Table S2. Calculated XRD *d*-Spacings (A) and Relative Intensities of α-$Ca_5Si_2N_6$[13] and β-$Ca_5Si_2N_6$, Observed XRD *d*-Spacings and Relative Intensities of $Ca_5Si_2N_6$[9]

calculated α-$Ca_5Si_2N_6$[13]					calculated β-$Ca_5Si_2N_6$					observed β-$Ca_5Si_2N_6$[9]	
h	*k*	*l*	*d* (Å)	I/I_1	*h*	*k*	*l*	*d* (Å)	I/I_1	*d* (Å)	I/I_1
					0	0	1	11.870	3		
0	0	2	6.278	2							
					0	0	2	5.935	2		
					1	1	0	5.265	11		
1	1	0	5.132	6							
					1	1	-1	5.079	2		
					0	2	0	5.009	0		
1	1	-1	4.915	24							
2	0	0	4.840	0							
1	1	1	4.601	5	0	2	1	4.615	0		
					1	1	1	4.585	0		
2	0	-2	4.211	1	1	1	-2	4.239	21		
1	1	-2	4.170	8						4.18	20
					0	0	3	3.957	0		
					0	2	2	3.828	0		
1	1	2	3.802	2							
					1	1	2	3.695	8	3.67	10
2	0	2	3.542	2							
1	1	-3	3.404	15							
					1	1	-3	3.395	18	3.35	20
0	0	4	3.139	31	2	0	-1	3.120	11		
1	1	3	3.104	14	0	2	3	3.105	11		
0	2	0	3.026	1	2	0	0	3.094	16	3.07	20
					1	1	3	2.973	6		
					0	0	4	2.968	19		
0	2	1	2.942	23	2	0	-2	2.946	0	2.93	10
					1	3	0	2.939	0		
					1	3	-1	2.905	21		
					2	0	1	2.883	9		
2	0	-4	2.876	0							
3	1	-1	2.875	9						2.86	10
3	1	0	2.847	21	1	3	1	2.803	0		
1	1	-4	2.797	16							
3	1	-2	2.760	19	1	1	-4	2.752	3		
0	2	2	2.726	49	1	3	-2	2.718	59		
3	1	1	2.688	100						2.68	30
					2	0	-3	2.655	13		
					2	2	-1	2.648	0		
					2	2	0	2.633	26		
1	1	4	2.572	2	2	0	2	2.578	0		
2	2	0	2.566	14	1	3	2	2.557	100	2.54	100
2	2	-1	2.561	0	0	2	4	2.553	26		
3	1	-3	2.547	92	2	2	-2	2.539	1		
					0	4	0	2.504	9		
					2	2	1	2.498	0		

2	2	1	2.469	9							
2	2	-2	2.457	3	1	3	-3	2.451	0		
3	1	2	2.453	20	0	4	1	2.450	6		
0	2	3	2.452	57	1	1	4	2.445	6		
2	0	4	2.443	41						2.42	25
4	0	0	2.420	0							
4	0	-2	2.406	1							
					0	0	5	2.374	0	2.38	20
1	1	-5	2.344	1	2	2	-3	2.346	2		
					2	0	-4	2.339	36		
2	2	2	2.301	11	0	4	2	2.307	11	2.31	35
3	1	-4	2.295	20	2	2	2	2.292	20		
2	2	-3	2.285	3	1	1	-5	2.285	0		
					1	3	3	2.277	7	2.27	30
3	1	3	2.200	1	2	0	3	2.266	5		
0	2	4	2.178	14	1	3	-4	2.173	0		
1	1	5	2.176	5	0	2	5	2.145	3		
4	0	2	2.135	5	2	2	-4	2.119	17		
4	0	-4	2.105	7	0	4	3	2.116	0		
2	2	3	2.101	0							
0	0	6	2.093	1							
2	2	-4	2.085	19						2.09	15
2	0	-6	2.058	16	2	2	3	2.065	1		
3	1	-5	2.049	1	1	1	5	2.061	2		
1	1	-6	2.005	9	2	0	-5	2.050	2		
					3	1	-1	2.046	0		
					3	1	0	2.021	3		
					3	1	-2	2.012	20		
					1	3	4	2.012	14	1.99	35
					2	0	4	1.987	17		
1	3	0	1.975	1	0	0	6	1.978	1		
3	1	4	1.962	13	2	4	-1	1.953	4	1.97	15
1	3	-1	1.962	14	2	4	0	1.947	2		
1	3	1	1.940	16	1	1	-6	1.942	15		
					3	1	1	1.942	1		
0	2	5	1.932	6						1.93	20
					3	1	-3	1.927	0		
					1	3	-5	1.920	4		
					0	4	4	1.914	2		
4	2	-1	1.908	0	2	4	-2	1.908	5		
1	3	-2	1.904	0	1	5	0	1.906	0		
2	2	4	1.901	1	2	2	-5	1.898	0		
4	2	0	1.890	1	1	5	-1	1.897	0		
2	2	-5	1.885	0	2	4	1	1.891	0		
4	2	-2	1.883	0	1	5	1	1.868	0		
1	1	6	1.877	7	2	2	4	1.847	6	1.84	15
5	1	-1	1.870	0	1	5	-2	1.842	1		
1	3	2	1.865	1	0	2	6	1.840	7		
5	1	-2	1.856	0	3	1	2	1.827	1		
5	1	0	1.844	0	2	4	-3	1.822	0		
4	2	1	1.832	1							

3	1	-6	1.828	13							
4	2	-3	1.819	2							
1	3	-3	1.811	0							
2	0	6	1.808	0	3	1	-4	1.809	1		
5	1	-3	1.803	1	2	0	-6	1.804	2		
5	1	1	1.782	7	2	4	2	1.796	1		
					1	5	2	1.789	2		
					1	3	5	1.781	0		
4	0	4	1.771	5	1	1	6	1.773	2		
					3	3	-1	1.772	16	1.76	15
1	3	3	1.762	1							
3	1	5	1.752	3	3	3	0	1.755	4		
					2	0	5	1.752	1		
					1	5	-3	1.752	2		
1	1	-7	1.745	17	3	3	-2	1.750	2		
4	2	2	1.744	5						1.73	10
4	0	-6	1.743	4							
4	2	-4	1.728	1	0	4	5	1.723	6		
5	1	-4	1.722	0							
0	2	6	1.721	6							
3	3	-1	1.717	20							
2	2	5	1.716	8							
3	3	0	1.711	5	2	4	-4	1.709	0		
2	2	-6	1.702	0	1	3	-6	1.703	7		
					3	3	1	1.703	4		
1	3	-4	1.699	6	2	2	-6	1.698	1		
5	1	2	1.694	4	0	0	7	1.696	0		
3	3	-2	1.691	3	3	1	3	1.694	0		
					3	3	-3	1.693	1		
					1	5	3	1.685	2		
					1	1	-7	1.683	1		
					2	4	3	1.680	1	1.68	25
3	3	1	1.674	3	3	1	-5	1.675	0		
					0	6	0	1.670	13		
					2	2	5	1.654	1		
					0	6	1	1.653	2		
1	1	7	1.646	4	1	5	-4	1.641	0		
1	3	4	1.645	0							
4	2	3	1.640	0							
3	3	-3	1.638	4							
3	1	-7	1.637	3							
6	0	-2	1.634	29						1.62	10
5	1	-5	1.623	4	3	3	2	1.623	0		
4	2	-5	1.622	0							
6	0	0	1.613	0							
3	3	2	1.612	1	3	3	-4	1.611	1		
					0	6	2	1.607	3		