Supplementary Materials for: Effect of chemical environment on the hydrogen-related defect chemistry in wadsleyite by Yu Nishihara,[1,2,3,*] Toru Shinmei,[1,4] and Shun-ichiro Karato[1]

Table S1. Exponents for concentration of point defects in $(Mg,Fe)_2SiO_4$ minerals

Charge neutrality	A			B			C			D			E			F		
condition	$[Fe_M^{\cdot}] = [H_M']$			$[H^{\cdot}] = [H_M']$			$[(3H)_M^{\cdot}] = [H_M']$			$2[Si_M^{\cdot\cdot}] = [H_M']$			$[h^{\cdot}] = [H_M']$			$[Fe_M^{\cdot}] = 2[V_M'']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	−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
$[M_i^{\cdot\cdot}]$	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
$[V_O^{\cdot\cdot}]$	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
$[O_i'']$	−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
$[V_{Si}'''']$	−1	1/2	4	0	0	4	2	0	2	−2/3	0	−2/3	−1	1/2	4	0	1/3	10/3
$[Si_i''''']$	1	−1/2	−4	0	0	−4	−2	0	−2	2/3	0	2/3	1	−1/2	−4	0	−1/3	−10/3
$[H^{\cdot}]$	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
$[H_M']$	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
$[H_{Si}''']$	−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
$[(2H)_{Si}'']$	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
$[(3H)_{Si}']$	5/4	1/8	5/2	3/2	0	5/2	2	0	2	4/3	0	4/3	5/4	1/8	5/2	3/2	1/12	7/3
$[(OH)_O^{\cdot}]$	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
$[(OH)_i']$	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
$[Fe_M^{\cdot}]$	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
$[M_{Si}'']$	−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
$[Fe_{Si}']$	−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
$[Si_M^{\cdot\cdot}]$	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
$[h^{\cdot}]$	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
$[e']$	−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 neutrality	G			H			I			J			K			L		
condition	$[H^{\bullet}] = 2[V_M'']$			$[(3H)_M^{\bullet}] = 2[V_M'']$			$2[Si_M^{\bullet\bullet}] = 2[V_M'']$			$[h^{\bullet}] = 2[V_M'']$			$[Fe_M^{\bullet}] = [Fe_{Si}']$			$[H^{\bullet}] = [Fe_{Si}']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	1/3	0	−1/3	1	0	−1	0	0	−2	0	1/6	−1/3	0	0	−4	1/2	−1/4	−4
$[M_i^{\bullet\bullet}]$	−1/3	0	1/3	−1	0	1	0	0	2	0	−1/6	1/3	0	0	4	−1/2	1/4	4
$[V_O^{\bullet\bullet}]$	−1/3	0	−2/3	−1	0	0	0	0	1	0	−1/6	−2/3	0	0	3	−1/2	1/4	3
$[O_i'']$	1/3	0	2/3	1	0	0	0	0	−1	0	1/6	2/3	0	0	−3	1/2	−1/4	−3
$[V_{Si}'''']$	2/3	0	10/3	2	0	2	0	0	0	0	1/3	10/3	0	0	−4	1	−1/2	−4
$[Si_i^{\bullet\bullet\bullet\bullet}]$	−2/3	0	−10/3	−2	0	−2	0	0	0	0	−1/3	−10/3	0	0	4	−1	1/2	4
$[H^{\bullet}]$	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
$[H_M']$	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
$[H_{Si}''']$	1	0	3	2	0	2	1/2	0	1/2	1/2	1/4	3	1/2	0	−5/2	5/4	−3/8	−5/2
$[(2H)_{Si}'']$	4/3	0	8/3	2	0	2	1	0	1	1	1/6	8/3	1	0	−1	3/2	−1/4	−1
$[(3H)_{Si}']$	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
$[(OH)_O^{\bullet}]$	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
$[(OH)_i']$	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
$[Fe_M^{\bullet}]$	−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
$[M_{Si}'']$	1/3	0	11/3	1	0	3	0	0	2	0	1/6	11/3	0	0	0	1/2	−1/4	0
$[Fe_{Si}']$	1/6	1/4	10/3	1/2	1/4	3	0	1/4	5/2	0	1/3	10/3	0	1/4	3/2	1/4	1/8	3/2
$[Si_M^{\bullet\bullet}]$	−1/3	0	−11/3	−1	0	−3	0	0	−2	0	−1/6	−11/3	0	0	0	−1/2	1/4	0
$[h^{\bullet}]$	−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	−1/4	−1/2	0	−1/6	1/3	0	−1/4	−3/2	1/4	−3/8	−3/2

Charge neutrality	M			N			O			P			Q			R		
condition	$[(3H)_M^{\bullet}] = [Fe_{Si}']$			$2[Si_M^{\bullet\bullet}] = [Fe_{Si}']$			$[h^{\bullet}] = [Fe_{Si}']$			$[Fe_M^{\bullet}] = 3[H_{Si}''']$			$[H^{\bullet}] = 3[H_{Si}''']$			$[(3H)_M^{\bullet}] = 3[H_{Si}''']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	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
$[M_i^{\bullet\bullet}]$	−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
$[V_O^{\bullet\bullet}]$	−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
$[O_i'']$	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
$[V_{Si}'''']$	3	−1/2	−6	0	−1/3	−6	0	0	−4	−1/2	1/4	0	0	0	0	1	0	−1
$[Si_i^{\bullet\bullet\bullet\bullet}]$	−3	1/2	6	0	1/3	6	0	0	4	1/2	−1/4	0	0	0	0	−1	0	1
$[H^{\bullet}]$	−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
$[H_M']$	5/4	−1/8	−3	1/2	−1/12	−3	1/2	0	−5/2	3/8	1/16	−3/2	1/2	0	−3/2	3/4	0	−7/4
$[H_{Si}''']$	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
$[(2H)_{Si}'']$	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
$[(3H)_{Si}']$	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
$[(OH)_O^{\bullet}]$	−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
$[(OH)_i']$	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
$[Fe_M^{\bullet}]$	−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
$[M_{Si}'']$	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
$[Fe_{Si}']$	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
$[Si_M^{\bullet\bullet}]$	−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
$[h^{\bullet}]$	−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
$[e']$	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

Notes: Table shows dependence of concentrations of point defects in $(Mg,Fe)_2SiO_4$ minerals on chemical environment: $[X] \propto f_{H_2O}^{\,q} f_{O_2}^{\,r} a_{MO}^{\,s}$. The name of each charge neutrality condition (e.g., A, B) is defined in Table 3.

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TABLE S1.—*Continued*

Charge neutrality condition	S			T			U			V			W			X		
	$2[Si_M^{\bullet\bullet}] = 3[H_{Si}'''']$			$[h^{\bullet}] = 3[H_{Si}'''']$			$[Fe_M^{\bullet}] = 2[(2H)_{Si}'']$			$[H^{\bullet}] = 2[(2H)_{Si}'']$			$[(3H)_M^{\bullet}] = 2[(2H)_{Si}'']$			$2[Si_M^{\bullet\bullet}] = 2[(2H)_{Si}'']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	−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
$[M_i^{\bullet\bullet}]$	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
$[V_O^{\bullet\bullet}]$	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
$[O_i'']$	−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
$[V_{Si}'''']$	−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
$[Si_i^{\bullet\bullet\bullet\bullet}]$	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
$[H^{\bullet}]$ 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	
$[H_M']$	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
$[H_{Si}'''']$	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
$[(2H)_{Si}'']$	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
$[(3H)_{Si}']$	7/5	0	1	11/8	1/16	3/2	7/6	1/12	4/3	4/3	0	4/3	5/3	0	1	5/4	0	3/4
$[(OH)_O^{\bullet}]$	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
$[(OH)_i']$	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
$[Fe_M^{\bullet}]$	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
$[M_{Si}'']$	−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
$[Fe_{Si}']$	−1/10	1/4	2	−1/8	5/16	5/2	−1/3	1/3	7/3	−1/6	1/4	7/3	1/6	1/4	2	−1/4	1/4	7/4
$[Si_M^{\bullet\bullet}]$	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
$[h^{\bullet}]$ 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	

Charge neutrality condition	Y			Z			AA			AB			AC			AD		
	$[h^{\bullet}] = 2[(2H)_{Si}'']$			$[Fe_M^{\bullet}] = [(3H)_{Si}']$			$[H^{\bullet}] = [(3H)_{Si}']$			$[(3H)_M^{\bullet}] = [(3H)_{Si}']$			$2[Si_M^{\bullet\bullet}] = [(3H)_{Si}']$			$[h^{\bullet}] = [(3H)_{Si}']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	−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
$[M_i^{\bullet\bullet}]$	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
$[V_O^{\bullet\bullet}]$	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
$[O_i'']$	−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
$[V_{Si}'''']$	−4/3	1/3	−2/3	−3	1/2	−2	−2	0	−2	0	0	−4	−2	0	−14/3	−3	1/2	−2
$[Si_i^{\bullet\bullet\bullet\bullet}]$	4/3	−1/3	2/3	3	−1/2	2	2	0	2	0	0	4	2	0	14/3	3	−1/2	2
$[H^{\bullet}]$ 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	
$[H_M']$	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
$[H_{Si}'''']$	−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
$[(2H)_{Si}'']$	1/3	1/6	2/3	−1/2	1/4	0	0	0	0	1	0	−1	0	0	−4/3	−1/2	1/4	0
$[(3H)_{Si}']$	7/6	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
$[(OH)_O^{\bullet}]$	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
$[(OH)_i']$	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
$[Fe_M^{\bullet}]$	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
$[M_{Si}'']$	−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
$[Fe_{Si}']$	−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
$[Si_M^{\bullet\bullet}]$	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
$[h^{\bullet}]$ 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	
$[e']$ −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	

Charge neutrality condition	AE			AF			AG			AH			AI		
	$[Fe_M^{\bullet}] = [e']$			$[H^{\bullet}] = [e']$			$[(3H)_M^{\bullet}] = [e']$			$2[Si_M^{\bullet\bullet}] = [e']$			$[h^{\bullet}] = [e']$		
Defect	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*	*q*	*r*	*s*
$[V_M'']$	0	1/2	−1	1/2	1/4	−1	3/2	1/4	−2	0	1/6	−3	0	1/2	−1
$[M_i^{\bullet\bullet}]$	0	−1/2	1	−1/2	−1/4	1	−3/2	−1/4	2	0	−1/6	3	0	−1/2	1
$[V_O^{\bullet\bullet}]$	0	−1/2	0	−1/2	−1/4	0	−3/2	−1/4	1	0	−1/6	2	0	−1/2	0
$[O_i'']$	0	1/2	0	1/2	1/4	0	3/2	1/4	−1	0	1/6	−2	0	1/2	0
$[V_{Si}'''']$	0	1	2	1	1/2	2	3	1/2	0	0	1/3	−2	0	1	2
$[Si_i^{\bullet\bullet\bullet\bullet}]$	0	−1	−2	−1	−1/2	−2	−3	−1/2	0	0	−1/3	2	0	−1	−2
$[H^{\bullet}]$ 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	
$[H_M']$	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
$[H_{Si}'''']$	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
$[(2H)_{Si}'']$	1	1/2	2	3/2	1/4	2	5/2	1/4	1	1	1/6	0	1	1/2	2
$[(3H)_{Si}']$	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
$[(OH)_O^{\bullet}]$	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
$[(OH)_i']$	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
$[Fe_M^{\bullet}]$	0	0	0	−1/4	1/8	0	−3/4	1/8	1/2	0	1/6	1	0	0	0
$[M_{Si}'']$	0	1/2	3	1/2	1/4	3	3/2	1/4	2	0	1/6	1	0	1/2	3
$[Fe_{Si}']$	0	1/2	3	1/4	3/8	3	3/4	3/8	5/2	0	1/3	2	0	1/2	3
$[Si_M^{\bullet\bullet}]$	0	−1/2	−3	−1/2	−1/4	−3	−3/2	−1/4	−2	0	−1/6	−1	0	−1/2	−3
$[h^{\bullet}]$	0	0	0	−1/4	1/8	0	−3/4	1/8	1/2	0	1/6	1	0	0	0
$[e']$	0	0	0	1/4	−1/8	0	3/4	−1/8	−1/2	0	−1/6	−1	0	0	0

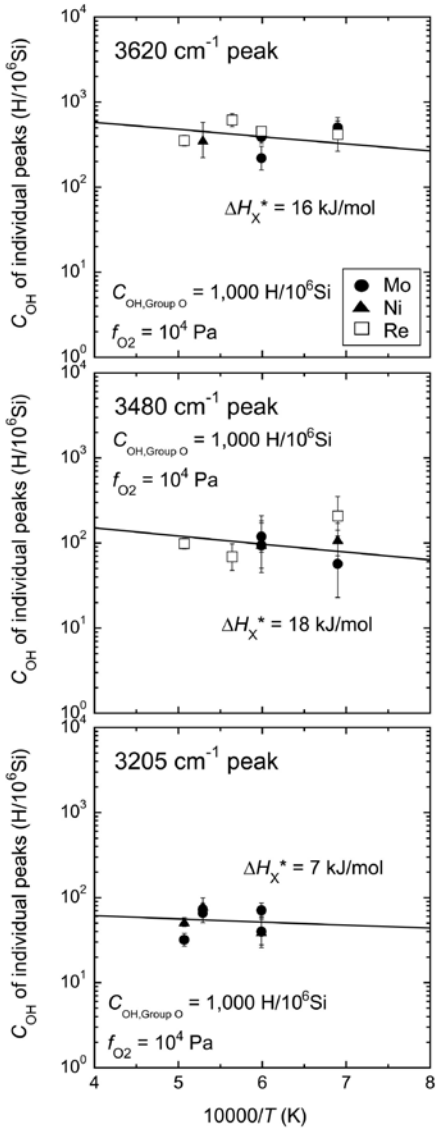

FIGURE S1. OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm^{-1} plotted as a function of OH concentration of Group O (COH,Group O). Data are normalized to f_{O_2} = 104 Pa and T = 1773 K using parameters derived by the fit without any constraint on q and r (Table 2). Solid circles, 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.

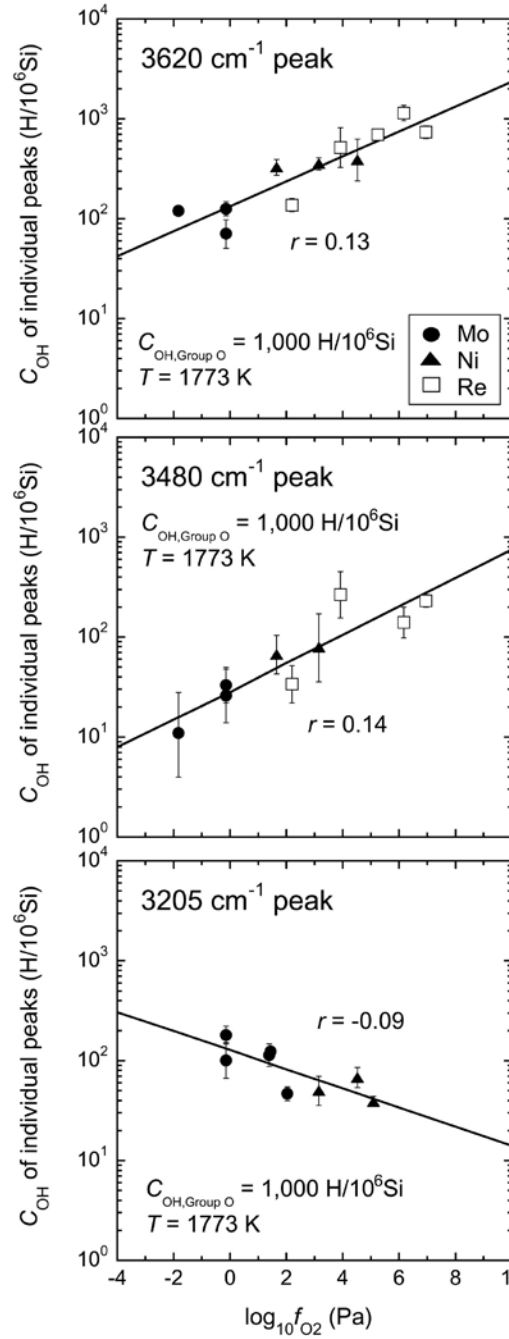

FIGURE S2. OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm^{-1} plotted as a function of oxygen fugacity. Data are normalized to COH,Group O = 1000 H/106Si and T = 1773 K using parameters derived by the fit without any constraint on q and r (Table 2). Same symbols as Figure S1 are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

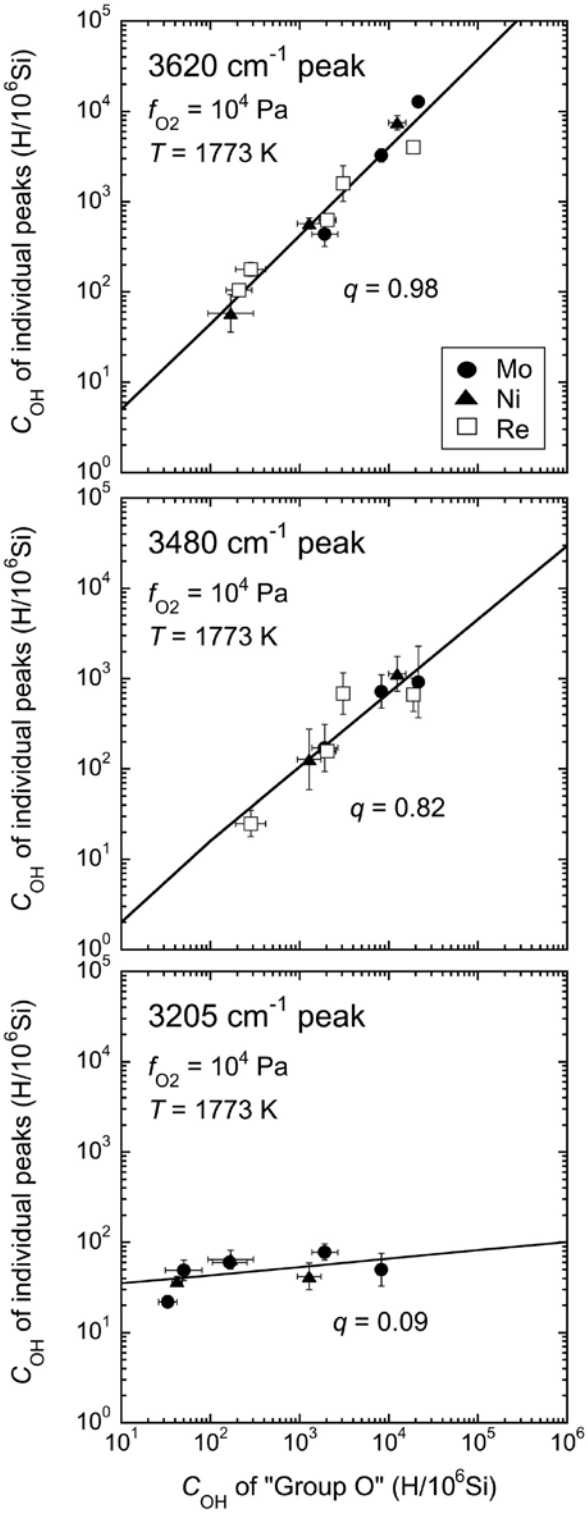

FIGURE S3. OH concentrations corresponding to peaks at 3620, 3480, and 3205 cm^{-1} plotted as a function of reciprocal temperature. Data are normalized to COH,Group O = 1000 H/106Si and f_{O_2} = 104 Pa using parameters derived by the fit without any constraint on q and r (Table 2). Same symbols as Figures S1 and S2 are used for each capsule material. Fits of Equation 5 are shown as solid lines.