

Synthesis and crystal and defect structures of polycrystalline Cu₂SrSnS₄ and Cu_{1.9}SrSnS₄ powders

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Table S1 Full Raman spectrum of Cu₂SrSnS₄

Cu ₂ SrSnS ₄					
This paper		Cu ₂ SrSnS ₄ in ^{S1}			
Raman shift, cm ⁻¹	I, a.u.	Raman shift, cm ⁻¹ , exp.	Raman shift, cm ⁻¹ , theor.	I, a.u., theor.	Symmetry, theor.
66	1035	66	41.6 47.3 53.5 58.7 69.4 70.3	45 46 402 0.2 3004 558	A E A A E E
76	730	-	71.2 73.2 77.7	603 83 2914	A E A
82	690	81	82.4 82.5 87.1 90.4	730 443 854 16	A E E A
98	780	98	92.9 93.4 100.3 111.4 116.6	544 2 236 1431 1001	E A E A E
128	815	128	120.8 128.8 141.7 141.9	17 341 15 151	A E A E
158	725	158	154.9 156.2 164.5 164.8 170.2 176.0	1536 341 1185 604 128 4051	E A A E A E
186	925	179 194	184.8 184.9	3307 4145	A E

275	1205	273	273.2 275.7 279.7	2 3651 298577	A E A
-		285	281.1 283.9 285.6	600 4114 1676	E E A
-		308	310.4 317.3	1325 2807	E A
346	6005	347	317.8 323.5	826363 9492	A E
366	1470	364	340.4 341.1	59354 580	E A
379	1586	377	352.9 353.1 355.2 365.2	15172 7146 26 9773	A E A E
414	1000	410	n/a	n/a	n/a
-	-	464	n/a	n/a	n/a
631	1205	n/a	n/a	n/a	n/a
694	1470	n/a	n/a	n/a	n/a

Table 2 Raman spectra of $\text{Cu}_{1.9}\text{SrSnS}_4$ powder

$\text{Cu}_{1.9}\text{SrSnS}_4$					
This paper		$\text{Cu}_2\text{SrSnS}_4$ in ^{S1}			
Raman shift, cm^{-1}	I, a.u.	Raman shift, cm^{-1}, exp.	Raman shift, cm^{-1}, theor.	I, a.u., theor ⁹	Symmetry, theor.
66	1205	66	41.6 47.3 53.5 58.7 69.4 70.3	45 46 402 0.2 3004 558	A E A A E E
76	960	-	71.2 73.2 77.7	603 83 2914	A E A
82	945	81	82.4 82.5 87.1 90.4	730 443 854 16	A E E A
98	975	98	92.9 93.4 100.3 111.4 116.6	544 2 236 1431 1001	E A E A E

128	1020	128	120.8 128.8 141.7 141.9	17 341 15 151	A E A E
158	960	158	154.9 156.2 164.5 164.8 170.2 176.0	1536 341 1185 604 128 4051	E A A E A E
185	1370	179 194	184.8 184.9	3307 4145	A E
275	1515	273	273.2 275.7 279.7	2 3651 298577	A E A
-		285	281.1 283.9 285.6	600 4114 1676	E E A
-		308	310.4 317.3	1325 2805	E A
345.5	8011	347	317.8 323.5	826363 9492	A E
364	1890	364	340.4 341.1	59354 580	E A
379	2280	377	352.9 353.1 355.2 365.2	15172 7146 26 9773	A E A E
414	1310	410	n/a	n/a	n/a
-	-	464	n/a	n/a	n/a
628.5	1655	n/a	n/a	n/a	n/a
694	2040	n/a	n/a	n/a	n/a

References

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