Electronic Supplementary Information for Dalton Transactions

Supplementary information

Crystal structure and transport properties of $Ba_8Ge_{43}\square_3$

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Table S1: Interatomic distances for $Ba_8Ge_{43}\square_3$.

Atoms			*d* / Å (quenched)	*d* / Å (annealed)
Ba1	– Ge21	2 ×	3.3766(4)	3.3768(6)
	– Ge22	6 ×	3.3923(4)	3.3914(6)
	– Ge322	6 ×	3.48(1)	3.46(1)
	– Ge311	6 ×	3.4809(6)	3.482(1)
	– Ge321	6 ×	3.8165(7)	3.815(1)
	– Ge312	6 ×	3.85(1)	3.87(1)
Ba2	– Ge321	2 ×	3.4284(8)	3.432(1)
	– Ge312	2 ×	3.466(9)	3.46(1)
	– Ge322	2 ×	3.50(1)	3.52(1)
	– Ge321	2 ×	3.5122(8)	3.511(1)
	– Ge311	2 ×	3.5546(7)	3.555(1)
	– Ge312	2 ×	3.557(9)	3.54(1)
	– Ge322	2 ×	3.59(1)	3.59(1)
	– Ge311	2 ×	3.6306(7)	3.626(1)
	– Ge12	2 ×	3.7304(3)	3.7328(5)
	– Ge11	2 ×	3.8041(3)	3.8012(5)
	– Ge21	2 ×	3.8946(6)	3.899(1)
	– Ge11	2 ×	3.8041(3)	3.930(1)
	– Ge22	2 ×	3.9285(6)	3.9285(6)
	– Ge22	2 ×	3.9296(6)	3.931(1)
	– Ge321	2 ×	3.9819(8)	3.986(1)
	– Ge312	2 ×	4.06(1)	4.06(1)
	– Ge22	2 ×	4.0932(6)	4.085(1)
Ge11	– Ge312	4 ×	2.14(1)	2.13(1)
	– Ge311	4 ×	2.5264(6)	2.5250(9)
Ge12	– Ge321	4 ×	2.1818(6)	2.183(1)
	– Ge322	4 ×	2.54(1)	2.55(1)
Ge21	– Ge322	3 ×	2.46(1)	2.46(1)
	– Ge21	1 ×	2.4736(6)	2.4726(9)
	– Ge321	3 ×	2.5697(9)	2.569(1)
Ge22	– Ge322	1 ×	2.44(1)	2.42(1)
	– Ge22	1 ×	2.4439(6)	2.4449(9)
	– Ge311	1 ×	2.5055(8)	2.504(1)
	– Ge311	1 ×	2.5095(8)	2.507(1)
	– Ge321	1 ×	2.5358(9)	2.538(1)
	– Ge312	1 ×	2.63(1)	2.63(1)
	– Ge312	1 ×	2.64(1)	2.64(1)
Ge311	– Ge322	1 ×	2.38(1)	2.38(1)
	– Ge22	1 ×	2.5055(8)	2.504(1)
	– Ge22	1 ×	2.5095(8)	2.507(1)
	– Ge11	1 ×	2.5264(6)	2.5250(9)
	– Ge11	1 ×	2.6099(9)	2.609(1)
Ge312	– Ge11	1 ×	2.14(1)	2.13(1)
	– Ge322	1 ×	2.62(1)	2.63(2)
	– Ge22	1 ×	2.63(1)	2.63(1)
	– Ge22	1 ×	2.64(1)	2.64(1)

	– Ge321	1 ×	2.82(1)	2.82(1)
Ge321	– Ge12	1 ×	2.1818(8)	2.183(1)
	– Ge22	1 ×	2.5358(8)	2.538(1)
	– Ge21	1 ×	2.5696(9)	2.569(1)
	– Ge311	1 ×	2.6099(9)	2.609(1)
	– Ge312	1 ×	2.82(1)	2.82(1)
Ge322	– Ge311	1 ×	2.38(1)	2.38(1)
	– Ge22	1 ×	2.44(1)	2.42(1)
	– Ge21	1 ×	2.46(1)	2.46(1)
	– Ge12	1 ×	2.54(1)	2.55(1)
	– Ge312	1 ×	2.62(1)	2.63(1)