

Experimental and Theoretical Infrared Signatures of REMO_3 (RE = La, Pr, Nd, Sm and M = Co, Fe) Perovskites

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Table S1: Calculated wavenumbers (cm⁻¹), IR intensities (km.mol⁻¹) and symmetry of IR active normal modes for ReMO₃ systems.

N°	LaFeO3			PrFeO3			NdFeO3			SmFeO3			LaCoO3			PrCoO3			NdCoO3			SmCoO3		
	v	Sym	I	v	Sym	I	v	Sym	I	v	Sym	I	v	Sym	I	v	Sym	I	v	Sym	I	v	Sym	I
1	120	Bu	27	114	Bu	28	114	Bu	31	110	Au	27	193	A2u	399	140	B1u	17	140	B1u	21	140	B1u	27
2	133	Au	71	116	Au	39	115	Au	38	113	Bu	34	202	Eu	581	154	B2u	115	153	B2u	124	145	B2u	109
3	178	Au	1375	176	Bu	77	176	Bu	74	174	Bu	6	273	Eu	273	187	B2u	902	188	B2u	868	195	B2u	714
4	186	Bu	149	180	Bu	1040	179	Bu	1030	177	Bu	917	320	A2u	1455	195	B3u	736	195	B3u	738	197	B3u	743
5	191	Bu	917	187	Bu	800	187	Bu	784	186	Bu	776	352	Eu	3426	204	B1u	691	203	B1u	683	201	B1u	698
6	201	Bu	613	191	Au	774	192	Au	702	198	Au	339	426	Eu	360	222	B3u	2	222	B3u	2	222	B3u	0
7	256	Au	59	244	Au	1305	245	Au	1402	244	Au	2018	548	A2u	1946	268	B2u	78	271	B2u	92	289	B2u	6
8	259	Bu	8	259	Bu	3317	260	Bu	3326	259	Bu	3397	557	Eu	3380	275	B1u	38	278	B1u	46	292	B2u	251
9	271	Au	1435	268	Bu	2782	269	Bu	2733	274	Bu	2199				287	B2u	71	288	B2u	83	298	B1u	126
10	280	Bu	3576	269	Au	2027	272	Au	2004	282	Au	1619				324	B1u	1345	323	B1u	1238	330	B1u	682
11	288	Bu	3407	273	Bu	232	274	Bu	234	284	Bu	246				334	B3u	1168	334	B3u	1173	343	B3u	1008
12	302	Au	2418	303	Au	1838	305	Au	1825	310	Au	1910				343	B2u	2093	346	B2u	1942	354	B2u	152
13	315	Bu	705	315	Bu	538	316	Bu	426	317	Bu	146				354	B2u	36	355	B2u	133	373	B1u	557
14	328	Au	57	326	Au	2	327	Au	4	327	Bu	26				372	B3u	712	373	B1u	844	376	B3u	327
15	341	Bu	343	328	Bu	90	328	Bu	100	334	Au	4				373	B1u	851	374	B3u	663	377	B2u	1599
16	351	Bu	1829	335	Bu	1622	337	Bu	1766	346	Bu	2539				404	B1u	4	406	B1u	2	415	B1u	0
17	352	Bu	361	350	Bu	1294	351	Bu	1198	357	Bu	739				437	B1u	215	442	B1u	205	486	B1u	117
18	367	Bu	4	370	Bu	1034	373	Bu	1081	390	Bu	1386				445	B3u	760	449	B3u	784	489	B3u	888
19	427	Bu	0	422	Au	216	423	Au	231	424	Au	342				468	B1u	1707	469	B1u	1737	498	B1u	2110
20	442	Au	55	440	Bu	2	443	Bu	2	464	Bu	6				488	B2u	81	489	B2u	91	507	B2u	196
21	553	Au	184	518	Bu	43	518	Bu	43	512	Bu	51				534	B2u	124	536	B2u	155	556	B3u	582
22	559	Bu	47	529	Au	862	530	Au	873	530	Au	807				547	B3u	656	548	B3u	734	559	B2u	2634
23	572	Bu	1157	544	Au	132	545	Au	94	550	Bu	902				549	B2u	3447	550	B2u	3395	566	B2u	573
24	572	Au	1202	546	Bu	963	548	Bu	971	554	Au	0				556	B3u	2606	558	B3u	2519	567	B3u	2500
25	598	Bu	1024	563	Bu	608	562	Bu	594	561	Bu	479				565	B1u	2588	566	B1u	2588	576	B1u	2135

Although being indexed in Pnma space group (n° 62), to model the spin ordering in ReFeO₃ systems, the symmetry of these compounds has been reduced to P2₁/c (n°14) for the calculation of their vibrational properties. The number of active modes is then increased to 33 with the irreducible representation: $\Gamma = 17 A_u + 16 B_u$. However, since the structure remains very close to the one in Pnma only 25 of those modes possess non null IR intensities (> 0.1 km.mol⁻¹). These 25 modes have been reported in the table to ease the comparison with the other compounds although some of them display very small IR intensities. LaCoO₃ is indexed in R $\bar{3}$ c space group (n°167) with the irreducible representation: $\Gamma = 3 A_{2u} + 5 E_u$.

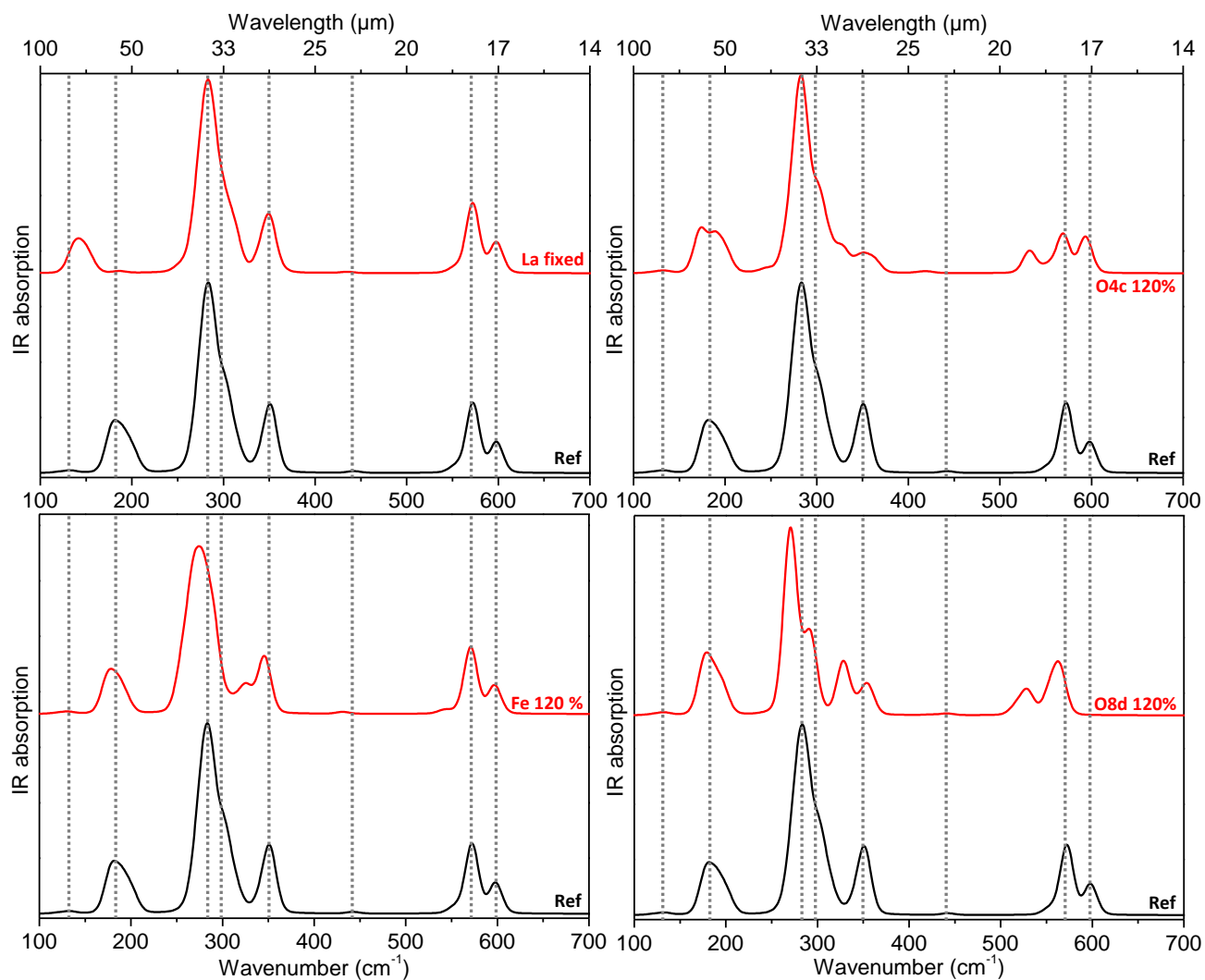


Figure S1.: Influence of isotopic substitution on the simulated IR spectrum of LaFeO_3 . Each panel corresponds to a particular isotopic substitution, where the atomic mass of the considered element is increased by 20% (except for La, which mass is fixed at 10 000 u, in order to remove all coupling with other modes and thus reveal its participation in those modes). The IR spectrum is then reconstructed from the same Hessian matrix than the former calculation.