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Table S6: Rietveld refinement data with substitution of Si on site 18 (polar) for B, site 18 (equatorial) for B, site 6 (chain end) for C and site 3 (chain center).

Site 18 (Polar): **R = 7.76%**

ID	Site	Occupancy	x	y	z	Biso
B	18	1	0.16104	0.83896	0.64095	1.33
B	18	0.9686	0.22337	0.77662	0.78065	1.53
Si	18	0.03	0.22337	0.77662	0.78065	0.5
C	6	1	0	0	0.6188	1.12
B	3	1	0	0	0.5	1.65

Site 18 (Equatorial): **R = 8.83%**

ID	Site	Occupancy	x	y	z	Biso
B	18	0.9686	0.16104	0.83896	0.64095	1.33
B	18	1	0.22337	0.77662	0.78065	1.53
Si	18	0.03	0.16104	0.83896	0.64095	0.5
C	6	1	0	0	0.6188	1.12
B	3	1	0	0	0.5	1.65

Site 6 (Chain end): **R = 7.18%**

ID	Site	Occupancy	x	y	z	Biso
B	18	1	0.16411	0.83589	0.64188	1.07
B	18	1	0.22414	0.77585	0.78574	1.47
Si	6	0.0337	0	0	0.61957	3.27
C	6	0.9686	0	0	0.61957	1.12
B	3	1	0	0	0.5	1.22

Site 3 (Chain center): **R = 7.35%**

ID	Site	Occupancy	x	y	z	Biso
B	18	1	0.16386	0.83614	0.64179	1.62
B	18	0.9686	0.22448	0.77551	0.78553	1.96
Si	3	0.03255	0	0	0.5	9.73
C	6	1	0	0	0.62113	0.73
B	3	0.968	0	0	0.5	1.22