exp(-26500/T_g)$	[8]	(a)
N03	$\text{CO}_2\text{v} + \text{O} \rightarrow \text{CO} + \text{O}_2$	$k_R(E_v, T_g)$	[8]	(b)
N04	$\text{CO}_2 + \text{C} \rightarrow 2\text{CO}$	1.0×10^{-15}	[8]	
N05	$\text{O} + \text{O}_2 + \text{CO}_2 \rightarrow \text{O}_3 + \text{CO}_2$	$1.7 \times 10^{-30} T_g^{-1.2}$	[13]	
N06	$\text{O} + \text{O} + \text{CO}_2 \rightarrow \text{O}_2 + \text{CO}_2$	$3.81 \times 10^{-30} T_g^{-1} \exp(-529/T_g)$	[13]	
N07	$\text{CO}_2 + \text{CO}_2 \rightarrow \text{CO} + \text{O} + \text{CO}_2$	$3.91 \times 10^{-10} T_g^{-1} \exp(-49430/T_g)$	[19]	(a)
N08	$\text{CO}_2\text{v} + \text{CO}_2 \rightarrow \text{CO} + \text{O} + \text{CO}_2$	$k_R(E_v, T_g)$	[19]	(b)

(a) 振动激发态 CO₂ 分子除外。

(b) 由于涉及振动激发态的反应活化能的变化，速率系数有所改变。

表 5 CO₂ 放电初始反应集中包含的振动能量交换反应，以及相应的速率系数和参考文献

Tab. 5 The vibrational energy exchange reactions included in the initial reaction set of CO₂ discharges, as well as the corresponding rate coefficients and references

序号	反应	速率系数	参考文献	备注
V01	CO ₂ v _a + M → CO ₂ + M	$7.14 \times 10^{-8} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V02	CO ₂ v _b + M → CO ₂ + M	$1.071 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V03	CO ₂ v _b + M → CO ₂ v _a + M	$1.438 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V04	CO ₂ v _c + M → CO ₂ v _a + M	$1.071 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V05	CO ₂ v _c + M → CO ₂ v _b + M	$2.897 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V06	CO ₂ v _d + M → CO ₂ v _b + M	$1.528 \times 10^{-5} \exp(-272T_g^{-1/3} + 437T_g^{-2/3})$	[20]	(b)
V07 _i	CO ₂ v _d + M → CO ₂ v _c + M	$4.321 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V08	CO ₂ v _d + M → CO ₂ v ₁ + M	$1.775 \times 10^{-11} \exp(-108T_g^{-1/3} + 165T_g^{-2/3})$	[20]	(c)
V09	CO ₂ v _{1a} + M → CO ₂ v _c + M	$8.57 \times 10^{-1} \exp(-404T_g^{-1/3} + 1096T_g^{-2/3})$	[20]	(d)
V10	CO ₂ v _{1a} + M → CO ₂ v _d + M	$1.431 \times 10^{-5} \exp(-252T_g^{-1/3} + 685T_g^{-2/3})$	[20]	(d)
V11	CO ₂ v _{1a} + M → CO ₂ v ₁ + M	$7.14 \times 10^{-8} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V12	CO ₂ v _{1b} + M → CO ₂ v _c + M	$3.218 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V13	CO ₂ v _{1b} + M → CO ₂ v _d + M	$6.447 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V14	CO ₂ v _{1b} + M → CO ₂ v _{1a} + M	$6.447 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V15	CO ₂ v _{1b} + M → CO ₂ v ₁ + M	$1.071 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V16	CO ₂ v _{1c} + M → CO ₂ v _{1a} + M	$1.071 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V17	CO ₂ v _{1c} + M → CO ₂ v _{1b} + M	$2.897 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V18	CO ₂ v _s + M → CO ₂ v _a + M	$1.071 \times 10^{-9} \exp(-137T_g^{-1/3})$	[20]	(b)
V19	CO ₂ v _s + M → CO ₂ v _b + M	$2.897 \times 10^{-7} \exp(-177T_g^{-1/3} + 451T_g^{-2/3})$	[20]	(a)
V20	CO ₂ v ₁ + M → CO ₂ v _a + M	$4.25 \times 10^{-1} \exp(-407T_g^{-1/3} - 824T_g^{-2/3})$	[20]	(d)
V21	CO ₂ v ₁ + M → CO ₂ v _b + M	$8.568 \times 10^{-1} \exp(-404T_g^{-1/3} - 1096T_g^{-2/3})$	[20]	(d)
V22	CO ₂ v ₁ + M → CO ₂ v _c + M	$1.43 \times 10^{-5} \exp(-252T_g^{-1/3} - 685T_g^{-2/3})$	[20]	(d)
V23	CO ₂ v ₁ + M → CO ₂ v _s + M	$1.43 \times 10^{-5} \exp(-252T_g^{-1/3} - 685T_g^{-2/3})$	[20]	(d)
V24	CO ₂ v ₁ + M → CO ₂ v _{1a} + M	$8.568 \times 10^{-1} \exp(-406T_g^{-1/3} - 829T_g^{-2/3})$	[20]	(d)
V25	CO ₂ v ₂ + M → CO ₂ v _{1b} + M	$1.725 \times 10^{-1} \exp(-404T_g^{-1/3} - 1098T_g^{-2/3})$	[20]	(d)
V26	CO ₂ v ₂ + M → CO ₂ v _{1c} + M	$2.882 \times 10^{-5} \exp(-253T_g^{-1/3} - 683T_g^{-2/3})$	[20]	(d)
V27 _i	CO ₂ v _i + M → CO ₂ v _{i-1} + M	$f(k(VT_{v_1-v_a}), k(VT_{v_1-v_b}))$	[20]	(e) i=1, ..., 8
V28	CO ₂ v _b + CO ₂ → CO ₂ v _a + CO ₂ v _a	$2.157 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V29	CO ₂ v _c + CO ₂ → CO ₂ v _a + CO ₂ v _b	$5.305 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V30	CO ₂ v _d + CO ₂ → CO ₂ v _a + CO ₂ v _c	$6.48 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V31	CO ₂ v _d + CO ₂ → CO ₂ v _b + CO ₂ v _b	$2.384 \times 10^{-9} \exp(-89T_g^{-1/3} - 234T_g^{-2/3})$	[20]	
V32	CO ₂ v _{1a} + CO ₂ → CO ₂ v ₁ + CO ₂ v _a	$1.071 \times 10^{-9} \exp(-88T_g^{-1/3} - 230T_g^{-2/3})$	[20]	

续表 5 CO₂ 放电初始反应集合中包含的振动能量交换反应，以及相应的速率系数和参考文献

Tab. 5 The vibrational energy exchange reactions included in the initial reaction set of CO₂ discharges, as well as the corresponding rate coefficients and references (continued)

序号	反应	速率系数	参考文献	备注
V33	$\text{CO}_2\text{V}_{1b} + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_a + \text{CO}_2\text{V}_d$	$9.667 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V34	$\text{CO}_2\text{V}_{1c} + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_a + \text{CO}_2\text{V}_d$	$2.378 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V35	$\text{CO}_2\text{V}_s + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_a + \text{CO}_2\text{V}_b$	$5.305 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V36	$\text{CO}_2\text{V}_1 + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_a + \text{CO}_2\text{V}_b$	$1.06 \times 10^{-5} \exp(-242T_g^{-1/3} - 633T_g^{-2/3})$	[20]	
V37	$\text{CO}_2\text{V}_2 + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_a + \text{CO}_2\text{V}_{1b}$	$4.299 \times 10^{-5} \exp(-241T_g^{-1/3} - 635T_g^{-2/3})$	[20]	
V38	$\text{CO}_2\text{V}_2 + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_b$	$4.299 \times 10^{-5} \exp(-241T_g^{-1/3} - 637T_g^{-2/3})$	[20]	
V39 _i	$\text{CO}_2\text{V}_i + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_{i-1} + \text{CO}_2\text{V}_a$	$2.03 \times 10^{-5} \exp(-242T_g^{-1/3} - 633T_g^{-2/3})$	[20]	$i=1, \dots, 8$
V40 _i	$\text{CO}_2\text{V}_i + \text{CO}_2 \rightarrow \text{CO}_2\text{V}_{i-1} + \text{CO}_2\text{V}_b$	$2.03 \times 10^{-5} \exp(-242T_g^{-1/3} - 633T_g^{-2/3})$	[20]	$i=1, \dots, 8$
V41	$\text{CO}_2\text{V}_c + \text{CO}_2\text{V}_a \rightarrow \text{CO}_2\text{V}_b + \text{CO}_2\text{V}_b$	$5.305 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V42	$\text{CO}_2\text{V}_d + \text{CO}_2\text{V}_a \rightarrow \text{CO}_2\text{V}_b + \text{CO}_2\text{V}_c$	$1.442 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V43	$\text{CO}_2\text{V}_d + \text{CO}_2\text{V}_b \rightarrow \text{CO}_2\text{V}_c + \text{CO}_2\text{V}_c$	$2.628 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V44	$\text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_a \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_b$	$2.157 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V45	$\text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_b \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_c$	$4.344 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V46	$\text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_c \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_d$	$6.48 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V47	$\text{CO}_2\text{V}_{1b} + \text{CO}_2\text{V}_a \rightarrow \text{CO}_2\text{V}_b + \text{CO}_2\text{V}_d$	$9.667 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V48	$\text{CO}_2\text{V}_{1b} + \text{CO}_2\text{V}_b \rightarrow \text{CO}_2\text{V}_c + \text{CO}_2\text{V}_d$	$4.332 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V49	$\text{CO}_2\text{V}_{1b} + \text{CO}_2\text{V}_c \rightarrow \text{CO}_2\text{V}_d + \text{CO}_2\text{V}_d$	$5.848 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V50	$\text{CO}_2\text{V}_{1c} + \text{CO}_2\text{V}_a \rightarrow \text{CO}_2\text{V}_b + \text{CO}_2\text{V}_d$	$5.292 \times 10^{-8} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V51	$\text{CO}_2\text{V}_{1c} + \text{CO}_2\text{V}_b \rightarrow \text{CO}_2\text{V}_b + \text{CO}_2\text{V}_d$	$1.066 \times 10^{-7} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V52	$\text{CO}_2\text{V}_{1c} + \text{CO}_2\text{V}_c \rightarrow \text{CO}_2\text{V}_d + \text{CO}_2\text{V}_d$	$1.438 \times 10^{-7} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V53	$\text{CO}_2\text{V}_{1c} + \text{CO}_2\text{V}_{1a} \rightarrow \text{CO}_2\text{V}_{1b} + \text{CO}_2\text{V}_{1b}$	$5.308 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V54	$\text{CO}_2\text{V}_{1b} + \text{CO}_2\text{V}_1 \rightarrow \text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_{1a}$	$2.157 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V55	$\text{CO}_2\text{V}_{1c} + \text{CO}_2\text{V}_1 \rightarrow \text{CO}_2\text{V}_{1a} + \text{CO}_2\text{V}_{1b}$	$5.305 \times 10^{-9} \exp(-88T_g^{-1/3} - 233T_g^{-2/3})$	[20]	
V56 _{i,j}	$\text{CO}_2\text{V}_i + \text{CO}_2\text{V}_j \rightarrow \text{CO}_2\text{V}_{i+1} + \text{CO}_2\text{V}_{j-1}$	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	$i=1, \dots, 6$ $j=3, \dots, 8$ $j \geq i+2$
V57	$\text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_1 \rightarrow \text{CO}_2 + \text{CO}_2\text{V}_2$	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V58	$\text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_2 \rightarrow \text{CO}_2 + \text{CO}_2\text{V}_3$	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V59	$\text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_3 \rightarrow \text{CO}_2 + \text{CO}_2\text{V}_4$	$4.825 \times 10^{-11} \exp(-20.1T_g^{-1/3} - 65T_g^{-2/3})$	[20]	
V60	$\text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_4 \rightarrow \text{CO}_2 + \text{CO}_2\text{V}_5$	$7.199 \times 10^{-11} \exp(-1.84T_g^{-1/3} - 76T_g^{-2/3})$	[20]	
V61	$\text{CO}_2\text{V}_2 + \text{CO}_2\text{V}_2 \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_4$	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V62	$\text{CO}_2\text{V}_2 + \text{CO}_2\text{V}_3 \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_5$	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V63	$\text{CO}_2\text{V}_2 + \text{CO}_2\text{V}_4 \rightarrow \text{CO}_2\text{V}_1 + \text{CO}_2\text{V}_6$	$4.825 \times 10^{-11} \exp(-20.1T_g^{-1/3} - 65T_g^{-2/3})$	[20]	

续表 5 CO₂ 放电初始反应集合中包含的振动能量交换反应，以及相应的速率系数和参考文献

Tab. 5 The vibrational energy exchange reactions included in the initial reaction set of CO₂ discharges, as well as the corresponding rate coefficients and references (continued)

序号	反应	速率系数	参考文献	备注
V64	CO ₂ v ₂ + CO ₂ v ₅ → CO ₂ v ₁ + CO ₂ v ₇	$7.199 \times 10^{-11} \exp(-1.84T_g^{-1/3} - 76T_g^{-2/3})$	[20]	
V65	CO ₂ v ₃ + CO ₂ v ₃ → CO ₂ v ₂ + CO ₂ v ₄	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V66	CO ₂ v ₃ + CO ₂ v ₄ → CO ₂ v ₂ + CO ₂ v ₅	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V67	CO ₂ v ₃ + CO ₂ v ₅ → CO ₂ v ₂ + CO ₂ v ₆	$4.825 \times 10^{-11} \exp(-20.1T_g^{-1/3} - 65T_g^{-2/3})$	[20]	
V68	CO ₂ v ₃ + CO ₂ v ₆ → CO ₂ v ₂ + CO ₂ v ₇	$7.199 \times 10^{-11} \exp(-1.84T_g^{-1/3} - 76T_g^{-2/3})$	[20]	
V69	CO ₂ v ₄ + CO ₂ v ₄ → CO ₂ v ₃ + CO ₂ v ₅	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V70	CO ₂ v ₄ + CO ₂ v ₅ → CO ₂ v ₃ + CO ₂ v ₆	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V71	CO ₂ v ₄ + CO ₂ v ₆ → CO ₂ v ₃ + CO ₂ v ₇	$4.825 \times 10^{-11} \exp(-20.1T_g^{-1/3} - 65T_g^{-2/3})$	[20]	
V72	CO ₂ v ₄ + CO ₂ v ₇ → CO ₂ v ₃ + CO ₂ v ₅	$7.199 \times 10^{-11} \exp(-1.84T_g^{-1/3} - 76T_g^{-2/3})$	[20]	
V73	CO ₂ v ₅ + CO ₂ v ₅ → CO ₂ v ₄ + CO ₂ v ₈	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V74	CO ₂ v ₅ + CO ₂ v ₆ → CO ₂ v ₄ + CO ₂ v ₆	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V75	CO ₂ v ₅ + CO ₂ v ₇ → CO ₂ v ₄ + CO ₂ v ₇	$4.825 \times 10^{-11} \exp(-20.1T_g^{-1/3} - 65T_g^{-2/3})$	[20]	
V76	CO ₂ v ₆ + CO ₂ v ₆ → CO ₂ v ₅ + CO ₂ v ₈	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	
V77	CO ₂ v ₆ + CO ₂ v ₇ → CO ₂ v ₅ + CO ₂ v ₈	$2.927 \times 10^{-11} \exp(-21.4T_g^{-1/3} - 53T_g^{-2/3})$	[20]	
V78	CO ₂ v ₇ + CO ₂ v ₇ → CO ₂ v ₆ + CO ₂ v ₈	$1.453 \times 10^{-11} \exp(-22.1T_g^{-1/3} - 40.3T_g^{-2/3})$	[20]	

- (a) 当 M 为 CO₂、CO 和 O₂ 时，反应速率系数分别乘以 1.0、0.7 和 0.7。
- (b) 当 M 为 CO₂、CO 和 O₂ 时，反应速率系数分别乘以 1.0、3.1 和 3.1。
- (c) 当 M 为 CO₂、CO 和 O₂ 时，反应速率系数分别乘以 1.0、1.2 和 1.2。
- (d) 当 M 为 CO₂、CO 和 O₂ 时，反应速率系数分别乘以 1.0、0.3 和 0.4。
- (e) 反应速率系数由基于 SSH 理论的缩放定律给出。

注：表中 CO₂v_x 表示对称拉伸模式和弯曲模式，CO₂v_i 和 CO₂v_j 表示非对称拉伸模式，CO₂e_i 表示电子激发态。在速率系数表达式中，T_e 是以 eV 为单位的电子温度，T_g 是以 K 为单位的气体温度。双体反应的速率系数的单位为 cm³s⁻¹，三体反应的速率系数的单位为 cm⁶s⁻¹。

参考文献

- [1] GROFULOVIĆ M, ALVES L L, GUERRA V. Electron-neutral scattering cross sections for CO₂: A complete and consistent set and an assessment of dissociation[J]. Journal of Physics D: Applied Physics, 2016, 49(39): 395207.
- [2] OGLOBLINA P, TEJERO-DEL-CAZ A, GUERRA V, et al. Electron impact cross sections for carbon monoxide and their importance in the electron kinetics of CO₂-CO mixtures[J]. Plasma Sources Science and Technology, 2019, 29(1): 015002.
- [3] WANG Y, ZATSARINNY O, BARTSCHAT K. B-spline R-matrix-with-pseudostates calculations for electron-impact excitation and ionization of carbon[J]. Physical Review A, 2013, 87(1): 012704.
- [4] ALVES L L, COCHE P, RIDENTI M A, et al. Electron scattering cross sections for the modelling of oxygen-containing plasmas[J]. The European Physical Journal D, 2016, 70: 1-9.
- [5] GOUSSET G, FERREIRA C M, PINHEIRO M, et al. Electron and heavy-particle kinetics in the low pressure oxygen positive column[J]. Journal of Physics D: Applied Physics, 1991, 24(3): 290.
- [6] MATEJCIK S, KIENDLER A, CICMAN P, et al. Electron attachment to molecules and clusters of atmospheric relevance: Oxygen and ozone[J]. Plasma Sources Science and Technology, 1997, 6(2): 140.
- [7] ELIASSON B. Basic data for modeling of electrical discharges in gases: Oxygen[J]. Asea Brown Boveri Corporate Research Report, 1986: KLR86-11C.
- [8] SUN S, WANG H, BOGAERTS A. Chemistry reduction of complex CO₂ chemical kinetics: Application to a gliding arc plasma[J]. Plasma Sources Science and Technology, 2020, 29(2): 025012.
- [9] KOZÁK T, BOGAERTS A. Splitting of CO₂ by vibrational excitation in non-equilibrium plasmas: A reaction kinetics model[J]. Plasma Sources Science and Technology, 2014, 23(4): 045004.
- [10] BEUTHE T G, CHANG J S. Chemical kinetic modelling of non-equilibrium Ar-CO₂ thermal plasmas[J]. Japanese Journal of Applied Physics, 1997, 36(7S): 4997.
- [11] WANG W, SNOECKX R, ZHANG X, et al. Modeling plasma-based CO₂ and CH₄ conversion in mixtures with N₂, O₂, and H₂O: The bigger plasma chemistry picture[J]. The Journal of Physical Chemistry C, 2018, 122(16): 8704-8723.
- [12] SNOECKX R, BOGAERTS A. Plasma technology-a novel solution for CO₂ conversion?[J].

- Chemical Society Reviews, 2017, 46(19): 5805-5863.
- [13] PONDURI S, BECKER M, WELZEL S, et al. Fluid modelling of CO₂ dissociation in a dielectric barrier discharge[J]. Journal of Applied Physics, 2016, 119(9): 093301.
- [14] AERTS R, SOMERS W, BOGAERTS A. Carbon dioxide splitting in a dielectric barrier discharge plasma: A combined experimental and computational study[J]. ChemSusChem, 2015, 8(4): 702-716.
- [15] CHENG H, MA M, ZHANG Y, et al. The plasma enhanced surface reactions in a packed bed dielectric barrier discharge reactor[J]. Journal of Physics D: Applied Physics, 2020, 53(14): 144001.
- [16] VERMEIREN V, BOGAERTS A. Supersonic microwave plasma: Potential and limitations for energy-efficient CO₂ conversion[J]. The Journal of Physical Chemistry C, 2018, 122(45): 25869-25881.
- [17] BERTHELOT A, BOGAERTS A. Modeling of CO₂ plasma: Effect of uncertainties in the plasma chemistry[J]. Plasma Sources Science and Technology, 2017, 26(11): 115002.
- [18] BERTHELOT A, BOGAERTS A. Modeling of plasma-based CO₂ conversion: Lumping of the vibrational levels[J]. Plasma Sources Science and Technology, 2016, 25(4): 045022.
- [19] MOSS M S, YANALLAH K, ALLEN R W K, et al. An investigation of CO₂ splitting using nanosecond pulsed corona discharge: effect of argon addition on CO₂ conversion and energy efficiency[J]. Plasma Sources Science and Technology, 2017, 26(3): 035009.
- [20] BLAUER J, NICKERSON G. A survey of vibrational relaxation rate data for processes important to CO₂-N₂-H₂O infrared plume radiation; proceedings of the 7th Fluid and Plasma Dynamics Conference, F, 1974[C].