An Insight into Local environment of lanthanide ions in Sr_2SiO_4:Ln (Ln=Sm, Eu and Dy)

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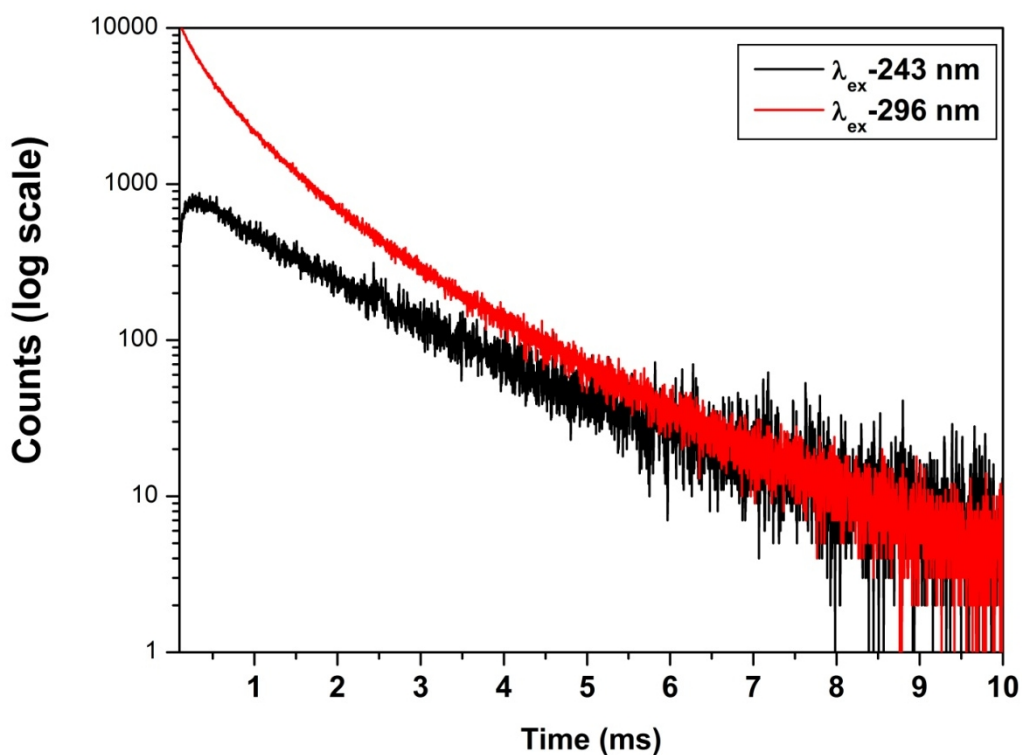
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Fig. S1: Luminescence decay time profile of Eu^{3+} doped Sr_2SiO_4 with λ_{ex}-243 and 296 nm respectively.
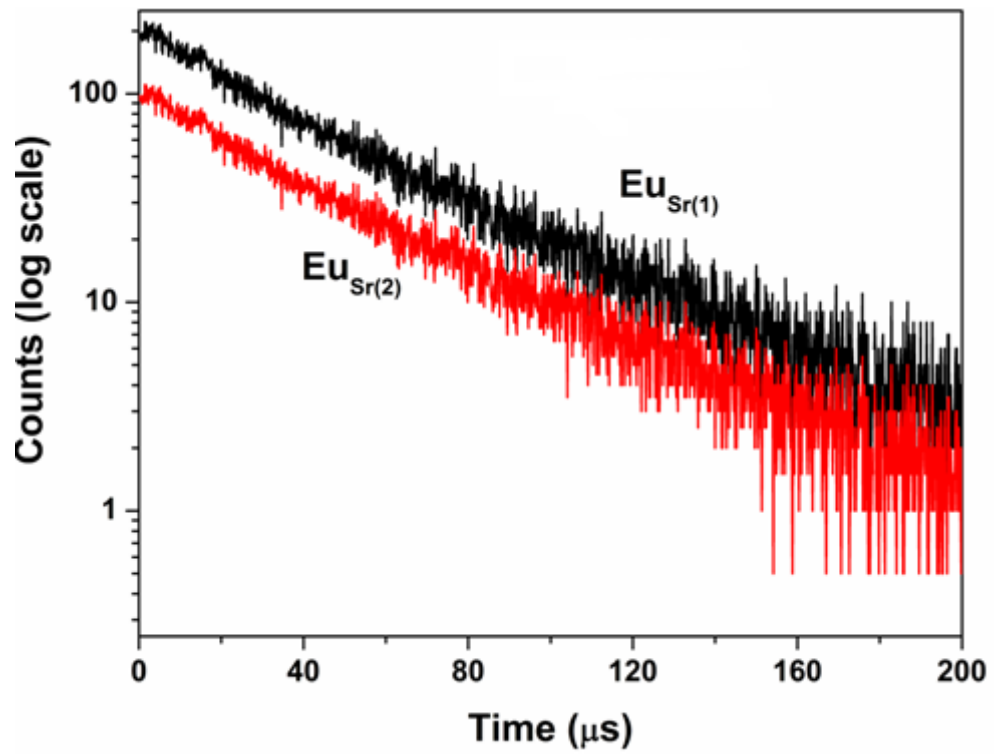
Fig. S2: Luminescence decay time profile of Sr_2SiO_4:Eu^{2+} with λ_{ex}-340 nm under λ_{em} − 490 and 560 nm
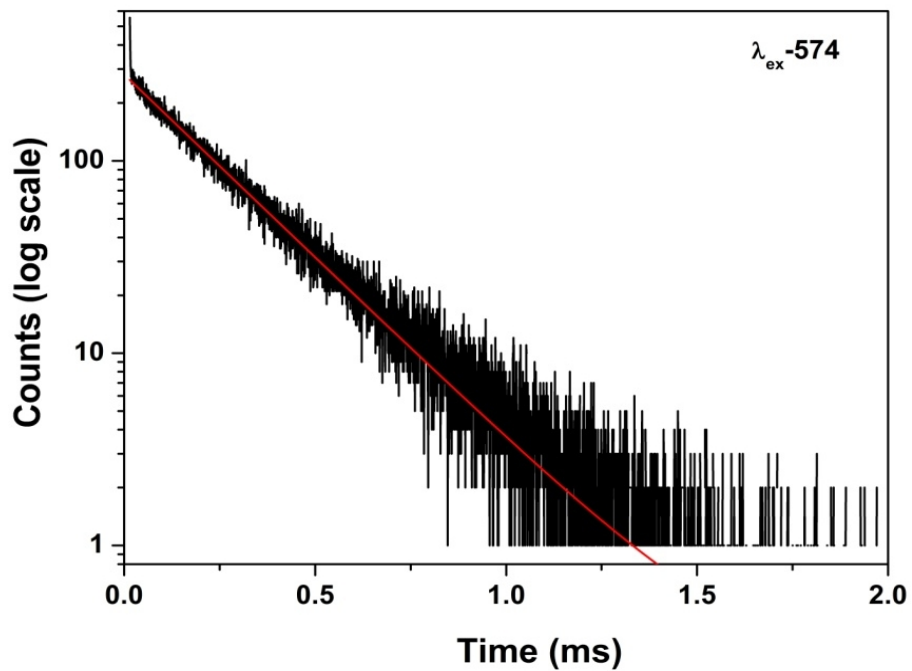

Fig. S3: PL decay curve for the Sr_2SiO_4:Dy^{3+} sample. Black curve is experimentally observed decay and the red one is exponentially fit one.
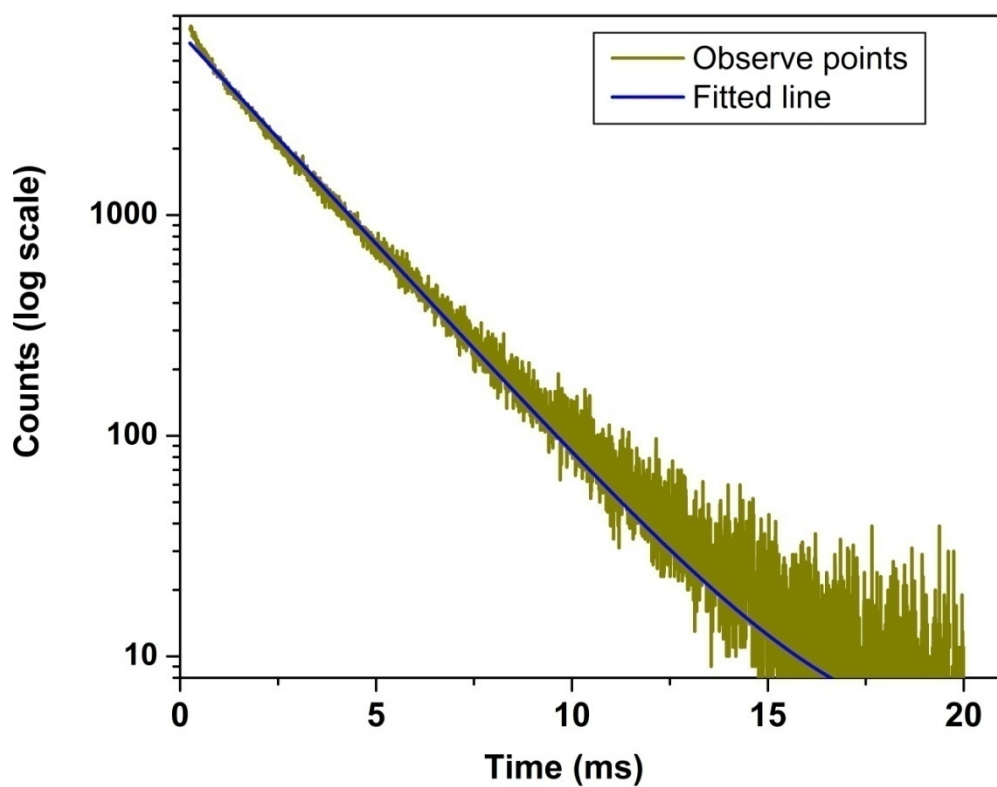
Fig. S4: PL decay curve for the Sr$_2$SiO$_4$:Sm^{3+} sample. Brown curve is experimentally observed decay and the blue one is exponentially fitted.
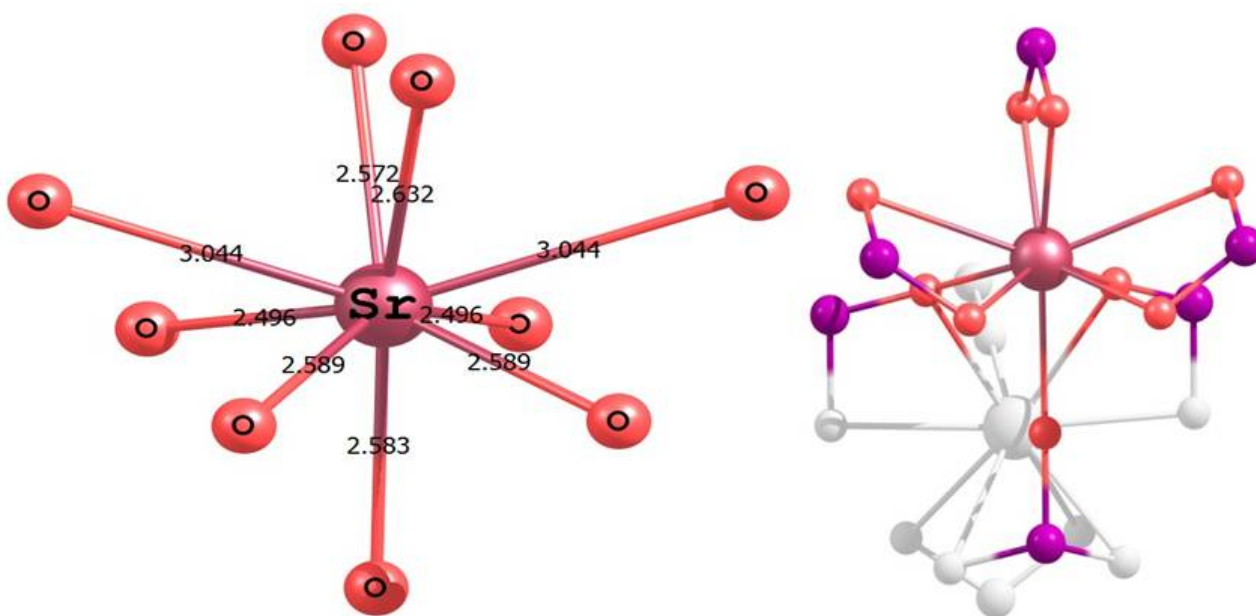
Fig. S5: Various Sr-O bond lengths in SrO_9 polyhedra and their linkage in $\alpha'Sr_2SiO_4$

Shortest bond: 2.50 Å, largest bond: 3.04 Å, Average Sr-O bond length: 2.68 Å, Experimental value: 2.70 Å
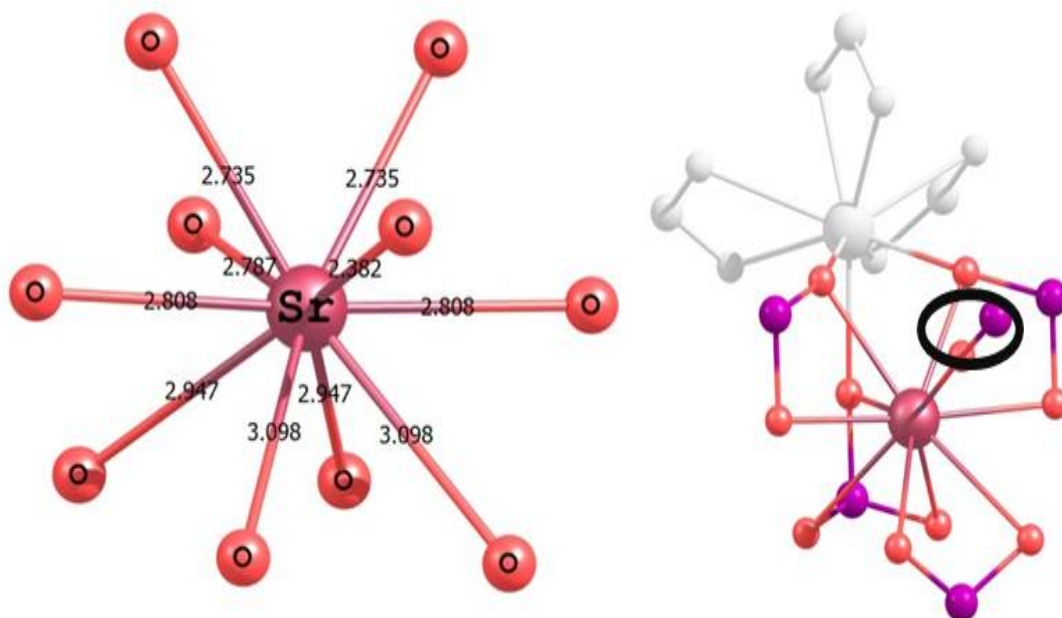
Fig. S6: Various Sr-O bond lengths in SrO_{10} polyhedra and their linkage in $\alpha'Sr_2SiO_4$

Shortest bond: 2.38 Å, largest bond: 3.10 Å, Average Sr-O bond length: 2.84 Å, Experimental value: 2.85 Å

Fig. S7: Eu incorporation at SrO$_{10}$ polyhedra

Fig. S8: Sm incorporation at SrO$_{10}$ polyhedra

Fig. S9: Dy incorporation at SrO$_{10}$ polyhedra

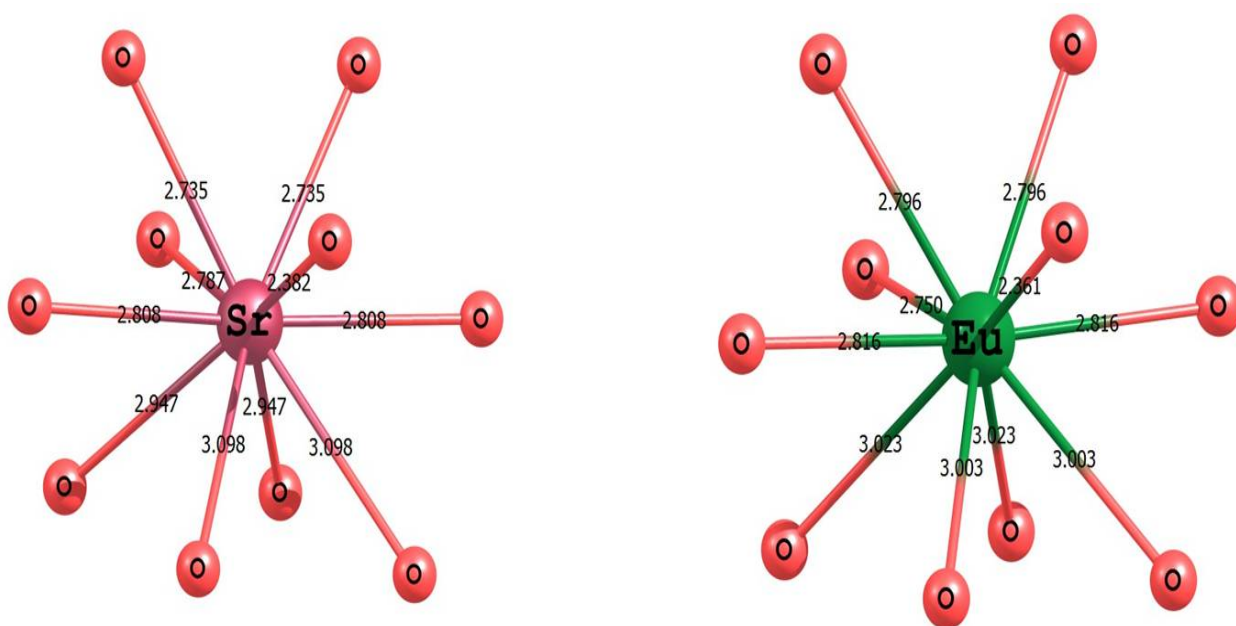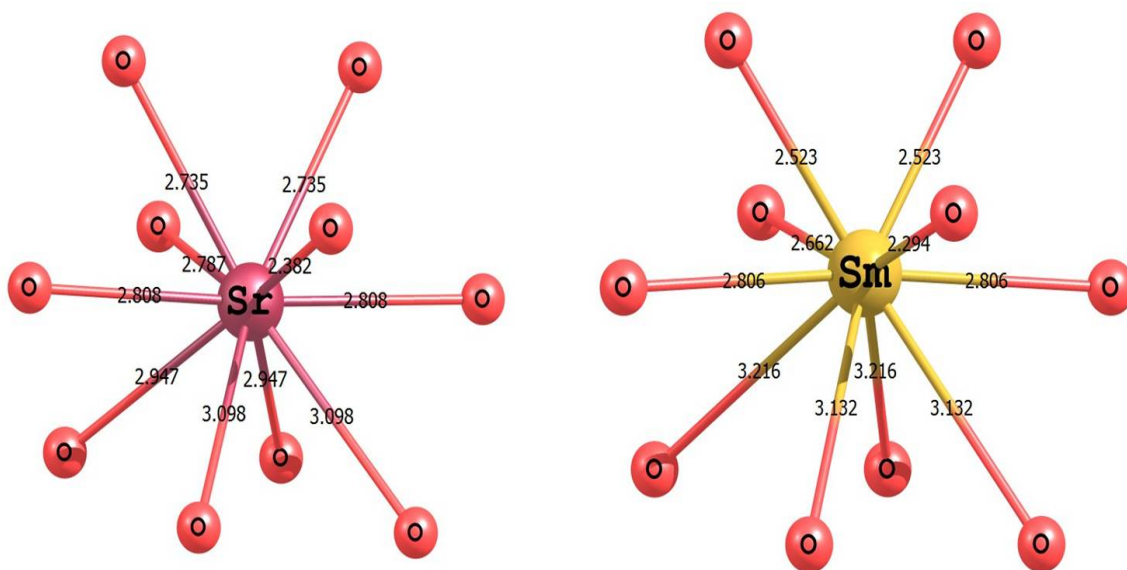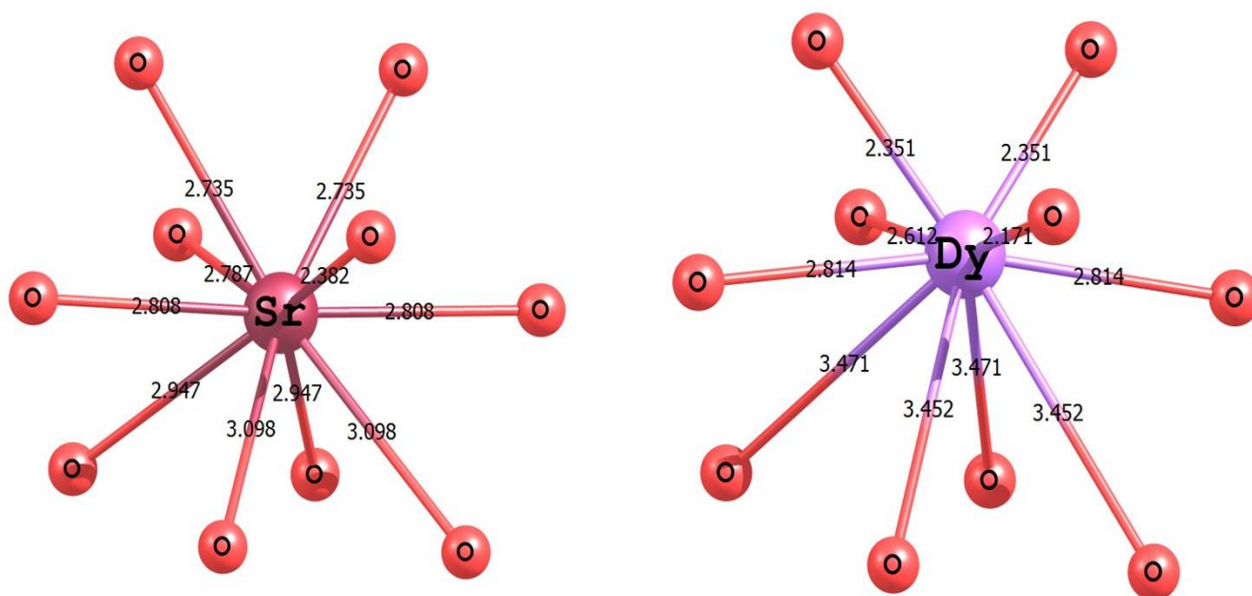**Table T1: XRD data of strontium silicate (λ= 0.15406 nm)**

2θ	d value (Å)	I/I₀	h k l
27.198	3.2760	39	1 1 2
29.736	3.0020	24	2 1 0
30.241	2.9530	17	1 0 3
31.137	2.8700	100	2 1 1
31.204	2.8640	30	2 0 2
31.52	2.8360	76	0 2 0
31.738	2.8170	92	0 1 3
37.554	2.3930	24	2 0 3
38.85	2.3161	25	1 2 2
39.077	2.3032	25	1 0 4
39.249	2.2935	44	3 0 1
42.32	2.1339	19	1 1 4
44.252	2.0451	20	1 2 3
45.136	2.0071	23	2 0 4
48.413	1.8786	18	1 0 5
49.849	1.8278	22	2 2 3
51.191	1.7830	26	1 1 5
55.157	1.6638	28	4 1 1
56.281	1.6332	21	0 3 3
56.659	1.6232	35	3 1 4

Table T2: Procedure data slicing in TRES

❖ Supposing there are two components A (short lived) and B (long lived), first we record the composite spectrum (A+B) with very short delay (just to avoid the lamp profile).

❖ Then give sufficient delay and record with identical integration times so that there is only B component in the spectrum (let's say B'; A is already decayed).

❖ But the intensity of the B' which we would get is not the same as the original B in the composite spectrum (A+B).

❖ So we multiply a suitable multiplying factor (exp factor, $e^{-t/\tau}$) so as to get the original intensity of B.

- ❖ Then if we subtract this B from the composite spectrum (A+B), it is possible to get the short lived component A.

- ❖ One has to maintain however same gate widths while dealing with this type of procedure.

Table T3: Structural parameters obtained from EXAFS fitting.

	Parameter	Sr_2SiO_4	Sr_2SiO_4:Dy	Sr_2SiO_4:Eu	Sr_2SiO_4:Sm
Sr(1)-O	R (Å) (2.38)	2.45	2.45	2.38	2.41
	N (1)	1*0.5	1*0.5	1*0.5	1*0.5
	σ^2	0.001	0.001	0.002	0.001
Sr(2)-O	R (Å) (2.51)	2.58	2.46	2.55	2.57
	N (2)	2*0.5	2*0.5	2*0.5	2*0.5
	σ^2	0.001	0.001	0.002	0.003
Sr(2)-O	R (Å) (2.60)	2.58	2.56	2.57	2.58
	N (5)	5*0.5	5*0.5	5*0.5	5*0.5
	σ^2	0.001	0.001	0.007	0.001
Sr(1)-O	R (Å) (2.85)	2.85	2.86	2.84	2.84
	N (5)	5*0.5	5*0.5	5*0.5	5*0.5
	σ^2	0.001	0.001	0.004	0.001
Sr(1)-O	R (Å) (3.07)	3.07	3.08	3.07	3.00
	N (4)	4*0.5	4*0.5	4*0.5	4*0.5
	σ^2	0.001	0.001	0.0044	0.001
Sr(2)-O	R (Å) (3.11)	3.07	3.08	3.07	2.78
	N (2)	2*0.5	2*0.5	2*0.5	2*0.5
	σ^2	0.001	0.001	0.006	0.004

Sr-Si	R (Å) (3.33)	3.14	3.14	3.15	3.06
	N (4)	4*0.689	4*0.8	4*0.76	4*0.68
	σ^2	0.01	0.017	0.013	0.01
Average Sr(1)-O (10 Coordinated)		2.90	2.91	2.90	2.86
Average Sr(2)-O (9 Coordinated)		2.69	2.65	2.68	2.62

Table T4: Energetics for various lanthanides in Sr_2SiO_4 for two different sites of Sr

	Total Energy (eV)		
M= Sm/Dy/Eu	Sm	Dy	Eu
M at9-coordinated Site	-200.64246	-200.65750	-207.56386
M at10-coordinated Site	-200.06394	-199.93745	-207.53293
Relative stability $\Delta E(10-9)$	0.57852	0.72005	0.03093

Table T5: Point symmetry and local structure around Eu ion in SrO_9 and SrO_{10}

SrO_9	SrO_{10}
symmetry: C_{2V}	symmetry: C_{3V}
Distorted local environment	A site distorted from perfect O_h symmetry, will be a D_3 or C_{3v}.