HIGH TEMPERATURE CONDENSATES AND WATER VAPOUR IN THE SOLAR NEBULA

F. C. Pignatale[1], S. T. Maddison[1], K. Liffman[2], G. Brooks[3], [1]Centre for Astrophysics & Supercomputing, Swinburne University, H30, PO Box 218, Hawthorn, VIC 3122, Australia (fpignatale@astro.swin.edu.au), [2]CSIRO/MSE, PO Box 56, Heightt, VIC 3190, Australia, [3]Departments of Mathematics, FEIS, Swinburne University

Introduction: The study of primitive bodies in our solar system, such as asteroids, meteorites and comets, provide direct evidence of the chemistry of the young solar nebula. Meteorites and comets are characterised by heterogeneous compositions [1], comprising compounds which formed or condensed in different locations and at different times during the protoplanetary disc phase [2]. The distribution of $\delta^{18}O$ and $\delta^{17}O$ in the three isotopes diagram for high refractory compounds forming the CAIs defines the well known slope-1 line [3]. One possible explanation of this behaviour has been traced back to the photodissociation of CO(g) molecules combined with self-shielding [4] in the molecular cloud out of which the solar nebula formed. According to this model, $C^{16}O$ will be depleted in the gas nearest the exterior UV source and the environment will be ^{16}O-rich. Due to the self-shielding, deep inside the molecular cloud the gas will be $C^{16}O$-rich and ^{16}O-poor. As such, we should expect the water in the solar nebula to be ^{16}O-poor [5]. Similarly, in the inner region of the nebula, the protostar will also dissociate $C^{16}O$-rich resulting in heterogeneity in the oxygen isotopes compositions. Analysis of the oxygen isotopic distribution in CAIs from the Allende meteorite shows the important role of remelting processes in the redistribution of ^{16}O within samples with ^{16}O-rich initial compositions [6]. More recent studies [3,7] also highlight the major role water can have in the mixing of oxygen isotopes.

Here we investigate the relation between the water vapour distribution and the high temperature condensates in the solar nebula in order to (1) understand the role of water vapour in the condensation of these compounds, (2) derive the possible stoichiometry of equilibrium reactions, and (3) obtain further clues of the origin of the different ^{16}O distribution in these condensates.

Method: Using a chemical equilibrium code [8], we study the condensation sequence of 59 compounds derived from the fifteen most abundant elements of the Sun with abundances from [9], in the pressure and temperature range appropriate for the solar nebula midplane. We use the disc model of [10] of a typical T Tauri star with $M_* = 0.5\,M_\odot$, $R_* = 2\,R_\odot$, $T_* = 4000$ K, and $\dot{M} = 10^{-8}\,M_\odot\mathrm{yr}^{-1}$ assuming an irradiated disc and we consider only the inner 5 AU. Typical disc mid-plane values for the temperature and pressure range from $(60 < T(\mathrm{K}) < 1900$ and $9.4 \times 10^{-9} < P(\mathrm{bar}) < 2.1 \times 10^{-3}$

between 5 and 0.05 AU. We assume that solid species can mix together to form solid solutions and apply the Gibbs free energy minimization technique [8 and ref. within]. We solve for the condensation sequence using the regular solution model [11], with activity coefficient polynomials from experimental data of activities [12]. We include the following phases and compounds: magnesiowustite (MgO & FeO), olivine (Mg_2SiO_4 forsterite & Fe_2SiO_4 fayalite), orthopyroxene ($MgSiO_3$ enstatite & $FeSiO_3$ ferrosilite), plagioclase ($CaAl_2Si_2O_8$ anorthite & $NaAlSi_3O_8$ albite), melilite ($Ca_2Al_2SiO_7$ gehlenite & $Ca_2MgSi_2O_7$ akermanite), fassaite ($CaAl_2SiO_6$ calcium tschermak & $CaMgSi_2O_6$ diopside), spinel ($MgAl_2O_4$ & $FeAl_2O_4$) and metal alloy (Fe, Ni, Si, Al).

Results: The water vapour in the condensation sequence show a distinctive distribution, and in the high temperature region we can see specific transition zones – see Fig. 1(a). Fig. 1(b) shows the condensation sequence in the high temperature zone for the most refractory compounds in our system. Tab. 1 lists the possible stoichiometry of the condensation sequence. Hibonite ($CaAl_{12}O_{19}$) is the most refractory compound, condensing at $T = 1734$ K (reaction (*i*), Tab. 1), followed by gehlenite ($Ca_2Al_2SiO_7$) (*ii*). According to our calculations the conversion from hibonite and ghelenite to Mg-spinel ($MgAl_2O_4$) and akermanite ($Ca_2MgSi_2O_7$) is driven by reactions (*iii*) and (*iv*). [14] propose a conversion from gehlenite to akermanite and Mg-Spinel (*v*). This reaction takes place at $T = 1458$ K and ends where akermanite reaches its maximum amount at $T = 1450$ K. The transition from the melilite phase (gehlenite, akermanite) to the fassaite phase, Ca-Tchermak ($CaAl_2SiO_6$) and diopside ($CaMgSi_2O_6$), starts at $T = 1450$ K and is driven by three reactions in which gehlenite is converted to diopside and Mg-spinel (*vi*), ghelenite is converted to diopside and Ca-Tchermak (*vii*), and akermanite is converted to diopside (*viii*). Then a conversion from Ca-Ts to Mg-spinel and diopside starts at $T = 1435$ K and ends at $T \sim 1415$ K (*ix*).

Discussion: The sequence of compounds and phases on the slope-1 line in the three isotopes diagram resembles our condensation sequence (Fig.1 (b)) of refractory compounds in the solar nebula. Our proposed stoichiometry of the equilibrium reactions stress the key role of water vapour in the formation of these refractories. If the initial ^{16}O distribution within the condensates was

2

Table 1: Chemical path in the high temperatures region

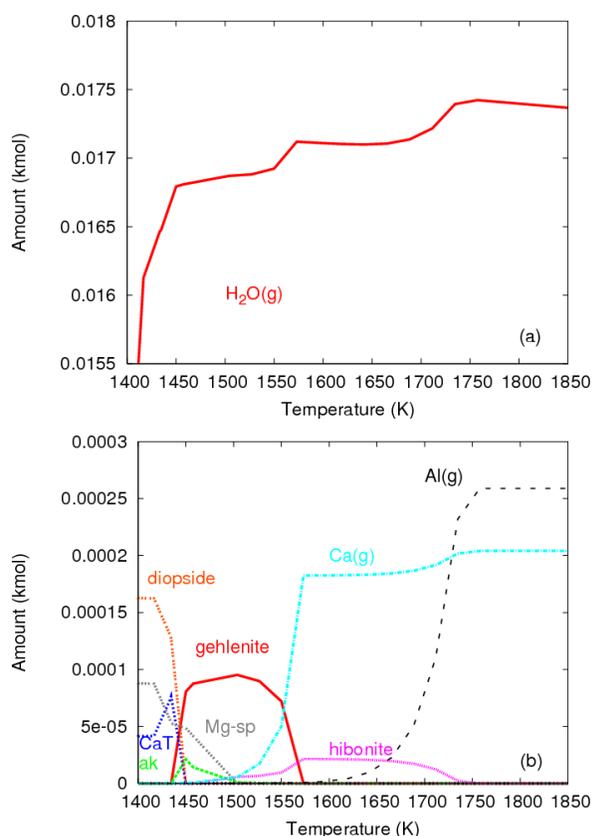| n	T(K)	reactions	reference
i	1735	$Ca(g) + 12Al(g) + 19H_2O(g) \rightarrow CaAl_{12}O_{19} + 19H_2(g)$	[13]
ii	1573	$11Ca(g) + CaAl_{12}O_{19} + 6SiO(g) + 17H_2O(g) \rightarrow 6Ca_2Al_2SiO_7 + 17H_2(g)$	[13]
iii	1503	$Ca_2Al_2SiO_7 + 2Mg(g) + SiO(g) + 3H_2O(g) \rightarrow MgAl_2O_4 + Ca_2MgSi_2O_7 + 3H_2(g)$	[13]
iv	1503	$2CaAl_{12}O_{19} + 13Mg(g) + 2SiO(g) + 15H_2O(g) \rightarrow 12MgAl_2O_4 + Ca_2MgSi_2O_7 + 15H_2(g)$	[13]
v	1458	$4Ca_2Al_2SiO_7 + 5Mg(g) + 4SiO(g) \rightarrow 4Ca_2MgSi_2O_7 + MgAl_2O_4$	[14]
vi	1450	$Ca_2Al_2SiO_7 + 3Mg(g) + 3SiO(g) + 6H_2O(g) \rightarrow 2CaMgSi_2O_6 + MgAl_2O_4 + 6H_2(g)$	[15]
vii	1450	$Ca_2Al_2SiO_7 + Mg(g) + 2SiO(g) + 3H_2O(g) \rightarrow CaMgSi_2O_6 + CaAl_2SiO_6 + 6H_2(g)$	[16]
viii	1450	$Ca_2MgSi_2O_7 + Mg(g) + 2SiO(g) + 3H_2O(g) \rightarrow 2CaMgSi_2O_6 + 3H_2(g)$	[13]
ix	1435	$CaAl_2SiO_6 + 2Mg(g) + SiO(g) + 3H_2O(g) \rightarrow CaMgSi_2O_6 + MgAl_2O_4 + 3H_2(g)$	[13]

Figure 1: (a) Water vapour distribution and (b) condensation sequence for refractories [13] using the regular solution model [12] at fixed pressure, $P = 10^{-3}$ bar.

condenses via three reactions, (*iii*), (*iv*) and (*v*). Reactions (*iii*) and (*iv*) require water vapour and produce 2 moles of akermanite, while reaction (*v*), produces 4 moles of akermanite without the use of water vapour. This could lead to a difference in the [16]O distribution in the akermanite before the remelting processes, described by [6], occurred. Mg-spinel results from reactions (*iii*) to (*vi*) and (*ix*), and since (*v*) does not use water vapour, we might therefore expect different oxygen isotope content in the formation of spinel similar to akermanite. However, the number of moles produced via the water vapour reactions is 15 while the number of moles produced without water vapour is 1.

Conclusion: We have presented a series of reactions demonstrating the importance of water vapour in the condensation of refractory grains in the solar nebula. If the initial [16]O content in these refractories was ^{16}O-rich [6], then the water vapour in the CAI formation region must also have been ^{16}O-rich.

References: [1] Krot A. N., et al. (2005) *Classification of Meteorites*, Davis, A. M., Holland, H. D., & Turekian, K. K., ed., Elsevier B, 83 **[2]** Scott E., Krot A. (2006) *Meteorites, Comets, and Planets: Treatise on Geochemistry*, Davis A., ed., Vol. 1, Elsevier, 143 **[3]** McKeegan, K. D., et al. (2011), *Science*, 332, 1528 **[4]** Thiemens and Heidenreich (1983) *Science*, 219,1073 **[5]** Young E.D. (2007), *Science*, 317, 211 **[6]** Ito, M., et al. (2004), *Geochimica Cosmochimica Acta*, 68, 2905 **[7]** Lyons, J. R., & Young, E. D. (2005) *Chondrites and the Protoplanetary Disk*, 341, 193 **[8]** Roine A. (2007) HSC Chemistry 6, version 6.12. Outokumpu Research Oy, Pori, Finland **[9]** Asplund, M., et al. (2009) *ARA&A*, 47, 481 **[10]** D'Alessio, P., et al. (1998) *ApJ*, 500, 411 **[11]** DeHoff R. (1993) *Thermodynamics in materials science*, McGraw-Hill International Editions **[12]** Pignatale, et. al. (2011) *MNRAS*, 414, 2386 **[13]** Pignatale, et. al. (2011b) *in prep* **[14]** Yoneda, S., & Grossman, L. (1995) *Geochimica Cosmochimica Acta*, 59, 3413 **[15]** Gail, H.-P. (1998), *A&A*, 332, 1099 **[16]** Krot, A. N., et. al. (2003) *Lunar and Planetary Institute Science Conference Abstracts*, 34, 1441

high and similar for each compound as reported by [6], the water vapour involved in reactions in Tab. 1 had to be formed from an ^{16}O-rich reservoir. Analyzing the oxygen isotope content in akermanite, [6] also found two groups of melilites, one ^{16}O-rich and one ^{16}O-poor. In our condensation sequence akermanite ($Ca_2MgSi_2O_7$)