

APPENDIX A: CHEMICAL NETWORK

In Tables A1–A14 we list the chemical reactions included in our model of primordial gas, along with the rate coefficients adopted and the references from which these rate coefficients were taken. Some of these reactions are discussed in more detail in Section 3.1. In these tables, T is the gas temperature in K, $T_3 = T/300$ K, and T_e is the gas temperature in units of eV.

Table A1. Chemical processes: collisional ionization (CI).

No.	Reaction	Rate coefficient ($\text{cm}^3 \text{s}^{-1}$)	Ref.
CI1	$\text{H} + \text{e}^- \rightarrow \text{H}^+ + \text{e}^- + \text{e}^-$	$k_{\text{CI1}} = \exp[-3.271396786 \times 10^1 + 1.35365560 \times 10^1 \ln T_e - 5.73932875 \times 10^0 (\ln T_e)^2 + 1.56315498 \times 10^0 (\ln T_e)^3 - 2.87705600 \times 10^{-1} (\ln T_e)^4 + 3.48255977 \times 10^{-2} (\ln T_e)^5 - 2.63197617 \times 10^{-3} (\ln T_e)^6 + 1.11954395 \times 10^{-4} (\ln T_e)^7 - 2.03914985 \times 10^{-6} (\ln T_e)^8]$	1
CI2	$\text{D} + \text{e}^- \rightarrow \text{D}^+ + \text{e}^- + \text{e}^-$	$k_{\text{CI2}} = k_{\text{CI1}}$	1
CI3	$\text{He} + \text{e}^- \rightarrow \text{He}^+ + \text{e}^- + \text{e}^-$	$k_{\text{CI3}} = \exp[-4.409864886 \times 10^1 + 2.391596563 \times 10^1 \ln T_e - 1.07532302 \times 10^1 (\ln T_e)^2 + 3.05803875 \times 10^0 (\ln T_e)^3 - 5.68511890 \times 10^{-1} (\ln T_e)^4 + 6.79539123 \times 10^{-2} (\ln T_e)^5 - 5.00905610 \times 10^{-3} (\ln T_e)^6 + 2.06723616 \times 10^{-4} (\ln T_e)^7 - 3.64916141 \times 10^{-6} (\ln T_e)^8]$	1
CI4	$\text{Li} + \text{e}^- \rightarrow \text{Li}^+ + \text{e}^- + \text{e}^-$	$k_{\text{CI4}} = 3.11 \times 10^{-8} T_3^{0.163} \exp\left(-\frac{62700}{T}\right)$	2

Notes: T is the gas temperature in K, $T_3 = T/300$ K, and T_e is the gas temperature in eV.

References: 1 – Janev et al.(1987); 2 – Voronov (1997).

Table A2. Chemical processes: photorecombination (PR).

No.	Reaction	Rate coefficient ($\text{cm}^3 \text{s}^{-1}$)	Notes	Ref.
PR1	$\text{H}^+ + \text{e}^- \rightarrow \text{H} + \gamma$	$k_{\text{PR1}} = 2.753 \times 10^{-14} \left(\frac{315614}{T}\right)^{1.500} \left[1.0 + \left(\frac{115188}{T}\right)^{0.407}\right]^{-2.242}$		1
PR2	$\text{D}^+ + \text{e}^- \rightarrow \text{D} + \gamma$	$k_{\text{PR2}} = k_{\text{PR1}}$		1
PR3	$\text{He}^+ + \text{e}^- \rightarrow \text{He} + \gamma$	$k_{\text{PR3,rr,A}} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T - 0.3162(\log T)^2 + 0.0493(\log T)^3]$ $k_{\text{PR3,rr,B}} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T - 0.2852(\log T)^2 + 0.04433(\log T)^3]$ $k_{\text{PR3,di}} = T^{-1.5} \left[5.966 \times 10^{-4} \exp\left(\frac{-455600}{T}\right) + 1.613 \times 10^{-4} \exp\left(\frac{-555200}{T}\right) - 2.223 \times 10^{-5} \exp\left(\frac{-898200}{T}\right)\right]$	Case A Case B	2 2
PR4	$\text{Li}^+ + \text{e}^- \rightarrow \text{Li} + \gamma$	$k_{\text{PR4,rr}} = 1.036 \times 10^{-11} \left(\frac{T}{107.7}\right)^{-0.5} \left[1.0 + \left(\frac{T}{107.7}\right)^{0.5}\right]^{-0.612} \times \left[1.0 + \left(\frac{T}{1.177 \times 10^7}\right)^{0.5}\right]^{-1.388}$ $k_{\text{PR4,di}} = T^{-1.5} \left[2.941 \times 10^{-5} \exp\left(\frac{-634500}{T}\right) + 6.068 \times 10^{-5} \exp\left(\frac{-702400}{T}\right) - 7.753 \times 10^{-7} \exp\left(\frac{-827100}{T}\right)\right]$		4 5

Notes: T is the gas temperature in K. Note that the recently revised values for PR1 and for the radiative recombination portions of PR3 and PR4 presented by Badnell (2006b) do not differ from the older rate coefficients quoted here by more than a couple of percent at the temperatures of interest in this study.

References: 1 – Ferland et al. (1992); 2 – Hummer & Storey (1998); 3 – Badnell (2006a); 4 – Verner & Ferland (1996); 5 – Bautista & Badnell (2007).

Table A3. Chemical processes: dissociative recombination (DR).

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
DR1	Htp + e ⁻ → H + H	$k_{\text{DR1}} = 1.0 \times 10^{-8}$ $= 1.32 \times 10^{-6} T^{-0.76}$	$T \leq 617$ K $T > 617$ K	1
DR2	HD ⁺ + e ⁻ → H + D	$k_{\text{DR2}} = 7.2 \times 10^{-8} T_3^{-0.5}$		2
DR3	D ₂ ⁺ + e ⁻ → D + D	$k_{\text{DR3}} = 3.4 \times 10^{-9} T_3^{-0.4}$		3
DR4	H ₃ ⁺ + e ⁻ → Ht + H	$k_{\text{DR4}} = 2.34 \times 10^{-8} T_3^{-0.52}$		4
DR5	H ₃ ⁺ + e ⁻ → H + H + H	$k_{\text{DR5}} = 4.36 \times 10^{-8} T_3^{-0.52}$		4
DR6	H ₂ D ⁺ + e ⁻ → H + H + D	$k_{\text{DR6}} = 4.38 \times 10^{-8} T_3^{-0.5}$		5
DR7	H ₂ D ⁺ + e ⁻ → Ht + D	$k_{\text{DR7}} = 4.2 \times 10^{-9} T_3^{-0.5}$		5
DR8	H ₂ D ⁺ + e ⁻ → H + HD	$k_{\text{DR8}} = 1.2 \times 10^{-8} T_3^{-0.5}$		5
DR9	HD ₂ ⁺ + e ⁻ → D + D + H	$k_{\text{DR9}} = 4.38 \times 10^{-8} T_3^{-0.5}$		6
DR10	HD ₂ ⁺ + e ⁻ → D ₂ + H	$k_{\text{DR10}} = 4.2 \times 10^{-9} T_3^{-0.5}$		6
DR11	HD ₂ ⁺ + e ⁻ → HD + D	$k_{\text{DR11}} = 1.2 \times 10^{-8} T_3^{-0.5}$		6
DR12	D ₃ ⁺ + e ⁻ → D ₂ + D	$k_{\text{DR12}} = 5.4 \times 10^{-9} T_3^{-0.5}$		7
DR13	D ₃ ⁺ + e ⁻ → D + D + D	$k_{\text{DR13}} = 2.16 \times 10^{-8} T_3^{-0.5}$		7
DR14	HeH ⁺ + e ⁻ → He + H	$k_{\text{DR14}} = 3.0 \times 10^{-8} T_3^{-0.47}$		8
DR15	HeD ⁺ + e ⁻ → He + D	$k_{\text{DR15}} = 3.0 \times 10^{-8} T_3^{-0.47}$		9
DR16	He ₂ ⁺ + e ⁻ → He + He	$k_{\text{DR16}} = 6.1 \times 10^{-11} T_3^{-0.9}$		10
DR17	LiH ⁺ + e ⁻ → Li + H	$k_{\text{DR17}} = 3.8 \times 10^{-7} T_3^{-0.47}$		11
DR18	LiD ⁺ + e ⁻ → Li + D	$k_{\text{DR18}} = 3.8 \times 10^{-7} T_3^{-0.47}$		12
DR19	LiH ₂ ⁺ + e ⁻ → Li + Ht	$k_{\text{DR19}} = 1.6 \times 10^{-7} T_3^{-0.5}$		13
DR20	LiH ₂ ⁺ + e ⁻ → LiH + H	$k_{\text{DR20}} = 2.0 \times 10^{-8} T_3^{-0.5}$		13
DR21	LiH ₂ ⁺ + e ⁻ → Li + H + H	$k_{\text{DR21}} = 2.0 \times 10^{-8} T_3^{-0.5}$		13

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Schneider et al. (1994); 2 – Stromhölm et al. (1995); 3 – Walmsley et al. (2004); 4 – McCall et al. (2004); 5 – Larsson et al. (1996); 6 – Roberts et al. (2004), based on Larsson et al. (1996); 7 – Larsson et al. (1997); 8 – Guberman (1994); 9 – Stancil et al. (1998), based on Guberman (1994); 10 – Carata et al. (1999); 11 – Krohn et al. (2001); 12 – same as corresponding H reaction; 13 – Thomas et al. (2006), C. Greene (private communication).

Table A4. Chemical processes: charge transfer (CT).

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
CT1	H + D ⁺ → D + H ⁺	$k_{CT1} = 2.06 \times 10^{-10} T^{0.396} \exp\left(-\frac{33}{T}\right) + 2.03 \times 10^{-9} T^{-0.332}$		1
CT2	H + D ⁻ → D + H ⁻	$k_{CT2} = 6.4 \times 10^{-9} T_3^{0.41}$		2
CT3	H + Htp → Ht + H ⁺	$k_{CT3} = 6.4 \times 10^{-10}$		3
CT4	H + HD ⁺ → HD + H ⁺	$k_{CT4} = 6.4 \times 10^{-10}$		4
CT5	H + D ₂ ⁺ → D ₂ + H ⁺	$k_{CT5} = 6.4 \times 10^{-10}$		4
CT6	H + Hep → He + H ⁺ + γ	$k_{CT6} = 1.25 \times 10^{-15} T_3^{0.25}$		5
CT7	H + He ₂ ⁺ → He + He + H ⁺	$k_{CT7} = 1.0 \times 10^{-9}$		6
CT8	H + LiH ⁺ → LiH + H ⁺	$k_{CT8} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		7
CT9	H + LiD ⁺ → LiD + H ⁺	$k_{CT9} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT10	D + H ⁺ → H + D ⁺	$k_{CT10} = 2.0 \times 10^{-10} T^{0.402} \exp\left(-\frac{37.1}{T}\right) - 3.31 \times 10^{-17} T^{1.48}$		1
CT11	D + H ⁻ → H + D ⁻	$k_{CT11} = 6.4 \times 10^{-9} T_3^{0.41}$		2
CT12	D + Htp → Ht + D ⁺	$k_{CT12} = 6.4 \times 10^{-10}$		4
CT13	D + HD ⁺ → HD + D ⁺	$k_{CT13} = 6.4 \times 10^{-10}$		4
CT14	D + D ₂ ⁺ → D ₂ + D ⁺	$k_{CT14} = 6.4 \times 10^{-10}$		4
CT15	D + Hep → He + D ⁺ + γ	$k_{CT15} = 1.1 \times 10^{-15} T_3^{0.25}$		8
CT16	D + He ₂ ⁺ → He + He + D ⁺	$k_{CT16} = 7.5 \times 10^{-10}$		9
CT17	D + LiH ⁺ → LiH + D ⁺	$k_{CT17} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT18	D + LiD ⁺ → LiD + D ⁺	$k_{CT18} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT19	Ht + H ⁺ → H + Htp	$k_{CT19} = [-3.3232183 \times 10^{-7} + 3.3735382 \times 10^{-7} \ln T - 1.4491368 \times 10^{-7} (\ln T)^2 + 3.4172805 \times 10^{-8} (\ln T)^3 - 4.7813720 \times 10^{-9} (\ln T)^4 + 3.9731542 \times 10^{-10} (\ln T)^5 - 1.8171411 \times 10^{-11} (\ln T)^6 + 3.5311932 \times 10^{-13} (\ln T)^7] \times \exp\left(-\frac{21237.15}{T}\right)$		10
CT20	Ht + D ⁺ → D + Htp	$k_{CT20} = k_{CT19}$		4
CT21	Ht + Hep → He + Htp	$k_{CT21} = 7.2 \times 10^{-15}$		11
CT22	Ht + Hep → He + H + H ⁺	$k_{CT22} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		11
CT23	Ht + Li ⁺ → Li + Htp	$k_{CT23} = 3.0 \times 10^{-10} T_3^{-1.5} \exp\left(-\frac{116000}{T}\right)$		12
CT24	HD + H ⁺ → H + HD ⁺	$k_{CT24} = k_{CT19}$		4
CT25	HD + D ⁺ → D + HD ⁺	$k_{CT25} = k_{CT19}$		4
CT26	HD + Hep → He + HD ⁺	$k_{CT26} = 7.2 \times 10^{-15}$		4
CT27	HD + Hep → He + H ⁺ + D	$k_{CT27} = 1.85 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		13
CT28	HD + Hep → He + H + D ⁺	$k_{CT28} = 1.85 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		13
CT29	HD + Li ⁺ → Li + HD ⁺	$k_{CT29} = k_{CT23}$		4
CT30	D ₂ + H ⁺ → H + D ₂ ⁺	$k_{CT30} = k_{CT19}$		4
CT31	D ₂ + D ⁺ → D + D ₂ ⁺	$k_{CT31} = k_{CT19}$		4
CT32	D ₂ + Hep → He + D ₂ ⁺	$k_{CT32} = 2.5 \times 10^{-14}$		14
CT33	D ₂ + Hep → He + D ⁺ + D	$k_{CT33} = 1.1 \times 10^{-13} T_3^{-0.24}$		14
CT34	D ₂ + Li ⁺ → Li + D ₂ ⁺	$k_{CT34} = k_{CT23}$		4
CT35	He + H ⁺ → H + Hep	$k_{CT35} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right) = 4.0 \times 10^{-37} T^{4.74}$	$T \leq 10000$ K $T > 10000$ K	15
CT36	He + D ⁺ → D + Hep	$k_{CT36} = k_{CT35}$		4

Table A4 – continued

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
CT37	Li + H ⁺ → H + Li ⁺	$k_{CT37} = 2.5 \times 10^{-40} T^{7.9} \exp\left(-\frac{T}{1210}\right)$		16
CT38	Li + H ⁺ → H + Li ⁺ + γ	$k_{CT38} = 1.7 \times 10^{-13} T^{-0.051} \exp\left(-\frac{T}{282000}\right)$		17
CT39	Li + D ⁺ → D + Li ⁺	$k_{CT39} = 8.0 \times 10^{-22} T_3^{6.8} \exp\left(-\frac{T}{1800}\right)$		18
CT40	Li + D ⁺ → D + Li ⁺ + γ	$k_{CT40} = 1.1 \times 10^{-13} T_3^{-0.051} \exp\left(-\frac{T}{282000}\right)$		19
CT41	Li + Ht ^p → Ht + Li ⁺	$k_{CT41} = 3.0 \times 10^{-10} T_3^{-1.5}$		20
CT42	Li + HD ⁺ → HD + Li ⁺	$k_{CT42} = k_{CT41}$		4
CT43	Li + D ₂ ⁺ → D ₂ + Li ⁺	$k_{CT43} = k_{CT41}$		4
CT44	LiH + H ⁺ → H + LiH ⁺	$k_{CT44} = 2.0 \times 10^{-15}$		21
CT45	LiH + D ⁺ → D + LiH ⁺	$k_{CT45} = 2.0 \times 10^{-15}$		21
CT46	LiD + H ⁺ → H + LiD ⁺	$k_{CT46} = 2.0 \times 10^{-15}$		21
CT47	LiD + D ⁺ → D + LiD ⁺	$k_{CT47} = 2.0 \times 10^{-15}$		21

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Savin (2002); 2 – Dalgarno & McDowell (1956), scaled by D reduced mass; 3 – Karpas, Anicich & Huntress (1979); 4 – same as corresponding H reaction; 5 – Zygelman et al. (1989); 6 – Estimate by Stancil et al. (1998), based on Stancil et al. (1993); 7 – Stancil et al. (1996); 8 – Zygelman et al. (1989), scaled by D reduced mass; 9 – As ref. 6, but scaled by D reduced mass; 10 – Savin et al. (2004); 11 – Barlow (1984); 12 – Estimate, based on low-energy extrapolation of cross-section in Wutte et al. (1997); 13 – total rate coefficient from Barlow (1984), branching ratios from Pineau des Forets et al. (1989); 14 – Walmsley, Flower, & Pineau des Forets (2004); 15 – Kimura et al. (1993); 16 – Kimura, Dutta, & Shimakura (1994); 17 – Stancil & Zygelman (1996); 18 – Kimura, Dutta & Shimakura (1994), scaled by D reduced mass; 19 – Stancil & Zygelman (1996), scaled by D reduced mass; 20 – From detailed balance applied to inverse reaction; 21 – Bodo et al. (2001).

Table A5. Chemical processes: radiative attachment and radiative association (RA) .

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
RA1	H + e ⁻ → H ⁻ + γ	$k_{\text{RA1}} = \text{dex}[-17.845 + 0.762 \log T + 0.1523(\log T)^2 - 0.03274(\log T)^3]$ $= \text{dex}[-16.420 + 0.1998(\log T)^2 - 5.447 \times 10^{-3}(\log T)^4 + 4.0415 \times 10^{-5}(\log T)^6]$	$T \leq 6000$ K $T > 6000$ K	1
RA2	D + e ⁻ → D ⁻ + γ	$k_{\text{RA2}} = k_{\text{RA1}}$		1
RA3	H + H ⁺ → Htp + γ	$k_{\text{RA3}} = \text{dex}[-19.38 - 1.523 \log T + 1.118(\log T)^2 - 0.1269(\log T)^3]$		2
RA4	H + D ⁺ → HD ⁺ + γ	$k_{\text{RA4}} = 3.9 \times 10^{-19} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		3
RA5	H + D → HD + γ	$k_{\text{RA5}} = 10^{-25} [2.80202 - 6.63697 \ln T + 4.75619(\ln T)^2 - 1.39325(\ln T)^3 + 0.178259(\ln T)^4 - 0.00817097(\ln T)^5]$ $= 10^{-25} \exp [507.207 - 370.889 \ln T + 104.854(\ln T)^2 - 14.4192(\ln T)^3 + 0.971469(\ln T)^4 - 0.0258076(\ln T)^5]$	$10 < T \leq 200$ K $T > 200$ K	4
RA6	H + Htp → H ₃ ⁺ + γ	$k_{\text{RA6}} = 1.5 \times 10^{-17} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		5
RA7	H + HD ⁺ → H ₂ D ⁺ + γ	$k_{\text{RA7}} = 1.2 \times 10^{-17} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		6
RA8	H + D ₂ ⁺ → HD ₂ ⁺ + γ	$k_{\text{RA8}} = 1.1 \times 10^{-17} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		6
RA9	H + Hep → HeH ⁺ + γ	$k_{\text{RA9}} = 4.16 \times 10^{-16} T_3^{-0.37} \exp\left(-\frac{T}{87600}\right)$		7
RA10	H + Li ⁺ → LiH ⁺ + γ	$k_{\text{RA10}} = \text{dex}[-22.4 + 0.999 \log T - 0.351(\log T)^2]$		8
RA11	D + H ⁺ → HD ⁺ + γ	$k_{\text{RA11}} = 3.9 \times 10^{-19} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		3
RA12	D + D ⁺ → D ₂ ⁺ + γ	$k_{\text{RA12}} = 1.9 \times 10^{-19} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		3
RA13	D + Htp → H ₂ D ⁺ + γ	$k_{\text{RA13}} = 7.0 \times 10^{-18} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		6
RA14	D + HD ⁺ → HD ₂ ⁺ + γ	$k_{\text{RA14}} = 5.2 \times 10^{-18} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		6
RA15	D + D ₂ ⁺ → D ₃ ⁺ + γ	$k_{\text{RA15}} = 4.3 \times 10^{-18} T_3^{1.8} \exp\left(\frac{20}{T}\right)$		6
RA16	D + Hep → HeD ⁺ + γ	$k_{\text{RA16}} = 5.0 \times 10^{-16} T_3^{-0.37} \exp\left(-\frac{T}{87600}\right)$		6
RA17	D + Li ⁺ → LiD ⁺ + γ	$k_{\text{RA17}} = 1.5 \times 10^{-22} T_3^{-0.9} \exp\left(-\frac{T}{7000}\right)$		9
RA18	Ht + H ⁺ → H ₃ ⁺ + γ	$k_{\text{RA18}} = 1.0 \times 10^{-16}$		10
RA19	Ht + D ⁺ → H ₂ D ⁺ + γ	$k_{\text{RA19}} = 1.0 \times 10^{-16}$		11
RA20	Li ⁺ + Ht → LiH ₂ ⁺ + γ	$k_{\text{RA20}} = 1.0 \times 10^{-22}$		12
RA21	HD + H ⁺ → H ₂ D ⁺ + γ	$k_{\text{RA21}} = 1.0 \times 10^{-16}$		11
RA22	HD + D ⁺ → HD ₂ ⁺ + γ	$k_{\text{RA22}} = 1.0 \times 10^{-16}$		11
RA23	D ₂ + H ⁺ → HD ₂ ⁺ + γ	$k_{\text{RA23}} = 1.0 \times 10^{-16}$		11
RA24	D ₂ + D ⁺ → D ₃ ⁺ + γ	$k_{\text{RA24}} = 1.0 \times 10^{-16}$		11
RA25	He + H ⁺ → HeH ⁺ + γ	$k_{\text{RA25}} = 8.0 \times 10^{-20} T_3^{-0.24} \exp\left(-\frac{T}{40000}\right)$		13
RA26	He + D ⁺ → HeD ⁺ + γ	$k_{\text{RA26}} = 1.0 \times 10^{-19} T_3^{-0.24} \exp\left(-\frac{T}{40000}\right)$		6
RA27	He + Hep → He ₂ ⁺ + γ	$k_{\text{RA27}} = 4.76 \times 10^{-20} T_3^{1.82} \exp\left(\frac{29}{T}\right)$		14
RA28	Li + e ⁻ → Li ⁻ + γ	$k_{\text{RA28}} = 6.1 \times 10^{-17} T^{0.58} \exp\left(-\frac{T}{17200}\right)$		15
RA29	Li + H ⁺ → LiH ⁺ + γ	$k_{\text{RA29}} = 4.8 \times 10^{-14} T^{-0.49}$		16
RA30	Li + D ⁺ → LiD ⁺ + γ	$k_{\text{RA30}} = 6.4 \times 10^{-14} T^{-0.49}$		6
RA31	Li + H → LiH + γ	$k_{\text{RA31}} = 10^{-20} \left\{ 3.22 + [0.0657(T/1000)^{-2.45} + 6.3 \times 10^{-3}(T/1000)^{0.837}]^{-1} \right\}$		17
RA32	Li + D → LiD + γ	$k_{\text{RA32}} = 5.5 \times 10^{-20} T_3^{-0.28} \exp\left(-\frac{T}{3300}\right)$		9

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Wishart (1979); 2 – Ramaker & Peek (1976); 3 – Ramaker & Peek (1976) and Frommhold & Pickett (1978), scaled by D reduced mass; 4 – Dickinson (2005); 5 – Dalgarno & McDowell (1956); 6 – Same as corresponding H reaction, but scaled by D reduced mass; 7 – Kraemer, Špirko & Južek (1995); 8 – Dalgarno et al. (1996); Gianturco & Gori Giorgi (1996); 9 – Stancil et al. (1996), scaled by D reduced mass; 10 – Gerlich & Horning (1992); 11 – estimate, based on Gerlich & Horning (1992); highly uncertain; 12 – estimate - see also Section 3.1.11; 13 – Južek, Špirko & Kraemer (1995); 14 – Stancil et al. (1993); 15 – Ramsbottom et al. (1994); 16 – Dalgarno et al. (1996); 17 – Bennett et al. (2003).

Table A6. Chemical processes: associative detachment, dissociative attachment and associative ionization (AD) .

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
AD1	H + H ⁻ → Ht + e ⁻	$k_{AD1} = 1.5 \times 10^{-9} T_3^{-0.1}$		1
AD2	D + H ⁻ → HD + e ⁻	$k_{AD2} = 1.5 \times 10^{-9} T_3^{-0.1}$		2
AD3	H + D ⁻ → HD + e ⁻	$k_{AD3} = 1.5 \times 10^{-9} T_3^{-0.1}$		2
AD4	D + D ⁻ → D ₂ + e ⁻	$k_{AD4} = 1.6 \times 10^{-9} T_3^{-0.1}$		2
AD5	Ht + e ⁻ → H + H ⁻	$k_{AD5} = 2.7 \times 10^{-8} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		3
AD6	HD + e ⁻ → H + D ⁻	$k_{AD6} = 1.35 \times 10^{-9} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD7	HD + e ⁻ → D + H ⁻	$k_{AD7} = 1.35 \times 10^{-9} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD8	D ₂ + e ⁻ → D + D ⁻	$k_{AD8} = 6.7 \times 10^{-11} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD9	H ⁺ + H ⁻ → Htp + e ⁻	$k_{AD9} = 6.9 \times 10^{-9} T^{-0.35}$ $= 9.6 \times 10^{-7} T^{-0.90}$	$T \leq 8000$ K $T > 8000$ K	5
AD10	H ⁺ + D ⁻ → HD ⁺ + e ⁻	$k_{AD10} = 1.1 \times 10^{-9} T_3^{-0.4}$		2
AD11	D ⁺ + H ⁻ → HD ⁺ + e ⁻	$k_{AD11} = 1.1 \times 10^{-9} T_3^{-0.4}$		2
AD12	D ⁺ + D ⁻ → D ₂ ⁺ + e ⁻	$k_{AD12} = 1.3 \times 10^{-9} T_3^{-0.4}$		2
AD13	Htp + H ⁻ → H ₃ ⁺ + e ⁻	$k_{AD13} = 2.7 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		6
AD14	Htp + D ⁻ → H ₂ D ⁺ + e ⁻	$k_{AD14} = 2.24 \times 10^{-10} T_3^{-0.49} \exp\left(\frac{T}{43600}\right)$		6
AD15	HD ⁺ + H ⁻ → H ₂ D ⁺ + e ⁻	$k_{AD15} = 2.9 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD16	HD ⁺ + D ⁻ → HD ₂ ⁺ + e ⁻	$k_{AD16} = 3.7 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD17	D ₂ ⁺ + H ⁻ → HD ₂ ⁺ + e ⁻	$k_{AD17} = 3.0 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD18	D ₂ ⁺ + D ⁻ → D ₃ ⁺ + e ⁻	$k_{AD18} = 3.9 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD19	Li + H ⁻ → LiH + e ⁻	$k_{AD19} = 4.0 \times 10^{-10}$		7
AD20	Li + D ⁻ → LiD + e ⁻	$k_{AD20} = 4.0 \times 10^{-10}$		2
AD21	Li ⁻ + H → LiH + e ⁻	$k_{AD21} = 4.0 \times 10^{-10}$		7
AD22	Li ⁻ + D → LiD + e ⁻	$k_{AD22} = 4.0 \times 10^{-10}$		2

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Launay et al. (1991); 2 – Same as corresponding H reaction, but scaled by D reduced mass; 3 – Schulz & Asundi (1967); 4 – Xu & Fabrikant (2001); 5 – Poulaert et al. (1978); 6 – Naji et al. (1998); 7 – Stancil et al. (1996).

Table A7. Chemical processes: collisional detachment and collisional dissociation (CD) .

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
CD1	$\text{H}^- + \text{e}^- \rightarrow \text{H} + \text{e}^- + \text{e}^-$	$k_{\text{CD1}} = \exp[-1.801849334 \times 10^1 + 2.36085220 \times 10^0 \ln T_e - 2.82744300 \times 10^{-1} (\ln T_e)^2 + 1.62331664 \times 10^{-2} (\ln T_e)^3 - 3.36501203 \times 10^{-2} (\ln T_e)^4 + 1.17832978 \times 10^{-2} (\ln T_e)^5 - 1.65619470 \times 10^{-3} (\ln T_e)^6 + 1.06827520 \times 10^{-4} (\ln T_e)^7 - 2.63128581 \times 10^{-6} (\ln T_e)^8]$		1
CD2	$\text{H}^- + \text{H} \rightarrow \text{H} + \text{H} + \text{e}^-$	$k_{\text{CD2}} = 2.5634 \times 10^{-9} T_e^{1.78186} = \exp[-2.0372609 \times 10^1 + 1.13944933 \times 10^0 \ln T_e - 1.4210135 \times 10^{-1} (\ln T_e)^2 + 8.4644554 \times 10^{-3} (\ln T_e)^3 - 1.4327641 \times 10^{-3} (\ln T_e)^4 + 2.0122503 \times 10^{-4} (\ln T_e)^5 + 8.6639632 \times 10^{-5} (\ln T_e)^6 - 2.5850097 \times 10^{-5} (\ln T_e)^7 + 2.4555012 \times 10^{-6} (\ln T_e)^8 - 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e \leq 0.1 \text{ eV}$ $T_e > 0.1 \text{ eV}$	1
CD3	$\text{H}^- + \text{D} \rightarrow \text{H} + \text{D} + \text{e}^-$	$k_{\text{CD3}} = k_{\text{CD2}}$		2
CD4	$\text{H}^- + \text{He} \rightarrow \text{H} + \text{He} + \text{e}^-$	$k_{\text{CD4}} = 4.1 \times 10^{-17} T^2 \exp\left(-\frac{19870}{T}\right)$		3
CD5	$\text{D}^- + \text{e}^- \rightarrow \text{D} + \text{e}^- + \text{e}^-$	$k_{\text{CD5}} = k_{\text{CD1}}$		2
CD6	$\text{D}^- + \text{H} \rightarrow \text{D} + \text{H} + \text{e}^-$	$k_{\text{CD6}} = k_{\text{CD2}}$		2
CD7	$\text{D}^- + \text{D} \rightarrow \text{D} + \text{D} + \text{e}^-$	$k_{\text{CD7}} = k_{\text{CD2}}$		2
CD8	$\text{D}^- + \text{He} \rightarrow \text{D} + \text{He} + \text{e}^-$	$k_{\text{CD8}} = 1.5 \times 10^{-17} T^2 \exp\left(-\frac{19870}{T}\right)$		4
CD9	$\text{Ht} + \text{H} \rightarrow \text{H} + \text{H} + \text{H}$	$k_{\text{CD9}} = 6.67 \times 10^{-12} T^{0.5} \exp\left[-\left(1 + \frac{63593}{T}\right)\right]$ $= k_{\text{TB1}}/K$	$v=0$ LTE	5 6
CD10	$\text{Ht} + \text{Ht} \rightarrow \text{H} + \text{H} + \text{Ht}$	$k_{\text{CD10}} = \frac{5.996 \times 10^{-30} T^{4.1881}}{(1.0 + 6.761 \times 10^{-6} T)^{5.6881}} \exp\left(-\frac{54657.4}{T}\right)$ $= k_{\text{TB2}}/K$	$v = 0$ LTE	7 6
CD11	$\text{Ht} + \text{He} \rightarrow \text{H} + \text{H} + \text{He}$	$k_{\text{CD11}} = \text{dex}\left[-27.029 + 3.801 \log T - \frac{29487}{T}\right]$ $= 6.6 \times 10^{-10} T^{0.115} \exp\left(-\frac{52000}{T}\right)$	$v = 0$ LTE	8 9
CD12	$\text{Ht} + \text{e}^- \rightarrow \text{H} + \text{H} + \text{e}^-$	$k_{\text{CD12}} = 4.49 \times 10^{-9} T^{0.11} \exp\left(-\frac{101858}{T}\right)$ $= 1.91 \times 10^{-9} T^{0.136} \exp\left(-\frac{53407.1}{T}\right)$	$v = 0$ LTE	10 10
CD13	$\text{HD} + \text{H} \rightarrow \text{H} + \text{D} + \text{H}$	$k_{\text{CD13}} = k_{\text{CD9}}$	See §??	2
CD14	$\text{HD} + \text{Ht} \rightarrow \text{H} + \text{D} + \text{Ht}$	$k_{\text{CD14}} = k_{\text{CD10}}$	See §??	2
CD15	$\text{HD} + \text{He} \rightarrow \text{H} + \text{D} + \text{He}$	$k_{\text{CD15}} = k_{\text{CD11}}$	See §??	2
CD16	$\text{HD} + \text{e}^- \rightarrow \text{H} + \text{D} + \text{e}^-$	$k_{\text{CD16}} = 5.09 \times 10^{-9} T^{0.128} \exp\left(-\frac{103258}{T}\right)$ $= 1.04 \times 10^{-9} T^{0.218} \exp\left(-\frac{53070.7}{T}\right)$	$v = 0$ LTE	11 11
CD17	$\text{D}_2 + \text{H} \rightarrow \text{D} + \text{D} + \text{H}$	$k_{\text{CD17}} = k_{\text{CD9}}$		2
CD18	$\text{D}_2 + \text{Ht} \rightarrow \text{D} + \text{D} + \text{Ht}$	$k_{\text{CD18}} = k_{\text{CD10}}$		2
CD19	$\text{D}_2 + \text{He} \rightarrow \text{D} + \text{D} + \text{He}$	$k_{\text{CD19}} = k_{\text{CD11}}$		2
CD20	$\text{D}_2 + \text{e}^- \rightarrow \text{D} + \text{D} + \text{e}^-$	$k_{\text{CD20}} = 8.24 \times 10^{-9} T^{0.126} \exp\left(-\frac{105388}{T}\right)$ $= 2.75 \times 10^{-9} T^{0.163} \exp\left(-\frac{53339.7}{T}\right)$	$v = 0$ LTE	10 10
CD21	$\text{LiH}^+ + \text{D} \rightarrow \text{Li}^+ + \text{H} + \text{D}$	$k_{\text{CD21}} = 1.0 \times 10^{-9} \exp\left(-\frac{1400}{T}\right)$		12
CD22	$\text{LiH}^+ + \text{D} \rightarrow \text{Li} + \text{H}^+ + \text{D}$	$k_{\text{CD22}} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD23	$\text{LiH}^+ + \text{D} \rightarrow \text{Li} + \text{H} + \text{D}^+$	$k_{\text{CD23}} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD24	$\text{LiD}^+ + \text{D} \rightarrow \text{Li}^+ + \text{D} + \text{D}$	$k_{\text{CD24}} = 1.0 \times 10^{-9} \exp\left(-\frac{1400}{T}\right)$		12
CD25	$\text{LiD}^+ + \text{D} \rightarrow \text{Li} + \text{D}^+ + \text{D}$	$k_{\text{CD25}} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD26	$\text{LiH}_2^+ + \text{Ht} \rightarrow \text{Li}^+ + \text{Ht} + \text{Ht}$	$k_{\text{CD26}} = 1.0 \times 10^{-9} \exp\left(-\frac{3000}{T}\right)$		13

Notes: T is the gas temperature in K and T_e is the gas temperature in eV. K is the equilibrium constant relating reactions TB1 and CD9, and reactions TB2 and CD10; its value is given in §??.

References: 1 – Janev et al. (1987); 2 – Assumed same as corresponding H reaction; 3 – Huq et al. (1982); 4 – Same as corresponding H reaction, but scaled by D reduced mass; 5 – Mac Low & Shull (1986); 6 – determined from three-body rate coefficient by detailed balance (see Section 3.1.7); 7 – Martin, Keogh, & Mandy (1998); 8 – Dove et al. (1987); 9 – determined from the Walkauskas & Kaufman (1975) rate coefficient for reaction TB3 by detailed balance; 10 – Trevisan & Tennyson (2002a); 11 – Trevisan & Tennyson (2002b); 13 – estimate – see also Section 3.1.11.

Table A8. Chemical processes: mutual neutralization (MN).

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Ref.
MN1	H ⁺ + H ⁻ → H + H	$k_{\text{MN1}} = 2.4 \times 10^{-6} T^{-1/2} (1.0 + 5.0 \times 10^{-5} T)$	1
MN2	D ⁺ + H ⁻ → D + H	$k_{\text{MN2}} = 1.1 \times k_{\text{MN1}}$	2
MN3	H ⁺ + D ⁻ → D + H	$k_{\text{MN3}} = 1.1 \times k_{\text{MN1}}$	2
MN4	D ⁺ + D ⁻ → D + D	$k_{\text{MN4}} = 1.3 \times k_{\text{MN1}}$	2
MN5	Ht _p + H ⁻ → Ht + H	$k_{\text{MN5}} = 1.4 \times 10^{-7} T_3^{-0.5}$	3
MN6	Ht _p + H ⁻ → H + H + H	$k_{\text{MN6}} = 1.4 \times 10^{-7} T_3^{-0.5}$	3
MN7	Ht _p + D ⁻ → Ht + D	$k_{\text{MN7}} = 1.7 \times 10^{-7} T_3^{-0.5}$	2
MN8	Ht _p + D ⁻ → H + H + D	$k_{\text{MN8}} = 1.7 \times 10^{-7} T_3^{-0.5}$	2
MN9	HD ⁺ + H ⁻ → HD + H	$k_{\text{MN9}} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN10	HD ⁺ + H ⁻ → D + H + H	$k_{\text{MN10}} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN11	HD ⁺ + D ⁻ → HD + D	$k_{\text{MN11}} = 1.9 \times 10^{-7} T_3^{-0.5}$	2
MN12	HD ⁺ + D ⁻ → D + H + D	$k_{\text{MN12}} = 1.9 \times 10^{-7} T_3^{-0.5}$	2
MN13	D ₂ ⁺ + H ⁻ → D ₂ + H	$k_{\text{MN13}} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN14	D ₂ ⁺ + H ⁻ → D + D + H	$k_{\text{MN14}} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN15	D ₂ ⁺ + D ⁻ → D ₂ + D	$k_{\text{MN15}} = 2.0 \times 10^{-7} T_3^{-0.5}$	2
MN16	D ₂ ⁺ + D ⁻ → D + D + D	$k_{\text{MN16}} = 2.0 \times 10^{-7} T_3^{-0.5}$	2
MN17	H ₃ ⁺ + H ⁻ → Ht + H + H	$k_{\text{MN17}} = 2.3 \times 10^{-7} T_3^{-0.5}$	4
MN18	H ₃ ⁺ + H ⁻ → Ht + Ht	$k_{\text{MN18}} = 2.3 \times 10^{-7} T_3^{-0.5}$	5
MN19	H ₃ ⁺ + D ⁻ → Ht + H + D	$k_{\text{MN19}} = 2.9 \times 10^{-7} T_3^{-0.5}$	6
MN20	H ₃ ⁺ + D ⁻ → Ht + HD	$k_{\text{MN20}} = 2.9 \times 10^{-7} T_3^{-0.5}$	6
MN21	H ₂ D ⁺ + H ⁻ → Ht + H + D	$k_{\text{MN21}} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN22	H ₂ D ⁺ + H ⁻ → Ht + HD	$k_{\text{MN22}} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN23	H ₂ D ⁺ + H ⁻ → HD + H + H	$k_{\text{MN23}} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN24	H ₂ D ⁺ + D ⁻ → Ht + D + D	$k_{\text{MN24}} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN25	H ₂ D ⁺ + D ⁻ → Ht + D ₂	$k_{\text{MN25}} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN26	H ₂ D ⁺ + D ⁻ → HD + H + D	$k_{\text{MN26}} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN27	H ₂ D ⁺ + D ⁻ → HD + HD	$k_{\text{MN27}} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN28	HD ₂ ⁺ + H ⁻ → Ht + D ₂	$k_{\text{MN28}} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN29	HD ₂ ⁺ + H ⁻ → HD + H + D	$k_{\text{MN29}} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN30	HD ₂ ⁺ + H ⁻ → HD + HD	$k_{\text{MN30}} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN31	HD ₂ ⁺ + H ⁻ → D ₂ + H + H	$k_{\text{MN31}} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN32	HD ₂ ⁺ + D ⁻ → HD + D + D	$k_{\text{MN32}} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN33	HD ₂ ⁺ + D ⁻ → HD + D ₂	$k_{\text{MN33}} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN34	HD ₂ ⁺ + D ⁻ → D ₂ + H + D	$k_{\text{MN34}} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN35	D ₃ ⁺ + H ⁻ → HD + D ₂	$k_{\text{MN35}} = 2.4 \times 10^{-7} T_3^{-0.5}$	6
MN36	D ₃ ⁺ + H ⁻ → D ₂ + H + D	$k_{\text{MN36}} = 2.4 \times 10^{-7} T_3^{-0.5}$	6
MN37	D ₃ ⁺ + D ⁻ → D ₂ + D + D	$k_{\text{MN37}} = 3.3 \times 10^{-7} T_3^{-0.5}$	2
MN38	D ₃ ⁺ + D ⁻ → D ₂ + D ₂	$k_{\text{MN38}} = 3.3 \times 10^{-7} T_3^{-0.5}$	2
MN39	Hep + H ⁻ → He + H	$k_{\text{MN39}} = 2.32 \times 10^{-7} T_3^{-0.52} \exp\left(\frac{T}{22400}\right)$	7
MN40	Hep + D ⁻ → He + D	$k_{\text{MN40}} = 3.03 \times 10^{-7} T_3^{-0.52} \exp\left(\frac{T}{22400}\right)$	2
MN41	Li ⁺ + H ⁻ → Li + H	$k_{\text{MN41}} = 2.93 \times 10^{-7} T_3^{-0.477} \exp\left(\frac{T}{23200}\right)$	1
MN42	Li ⁺ + D ⁻ → Li + D	$k_{\text{MN42}} = 2.06 \times 10^{-7} T_3^{-0.5} \exp\left(\frac{T}{18300}\right)$	7
MN43	Li ⁻ + H ⁺ → Li + H	$k_{\text{MN43}} = 1.8 \times 10^{-7} T_3^{-0.477} \exp\left(\frac{T}{23200}\right)$	1
MN44	Li ⁻ + D ⁺ → Li + D	$k_{\text{MN44}} = 2.06 \times 10^{-7} T_3^{-0.5} \exp\left(\frac{T}{18300}\right)$	7

Notes: T is the gas temperature in K, and $T_3 = T/300$ K. Some of the mutual neutralization reactions listed here also include dissociation or transfer in the process.

References: 1 – Croft et al. (1999); 2 – Same as corresponding H reaction, but scaled by D reduced mass; 3 – Dalgarno & Lepp (1987); 4 – Dalgarno & McDowell (1956); 5 – Le Teuff et al. (2000); 6 – As 2, with the additional assumption of equally probable outcomes; 7 – Peart & Hayton (1994).

Table A9. Chemical processes: three-body association (TB).

No.	Reaction	Rate coefficient ($\text{cm}^6 \text{s}^{-1}$)	Ref.
TB1	$\text{H} + \text{H} + \text{H} \rightarrow \text{Ht} + \text{H}$	See §??	—
TB2	$\text{H} + \text{H} + \text{Ht} \rightarrow \text{Ht} + \text{Ht}$	See §??	—
TB3	$\text{H} + \text{H} + \text{He} \rightarrow \text{Ht} + \text{He}$	$k_{\text{TB3}} = 6.9 \times 10^{-32} T^{-0.4}$	1
TB4	$\text{H} + \text{D} + \text{H} \rightarrow \text{HD} + \text{H}$	See §??	—
TB5	$\text{H} + \text{D} + \text{Ht} \rightarrow \text{HD} + \text{Ht}$	See §??	—
TB6	$\text{H} + \text{D} + \text{He} \rightarrow \text{HD} + \text{He}$	$k_{\text{TB6}} = 6.9 \times 10^{-32} T^{-0.4}$	2
TB7	$\text{D} + \text{D} + \text{H} \rightarrow \text{D}_2 + \text{H}$	See §??	—
TB8	$\text{D} + \text{D} + \text{Ht} \rightarrow \text{D}_2 + \text{Ht}$	See §??	—
TB9	$\text{D} + \text{D} + \text{He} \rightarrow \text{D}_2 + \text{He}$	$k_{\text{TB9}} = 6.9 \times 10^{-32} T^{-0.4}$	2
TB10	$\text{H}^+ + \text{H} + \text{H} \rightarrow \text{Htp} + \text{H}$	$k_{\text{TB10}} = 1.203 \times 10^{-29} T^{-1.041}$	3
TB11	$\text{D}^+ + \text{H} + \text{H} \rightarrow \text{HD}^+ + \text{H}$	$k_{\text{TB11}} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB12	$\text{H}^+ + \text{D} + \text{H} \rightarrow \text{HD}^+ + \text{H}$	$k_{\text{TB12}} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB13	$\text{D}^+ + \text{D} + \text{H} \rightarrow \text{D}_2^+ + \text{H}$	$k_{\text{TB13}} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB14	$\text{H}^+ + \text{Ht} + \text{H} \rightarrow \text{H}_3^+ + \text{H}$	$k_{\text{TB14}} = 1.0 \times 10^{-28}$	4
TB15	$\text{H}^+ + \text{Ht} + \text{Ht} \rightarrow \text{H}_3^+ + \text{Ht}$	$k_{\text{TB15}} = 5.4 \times 10^{-29}$	5
TB16	$\text{H}^+ + \text{Ht} + \text{He} \rightarrow \text{H}_3^+ + \text{He}$	$k_{\text{TB16}} = 1.07 \times 10^{-28}$	5
TB17	$\text{D}^+ + \text{Ht} + \text{H} \rightarrow \text{H}_2\text{D}^+ + \text{H}$	$k_{\text{TB17}} = 1.0 \times 10^{-28}$	4
TB18	$\text{D}^+ + \text{Ht} + \text{Ht} \rightarrow \text{H}_2\text{D}^+ + \text{Ht}$	$k_{\text{TB18}} = 5.4 \times 10^{-29}$	2
TB19	$\text{D}^+ + \text{Ht} + \text{He} \rightarrow \text{H}_2\text{D}^+ + \text{He}$	$k_{\text{TB19}} = 1.07 \times 10^{-28}$	2
TB20	$\text{H}^+ + \text{HD} + \text{H} \rightarrow \text{H}_2\text{D}^+ + \text{H}$	$k_{\text{TB20}} = 1.0 \times 10^{-28}$	4
TB21	$\text{H}^+ + \text{HD} + \text{Ht} \rightarrow \text{H}_2\text{D}^+ + \text{Ht}$	$k_{\text{TB21}} = 5.4 \times 10^{-29}$	2
TB22	$\text{H}^+ + \text{HD} + \text{He} \rightarrow \text{H}_2\text{D}^+ + \text{He}$	$k_{\text{TB22}} = 1.07 \times 10^{-28}$	2
TB23	$\text{D}^+ + \text{HD} + \text{H} \rightarrow \text{HD}_2^+ + \text{H}$	$k_{\text{TB23}} = 1.0 \times 10^{-28}$	4
TB24	$\text{D}^+ + \text{HD} + \text{Ht} \rightarrow \text{HD}_2^+ + \text{Ht}$	$k_{\text{TB24}} = 5.4 \times 10^{-29}$	2
TB25	$\text{D}^+ + \text{HD} + \text{He} \rightarrow \text{HD}_2^+ + \text{He}$	$k_{\text{TB25}} = 1.07 \times 10^{-28}$	2
TB26	$\text{H}^+ + \text{D}_2 + \text{H} \rightarrow \text{HD}_2^+ + \text{H}$	$k_{\text{TB26}} = 1.0 \times 10^{-28}$	4
TB27	$\text{H}^+ + \text{D}_2 + \text{Ht} \rightarrow \text{HD}_2^+ + \text{Ht}$	$k_{\text{TB27}} = 5.4 \times 10^{-29}$	2
TB28	$\text{H}^+ + \text{D}_2 + \text{He} \rightarrow \text{HD}_2^+ + \text{He}$	$k_{\text{TB28}} = 1.07 \times 10^{-28}$	2
TB29	$\text{D}^+ + \text{D}_2 + \text{H} \rightarrow \text{D}_3^+ + \text{H}$	$k_{\text{TB29}} = 1.0 \times 10^{-28}$	4
TB30	$\text{D}^+ + \text{D}_2 + \text{Ht} \rightarrow \text{D}_3^+ + \text{Ht}$	$k_{\text{TB30}} = 5.4 \times 10^{-29}$	2
TB31	$\text{D}^+ + \text{D}_2 + \text{He} \rightarrow \text{D}_3^+ + \text{He}$	$k_{\text{TB31}} = 1.07 \times 10^{-28}$	2
TB32	$\text{Li} + \text{H} + \text{H} \rightarrow \text{LiH} + \text{H}$	$k_{\text{TB32}} = 2.5 \times 10^{-29} T^{-1}$	6
TB33	$\text{Li} + \text{H} + \text{Ht} \rightarrow \text{LiH} + \text{Ht}$	$k_{\text{TB33}} = 4.1 \times 10^{-30} T^{-1}$	6
TB34	$\text{Li} + \text{D} + \text{H} \rightarrow \text{LiD} + \text{H}$	$k_{\text{TB34}} = 2.5 \times 10^{-29} T^{-1}$	2
TB35	$\text{Li} + \text{D} + \text{Ht} \rightarrow \text{LiD} + \text{Ht}$	$k_{\text{TB35}} = 4.1 \times 10^{-30} T^{-1}$	2

Notes: T is the gas temperature in K.

References: 1 – Walkauskas & Kaufman (1975); 2 – Same as corresponding H reaction; 3 – Krstić, Janev, & Schultz (2003); 4 – Estimate; 5 – Gerlich & Horning (1992); 6 – Mizusawa, Omukai, & Nishi (2005).

Table A10. Chemical processes: isotopic exchange (IX).

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
IX1	Htp + D → HD ⁺ + H	$k_{\text{IX1}} = 1.07 \times 10^{-9} T_3^{0.062} \exp\left(-\frac{T}{41400}\right)$		1
IX2	Htp + D → HD + H ⁺	$k_{\text{IX2}} = 1.0 \times 10^{-9}$		2
IX3	HD ⁺ + H → Htp + D	$k_{\text{IX3}} = 1.0 \times 10^{-9} \exp\left(-\frac{154}{T}\right)$		3
IX4	HD ⁺ + H → Ht + D ⁺	$k_{\text{IX4}} = 1.0 \times 10^{-9}$		2
IX5	HD ⁺ + D → D ₂ ⁺ + H	$k_{\text{IX5}} = 1.0 \times 10^{-9}$		4
IX6	HD ⁺ + D → D ₂ + H ⁺	$k_{\text{IX6}} = 1.0 \times 10^{-9}$		2
IX7	D ₂ ⁺ + H → HD ⁺ + D	$k_{\text{IX7}} = 1.0 \times 10^{-9} \exp\left(-\frac{472}{T}\right)$		4
IX8	D ₂ ⁺ + H → HD + D ⁺	$k_{\text{IX8}} = 1.0 \times 10^{-9}$		2
IX9	Ht + D ⁺ → HD + H ⁺	$k_{\text{IX9}} = 4.17 \times 10^{-10} + 8.46 \times 10^{-10} \log T$ $- 1.37 \times 10^{-10} (\log T)^2$		5
IX10	Ht + D ⁺ → HD ⁺ + H	$k_{\text{IX10}} = \left[1.04 \times 10^{-9} + 9.52 \times 10^{-9} \left(\frac{T}{10000}\right) - 1.81 \times 10^{-9} \left(\frac{T}{10000}\right)^2\right] \exp\left(-\frac{21000}{T}\right)$		6
IX11	HD + H ⁺ → Ht + D ⁺	$k_{\text{IX11}} = 1.1 \times 10^{-9} \exp\left(-\frac{488}{T}\right)$		5
IX12	HD + H ⁺ → Htp + D	$k_{\text{IX12}} = 1.0 \times 10^{-9} \exp\left(-\frac{21600}{T}\right)$		2
IX13	HD + D ⁺ → D ₂ + H ⁺	$k_{\text{IX13}} = 1.0 \times 10^{-9}$		4
IX14	HD + D ⁺ → D ₂ ⁺ + H	$k_{\text{IX14}} = \left[3.54 \times 10^{-9} + 7.50 \times 10^{-10} \left(\frac{T}{10000}\right) - 2.92 \times 10^{-10} \left(\frac{T}{10000}\right)^2\right] \exp\left(-\frac{21100}{T}\right)$		6
IX15	D ₂ + H ⁺ → HD + D ⁺	$k_{\text{IX15}} = 2.1 \times 10^{-9} \exp\left(-\frac{491}{T}\right)$		4
IX16	D ₂ + H ⁺ → HD ⁺ + D	$k_{\text{IX16}} = \left[5.18 \times 10^{-11} + 3.05 \times 10^{-9} \left(\frac{T}{10000}\right) - 5.42 \times 10^{-10} \left(\frac{T}{10000}\right)^2\right] \exp\left(-\frac{20100}{T}\right)$		6
IX17	Ht + D → HD + H	$k_{\text{IX17}} = \text{dex}[-56.4737 + 5.88886 \log T$ $+ 7.19692(\log T)^2$ $+ 2.25069(\log T)^3$ $- 2.16903(\log T)^4$ $+ 0.317887(\log T)^5]$ $= 3.17 \times 10^{-10} \exp\left(-\frac{5207}{T}\right)$	$T \leq 2000$ K $T > 2000$ K	7
IX18	HD + H → Ht + D	$k_{\text{IX18}} = 5.25 \times 10^{-11} \exp\left(-\frac{4430}{T}\right)$ $= 5.25 \times 10^{-11} \exp\left(-\frac{4430}{T} + \frac{173900}{T^2}\right)$	$T \leq 200$ K $T > 200$ K	8
IX19	HD + D → D ₂ + H	$k_{\text{IX19}} = 1.15 \times 10^{-11} \exp\left(-\frac{3220}{T}\right)$		8
IX20	D ₂ + H → HD + D	$k_{\text{IX20}} = \text{dex}[-86.1558 + 4.53978 \log T$ $+ 33.5707(\log T)^2$ $- 13.0449(\log T)^3$ $+ 1.22017(\log T)^4$ $+ 0.0482453(\log T)^5]$ $= 2.67 \times 10^{-10} \exp\left(-\frac{5945}{T}\right)$	$T \leq 2200$ K $T > 2200$ K	7
IX21	H ₃ ⁺ + D → H ₂ D ⁺ + H	$k_{\text{IX21}} = 1.0 \times 10^{-9}$		9
IX22	H ₂ D ⁺ + H → H ₃ ⁺ + D	$k_{\text{IX22}} = 1.0 \times 10^{-9} \exp\left(-\frac{632}{T}\right)$		10
IX23	H ₂ D ⁺ + D → HD ₂ ⁺ + H	$k_{\text{IX23}} = 1.0 \times 10^{-9}$		4
IX24	HD ₂ ⁺ + H → H ₂ D ⁺ + D	$k_{\text{IX24}} = 1.0 \times 10^{-9} \exp\left(-\frac{600}{T}\right)$		4
IX25	HD ₂ ⁺ + D → D ₃ ⁺ + H	$k_{\text{IX25}} = 1.0 \times 10^{-9}$		4
IX26	D ₃ ⁺ + H → HD ₂ ⁺ + D	$k_{\text{IX26}} = 1.0 \times 10^{-9} \exp\left(-\frac{655}{T}\right)$		4
IX27	H ₃ ⁺ + HD → H ₂ D ⁺ + Ht	$k_{\text{IX27}} = 3.5 \times 10^{-10}$		4
IX28	H ₃ ⁺ + D ₂ → H ₂ D ⁺ + HD	$k_{\text{IX28}} = 3.5 \times 10^{-11} T_3^{-0.19}$		11
IX29	H ₃ ⁺ + D ₂ → HD ₂ ⁺ + Ht	$k_{\text{IX29}} = 9.64 \times 10^{-10} T_3^{-0.024}$		11
IX30	H ₂ D ⁺ + Ht → H ₃ ⁺ + HD	$k_{\text{IX30}} = 1.4 \times 10^{-10} \exp\left(-\frac{232}{T}\right)$		4
IX31	H ₂ D ⁺ + HD → H ₃ ⁺ + D ₂	$k_{\text{IX31}} = 1.75 \times 10^{-11} T_3^{-0.19} \exp\left(-\frac{153}{T}\right)$		12
IX32	H ₂ D ⁺ + HD → HD ₂ ⁺ + Ht	$k_{\text{IX32}} = 2.6 \times 10^{-10}$		4
IX33	H ₂ D ⁺ + D ₂ → HD ₂ ⁺ + HD	$k_{\text{IX33}} = 8.5 \times 10^{-10}$		4
IX34	H ₂ D ⁺ + D ₂ → D ₃ ⁺ + Ht	$k_{\text{IX34}} = 8.5 \times 10^{-10}$		4
IX35	HD ₂ ⁺ + Ht → H ₃ ⁺ + D ₂	$k_{\text{IX35}} = 2.0 \times 10^{-10} \exp\left(-\frac{340.2}{T}\right)$		13

Table A10 – *continued*

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Notes	Ref.
IX36	HD ₂ ⁺ + Ht → H ₂ D ⁺ + HD	$k_{\text{IX36}} = 1.0 \times 10^{-10} \exp\left(-\frac{187.2}{T}\right) \times \left[1.0 + \exp\left(-\frac{87}{T}\right)\right]$		13
IX37	HD ₂ ⁺ + HD → H ₂ D ⁺ + D ₂	$k_{\text{IX37}} = 1.0 \times 10^{-10} \exp\left(-\frac{108.4}{T}\right) \times \left[1.0 + \exp\left(-\frac{86.5}{T}\right)\right]$		13
IX38	HD ₂ ⁺ + HD → D ₃ ⁺ + Ht	$k_{\text{IX38}} = 2.0 \times 10^{-10}$		4
IX39	HD ₂ ⁺ + D ₂ → D ₃ ⁺ + HD	$k_{\text{IX39}} = 8.7 \times 10^{-10}$		14
IX40	D ₃ ⁺ + Ht → H ₂ D ⁺ + D ₂	$k_{\text{IX40}} = 1.5 \times 10^{-9} \exp\left(-\frac{342.2}{T}\right)$		13
IX41	D ₃ ⁺ + Ht → HD ₂ ⁺ + HD	$k_{\text{IX41}} = 1.5 \times 10^{-9} \exp\left(-\frac{233.8}{T}\right)$		13
IX42	D ₃ ⁺ + HD → HD ₂ ⁺ + D ₂	$k_{\text{IX42}} = 3.75 \times 10^{-10} \exp\left(-\frac{155}{T}\right) \times \left[1.0 + 2.0 \exp\left(-\frac{50.4}{T}\right) + \exp\left(-\frac{86}{T}\right)\right]$		13
IX43	HeH ⁺ + D → HeD ⁺ + H	$k_{\text{IX43}} = 1.0 \times 10^{-9}$		3
IX44	HeD ⁺ + H → HeH ⁺ + D	$k_{\text{IX44}} = 8.0 \times 10^{-10} \exp\left(-\frac{468}{T}\right)$		3
IX45	LiH ⁺ + D → LiD ⁺ + H	$k_{\text{IX45}} = 1.0 \times 10^{-9}$		2
IX46	LiD ⁺ + H → LiH ⁺ + D	$k_{\text{IX46}} = 1.0 \times 10^{-9} \exp\left(-\frac{64}{T}\right)$		2

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Linder, Janev & Botero (1995); 2 – estimate; 3 – Dalgarno & McDowell (1956), scaled as in Stancil et al. (1998); 4 – Walmsley, Flower & Pineau des Forêts (2004); 5 – Gerlich (1982); 6 – Our fits to cross-sections from Wang & Stancil (2002); 7 – Our fits to Mielke et al. (2003); 8 – Shavitt (1959); 9 – Millar, Bennett & Herbst (1989); 10 – Pineau des Forêts et al. (1989); 11 – Moyano & Collins (2003); 12 – Derived from forward reaction, using equilibrium constant from Ramanlal & Tennyson (2004); 13 – Flower, Pineau des Forêts & Walmsley (2004); 14 – Derived from inverse reaction in Walmsley, Flower & Pineau des Forêts (2004).

Table A11. Chemical processes: transfer reactions (TR).

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Ref.
TR1	Htp + Ht → H ₃ ⁺ + H	$k_{\text{TR1}} = 2.24 \times 10^{-9} T_3^{0.042} \exp\left(-\frac{T}{46600}\right)$	1
TR2	Htp + HD → H ₃ ⁺ + D	$k_{\text{TR2}} = 1.05 \times 10^{-9}$	2
TR3	Htp + HD → H ₂ D ⁺ + H	$k_{\text{TR3}} = 1.05 \times 10^{-9}$	2
TR4	Htp + D ₂ → H ₂ D ⁺ + D	$k_{\text{TR4}} = 1.05 \times 10^{-9}$	3
TR5	Htp + D ₂ → HD ₂ ⁺ + H	$k_{\text{TR5}} = 1.05 \times 10^{-9}$	3
TR6	HD ⁺ + Ht → H ₃ ⁺ + D	$k_{\text{TR6}} = 0.5 \times k_{\text{TR1}}$	1
TR7	HD ⁺ + Ht → H ₂ D ⁺ + H	$k_{\text{TR7}} = 0.5 \times k_{\text{TR1}}$	1
TR8	HD ⁺ + HD → H ₂ D ⁺ + D	$k_{\text{TR8}} = 1.05 \times 10^{-9}$	3
TR9	HD ⁺ + HD → HD ₂ ⁺ + H	$k_{\text{TR9}} = 1.05 \times 10^{-9}$	3
TR10	HD ⁺ + D ₂ → HD ₂ ⁺ + D	$k_{\text{TR10}} = 1.05 \times 10^{-9}$	3
TR11	HD ⁺ + D ₂ → D ₃ ⁺ + H	$k_{\text{TR11}} = 1.05 \times 10^{-9}$	3
TR12	D ₂ ⁺ + Ht → H ₂ D ⁺ + D	$k_{\text{TR12}} = 1.05 \times 10^{-9}$	3
TR13	D ₂ ⁺ + Ht → HD ₂ ⁺ + H	$k_{\text{TR13}} = 1.05 \times 10^{-9}$	3
TR14	D ₂ ⁺ + HD → HD ₂ ⁺ + D	$k_{\text{TR14}} = 1.05 \times 10^{-9}$	3
TR15	D ₂ ⁺ + HD → D ₃ ⁺ + H	$k_{\text{TR15}} = 1.05 \times 10^{-9}$	3
TR16	D ₂ ⁺ + D ₂ → D ₃ ⁺ + D	$k_{\text{TR16}} = 2.1 \times 10^{-9}$	3
TR17	H ₃ ⁺ + H → Htp + Ht	$k_{\text{TR17}} = 7.7 \times 10^{-9} \exp\left(-\frac{17560}{T}\right)$	4
TR18	H ₃ ⁺ + D → Htp + HD	$k_{\text{TR18}} = 0.5 \times k_{\text{TR17}}$	5
TR19	H ₃ ⁺ + D → HD ⁺ + Ht	$k_{\text{TR19}} = 0.5 \times k_{\text{TR17}}$	5
TR20	H ₂ D ⁺ + H → Htp + HD	$k_{\text{TR20}} = 0.5 \times k_{\text{TR17}}$	5
TR21	H ₂ D ⁺ + H → HD ⁺ + Ht	$k_{\text{TR21}} = 0.5 \times k_{\text{TR17}}$	5
TR22	H ₂ D ⁺ + D → Htp + D ₂	$k_{\text{TR22}} = 0.333 \times k_{\text{TR17}}$	5
TR23	H ₂ D ⁺ + D → HD ⁺ + HD	$k_{\text{TR23}} = 0.333 \times k_{\text{TR17}}$	5
TR24	H ₂ D ⁺ + D → D ₂ ⁺ + Ht	$k_{\text{TR24}} = 0.333 \times k_{\text{TR17}}$	5
TR25	HD ₂ ⁺ + H → Htp + D ₂	$k_{\text{TR25}} = 0.333 \times k_{\text{TR17}}$	5
TR26	HD ₂ ⁺ + H → HD ⁺ + HD	$k_{\text{TR26}} = 0.333 \times k_{\text{TR17}}$	5
TR27	HD ₂ ⁺ + H → D ₂ ⁺ + Ht	$k_{\text{TR27}} = 0.333 \times k_{\text{TR17}}$	5
TR28	HD ₂ ⁺ + D → HD ⁺ + D ₂	$k_{\text{TR28}} = 0.5 \times k_{\text{TR17}}$	5
TR29	HD ₂ ⁺ + D → D ₂ ⁺ + HD	$k_{\text{TR29}} = 0.5 \times k_{\text{TR17}}$	5
TR30	D ₃ ⁺ + H → HD ⁺ + D ₂	$k_{\text{TR30}} = 0.5 \times k_{\text{TR17}}$	5
TR31	D ₃ ⁺ + H → D ₂ ⁺ + HD	$k_{\text{TR31}} = 0.5 \times k_{\text{TR17}}$	5
TR32	D ₃ ⁺ + D → D ₂ ⁺ + D ₂	$k_{\text{TR32}} = k_{\text{TR17}}$	5
TR33	He + Htp → HeH ⁺ + H	$k_{\text{TR33}} = 3.0 \times 10^{-10} \exp\left(-\frac{6717}{T}\right)$	6
TR34	He + HD ⁺ → HeH ⁺ + D	$k_{\text{TR34}} = k_{\text{TR33}}$	7
TR35	He + HD ⁺ → HeD ⁺ + H	$k_{\text{TR35}} = k_{\text{TR33}}$	7
TR36	He + D ₂ ⁺ → HeD ⁺ + D	$k_{\text{TR36}} = k_{\text{TR33}}$	8
TR37	HeH ⁺ + H → Htp + He	$k_{\text{TR37}} = 1.04 \times 10^{-9} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	1
TR38	HeH ⁺ + D → HD ⁺ + He	$k_{\text{TR38}} = 8.5 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	9
TR39	HeH ⁺ + Ht → H ₃ ⁺ + He	$k_{\text{TR39}} = 1.53 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	1
TR40	HeH ⁺ + HD → H ₂ D ⁺ + He	$k_{\text{TR40}} = 1.20 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	2
TR41	HeH ⁺ + D ₂ → HD ₂ ⁺ + He	$k_{\text{TR41}} = 1.1 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR42	HeD ⁺ + H → HD ⁺ + He	$k_{\text{TR42}} = 9.1 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	9
TR43	HeD ⁺ + D → D ₂ ⁺ + He	$k_{\text{TR43}} = 8.5 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	11
TR44	HeD ⁺ + Ht → H ₂ D ⁺ + He	$k_{\text{TR44}} = 1.24 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	2
TR45	HeD ⁺ + HD → HD ₂ ⁺ + He	$k_{\text{TR45}} = 1.2 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR46	HeD ⁺ + D ₂ → D ₃ ⁺ + He	$k_{\text{TR46}} = 1.1 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR47	LiH ⁺ + H → Li ⁺ + Ht	$k_{\text{TR47}} = 3.0 \times 10^{-10}$	12
TR48	LiH ⁺ + D → Li ⁺ + HD	$k_{\text{TR48}} = 3.0 \times 10^{-10}$	13
TR49	LiD ⁺ + H → Li ⁺ + HD	$k_{\text{TR49}} = 3.0 \times 10^{-10}$	14
TR50	LiD ⁺ + D → Li ⁺ + D ₂	$k_{\text{TR50}} = 3.0 \times 10^{-10}$	14
TR51	LiH ⁺ + H → Li + Htp	$k_{\text{TR51}} = 9.0 \times 10^{-10} \exp\left(-\frac{66400}{T}\right)$	12
TR52	LiH ⁺ + D → Li + HD ⁺	$k_{\text{TR52}} = k_{\text{TR51}}$	13
TR53	LiD ⁺ + H → Li + HD ⁺	$k_{\text{TR53}} = k_{\text{TR51}}$	14
TR54	LiD ⁺ + D → Li + D ₂ ⁺	$k_{\text{TR54}} = k_{\text{TR51}}$	14

Table A11 – *continued*

No.	Reaction	Rate coefficient (cm ³ s ⁻¹)	Ref.
TR55	LiH + H ⁺ → Li ⁺ + Ht	$k_{\text{TR55}} = 2.0 \times 10^{-15}$	15
TR56	LiH + D ⁺ → Li ⁺ + HD	$k_{\text{TR56}} = 2.0 \times 10^{-15}$	16
TR57	LiD + H ⁺ → Li ⁺ + HD	$k_{\text{TR57}} = 2.0 \times 10^{-15}$	16
TR58	LiD + D ⁺ → Li ⁺ + D ₂	$k_{\text{TR58}} = 2.0 \times 10^{-15}$	16
TR59	LiH + H ⁺ → Li + Htp	$k_{\text{TR59}} = 1.0 \times 10^{-9}$	12
TR60	LiH + D ⁺ → Li + HD ⁺	$k_{\text{TR60}} = 1.0 \times 10^{-9}$	16
TR61	LiD + H ⁺ → Li + HD ⁺	$k_{\text{TR61}} = 1.0 \times 10^{-9}$	16
TR62	LiD + D ⁺ → Li + D ₂ ⁺	$k_{\text{TR62}} = 1.0 \times 10^{-9}$	16
TR63	LiH + H → Li + Ht	$k_{\text{TR63}} = 1.55 \times 10^{-11} T^{0.4247}$	17
TR64	LiH + D → Li + HD	$k_{\text{TR64}} = 1.2 \times 10^{-11} T^{0.4247}$	11
TR65	LiD + H → Li + HD	$k_{\text{TR65}} = 1.54 \times 10^{-11} T^{0.4247}$	11
TR66	LiD + D → Li + D ₂	$k_{\text{TR66}} = 1.2 \times 10^{-11} T^{0.4247}$	11

Notes: T is the gas temperature in K, and $T_3 = T/300$ K.

References: 1 – Linder, Janev & Botero (1995); 2 – Stancil et al. (1998); 3 – Walmsley, Flower & Pineau des Forêts (2004); 4 – Sidhu, Miller & Tennyson (1992); 5 – estimate, based on Sidhu, Miller & Tennyson (1992); 6 – Black (1978); 7 – Stancil et al. (1998), based on Black (1978); 8 estimate, based on Black (1978); 9 – Linder, Janev & Botero (1995), scaled as in Stancil et al. (1998); 10 – Estimate, based on Stancil et al. (1998); 11 – Same as corresponding H reaction, but scaled by D reduced mass; 12 – Stancil et al. (1996); 13 – Stancil et al. (1998), based on corresponding H reaction in Stancil et al. (1996); 14 – estimate, based on Stancil et al. (1996); 15 – Bodo et al. (2001); 16 – same as corresponding H reaction; 17 – Defazio et al. (2005).

Table A12. Chemical processes: background radiation induced photodetachment, photodissociation and photoionization (BP).

No.	Reaction	Rate ($J_{21}^{-1} \text{ s}^{-1}$)	Ref.
BP1	$\text{H}^- + \gamma \rightarrow \text{H} + \text{e}^-$	$R_{\text{BP1}} = 1.36 \times 10^{-11}$	1
BP2	$\text{D}^- + \gamma \rightarrow \text{D} + \text{e}^-$	$R_{\text{BP2}} = 1.36 \times 10^{-11}$	2
BP3	$\text{Htp} + \gamma \rightarrow \text{H} + \text{H}^+$	$R_{\text{BP3}} = 4.11 \times 10^{-12}$	3
BP4	$\text{HD}^+ + \gamma \rightarrow \text{H} + \text{D}^+$	$R_{\text{BP4}} = 2.05 \times 10^{-12}$	2
BP5	$\text{HD}^+ + \gamma \rightarrow \text{D} + \text{H}^+$	$R_{\text{BP5}} = 2.05 \times 10^{-12}$	2
BP6	$\text{D}_2^+ + \gamma \rightarrow \text{D} + \text{D}^+$	$R_{\text{BP6}} = 4.11 \times 10^{-12}$	2
BP7	$\text{Ht} + \gamma \rightarrow \text{H} + \text{H}$	$R_{\text{BP7}} = 1.3 \times 10^{-12} f_{\text{sh,Ht}}$	5
BP8	$\text{HD} + \gamma \rightarrow \text{H} + \text{D}$	$R_{\text{BP8}} = 1.45 \times 10^{-12} f_{\text{sh,HD}}$	6
BP9	$\text{D}_2 + \gamma \rightarrow \text{D} + \text{D}$	$R_{\text{BP9}} = 1.3 \times 10^{-12}$	7
BP10	$\text{H}_3^+ + \gamma \rightarrow \text{Htp} + \text{H}$	$R_{\text{BP10}} = 2.4 \times 10^{-16}$	8
BP11	$\text{H}_3^+ + \gamma \rightarrow \text{Ht} + \text{H}^+$	$R_{\text{BP11}} = 2.4 \times 10^{-16}$	8
BP12	$\text{H}_2\text{D}^+ + \gamma \rightarrow \text{Htp} + \text{D}$	$R_{\text{BP12}} = 1.2 \times 10^{-16}$	9
BP13	$\text{H}_2\text{D}^+ + \gamma \rightarrow \text{Ht} + \text{D}^+$	$R_{\text{BP13}} = 1.2 \times 10^{-16}$	9
BP14	$\text{H}_2\text{D}^+ + \gamma \rightarrow \text{HD}^+ + \text{H}$	$R_{\text{BP14}} = 1.2 \times 10^{-16}$	9
BP15	$\text{H}_2\text{D}^+ + \gamma \rightarrow \text{HD} + \text{H}^+$	$R_{\text{BP15}} = 1.2 \times 10^{-16}$	9
BP16	$\text{HD}_2^+ + \gamma \rightarrow \text{HD}^+ + \text{D}$	$R_{\text{BP16}} = 1.2 \times 10^{-16}$	9
BP17	$\text{HD}_2^+ + \gamma \rightarrow \text{HD} + \text{D}^+$	$R_{\text{BP17}} = 1.2 \times 10^{-16}$	9
BP18	$\text{HD}_2^+ + \gamma \rightarrow \text{D}_2^+ + \text{H}$	$R_{\text{BP18}} = 1.2 \times 10^{-16}$	9
BP19	$\text{HD}_2^+ + \gamma \rightarrow \text{D}_2 + \text{H}^+$	$R_{\text{BP19}} = 1.2 \times 10^{-16}$	9
BP20	$\text{D}_3^+ + \gamma \rightarrow \text{D}_2^+ + \text{D}$	$R_{\text{BP20}} = 2.4 \times 10^{-16}$	9
BP21	$\text{D}_3^+ + \gamma \rightarrow \text{D}_2 + \text{D}^+$	$R_{\text{BP21}} = 2.4 \times 10^{-16}$	9
BP22	$\text{HeH}^+ + \gamma \rightarrow \text{He} + \text{H}^+$	$R_{\text{BP22}} = 1.0 \times 10^{-17}$	10
BP23	$\text{HeD}^+ + \gamma \rightarrow \text{He} + \text{D}^+$	$R_{\text{BP23}} = 1.0 \times 10^{-17}$	10
BP24	$\text{He}_2^+ + \gamma \rightarrow \text{He} + \text{Hep}$	$R_{\text{BP24}} = 1.0 \times 10^{-12}$	11
BP25	$\text{Li} + \gamma \rightarrow \text{Li}^+ + \text{e}^-$	$R_{\text{BP25}} = 1.4 \times 10^{-12}$	12
BP26	$\text{Li}^- + \gamma \rightarrow \text{Li} + \text{e}^-$	$R_{\text{BP26}} = 1.2 \times 10^{-11}$	13
BP27	$\text{LiH}^+ + \gamma \rightarrow \text{Li}^+ + \text{H}$	$R_{\text{BP27}} = 5.0 \times 10^{-18}$	13
BP28	$\text{LiH}^+ + \gamma \rightarrow \text{Li} + \text{H}^+$	$R_{\text{BP28}} = 9.3 \times 10^{-9}$	13
BP29	$\text{LiD}^+ + \gamma \rightarrow \text{Li}^+ + \text{D}$	$R_{\text{BP29}} = 5.0 \times 10^{-18}$	2
BP30	$\text{LiD}^+ + \gamma \rightarrow \text{Li} + \text{D}^+$	$R_{\text{BP30}} = 9.3 \times 10^{-9}$	2
BP31	$\text{LiH} + \gamma \rightarrow \text{Li} + \text{H}$	$R_{\text{BP31}} = 4.4 \times 10^{-14}$	14
BP32	$\text{LiD} + \gamma \rightarrow \text{Li} + \text{D}$	$R_{\text{BP32}} = 4.4 \times 10^{-14}$	2

Notes: γ represents a photon from the external background radiation field. The listed reaction rates were computed assuming that this background has the spectrum of a 10^5 K diluted black-body, cut-off above $h\nu = 13.6$ eV, as described in Section 3. With this spectrum, reactions with threshold energies greater than 13.6 eV do not occur and are not listed in the table. $f_{\text{sh,Ht}}$ and $f_{\text{sh,HD}}$ are the self-shielding factors for Ht and HD photodissociation, respectively (see e.g. Glover & Jappsen 2007). Note that in this paper, we consider only the limiting cases $f_{\text{sh,Ht}} = f_{\text{sh,HD}} = 0$ and $f_{\text{sh,Ht}} = f_{\text{sh,HD}} = 1$.

References: 1 – Wishart (1979); 2 – assumed same as for corresponding H reaction; 3 – Dunn (1968); 4 – total rate assumed same as for corresponding H reaction, individual outcomes assumed equally probable; 5 – Draine & Bertoldi (1996); 6 – Abgrall & Roueff (2006); 7 – estimate; 8 – van Dishoeck (1988); 9 – estimate, based on van Dishoeck (1988); 10 – Roberge & Dalgarno (1982); 11 – Stancil (1994); 12 – Verner & Ferland (1996); 13 – Galli & Palla (1998); 14 – Kirby & Dalgarno (1978).

Table A13. Chemical processes: cosmic ray ionization (CR).

No.	Process	Rate (ζ_i/ζ_H)	Reference
CR1	$H + \text{C.R.} \rightarrow H^+ + e^-$	1.0	—
CR2	$\text{Ht} + \text{C.R.} \rightarrow \text{Htp} + e^-$	2.09	1
CR3	$\text{Ht} + \text{C.R.} \rightarrow H + H^+ + e^-$	0.09	1
CR4	$\text{Ht} + \text{C.R.} \rightarrow H + H$	3.26	1
CR5	$\text{He} + \text{C.R.} \rightarrow \text{Hep} + e^-$	1.09	1
CR6	$D + \text{C.R.} \rightarrow D^+ + e^-$	1.0	2
CR7	$\text{HD} + \text{C.R.} \rightarrow \text{HD}^+ + e^-$	2.09	2
CR8	$\text{HD} + \text{C.R.} \rightarrow H + D^+ + e^-$	0.04	2
CR9	$\text{HD} + \text{C.R.} \rightarrow H^+ + D + e^-$	0.04	2
CR10	$\text{HD} + \text{C.R.} \rightarrow H + D$	3.26	2
CR11	$D_2 + \text{C.R.} \rightarrow D_2^+ + e^-$	2.09	2
CR12	$D_2 + \text{C.R.} \rightarrow D + D^+ + e^-$	0.09	2
CR13	$D_2 + \text{C.R.} \rightarrow D + D$	3.26	2

Notes: C.R. represents a cosmic ray. ζ_H , the cosmic ray ionization rate of atomic hydrogen, is an adjustable parameter in our models.

References: 1 – Walmsley, Flower, & Pineau des Forêts (2004); 2 – assumed same as corresponding H process.

Table A14. Chemical processes: cosmic ray induced photodetachment, photodissociation and photoionization (CP) .

No.	Reaction	$\sigma_{X,\text{eff,Ht}}$ (Mb)	$\sigma_{X,\text{eff,H}}$ (Mb)	Ref.
CP1	$H^- + \gamma_{\text{cr}} \rightarrow H + e^-$	5.0	5.8	1
CP2	$D^- + \gamma_{\text{cr}} \rightarrow D + e^-$	5.0	5.8	2
CP3	$\text{Htp} + \gamma_{\text{cr}} \rightarrow H + H^+$	5.0	6.6	3
CP4	$\text{HD}^+ + \gamma_{\text{cr}} \rightarrow H + D^+$	2.5	3.3	2
CP5	$\text{HD}^+ + \gamma_{\text{cr}} \rightarrow D + H^+$	2.5	3.3	2
CP6	$D_2^+ + \gamma_{\text{cr}} \rightarrow D + D^+$	5.0	6.6	2
CP7	$\text{Li} + \gamma_{\text{cr}} \rightarrow \text{Li}^+ + e^-$	1.0	1.3	4
CP8	$\text{Li}^- + \gamma_{\text{cr}} \rightarrow \text{Li} + e^-$	1.0	1.0	5
CP9	$\text{He}_2^+ + \gamma_{\text{cr}} \rightarrow \text{He} + \text{Hep}$	5.0	5.0	6
CP10	$\text{LiH}^+ + \gamma_{\text{cr}} \rightarrow \text{Li} + H^+$	100	100	7
CP11	$\text{LiD}^+ + \gamma_{\text{cr}} \rightarrow \text{Li} + D^+$	100	100	2

Notes: γ_{cr} represents a secondary photon, produced by cosmic-ray induced excitation of H or Ht, as described in Section 3.3. The references listed are the sources from which we have taken our photodissociation or photoionization cross-sections. The emission probabilities $P_{\text{Ht}}(\nu)$ used to calculate $\sigma_{X,\text{eff,Ht}}$ are rough estimates based on the emission spectra given in Sternberg, Dalgarno, & Lepp (1987) and are likely accurate only to within a factor of a few.

References: 1 – Wishart (1979); 2 – assumed same as for corresponding H reaction; 3 – Dunn (1968); 4 – Verner & Ferland (1996); 5 – order of magnitude estimate; 6 – estimate, based on Stancil (1994); 7 – rough estimate, based on thermal rate in Galli & Palla (1998).