

Supplementary materials

A comparative EPR study of non-substituted and Mg-substituted hydroxyapatite behaviour in model media and during accelerated ageing

Monica Vidotto¹, Timor Grego^{2,3&}, Božana Petrović⁴, Nicolas Somers⁵, Tatjana Antonić Jelić⁶, Damir Kralj⁷, Nives Matijaković Mlinarić⁷, Anne Leriche⁵, Maja Dutour Sikirić⁸, Ina Erceg^{8*}, Nadica Maltar-Strmečki^{1*}

¹Laboratory for Electron Spin Spectroscopy, Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia; Monica.Vidotto@irb.hr, nstrm@irb.hr

²Department of Occupational Safety and Health, Fire and Radiation Protection Ruđer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia; Timor.Gregor@irb.hr

³University Hospital Centre Zagreb, Kišpatićeva 12, Zagreb, Croatia; Timor.Gregor@irb.hr

⁴Laboratory for Atomic Physics, Vinča Institute of Nuclear Sciences- National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, 11351 Vinča, Belgrade, Serbia; bozana@vin.bg.ac.rs

⁵Université Polytechnique Hauts-de-France (UPHF), FR CERAMATHS Département Matériaux et Procédés 59600 Maubeuge, France; anne.leriche@uphf.fr, nicolas.somers@uphf.fr

⁶Laboratory for synthesis of new materials, Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia; Tatjana.Antonic.Jelic@irb.hr

⁷Laboratory for Precipitation Processes, Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia; Damir.Kralj@irb.hr, Nives.Matijakovic.Mlinaric@irb.hr

⁸Laboratory for Biocolloids and Surface Chemistry, Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia; ierceg@irb.hr, sikiric@irb.hr

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* Correspondence: ierceg@irb.hr, I.E.; nstrm@irb.hr, N.M.S.

& Monica Vidotto and Timor Grego contributed equally to this work and share co-first authorship

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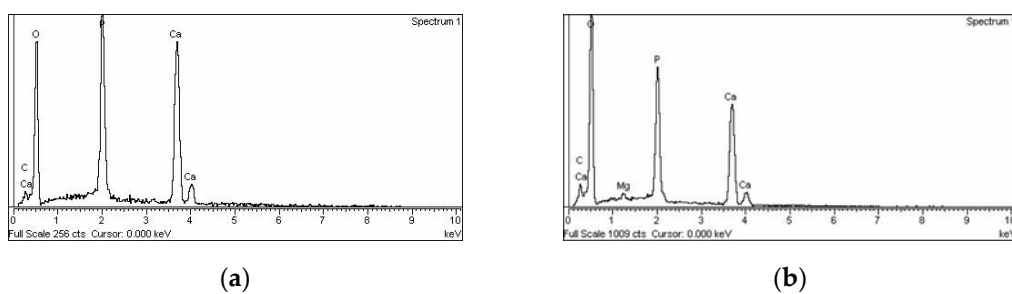


Figure S1. EDS images of a) hydroxyapatite (HAP) and b) Mg-substituted.

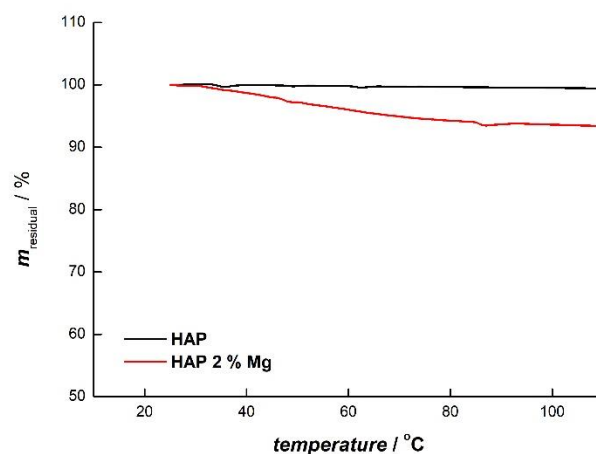
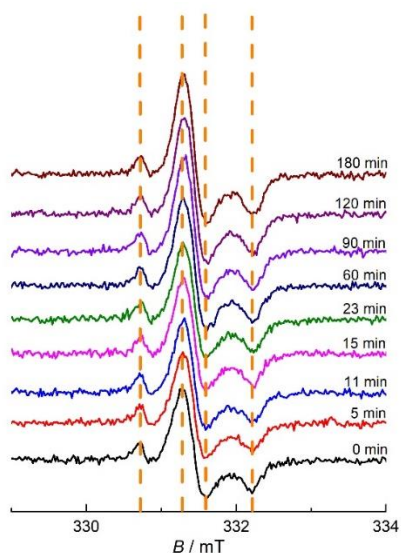
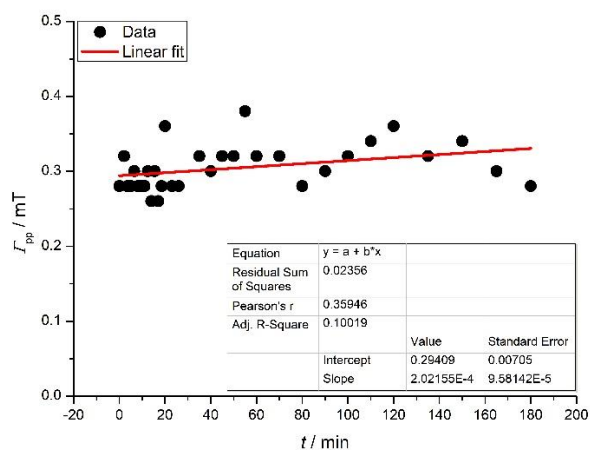


Figure S2. TGA curves of non-substituted hydroxyapatite (HAP) and Mg-substituted HAP (Mg HAP).



(a)



(b)

Figure S3. a) EPR spectra of irradiated hydroxyapatite substituted with 0.25% Mg heated at 373 K at different times and b) relation between the relative distance of EPR peaks and time of heating for sample Mg-HAP at 373 K.

Table S1. Assignment of peaks in PXRD patterns of hydroxyapatite (HAP), the initial powder, powder obtained after the irradiation, and after immersion in corrected simulated body fluid (c-SBF) and saline solution (SS) for 1 - 28 days at 37 °C.

Assignment	HAP		c-SBF			SS		
	untreated	irradiated	1d	14d	28d	1d	14d	28d
100	10.86	10.76	10.86	10.86	10.81	10.80	10.89	10.90
				13.67	13.47		13.72	13.67
101	16.9	16.76	16.87	16.89	16.8	16.83	16.91	16.86
110	18.86	18.82	18.86	19.32	18.79	18.74		
200	21.83	21.71	21.82	21.87	21.74	21.73	21.81	21.78
111	22.9	22.77	22.88	22.95	22.82	22.83	22.94	22.85
002	25.91	25.79	25.90	25.97	25.85	25.85	25.95	25.91
102	28.18	28.05	28.12	28.19	28.11	28.10	28.20	28.13
210	28.97	28.84	28.93	29.02	28.91	28.89	28.98	28.97
	31.17	31.02	31.14	31.19		31.20		
211	31.81	31.69	31.78	31.85	31.75	31.74	31.82	31.80
112	32.25	32.11	32.2	32.27	32.17	32.16	32.25	32.21
300	32.95	32.83	32.96	23.99	32.89	32.88	32.97	32.94
202	34.11	33.99	34.07	34.13	34.05	34.03	34.12	34.08
311	35.51	35.86	35.49	35.52	35.42	35.45	35.51	35.46
212	39.24	39.11	39.22	39.25	39.2	39.20	39.20	39.24
310	39.85	39.72	39.82	39.89	39.78	39.77	39.86	39.84
311	42.07	41.93	42.01	42.08	41.95	41.95	42.05	42.00
113	43.95	43.79	43.90	43.87	43.83	43.82	43.92	43.92
203	45.34	45.23	45.43	45.46	45.43	45.35	45.49	45.46
222	46.75	46.61	46.70	46.78	46.68	46.66	46.76	46.71
312	48.12	48.00	48.09	48.16	48.07	48.06	48.14	48.11
320	48.63	48.52	48.58	48.60	48.58	48.57	48.63	48.67
213	49.53	49.40	49.51	49.56	49.45	49.44	49.54	49.51
321	50.54	50.42	50.50	50.58	50.46	50.45	50.53	50.51
410	51.31	51.19	51.31	51.35	51.25	51.25	51.31	51.28
402, 303	52.13	52.01	52.11	52.15	52.07	52.06	52.16	52.09
004, 411	53.24	53.11	53.21	53.26	53.17	53.16	53.25	53.23
322, 223	55.93	55.79	55.90	55.98	55.84	55.82	55.92	55.99
313	57.13	57.05	57.16	57.14	57.09	57.07	56.53	57.14
420	59.98	59.98	59.96	59.99	59.89	59.92	60.01	59.99
214, 421	61.61	61.62	61.77	61.69	61.62	61.37	64.74	61.68
405	63.02	62.92	62.98	63.09	62.97	62.94	63.04	63.03
304, 323	64.15	64.09	64.03	64.09	64.12	64.12	64.20	64.18
511	65.05	64.94	65.02	65.1	65.01	64.99	65.03	65.05
422	66.45	66.26	66.36	66.39	66.39	66.39	66.41	66.39

Table S2. Assignment of IR bands in FTIR spectra of hydroxyapatite (HAP), the initial powder, powder obtained after the irradiation, and after immersion corrected simulated body fluid (c-SBF) and saline solution (SS) for 1 - 28 days at 37 °C.

Assignment	HAP		c-SBF			SS		
	untreated	irradiated	1d	14d	28d	1d	14d	28d
OH ⁻	3573	3573	3573	3573	3573	3573	3573	3573
PO ₄ ³⁻ v _{3a}	1087	1087	1087	1087	1087	1087	1087	1087
PO ₄ ³⁻ v _{3c}	1024	1026	1028	1024	1027	1024	1024	1024
PO ₄ ³⁻ v ₁	963	963	963	963	963	963	963	963
OH ⁻	629	630	630	629	630	630	629	630
PO ₄ ³⁻ v _{4a}	599	599	599	599	599	599	599	599
PO ₄ ³⁻ v _{4c}	564	565	566	562	565	564	564	562
PO ₄ ³⁻ v _{2b}	474	474	473	473	473	474	474	474

Table S3. Assignment of peaks in PXRD patterns of Mg-substituted hydroxyapatite (Mg-HAP), the initial powder, powder obtained after the irradiation, and after immersion in corrected simulated body fluid (c-SBF) and saline solution (SS) for 1 - 28 days at 37 °C.

Assignment	Mg - HAP		c-SBF			SS		
	untreated	irradiated	1d	14d	28d	1d	14d	28d
				12.14- 15.18			12.06- 14.49	12.47- 15.18
HAP (110)	18.1	18.04						
HAP (111)	22.54	22.49						
HAP (002)	25.90	25.94	25.90	25.86 27.34	25.87	25.83	25.86 27.43	25.97 27.41
HAP (210)	29.01	28.91	28.32					
HAP (211)	31.19	31.84	31.77	31.70	31.63	31.71	31.74	31.75
HAP (112)	32.17	32.89						
MgOH ₂	37.71	37.74						
HAP (310)	39.96	39.85						
HAP (203)				45.42	45.39	45.44	45.46	45.45
HAP (222)	46.73	46.6	46.71	46.70	46.66	46.58	46.67	46.62
HAP (213)	49.34	49.43	49.4	49.56	49.79	49.52	49.47	49.46
HAP (004)	53.17	53.17	53.07	53.17	53.14	53.07	53.19	53.31
HAP				56.48			56.5	56.48

Table S4. Assignment of IR bands in FTIR spectra of Mg-substituted hydroxyapatite (Mg-HAP), the initial powder, powder obtained after the irradiation, and after immersion in corrected simulated body fluid (c-SBF) and saline solution (SS) for 1 - 28 days at 37 °C.

Assignment	Mg-HAP		SBF			Physiological		
	untreated	irradiated	1d	14d	28d	1d	14d	28d
H ₂ O	3564 - 3000	3560 - 2812						
H ₂ O	1633	1633						
CO ₃ ²⁻	1417	1416	1448	1451	1450	1447	1448	1449
CO ₃ ²⁻	1329	1326	1418	1417	1417	1418	1417	1417
PO ₄ ³⁻ v _{3a}	1092	1086	1107	1098	1104	1100	1090	1104
PO ₄ ³⁻ v _{3c}	1022	1021	1022	1020	1020	1022	1020	1022
PO ₄ ³⁻ v ₁	961	961	961	961	961	961	961	961
CO ₃ ²⁻	873	873	873	873	873	874	873	873
	828	828						
P ₂ O ₇ ⁴⁻	715	715						
PO ₄ ³⁻ v _{4a}	601	600	601	600	601	601	600	601
PO ₄ ³⁻ v _{4c}	561	561	561	560	560	561	560	561
PO ₄ ³⁻ v _{2b}	472	473	470	471	471	465	471	471