Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

V. SUPPLEMENTARY MATERIAL

TABLE VI: Energy levels (cm^{-1}) of the $4f$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1\ 1\Gamma_5$ ground state, as calculated for the $(CeO_8)^{13-}$ clusters embedded in a common cubic confinement potential.

	Garnet	$4f_2\ 2\Gamma_5$	$4f_3\ 3\Gamma_5$	$4f_4\ 4\Gamma_5$	$4f_5\ 5\Gamma_5$	$4f_6\ 6\Gamma_5$	$4f_7\ 7\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	378	1068	2284	2527	2751	5879
			$A_3B'_2Si_3O_{12}$ garnets				
2	Pyrope	279	1029	2270	2438	2639	6063
3	Almandine	348	1079	2290	2491	2725	6003
4	Spessartine	401	1120	2306	2526	2804	5920
5	Grossular	486	1179	2334	2560	2968	5691
6	Andradite	498	1205	2327	2558	3029	5678
7	$Ca_3Sc_2Si_3O_{12}$	564	1288	2331	2614	3135	5701
			$A_3Al_5O_{12}$ garnets				
8	LuAG	82	863	2191	2286	2500	5788
9	YbAG	93	870	2212	2287	2508	5744
10	ErAG	127	876	2266	2293	2519	5637
11	YAG	144	899	2284	2301	2537	5654
12	GdAG	144	867	2290	2309	2517	5539
			$A_3Ga_5O_{12}$ garnets				
13	LuGG	331	1043	2123	2544	2734	5920
14	YbGG	233	1000	2142	2448	2679	5849
15	YGG	204	919	2159	2434	2601	5648
16	HoGG	193	916	2160	2422	2596	5657
17	DyGG	178	895	2165	2410	2575	5615
18	TbGG	169	873	2171	2406	2555	5559
19	GdGG	137	841	2186	2374	2522	5489
20	SmGG	126	840	2209	2356	2523	5421
21	NdGG	118	818	2235	2342	2502	5337

TABLE VII: Energy levels (cm^{-1}) of the $4f$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1$ $1\Gamma_5$ ground state, as calculated for the $(CeO_8)^{13-}$ clusters embedded in the embedding potentials of the undistorted garnets. Available experimental data are shown in parentheses.

	Garnet	$4f_2$ $2\Gamma_5$	$4f_3$ $3\Gamma_5$	$4f_4$ $4\Gamma_5$	$4f_5$ $5\Gamma_5$	$4f_6$ $6\Gamma_5$	$4f_7$ $7\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	413	744	2302	2433	2738	4391
			$A_3B'_2Si_3O_{12}$ garnets				
2	Pyrope	419	837	2166	2613	2662	5002
3	Almandine	330	760	2192	2534	2560	4782
4	Spessartine	260	692	2220	2440	2513	4574
5	Grossular	319	644	2325	2364	2597	4244
6	Andradite	383	702	2310	2404	2719	4227
7	$Ca_3Sc_2Si_3O_{12}$	440	785	2282	2457	2841	4199
			$A_3Al_5O_{12}$ garnets				
8	LuAG	269	809	2246	2362	2634	4710
9	YbAG	267	790	2264	2346	2625	4643
10	ErAG	293	764	2270	2377	2624	4511
11	YAG	300	754	2266	2387	2615	4508
12	GdAG	323	748	2268	2421	2634	4394
			$A_3Ga_5O_{12}$ garnets				
13	LuGG	547	1068	2151	2759	2889	4798
14	YbGG	448	972	2156	2654	2794	4691
15	YGG	347	880	2188	2545	2722	4478
16	HoGG	344	878	2187	2543	2719	4491
17	DyGG	325	859	2194	2521	2706	4442
18	TbGG	300	833	2206	2493	2686	4386
19	GdGG	268	792	2222	2451	2655	4296
		(198)[a]		(2145)[a]	(2245)[a]	(2403)[a]	(3639)[a]
20	SmGG	235	746	2238	2408	2621	4192
21	NdGG	222	710	2267	2377	2600	4098

[a]Reference 46.

TABLE VIII: Unrelaxed host effect (cm^{-1}) on the energy levels of the $4f$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1$ $1\Gamma_5$ ground state.

	Garnet	$4f_2$ $2\Gamma_5$	$4f_3$ $3\Gamma_5$	$4f_4$ $4\Gamma_5$	$4f_5$ $5\Gamma_5$	$4f_6$ $6\Gamma_5$	$4f_7$ $7\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	35	-324	18	-94	-13	-1488
			$A_3B'_2Si_3O_{12}$ garnets				
2	Pyrope	140	-192	-104	175	23	-1061
3	Almandine	-19	-320	-98	43	-16	-1221
4	Spessartine	-141	-427	-86	-86	-291	-1346
5	Grossular	-166	-535	-9	-196	-371	-1447
6	Andradite	-115	-503	-17	-154	-311	-1450
7	$Ca_3Sc_2Si_3O_{12}$	-124	-504	-49	-157	-294	-1503
			$A_3Al_5O_{12}$ garnets				
8	LuAG	187	-54	56	75	134	-1078
9	YbAG	174	-80	52	59	116	-1101
10	ErAG	166	-112	4	83	105	-1126
11	YAG	156	-144	-18	86	78	-1147
12	GdAG	179	-119	-21	111	117	-1144
			$A_3Ga_5O_{12}$ garnets				
13	LuGG	216	25	28	215	155	-1122
14	YbGG	215	-28	14	207	116	-1158
15	YGG	142	-40	29	111	121	-1170
16	HoGG	151	-38	27	120	123	-1166
17	DyGG	147	-37	29	111	130	-1173
18	TbGG	131	-40	35	87	131	-1173
19	GdGG	131	-49	36	77	133	-1193
20	SmGG	109	-94	29	52	98	-1229
21	NdGG	104	-108	32	35	97	-1239

TABLE IX: Energy levels (cm^{-1}) of the $5d$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1$ $1\Gamma_5$ ground state, as calculated for the $(CeO_8)^{13-}$ clusters embedded in a common cubic confinement potential.

	Garnet	$5d_1$ $8\Gamma_5$	$5d_2$ $9\Gamma_5$	$5d_3$ $10\Gamma_5$	$5d_4$ $11\Gamma_5$	$5d_5$ $12\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	25236	29997	50986	55722	58664
			$A_3B'_2Si_3O_{12}$ garnets			
2	Pyrope	22745	28568	53621	57241	62112
3	Almandine	23381	29271	52591	56896	61093
4	Spessartine	24101	29971	51555	56311	59944
5	Grossular	25666	31415	49381	54856	56797
6	Andradite	26214	31578	48631	54623	55831
7	$Ca_3Sc_2Si_3O_{12}$	26577	31864	47324	54060	55230
			$A_3Al_5O_{12}$ garnets			
8	LuAG	24913	28703	53752	54519	60223
9	YbAG	25144	28972	53407	54159	59868
10	ErAG	25711	29589	52616	53501	58751
11	YAG	25680	29676	52354	53556	58900
12	GdAG	26340	30079	51856	52921	57584
			$A_3Ga_5O_{12}$ garnets			
13	LuGG	25871	28446	51957	55223	60529
14	YbGG	25862	28712	52109	54184	60555
15	YGG	26636	29395	51597	53536	58468
16	HoGG	26607	29357	51691	53516	58589
17	DyGG	26741	29497	51621	53319	58177
18	TbGG	26981	29683	51427	53074	57567
19	GdGG	27174	29929	51299	52590	56963
20	SmGG	27414	30257	50875	51806	56496
21	NdGG	27723	30588	50458	51196	55568

TABLE X: Energy levels (cm^{-1}) of the $5d$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1$ $1\Gamma_5$ ground state, as calculated for the $(CeO_8)^{13-}$ clusters embedded in the embedding potentials of the undistorted garnets. Available experimental data are shown in parentheses.

	Garnet	$5d_1$ $8\Gamma_5$	$5d_2$ $9\Gamma_5$	$5d_3$ $10\Gamma_5$	$5d_4$ $11\Gamma_5$	$5d_5$ $12\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	21719	31112	49946	52451	54904
		$(21300)^a$	$(32800)^a$			
			$A_3B'_2Si_3O_{12}$ garnets			
2	Pyrope	22210	27952	52449	53309	58981
3	Almandine	22365	28626	51426	52392	57051
4	Spessartine	22710	29365	50405	51712	55932
5	Grossular	23873	31573	48378	51170	53217
6	Andradite	24092	31972	47693	51680	52861
7	$Ca_3Sc_2Si_3O_{12}$	24367	32349	46374	51516	52591
		$(22200)^b$				
			$A_3Al_5O_{12}$ garnets			
8	LuAG	22102	27807	50006	52423	54540
		$(22470)^c$	$(29410)^c$			
		$(21138)^d$	$(28233)^d$			
9	YbAG	22249	28199	49827	51966	54241
10	ErAG	22493	29052	49522	51114	53550
11	YAG	22523	29242	49673	50906	53835
		$(22000)^e$	$(29400)^e$	$(44000)^e$		
		$(20440)^f$	$(28800)^f$			
12	GdAG	23001	29789	49399	50540	53063
			$A_3Ga_5O_{12}$ garnets			
13	LuGG	24112	26367	47788	53183	54404
14	YbGG	24102	26852	47979	52367	54293
15	YGG	24446	27883	47786	51804	53308
		$(23800)^e$	$(28100)^e$			
16	HoGG	24416	27863	48023	51882	53519
17	DyGG	24497	28068	47926	51674	53149
18	TbGG	24627	28390	47975	51513	52969
19	GdGG	24773	28779	47872	51037	52421
		$(23500)^g$	$(28700)^g$			
20	SmGG	24977	29332	47690	50359	52105
21	NdGG	25145	29956	47656	49829	51643

[a] Reference 9, excitation band maximum.
[b] Reference 10, excitation band maximum.
[c] Reference 54, excitation band maximum.
[d] Reference 54, zero-phonon line.
[e] Reference 1, excitation band maximum.
[f] Reference 8, zero-phonon line.
[g] Reference 46, excitation band maximum.

TABLE XI: Energy levels (cm^{-1}) of the $5d$ configuration of Ce^{3+} in 21 selected garnets referred to the $5d_1$ $8\Gamma_5$ state, as calculated for the $(CeO_8)^{13-}$ clusters embedded in the embedding potentials of the undistorted garnets. Available experimental data are shown in parentheses.

	Garnet	$5d_1$ $8\Gamma_5$	$5d_2$ $9\Gamma_5$	$5d_3$ $10\Gamma_5$	$5d_4$ $11\Gamma_5$	$5d_5$ $12\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	0	9393	28227	30732	33185
			(11500)[a]			
			$A_3B'_2Si_3O_{12}$ garnets			
2	Pyrope	0	5742	30239	31098	36771
3	Almandine	0	6261	29061	30027	34685
4	Spessartine	0	6655	27695	29002	33223
5	Grossular	0	7700	24505	27297	29344
6	Andradite	0	7880	23602	27588	28770
7	$Ca_3Sc_2Si_3O_{12}$	0	7982	22007	27149	28224
			$A_3Al_5O_{12}$ garnets			
8	LuAG	0	5704	27904	30321	32438
			(6940)[b]			
			(7100)[c]			
9	YbAG	0	5950	27578	29716	31991
10	ErAG	0	6559	27029	28621	31057
11	YAG	0	6718	27150	28383	31312
			(7470)[d]	(22000)[d]		
			(8360)[e]			
12	GdAG	0	6788	26398	27539	30062
			$A_3Ga_5O_{12}$ garnets			
13	LuGG	0	2256	23676	29071	30292
14	YbGG	0	2750	23877	28265	30192
15	YGG	0	3437	23340	27358	28862
			(4300)[d]			
16	HoGG	0	3447	23608	27467	29103
17	DyGG	0	3571	23429	27177	28653
18	TbGG	0	3763	23348	26886	28342
19	GdGG	0	4007	23099	26264	27648
			(5200)[f]			
20	SmGG	0	4356	22713	25383	27129
21	NdGG	0	4811	22511	24685	26498

[a] Reference 9, excitation band maximum.
[b] Reference 54, excitation band maximum.
[c] Reference 54, zero-phonon line.
[d] Reference 1, excitation band maximum.
[e] Reference 8, zero-phonon line.
[f] Reference 46, excitation band maximum.

TABLE XII: Unrelaxed host effect (cm^{-1}) on the energy levels of the $5d$ configuration of Ce^{3+} in 21 selected garnets referred to the $4f_1$ $1\Gamma_5$ ground state.

	Garnet	$5d_1$ $8\Gamma_5$	$5d_2$ $9\Gamma_5$	$5d_3$ $10\Gamma_5$	$5d_4$ $11\Gamma_5$	$5d_5$ $12\Gamma_5$
1	$Lu_2CaMg_2Si_3O_{12}$	-3517	1115	-1040	-3271	-3760
			$A_3B'_2Si_3O_{12}$ garnets			
2	Pyrope	-534	-616	-1173	-3932	-3131
3	Almandine	-1016	-645	-1164	-4504	-4042
4	Spessartine	-1392	-607	-1151	-4599	-4012
5	Grossular	-1792	158	-1003	-3686	-3579
6	Andradite	-2122	395	-938	-2944	-2970
7	$Ca_3Sc_2Si_3O_{12}$	-2210	485	-950	-2544	-2639
			$A_3Al_5O_{12}$ garnets			
8	LuAG	-2811	-896	-3746	-2096	-5682
9	YbAG	-2895	-773	-3579	-2193	-5627
10	ErAG	-3218	-537	-3093	-2387	-5201
11	YAG	-3157	-435	-2681	-2650	-5065
12	GdAG	-3339	-290	-2457	-2380	-4521
			$A_3Ga_5O_{12}$ garnets			
13	LuGG	-1759	-2078	-4169	-2040	-6125
14	YbGG	-1760	-1861	-4130	-1817	-6262
15	YGG	-2191	-1513	-3811	-1732	-5160
16	HoGG	-2192	-1494	-3668	-1634	-5070
17	DyGG	-2244	-1429	-3695	-1645	-5028
18	TbGG	-2354	-1292	-3452	-1560	-4597
19	GdGG	-2401	-1150	-3427	-1553	-4542
20	SmGG	-2437	-925	-3185	-1447	-4391
21	NdGG	-2578	-632	-2803	-1366	-3925

Supplementary material figure captions

FIG. 8: Centroid energy component of the $4f \to 5d$ transition, $\Delta E_{\text{centroid}}(fd)$ (Eq. 2), of Ce^{3+} doped in 21 selected garnets. See Fig. 2 caption.

FIG. 9: Crystal field splitting component of the $4f_1 \to 5d_1$ transition, $\Delta E_{\text{LF}}(4f_1 \to 5d_1)$ (Eq. 3), of Ce^{3+} doped in 21 selected garnets. See Fig. 2 caption.

FIG. 10: Energy levels of the $4f$ configuration (referred to the $4f_1$ $1\Gamma_5$ ground state) of Ce^{3+} in 21 selected garnets, as calculated for the $(CeO_8)^{13-}$ clusters embedded in a common cubic confinement potential. See Fig. 6 caption.

FIG. 11: Unrelaxed host effect on the energy levels of the $4f$ configuration (referred to the $4f_1$ $1\Gamma_5$ ground state) of Ce^{3+} in 21 selected garnets. See Fig. 6 caption.

FIG. 12: Energy levels of the $5d$ configuration (referred to the $5d_1$ $8\Gamma_5$ level) of Ce^{3+} in 21 selected garnets. as calculated for the $(CeO_8)^{13-}$ clusters embedded in a common cubic confinement potential. See Fig. 7 caption.

FIG. 13: Unrelaxed host effect on the energy levels of the $5d$ configuration (referred to the $5d_1$ $8\Gamma_5$ level) of Ce^{3+} in 21 selected garnets. See Fig. 7 caption.

FIG. 14: Energy levels of the $5d$ configuration (referred to the $4f_1$ $1\Gamma_5$ ground state) of Ce^{3+} in 21 selected garnets, as calculated for the $(CeO_8)^{13-}$ clusters embedded in the embedding potentials of the undistorted garnets. See Fig. 7 caption.

FIG. 15: Energy levels of the $5d$ configuration (referred to the $4f_1$ $1\Gamma_5$ ground state) of Ce^{3+} in 21 selected garnets, as calculated for the $(CeO_8)^{13-}$ clusters embedded in a common cubic confinement potential. See Fig. 7 caption.

FIG. 16: Unrelaxed host effect on the energy levels of the $5d$ configuration (referred to the $4f_1$ $1\Gamma_5$ ground state) of Ce^{3+} in 21 selected garnets. See Fig. 7 caption.

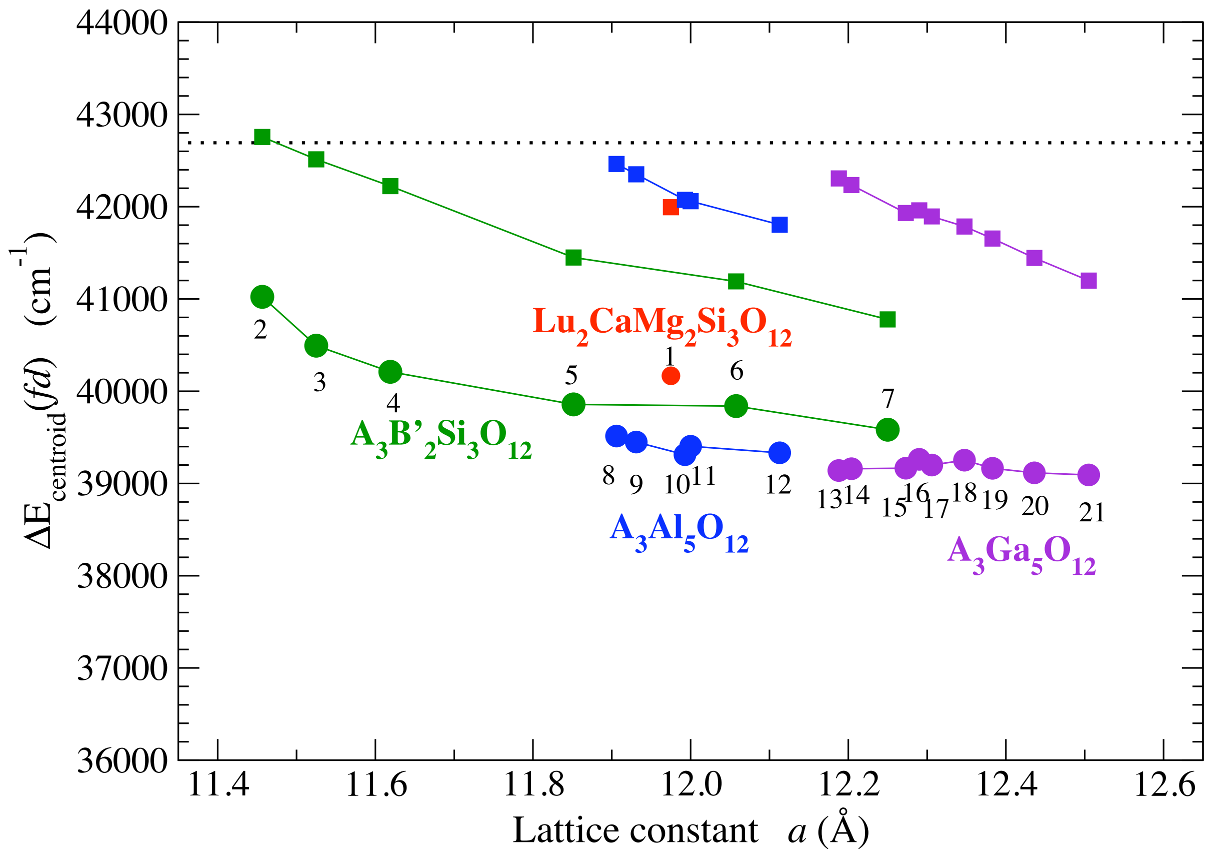

Figure 8. Seijo and Barandiarán

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

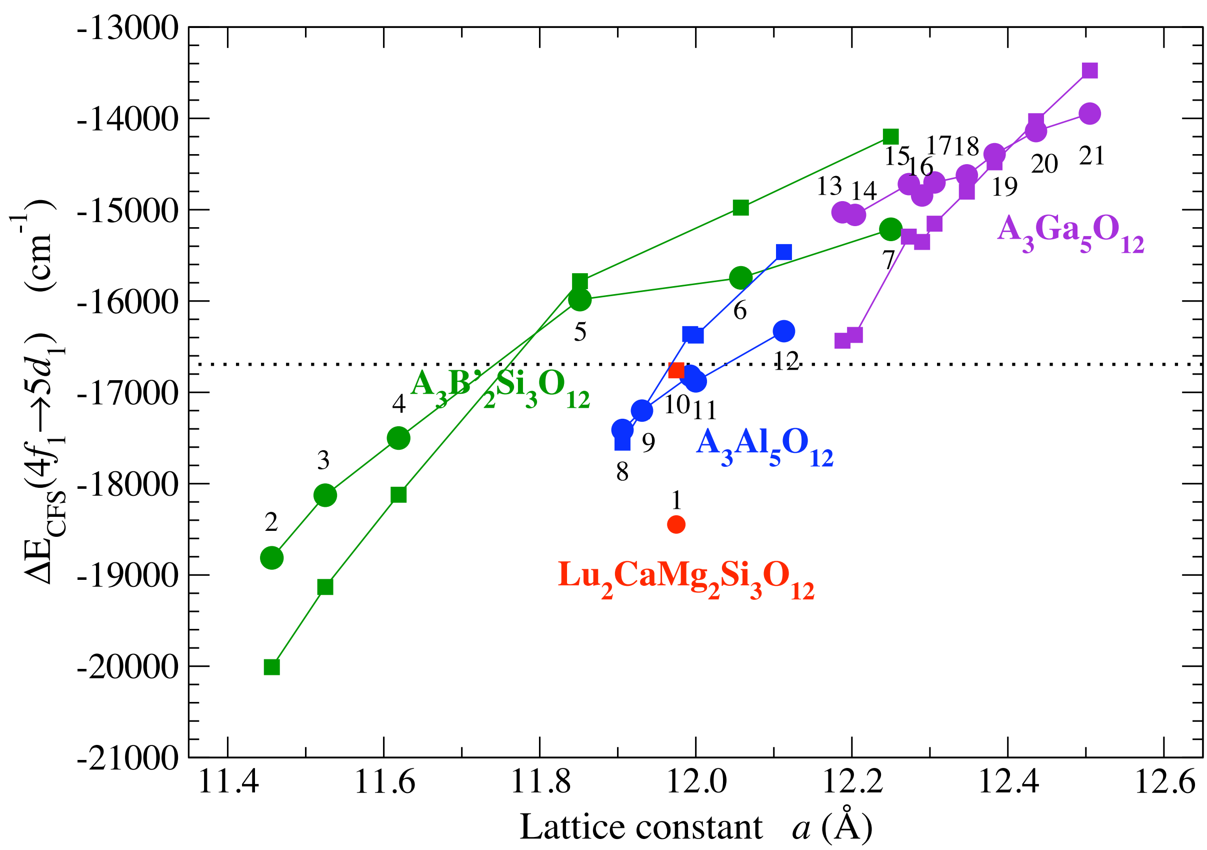

Figure 9. Seijo and Barandiarán

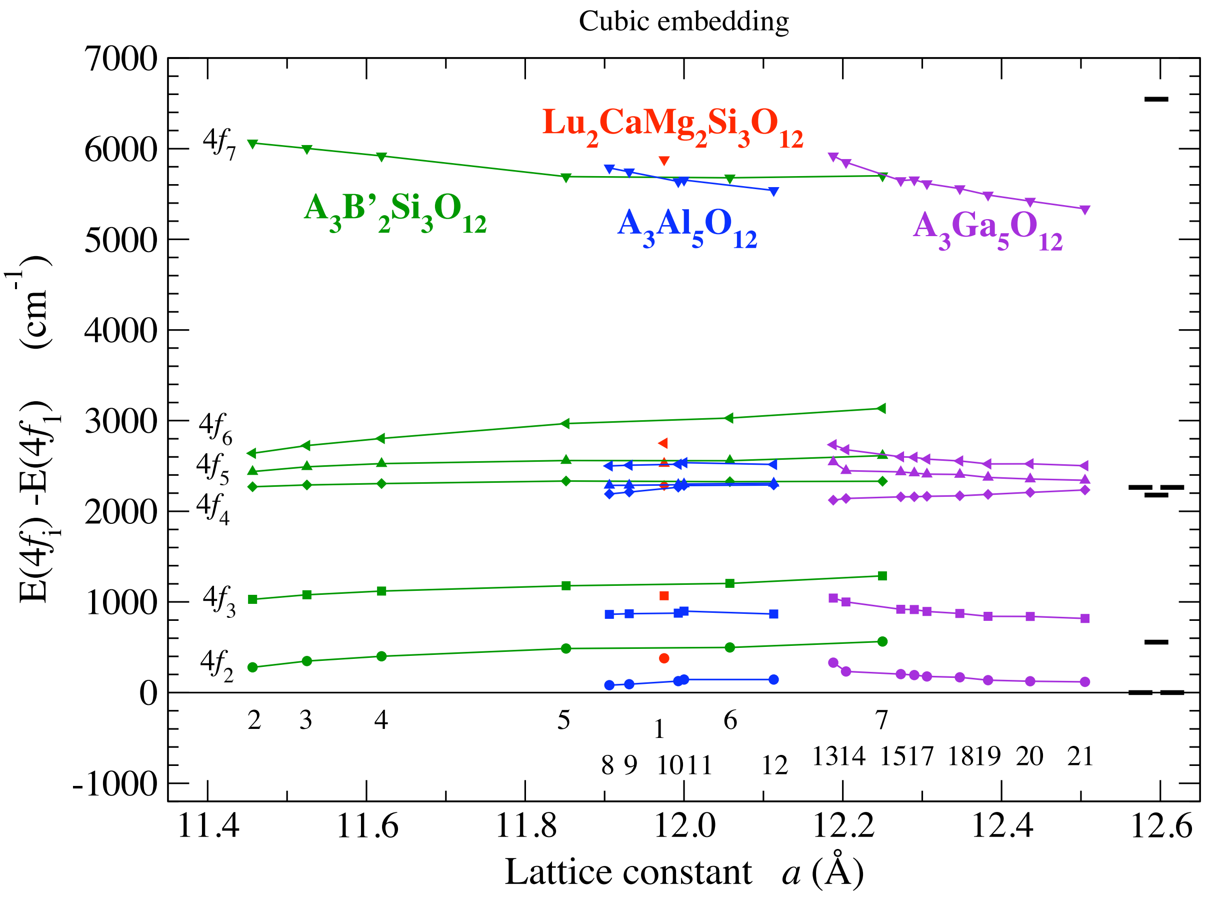

Figure 10. Seijo and Barandiarán

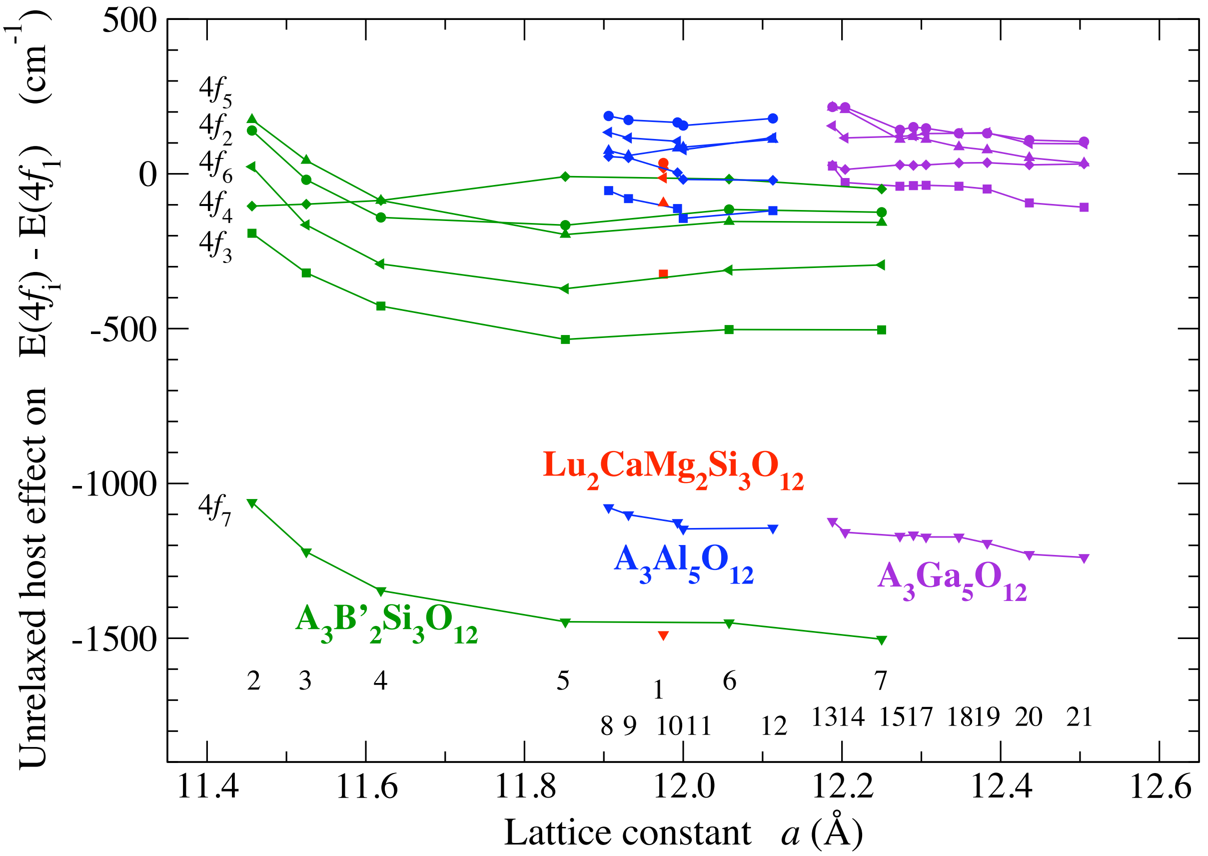

Figure 11. Seijo and Barandiarán

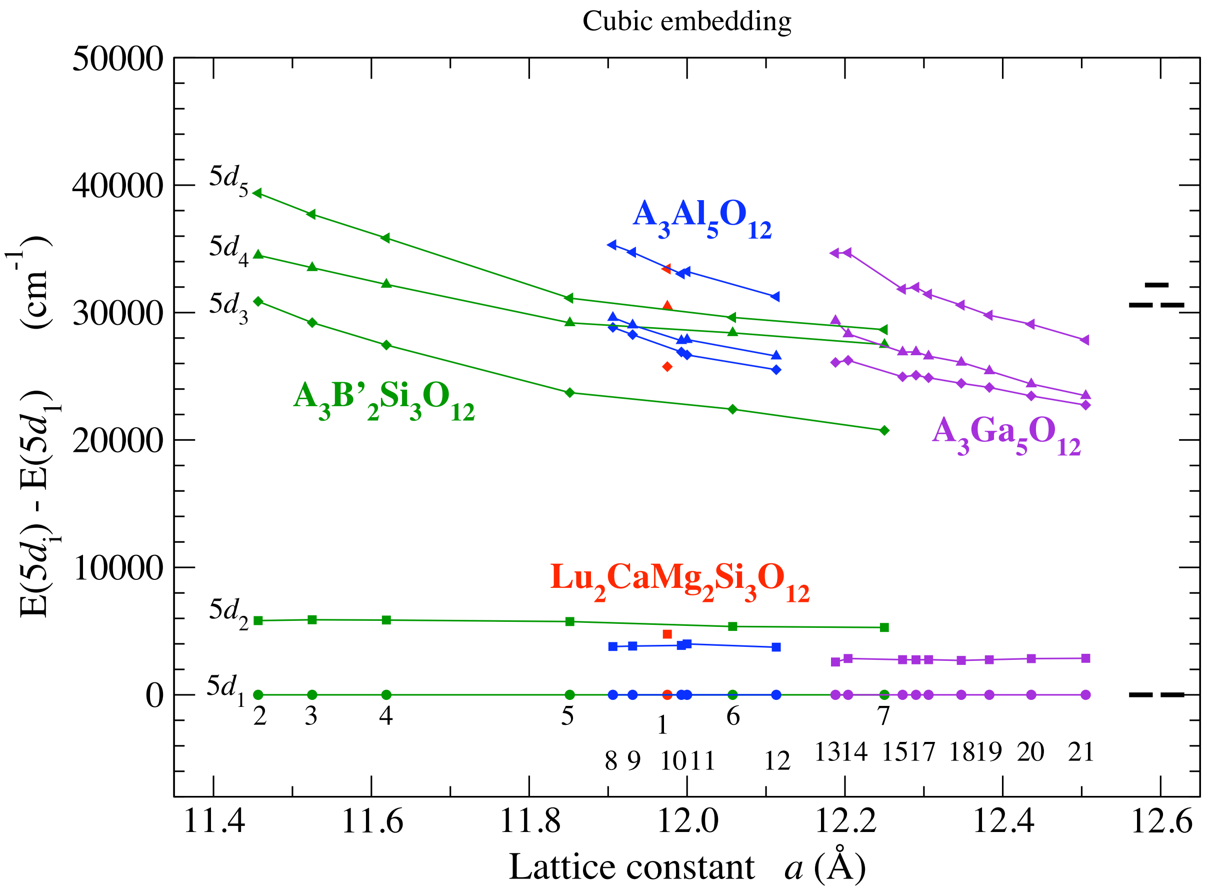

Figure 12. Seijo and Barandiarán

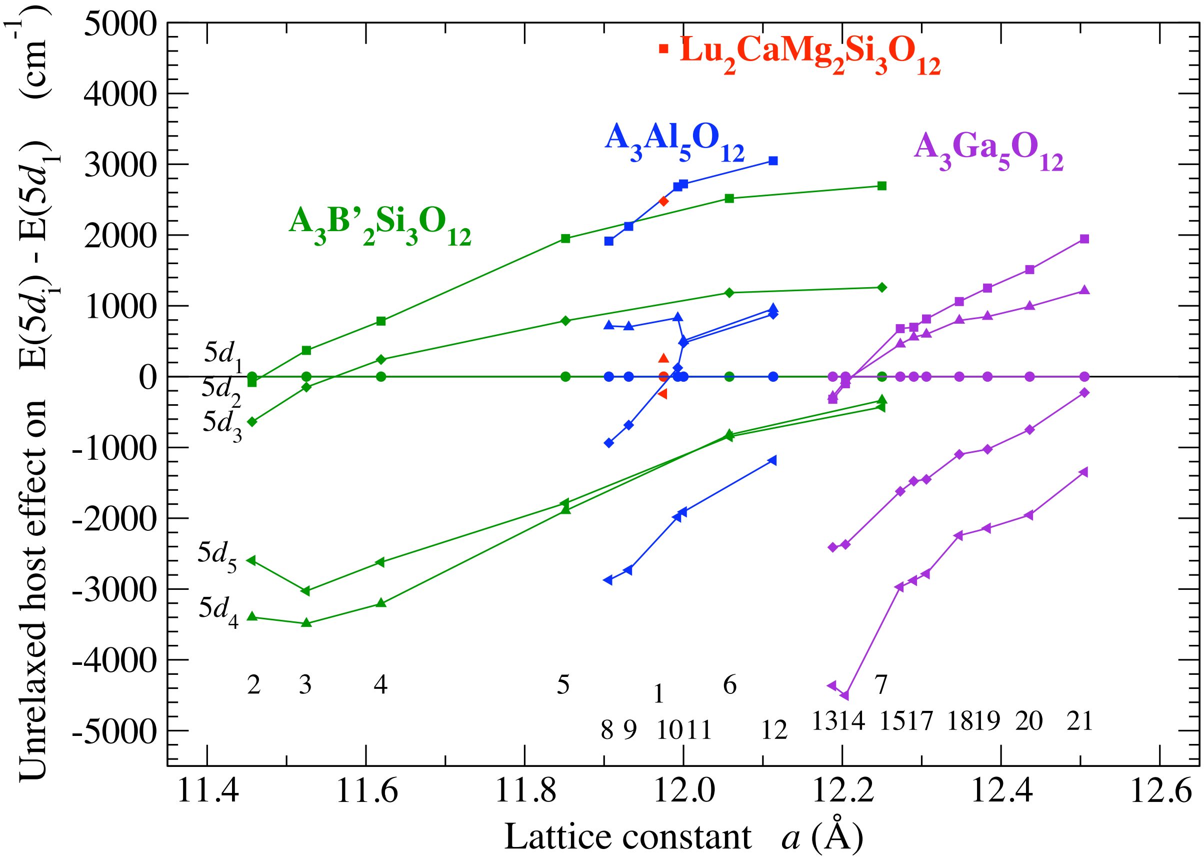

Figure 13. Seijo and Barandiarán

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2013

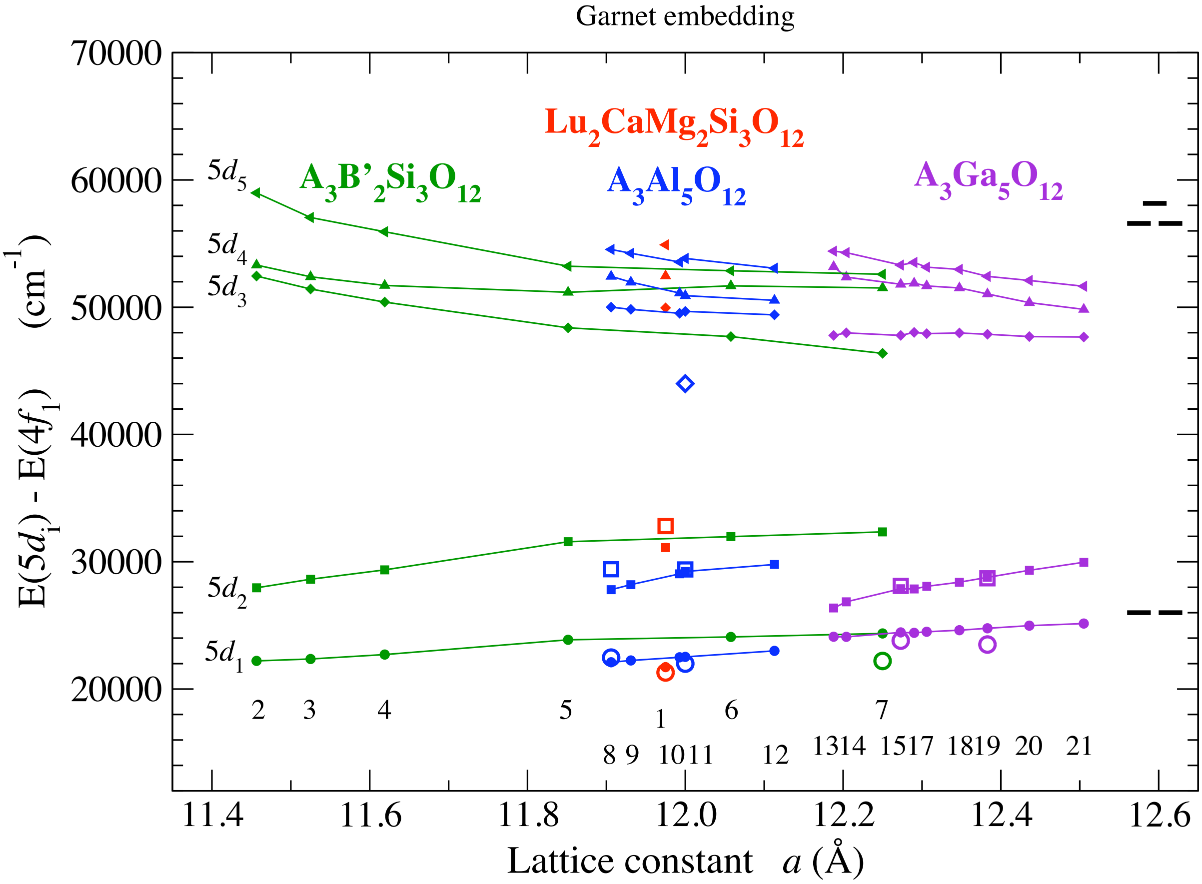

Figure 14. Seijo and Barandiarán

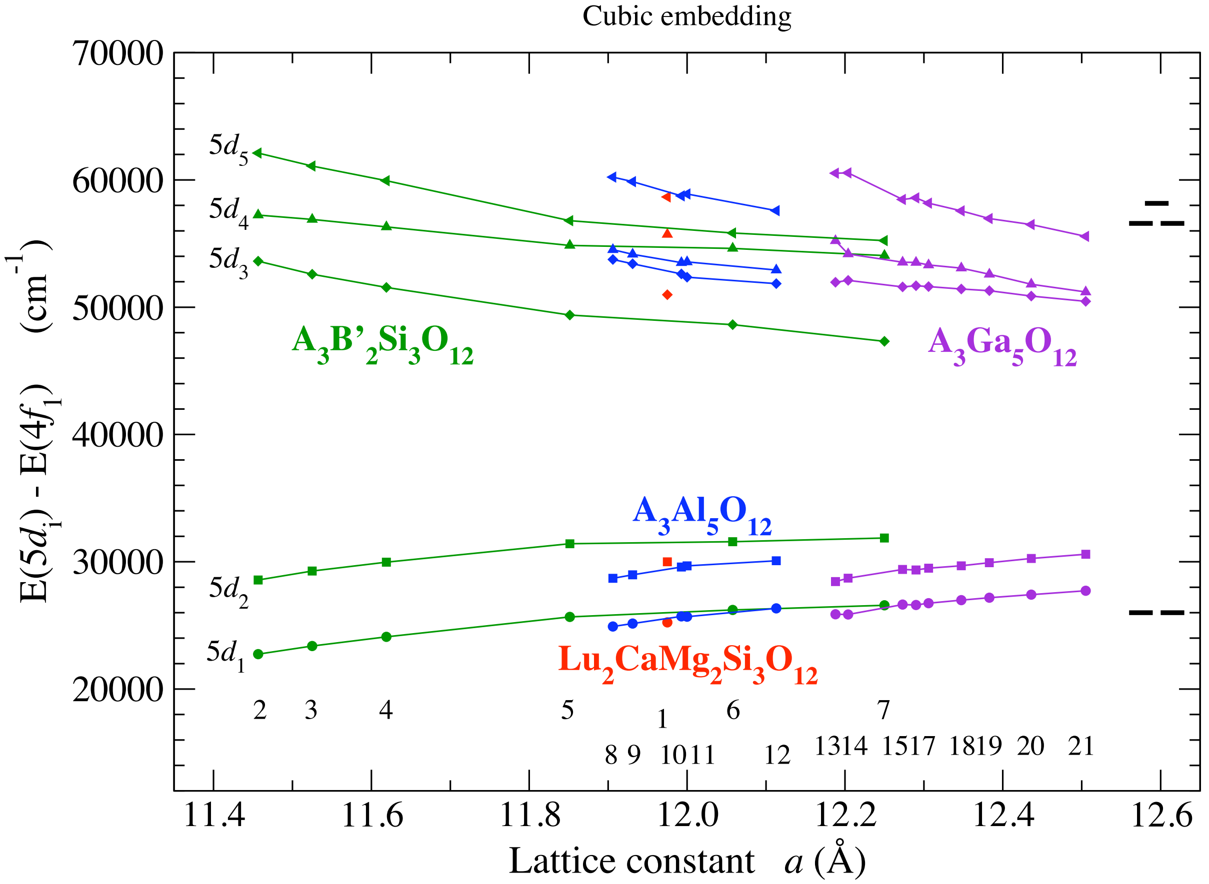

Figure 15. Seijo and Barandiarán

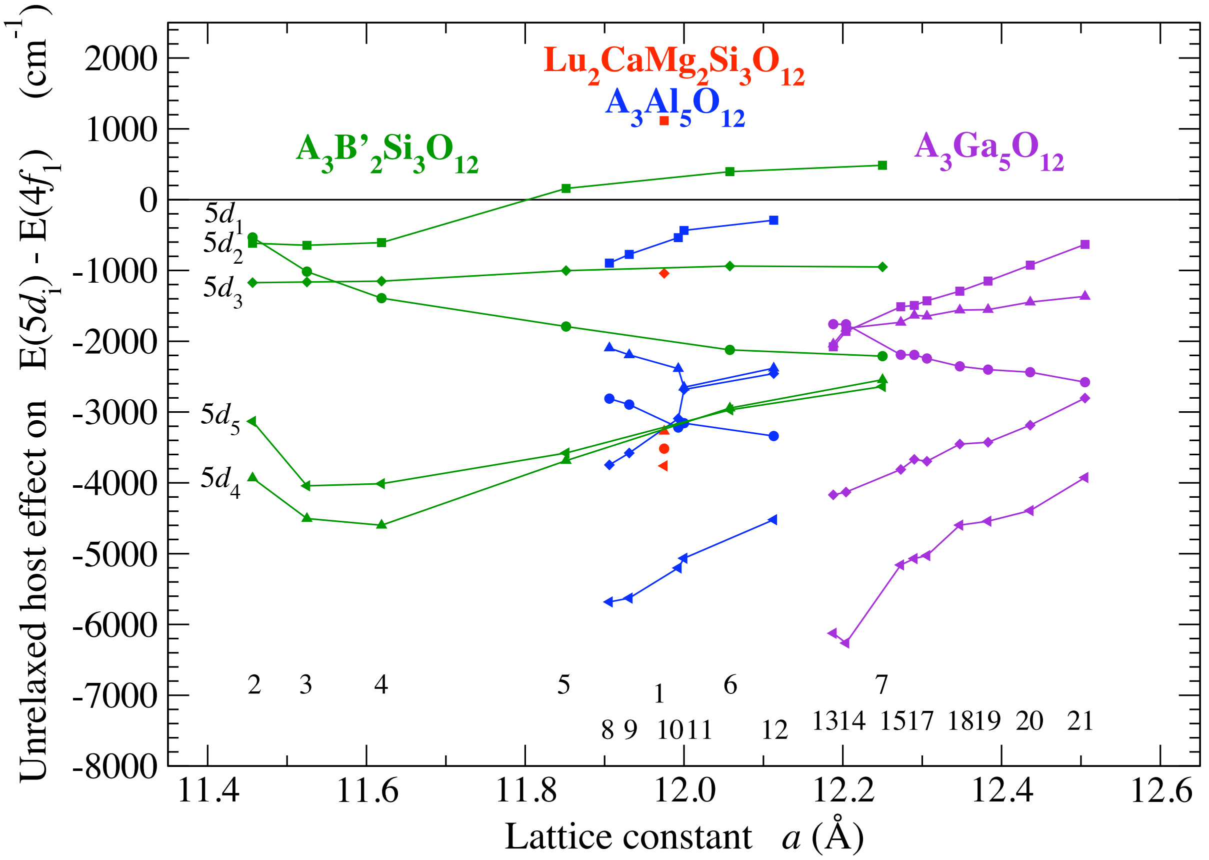

Figure 16. Seijo and Barandiarán