Supplementary material

Fructose-based Metal Organic Framework as a means to synthesize chitosan nanospheres loaded with Sr with NLO properties for theranostic applications in radiotherapy

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X-ray diffraction structure of the SrFruCl MOF.

The asymmetric unit of the SrFruCl MOF contains one fructose molecule, one-half of a calcium ion, one chloride, one water molecule coordinated to the calcium ion, and one-half of a free water molecule. In the crystal packing, two fructose molecules bridge two metal ions, and an infinite thread of fructose and calcium ions develops in the [010] direction (Figure 1s). Consequently, this compound is an uni-dimensional Metal Organic Framework (1D-MOF) of a particular type, since the multi-dentate ligand is a neutral molecule (fructose), while the metal atom is charged +2. The halogen ions and the free water molecules are inserted between the Ca-fructose threads, strictly connected through strong hydrogen bonds to the sugar molecules and to the water molecules coordinated to the metal. Those bonds contribute to stabilize the crystal.

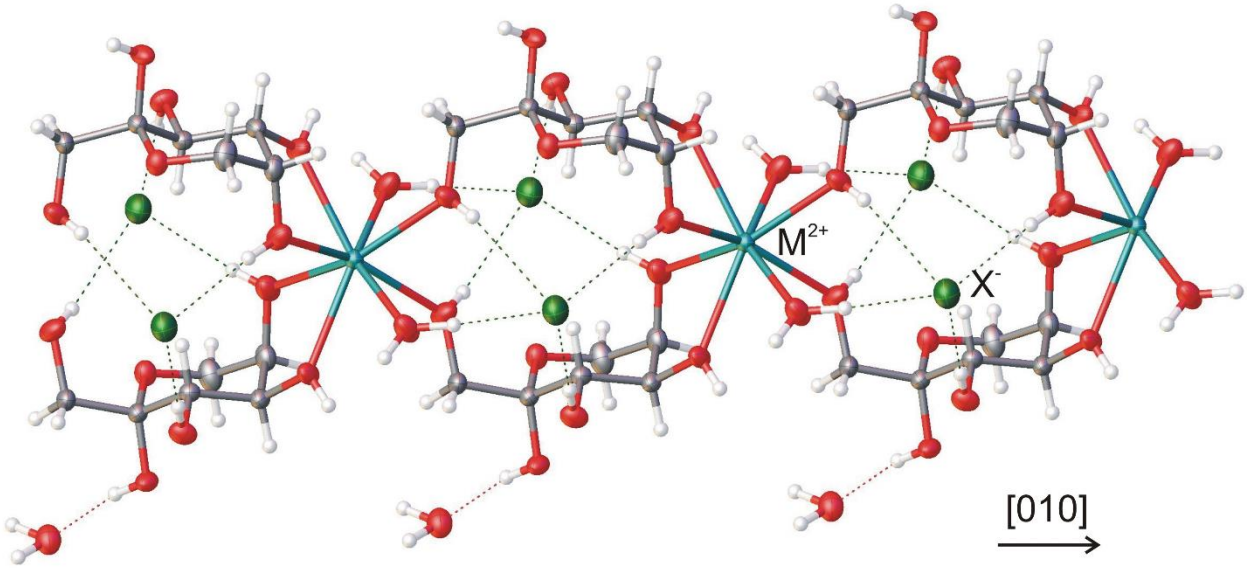

Figure 1S. *The infinite network of metal and halogen ions and sugar molecules for the structure of the SrFruCl MOF. Red=oxygen, grey=carbon, white=hydrogen, light blue=Sr, green=Cl*

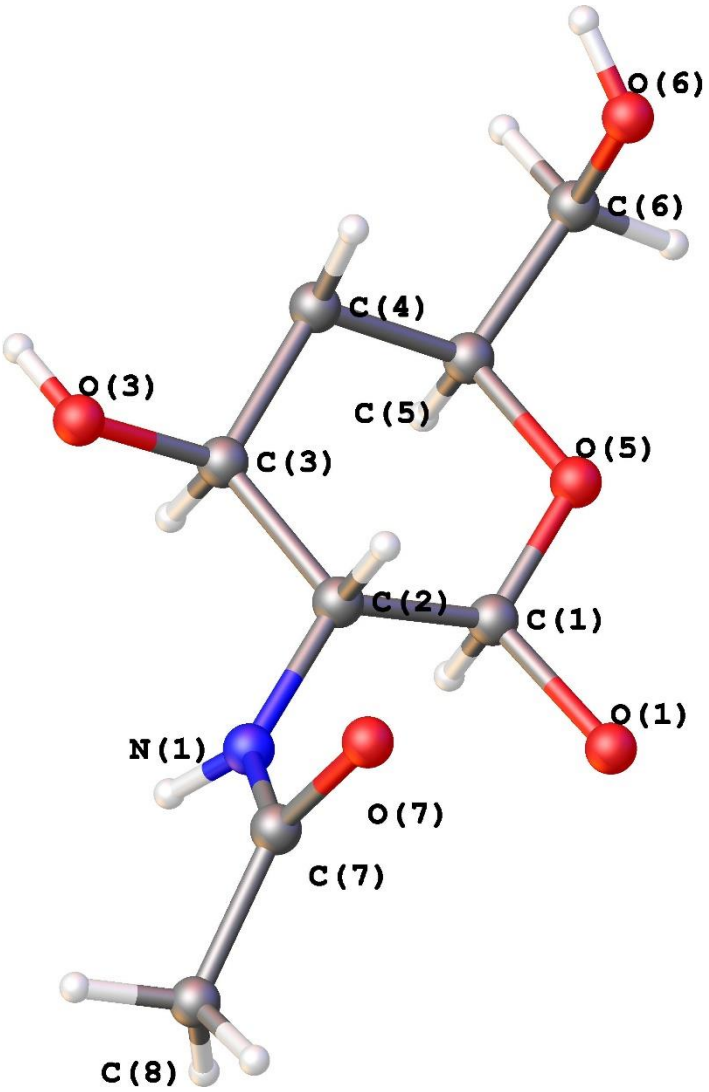

Figure 2S. X-ray molecular structure of chitin, downloaded from the crystallographic CSD databank (CCDC 1425611), with non-hydrogen atoms labelled.

Table 1S. Crystal data of chitin (CCDC 1425611).

Crystal system	monoclinic
Space group	$P112_1$
a/Å	4.8190(10)
b/Å	9.239(2)
c/Å	10.384(2)
α/°	90.00
β/°	90.00
γ/°	97.16(5)
Z	2

Computational Details

Table 3S. Computational optimized coordinates (Å) for **FRAG1** (E(RB3LYP) = -1410.81134050)

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1,992575	-2,49954	-1,79752
2	1	0	2,456324	-3,15381	-1,04928
3	6	0	0,733812	-1,87151	-1,17277
4	1	0	-0,02303	-3,56253	-1,64011
5	6	0	1,087744	-1,12964	0,135741
6	1	0	0,959668	-1,83291	0,971222
7	6	0	2,560932	-0,67045	0,090846
8	1	0	3,202249	-1,49847	0,420288
9	8	0	-4,81781	0,716421	0,050153
10	8	0	-0,21722	-2,90363	-0,93731
11	8	0	2,932683	-0,30893	-1,25565
12	6	0	2,894351	0,545277	0,949976
13	1	0	2,622987	0,355339	1,992643
14	8	0	4,286995	0,808129	0,923987
15	6	0	3,012795	-1,40775	-2,14699
16	8	0	4,280944	-2,02142	-2,13575
17	6	0	-0,94354	-0,17424	1,060698
18	6	0	-1,40941	1,218378	1,555013
19	1	0	-1,0116	1,967365	0,866345
20	6	0	-2,94911	1,278047	1,504056
21	6	0	-3,45213	1,110308	0,065972
22	1	0	-3,33626	2,081998	-0,44122
23	6	0	-2,57703	0,069765	-0,66075
24	1	0	-1,78925	0,596906	-1,21409
25	6	0	-3,29545	-0,85271	-1,64032
26	1	0	-3,83856	-0,25475	-2,37859
27	8	0	0,26199	0,020834	0,355667
28	8	0	-3,45511	2,519273	1,982158
29	8	0	-1,94371	-0,80025	0,300653
30	8	0	-2,36608	-1,65543	-2,34246
31	7	0	1,581168	-3,36904	-2,90045
32	1	0	1,294206	-2,81957	-3,71059
33	1	0	2,352464	-3,96428	-3,19295
34	1	0	4,518115	0,887054	-0,01589
35	1	0	-1,83814	-2,14587	-1,67804
36	1	0	-3,20631	2,590031	2,918362
37	7	0	-0,89514	1,514133	2,882047
38	1	0	-0,96091	0,790147	3,590101
39	6	0	-0,24911	2,648429	3,335277
40	6	0	-0,07033	3,787402	2,345045
41	1	0	0,598945	3,497636	1,526375
42	1	0	0,371132	4,628068	2,881082

43	1	0	-1,02775	4,088881	1,907273
44	1	0	2,310732	1,405533	0,597609
45	1	0	-4,03225	-1,45329	-1,08976
46	1	0	4,935496	-1,35779	-2,40773
47	8	0	0,140711	2,711461	4,492098
48	1	0	0,316148	-1,12928	-1,86978
49	1	0	-5,30186	1,392904	0,551499
50	1	0	-3,35832	0,443137	2,092538
51	1	0	-0,77292	-0,85449	1,907343
52	1	0	2,795904	-0,97447	-3,13466

Table 4S. Computational optimized coordinates (Å) for **FRAG2** (E(RB3LYP) = -1871.63065312)

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	8	0	0	0	0
2	6	0	0	0	1,416637
3	6	0	1,443821	0	1,976571
4	6	0	2,412122	0,485746	0,881744
5	6	0	2,390569	-0,46532	-0,31718
6	6	0	0,937713	-0,91885	-0,58489
7	8	0	-0,66212	-1,10655	1,970498
8	6	0	-2,09756	-1,07478	1,991089
9	6	0	-2,69473	-1,73349	0,72528
10	6	0	-4,10278	-2,24255	1,045886
11	6	0	-4,09674	-3,32575	2,165882
12	8	0	-2,91544	-3,18377	2,920487
13	6	0	-2,61355	-1,81277	3,247454
14	7	0	-4,74303	-2,74894	-0,20318
15	8	0	-2,82369	-0,85798	-0,37967
16	6	0	-1,6519	-1,8791	4,429518
17	8	0	-2,29097	-2,44517	5,554987
18	8	0	-5,19121	-3,22466	3,011953
19	7	0	1,549482	0,798486	3,184289
20	6	0	2,06742	0,450305	4,421508
21	8	0	2,040608	1,254789	5,339187
22	8	0	3,75675	0,53887	1,335771
23	8	0	2,930747	0,161398	-1,47274
24	6	0	0,589442	-1,01129	-2,05861
25	8	0	-0,72783	-1,57243	-2,1411
26	6	0	2,666992	-0,93854	4,55831
27	17	0	-7,38674	-3,45361	0,744754
28	1	0	-4,73414	-1,40939	1,370005
29	1	0	-1,97741	-0,85678	-0,87514
30	1	0	-2,4309	-0,02801	2,020922
31	1	0	-3,53602	-1,32893	3,591349
32	1	0	-1,32815	-0,87233	4,711372

33	1	0	1,701502	-1,03044	2,232599
34	1	0	2,993014	-1,34858	-0,05238
35	1	0	0,782682	-1,90632	-0,13051
36	1	0	1,319756	-1,64901	-2,57115
37	1	0	-4,62368	-2,03093	-0,92668
38	1	0	-2,7385	-3,2475	5,236063
39	1	0	-1,03322	-1,49213	-3,05743
40	1	0	3,790685	1,178885	2,065954
41	1	0	1,141804	1,728014	3,178976
42	1	0	1,900003	-1,71319	4,442242
43	1	0	3,098919	-1,01719	5,556289
44	1	0	3,443674	-1,11481	3,8063
45	1	0	-0,76182	-2,45165	4,12998
46	1	0	0,626856	-0,01172	-2,50422
47	1	0	-6,0182	-3,35153	2,47994
48	1	0	-2,05168	-2,59017	0,474818
49	1	0	3,818204	0,470888	-1,22702
50	1	0	2,083953	1,473925	0,52467
51	1	0	-0,52404	0,927737	1,682133
52	1	0	-4,01968	-4,32716	1,708499
53	1	0	-5,82605	-2,98593	0,011315
54	1	0	-4,2933	-3,60712	-0,53412