## Supplementary Materials for: Effect of chemical environment on the hydrogen-related defect chemistry in wadsleyite by YU NISHIHARA,<sup>1,2,3,\*</sup> TORU SHINMEI,<sup>1,4</sup> AND SHUN-ICHIRO KARATO<sup>1</sup>

<u>cı</u>	1			6		
Charge neutr	ality A	В	C	D	E	F
condition	$[Fe_M] = [H_M]$	$[H^{-}] = [H_{M}]$	$[(3H)_{M}] = [H_{M}]$	$2[Si_{M}] = [H_{M}]$	$[h] = [H_{M}]$	$[Fe_{M'}] = 2[V_{M''}]$
Defect	q r s	q r s	q r s	q r s	q r s	q r s
[] ( // // ]	1/2 1/4 0	, , ,	, , , ,	1/2 0 7/2	1/2 1/4 0	0 1/6 1/2
[V <sub>M</sub> ]	-1/2 1/4 0	0 0 0	1 0 -1	-1/3 0 -//3	-1/2 1/4 0	0 1/6 -1/3
[M <sub>1</sub> "]	1/2 -1/4 0	0 0 0	-1 0 1	1/3 0 7/3	1/2 -1/4 0	0 –1/6 1/3
[V_"]	1/2 -1/4 -1	0 0 -1	-1 0 0	1/3 0 4/3	1/2 -1/4 -1	0 -1/6 -2/3
[O"]	1/2 1/4 1	0 0 1	1 0 0	1/2 0 4/2	1/2 1/4 1	0 1/6 2/2
	-1/2 1/4 1	0 0 1	1 0 0	-1/3 0 -4/3	-1/2 1/4 1	0 1/0 2/3
[V <sub>si</sub> ""]	-1 1/2 4	0 0 4	2 0 2	-2/3 0 -2/3	-1 1/2 4	0 1/3 10/3
[Si,***]	1 -1/2 -4	0 0 -4	-2 0 -2	2/3 0 2/3	1 -1/2 -4	0 -1/3 -10/3
[H-]	3/1 _1/8 _1/2	1/2 0 _1/2	0 0 0	2/3 0 2/3	3/4 _1/8 _1/2	1/2 _1/12 _1/3
	5/4 -1/6 -1/2	1/2 0 -1/2	0 0 0	2/3 0 2/3	3/4 -1/8 -1/2	1/2 -1/12 -1/3
[H <sub>M</sub> ]	1/4 1/8 -1/2	1/2 0 -1/2	1 0 -1	1/3 0 -5/3	1/4 1/8 -1/2	1/2 1/12 -2/3
[H <sub>si</sub> "']	-1/4 3/8 7/2	1/2 0 7/2	2 0 2	0 0 0	-1/4 3/8 7/2	1/2 1/4 3
[(2H),,"]	1/2 1/4 3	1 0 3	2 0 2	2/3 0 2/3	1/2 1/4 3	1 1/6 8/3
[(21)]	E/A 1/9 E/2		2 0 2	4/2 0 4/2	E/A 1/9 E/0	2/2 1/12 7/2
	J/4 1/8 J/2	3/2 0 3/2	2 0 2	4/3 0 4/3	3/4 1/8 3/2	3/2 1/12 //3
[(OH) <sub>0</sub> ']	3/4 -1/8 -1/2	1/2 0 -1/2	0 0 0	2/3 0 2/3	3/4 -1/8 -1/2	1/2 -1/12 -1/3
[(OH),']	1/4 1/8 1/2	1/2 0 1/2	1 0 0	1/3 0 -2/3	1/4 1/8 1/2	1/2 1/12 1/3
[Feut]	1/4 1/8 -1/2	0 1/4 -1/2	-1/2 1/4 0	1/6 1/4 2/3	1/4 1/8 -1/2	0.00 1/6 -1/3
	1/2 1/4 4	0 1/4 1/2	1/2 1/4 0	1/2 0 5/2	1/2 1/4 4	0.00 1/0 1/5
[IVI <sub>Si</sub> "]	-1/2 1/4 4	0 0 4	1 0 3	-1/3 0 5/3	-1/2 1/4 4	0.00 1/6 11/3
[Fe <sub>si</sub> ']	-1/4 3/8 7/2	0 1/4 7/2	1/2 1/4 3	-1/6 1/4 7/3	-1/4 3/8 7/2	0.00 1/3 10/3
[Si,]	1/2 -1/4 -4	0 0 -4	-1 0 -3	1/3 0 -5/3	1/2 -1/4 -4	0.00 -1/6 -11/3
[b·]	1/4 1/9 1/2	0 1/4 1/2	1/2 1/4 0	1/6 1/4 2/2	1/4 1/9 1/2	0.00 1/6 1/2
[[1]]	1/4 1/6 -1/2	0 1/4 -1/2	-1/2 1/4 0	1/0 1/4 2/3	1/4 1/6 -1/2	0.00 1/6 -1/5
[e']	-1/4 -1/8 1/2	0 -1/4 1/2	1/2 -1/4 0	-1/6 -1/4 -2/3	-1/4 -1/8 1/2	0.00 -1/6 1/3
Charge neutr	ality G	н	1	1	к	1
charge neuth						
condition	$[H^{-}] = 2[V_{M}^{-}]$	$[(3\Pi)_{M}] = 2[V_{M}]$	$2[SI_M^{-1}] = 2[V_M^{-1}]$	$[n^{-}] = 2[V_{M}^{-}]$	$[Fe_M] = [Fe_{Si}]$	$[H^{-}] = [Fe_{Si}]$
Defect	q r s	q r s	q r s	q r s	q r s	q r s
[V <sub>M</sub> "]	1/3 0 -1/3	1 0 -1	0 0 -2	0 1/6 -1/3	0 0 -4	1/2 -1/4 -4
[N/ ••]	1/2 0 1/2	1 0 1		0 1/6 1/2		1/2 1/4 4
	-1/3 0 1/3	-1 0 1	0 0 2	0 -1/0 1/3	0 0 4	-1/2 1/4 4
[V <sub>o</sub> ••]	-1/3 0 -2/3	-1 0 0	0 0 1	0 -1/6 -2/3	0 0 3	-1/2 1/4 3
[O <sub>1</sub> "]	1/3 0 2/3	1 0 0	0 0 -1	0 1/6 2/3	0 0 -3	1/2 -1/4 -3
[V.,""]	2/3 0 10/3	2 0 2	0 0 0	0 1/3 10/3	0 0 -4	1 _1/2 _4
[C: eeee]	2/3 0 10/3	2 0 2		0 1/2 10/2		1 1/2 4
[SI <sub>1</sub> ]	-2/3 0 -10/3	-2 0 -2	0 0 0	0 -1/3 -10/3	0 0 4	-1 1/2 4
[H•]	1/3 0 –1/3	0 0 0	1/2 0 1/2	1/2 -1/12 -1/3	1/2 0 3/2	1/4 1/8 3/2
[H <sub>4</sub> /]	2/3 0 -2/3	1 0 -1	1/2 0 -3/2	1/2 1/12 -2/3	1/2 0 -5/2	3/4 -1/8 -5/2
[H ""]	1 0 3	2 0 2	1/2 0 1/2	1/2 1/4 3	1/2 0 -5/2	5/1 _3/8 _5/2
		2 0 2	1/2 0 1/2	1/2 1/4 5	1/2 0 -5/2	3/4 -3/8 -3/2
[(2H) <sub>si</sub> "]	4/3 0 8/3	2 0 2	1 0 1	1 1/6 8/3	1 0 -1	3/2 -1/4 -1
[(3H) <sub>si</sub> /]	5/3 0 7/3	2 0 2	3/2 0 3/2	3/2 1/12 7/3	3/2 0 1/2	7/4 -1/8 1/2
[(OH).•]	1/3 0 -1/3	0 0 0	1/2 0 1/2	1/2 -1/12 -1/3	1/2 0 3/2	1/4 1/8 3/2
	2/2 0 1/2	1 0 0	1/2 0 1/2	1/2 1/12 1/2	1/2 0 3/2	2/4 1/0 2/2
[(OH) <sub>1</sub> ]	2/3 0 1/3	1 0 0	1/2 0 -1/2	1/2 1/12 1/3	1/2 0 -3/2	3/4 -1/8 -3/2
[Fe <sub>M</sub> •]	-1/6 1/4 -1/3	-1/2 1/4 0	0 1/4 1/2	0 1/6 -1/3	0 1/4 3/2	-1/4 3/8 3/2
[Mc:"]	1/3 0 11/3	1 0 3	0 0 2	0 1/6 11/3	0 0 0	1/2 -1/4 0
[Eo /]	1/6 1/4 10/2	1/2 1/4 2	0 1/4 5/2	0 1/2 10/2	0 1/4 2/2	1/4 1/9 2/2
	1/0 1/4 10/3	1/2 1/4 3	0 1/4 3/2	0 1/3 10/3	0 1/4 3/2	1/4 1/8 3/2
[SI <sub>M</sub> **]	-1/3 0 -11/3	-1 0 -3	0 0 -2	0 -1/6 -11/3	0 0 0	-1/2 1/4 0
[h•]	-1/6 1/4 -1/3	-1/2 1/4 0	0 1/4 1/2	0 1/6 -1/3	0 1/4 3/2	-1/4 3/8 3/2
[e']	1/6 -1/4 1/3	1/2 -1/4 0	$0 -\frac{1}{4} -\frac{1}{2}$	0 -1/6 1/3	$0 -\frac{1}{4} -\frac{3}{2}$	1/4 -3/8 -3/2
[0]	1/6 1/1 1/5	1/2 1/1 0	0 1/1 1/2	0 1/0 1/5	0 1/1 3/2	1,1 5,6 5,2
			_	_	_	_
Charge neutr	ality M	N	0	Ρ	Q	R
condition	$[(3H)_{M}^{\bullet}] = [Fe_{Si}']$	$2[Si_M^{\bullet\bullet}] = [Fe_{Si}']$	$[h^{\bullet}] = [Fe_{si}]$	$[Fe_{M}] = 3[H_{Si}]$	$[H^{\bullet}] = 3[H_{si}''']$	$[(3H)_{M}] = 3[H_{Si}]$
Defect	a r s	ars	a r s	a r s	ars	a r s
[\/ "]	2/2 1/4 5	0 1/6 5	0 0 1	1/1 1/0 2	0 0 2	1/2 0 5/2
LV <sub>M</sub> J	5/2 -1/4 -5	0 -1/6 -5	0 0 -4	-1/4 1/6 -2	0 0 -2	1/2 0 -5/2
[Mi••]	-3/2 1/4 5	0 1/6 5	0 0 4	1/4 -1/8 2	0 0 2	-1/2 0 5/2
[V <sub>0</sub> ••]	-3/2 1/4 4	0 1/6 4	0 0 3	1/4 -1/8 1	0 0 1	-1/2 0 3/2
[O"]	3/2 _1/4 _4	0 -1/6 -4	0 0 -3	_1/4 1/8 _1	0 0 -1	1/2  0  -3/2
	2 1/2 4	0 1/2 (	0 0 -5	1/2 1/4 0	0 0 -1	1/2 0 -3/2
[V <sub>Si</sub> <sup>m</sup> ]	3 -1/2 -6	0 -1/3 -6	0 0 -4	-1/2 1/4 0	0 0 0	i 0 –1
[Si <sub>I</sub> ••••]	-3 1/2 6	0 1/3 6	0 0 4	1/2 -1/4 0	0 0 0	-1 0 1
[H•]	-1/4 1/8 2	1/2 1/12 2	1/2 0 3/2	5/8 -1/16 1/2	1/2 0 1/2	1/4 0 3/4
[] /]	5/A 1/9 3	1/2 1/12 2	1/2 0 5/2	2/0 1/16 2/2	1/2 0 3/2	2/4 0 7/4
	3/4 -1/0 -3	1/2 -1/12 -3	1/2 U -5/2	5/0 1/10 -3/2	1/2 U -3/2	5/4 U -//4
[H <sub>si</sub> ‴]	11/4 -3/8 -4	1/2 -1/4 -4	1/2 0 -5/2	1/8 3/16 1/2	1/2 0 1/2	5/4 0 -1/4
[(2H) <sub>si</sub> "]	5/2 -1/4 -2	1 -1/6 -2	1 0 -1	3/4 1/8 1	1 0 1	3/2 0 1/2
[(3H) <sub>0</sub> /]	9/4 _1/8 0	3/2 _1/12 0	3/2 0 1/2	11/8 1/16 3/2	3/2 0 3/2	7/4 0 5/4
	J, T = 1/0 U	J/Z = 1/1Z = 0	J/2 0 1/2	F/0 1/10 3/2	J/2 U J/2	1/4 0 5/4
[(UH) <sub>0</sub> •]	-1/4 1/8 2	1/2 1/12 2	1/2 0 3/2	5/8 -1/16 1/2	1/2 0 1/2	1/4 0 3/4
[(OH) <sub>I</sub> ']	5/4 -1/8 -2	1/2 -1/12 -2	1/2 0 -3/2	3/8 1/16 -1/2	1/2 0 -1/2	3/4 0 -3/4
[Feu•]	-3/4 3/8 2	0 1/3 2	0 1/4 3/2	1/8 3/16 1/2	0 1/4 1/2	-1/4 1/4 2/4
[NA "]	2/2  1/4  1	0 1/2 1	0 0 0	1/4 1/0 2		1/2 0 2/2
LIVI <sub>Si</sub> J	5/2 -1/4 -1	0 -1/6 -1	0 0 0	-1/4 1/8 2	0 0 2	1/2 U 3/2
[Fe <sub>si</sub> ']	3/4 1/8 1	0 1/6 1	0 1/4 3/2	-1/8 5/16 5/2	0 1/4 5/2	1/4 1/4 9/4
[Si <sub>M</sub> ••]	-3/2 1/4 1	0 1/6 1	0 0 0	1/4 -1/8 -2	0 0 -2	-1/2 0 -3/2
[h•]	_3/4 3/8 2	0 1/3 2	0 1/4 3/2	1/8 3/16 1/2		_1/4 1/4 2/4
[]		0 1/3 2	0 1/7 3/2	1/0 3/10 1/2	0 1/4 1/2	-1/4 1/4 5/4
[e]	3/4 -3/8 -2	0 -1/3 -2	0 -1/4 -3/2	-1/8 -3/16 -1/2	0 -1/4 -1/2	1/4 -1/4 -3/4
Notoci Tablad	hour donondon co of cor	contrations of point dat	acts in (Ma Fa) SiO min	orals on chamical anviron	monte [V] fill Of fO [ a	The name of each charge

**TABLE S1.** Exponents for concentration of point defects in (Mg,Fe)<sub>2</sub>SiO<sub>4</sub> minerals

Notes: Table shows dependence of concentrations of point defects in  $(Mg,Fe)_2SiO_4$  minerals on chemical environment:  $[X] \propto fH_2O^q fO_2 r a_{MO}^s$ . The name of each charge neutrality condition (e.g., A, B) is defined in Table 3.

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TABLE S1.—Continued

Chargo nout		т		V	14/	v
Charge neut	railty S					X
condition	$2[SI_{M}^{**}] = 3[H_{Si}^{**}]$	$[h^{\bullet}] = 3[H_{Si}^{m}]$	$[Fe_{M}] = 2[(2H)_{Si}]$	$[H^{\bullet}] = 2[(2H)_{Si}]$	$[(3H)_{M}] = 2[(2H)_{Si}]$	$2[SI_{M}^{\bullet\bullet}] = 2[(2H)_{Si}^{"}]$
Defect	q r s	q r s	q r s	q r s	q r s	q r s
[V"]	-1/5 0 -3	-1/4 1/8 -2	-2/3 1/6 -7/3	-1/3 0 -7/3	1/3 0 -3	-1/2 0 -7/2
[NA ••]	1/5 0 2	1/4 1/9 2	2/3 1/6 7/3	1/2 0 7/2	1/2 0 2	1/2 0 7/2
	1/3 0 3	1/4 =1/8 2	2/3 =1/0 //3	1/3 0 //3	-1/3 0 3	1/2 0 7/2
[Vo"]	1/5 0 2	1/4 -1/8 1	2/3 -1/6 4/3	1/3 0 4/3	-1/3 0 2	1/2 0 5/2
[O <sub>1</sub> "]	-1/5 0 -2	-1/4 1/8 -1	-2/3 1/6 -4/3	-1/3 0 -4/3	1/3 0 –2	-1/2 0 -5/2
[V <sub>si</sub> ""]	-2/5 0 -2	-1/2 1/4 0	-4/3 1/3 -2/3	-2/3 0 -2/3	2/3 0 -2	-1 0 -3
[51.***]	2/5 0 2	1/2 -1/4 0	4/3 -1/3 2/3	2/3 0 2/3	-2/3 0 2	1 0 3
		1/2 1/4 0	1/12 2/2 2/3	2/3 0 2/3	2/3 0 2	
[H <sup>-</sup> ] 3/5	0 1 5/8	-1/10 1/2 5/0	-1/12 2/3 2/3	0 2/3 1/3	0 1 3/4	0 5/4
[H <sub>M</sub> ′]	2/5 0 -2	3/8 1/16 -3/2	1/6 1/12 -5/3	1/3 0 -5/3	2/3 0 -2	1/4 0 -9/4
[H <sub>si</sub> "']	1/5 0 -1	1/8 3/16 1/2	-1/2 1/4 0	0 0 0	1 0 -1	-1/4 0 -7/4
[(2H),,"]	4/5 0 0	3/4 1/8 1	1/3 1/6 2/3	2/3 0 2/3	4/3 0 0	1/2 0 -1/2
[(2L) /]	7/5 0 1	11/9 1/16 2/2	7/6 1/12 4/2	1/2 0 1/2	5/2 0 1	5/4 0 2/4
	7/3 0 1	11/8 1/10 3/2	7/0 1/12 4/3	4/3 0 4/3	5/5 0 1	3/4 0 3/4
[(OH) <sub>0</sub> *]	3/5 0 1	5/8 -1/16 1/2	5/6 -1/12 2/3	2/3 0 2/3	1/3 0 1	3/4 0 5/4
[(OH) <sub>I</sub> ′]	2/5 0 -1	3/8 1/16 -1/2	1/6 1/12 –2/3	1/3 0 –2/3	2/3 0 -1	1/4 0 –5/4
[Fe <sub>M</sub> •]	1/10 1/4 1	1/8 3/16 1/2	1/3 1/6 2/3	1/6 1/4 2/3	-1/6 1/4 1	1/4 1/4 5/4
[M"]	-1/5 0 1	_1/4 1/8 2	_2/3 1/6 5/3	_1/3 0 5/3	1/3 0 1	_1/2 0 1/2
	-1/5 0 1	-1/4 1/0 2	-2/3 1/0 3/3	-1/5 0 5/5	1/5 0 1	-1/2 0 1/2
[Fe <sub>si</sub> ]	-1/10 1/4 2	-1/8 5/10 5/2	-1/3 1/3 //3	-1/6 1/4 //3	1/6 1/4 2	-1/4 1/4 //4
[Si <sub>M</sub> ••]	1/5 0 –1	1/4 -1/8 -2	2/3 -1/6 -5/3	1/3 0 –5/3	-1/3 0 -1	1/2 0 -1/2
[h•] 1/10	1/4 1 1/8	3/16 1/2 1/3	1/6 2/3 1/6	1/4 2/3 -1/6	1/4 1 1/4	1/4 5/4
[e'] _1/10	-1/4 -1 -1/8	-3/16 - 1/2 - 1/3	-1/6 -2/3 -1/6	-1/4 -2/3 1/6	-1/4 -1 -1/4	-1/4 -5/4
	1/4 1 1/0	5/10 1/2 1/5	1/6 2/5 1/6	1/4 2/5 1/0	1/4 1 1/4	1/4 5/4
<b>C1</b>		7		10	10	10
charge neut	гансу к	۷	AA	AB	AC	AD
condition	$[h^{\bullet}] = 2[(2H)_{Si}]$	$[Fe_{M}^{\bullet}] = [(3H)_{Si}']$	$[H^{\bullet}] = [(3H)_{Si}]$	$[(3H)_{M}] = [(3H)_{Si}]$	$2[Si_{M}^{\bullet\bullet}] = [(3H)_{Si}]$	[h•] = [(3H) <sub>si</sub> ']
Defect	q r s	q r s	q r s	q r s	q r s	q r s
[V.,"]	-2/3 1/6 -7/3	_3/2 1/4 _3	-1 0 -3	0 0 -4	_1 0 _13/3	_3/2 1/4 _3
[• M ]	2/3 1/6 7/3	3/2 1/4 3	1 0 2		1 0 13/3	3/2 1/4 3
	2/3 -1/0 //3	5/2 -1/4 5	1 0 5	0 0 4	1 0 15/5	5/2 -1/4 5
[V <sub>o</sub> ••]	2/3 -1/6 4/3	3/2 -1/4 2	1 0 2	0 0 3	1 0 10/3	3/2 -1/4 2
[O <sub>1</sub> "]	-2/3 1/6 -4/3	-3/2 1/4 -2	-1 0 -2	0 0 -3	-1 0 -10/3	-3/2 1/4 -2
[V.,""]	-4/3 1/3 -2/3	-3 1/2 -2	-2 0 -2	0 0 -4	-2 0 -14/3	-3 1/2 -2
[\$;••••]	1/3 _1/3 2/3	3 _1/2 2	2 0 2	0 0 1	2 0 14/3	3 _1/2 2
	4/3 -1/3 2/3	5 -1/2 2	2 0 2	0 0 4	2 0 14/3	5 -1/2 2
[H <sup>*</sup> ] 5/6	-1/12 2/3 5/4	-1/8 1 1	0 1 1/2	0 3/2 1	0 5/3 5/4	-1/8 1
[H <sub>M</sub> ']	1/6 1/12 –5/3	-1/4 1/8 -2	0 0 -2	1/2 0 -5/2	0 0 -8/3	-1/4 1/8 -2
[H <sub>s</sub> ,‴]	-1/2 1/4 0	-7/4 3/8 -1	-1 0 -1	1/2 0 -5/2	-1 0 -3	-7/4 3/8 -1
[(2H)."]	1/3 1/6 2/3	-1/2 1/4 0	0 0 0	1 0 _1	0 0 -1/3	-1/2 1/4 0
	7/5 1/10 2/5	-1/2 1/4 0		2/2 0 1/2	0 0 -4/3	-1/2 1/4 0
[(3H) <sub>Si</sub> ]	//6 1/12 4/3	3/4 1/8 1	1 0 1	3/2 0 1/2	1 0 1/3	3/4 1/8 1
[(OH) <sub>o</sub> •]	5/6 -1/12 2/3	5/4 –1/8 1	1 0 1	1/2 0 3/2	1 0 5/3	5/4 –1/8 1
[(OH) <sub>1</sub> /]	1/6 1/12 -2/3	-1/4 1/8 -1	0 0 -1	1/2 0 -3/2	0 0 -5/3	-1/4 1/8 -1
[Fe•]	1/3 1/6 2/3	3/4 1/8 1	1/2 1/4 1	0 1/4 3/2	1/2 1/4 5/3	3/4 1/8 1
		2/2 1/4 1	1 0 1	0 1/4 3/2	1/2 1/4 5/5	2/2 1/4 1
[IVI <sub>Si</sub> ]	-2/3 1/6 5/3	-3/2 1/4 1	-1 0 1	0 0 0	-1 0 -1/3	-3/2 1/4 1
[Fe <sub>si</sub> ']	-1/3 1/3 7/3	-3/4 3/8 2	-1/2 1/4 2	0 1/4 3/2	-1/2 1/4 4/3	-3/4 3/8 2
[Si <sub>M</sub> ••]	2/3 -1/6 -5/3	3/2 -1/4 -1	1 0 -1	0 0 0	1 0 1/3	3/2 -1/4 -1
[h•] 1/3	1/6 2/3 3/4	1/8 1 1/2	1/4 1 0	1/4 3/2 1/2	1/4 5/3 3/4	1/8 1
[0 <sup>'</sup> ] 1/2	1/6 2/2 2/4	1/9 1 1/2	1/4 1 0	1/4 2/2 1/2	1/4 5/2 2/4	1/0 1
[e] =1/5	=1/0 =2/3 = 3/4	-1/8 -1 -1/2	-1/4 -1 0	-1/4 -3/2 -1/2	-1/4 -3/3 -3/4	-1/8 -1
Charge neut	trality AE	AF	AG	AH	AI	
condition	$[Fe_{M}^{\bullet}] = [e']$	[H•] = [e']	$[(3H)_{M}] = [e']$	$2[Si_{M}^{**}] = [e']$	[h•] = [e']	
Defect	ar s	a r s	ar s	a r s	a r s	
[V"]	$0 \frac{1}{2} -1$	1/2 1/4 _1	3/2 1/4 -2	0 1/6 -3	$0 \frac{1}{2} -1$	
L V M J	0 1/2 1	1/2 1/4 -1	3/2 + 1/4 = -2		0 1/2 1	
	U -1/2 I	-1/2 -1/4 1	-3/2 -1/4 2	U -1/b 3	U -1/2 I	
[V <sub>o</sub> ••]	0 -1/2 0	-1/2 -1/4 0	-3/2 -1/4 1	0 -1/6 2	0 -1/2 0	
[O <sub>1</sub> "]	0 1/2 0	1/2 1/4 0	3/2 1/4 -1	0 1/6 -2	0 1/2 0	
[V.,""]	0 1 2	1 1/2 2	3 1/2 0	0 1/3 _2	0 1 2	
[VSI ] [C: ••••]		1 1/2 2	2 1/2 0	0 1/2 2		
	0 =1 =2	-1 -1/2 -2	-5 -1/2 0	0 -1/5 2	0 =1 =2	
[H•] 1/2	-1/4 0 1/4	-1/8 0 -1/4	-1/8 1/2 1/2	-1/12 1 1/2	-1/4 0	
[H <sub>M</sub> ′]	1/2 1/4 -1	3/4 1/8 -1	5/4 1/8 -3/2	1/2 1/12 -2	1/2 1/4 -1	
[He]"]	1/2 3/4 2	5/4 3/8 2	11/4 3/8 1/2	1/2 1/4 -1	1/2 3/4 2	
[()H) "	1 1/2 2	3/2 1/4 2	5/2 1/4 1	1 1/6 0	1 1/2 2	
[(ZΠ) <sub>Si</sub> ]	1 1/2 Z	5/2 1/4 Z	5/2 1/4 1	I I/O U	I 1/2 2	
[(3H) <sub>si</sub> ']	3/2 1/4 2	7/4 1/8 2	9/4 1/8 3/2	3/2 1/12 1	3/2 1/4 2	
[(OH) <sub>0</sub> •]	1/2 -1/4 0	1/4 -1/8 0	-1/4 -1/8 1/2	1/2 -1/12 1	1/2 -1/4 0	
[(OH),']	1/2 1/4 0	3/4 1/8 0	5/4 1/8 -1/2	1/2 1/12 -1	1/2 1/4 0	
[Eo•]	0 0 0	_1/4 1/9 0	_3/4 1/9 1/2	0 1/6 1	0 0 0	
		-1/4 1/0 U	-3/4 1/0 1/2			
[M <sub>si</sub> "]	0 1/2 3	1/2 1/4 3	3/2 1/4 2	0 1/6 1	0 1/2 3	
[Fe <sub>si</sub> ']	0 1/2 3	1/4 3/8 3	3/4 3/8 5/2	0 1/3 2	0 1/2 3	
[Si <sub>M</sub> ••]	0 -1/2 -3	-1/2 -1/4 -3	-3/2 -1/4 -2	0 -1/6 -1	0 -1/2 -3	
[h•]	0 0 0	-1/4 1/8 0	_3/4 1/8 1/2	0 1/6 1	0 0 0	
[0]		1/4 1/9 0	2/4 1/0 1/2			
[]	0 0 0	1/4 -1/0 U	3/4 -1/0 -1/2	0 -1/0 -1	0 0 0	



**FIGURE S1.** OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm<sup>-1</sup> plotted as a function of OH concentration of Group O (COH,Group O). Data are normalized to  $f_{O2} = 104$  Pa and T = 1773 K using parameters derived by the fit without any constraint on q and r (Table 2). Solid circles, solid triangles and open squares are experimental data collected using Mo, Ni and Re capsules, respectively. Fits of Equation 5 are shown as solid lines.



**FIGURE S2.** OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm<sup>-1</sup> plotted as a function of oxygen fugacity. Data are normalized to COH,Group O = 1000 H/106Si and T = 1773 K using parameters derived by the fit without any constraint on q and r (Table 2). Same symbols as Figure S1 are used for each capsule material. Fits of Equation 5 are shown as solid lines.



**FIGURE S3.** OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm<sup>-1</sup> plotted as a function of reciprocal temperature. Data are normalized to COH,Group O = 1000 H/106Si and  $f_{02}$  = 104 Pa using parameters derived by the fit without any constraint on q and r (Table 2). Same symbols as Figures S1 and S2 are used for each capsule material. Fits of Equation 5 are shown as solid lines.