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, $T_3 = T/300\,\mathrm{K}$, and T_{e} is the gas temperature in units of eV.

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

No.	Reaction	Rate coefficient ($cm^3\ s^{-1}$)	Ref.
CI1	$H + e^- \rightarrow H^+ + e^- + e^-$	$k_{CI1} = \exp[-3.271396786 \times 10^1 + 1.35365560 \times 10^1 \ln T_e - 5.73932875 \times 10^0 (\ln T_e)^2 + 1.56315498 \times 10^0 (\ln T_e)^3 - 2.87705600 \times 10^{-1} (\ln T_e)^4 + 3.48255977 \times 10^{-2} (\ln T_e)^5 - 2.63197617 \times 10^{-3} (\ln T_e)^6 + 1.11954395 \times 10^{-4} (\ln T_e)^7 - 2.03914985 \times 10^{-6} (\ln T_e)^8]$	1
CI2	$D + e^- \rightarrow D^+ + e^- + e^-$	$k_{CI2} = k_{CI1}$	1
CI3	$He + e^- \rightarrow Hep + e^- + e^-$	$k_{CI3} = \exp[-4.409864886 \times 10^1 + 2.391596563 \times 10^1 \ln T_e - 1.07532302 \times 10^1 (\ln T_e)^2 + 3.05803875 \times 10^0 (\ln T_e)^3 - 5.68511890 \times 10^{-1} (\ln T_e)^4 + 6.79539123 \times 10^{-2} (\ln T_e)^5 - 5.00905610 \times 10^{-3} (\ln T_e)^6 + 2.06723616 \times 10^{-4} (\ln T_e)^7 - 3.64916141 \times 10^{-6} (\ln T_e)^8]$	1
CI4	$Li + e^- \rightarrow Li^+ + e^- + e^-$	$k_{CI4} = 3.11 \times 10^{-8} T_3^{0.163} \exp\left(-\frac{62700}{T}\right)$	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 ($cm^3\ s^{-1}$)	Notes	Ref.
PR1	$H^+ + e^- \rightarrow H + \gamma$	$k_{PR1} = 2.753 \times 10^{-14} \left(\frac{315614}{T}\right)^{1.500} [1.0 + \left(\frac{115188}{T}\right)^{0.407}]^{-2.242}$		1
PR2	$D^+ + e^- \rightarrow D + \gamma$	$k_{PR2} = k_{PR1}$		1
PR3	$Hep + e^- \rightarrow He + \gamma$	$k_{PR3,rr,A} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T - 0.3162 (\log T)^2 + 0.0493 (\log T)^3]$	Case A	2
		$k_{PR3,rr,B} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T - 0.2852 (\log T)^2 + 0.04433 (\log T)^3]$	Case B	2
		$k_{PR3,di} = T^{-1.5} \left[5.966 \times 10^{-4} \exp\left(\frac{-455600}{T}\right) + 1.613 \times 10^{-4} \exp\left(\frac{-555200}{T}\right) - 2.223 \times 10^{-5} \exp\left(\frac{-898200}{T}\right)\right]$		3
PR4	$Li^+ + e^- \rightarrow Li + \gamma$	$k_{PR4,rr} = 1.036 \times 10^{-11} \left(\frac{T}{107.7}\right)^{-0.5} \left[1.0 + \left(\frac{T}{107.7}\right)^{0.5}\right]^{-0.612} \times \left[1.0 + \left(\frac{T}{1.177 \times 10^7}\right)^{0.5}\right]^{-1.388}$		4
		$k_{PR4,di} = T^{-1.5} \left[2.941 \times 10^{-5} \exp\left(\frac{-634500}{T}\right) + 6.068 \times 10^{-5} \exp\left(\frac{-702400}{T}\right) - 7.753 \times 10^{-7} \exp\left(\frac{-827100}{T}\right)\right]$		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	$Htp + e^- \rightarrow H + H$	$k_{DR1} = 1.0 \times 10^{-8}$	$T \leqslant 617\,K$	1
		$= 1.32 \times 10^{-6} T^{-0.76}$	$T > 617\,K$	
DR2	$HD^+ + e^- \rightarrow H + D$	$k_{DR2} = 7.2 \times 10^{-8} T^{-0.5}$		2
DR3	$D_2^+ + e^- \rightarrow D + D$	$k_{DR3} = 3.4 \times 10^{-9} T_3^{-0.4}$		3
DR4	$H_3^+ + e^- \rightarrow Ht + H$	$k_{DR4} = 2.34 \times 10^{-8} T_3^{-0.52}$		4
DR5	$H_3^+ + e^- \rightarrow H + H + H$	$k_{DR5} = 4.36 \times 10^{-8} T_3^{-0.52}$		4
DR6	$H_2D^+ + e^- \rightarrow H + H + D$	$k_{DR6} = 4.38 \times 10^{-8} T_3^{-0.5}$		5
DR7	$H_2D^+ + e^- \rightarrow Ht + D$	$k_{DR7} = 4.2 \times 10^{-9} T_3^{-0.5}$		5
DR8	$H_2D^+ + e^- \rightarrow H + HD$	$k_{DR8} = 1.2 \times 10^{-8} T_3^{-0.5}$		5
DR9	$HD_2^+ + e^- \rightarrow D + D + H$	$k_{DR9} = 4.38 \times 10^{-8} T_3^{-0.5}$		6
DR10	$HD_2^+ + e^- \rightarrow D_2 + H$	$k_{DR10} = 4.2 \times 10^{-9} T_3^{-0.5}$		6
DR11	$HD_2^+ + e^- \rightarrow HD + D$	$k_{DR11} = 1.2 \times 10^{-8} T_3^{-0.5}$		6
DR12	$D_3^+ + e^- \rightarrow D_2 + D$	$k_{DR12} = 5.4 \times 10^{-9} T_3^{-0.5}$		7
DR13	$D_3^+ + e^- \rightarrow D + D + D$	$k_{DR13} = 2.16 \times 10^{-8} T_3^{-0.5}$		7
DR14	$HeH^+ + e^- \rightarrow He + H$	$k_{DR14} = 3.0 \times 10^{-8} T_3^{-0.47}$		8
DR15	$HeD^+ + e^- \rightarrow He + D$	$k_{DR15} = 3.0 \times 10^{-8} T_3^{-0.47}$		9
DR16	$He_2^+ + e^- \rightarrow He + He$	$k_{DR16} = 6.1 \times 10^{-11} T_3^{-0.9}$		10
DR17	$LiH^+ + e^- \rightarrow Li + H$	$k_{DR17} = 3.8 \times 10^{-7} T_3^{-0.47}$		11
DR18	$LiD^+ + e^- \rightarrow Li + D$	$k_{DR18} = 3.8 \times 10^{-7} T_3^{-0.47}$		12
DR19	$LiH_2^+ + e^- \rightarrow Li + Ht$	$k_{DR19} = 1.6 \times 10^{-7} T_3^{-0.5}$		13
DR20	$LiH_2^+ + e^- \rightarrow LiH + H$	$k_{DR20} = 2.0 \times 10^{-8} T_3^{-0.5}$		13
DR21	$LiH_2^+ + e^- \rightarrow Li + H + H$	$k_{DR21} = 2.0 \times 10^{-8} T_3^{-0.5}$		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	$H + D^+ \rightarrow D + H^+$	$k_{CT1} = 2.06 \times 10^{-10} T^{0.396} \exp\left(-\frac{33}{T}\right)$ $+ 2.03 \times 10^{-9} T^{-0.332}$		1
CT2	$H + D^- \rightarrow D + H^-$	$k_{CT2} = 6.4 \times 10^{-9} T_3^{0.41}$		2
CT3	$H + Htp \rightarrow Ht + H^+$	$k_{CT3} = 6.4 \times 10^{-10}$		3
CT4	$H + HD^+ \rightarrow HD + H^+$	$k_{CT4} = 6.4 \times 10^{-10}$		4
CT5	$H + D_2^+ \rightarrow D_2 + H^+$	$k_{CT5} = 6.4 \times 10^{-10}$		4
CT6	$H + Hep \rightarrow He + H^+ + \gamma$	$k_{CT6} = 1.25 \times 10^{-15} T_3^{0.25}$		5
CT7	$H + He_2^+ \rightarrow He + He + H^+$	$k_{CT7} = 1.0 \times 10^{-9}$		6
CT8	$H + LiH^+ \rightarrow LiH + H^+$	$k_{CT8} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		7
CT9	$H + LiD^+ \rightarrow LiD + H^+$	$k_{CT9} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT10	$D + H^+ \rightarrow H + D^+$	$k_{CT10} = 2.0 \times 10^{-10} T^{0.402} \exp\left(-\frac{37.1}{T}\right)$ $- 3.31 \times 10^{-17} T^{1.48}$		1
CT11	$D + H^- \rightarrow H + D^-$	$k_{CT11} = 6.4 \times 10^{-9} T_3^{0.41}$		2
CT12	$D + Htp \rightarrow Ht + D^+$	$k_{CT12} = 6.4 \times 10^{-10}$		4
CT13	$D + HD^+ \rightarrow HD + D^+$	$k_{CT13} = 6.4 \times 10^{-10}$		4
CT14	$D + D_2^+ \rightarrow D_2 + D^+$	$k_{CT14} = 6.4 \times 10^{-10}$		4
CT15	$D + Hep \rightarrow He + D^+ + \gamma$	$k_{CT15} = 1.1 \times 10^{-15} T_3^{0.25}$		8
CT16	$D + He_2^+ \rightarrow He + He + D^+$	$k_{CT16} = 7.5 \times 10^{-10}$		9
CT17	$D + LiH^+ \rightarrow LiH + D^+$	$k_{CT17} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT18	$D + LiD^+ \rightarrow LiD + D^+$	$k_{CT18} = 1.0 \times 10^{-11} \exp\left(-\frac{67900}{T}\right)$		4
CT19	$Ht + H^+ \rightarrow H + Htp$	$k_{CT19} = [-3.3232183 \times 10^{-7}$ $+ 3.3735382 \times 10^{-7} \ln T$ $- 1.4491368 \times 10^{-7} (\ln T)^2$ $+ 3.4172805 \times 10^{-8} (\ln T)^3$ $- 4.7813720 \times 10^{-9} (\ln T)^4$ $+ 3.9731542 \times 10^{-10} (\ln T)^5$ $- 1.8171411 \times 10^{-11} (\ln T)^6$ $+ 3.5311932 \times 10^{-13} (\ln T)^7]$ $\times \exp\left(\frac{-21237.15}{T}\right)$		10
CT20	$Ht + D^+ \rightarrow D + Htp$	$k_{CT20} = k_{CT19}$		4
CT21	$Ht + Hep \rightarrow He + Htp$	$k_{CT21} = 7.2 \times 10^{-15}$		11
CT22	$Ht + Hep \rightarrow He + H + H^+$	$k_{CT22} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		11
CT23	$Ht + Li^+ \rightarrow Li + Htp$	$k_{CT23} = 3.0 \times 10^{-10} T_3^{-1.5} \exp\left(-\frac{116000}{T}\right)$		12
CT24	$HD + H^+ \rightarrow H + HD^+$	$k_{CT24} = k_{CT19}$		4
CT25	$HD + D^+ \rightarrow D + HD^+$	$k_{CT25} = k_{CT19}$		4
CT26	$HD + Hep \rightarrow He + HD^+$	$k_{CT26} = 7.2 \times 10^{-15}$		4
CT27	$HD + Hep \rightarrow He + H^+ + D$	$k_{CT27} = 1.85 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		13
CT28	$HD + Hep \rightarrow He + H + D^+$	$k_{CT28} = 1.85 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		13
CT29	$HD + Li^+ \rightarrow Li + HD^+$	$k_{CT29} = k_{CT23}$		4
CT30	$D_2 + H^+ \rightarrow H + D_2^+$	$k_{CT30} = k_{CT19}$		4
CT31	$D_2 + D^+ \rightarrow D + D_2^+$	$k_{CT31} = k_{CT19}$		4
CT32	$D_2 + Hep \rightarrow He + D_2^+$	$k_{CT32} = 2.5 \times 10^{-14}$		14
CT33	$D_2 + Hep \rightarrow He + D^+ + D$	$k_{CT33} = 1.1 \times 10^{-13} T_3^{-0.24}$		14
CT34	$D_2 + Li^+ \rightarrow Li + D_2^+$	$k_{CT34} = k_{CT23}$		4
CT35	$He + H^+ \rightarrow H + Hep$	$k_{CT35} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right)$ $= 4.0 \times 10^{-37} T^{4.74}$	$T \leqslant 10000$ K $T > 10000$ K	15
CT36	$He + D^+ \rightarrow D + Hep$	$k_{CT36} = k_{CT35}$		4

Table A4 – *continued*

No.	Reaction	Rate coefficient ($cm^3\ s^{-1}$)	Notes	Ref.
CT37	$Li + H^+ \rightarrow H + Li^+$	$k_{CT37} = 2.5 \times 10^{-40} T^{7.9} \exp\left(-\frac{T}{1210}\right)$		16
CT38	$Li + H^+ \rightarrow H + Li^+ + \gamma$	$k_{CT38} = 1.7 \times 10^{-13} T^{-0.051} \exp\left(-\frac{T}{282000}\right)$		17
CT39	$Li + D^+ \rightarrow D + Li^+$	$k_{CT39} = 8.0 \times 10^{-22} T_3^{6.8} \exp\left(-\frac{T}{1800}\right)$		18
CT40	$Li + D^+ \rightarrow D + Li^+ + \gamma$	$k_{CT40} = 1.1 \times 10^{-13} T_3^{-0.051} \exp\left(-\frac{T}{282000}\right)$		19
CT41	$Li + Htp \rightarrow Ht + Li^+$	$k_{CT41} = 3.0 \times 10^{-10} T_3^{-1.5}$		20
CT42	$Li + HD^+ \rightarrow HD + Li^+$	$k_{CT42} = k_{CT41}$		4
CT43	$Li + D_2^+ \rightarrow D_2 + Li^+$	$k_{CT43} = k_{CT41}$		4
CT44	$LiH + H^+ \rightarrow H + LiH^+$	$k_{CT44} = 2.0 \times 10^{-15}$		21
CT45	$LiH + D^+ \rightarrow D + LiH^+$	$k_{CT45} = 2.0 \times 10^{-15}$		21
CT46	$LiD + H^+ \rightarrow H + LiD^+$	$k_{CT46} = 2.0 \times 10^{-15}$		21
CT47	$LiD + D^+ \rightarrow D + LiD^+$	$k_{CT47} = 2.0 \times 10^{-15}$		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	$H + e^- \rightarrow H^- + \gamma$	$k_{RA1} = \mathrm{dex}[-17.845 + 0.762\log T + 0.1523(\log T)^2 - 0.03274(\log T)^3]$	$T \leqslant 6000$ K	1
		$= \mathrm{dex}[-16.420 + 0.1998(\log T)^2 - 5.447\times10^{-3}(\log T)^4 + 4.0415\times10^{-5}(\log T)^6]$	$T > 6000$ K	
RA2	$D + e^- \rightarrow D^- + \gamma$	$k_{RA2} = k_{RA1}$		1
RA3	$H + H^+ \rightarrow Htp + \gamma$	$k_{RA3} = \mathrm{dex}[-19.38 - 1.523\log T + 1.118(\log T)^2 - 0.1269(\log T)^3]$		2
RA4	$H + D^+ \rightarrow HD^+ + \gamma$	$k_{RA4} = 3.9\times10^{-19} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		3
RA5	$H + D \rightarrow HD + \gamma$	$k_{RA5} = 10^{-25}\,[2.80202 - 6.63697\ln T + 4.75619(\ln T)^2 - 1.39325(\ln T)^3 + 0.178259(\ln T)^4 - 0.00817097(\ln T)^5]$	$10 < T \leqslant 200$ K	4
		$= 10^{-25}\exp[507.207 - 370.889\ln T + 104.854(\ln T)^2 - 14.4192(\ln T)^3 + 0.971469(\ln T)^4 - 0.0258076(\ln T)^5]$	$T > 200$ K	
RA6	$H + Htp \rightarrow H_3^+ + \gamma$	$k_{RA6} = 1.5\times10^{-17} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		5
RA7	$H + HD^+ \rightarrow H_2D^+ + \gamma$	$k_{RA7} = 1.2\times10^{-17} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		6
RA8	$H + D_2^+ \rightarrow HD_2^+ + \gamma$	$k_{RA8} = 1.1\times10^{-17} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		6
RA9	$H + Hep \rightarrow HeH^+ + \gamma$	$k_{RA9} = 4.16\times10^{-16} T_3^{-0.37}\exp\left(-\frac{T}{87600}\right)$		7
RA10	$H + Li^+ \rightarrow LiH^+ + \gamma$	$k_{RA10} = \mathrm{dex}\,[-22.4 + 0.999\log T - 0.351(\log T)^2]$		8
RA11	$D + H^+ \rightarrow HD^+ + \gamma$	$k_{RA11} = 3.9\times10^{-19} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		3
RA12	$D + D^+ \rightarrow D_2^+ + \gamma$	$k_{RA12} = 1.9\times10^{-19} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		3
RA13	$D + Htp \rightarrow H_2D^+ + \gamma$	$k_{RA13} = 7.0\times10^{-18} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		6
RA14	$D + HD^+ \rightarrow HD_2^+ + \gamma$	$k_{RA14} = 5.2\times10^{-18} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		6
RA15	$D + D_2^+ \rightarrow D_3^+ + \gamma$	$k_{RA15} = 4.3\times10^{-18} T_3^{1.8}\exp\left(\frac{20}{T}\right)$		6
RA16	$D + Hep \rightarrow HeD^+ + \gamma$	$k_{RA16} = 5.0\times10^{-16} T_3^{-0.37}\exp\left(-\frac{T}{87600}\right)$		6
RA17	$D + Li^+ \rightarrow LiD^+ + \gamma$	$k_{RA17} = 1.5\times10^{-22} T_3^{-0.9}\exp\left(-\frac{T}{7000}\right)$		9
RA18	$Ht + H^+ \rightarrow H_3^+ + \gamma$	$k_{RA18} = 1.0\times10^{-16}$		10
RA19	$Ht + D^+ \rightarrow H_2D^+ + \gamma$	$k_{RA19} = 1.0\times10^{-16}$		11
RA20	$Li^+ + Ht \rightarrow LiH_2^+ + \gamma$	$k_{RA20} = 1.0\times10^{-22}$		12
RA21	$HD + H^+ \rightarrow H_2D^+ + \gamma$	$k_{RA21} = 1.0\times10^{-16}$		11
RA22	$HD + D^+ \rightarrow HD_2^+ + \gamma$	$k_{RA22} = 1.0\times10^{-16}$		11
RA23	$D_2 + H^+ \rightarrow HD_2^+ + \gamma$	$k_{RA23} = 1.0\times10^{-16}$		11
RA24	$D_2 + D^+ \rightarrow D_3^+ + \gamma$	$k_{RA24} = 1.0\times10^{-16}$		11
RA25	$He + H^+ \rightarrow HeH^+ + \gamma$	$k_{RA25} = 8.0\times10^{-20} T_3^{-0.24}\exp\left(-\frac{T}{4000}\right)$		13
RA26	$He + D^+ \rightarrow HeD^+ + \gamma$	$k_{RA26} = 1.0\times10^{-19} T_3^{-0.24}\exp\left(-\frac{T}{4000}\right)$		6
RA27	$He + Hep \rightarrow He_2^+ + \gamma$	$k_{RA27} = 4.76\times10^{-20} T_3^{1.82}\exp\left(\frac{29}{T}\right)$		14
RA28	$Li + e^- \rightarrow Li^- + \gamma$	$k_{RA28} = 6.1\times10^{-17} T^{0.58}\exp\left(-\frac{T}{17200}\right)$		15
RA29	$Li + H^+ \rightarrow LiH^+ + \gamma$	$k_{RA29} = 4.8\times10^{-14} T^{-0.49}$		16
RA30	$Li + D^+ \rightarrow LiD^+ + \gamma$	$k_{RA30} = 6.4\times10^{-14} T^{-0.49}$		6
RA31	$Li + H \rightarrow LiH + \gamma$	$k_{RA31} = 10^{-20}\left\{3.22 + [0.0657(T/1000)^{-2.45} + 6.3\times10^{-3}(T/1000)^{0.837}]^{-1}\right\}$		17
RA32	$Li + D \rightarrow LiD + \gamma$	$k_{RA32} = 5.5\times10^{-20} T_3^{-0.28}\exp\left(-\frac{T}{3300}\right)$		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 & Ju?rek (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 Juřek, 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	$H + H^- \rightarrow Ht + e^-$	$k_{AD1} = 1.5 \times 10^{-9} T_3^{-0.1}$		1
AD2	$D + H^- \rightarrow HD + e^-$	$k_{AD2} = 1.5 \times 10^{-9} T_3^{-0.1}$		2
AD3	$H + D^- \rightarrow HD + e^-$	$k_{AD3} = 1.5 \times 10^{-9} T_3^{-0.1}$		2
AD4	$D + D^- \rightarrow D_2 + e^-$	$k_{AD4} = 1.6 \times 10^{-9} T_3^{-0.1}$		2
AD5	$Ht + e^- \rightarrow H + H^-$	$k_{AD5} = 2.7 \times 10^{-8} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		3
AD6	$HD + e^- \rightarrow H + D^-$	$k_{AD6} = 1.35 \times 10^{-9} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD7	$HD + e^- \rightarrow D + H^-$	$k_{AD7} = 1.35 \times 10^{-9} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD8	$D_2 + e^- \rightarrow D + D^-$	$k_{AD8} = 6.7 \times 10^{-11} T^{-1.27} \exp\left(-\frac{43000}{T}\right)$		4
AD9	$H^+ + H^- \rightarrow Htp + e^-$	$k_{AD9} = 6.9 \times 10^{-9} T^{-0.35}$	$T \leqslant 8000\,K$	5
		$= 9.6 \times 10^{-7} T^{-0.90}$	$T > 8000\,K$	
AD10	$H^+ + D^- \rightarrow HD^+ + e^-$	$k_{AD10} = 1.1 \times 10^{-9} T_3^{-0.4}$		2
AD11	$D^+ + H^- \rightarrow HD^+ + e^-$	$k_{AD11} = 1.1 \times 10^{-9} T_3^{-0.4}$		2
AD12	$D^+ + D^- \rightarrow D_2^+ + e^-$	$k_{AD12} = 1.3 \times 10^{-9} T_3^{-0.4}$		2
AD13	$Htp + H^- \rightarrow H_3^+ + e^-$	$k_{AD13} = 2.7 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		6
AD14	$Htp + D^- \rightarrow H_2D^+ + e^-$	$k_{AD14} = 2.24 \times 10^{-10} T_3^{-0.49} \exp\left(\frac{T}{43600}\right)$		6
AD15	$HD^+ + H^- \rightarrow H_2D^+ + e^-$	$k_{AD15} = 2.9 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD16	$HD^+ + D^- \rightarrow HD_2^+ + e^-$	$k_{AD16} = 3.7 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD17	$D_2^+ + H^- \rightarrow HD_2^+ + e^-$	$k_{AD17} = 3.0 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD18	$D_2^+ + D^- \rightarrow D_3^+ + e^-$	$k_{AD18} = 3.9 \times 10^{-10} T_3^{-0.485} \exp\left(\frac{T}{31200}\right)$		2
AD19	$Li + H^- \rightarrow LiH + e^-$	$k_{AD19} = 4.0 \times 10^{-10}$		7
AD20	$Li + D^- \rightarrow LiD + e^-$	$k_{AD20} = 4.0 \times 10^{-10}$		2
AD21	$Li^- + H \rightarrow LiH + e^-$	$k_{AD21} = 4.0 \times 10^{-10}$		7
AD22	$Li^- + D \rightarrow LiD + e^-$	$k_{AD22} = 4.0 \times 10^{-10}$		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	$H^- + e^- \rightarrow H + e^- + e^-$	$k_{CD1} = \exp[-1.801849334 \times 10^1$ $+ 2.36085220 \times 10^0 \ln T_e$ $- 2.82744300 \times 10^{-1} (\ln T_e)^2$ $+ 1.62331664 \times 10^{-2} (\ln T_e)^3$ $- 3.36501203 \times 10^{-2} (\ln T_e)^4$ $+ 1.17832978 \times 10^{-2} (\ln T_e)^5$ $- 1.65619470 \times 10^{-3} (\ln T_e)^6$ $+ 1.06827520 \times 10^{-4} (\ln T_e)^7$ $- 2.63128581 \times 10^{-6} (\ln T_e)^8]$		1
CD2	$H^- + H \rightarrow H + H + e^-$	$k_{CD2} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leqslant 0.1$ eV	1
		$= \exp[-2.0372609 \times 10^1$ $+ 1.13944933 \times 10^0 \ln T_e$ $- 1.4210135 \times 10^{-1} (\ln T_e)^2$ $+ 8.4644554 \times 10^{-3} (\ln T_e)^3$ $- 1.4327641 \times 10^{-3} (\ln T_e)^4$ $+ 2.0122503 \times 10^{-4} (\ln T_e)^5$ $+ 8.6639632 \times 10^{-5} (\ln T_e)^6$ $- 2.5850097 \times 10^{-5} (\ln T_e)^7$ $+ 2.4555012 \times 10^{-6} (\ln T_e)^8$ $- 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e > 0.1$ eV	
CD3	$H^- + D \rightarrow H + D + e^-$	$k_{CD3} = k_{CD2}$		2
CD4	$H^- + He \rightarrow H + He + e^-$	$k_{CD4} = 4.1 \times 10^{-17} T^2 \exp\left(-\frac{19870}{T}\right)$		3
CD5	$D^- + e^- \rightarrow D + e^- + e^-$	$k_{CD5} = k_{CD1}$		2
CD6	$D^- + H \rightarrow D + H + e^-$	$k_{CD6} = k_{CD2}$		2
CD7	$D^- + D \rightarrow D + D + e^-$	$k_{CD7} = k_{CD2}$		2
CD8	$D^- + He \rightarrow D + He + e^-$	$k_{CD8} = 1.5 \times 10^{-17} T^2 \exp\left(-\frac{19870}{T}\right)$		4
CD9	$Ht + H \rightarrow H + H + H$	$k_{CD9} = 6.67 \times 10^{-12} T^{0.5} \exp\left[-(1 + \frac{63593}{T})\right]$	v=0	5
		$= k_{TB1}/K$	LTE	6
CD10	$Ht + Ht \rightarrow H + H + Ht$	$k_{CD10} = \frac{5.996\times10^{-30} T^{4.1881}}{(1.0+6.761\times10^{-6} T)^{5.6881}} \exp\left(-\frac{54657.4}{T}\right)$	$v = 0$	7
		$= k_{TB2}/K$	LTE	6
CD11	$Ht + He \rightarrow H + H + He$	$k_{CD11} = \mathrm{dex}\left[-27.029 + 3.801 \log T - \frac{29487}{T}\right]$	$v = 0$	8
		$= 6.6 \times 10^{-10} T^{0.115} \exp\left(-\frac{52000}{T}\right)$	LTE	9
CD12	$Ht + e^- \rightarrow H + H + e^-$	$k_{CD12} = 4.49 \times 10^{-9} T^{0.11} \exp\left(-\frac{101858}{T}\right)$	$v = 0$	10
		$= 1.91 \times 10^{-9} T^{0.136} \exp\left(-\frac{53407.1}{T}\right)$	LTE	10
CD13	$HD + H \rightarrow H + D + H$	$k_{CD13} = k_{CD9}$	See §??	2
CD14	$HD + Ht \rightarrow H + D + Ht$	$k_{CD14} = k_{CD10}$	See §??	2
CD15	$HD + He \rightarrow H + D + He$	$k_{CD15} = k_{CD11}$	See §??	2
CD16	$HD + e^- \rightarrow H + D + e^-$	$k_{CD16} = 5.09 \times 10^{-9} T^{0.128} \exp\left(-\frac{103258}{T}\right)$	$v = 0$	11
		$= 1.04 \times 10^{-9} T^{0.218} \exp\left(-\frac{53070.7}{T}\right)$	LTE	11
CD17	$D_2 + H \rightarrow D + D + H$	$k_{CD17} = k_{CD9}$		2
CD18	$D_2 + Ht \rightarrow D + D + Ht$	$k_{CD18} = k_{CD10}$		2
CD19	$D_2 + He \rightarrow D + D + He$	$k_{CD19} = k_{CD11}$		2
CD20	$D_2 + e^- \rightarrow D + D + e^-$	$k_{CD20} = 8.24 \times 10^{-9} T^{0.126} \exp\left(-\frac{105388}{T}\right)$	$v = 0$	10
		$= 2.75 \times 10^{-9} T^{0.163} \exp\left(-\frac{53339.7}{T}\right)$	LTE	10
CD21	$LiH^+ + D \rightarrow Li^+ + H + D$	$k_{CD21} = 1.0 \times 10^{-9} \exp\left(-\frac{1400}{T}\right)$		12
CD22	$LiH^+ + D \rightarrow Li + H^+ + D$	$k_{CD22} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD23	$LiH^+ + D \rightarrow Li + H + D^+$	$k_{CD23} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD24	$LiD^+ + D \rightarrow Li^+ + D + D$	$k_{CD24} = 1.0 \times 10^{-9} \exp\left(-\frac{1400}{T}\right)$		12
CD25	$LiD^+ + D \rightarrow Li + D^+ + D$	$k_{CD25} = 1.0 \times 10^{-9} \exp\left(-\frac{97500}{T}\right)$		12
CD26	$LiH_2^+ + Ht \rightarrow Li^+ + Ht + Ht$	$k_{CD26} = 1.0 \times 10^{-9} \exp\left(-\frac{3000}{T}\right)$		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	$H^+ + H^- \rightarrow H + H$	$k_{MN1} = 2.4 \times 10^{-6} T^{-1/2} \left(1.0 + 5.0 \times 10^{-5} T\right)$	1
MN2	$D^+ + H^- \rightarrow D + H$	$k_{MN2} = 1.1 \times k_{MN1}$	2
MN3	$H^+ + D^- \rightarrow D + H$	$k_{MN3} = 1.1 \times k_{MN1}$	2
MN4	$D^+ + D^- \rightarrow D + D$	$k_{MN4} = 1.3 \times k_{MN1}$	2
MN5	$Htp + H^- \rightarrow Ht + H$	$k_{MN5} = 1.4 \times 10^{-7} T_3^{-0.5}$	3
MN6	$Htp + H^- \rightarrow H + H + H$	$k_{MN6} = 1.4 \times 10^{-7} T_3^{-0.5}$	3
MN7	$Htp + D^- \rightarrow Ht + D$	$k_{MN7} = 1.7 \times 10^{-7} T_3^{-0.5}$	2
MN8	$Htp + D^- \rightarrow H + H + D$	$k_{MN8} = 1.7 \times 10^{-7} T_3^{-0.5}$	2
MN9	$HD^+ + H^- \rightarrow HD + H$	$k_{MN9} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN10	$HD^+ + H^- \rightarrow D + H + H$	$k_{MN10} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN11	$HD^+ + D^- \rightarrow HD + D$	$k_{MN11} = 1.9 \times 10^{-7} T_3^{-0.5}$	2
MN12	$HD^+ + D^- \rightarrow D + H + D$	$k_{MN12} = 1.9 \times 10^{-7} T_3^{-0.5}$	2
MN13	$D_2^+ + H^- \rightarrow D_2 + H$	$k_{MN13} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN14	$D_2^+ + H^- \rightarrow D + D + H$	$k_{MN14} = 1.5 \times 10^{-7} T_3^{-0.5}$	2
MN15	$D_2^+ + D^- \rightarrow D_2 + D$	$k_{MN15} = 2.0 \times 10^{-7} T_3^{-0.5}$	2
MN16	$D_2^+ + D^- \rightarrow D + D + D$	$k_{MN16} = 2.0 \times 10^{-7} T_3^{-0.5}$	2
MN17	$H_3^+ + H^- \rightarrow Ht + H + H$	$k_{MN17} = 2.3 \times 10^{-7} T_3^{-0.5}$	4
MN18	$H_3^+ + H^- \rightarrow Ht + Ht$	$k_{MN18} = 2.3 \times 10^{-7} T_3^{-0.5}$	5
MN19	$H_3^+ + D^- \rightarrow Ht + H + D$	$k_{MN19} = 2.9 \times 10^{-7} T_3^{-0.5}$	6
MN20	$H_3^+ + D^- \rightarrow Ht + HD$	$k_{MN20} = 2.9 \times 10^{-7} T_3^{-0.5}$	6
MN21	$H_2D^+ + H^- \rightarrow Ht + H + D$	$k_{MN21} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN22	$H_2D^+ + H^- \rightarrow Ht + HD$	$k_{MN22} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN23	$H_2D^+ + H^- \rightarrow HD + H + H$	$k_{MN23} = 1.6 \times 10^{-7} T_3^{-0.5}$	6
MN24	$H_2D^+ + D^- \rightarrow Ht + D + D$	$k_{MN24} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN25	$H_2D^+ + D^- \rightarrow Ht + D_2$	$k_{MN25} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN26	$H_2D^+ + D^- \rightarrow HD + H + D$	$k_{MN26} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN27	$H_2D^+ + D^- \rightarrow HD + HD$	$k_{MN27} = 1.5 \times 10^{-7} T_3^{-0.5}$	6
MN28	$HD_2^+ + H^- \rightarrow Ht + D_2$	$k_{MN28} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN29	$HD_2^+ + H^- \rightarrow HD + H + D$	$k_{MN29} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN30	$HD_2^+ + H^- \rightarrow HD + HD$	$k_{MN30} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN31	$HD_2^+ + H^- \rightarrow D_2 + H + H$	$k_{MN31} = 1.2 \times 10^{-7} T_3^{-0.5}$	6
MN32	$HD_2^+ + D^- \rightarrow HD + D + D$	$k_{MN32} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN33	$HD_2^+ + D^- \rightarrow HD + D_2$	$k_{MN33} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN34	$HD_2^+ + D^- \rightarrow D_2 + H + D$	$k_{MN34} = 2.1 \times 10^{-7} T_3^{-0.5}$	6
MN35	$D_3^+ + H^- \rightarrow HD + D_2$	$k_{MN35} = 2.4 \times 10^{-7} T_3^{-0.5}$	6
MN36	$D_3^+ + H^- \rightarrow D_2 + H + D$	$k_{MN36} = 2.4 \times 10^{-7} T_3^{-0.5}$	6
MN37	$D_3^+ + D^- \rightarrow D_2 + D + D$	$k_{MN37} = 3.3 \times 10^{-7} T_3^{-0.5}$	2
MN38	$D_3^+ + D^- \rightarrow D_2 + D_2$	$k_{MN38} = 3.3 \times 10^{-7} T_3^{-0.5}$	2
MN39	$Hep + H^- \rightarrow He + H$	$k_{MN39} = 2.32 \times 10^{-7} T_3^{-0.52} \exp\left(\frac{T}{22400}\right)$	7
MN40	$Hep + D^- \rightarrow He + D$	$k_{MN40} = 3.03 \times 10^{-7} T_3^{-0.52} \exp\left(\frac{T}{22400}\right)$	2
MN41	$Li^+ + H^- \rightarrow Li + H$	$k_{MN41} = 2.93 \times 10^{-7} T_3^{-0.477} \exp\left(\frac{T}{23200}\right)$	1
MN42	$Li^+ + D^- \rightarrow Li + D$	$k_{MN42} = 2.06 \times 10^{-7} T_3^{-0.5} \exp\left(\frac{T}{18300}\right)$	7
MN43	$Li^- + H^+ \rightarrow Li + H$	$k_{MN43} = 1.8 \times 10^{-7} T_3^{-0.477} \exp\left(\frac{T}{23200}\right)$	1
MN44	$Li^- + D^+ \rightarrow Li + D$	$k_{MN44} = 2.06 \times 10^{-7} T_3^{-0.5} \exp\left(\frac{T}{18300}\right)$	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 ($cm^6\ s^{-1}$)	Ref.
TB1	$H + H + H \rightarrow Ht + H$	See §??	—
TB2	$H + H + Ht \rightarrow Ht + Ht$	See §??	—
TB3	$H + H + He \rightarrow Ht + He$	$k_{TB3} = 6.9 \times 10^{-32} T^{-0.4}$	1
TB4	$H + D + H \rightarrow HD + H$	See §??	—
TB5	$H + D + Ht \rightarrow HD + Ht$	See §??	—
TB6	$H + D + He \rightarrow HD + He$	$k_{TB6} = 6.9 \times 10^{-32} T^{-0.4}$	2
TB7	$D + D + H \rightarrow D_2 + H$	See §??	—
TB8	$D + D + Ht \rightarrow D_2 + Ht$	See §??	—
TB9	$D + D + He \rightarrow D_2 + He$	$k_{TB9} = 6.9 \times 10^{-32} T^{-0.4}$	2
TB10	$H^+ + H + H \rightarrow Htp + H$	$k_{TB10} = 1.203 \times 10^{-29} T^{-1.041}$	3
TB11	$D^+ + H + H \rightarrow HD^+ + H$	$k_{TB11} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB12	$H^+ + D + H \rightarrow HD^+ + H$	$k_{TB12} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB13	$D^+ + D + H \rightarrow D_2^+ + H$	$k_{TB13} = 1.203 \times 10^{-29} T^{-1.041}$	2
TB14	$H^+ + Ht + H \rightarrow H_3^+ + H$	$k_{TB14} = 1.0 \times 10^{-28}$	4
TB15	$H^+ + Ht + Ht \rightarrow H_3^+ + Ht$	$k_{TB15} = 5.4 \times 10^{-29}$	5
TB16	$H^+ + Ht + He \rightarrow H_3^+ + He$	$k_{TB16} = 1.07 \times 10^{-28}$	5
TB17	$D^+ + Ht + H \rightarrow H_2D^+ + H$	$k_{TB17} = 1.0 \times 10^{-28}$	4
TB18	$D^+ + Ht + Ht \rightarrow H_2D^+ + Ht$	$k_{TB18} = 5.4 \times 10^{-29}$	2
TB19	$D^+ + Ht + He \rightarrow H_2D^+ + He$	$k_{TB19} = 1.07 \times 10^{-28}$	2
TB20	$H^+ + HD + H \rightarrow H_2D^+ + H$	$k_{TB20} = 1.0 \times 10^{-28}$	4
TB21	$H^+ + HD + Ht \rightarrow H_2D^+ + Ht$	$k_{TB21} = 5.4 \times 10^{-29}$	2
TB22	$H^+ + HD + He \rightarrow H_2D^+ + He$	$k_{TB22} = 1.07 \times 10^{-28}$	2
TB23	$D^+ + HD + H \rightarrow HD_2^+ + H$	$k_{TB23} = 1.0 \times 10^{-28}$	4
TB24	$D^+ + HD + Ht \rightarrow HD_2^+ + Ht$	$k_{TB24} = 5.4 \times 10^{-29}$	2
TB25	$D^+ + HD + He \rightarrow HD_2^+ + He$	$k_{TB25} = 1.07 \times 10^{-28}$	2
TB26	$H^+ + D_2 + H \rightarrow HD_2^+ + H$	$k_{TB26} = 1.0 \times 10^{-28}$	4
TB27	$H^+ + D_2 + Ht \rightarrow HD_2^+ + Ht$	$k_{TB27} = 5.4 \times 10^{-29}$	2
TB28	$H^+ + D_2 + He \rightarrow HD_2^+ + He$	$k_{TB28} = 1.07 \times 10^{-28}$	2
TB29	$D^+ + D_2 + H \rightarrow D_3^+ + H$	$k_{TB29} = 1.0 \times 10^{-28}$	4
TB30	$D^+ + D_2 + Ht \rightarrow D_3^+ + Ht$	$k_{TB30} = 5.4 \times 10^{-29}$	2
TB31	$D^+ + D_2 + He \rightarrow D_3^+ + He$	$k_{TB31} = 1.07 \times 10^{-28}$	2
TB32	$Li + H + H \rightarrow LiH + H$	$k_{TB32} = 2.5 \times 10^{-29} T^{-1}$	6
TB33	$Li + H + Ht \rightarrow LiH + Ht$	$k_{TB33} = 4.1 \times 10^{-30} T^{-1}$	6
TB34	$Li + D + H \rightarrow LiD + H$	$k_{TB34} = 2.5 \times 10^{-29} T^{-1}$	2
TB35	$Li + D + Ht \rightarrow LiD + Ht$	$k_{TB35} = 4.1 \times 10^{-30} T^{-1}$	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	$Htp + D \rightarrow HD^+ + H$	$k_{IX1} = 1.07\times10^{-9}T_3^{0.062}\exp\left(-\frac{T}{41400}\right)$		1
IX2	$Htp + D \rightarrow HD + H^+$	$k_{IX2} = 1.0\times10^{-9}$		2
IX3	$HD^+ + H \rightarrow Htp + D$	$k_{IX3} = 1.0\times10^{-9}\exp\left(-\frac{154}{T}\right)$		3
IX4	$HD^+ + H \rightarrow Ht + D^+$	$k_{IX4} = 1.0\times10^{-9}$		2
IX5	$HD^+ + D \rightarrow D_2^+ + H$	$k_{IX5} = 1.0\times10^{-9}$		4
IX6	$HD^+ + D \rightarrow D_2 + H^+$	$k_{IX6} = 1.0\times10^{-9}$		2
IX7	$D_2^+ + H \rightarrow HD^+ + D$	$k_{IX7} = 1.0\times10^{-9}\exp\left(-\frac{472}{T}\right)$		4
IX8	$D_2^+ + H \rightarrow HD + D^+$	$k_{IX8} = 1.0\times10^{-9}$		2
IX9	$Ht + D^+ \rightarrow HD + H^+$	$k_{IX9} = 4.17\times10^{-10} + 8.46\times10^{-10}\log T - 1.37\times10^{-10}(\log T)^2$		5
IX10	$Ht + D^+ \rightarrow HD^+ + H$	$k_{IX10} = \left[1.04\times10^{-9} + 9.52\times10^{-9}\left(\frac{T}{10000}\right) - 1.81\times10^{-9}\left(\frac{T}{10000}\right)^2\right]\exp\left(-\frac{21000}{T}\right)$		6
IX11	$HD + H^+ \rightarrow Ht + D^+$	$k_{IX11} = 1.1\times10^{-9}\exp\left(-\frac{488}{T}\right)$		5
IX12	$HD + H^+ \rightarrow Htp + D$	$k_{IX12} = 1.0\times10^{-9}\exp\left(-\frac{21600}{T}\right)$		2
IX13	$HD + D^+ \rightarrow D_2 + H^+$	$k_{IX13} = 1.0\times10^{-9}$		4
IX14	$HD + D^+ \rightarrow D_2^+ + H$	$k_{IX14} = \left[3.54\times10^{-9} + 7.50\times10^{-10}\left(\frac{T}{10000}\right) - 2.92\times10^{-10}\left(\frac{T}{10000}\right)^2\right]\exp\left(-\frac{21100}{T}\right)$		6
IX15	$D_2 + H^+ \rightarrow HD + D^+$	$k_{IX15} = 2.1\times10^{-9}\exp\left(-\frac{491}{T}\right)$		4
IX16	$D_2 + H^+ \rightarrow HD^+ + D$	$k_{IX16} = \left[5.18\times10^{-11} + 3.05\times10^{-9}\left(\frac{T}{10000}\right) - 5.42\times10^{-10}\left(\frac{T}{10000}\right)^2\right]\exp\left(-\frac{20100}{T}\right)$		6
IX17	$Ht + D \rightarrow HD + H$	$k_{IX17} = \mathrm{dex}\left[-56.4737 + 5.88886\log T + 7.19692(\log T)^2 + 2.25069(\log T)^3 - 2.16903(\log T)^4 + 0.317887(\log T)^5\right]$	$T \leqslant 2000$ K	7
		$= 3.17\times10^{-10}\exp\left(-\frac{5207}{T}\right)$	$T > 2000$ K	
IX18	$HD + H \rightarrow Ht + D$	$k_{IX18} = 5.25\times10^{-11}\exp\left(-\frac{4430}{T}\right)$	$T \leqslant 200$ K	8
		$= 5.25\times10^{-11}\exp\left(-\frac{4430}{T} + \frac{173900}{T^2}\right)$	$T > 200$ K	
IX19	$HD + D \rightarrow D_2 + H$	$k_{IX19} = 1.15\times10^{-11}\exp\left(-\frac{3220}{T}\right)$		8
IX20	$D_2 + H \rightarrow HD + D$	$k_{IX20} = \mathrm{dex}\left[-86.1558 + 4.53978\log T + 33.5707(\log T)^2 - 13.0449(\log T)^3 + 1.22017(\log T)^4 + 0.0482453(\log T)^5\right]$	$T \leqslant 2200$ K	7
		$= 2.67\times10^{-10}\exp\left(-\frac{5945}{T}\right)$	$T > 2200$ K	
IX21	$H_3^+ + D \rightarrow H_2D^+ + H$	$k_{IX21} = 1.0\times10^{-9}$		9
IX22	$H_2D^+ + H \rightarrow H_3^+ + D$	$k_{IX22} = 1.0\times10^{-9}\exp\left(-\frac{632}{T}\right)$		10
IX23	$H_2D^+ + D \rightarrow HD_2^+ + H$	$k_{IX23} = 1.0\times10^{-9}$		4
IX24	$HD_2^+ + H \rightarrow H_2D^+ + D$	$k_{IX24} = 1.0\times10^{-9}\exp\left(-\frac{600}{T}\right)$		4
IX25	$HD_2^+ + D \rightarrow D_3^+ + H$	$k_{IX25} = 1.0\times10^{-9}$		4
IX26	$D_3^+ + H \rightarrow HD_2^+ + D$	$k_{IX26} = 1.0\times10^{-9}\exp\left(-\frac{655}{T}\right)$		4
IX27	$H_3^+ + HD \rightarrow H_2D^+ + Ht$	$k_{IX27} = 3.5\times10^{-10}$		4
IX28	$H_3^+ + D_2 \rightarrow H_2D^+ + HD$	$k_{IX28} = 3.5\times10^{-11}T_3^{-0.19}$		11
IX29	$H_3^+ + D_2 \rightarrow HD_2^+ + Ht$	$k_{IX29} = 9.64\times10^{-10}T_3^{-0.024}$		11
IX30	$H_2D^+ + Ht \rightarrow H_3^+ + HD$	$k_{IX30} = 1.4\times10^{-10}\exp\left(-\frac{232}{T}\right)$		4
IX31	$H_2D^+ + HD \rightarrow H_3^+ + D_2$	$k_{IX31} = 1.75\times10^{-11}T_3^{-0.19}\exp\left(-\frac{153}{T}\right)$		12
IX32	$H_2D^+ + HD \rightarrow HD_2^+ + Ht$	$k_{IX32} = 2.6\times10^{-10}$		4
IX33	$H_2D^+ + D_2 \rightarrow HD_2^+ + HD$	$k_{IX33} = 8.5\times10^{-10}$		4
IX34	$H_2D^+ + D_2 \rightarrow D_3^+ + Ht$	$k_{IX34} = 8.5\times10^{-10}$		4
IX35	$HD_2^+ + Ht \rightarrow H_3^+ + D_2$	$k_{IX35} = 2.0\times10^{-10}\exp\left(-\frac{340.2}{T}\right)$		13

Table A10 – *continued*

No.	Reaction	Rate coefficient ($cm^3\,s^{-1}$)	Notes	Ref.
IX36	$HD_2^+ + Ht \rightarrow H_2D^+ + HD$	$k_{IX36} = 1.0 \times 10^{-10} \exp\left(-\frac{187.2}{T}\right) \times \left[1.0 + \exp\left(-\frac{87}{T}\right)\right]$		13
IX37	$HD_2^+ + HD \rightarrow H_2D^+ + D_2$	$k_{IX37} = 1.0 \times 10^{-10} \exp\left(-\frac{108.4}{T}\right) \times \left[1.0 + \exp\left(-\frac{86.5}{T}\right)\right]$		13
IX38	$HD_2^+ + HD \rightarrow D_3^+ + Ht$	$k_{IX38} = 2.0 \times 10^{-10}$		4
IX39	$HD_2^+ + D_2 \rightarrow D_3^+ + HD$	$k_{IX39} = 8.7 \times 10^{-10}$		14
IX40	$D_3^+ + Ht \rightarrow H_2D^+ + D_2$	$k_{IX40} = 1.5 \times 10^{-9} \exp\left(-\frac{342.2}{T}\right)$		13
IX41	$D_3^+ + Ht \rightarrow HD_2^+ + HD$	$k_{IX41} = 1.5 \times 10^{-9} \exp\left(-\frac{233.8}{T}\right)$		13
IX42	$D_3^+ + HD \rightarrow HD_2^+ + D_2$	$k_{IX42} = 3.75 \times 10^{-10} \exp\left(-\frac{155}{T}\right) \times \left[1.0 + 2.0 \exp\left(-\frac{50.4}{T}\right) + \exp\left(-\frac{86}{T}\right)\right]$		13
IX43	$HeH^+ + D \rightarrow HeD^+ + H$	$k_{IX43} = 1.0 \times 10^{-9}$		3
IX44	$HeD^+ + H \rightarrow HeH^+ + D$	$k_{IX44} = 8.0 \times 10^{-10} \exp\left(-\frac{468}{T}\right)$		3
IX45	$LiH^+ + D \rightarrow LiD^+ + H$	$k_{IX45} = 1.0 \times 10^{-9}$		2
IX46	$LiD^+ + H \rightarrow LiH^+ + D$	$k_{IX46} = 1.0 \times 10^{-9} \exp\left(-\frac{64}{T}\right)$		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	$Htp + Ht \rightarrow H_3^+ + H$	$k_{TR1} = 2.24 \times 10^{-9} T_3^{0.042} \exp\left(-\frac{T}{46600}\right)$	1
TR2	$Htp + HD \rightarrow H_3^+ + D$	$k_{TR2} = 1.05 \times 10^{-9}$	2
TR3	$Htp + HD \rightarrow H_2D^+ + H$	$k_{TR3} = 1.05 \times 10^{-9}$	2
TR4	$Htp + D_2 \rightarrow H_2D^+ + D$	$k_{TR4} = 1.05 \times 10^{-9}$	3
TR5	$Htp + D_2 \rightarrow HD_2^+ + H$	$k_{TR5} = 1.05 \times 10^{-9}$	3
TR6	$HD^+ + Ht \rightarrow H_3^+ + D$	$k_{TR6} = 0.5 \times k_{TR1}$	1
TR7	$HD^+ + Ht \rightarrow H_2D^+ + H$	$k_{TR7} = 0.5 \times k_{TR1}$	1
TR8	$HD^+ + HD \rightarrow H_2D^+ + D$	$k_{TR8} = 1.05 \times 10^{-9}$	3
TR9	$HD^+ + HD \rightarrow HD_2^+ + H$	$k_{TR9} = 1.05 \times 10^{-9}$	3
TR10	$HD^+ + D_2 \rightarrow HD_2^+ + D$	$k_{TR10} = 1.05 \times 10^{-9}$	3
TR11	$HD^+ + D_2 \rightarrow D_3^+ + H$	$k_{TR11} = 1.05 \times 10^{-9}$	3
TR12	$D_2^+ + Ht \rightarrow H_2D^+ + D$	$k_{TR12} = 1.05 \times 10^{-9}$	3
TR13	$D_2^+ + Ht \rightarrow HD_2^+ + H$	$k_{TR13} = 1.05 \times 10^{-9}$	3
TR14	$D_2^+ + HD \rightarrow HD_2^+ + D$	$k_{TR14} = 1.05 \times 10^{-9}$	3
TR15	$D_2^+ + HD \rightarrow D_3^+ + H$	$k_{TR15} = 1.05 \times 10^{-9}$	3
TR16	$D_2^+ + D_2 \rightarrow D_3^+ + D$	$k_{TR16} = 2.1 \times 10^{-9}$	3
TR17	$H_3^+ + H \rightarrow Htp + Ht$	$k_{TR17} = 7.7 \times 10^{-9} \exp\left(-\frac{17560}{T}\right)$	4
TR18	$H_3^+ + D \rightarrow Htp + HD$	$k_{TR18} = 0.5 \times k_{TR17}$	5
TR19	$H_3^+ + D \rightarrow HD^+ + Ht$	$k_{TR19} = 0.5 \times k_{TR17}$	5
TR20	$H_2D^+ + H \rightarrow Htp + HD$	$k_{TR20} = 0.5 \times k_{TR17}$	5
TR21	$H_2D^+ + H \rightarrow HD^+ + Ht$	$k_{TR21} = 0.5 \times k_{TR17}$	5
TR22	$H_2D^+ + D \rightarrow Htp + D_2$	$k_{TR22} = 0.333 \times k_{TR17}$	5
TR23	$H_2D^+ + D \rightarrow HD^+ + HD$	$k_{TR23} = 0.333 \times k_{TR17}$	5
TR24	$H_2D^+ + D \rightarrow D_2^+ + Ht$	$k_{TR24} = 0.333 \times k_{TR17}$	5
TR25	$HD_2^+ + H \rightarrow Htp + D_2$	$k_{TR25} = 0.333 \times k_{TR17}$	5
TR26	$HD_2^+ + H \rightarrow HD^+ + HD$	$k_{TR26} = 0.333 \times k_{TR17}$	5
TR27	$HD_2^+ + H \rightarrow D_2^+ + Ht$	$k_{TR27} = 0.333 \times k_{TR17}$	5
TR28	$HD_2^+ + D \rightarrow HD^+ + D_2$	$k_{TR28} = 0.5 \times k_{TR17}$	5
TR29	$HD_2^+ + D \rightarrow D_2^+ + HD$	$k_{TR29} = 0.5 \times k_{TR17}$	5
TR30	$D_3^+ + H \rightarrow HD^+ + D_2$	$k_{TR30} = 0.5 \times k_{TR17}$	5
TR31	$D_3^+ + H \rightarrow D_2^+ + HD$	$k_{TR31} = 0.5 \times k_{TR17}$	5
TR32	$D_3^+ + D \rightarrow D_2^+ + D_2$	$k_{TR32} = k_{TR17}$	5
TR33	$He + Htp \rightarrow HeH^+ + H$	$k_{TR33} = 3.0 \times 10^{-10} \exp\left(-\frac{6717}{T}\right)$	6
TR34	$He + HD^+ \rightarrow HeH^+ + D$	$k_{TR34} = k_{TR33}$	7
TR35	$He + HD^+ \rightarrow HeD^+ + H$	$k_{TR35} = k_{TR33}$	7
TR36	$He + D_2^+ \rightarrow HeD^+ + D$	$k_{TR36} = k_{TR33}$	8
TR37	$HeH^+ + H \rightarrow Htp + He$	$k_{TR37} = 1.04 \times 10^{-9} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	1
TR38	$HeH^+ + D \rightarrow HD^+ + He$	$k_{TR38} = 8.5 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	9
TR39	$HeH^+ + Ht \rightarrow H_3^+ + He$	$k_{TR39} = 1.53 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	1
TR40	$HeH^+ + HD \rightarrow H_2D^+ + He$	$k_{TR40} = 1.20 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	2
TR41	$HeH^+ + D_2 \rightarrow HD_2^+ + He$	$k_{TR41} = 1.1 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR42	$HeD^+ + H \rightarrow HD^+ + He$	$k_{TR42} = 9.1 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	9
TR43	$HeD^+ + D \rightarrow D_2^+ + He$	$k_{TR43} = 8.5 \times 10^{-10} T_3^{0.13} \exp\left(-\frac{T}{33100}\right)$	11
TR44	$HeD^+ + Ht \rightarrow H_2D^+ + He$	$k_{TR44} = 1.24 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	2
TR45	$HeD^+ + HD \rightarrow HD_2^+ + He$	$k_{TR45} = 1.2 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR46	$HeD^+ + D_2 \rightarrow D_3^+ + He$	$k_{TR46} = 1.1 \times 10^{-9} T_3^{0.24} \exp\left(-\frac{T}{14800}\right)$	10
TR47	$LiH^+ + H \rightarrow Li^+ + Ht$	$k_{TR47} = 3.0 \times 10^{-10}$	12
TR48	$LiH^+ + D \rightarrow Li^+ + HD$	$k_{TR48} = 3.0 \times 10^{-10}$	13
TR49	$LiD^+ + H \rightarrow Li^+ + HD$	$k_{TR49} = 3.0 \times 10^{-10}$	14
TR50	$LiD^+ + D \rightarrow Li^+ + D_2$	$k_{TR50} = 3.0 \times 10^{-10}$	14
TR51	$LiH^+ + H \rightarrow Li + Htp$	$k_{TR51} = 9.0 \times 10^{-10} \exp\left(-\frac{66400}{T}\right)$	12
TR52	$LiH^+ + D \rightarrow Li + HD^+$	$k_{TR52} = k_{TR51}$	13
TR53	$LiD^+ + H \rightarrow Li + HD^+$	$k_{TR53} = k_{TR51}$	14
TR54	$LiD^+ + D \rightarrow Li + D_2^+$	$k_{TR54} = k_{TR51}$	14

Table A11 – *continued*

No.	Reaction	Rate coefficient ($cm^3\ s^{-1}$)	Ref.
TR55	$LiH + H^+ \rightarrow Li^+ + Ht$	$k_{TR55} = 2.0 \times 10^{-15}$	15
TR56	$LiH + D^+ \rightarrow Li^+ + HD$	$k_{TR56} = 2.0 \times 10^{-15}$	16
TR57	$LiD + H^+ \rightarrow Li^+ + HD$	$k_{TR57} = 2.0 \times 10^{-15}$	16
TR58	$LiD + D^+ \rightarrow Li^+ + D_2$	$k_{TR58} = 2.0 \times 10^{-15}$	16
TR59	$LiH + H^+ \rightarrow Li + Htp$	$k_{TR59} = 1.0 \times 10^{-9}$	12
TR60	$LiH + D^+ \rightarrow Li + HD^+$	$k_{TR60} = 1.0 \times 10^{-9}$	16
TR61	$LiD + H^+ \rightarrow Li + HD^+$	$k_{TR61} = 1.0 \times 10^{-9}$	16
TR62	$LiD + D^+ \rightarrow Li + D_2^+$	$k_{TR62} = 1.0 \times 10^{-9}$	16
TR63	$LiH + H \rightarrow Li + Ht$	$k_{TR63} = 1.55 \times 10^{-11} T^{0.4247}$	17
TR64	$LiH + D \rightarrow Li + HD$	$k_{TR64} = 1.2 \times 10^{-11} T^{0.4247}$	11
TR65	$LiD + H \rightarrow Li + HD$	$k_{TR65} = 1.54 \times 10^{-11} T^{0.4247}$	11
TR66	$LiD + D \rightarrow Li + D_2$	$k_{TR66} = 1.2 \times 10^{-11} T^{0.4247}$	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} s^{-1})	Ref.
BP1	$H^- + \gamma \rightarrow H + e^-$	$R_{BP1} = 1.36 \times 10^{-11}$	1
BP2	$D^- + \gamma \rightarrow D + e^-$	$R_{BP2} = 1.36 \times 10^{-11}$	2
BP3	$Htp + \gamma \rightarrow H + H^+$	$R_{BP3} = 4.11 \times 10^{-12}$	3
BP4	$HD^+ + \gamma \rightarrow H + D^+$	$R_{BP4} = 2.05 \times 10^{-12}$	2
BP5	$HD^+ + \gamma \rightarrow D + H^+$	$R_{BP5} = 2.05 \times 10^{-12}$	2
BP6	$D_2^+ + \gamma \rightarrow D + D^+$	$R_{BP6} = 4.11 \times 10^{-12}$	2
BP7	$Ht + \gamma \rightarrow H + H$	$R_{BP7} = 1.3 \times 10^{-12} f_{sh,Ht}$	5
BP8	$HD + \gamma \rightarrow H + D$	$R_{BP8} = 1.45 \times 10^{-12} f_{sh,HD}$	6
BP9	$D_2 + \gamma \rightarrow D + D$	$R_{BP9} = 1.3 \times 10^{-12}$	7
BP10	$H_3^+ + \gamma \rightarrow Htp + H$	$R_{BP10} = 2.4 \times 10^{-16}$	8
BP11	$H_3^+ + \gamma \rightarrow Ht + H^+$	$R_{BP11} = 2.4 \times 10^{-16}$	8
BP12	$H_2D^+ + \gamma \rightarrow Htp + D$	$R_{BP12} = 1.2 \times 10^{-16}$	9
BP13	$H_2D^+ + \gamma \rightarrow Ht + D^+$	$R_{BP13} = 1.2 \times 10^{-16}$	9
BP14	$H_2D^+ + \gamma \rightarrow HD^+ + H$	$R_{BP14} = 1.2 \times 10^{-16}$	9
BP15	$H_2D^+ + \gamma \rightarrow HD + H^+$	$R_{BP15} = 1.2 \times 10^{-16}$	9
BP16	$HD_2^+ + \gamma \rightarrow HD^+ + D$	$R_{BP16} = 1.2 \times 10^{-16}$	9
BP17	$HD_2^+ + \gamma \rightarrow HD + D^+$	$R_{BP17} = 1.2 \times 10^{-16}$	9
BP18	$HD_2^+ + \gamma \rightarrow D_2^+ + H$	$R_{BP18} = 1.2 \times 10^{-16}$	9
BP19	$HD_2^+ + \gamma \rightarrow D_2 + H^+$	$R_{BP19} = 1.2 \times 10^{-16}$	9
BP20	$D_3^+ + \gamma \rightarrow D_2^+ + D$	$R_{BP20} = 2.4 \times 10^{-16}$	9
BP21	$D_3^+ + \gamma \rightarrow D_2 + D^+$	$R_{BP21} = 2.4 \times 10^{-16}$	9
BP22	$HeH^+ + \gamma \rightarrow He + H^+$	$R_{BP22} = 1.0 \times 10^{-17}$	10
BP23	$HeD^+ + \gamma \rightarrow He + D^+$	$R_{BP23} = 1.0 \times 10^{-17}$	10
BP24	$He_2^+ + \gamma \rightarrow He + Hep$	$R_{BP24} = 1.0 \times 10^{-12}$	11
BP25	$Li + \gamma \rightarrow Li^+ + e^-$	$R_{BP25} = 1.4 \times 10^{-12}$	12
BP26	$Li^- + \gamma \rightarrow Li + e^-$	$R_{BP26} = 1.2 \times 10^{-11}$	13
BP27	$LiH^+ + \gamma \rightarrow Li^+ + H$	$R_{BP27} = 5.0 \times 10^{-18}$	13
BP28	$LiH^+ + \gamma \rightarrow Li + H^+$	$R_{BP28} = 9.3 \times 10^{-9}$	13
BP29	$LiD^+ + \gamma \rightarrow Li^+ + D$	$R_{BP29} = 5.0 \times 10^{-18}$	2
BP30	$LiD^+ + \gamma \rightarrow Li + D^+$	$R_{BP30} = 9.3 \times 10^{-9}$	2
BP31	$LiH + \gamma \rightarrow Li + H$	$R_{BP31} = 4.4 \times 10^{-14}$	14
BP32	$LiD + \gamma \rightarrow Li + D$	$R_{BP32} = 4.4 \times 10^{-14}$	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. $f_{sh,Ht}$ and $f_{sh,HD}$ 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 $f_{sh,Ht} = f_{sh,HD} = 0$ and $f_{sh,Ht} = f_{sh,HD} = 1$.

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	$H + C.R. \rightarrow H^+ + e^-$	1.0	—
CR2	$Ht + C.R. \rightarrow Htp + e^-$	2.09	1
CR3	$Ht + C.R. \rightarrow H + H^+ + e^-$	0.09	1
CR4	$Ht + C.R. \rightarrow H + H$	3.26	1
CR5	$He + C.R. \rightarrow Hep + e^-$	1.09	1
CR6	$D + C.R. \rightarrow D^+ + e^-$	1.0	2
CR7	$HD + C.R. \rightarrow HD^+ + e^-$	2.09	2
CR8	$HD + C.R. \rightarrow H + D^+ + e^-$	0.04	2
CR9	$HD + C.R. \rightarrow H^+ + D + e^-$	0.04	2
CR10	$HD + C.R. \rightarrow H + D$	3.26	2
CR11	$D_2 + C.R. \rightarrow D_2^+ + e^-$	2.09	2
CR12	$D_2 + C.R. \rightarrow D + D^+ + e^-$	0.09	2
CR13	$D_2 + C.R. \rightarrow D + D$	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	$\sigma_{X,eff,Ht}$ (Mb)	$\sigma_{X,eff,H}$ (Mb)	Ref.
CP1	$H^- + \gamma_{cr} \rightarrow H + e^-$	5.0	5.8	1
CP2	$D^- + \gamma_{cr} \rightarrow D + e^-$	5.0	5.8	2
CP3	$Htp + \gamma_{cr} \rightarrow H + H^+$	5.0	6.6	3
CP4	$HD^+ + \gamma_{cr} \rightarrow H + D^+$	2.5	3.3	2
CP5	$HD^+ + \gamma_{cr} \rightarrow D + H^+$	2.5	3.3	2
CP6	$D_2^+ + \gamma_{cr} \rightarrow D + D^+$	5.0	6.6	2
CP7	$Li + \gamma_{cr} \rightarrow Li^+ + e^-$	1.0	1.3	4
CP8	$Li^- + \gamma_{cr} \rightarrow Li + e^-$	1.0	1.0	5
CP9	$He_2^+ + \gamma_{cr} \rightarrow He + Hep$	5.0	5.0	6
CP10	$LiH^+ + \gamma_{cr} \rightarrow Li + H^+$	100	100	7
CP11	$LiD^+ + \gamma_{cr} \rightarrow Li + D^+$	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 $P_{Ht}(\nu)$ used to calculate $\sigma_{X,eff,Ht}$ 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).