NOTICE DE TITRES ET TRAVAUX

1976-2015

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Septembre 2014

Index

Quelques chiffres

DR1 depuis 4 ans

1ère demande de promotion DR1-DRCE1

> 190 publications dont 35 depuis 2009

17 thésards/post-docs/stagiaires encadrés ou co-encadrés se traduisant par 38 publications

49 étudiants formés à distance aux méthodes SDPD
(Structure Determination by Powder Diffractometry)

147 publications dans le Web of Science

3680 citations, actuellement > 250 par an (Web of Science)
(respectivement 4400 et 350 sur Google Scholar)

1330 citations pour l'article le plus cité (Web of Science)
(1600 sur Google Scholar)

h-index = 28 (Web of Science)
(29 sur Google Scholar)

38 conférences invitées

Une dizaine de logiciels pour la cristallographie

~300.000 fichiers CIF dans COD (Crystallography Open Database)

> 1.000.000 fichiers CIF dans PCOD et P2D2 (Predicted Powder Diffraction Database)

64 ans

Curriculum-Vitæ

Age : 64 ans le 16 juin 2014

Diplômes : Doctorat de 3éme Cycle (1976, Rennes), Doctorat D'Etat (1985, Le Mans).

Carrière hors CNRS : 1977-1981, Maître-Assistant à l'Université d'ORAN (Algérie).

Carrière au CNRS : Octobre 1981, Attaché de Recherche ; Octobre 1985, CR1 ; Octobre 1990, DR2 ; Octobre 2010, DR1.

Hébergé par : Université du Maine, UMR 6283, Institut des Molécules et des Matériaux du Mans (IMMM), Département des Oxydes et Fluorures. Numérotations CNRS antérieures et successives : ERA 609, UA 449, URA 449, ESA 6010, UMR 6010. Précédemment : "Laboratoire des Oxydes et Fluorures ;" anciennement "Laboratoire des Fluorures ;" plus anciennement : "Laboratoire des Fluorures et Oxyfluorures ioniques."

Mobilité thématique : Le nombre de publications concernant le thème est indiqué. Certains textes (190 publications traditionnelles dénombrées) peuvent combiner plusieurs de ces thèmes.

1976-2005 Réseaux imparfaits (taille, distorsion)	20
1976-2014 Programmation FORTRAN	32
1981-2003 Verres fluorés, amorphes	22
1981-2015 Cristallochimie de fluorures	55
1981-1988 EXAFS	10
1987-2015 Détermination de structure *ab initio* sur poudre	50
1988-2015 Cristallochimie des oxydes	43
1988-2015 Problèmes de maclage	9
1989-2015 Grandes mailles, superstructures	8
1997-2015 Reverse Monte Carlo, recuit simulé	12
2003-2015 Prédiction de structures inorganiques	8
2003-2015 Bases de données COD/TCOD/PCOD/P2D2	5

Conférences invitées : 38

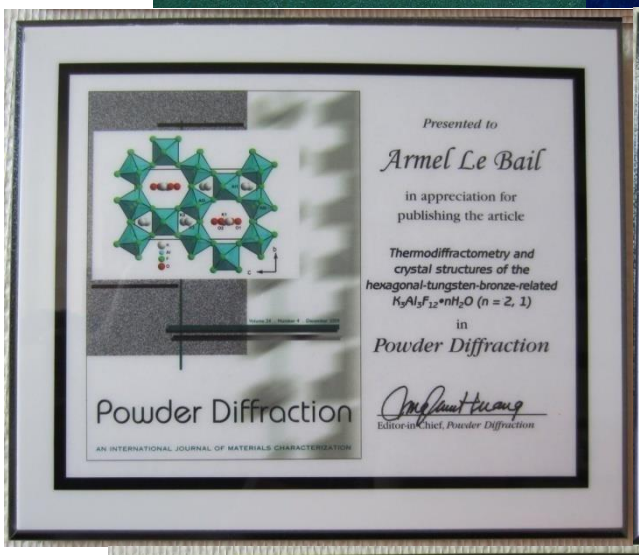
Principales activités d'enseignement :
- Créateur du Diplôme d'Université (D.U.) «Structure Determination by Powder Diffractometry», en EAD (Enseignement à Distance = ancêtre des MOOCs). Une cinquantaine d'étudiants de niveau PhD, post-doc ou professionnel inscrits dans la période 1999-2006. La formation est actuellement en accès libre (http://sdpd.univ-lemans.fr/du-sdpd/).
- Enseignement de cristallographie (diffraction de poudres) au niveau Master 2 recherche - certaines années.

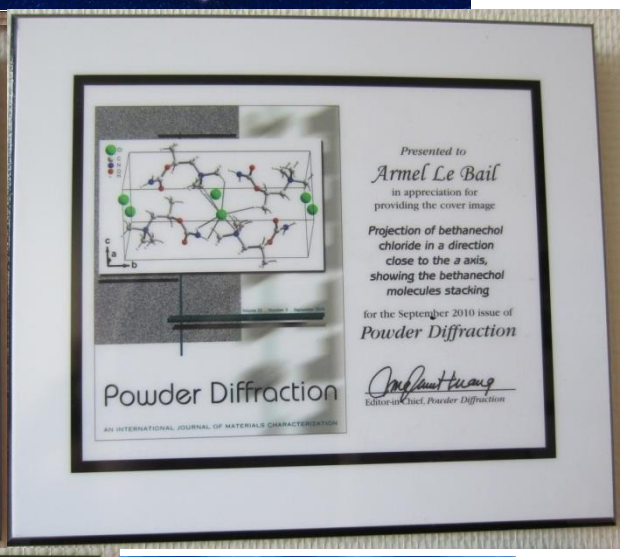
Encadrement ou co-encadrement : 17 thésard(e)s, post-docs ou stagiaires, se traduisant par 38 publications co-signées.

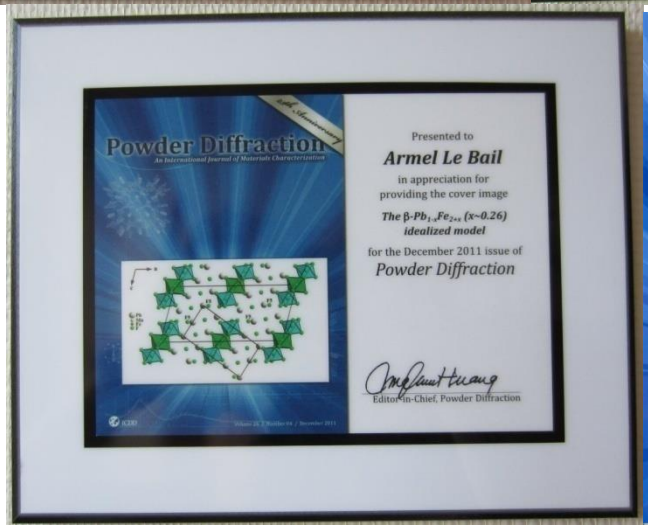
Global Activity Report

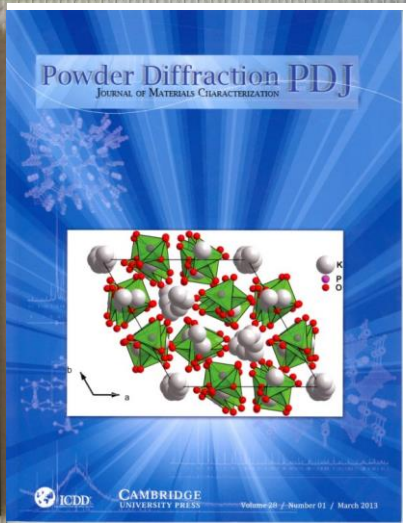
1976-2015

- **The devil's advocate :** Asking for a DRCE promotion at 64 ? Please tell us about your numerous awards as a smart scientist, any Nobel or something else which could shorten the discussion and place you inside of the very limited list of DRCEs ? Leader of a super-big lab ? Prestigious medals ?
- **The candidate :** Well, it is up to you, the examiners, to decide, according to the following evidences. I am proud to show these two plaques in simili gold from conferences in Egypt (2000 and 2004) and also these four first pages issues in the powder diffraction journal mounted on wood plaques :

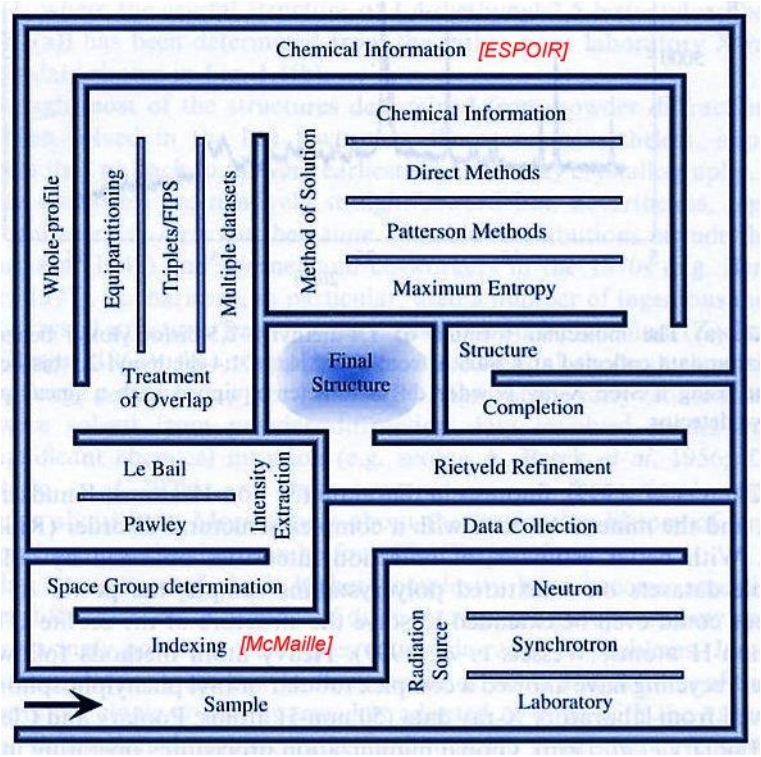








- **The devil's advocate :** Are you kidding ? The impact factor of the Powder Diffraction journal is ~0.5 !
- **The candidate :** No kidding at all ! Trying to find more evidences of exceptionnality, first of all, I have to point out that my name is visible everywhere in the recent books about my main discipline, powder diffraction. For instance in that book of which the content is summarized by a maze shown nowadays by all serious conferencers speaking about that topic. Intensity extraction by either the Pawley or the Le Bail method is an unavoidable step in the SDPD process (Structure Determination by Powder Diffractometry). Enter into the maze and find my name :



From the book "*Structure Determination from Powder Diffraction Data*", 2002, Oxford University Press, page 4. Added in red are the names of my ***ESPOIR*** and ***McMaille*** computer programs, respectively for structure solution in direct space and indexing showing that I have produced some software not only in the "Intensity Extraction" step.

- **The Devil's advocate :** Well, seriously, “powder diffraction” is nothing but exceptionnal, if you were Debye, but you are only Le Bail, you know, even not Daniel Louër.
- **The candidate :** Sure, I know. You should at least give a look at the exceptionnal results that people (including Daniel Louër) obtained using my tools or algorithms, this is really something. Do you think that > 1300 citations for one paper are nothing ? This paper is the ever most cited one in the "*Material Research Bulletin*." This is really exceptionnal and deserves the corresponding class.
- **The Devil's advotate :** Sorry but this is not convincing at all.
- **The candidate :** Note also that if I am exceptionnal, I should have been recognized as such already by other exceptionnal people. How to prove that ? Are the researchers using my algorithms all exceptionnal ? Well, many are certainly more exceptionnal than me, see the well known names of authors citing me (so having found some value in my published work) in some highly cited papers below. My own h index is currently 28, but there are H = 86 papers listed below, cited at least 86 times which are citing me (from ~3000 in the Web of Science), not too bad if not exceptionnal. And don't forget that the annual production in number of crystal structures from powder diffraction data is 200 times smaller than from single crystal data, so the number of citations should be rescaled. This is typically a "niche."

No	Reference	Times cited
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2	RECENT ADVANCES IN MAGNETIC-STRUCTURE DETERMINATION BY NEUTRON POWDER DIFFRACTION, RODRIGUEZCARVAJAL, J, PHYSICA B 192 (1993) 55-69.	4665
3	A Rietveld-analysis program RIETAN-98 and its applications to zeolites, Izumi, F; Ikeda, T, MATERIALS SCIENCE FORUM Volume: 321-3 (2000) 198-203.	1235
4	Charge, orbital, and magnetic ordering in La0.5Ca0.5MnO3, Radaelli, PG; Cox, DE; Marezio, M; et al., PHYSICAL REVIEW B 55 (1997) 3015-3023.	706
5	Rietveld refinement guidelines, McCusker, LB; Von Dreele, RB; Cox, DE; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 32 (1999) 36-50.	607

6	Powder pattern indexing with the dichotomy method, Boultif, A; Louer, D, JOURNAL OF APPLIED CRYSTALLOGRAPHY 37 (2004) 724-731.	604
7	FOX, 'free objects for crystallography': a modular approach to ab initio structure determination from powder diffraction, Favre-Nicolin, V; Cerny, R, JOURNAL OF APPLIED CRYSTALLOGRAPHY 35 (2002) 734-743.	533
8	Microporous solids: From organically templated inorganic skeletons to hybrid frameworks ... ecumenism in chemistry, Ferey, G, CHEMISTRY OF MATERIALS 13 (2001) 3084-3098.	512
9	Phenomenological model of anisotropic peak broadening in powder diffraction, Stephens, PW, JOURNAL OF APPLIED CRYSTALLOGRAPHY 32 (1999) 281-289.	497
10	The structure of malaria pigment beta-haematin, Pagola, S; Stephens, PW; Bohle, DS; et al., NATURE 404 (2000) 307-310.	497
11	EXPO: a program for full powder pattern decomposition and crystal structure solution, Altomare, A; Burla, MC; Camalli, M; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 32 (1999) 339-340.	380
12	Negative thermal expansion in ZrW2O8 and HfW2O8, Evans, JSO; Mary, TA; Vogt, T; et al., CHEMISTRY OF MATERIALS 8 (1996) 2809-2823.	370
13	STRUCTURAL AND ELECTROCHEMICAL PROPERTIES OF THE PROTON GAMMA-MNO2 SYSTEM, CHABRE, Y; PANNETIER, J, PROGRESS IN SOLID STATE CHEMISTRY 23 (1995) 1-130.	363
14	Crystallite size distribution and dislocation structure determined by diffraction profile analysis: principles and practical application to cubic and hexagonal crystals, Ungar, T; Gubicza, J; Ribarik, G; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 34 (2001) 298-310.	330
15	Aufbau principle of complex open-framework structures of metal phosphates with different dimensionalities, Rao, CNR; Natarajan, S; Choudhury, A; et al., ACCOUNTS OF CHEMICAL RESEARCH 34 (2001) 80-87.	322
16	Building units design and scale chemistry, Ferey, G, JOURNAL OF SOLID STATE CHEMISTRY 152 (2000) 37-48.	279
17	Quantitative texture analysis by Rietveld refinement, VonDreele, RB, JOURNAL OF APPLIED CRYSTALLOGRAPHY 30 (1997) 517-525.	269
18	EXTRA: A program for extracting structure factor amplitudes from powder diffraction data, Altomare, A; Burla, MC; Cascarano, G; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 28 (1995) 842-846	260
19	Compressibility, phase transitions, and oxygen migration in zirconium tungstate, ZrW2O8, Evans, JSO; Hu, Z; Jorgensen, JD; et al., SCIENCE 275 (1997) 61-65.	258
20	Powder diffraction, Langford, JI; Louer, D, REPORTS ON PROGRESS IN PHYSICS 59 (1996) 131-234.	246
21	Colossal magnetoresistance without Mn3+/Mn4+ double exchange in the stoichiometric pyrochlore Tl2Mn2O7, Subramanian, MA; Toby, BH; Ramirez, AP; et al., SCIENCE 273 (1996) 81-84.	238
22	Estimating grain-size distributions in nanocrystalline materials from X-ray diffraction profile analysis, Krill, CE; Birringer, R, PHILOSOPHICAL MAGAZINE A-PHYSICS OF CONDENSED MATTER STRUCTURE DEFECTS AND MECHANICAL PROPERTIES 77 (1998) 621-640.	234
23	CRYSTAL-STRUCTURES OF HIGH-TC OXIDES - THE YEARS 1987 AND 1988 , YVON, K; FRANCOIS, M, ZEITSCHRIFT FUR PHYSIK B-CONDENSED MATTER 76 (1989) 413-444.	229
24	The (hkl) dependence of diffraction-line broadening caused by strain and size for all Laue groups in Rietveld refinement, Popa, NC, JOURNAL OF APPLIED CRYSTALLOGRAPHY 31 (1998) 176-180.	218
25	OXOVANADIUM AND OXOMOLYBDENUM CLUSTERS AND SOLIDS INCORPORATING OXYGEN-DONOR LIGANDS, KHAN, MI; ZUBIETA, J, PROGRESS IN INORGANIC CHEMISTRY, 43 (1995) 1-149.	208
26	Combined texture and structure analysis of deformed limestone from time-of-flight neutron diffraction spectra, Lutterotti, L; Matthies, S; Wenk, HR; et al. JOURNAL OF APPLIED PHYSICS 81 (1997) 594-600.	193
27	The effect of dislocation contrast on X-ray line profiles in untextured polycrystals, Ungar, T; Tichy, G, PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 171 (1999) 425-434.	190
28	Microporous titanosilicates and other novel mixed octahedral-tetrahedral framework oxides , Rocha, J; Anderson, MW, EUROPEAN JOURNAL OF INORGANIC CHEMISTRY Issue: 5 (2000) 801-818.	185
29	Effect of a crystallite size distribution on X-ray diffraction line profiles and whole-powder-pattern fitting , Langford, JI; Louer, D; Scardi, P, JOURNAL OF APPLIED CRYSTALLOGRAPHY 33 (2000) 964-974.	184
30	Hydrogen physisorption in metal-organic porous crystals, Panella, B; Hirscher, M, ADVANCED MATERIALS 17 (2005) 538-+.	182
31	PowderSolve - a complete package for crystal structure solution from powder diffraction patterns, Engel, GE; Wilke, S; Konig, O; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 32 (1999) 1169-1179.	180
32	Structural chemistry of vanadium oxides with open frameworks, Zavalij, PY; Whittingham, MS, ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE 55 (1999) 627-663.	179
33	Magnetic excitations in the S=1/2 alternating chain compound (VO)(2)P2O7, Garrett, AW; Nagler, SE; Tennant, DA; et al., PHYSICAL REVIEW LETTERS 79 (1997) 745-748.	175
34	Fityk: a general-purpose peak fitting program, Wojdyr, Marcin, JOURNAL OF APPLIED CRYSTALLOGRAPHY 43 (2010) 1126-1128.	169
35	Crystal structure prediction from first principles, Woodley, Scott M.; Catlow, Richard, NATURE MATERIALS 7 (2008) 937-946.	169
36	Crystal structure determination from powder diffraction data, Harris, KDM; Tremayne, M, CHEMISTRY OF MATERIALS 8 (1996) 2554-2570.	159
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39	Size-dependent extinction coefficients of PbS quantum dots, Cademartiri, Ludovico; Montanari, Erica; Calestani, Gianluca; et al., JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (2006) 10337-10346.	153
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43	Superionics: crystal structures and conduction processes, Hull, S, REPORTS ON PROGRESS IN PHYSICS 67 (2004) 1233-1314.	136
44	Spin-1/2 kagome-like lattice in Volborthite Cu3V2O7(OH)(2)center dot 2H2O, Hiroi, Z; Hanawa, M; Kobayashi, N; et al., JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN 70 (2001) 3377-3384.	133

45	ALMEPO-ALPHA - A NOVEL OPEN-FRAMEWORK ALUMINUM METHYLPHOSPHONATE WITH ORGANO-LINED UNIDIMENSIONAL CHANNELS, MAEDA, K; AKIMOTO, J; KIYOZUMI, Y; et al., ANGEWANDTE CHEMIE-INTERNATIONAL EDITION IN ENGLISH 34 (1995)1199-1201.	132
46	Automatic structure determination from powder data with EXPO2004, Altomare, A; Caliandro, R; Camalli, M; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 37 (2004) 1025-1028.	131
47	SOLID-STATE DEFECT MECHANISM IN VANADYL PYROPHOSPHATE CATALYSTS - IMPLICATIONS FOR SELECTIVE OXIDATION, GAI, PL; KOURTAKIS, K, SCIENCE 267 (1995) 661-663.	129
48	VANADIUM PHOSPHATE FRAMEWORK SOLID CONSTRUCTED OF OCTAHEDRA, SQUARE PYRAMIDS, AND TETRAHEDRA WITH A CAVITY DIAMETER OF 18.4 ANGSTROM, SOGHOMONIAN, V; CHEN, Q; HAUSHALTER, RC; et al., ANGEWANDTE CHEMIE-INTERNATIONAL EDITION IN ENGLISH 32 (1993) 610-612.	129
49	Transformations of molecules and secondary building units to materials: A bottom-up approach, Murugavel, R; Walawalkar, MG; Dan, M; et al., ACCOUNTS OF CHEMICAL RESEARCH 37 (2004) 763-774.	126
50	In situ X-ray diffraction and solid-state NMR study of the fluorination of gamma-Al2O3 with HCF2Cl , Chupas, PJ; Ciraolo, MF; Hanson, JC; et al., JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 123 (2001) 1694-1702.	125
51	Structural studies of charge disproportionation and magnetic order in CaFeO3, Woodward, PM; Cox, DE; Moshopoulou, E; et al., PHYSICAL REVIEW B 62 (2000) 844-855.	125
52	Combined method for ab initio structure solution from powder diffraction data, Putz, H; Schon, JC; Jansen, M, JOURNAL OF APPLIED CRYSTALLOGRAPHY 32 (1999) 864-870.	124
53	X-Cell: a novel indexing algorithm for routine tasks and difficult cases, Neumann, MA, JOURNAL OF APPLIED CRYSTALLOGRAPHY 36 (2003) 356-365.	123
54	PROFILE ANALYSIS FOR MICROCRYSTALLINE PROPERTIES BY THE FOURIER AND OTHER METHODS, LANGFORD, JI; DELHEZ, R; DEKEIJSER, TH; et al., AUSTRALIAN JOURNAL OF PHYSICS 41 (1988) 173-187.	121
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59	Nanochannels of two distinct cross-sections in a porous Al-based coordination polymer , Comotti, Angiolina; Bracco, Silvia; Sozzani, Piero; et al., JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 130 (2008) 13664-13672.	112
60	Li2.5V2(PO4)(3): A room-temperature analogue to the fast-ion conducting high-temperature gamma-phase of Li3V2(PO4)(3) , Yin, SC; Strobel, PS; Grondey, H; et al., CHEMISTRY OF MATERIALS 16 (2004) 1456-1465.	112
61	Quantitative analysis of silicate glass in ceramic materials by the Rietveld method, Lutterotti, L; Ceccato, R; Dal Maschio, R; et al., MATERIALS SCIENCE FORUM Volume: 278-2 (1998) 87-92.	112
62	Single C-C bond in (C-60)(2)(2-) , Oszlanyi, G; Bortel, G; Faigel, G; et al., PHYSICAL REVIEW B 54 (1996) 11849-11852.	112
63	PHASE-TRANSITIONS IN KC60 - DIMER FORMATION VIA RAPID QUENCHING, ZHU, Q; COX, DE; FISCHER, JE, PHYSICAL REVIEW B 51 (1995) 3966-3969.	112
64	EXPO2009: structure solution by powder data in direct and reciprocal space, Altomare, Angela; Camalli, Mercedes; Cuocci, Corrado; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 42 (2009) 1197-1202.	109
65	Organically-templated metal sulfates, selenites and selenates, Rao, CNR; Behera, JN; Dan, M, CHEMICAL SOCIETY REVIEWS 35 (2006) 375-387.	109
66	POTENTIAL OF THE INEL X-RAY POSITION-SENSITIVE DETECTOR - A GENERAL STUDY OF THE DEBYE-SCHERRER SETTING, EVAIN, M; DENIARD, P; JOUANNEAUX, A; et al., JOURNAL OF APPLIED CRYSTALLOGRAPHY 26 (1993) 563-569.	109
67	How to determine structures when single crystals cannot be grown: opportunities for structure determination of molecular materials using powder diffraction data, Harris, KDM; Cheung, EY, CHEMICAL SOCIETY REVIEWS 33 (2004) 526-538.	108
68	(C2H10N2)[Cr(HPO3)F-3]: The first organically templated fluorochromium(III) phosphite, Fernandez, S; Mesa, JL; Pizarro, JL; et al., ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 41 (2002) 3683-3685.	108
69	Spin dynamics and transport in gapped one-dimensional Heisenberg antiferromagnets at nonzero temperatures, Damle, K; Sachdev, S, PHYSICAL REVIEW B 57 (1998) 8307-8339.	108
70	RMCProfile: reverse Monte Carlo for polycrystalline materials, Tucker, Matthew G.; Keen, David A.; Dove, Martin T.; et al., JOURNAL OF PHYSICS-CONDENSED MATTER 19, Issue: 33 (2007) Article Number: 335218.	106
71	SYNTHESIS AND STRUCTURE OF A NEW FAMILY OF CUPRATE SUPERCONDUCTORS - LNSR2CU2GAO7, VAUGHEY, JT; THIEL, JP; HASTY, EF; et al., CHEMISTRY OF MATERIALS 3 (1991) 935-940.	106
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73	Synthesis and structure of a layered titanosilicate catalyst with five-coordinate titanium, Roberts, MA; Sankar, G; Thomas, JM; et al., NATURE 381 (1996) 401-404.	104
74	Complex zeolite structure solved by combining powder diffraction and electron microscopy, Gramm, Fabian; Baerlocher, Christian; McCusker, Lynne B.; et al., NATURE 444 (2006) 79-81.	103
75	An approach to the synthesis of organically templated open-framework metal sulfates by the amine-sulfate route, Choudhury, A; Krishnamoorthy, J; Rao, CNR, CHEMICAL COMMUNICATIONS 24 (2001) 2610-2611.	103
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77	Characterization of the products of the heme detoxification pathway in malarial late trophozoites by X-ray diffraction, Bohle, DS; Dinnebier, RE; Madsen, SK; et al., JOURNAL OF BIOLOGICAL CHEMISTRY 272 (1997) 713-716.	103
78	Metal complexes of organophosphate esters and open-framework metal phosphates: Synthesis, structure, transformations, and applications, Murugavel, R.; Choudhury, Amitava; Walawalkar, M. G.; et al., CHEMICAL REVIEWS 108 (2008) 3549-3655.	101
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82	SOLID-STATE LITHIUM CYANOCOBALTATES WITH A HIGH-CAPACITY FOR REVERSIBLE DIOXYGEN BINDING - SYNTHESIS, REACTIVITY, AND STRUCTURES, RAMPRASAD, D; PEZ, GP; TOBY, BH; et al., JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 117 (1995) 10694-10701.	92
83	High-pressure structural study of the scheelite tungstates CaWO4 and SrWO4, Errandonea, D; Pellicer-Porres, J; Manjon, FJ; et al., PHYSICAL REVIEW B 72 (2005) article number: 174106.	91
84	Nanosize effects on hydrogen storage in palladium, Yamauchi, Miho; Ikeda, Ryuichi; Kitagawa, Hiroshi; et al., JOURNAL OF PHYSICAL CHEMISTRY C 112 (2008) 3294-3299.	86
85	Electronic structure and energetics of LaNi5, alpha-La2Ni10H and beta-La2Ni10H14, Nakamura, H; Nguyen-Manh, D; Pettifor, DG, JOURNAL OF ALLOYS AND COMPOUNDS 281 (1998) 81-91.	86
86	A general Monte Carlo approach to structure solution from powder-diffraction data: Application to poly(ethylene oxide)(3):LiN(SO2CF3)(2), Andreev, YG; Lightfoot, P; Bruce, PG, JOURNAL OF APPLIED CRYSTALLOGRAPHY 30 (1997) 294-305.	86

Other proofs (of my excellence) are some pictures of me at congress all over the world. For instance this one (I am on the left) with William L. Duax (IUCr president) (on the right) in Morocco, 2004 (nice food anyway) :

With Carmelo Giacovazzo in Egypt (2004). Waiting for an airplane at Cairo, I remember discussing with him about ambition. He declared he always had the target to build his own team, refusing to work on ideas coming from other brains than his own. I confess that I explained him to have limited drastically my own ambitions since 1995 when I understood that, in spite of any of my efforts, it would never be possible to build my own team at Le Mans. At least, working on my own ideas was also possible, fortunately.

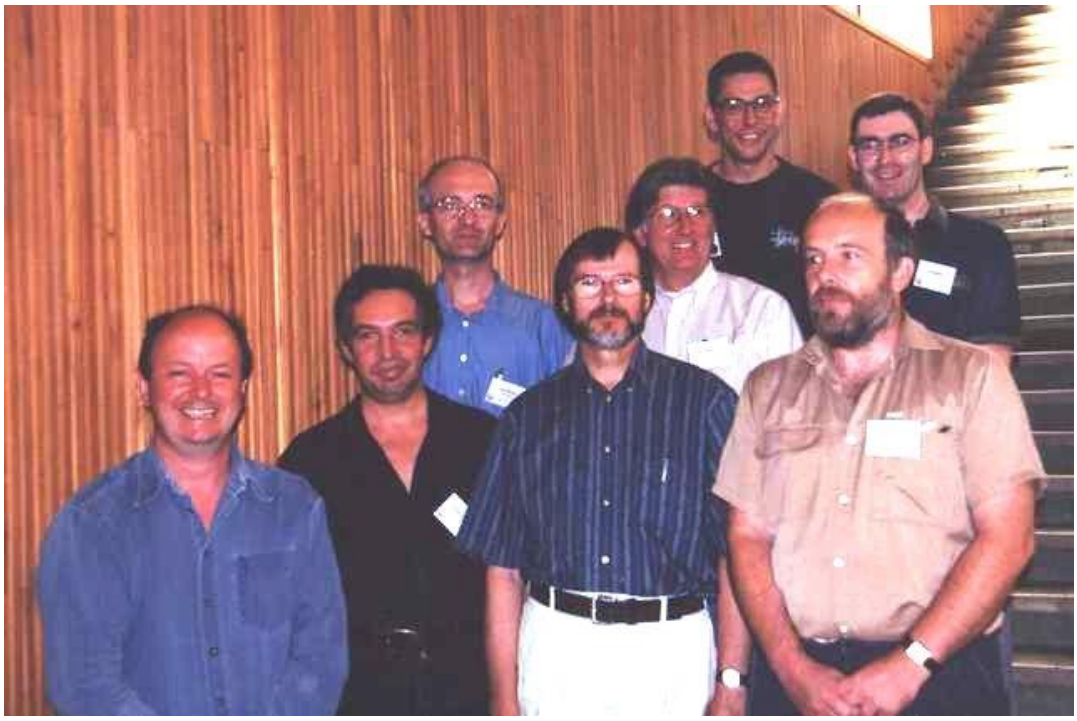
With Ray Young (yes, the famous editor of "*The Rietveld method*" book) (right) and Prof. Lin Shao Fan (left) navigating on the Dian lake at the south of Kunming in China (1999) after a workshop :

With Lachlan Cranswick visiting France in 1999. We were quite good, both of us, at organizing the three SDPD-RR (Structure Determination by Powder Diffractometry Round Robin) in 1998, 2002 and 2008 :

Picture of me (2nd from the right) becoming already quite excellent, with Gérard Férey (CNRS 2010 Gold medal), Le Mans, 1987. Gérard Férey has produced a text on the place of crystallography in his own scientific work. In this text, one can find : ″*Il* (Daniel Louër) *a formé des élèves à cette même rigueur. Leurs noms, à leur tour, deviennent incontournables : Nathalie Audebrand, Nathalie Guillou et surtout Armel Le Bail (la méthode de Le Bail) dont j'ai eu la chance de bénéficier des bienfaits lorsqu'il a rejoint notre laboratoire du Mans.*" Ahem... Please note that I joined Le Mans in 1981 for working on fluoride glasses. The "*Le Bail method*" was established much later, in 1987, and published in 1988. I left

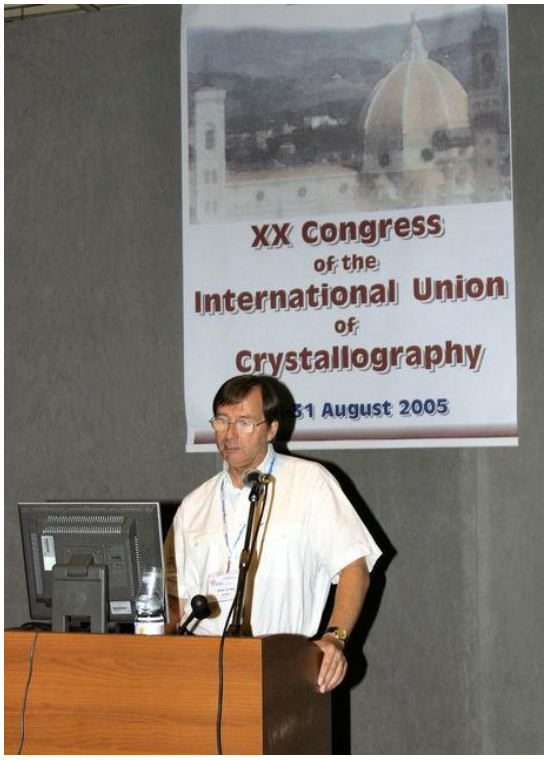
Rennes ten years earlier, after a 3rd cycle thesis (D. Louër director) in 1976, and at that time, no Rietveld fit of any powder pattern had been realized in that town, and very few all over the world. The DICVOL software was not able yet to index monoclinic or triclinic cells from powder patterns. To my knowledge, the extension of DICVOL to monoclinic cells was published in 1982, and to triclinic cells even much later. Anyway, I owe many thanks to Daniel Louër ! Thanks also to Yvon Laligant, Charles Jacoboni, Annie Hémon, Jean-Louis Fourquet, Huguette Duroy, Gérard Férey, Pedro Amoros, Dominique Bazin, Karim Adil (...) for all these fascinating problems which they expected to be solved. Thanks to Anne-Marie Mercier for 33 years of continuous help on the technical and chemistry sides. See all these names and many more (sorry for not giving them all here) as co-authors in the publication list, pages 45-57.

- Devil's advocate : I see... It was "*la vie de château*" ! Something else that would be seriously exceptionnal in your career, apart from having been snapshoted with a few famous guys ?
- The candidate : Am I not famous myself ? See more pictures from my ~40 conferences. For instance, Prague, ECM-18, 1998, with Bill David, Kenneth Shankland, Kenneth D.M. Harris, Rainer Rudert, Bob von Dreele, Lubomir Smrcok (etc) surely you recognize that some of them are really famous :



Durban, South Africa, ECM-21, 2003, with Robin Shirley, Juan Rodriguez-Carvajal, Vincent Favre-Nicolin, Lachlan Cranswick, (etc) :

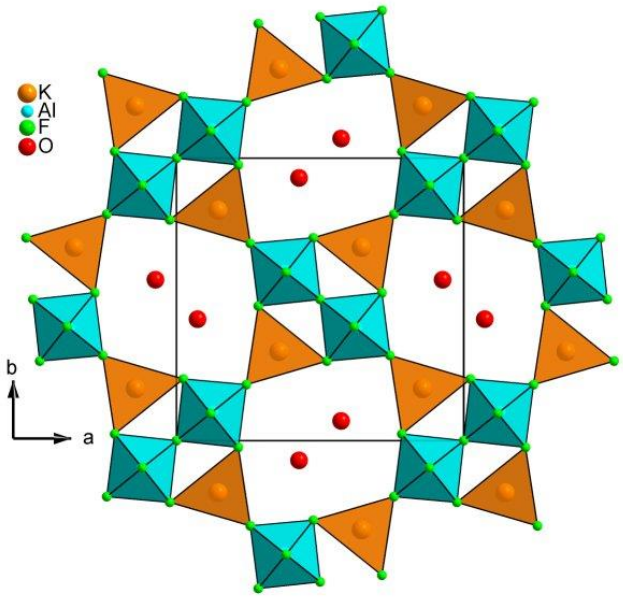
Florence, Italy, 2005, speaking about crystal structure prediction with the GRINSP software :



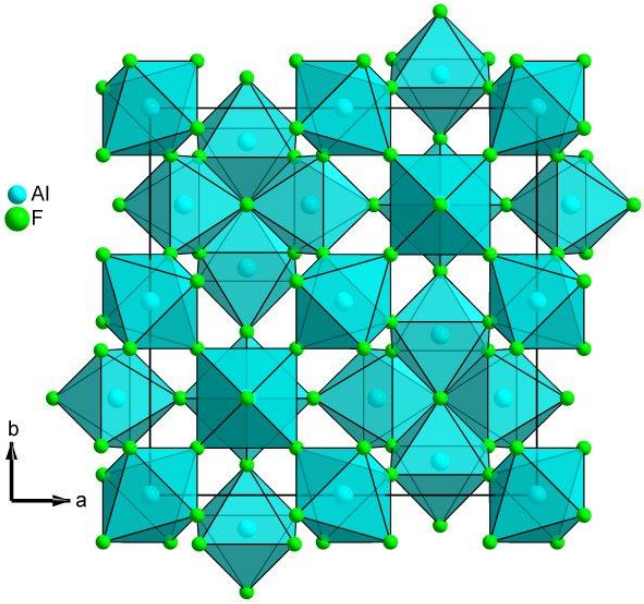
- Devil's advocate : Famous, maybe, perhaps insufficiently, known by less than 2000 researchers, not enough. And since you became DR1 in 2010, have you done some exceptionnal new sparks ? I notice that you sent 15 scientific reports before to obtain that DR1 promotion, one report each year during 15 years, a nice example of perseverance, but you stayed 20 years as a DR2, which is not a very good point !

- **The candidate :** Well, I have more pictures... Anyway, I think that being able to convince you would be more than exceptionnal. As sparks, let me show you the drawings of all the crystal structures I solved by using powder diffraction methodologies, in the past, and recently (1987-2015). Each of them was a performance, some requiring months if not years of efforts. First some interesting fluorides refusing to grow in large-enough single crystals (thermal decomposition or transition products, etc) - remember we were the "Laboratory of Fluorides". After all, 2014 is the International Year of Crystallography, so enjoy :

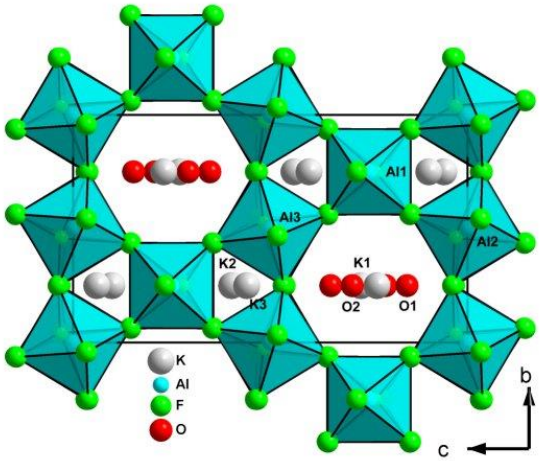
(numbers under brackets refer to the list of publication pages 45-57)



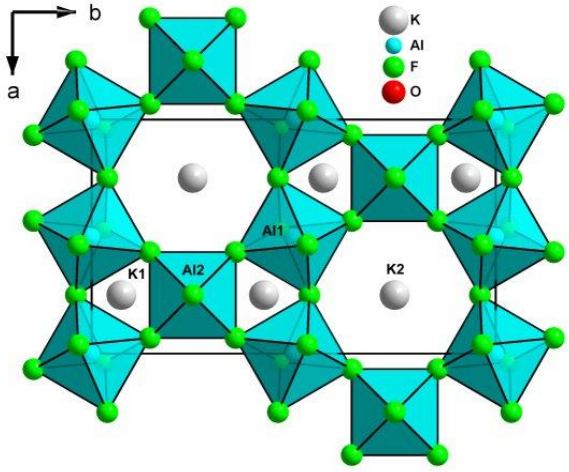
$K_2(H_5O_2)(Al_2F_9)$ obtained from a spontaneous decomposition of $K(H_3O)_2AlF_6$ in a drawer [78]



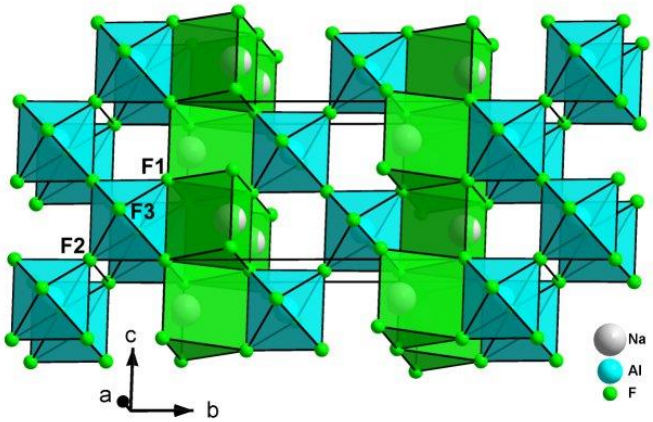
τ-AlF_3 [81] crystallizing from amorphous AlF_3, appearing scarcely in lists of MF_3 compounds !



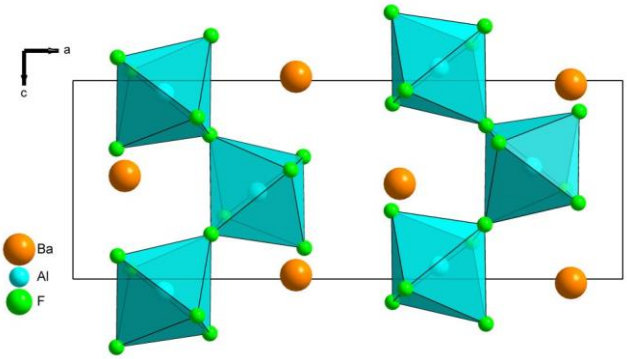
$K_3Al_3F_{12}.2H_2O$ [166]



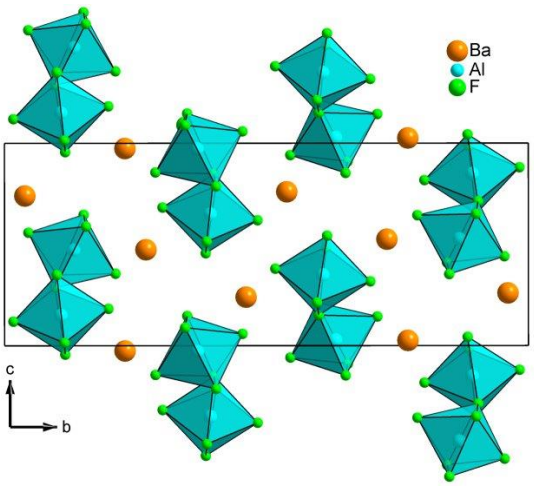
$K_3Al_3F_{12}.H_2O$ [166]



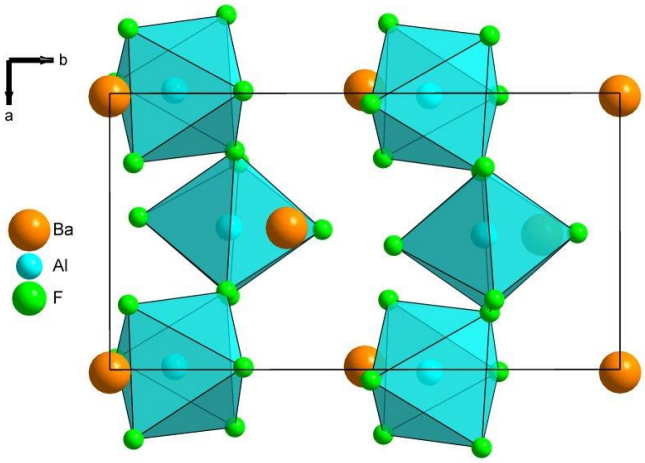
$NaAlF_4$ [165] structure solved dozens of years after it was supposed to exist



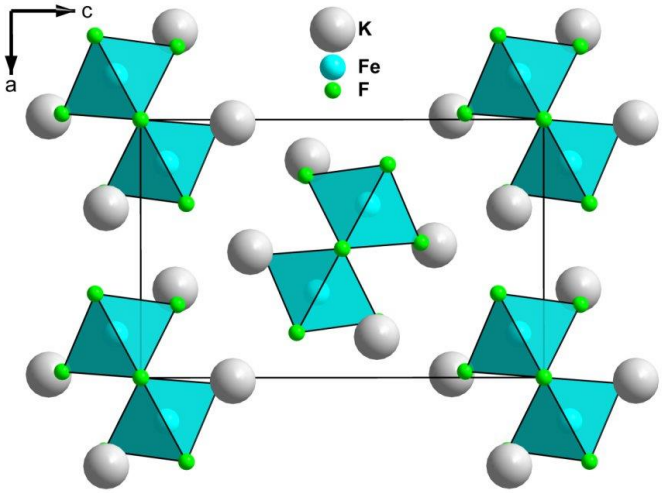
α-$BaAlF_5$ [62]



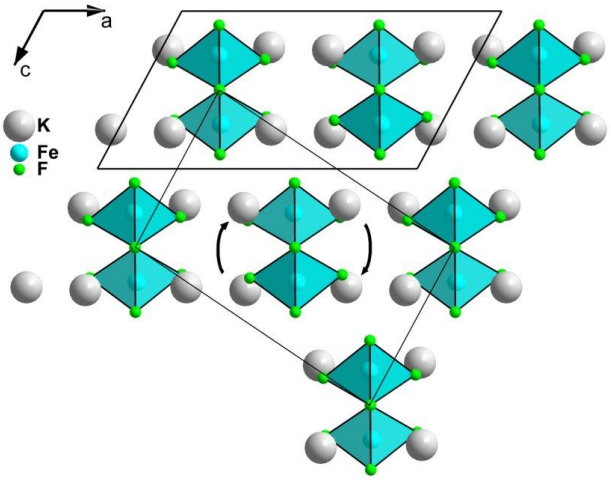
β-$BaAlF_5$ [62]



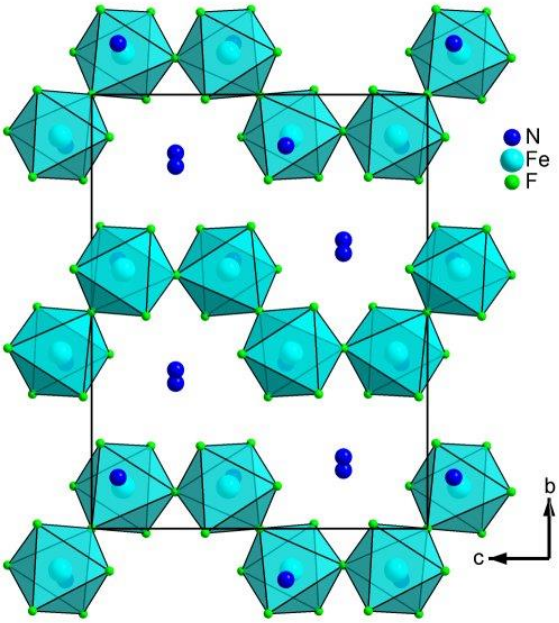
γ-$BaAlF_5$ [62]



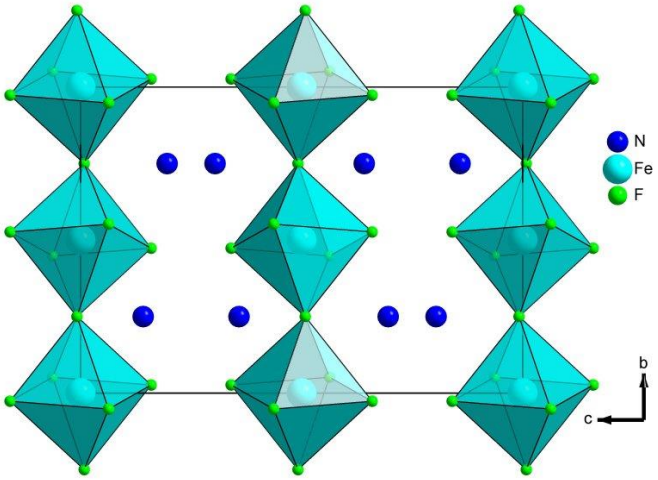
K_2FeF_5 form III [186]



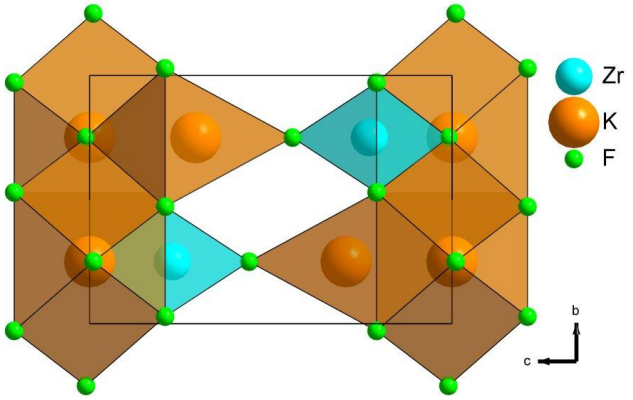
K_2FeF_5 form IV [186]



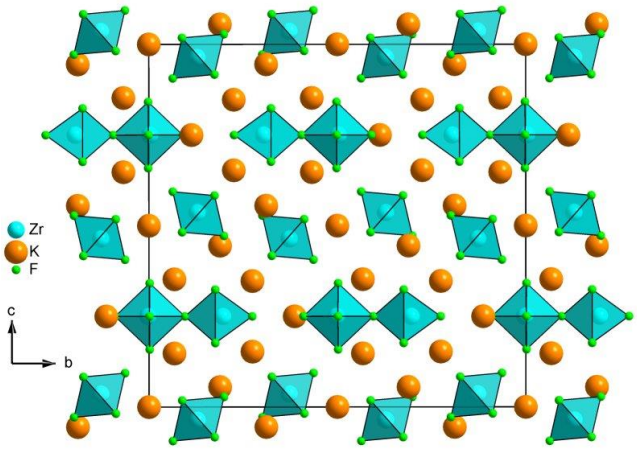
α-$(NH_4)_2FeF_5$ [50]



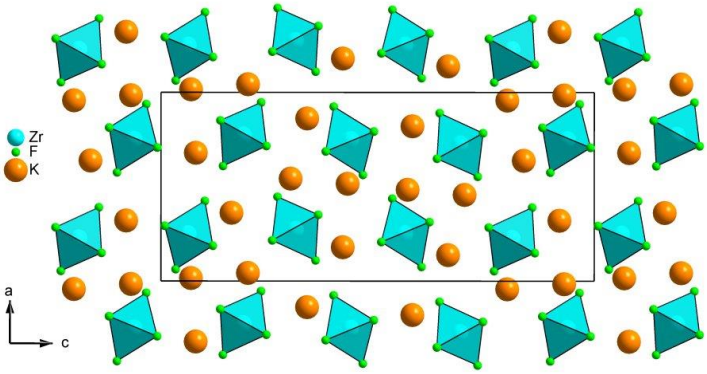
β-$(NH_4)_2FeF_5$ [50]



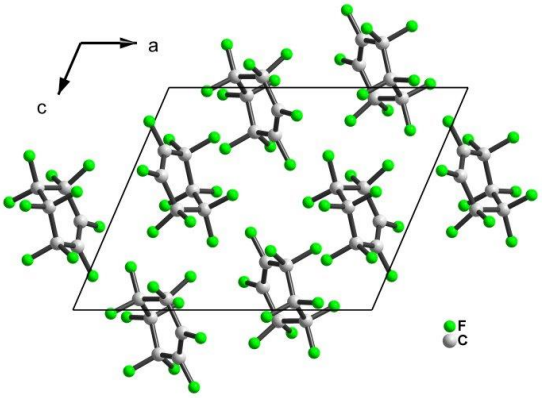
K_2ZrF_6 - form V [192]



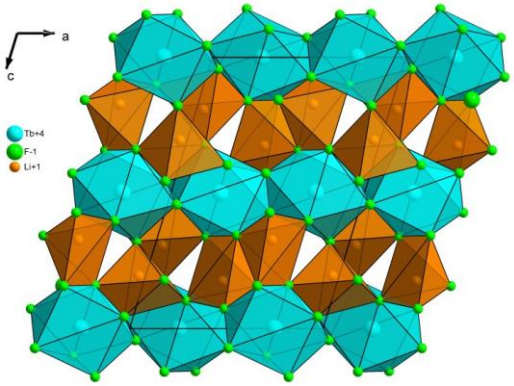
K_2ZrF_6 - form VI [192]



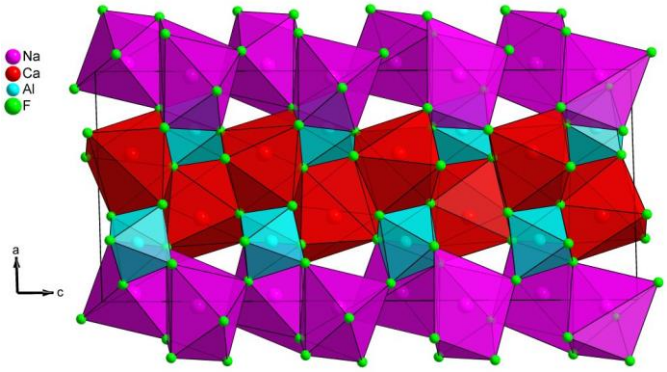
K_2ZrF_6 - form VII [192]



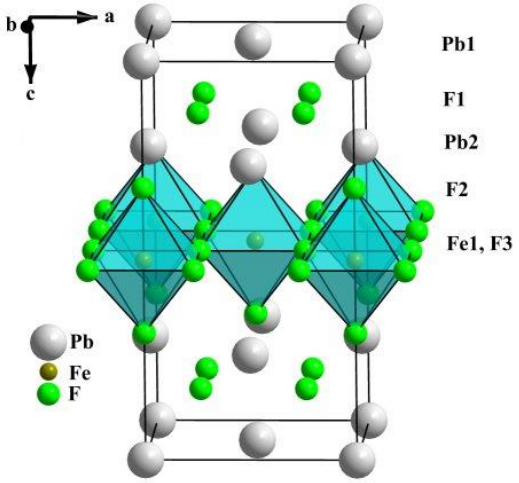
C_6F_{10} was waiting since 1981 [182]



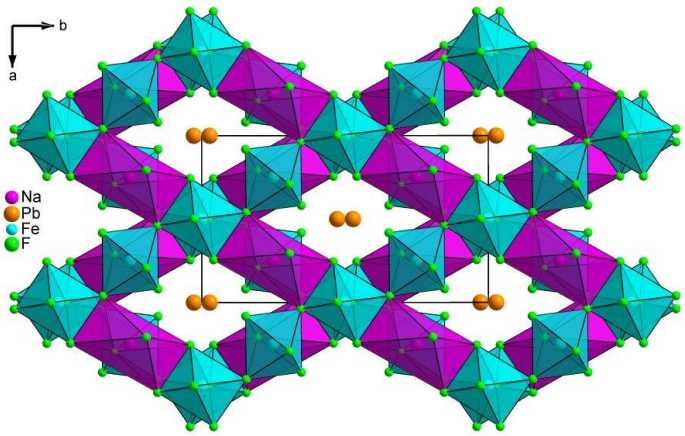
Li_2TbF_6 [39]



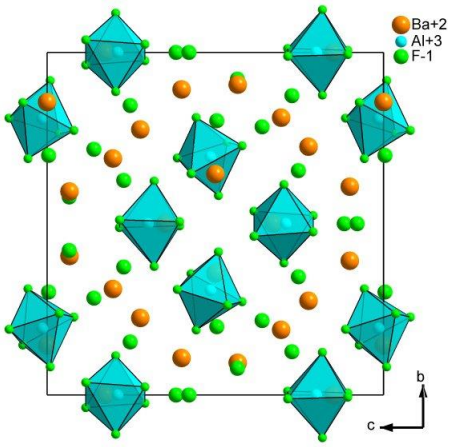
α-$NaCaAlF_6$ [109]



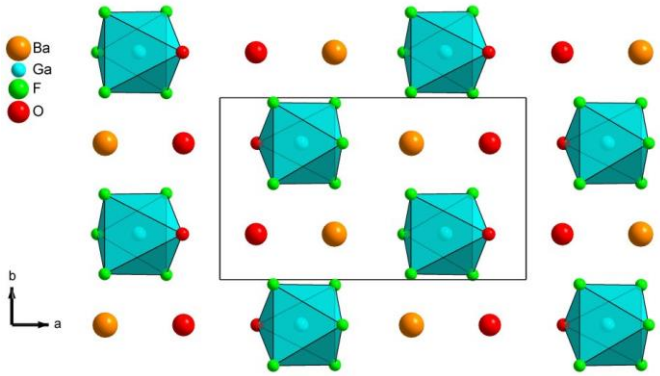
β-$Pb_{1-x}Fe_xF_{2+x}$ ($0.25 \leq x \leq 0.27$) (~Pb_3FeF_9) [177]



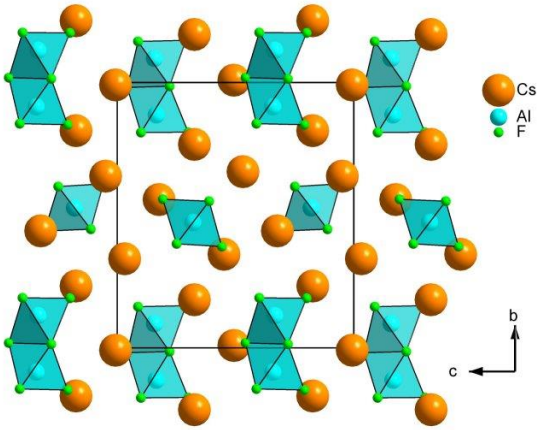
$NaPbFe_2F_9$ [52] one of my first SDPDs, the referee first refused to believe it



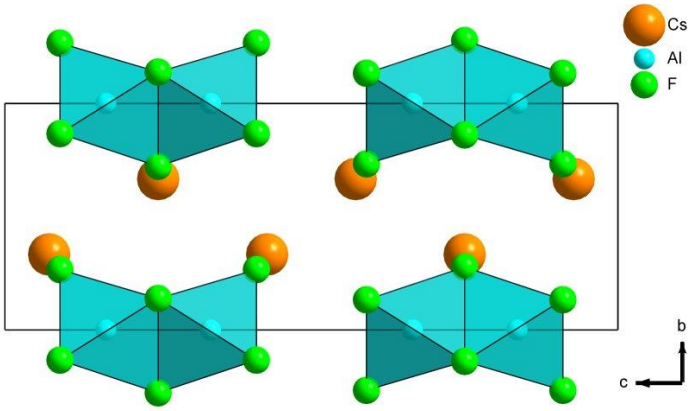
β-Ba_3AlF_9 with 29 independent atoms [88]



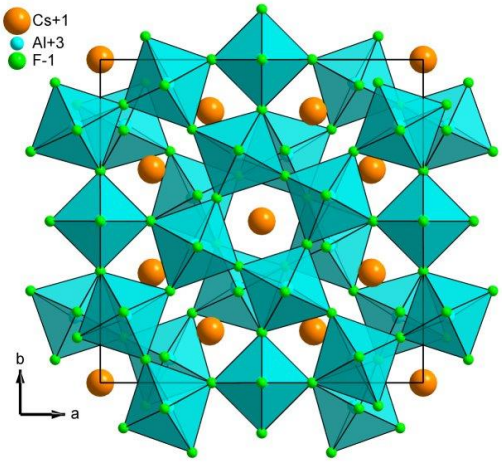
$BaGaF_5.2H_2O$ [104]



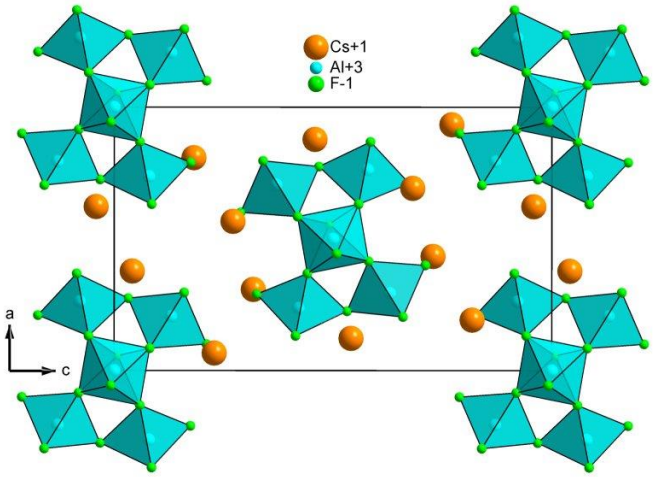
Cs_2AlF_5 : 20 years efforts [189]



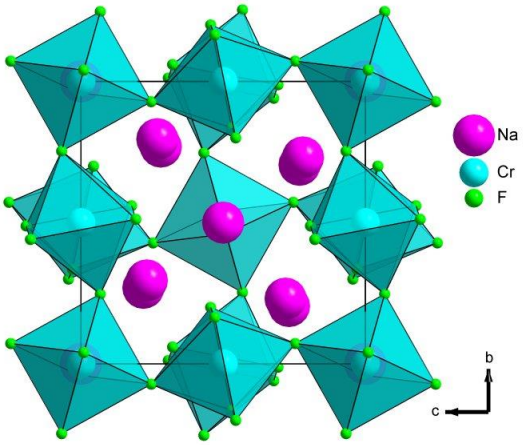
$Cs_3Al_2F_9$ [189]



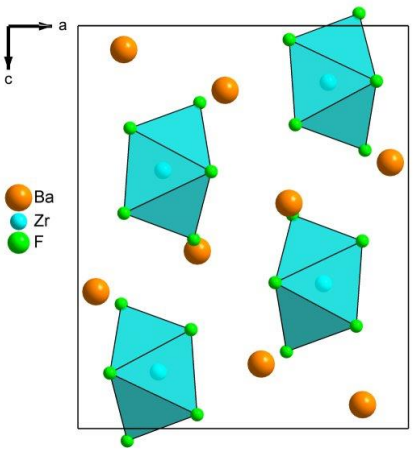
β-$CsAlF_4$ [77]



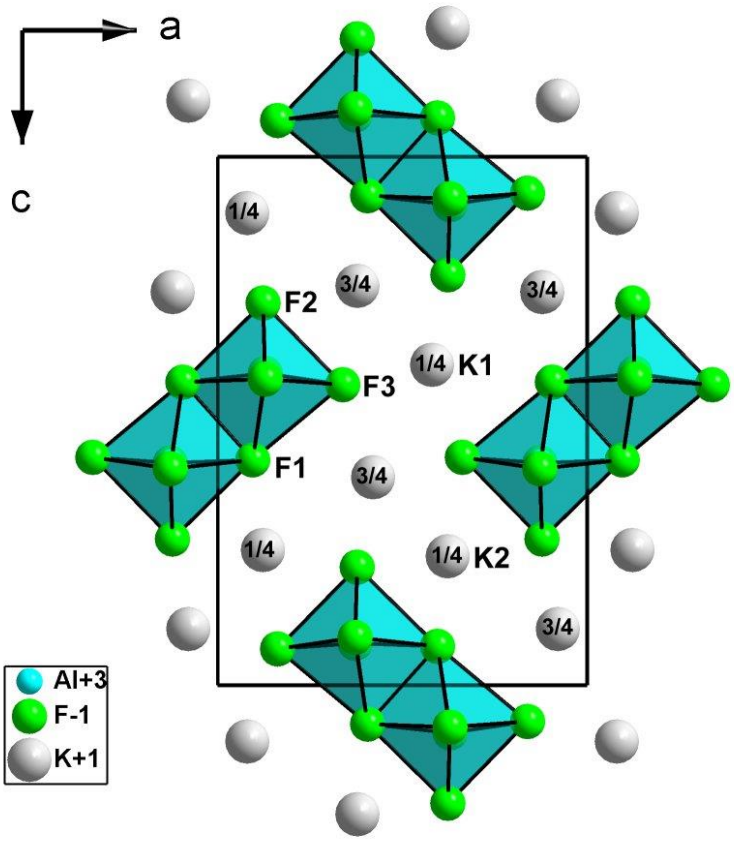
γ-$CsAlF_4$ [77]



$Na_5Cr_3F_{14}$ [131]

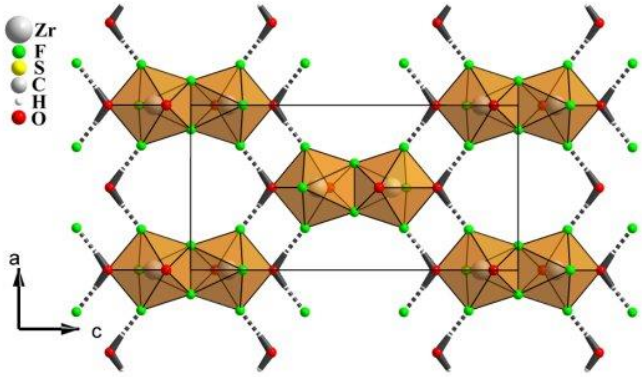


α-Ba_2ZrF_8 [107]

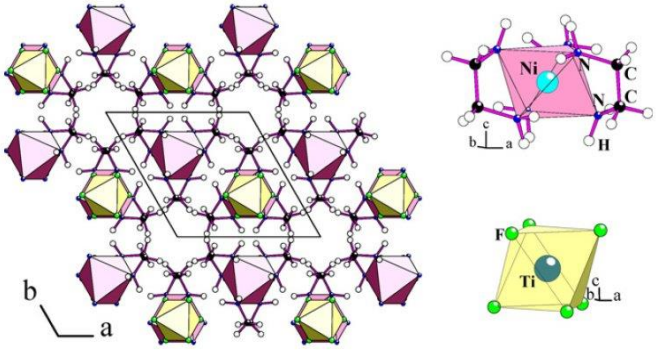


θ-$KAlF_4$
from the thermolysis of $K_2(H_5O_2)(Al_2F_9)$,solved after 20 years efforts [163]

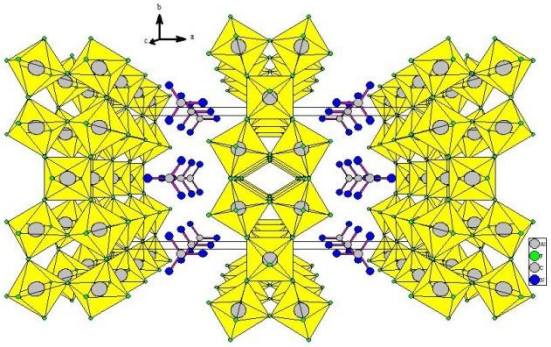
The candidate : A few hybrids containing fluorine ions, that were solved from powder diffraction data too :



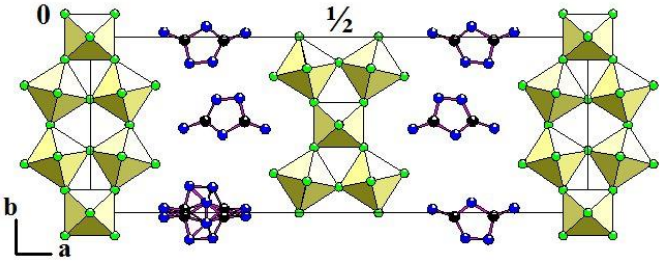
Di-mu-fluoro-bis[aqua-(dimethyl sulfoxide)
-trifluorozirconium(IV)] - $C_4H_{16}F_8O_4S_2Zr_2$ [172]



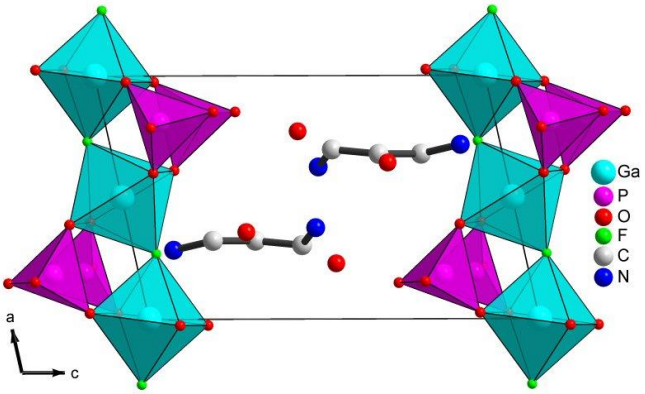
$[Ni(en)_3].(TiF_6)]$ [179]
(*en* = ethylene diamine)



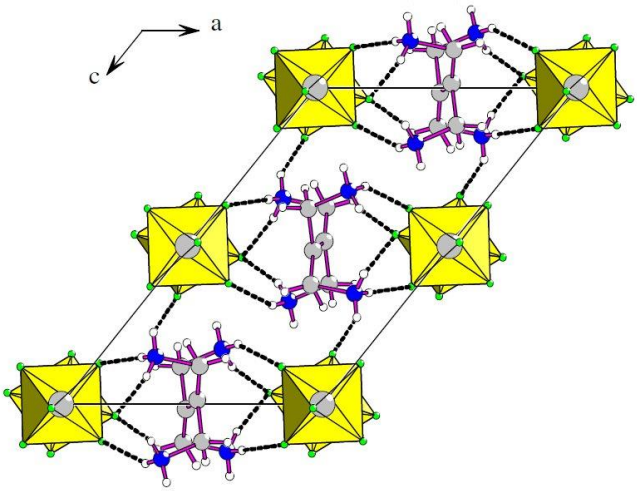
Layered hybrid fluoroaluminate $C_2H_{12}Al_5F_{17}N_6$ [167]



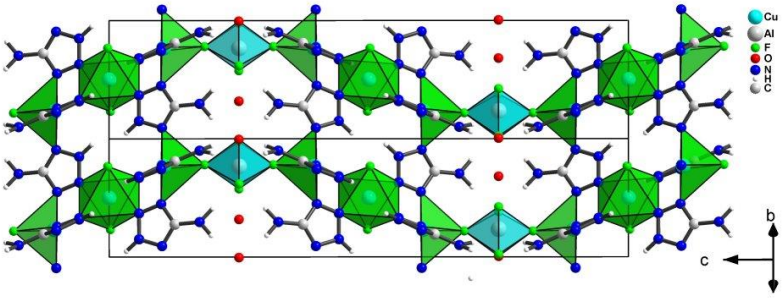
2D Guanazolium fluoroaluminate $C_4H_{12}Al_5F_{17}N_{10}$ [173]



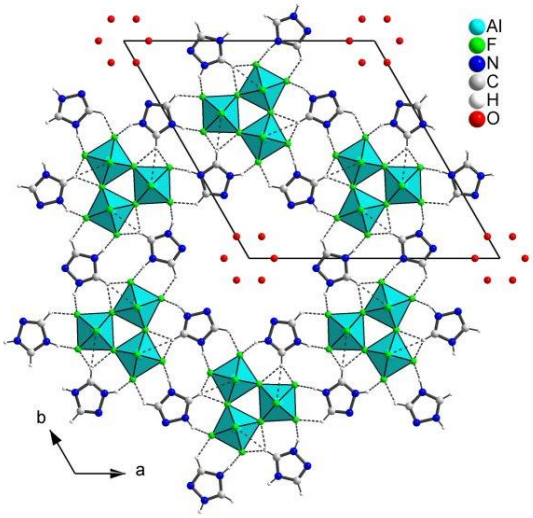
$Ga(HPO_4)_2F.H_3N(CH_2)_3NH_3.2H_2O$ [118]



1D hybrid fluoroaluminate $C_6N_4H_{20}Al_2F_{10}$ [149]

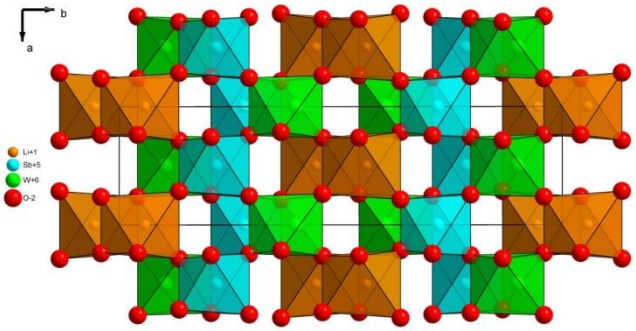


$Cu_3AlF_7O[CH_3N_5]_4.H_2O$ [194]

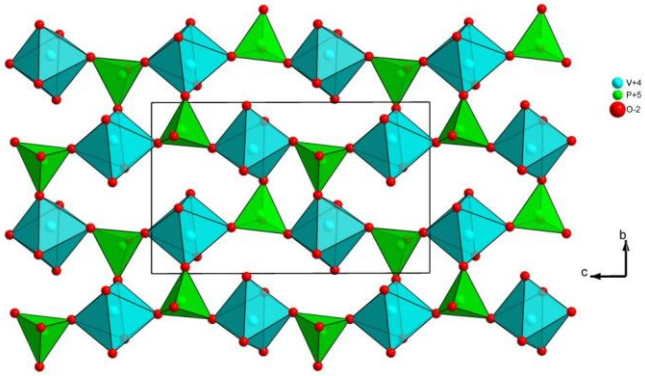


$[Htaz]_3•(Al_3F_{12})•3H_2O$ [191]

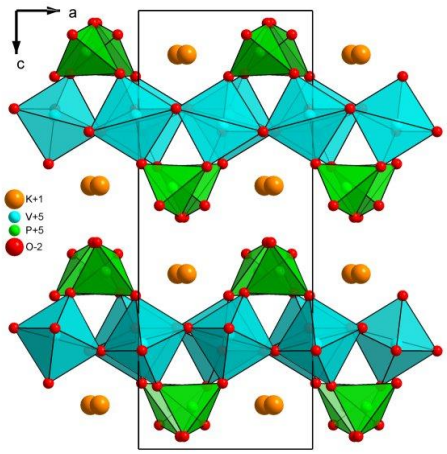
The candidate : Then some oxides, including phosphates (etc), as well solved *ab initio* from powder diffraction data :



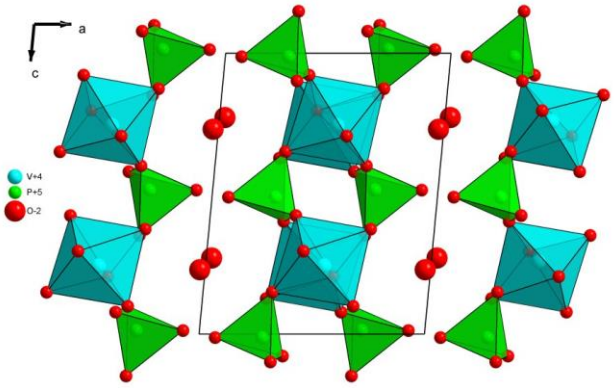
$LiSbWO_6$ [31] first case using the "Le Bail method" in 1988



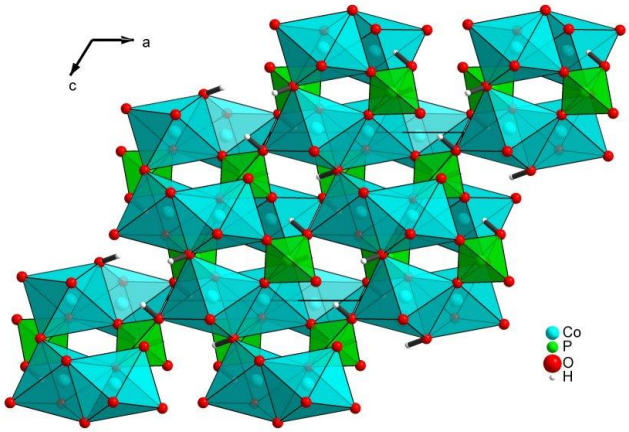
β-$VO(HPO_4).2H_2O$ [43], saving (with other structures below) the thesis of a future spanish PhD



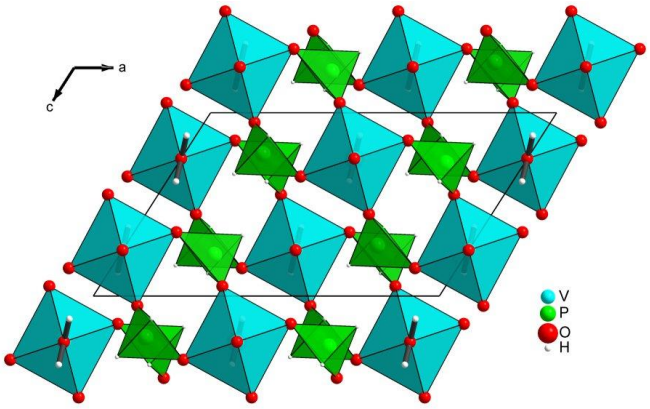
$KVO_2(HPO_4)$ [40]



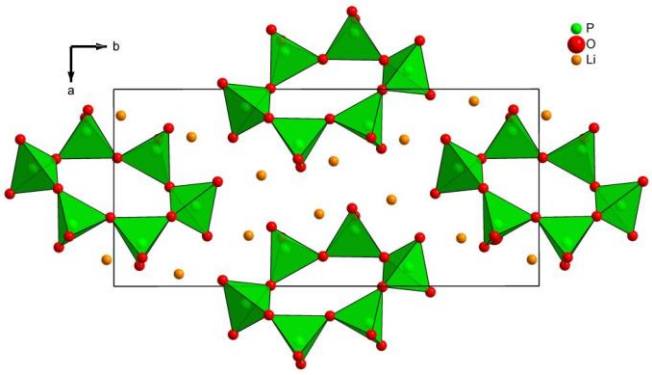
α-$VO(HPO_4).2H_2O$ [51]



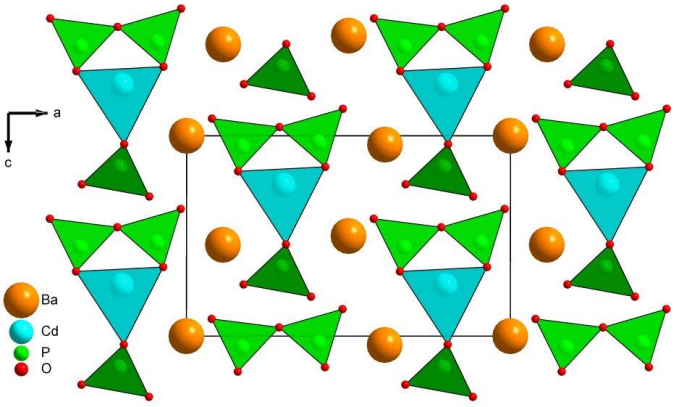
$Co_3(HPO_4)(OH)_2$ [68]



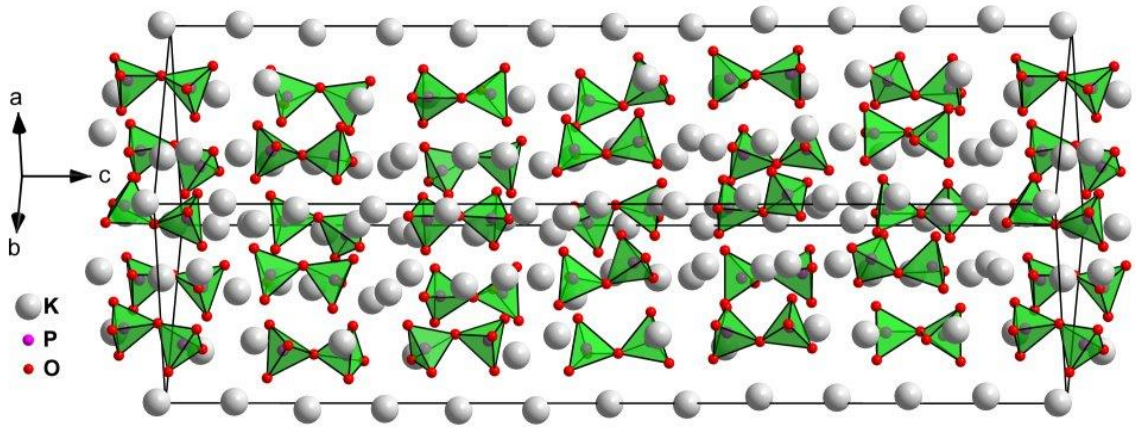
$(VO)(H_2PO_2)_2(H_2O)$ [92]



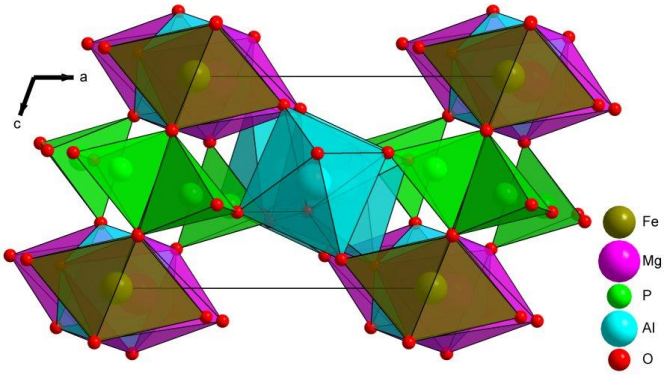
$Li_6P_6O_{18}$ [108]



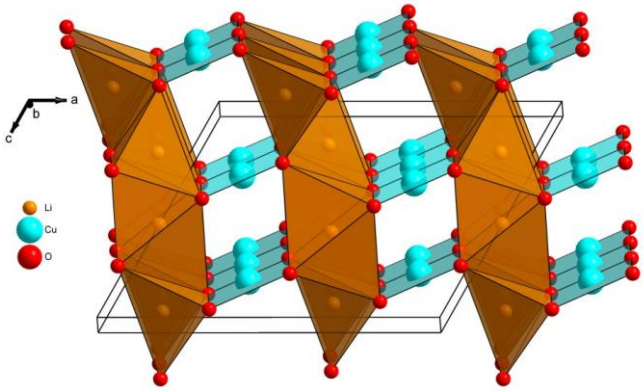
$CdBa_2(P_2O_7)(HPO_4)$ [115]



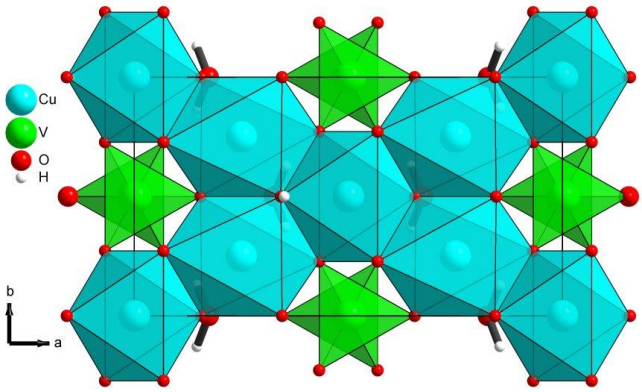
ó-$K_4P_2O_7$ [180]



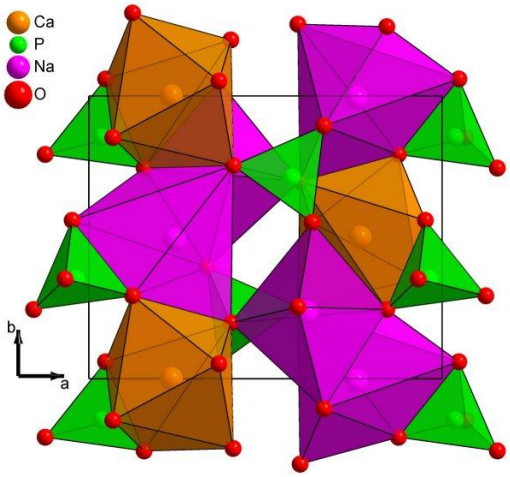
Gormanite : $(Fe,Mg)_3(Al,Fe)_4(PO_4)_4(OH)_6 \cdot 2H_2O$ [132]



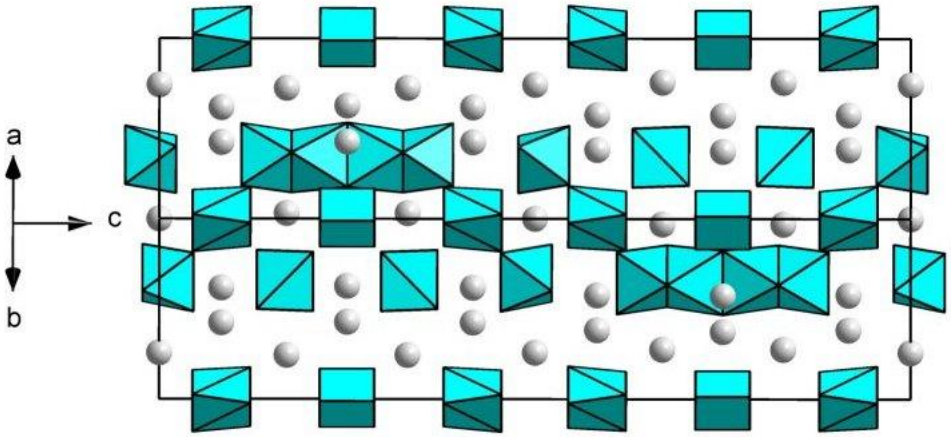
$Li_3Cu_2O_4$ [86]



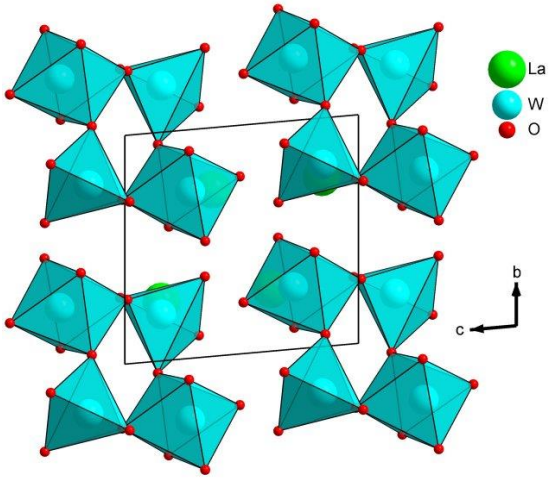
Volborthite : $Cu_3(V_2O_7)(OH)_2(H_2O)_2$ [53]



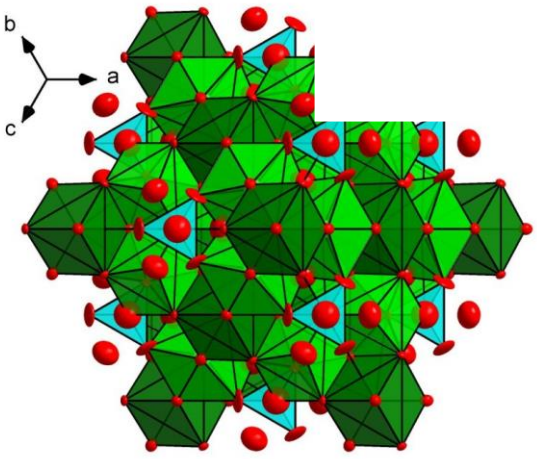
$Na_2Ca(HPO_4)_2$ [105]



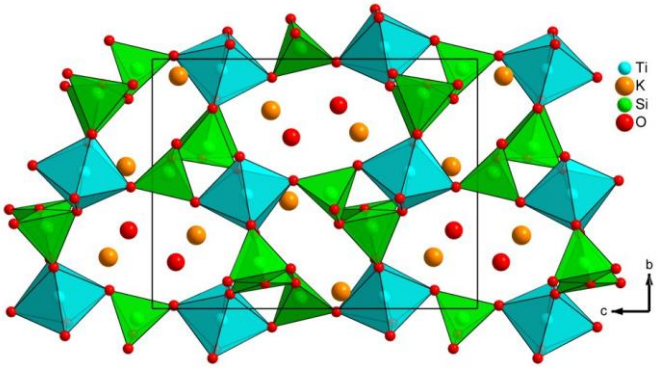
$La_{18}W_{10}O_{57}$ [164]



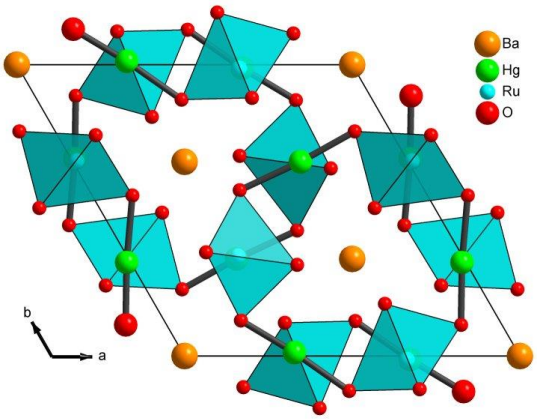
α-$La_2W_2O_9$ [124]



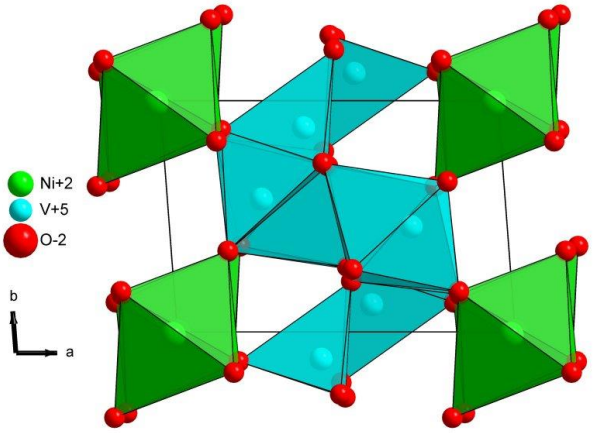
$La_{10}W_2O_{21}$ [187]



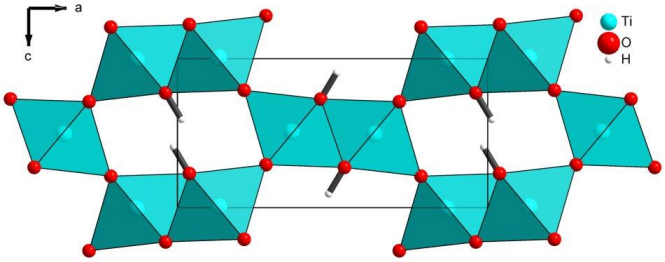
$K_2TiSi_3O_9.H_2O$ [103]



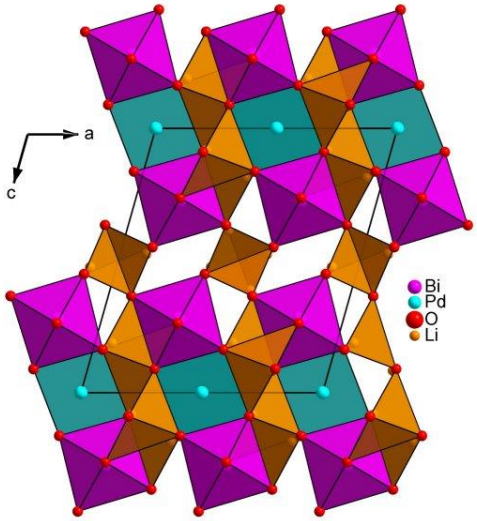
$BaHgRuO_5$ [99]



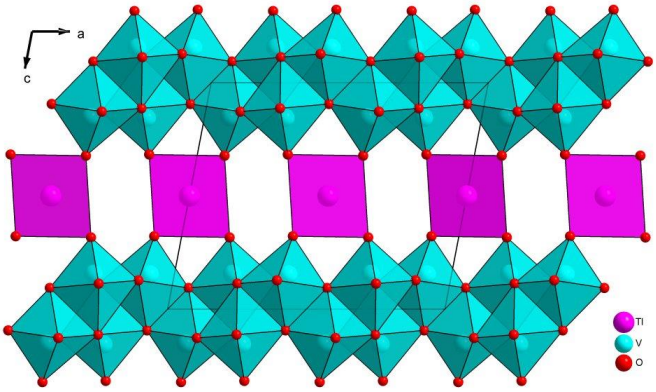
NiV_2O_6 [63]



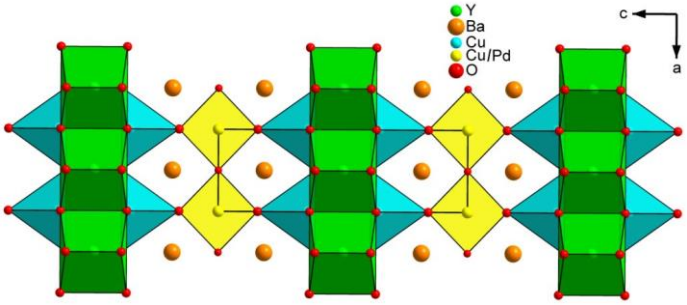
$H_2Ti_3O_7$ [80]



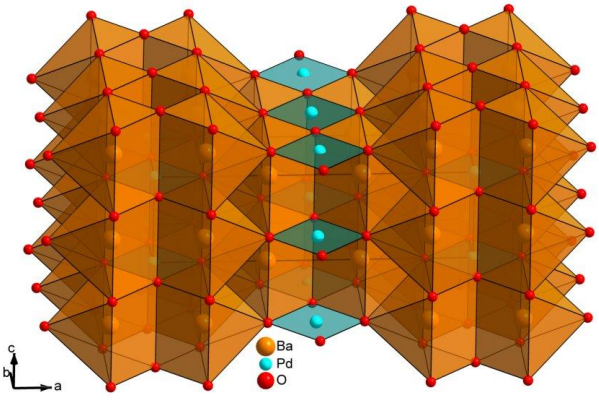
$Li_8Bi_2PdO_{10}$ [91]



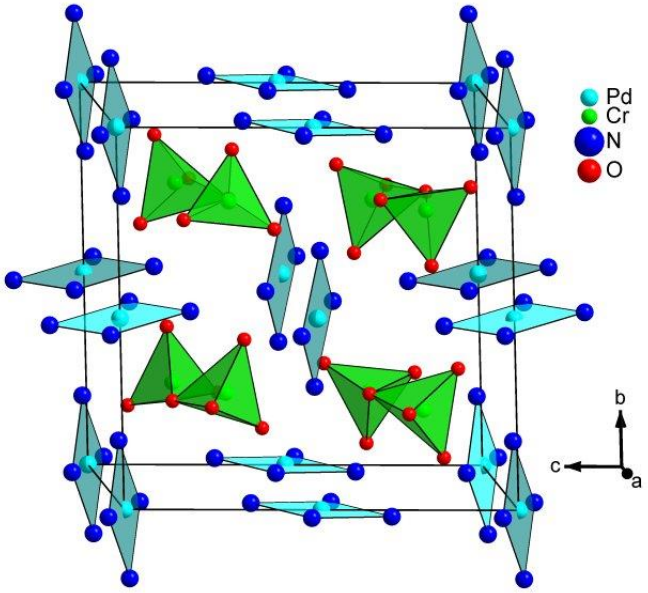
TlV_4O_{10} [75]



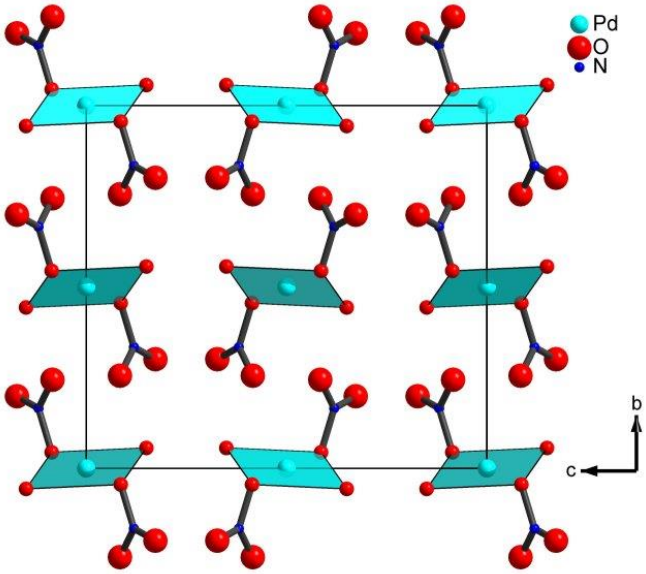
$YBa_2Pd_{0.5}Cu_{2.5}O_7$ [33]



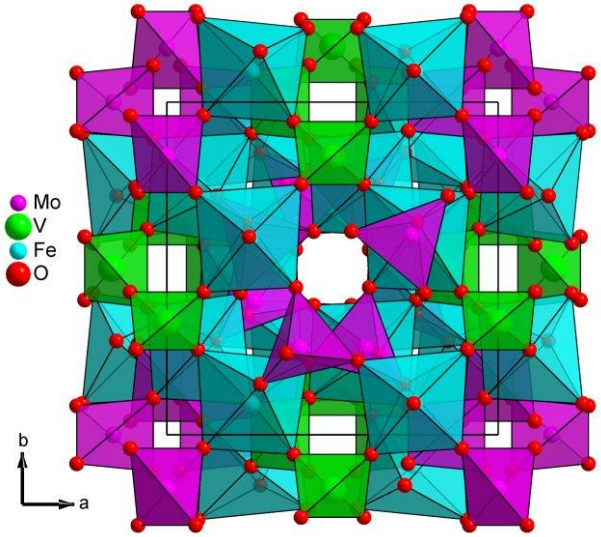
Ba_2PdO_3 [34]



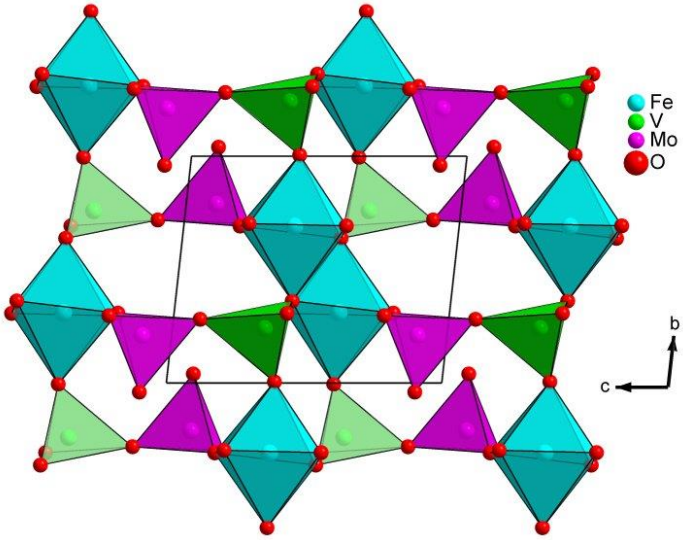
$Pd(NH_3)_4Cr_2O_7$ [93]



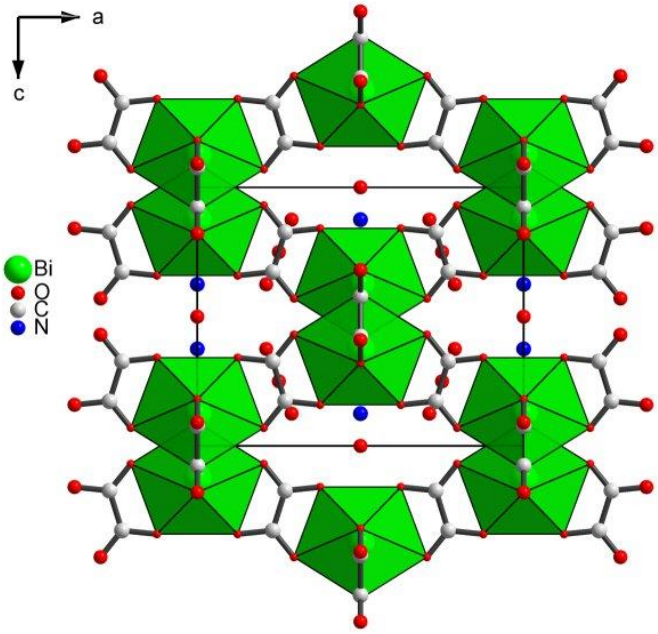
$Pd(NO_3)_2(H_2O)_2$ [67]



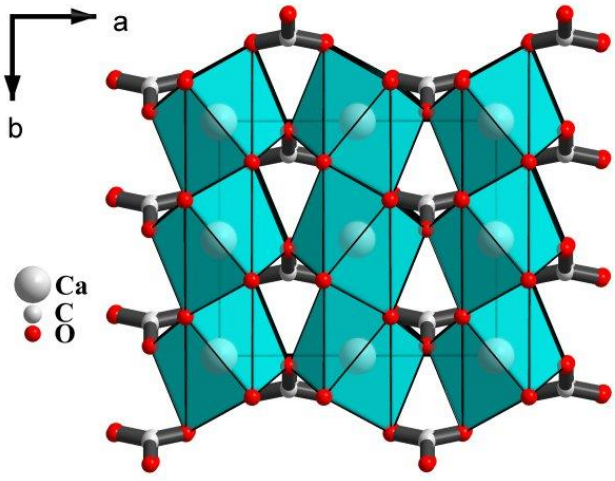
$Fe_4V_2Mo_3O_{20}$ [96]



$FeVMoO_7$ [98]

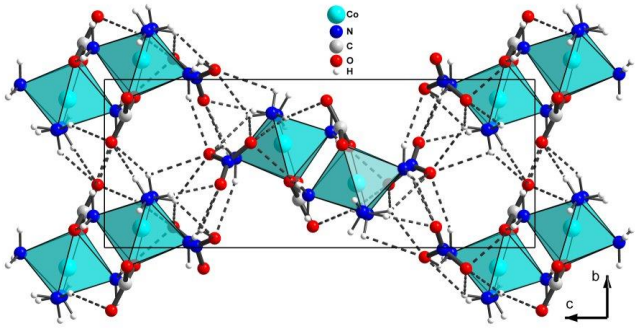


$Bi(NH_4)(C_2O_4)_2.xH_2O$ [137]

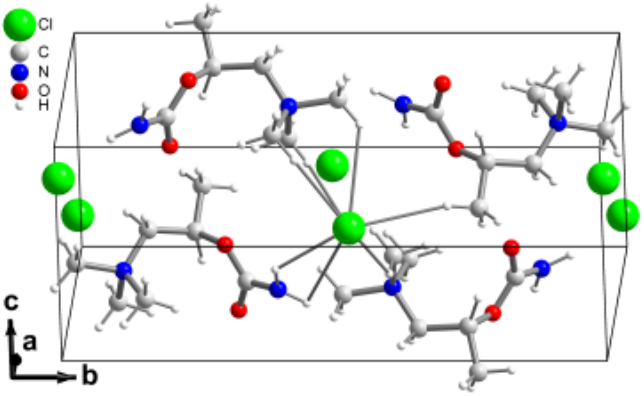


$CaCO_3$ Vaterite [174]

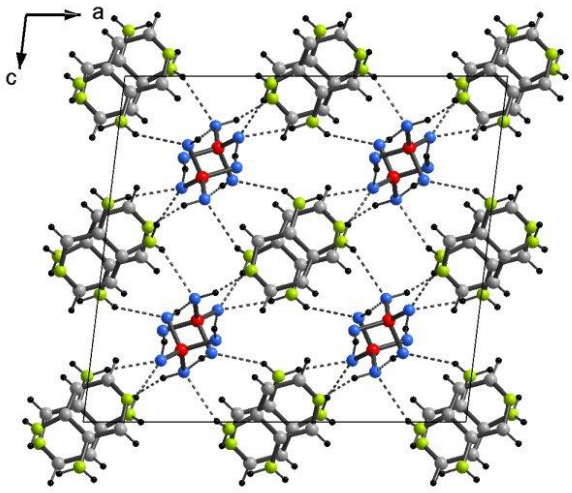
The candidate : Also some kidney stones, or pharmaceutical compounds, or (...) solved from powder diffraction data too :



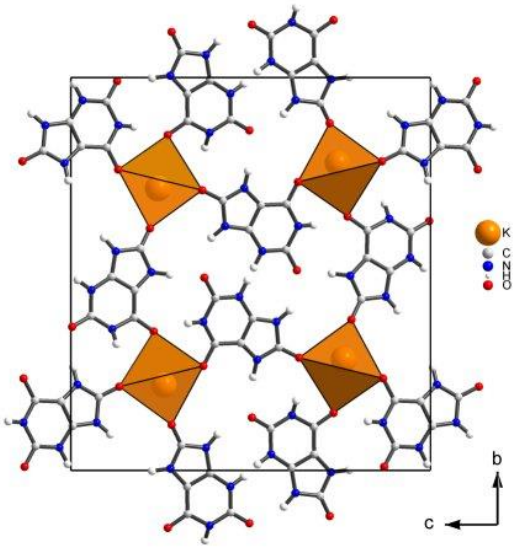
Tetrammine-Carbonatocobalt(III) Nitrate
$[Co(CO_3)(NH_3)_4]NO_3$ [183]



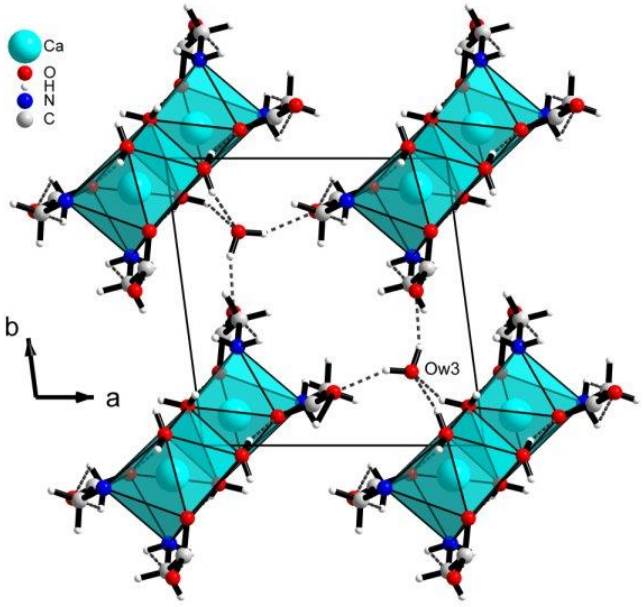
bethanechol chloride - $C_7H_{17}ClN_2O_2$
pharmaceutical compound [168]



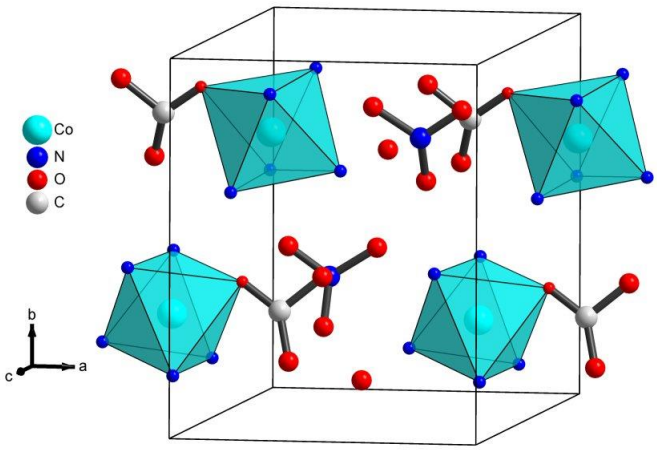
3,4-diaminopyridin-1-ium dihydrogen phosphate
$C_5H_8N_3(H_2PO_4)$ - pharmaceutical compound [176]



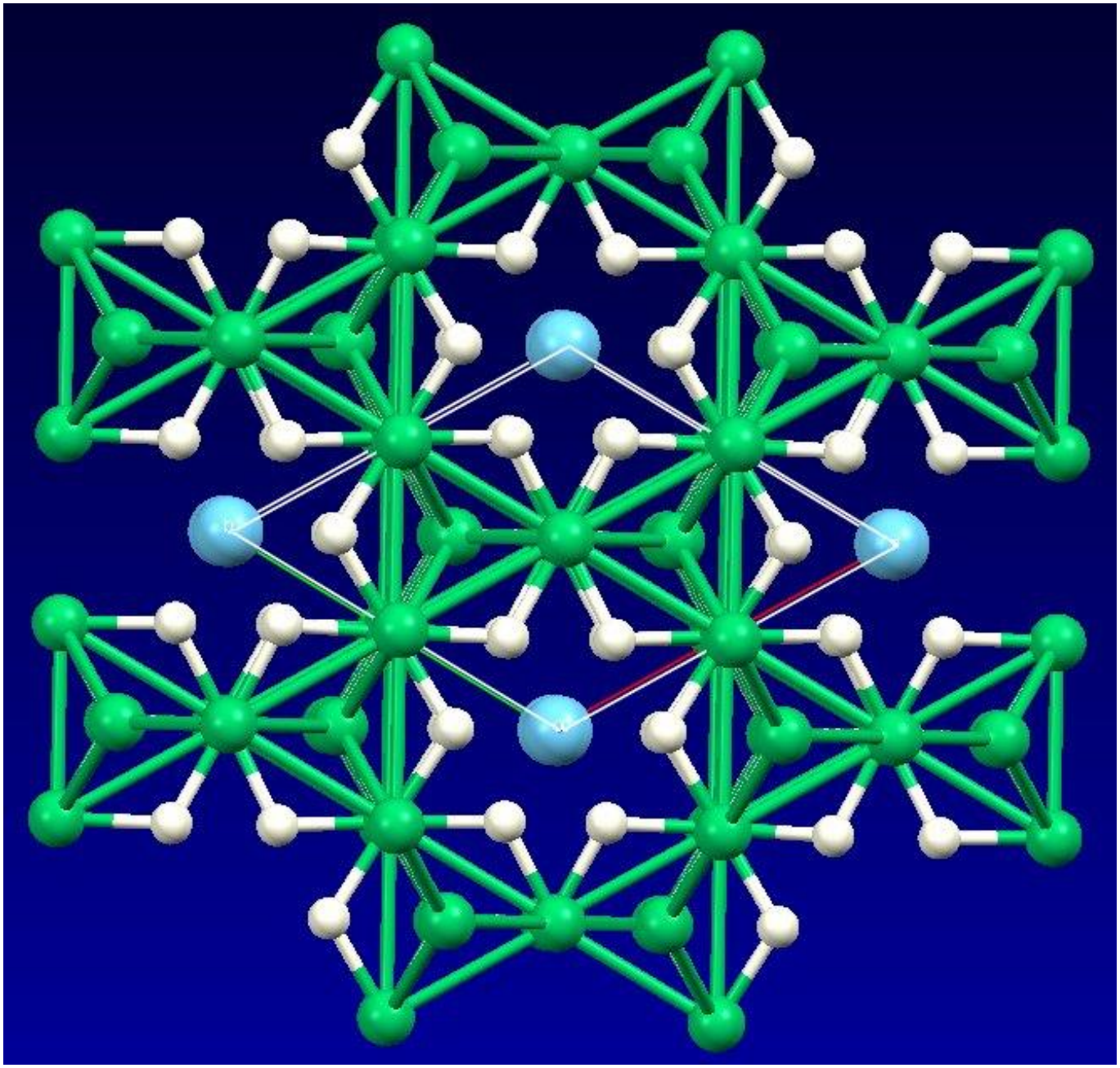
uric acid monopotassium urate [190]
$[C_5H_4N_4O_3]K[C_5H_3N_4O_3]$ - kidney stone



Calcium glycinate trihydrate [181]
$[Ca(C_2H_4NO_2)_2(H_2O)_2]H_2O$ - kidney stone

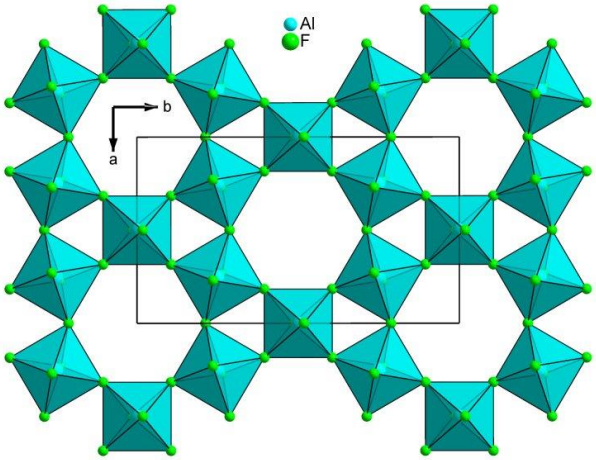


$[Co(NH_3)_5CO_3]NO_3.H_2O$ [111]

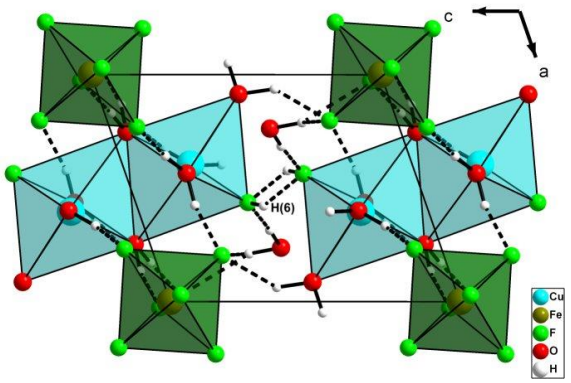


$LaNi_5D_{6.7}$ [26]

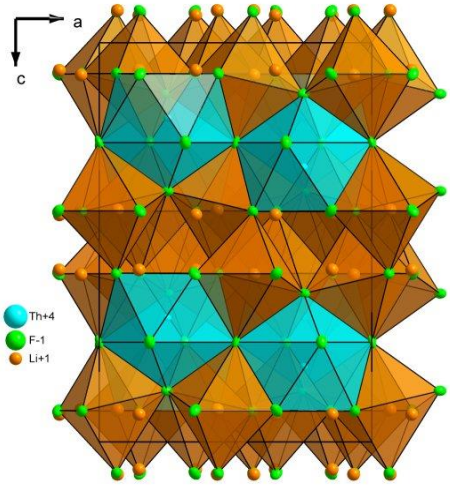
- **The candidate :** And also some crystal structures determined from single crystal data, generally easier than from powder, but not always, especially in case of systematic twinning. Many fluorides of course :



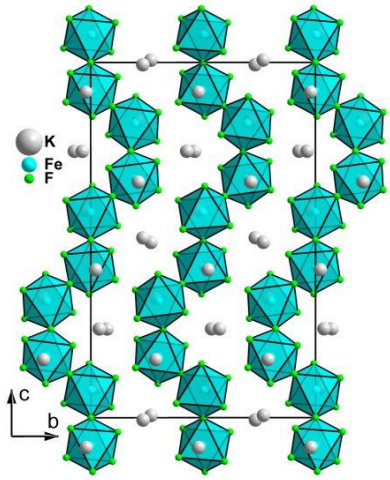
β-AlF_3 [37] orthorhombic pseudo-hexagonal, systematically twinned, three domains at 120°



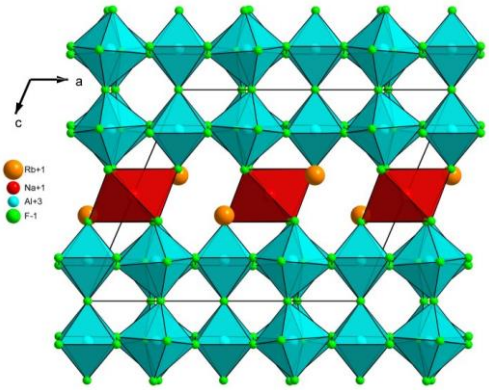
$[Cu_2(HF_2)(H_2O)_8][FeF_6].2H_2O$ [160]



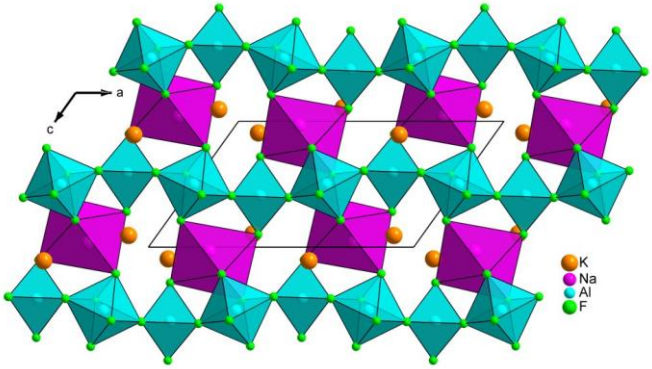
Li_3ThF_7 [44]



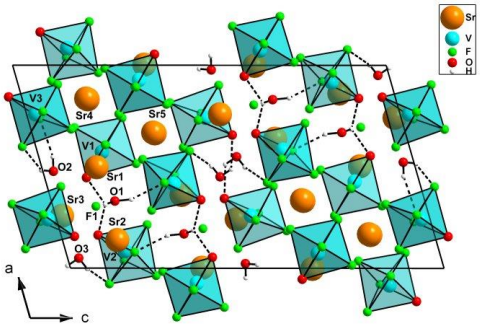
K_2FeF_5- form I [54]



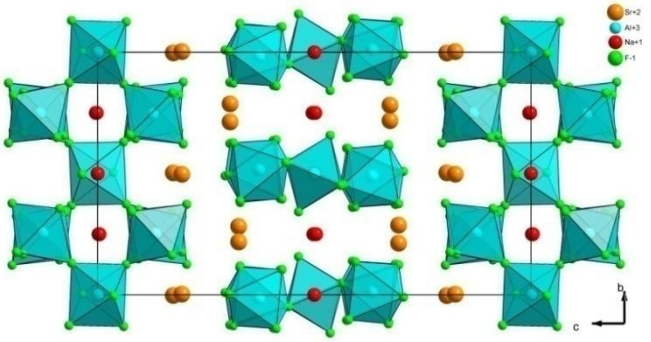
$Rb_2NaAl_6F_{21}$[48] twinned



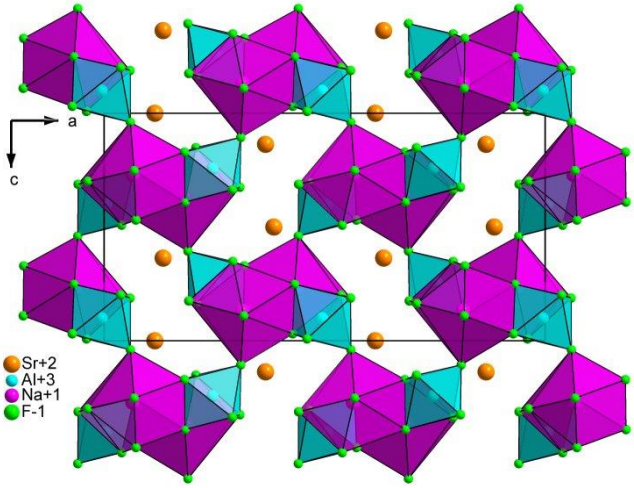
$K_2NaAl_3F_{12}$ [56] twinned



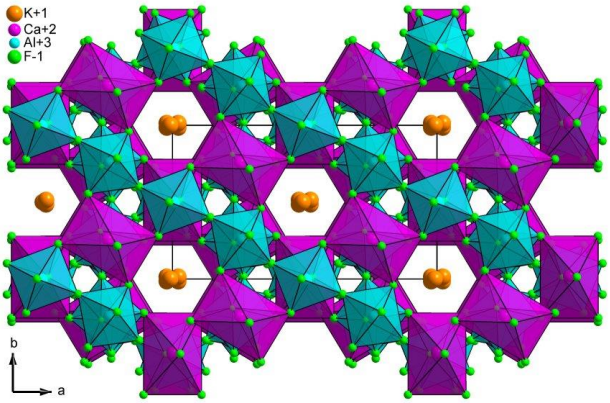
$Sr_5(V^{IV}OF_5)_3F.3H_2O$ [162] twinned



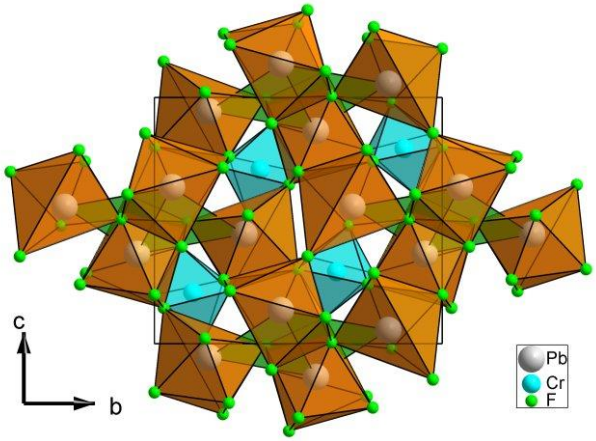
$Na_3Sr_4Al_5F_{26}$ [47] twinned



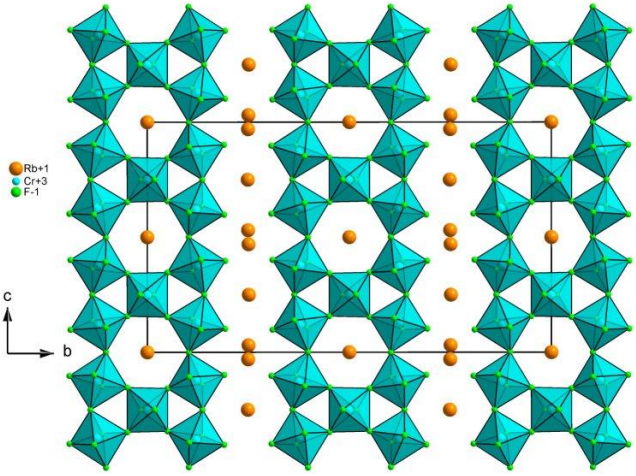
$NaSrAlF_6$ [65]



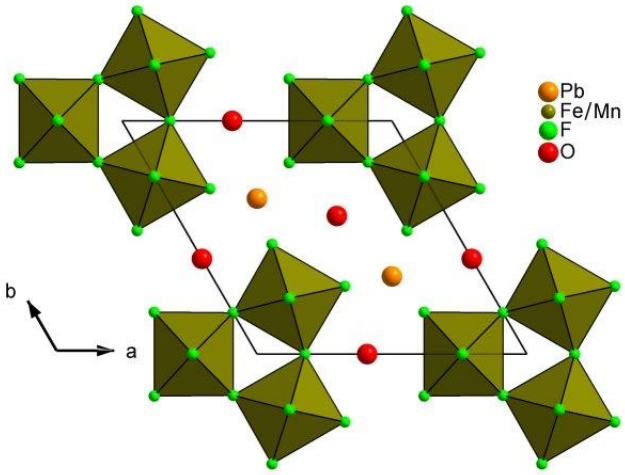
$KCaAl_2F_9$ [87]



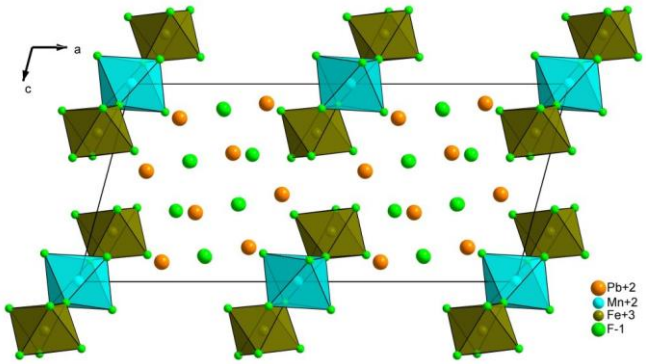
Pb_2CrF_7 [169)



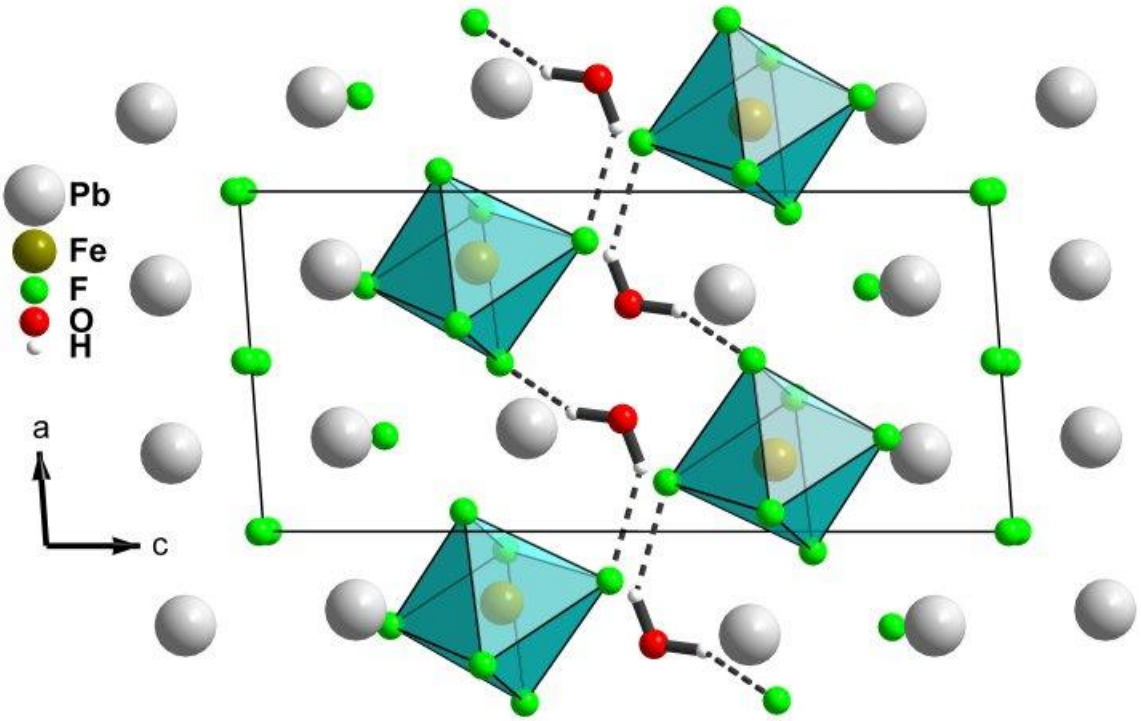
$Rb_2Cr_5F_{17}$ [49]



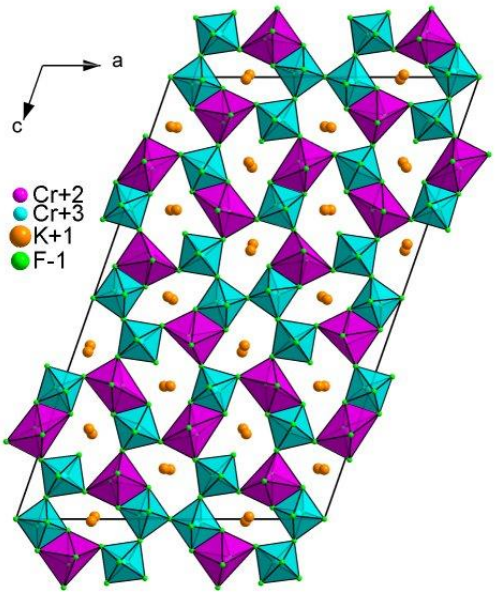
$Pb_2(MnFe_2)F_{12}.3H_2O$ [74]



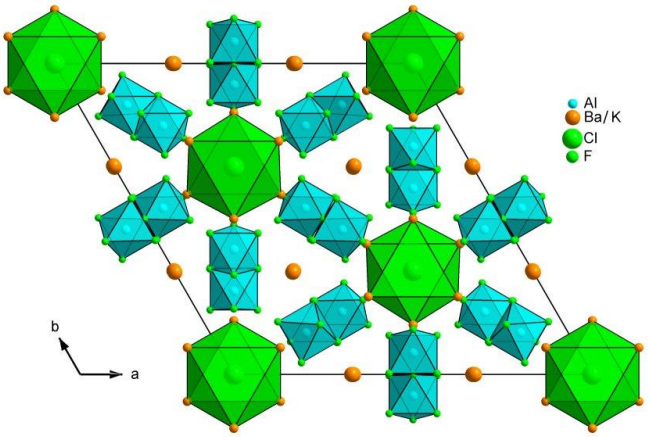
$Pb_8MnFe_2F_{24}$ [73]



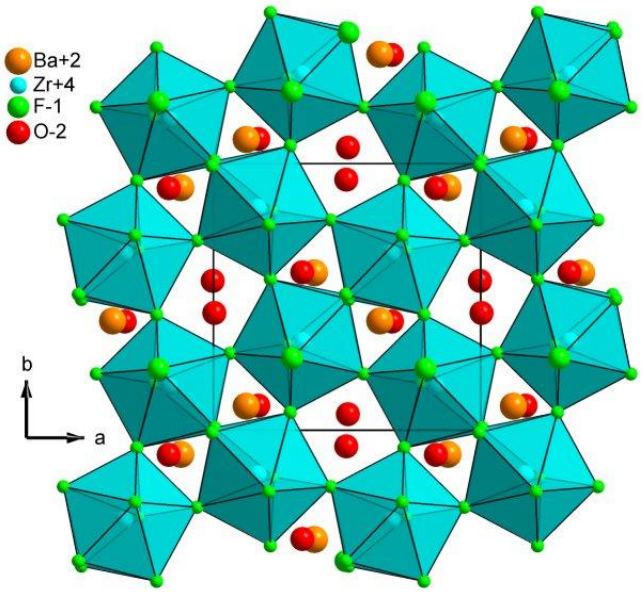
$Pb_3FeF_9.H_2O$ [193]



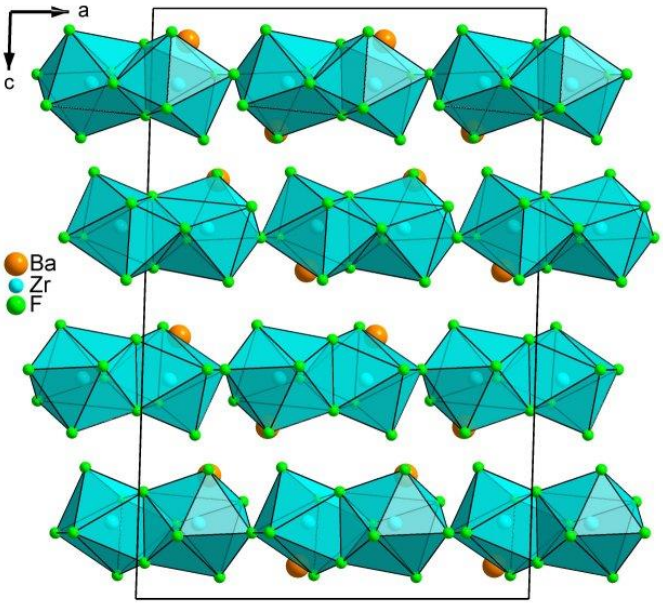
$K_5Cr_{10}F_{31}$ [57] ordered Cr^{2+} and Cr^{3+}



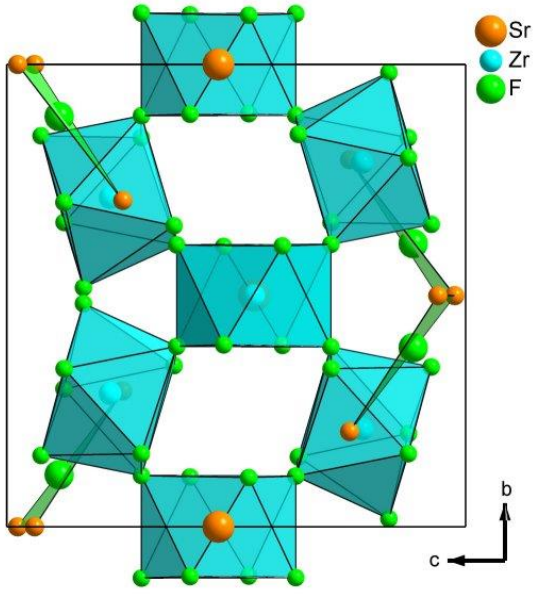
$K_3Ba_7Al_6F_{33}Cl_2$ [89]



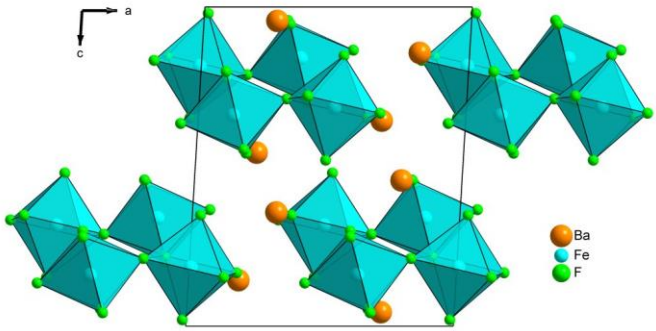
$BaZr_2F_{10}.2H_2O$ [76] twinned



γ-$BaZrF_6$ [82]

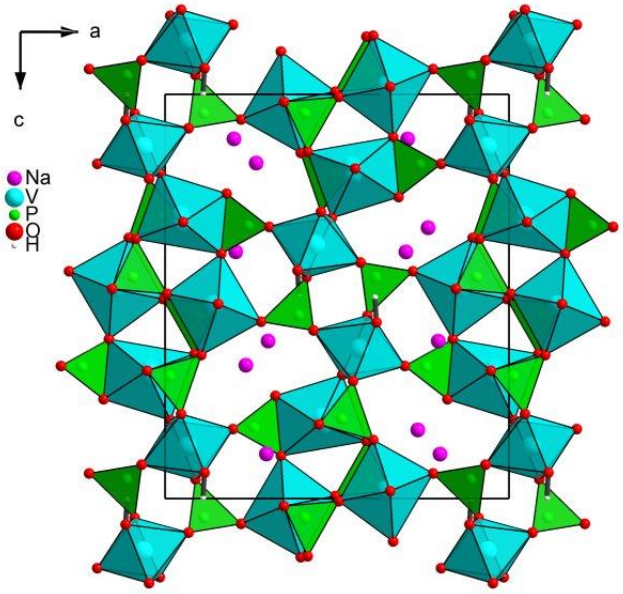


$Sr_5Zr_3F_{22}$ [100] with $[FSr_3]$ triangles

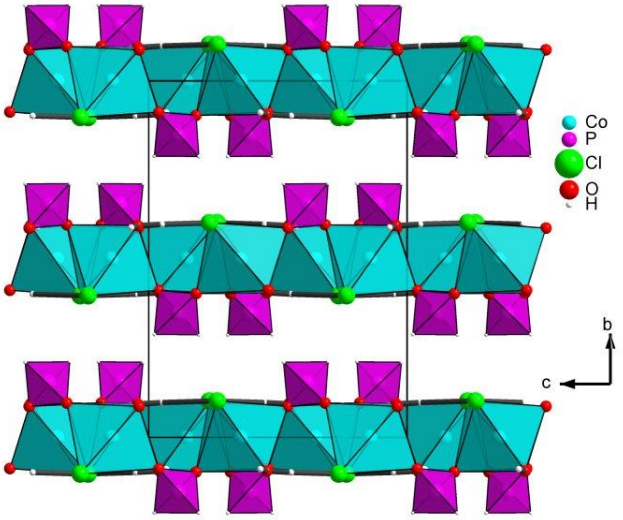


α'-$BaFeF_5$ [94]

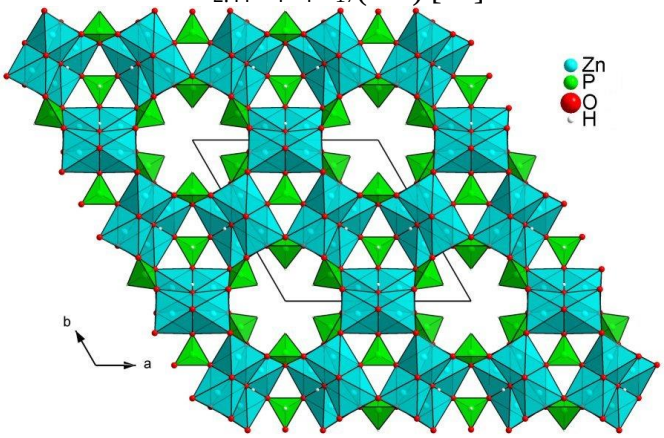
The candidate : Or some non-fluoride structures from single crystal data :



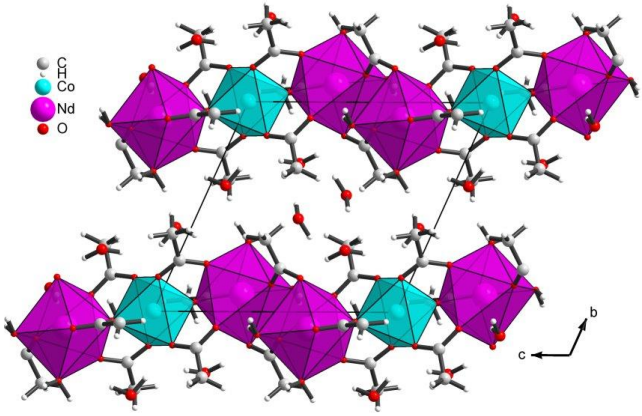
$Na_{2.44}V_4P_4O_{17}(OH)$ [59]



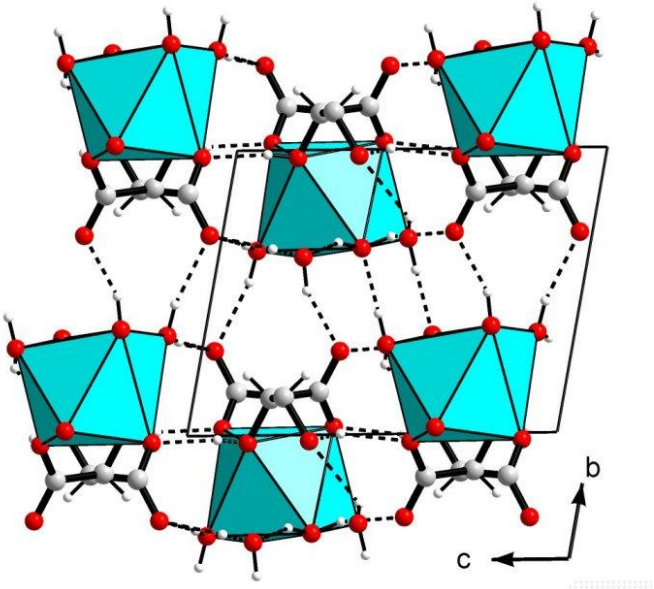
$Co(H_2PO_2)Cl(H_2O)$ [69]



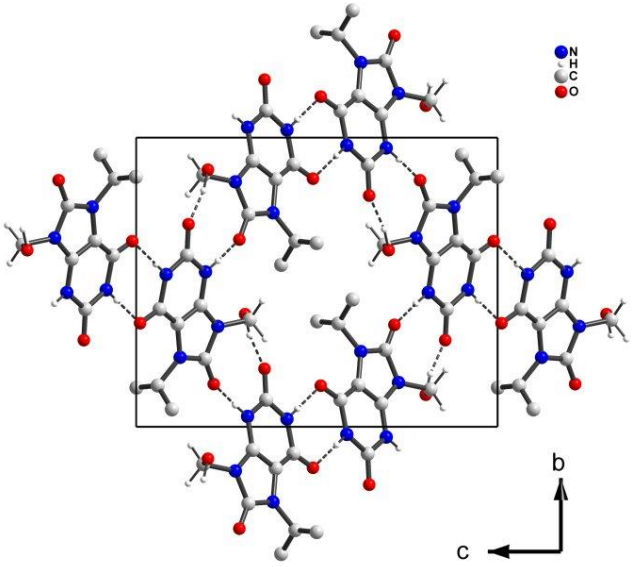
$Zn_{11}(HPO_3)_8(OH)_6$ [90]



$CoNd_2(\mu\text{-}C_2H_3O_2)_8(H_2O)_{10}$ [70]

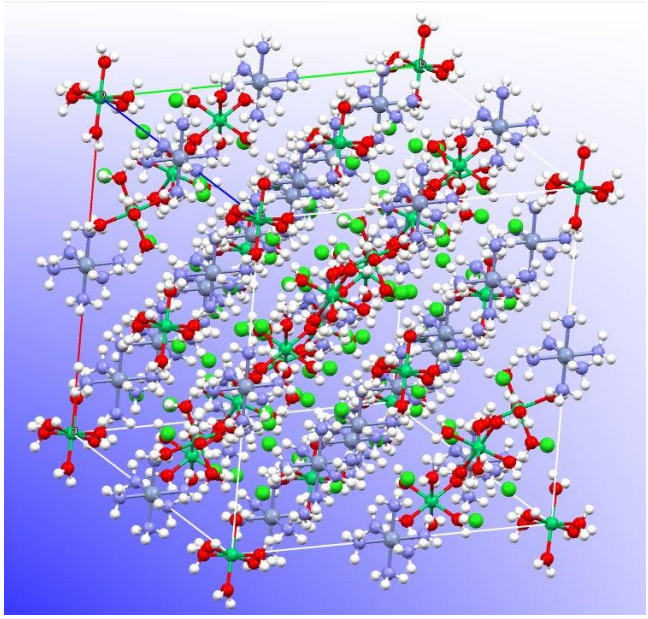


Calcium tartrate tetrahydrate form II
$C_4H_{12}CaO_{10}$ - kidney stone [158]

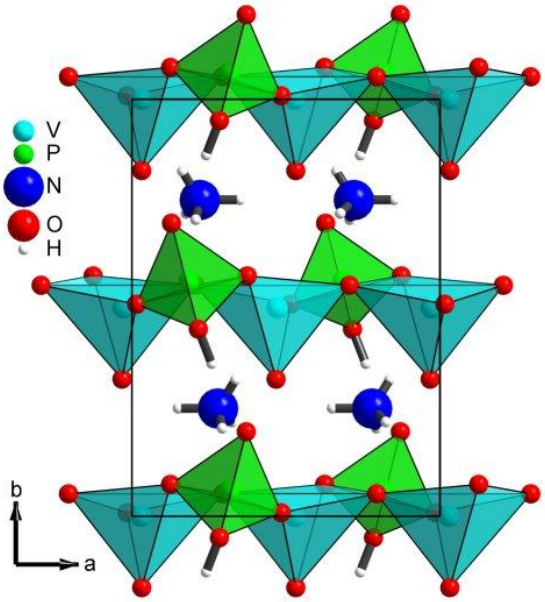


7,9-bis(hydroxymethyl)-uric acid
$C_7H_8N_4O$ - kidney stone [175]

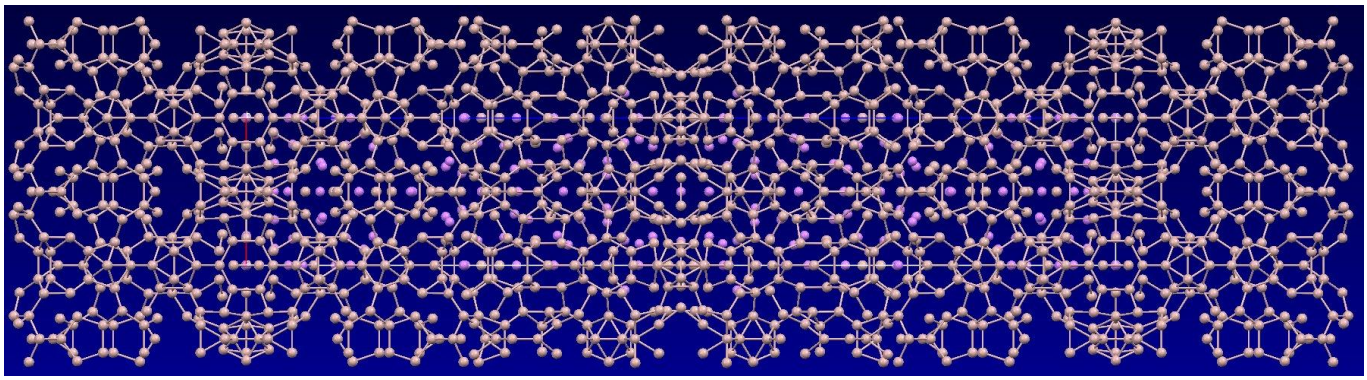
;



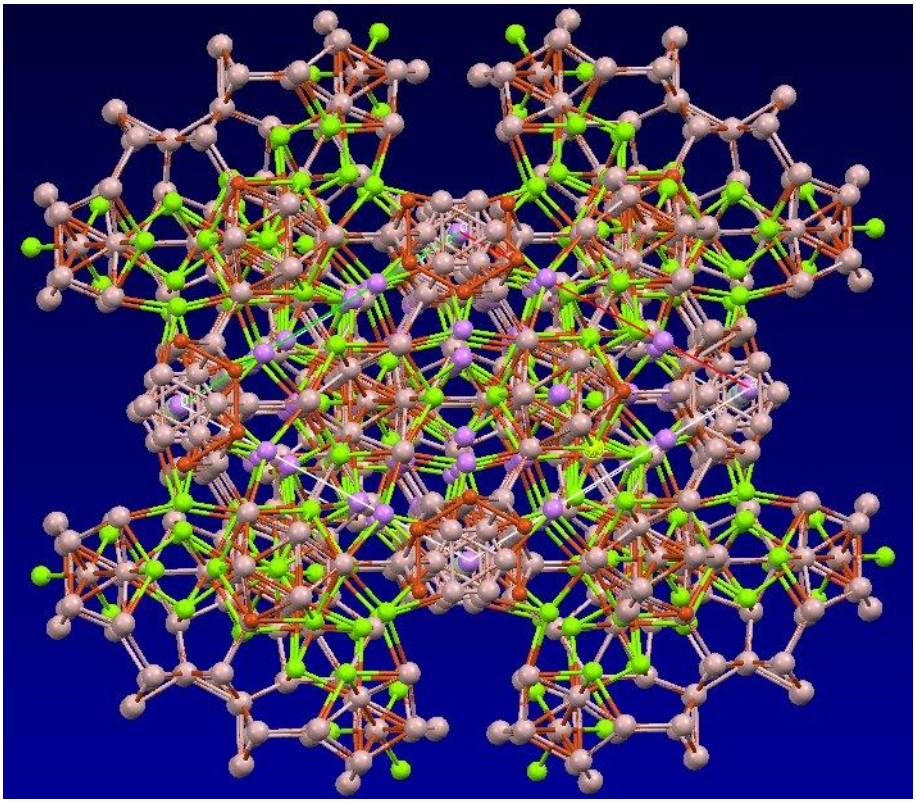
Cr $(NH_3)_6Ni(H_2O)_6Cl_5(NH_4)_{0.5}Cl_{0.5}$ [61]



α-$NH_4(VO_2)(HPO_4)$ [79]

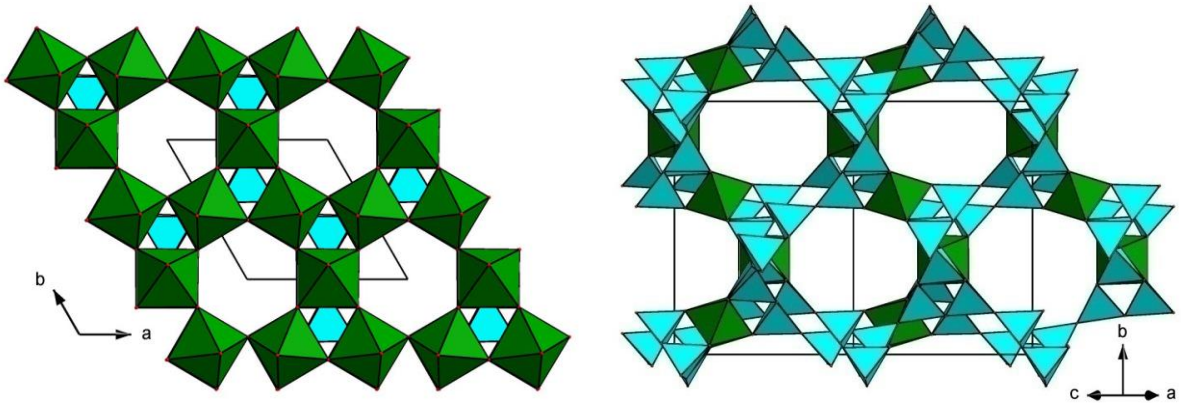


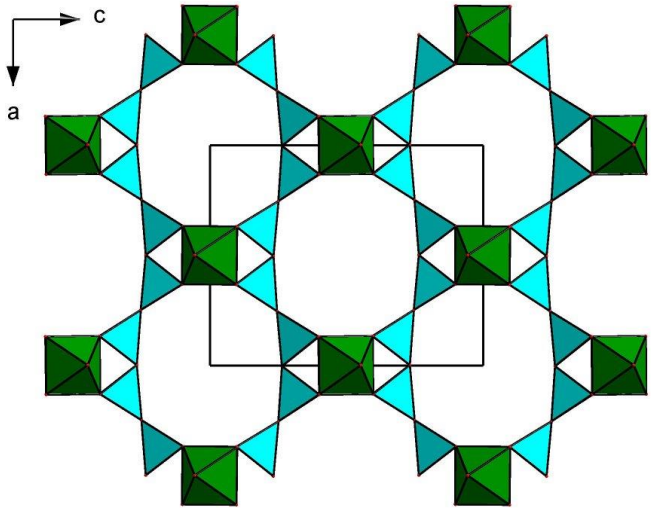
$Al_{56}(Cu,Zn)_{11}Li_{33}$, close to the quasi-crystals strange world [72]

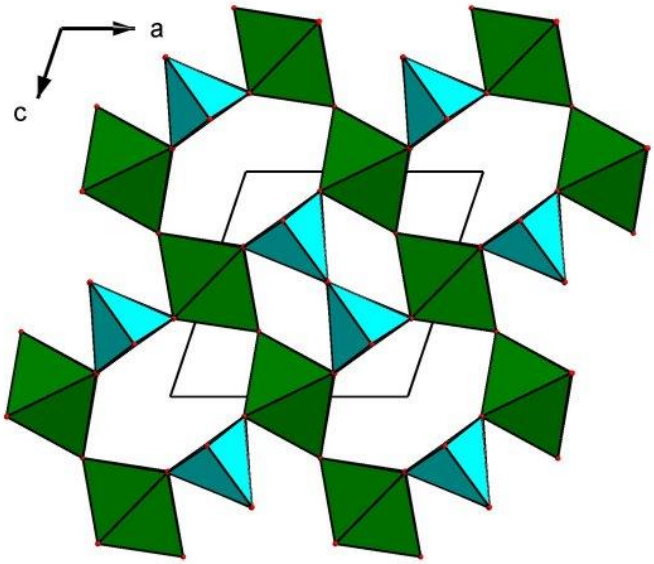


$Al_{59}Cu_5Li_{26}Mg_{10}$ [71]

- **Devil's advocate :** Small molecules, powders, crystallography... A simple press-button technique ! University Professors reserve half their working hours to teach, forming brilliant students, transferring their knowledge to many PhDs. What about teaching ?
- **The candidate :** A whole working life trying to solve complex problems in crystallography, succeeding many times, but not allways, building tools (software such as *ESPOIR*, *McMaille* or algorithms such as that one behind the "*Le Bail method*") for helping to attain the long expected solutions. Thanks a lot to the CNRS !
- **Devil's advocate :** OK, OK, you deserve first class, and you have it already, but you are certainly not exceptionnal. No "ultra big salary" for you. These are reserved to people much more brilliant than you are.
- **The candidate :** I suspected you would tell something like that. Well, I have participated to the formation of such brilliant students (seventeen or so), locally at Le Mans, or solved some of their most difficult problems, sometimes under their eyes. Moreover my SDPD Internet Course was followed by ~50 students all over the world. I used their subscription fees (and some money from industry) for financing my computers and congress (IUCr meetings, European Crystallography meetings, etc) costs (Osaka, Japan, 2008; Lausanne, Switzerland, 2008; Oran, Algeria, 2008; Campinas, Brazil, 2007; Wisla, Poland, 2006; Geneva, Switzerland, 2006; Anvers, Belgium, 2006; London, Great Brittain, 2006; Agadir, Morocco, 2006; Florence, Italy, 2005; Constantine, Algeria, 2005; Assiut, Egypt, 2004; El Jadida, Morocco, 2004; Durban, South Africa, 2003; Stara Lesla, Slovakia, 2003; Bonn, Germany, 2003; Geneva, Switzerland, 2002, Krakow, Poland, 2001; Barcelona, Spain, 2000; Ismailia, Egypt, 2000; Kunming, China, 1999; Glasgow, Scotland, 1999: Prague, Czek Republik, 1998; Colorado Spring, USA, 1998; St Louis, USA, 1997; Seattle, USA, 1996; Liptowski Mikulas, Slovakia, 1995; Gaithersburg, USA, 1992; Valencia, Spain, 1990, 1988; Hambourg, Germany, 1984; etc). These were generally invitations for presenting my software and results obtained with them by me or others. Paid for discovering the World, thanks again to the CNRS (even if I had to find by myself all the money) ! Let me finish now by some views of predicted inorganic compounds selected among the >100000 generated by my GRINSP software ("white" ANR project in 2005, rejected, then job done alone) :




c
a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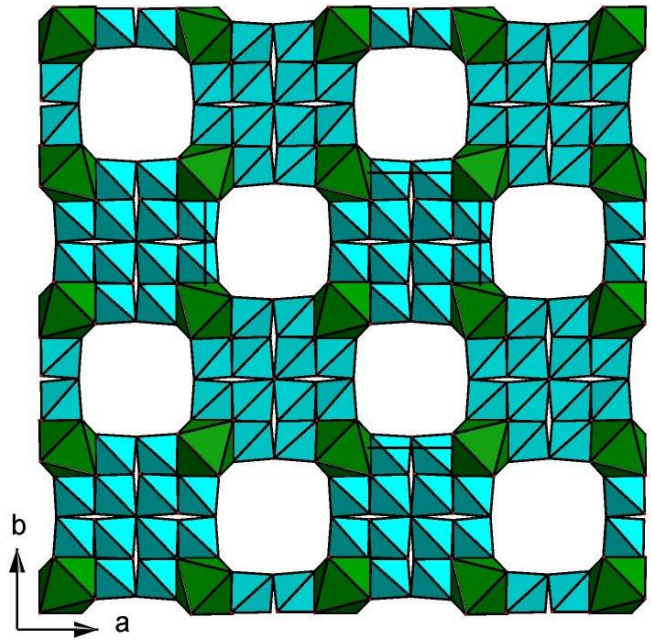
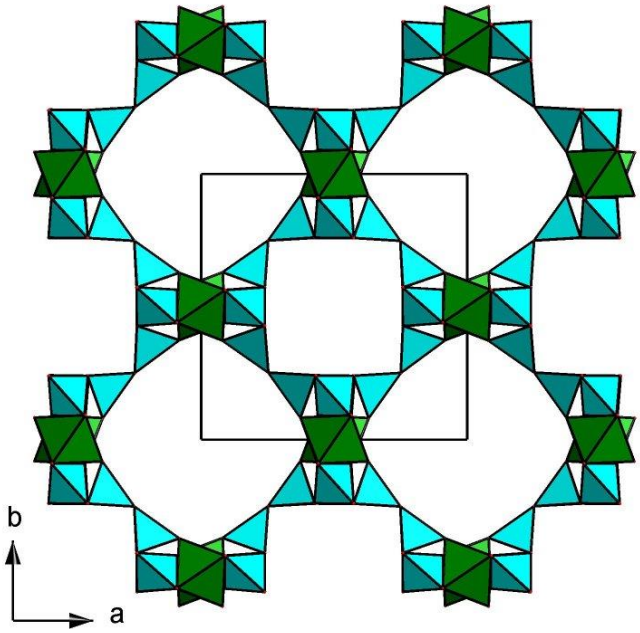

b
a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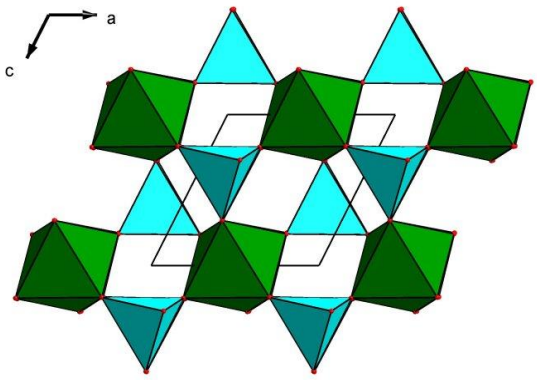
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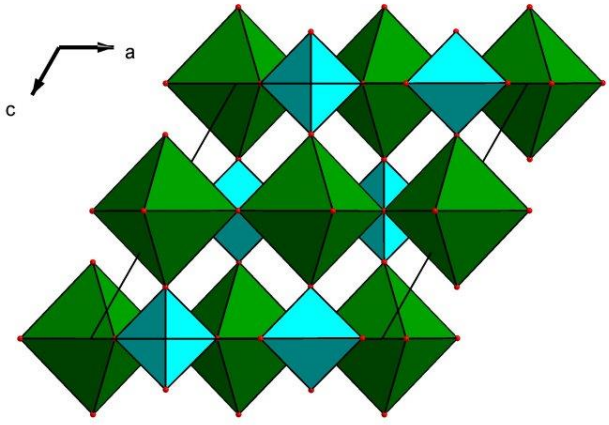
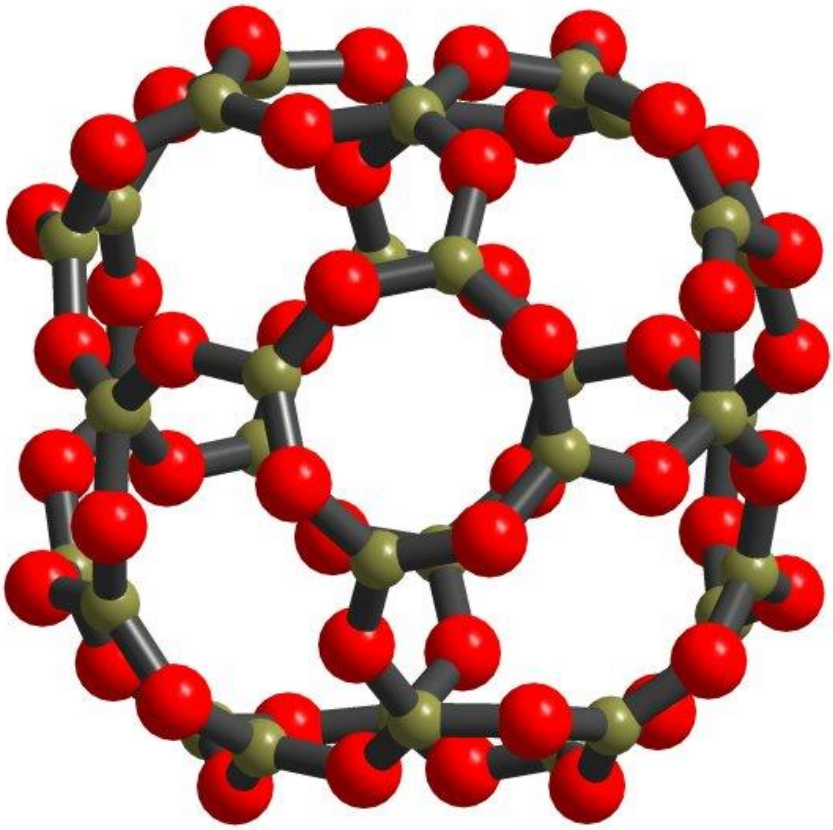
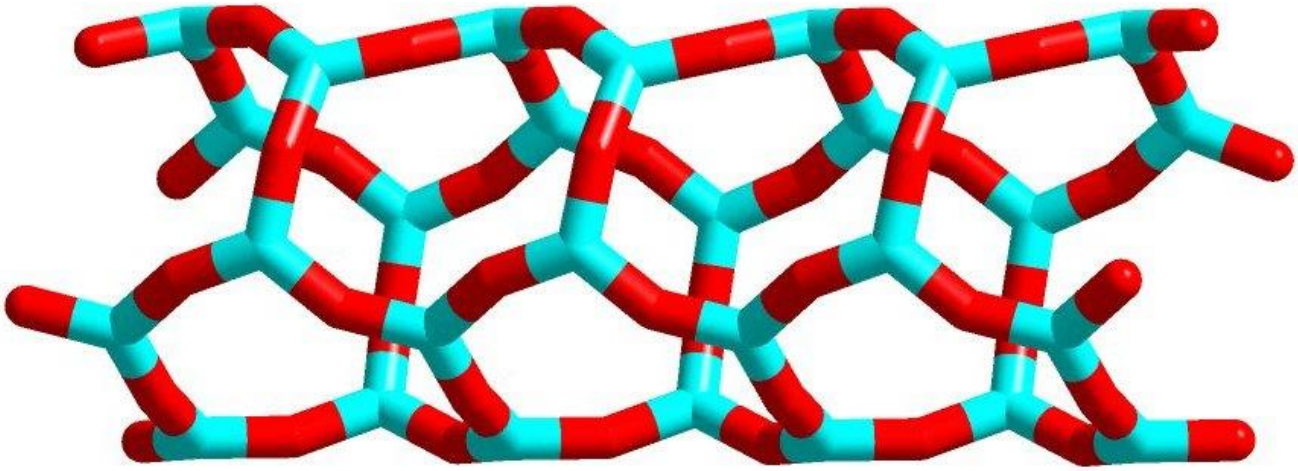
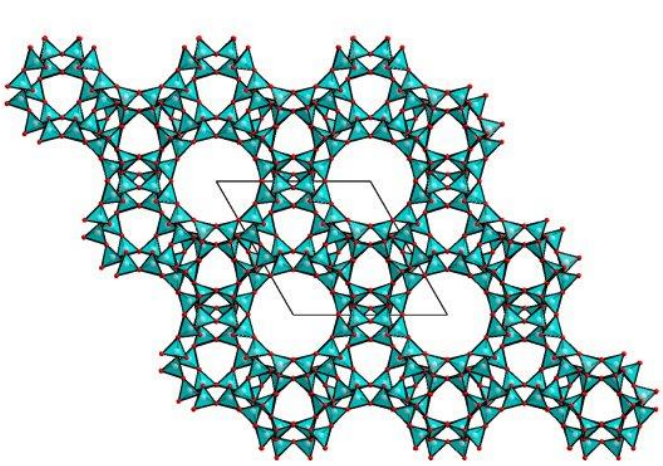

a
c

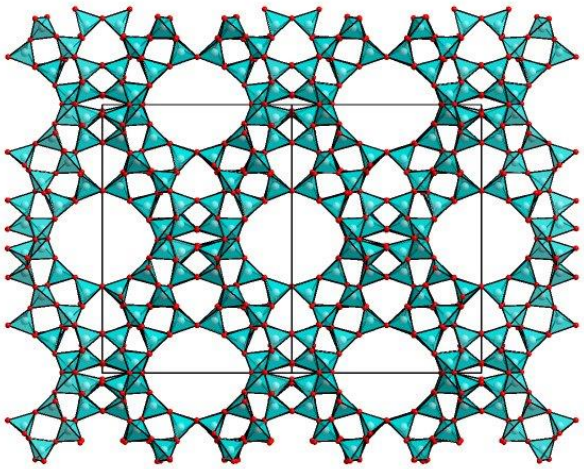


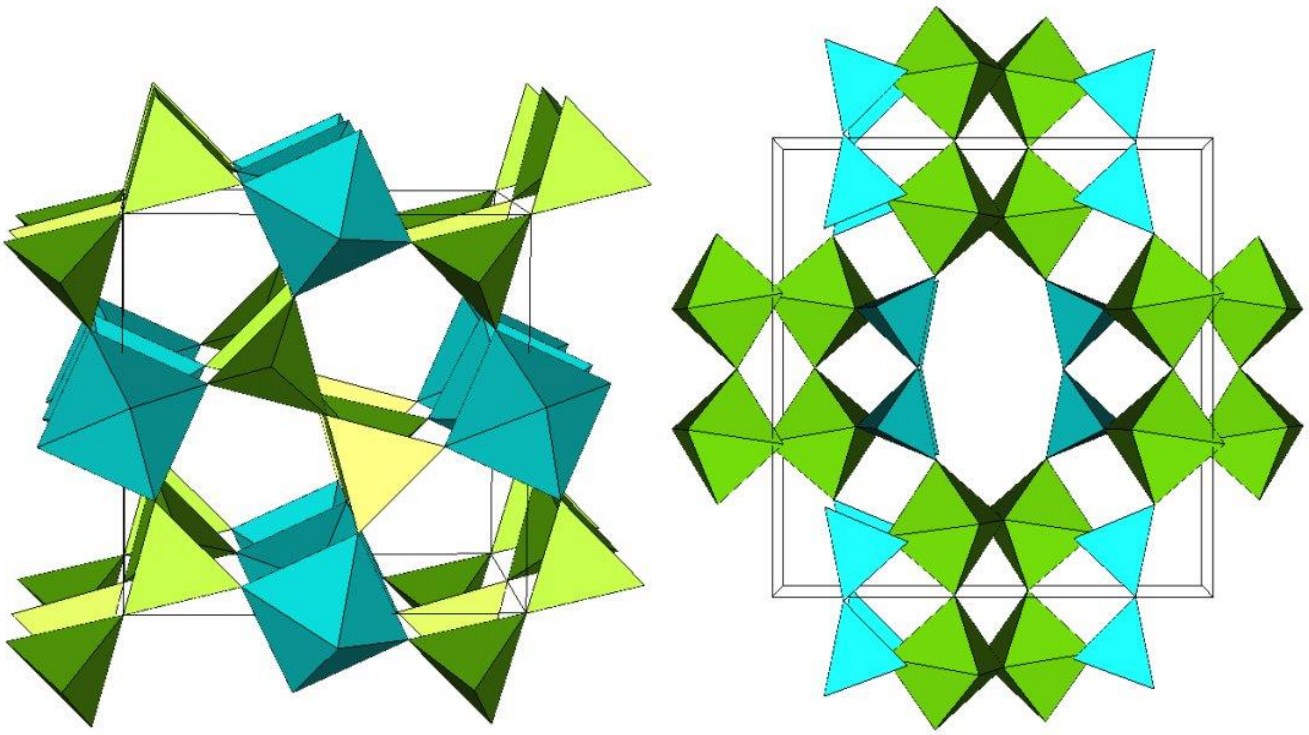
B_2O_3 nanosphere

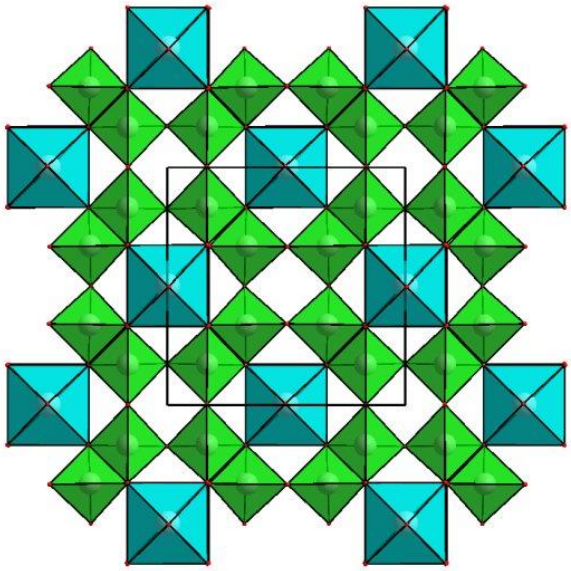


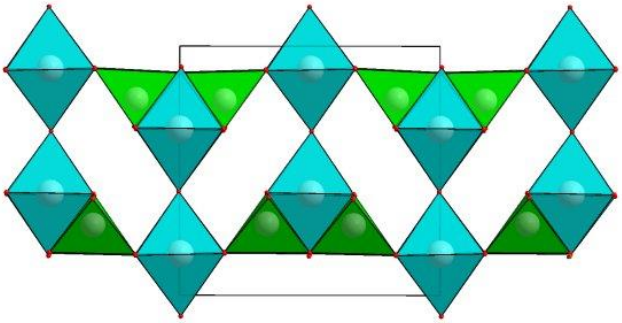
B_2O_3 nanotube

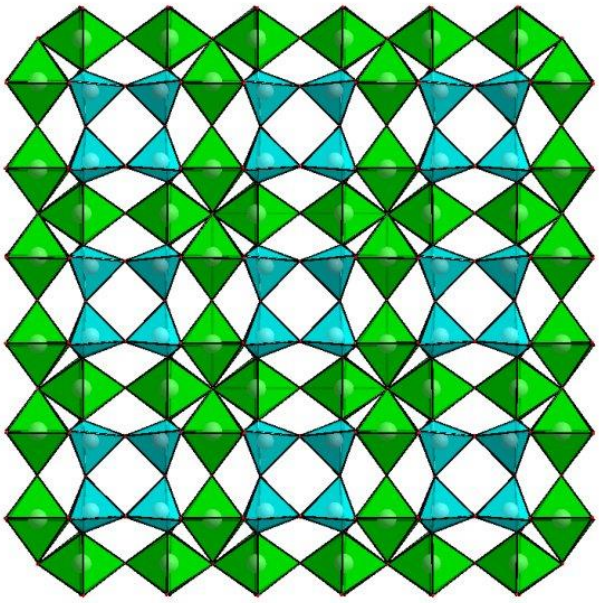


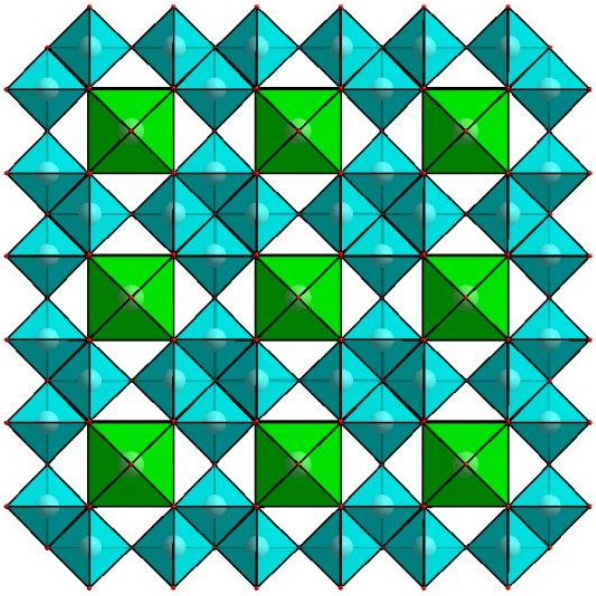


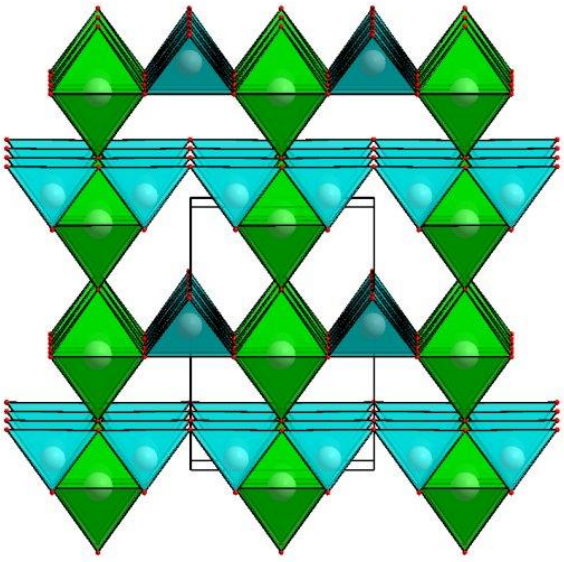


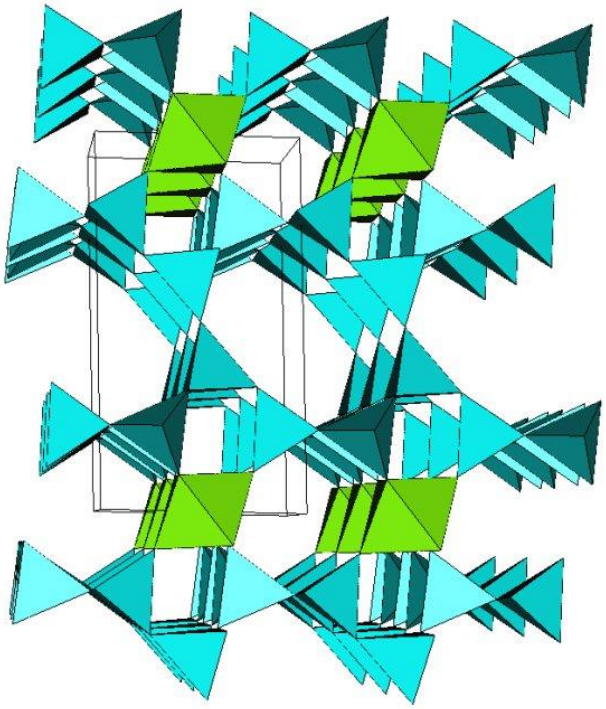


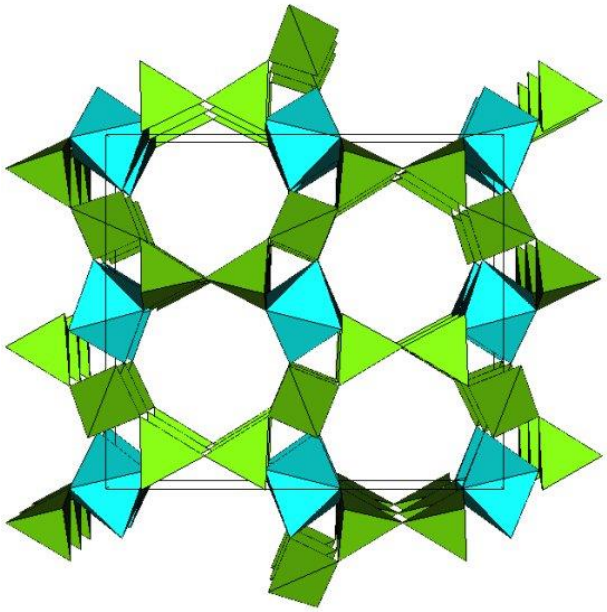
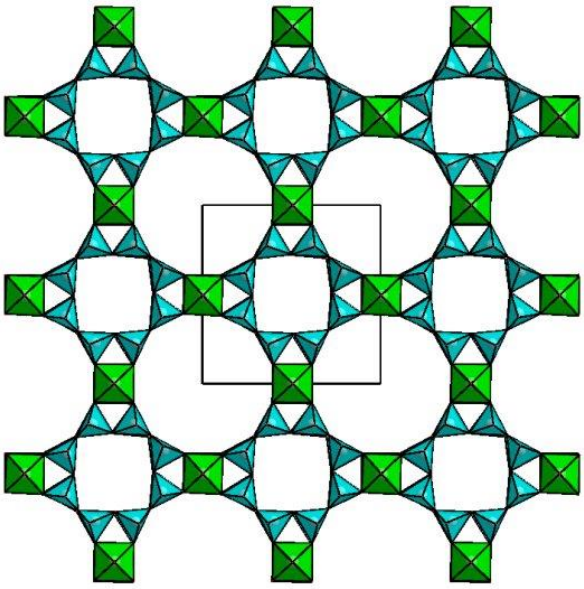
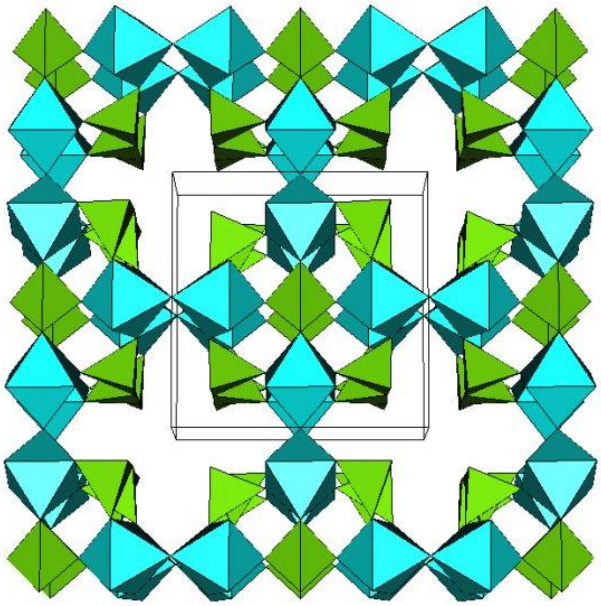
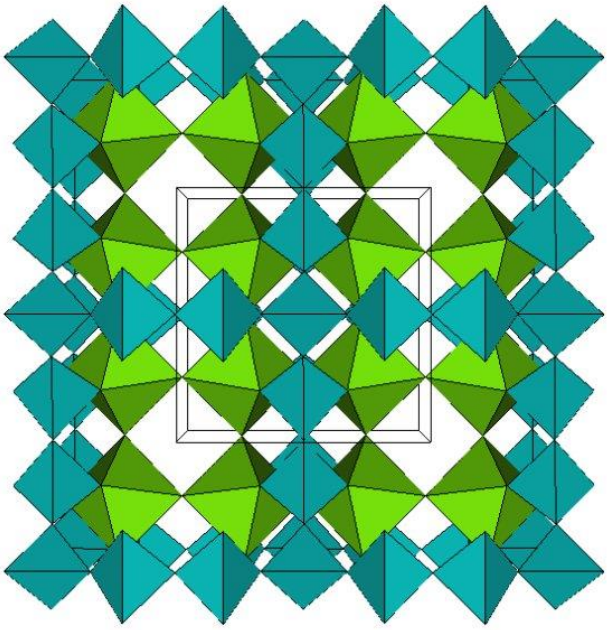
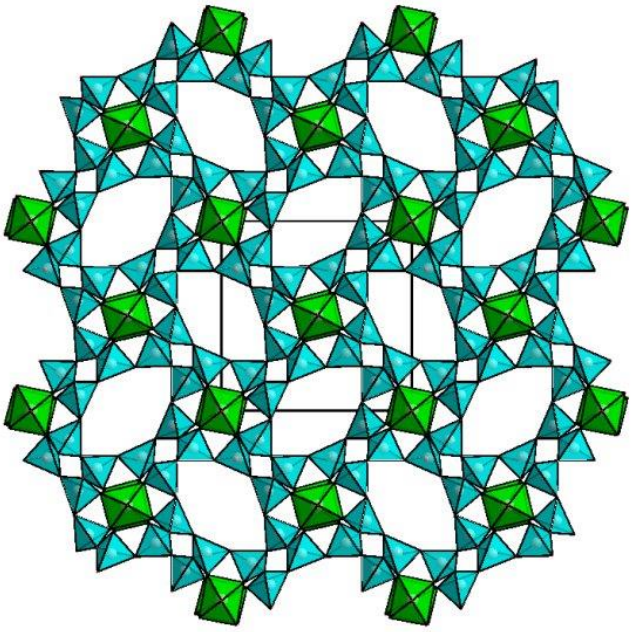
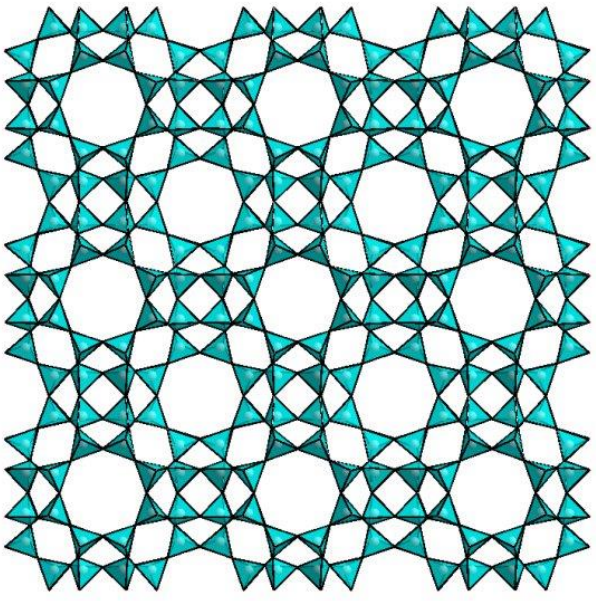


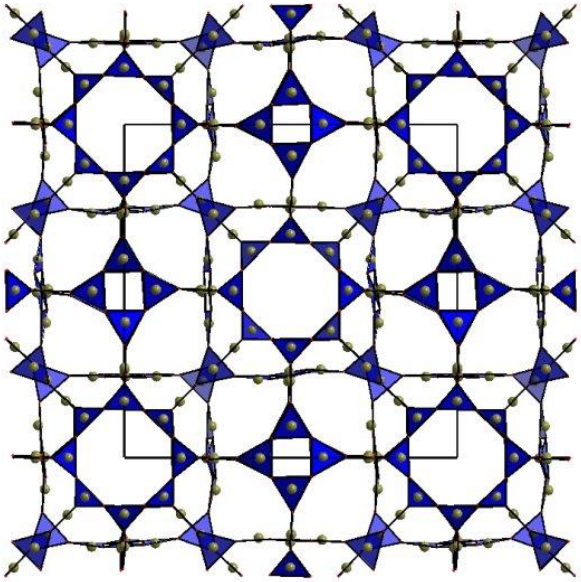


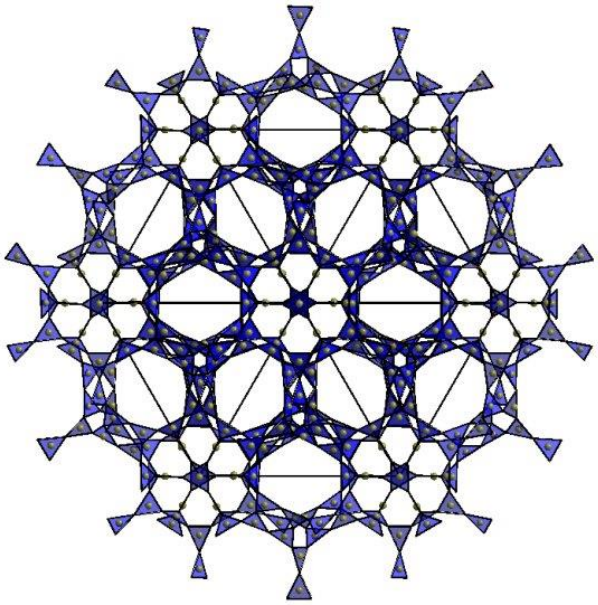


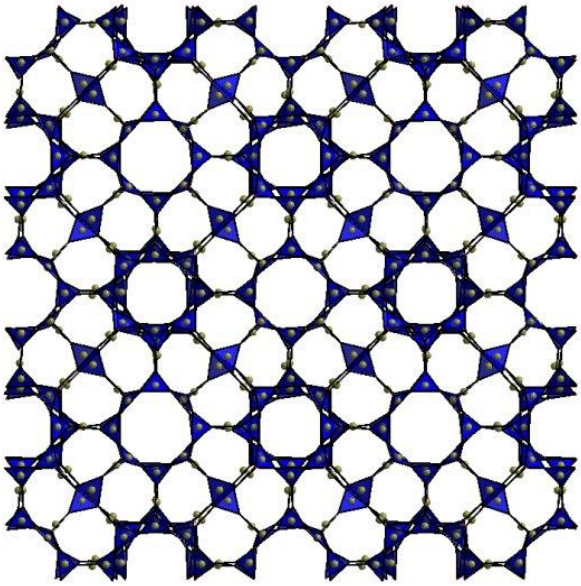


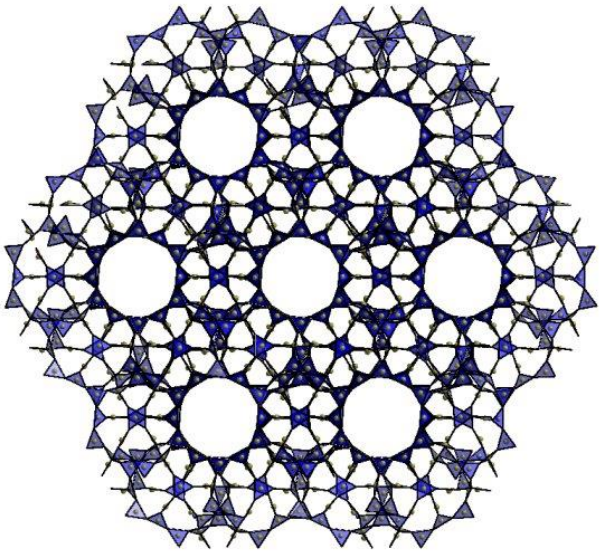


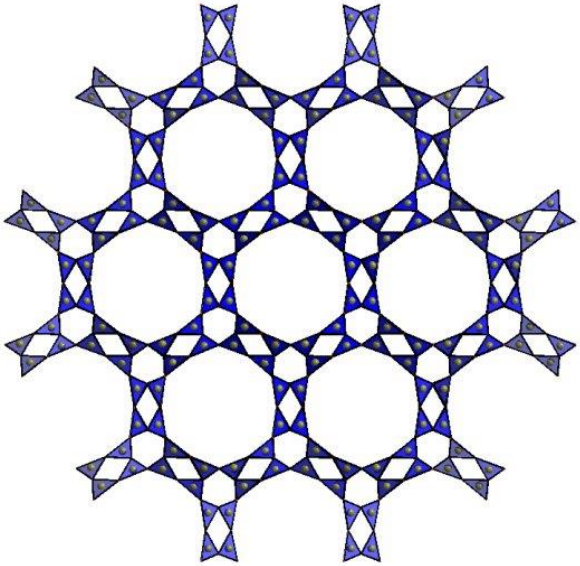







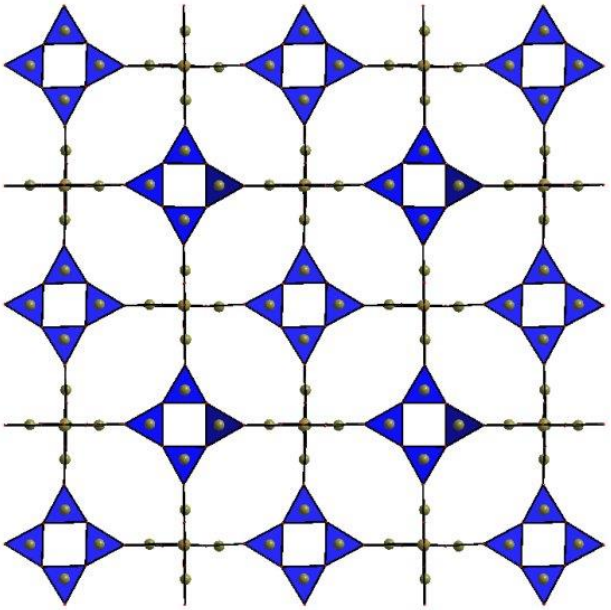


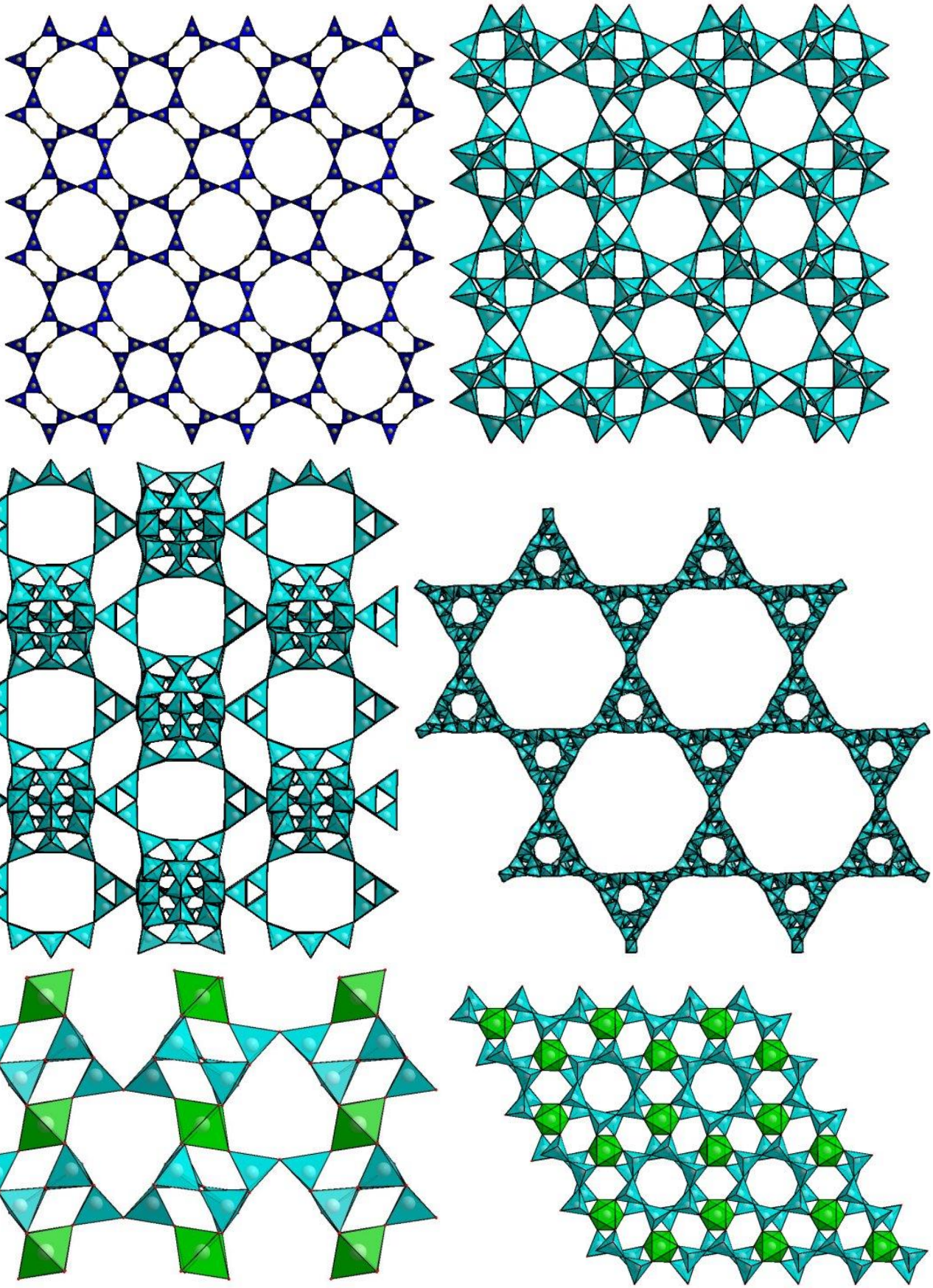


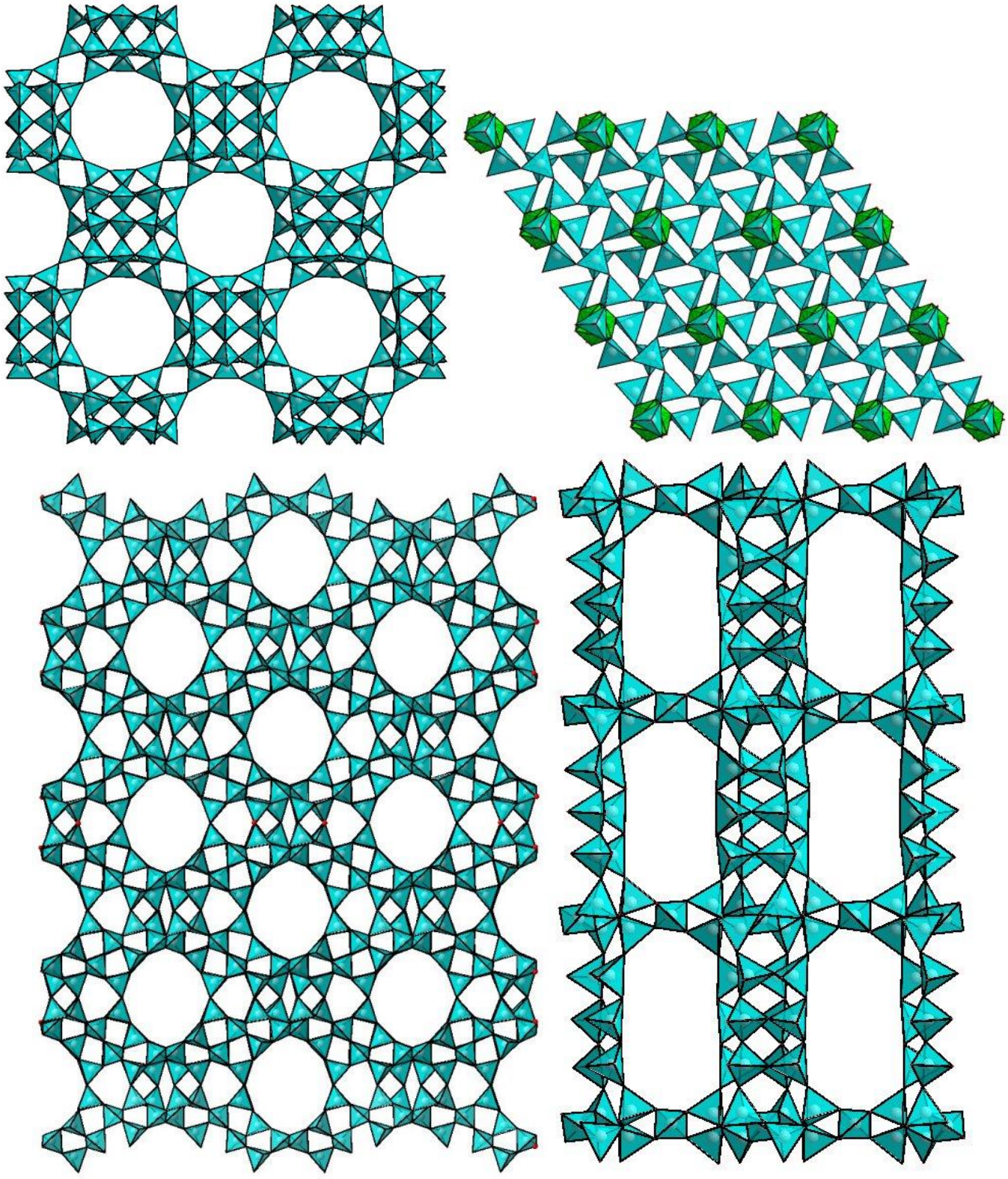


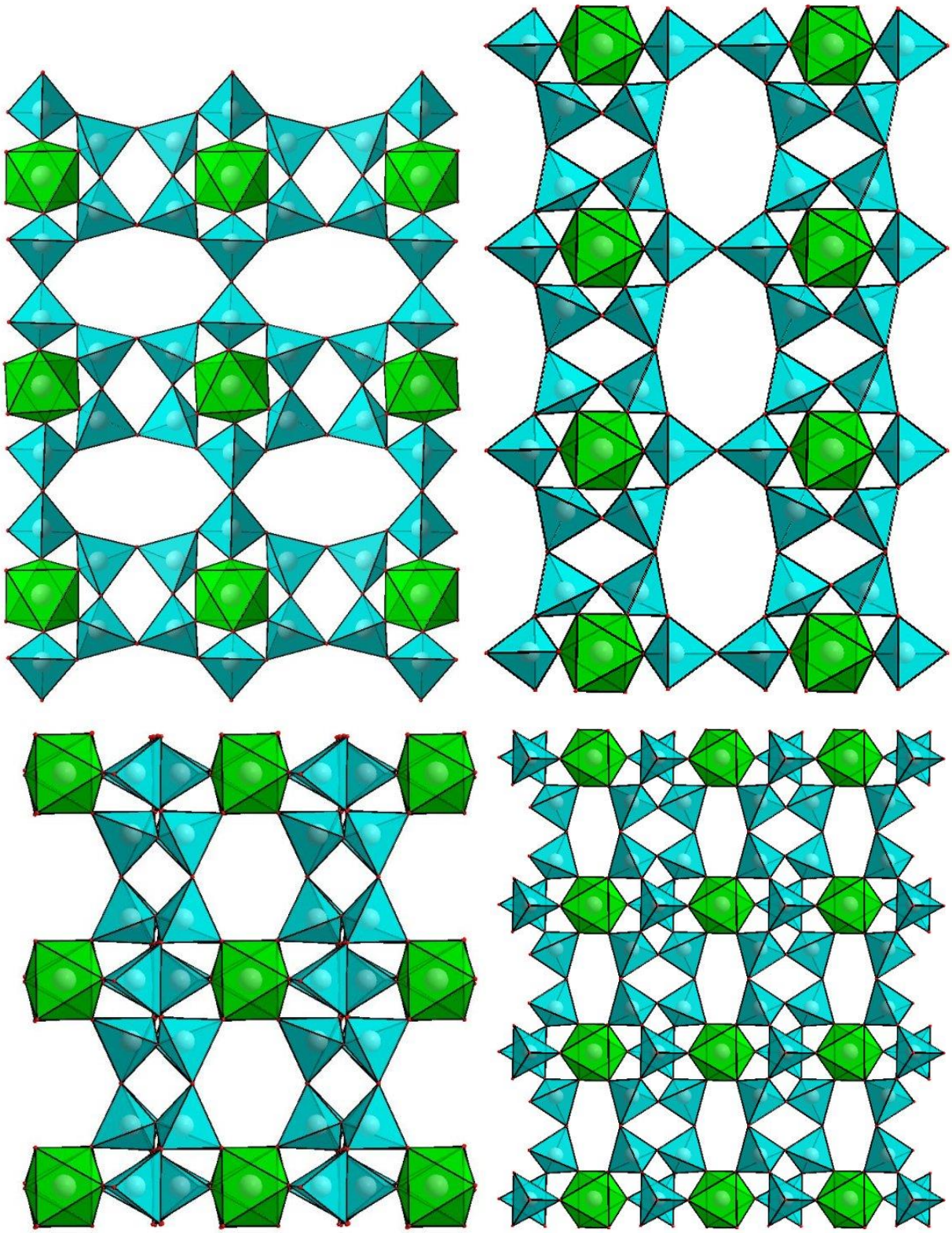


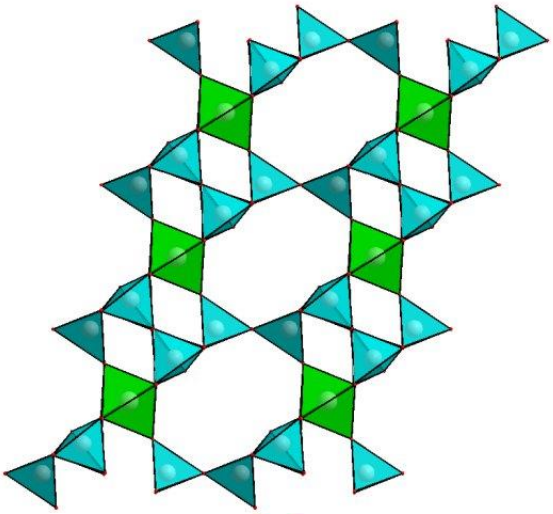


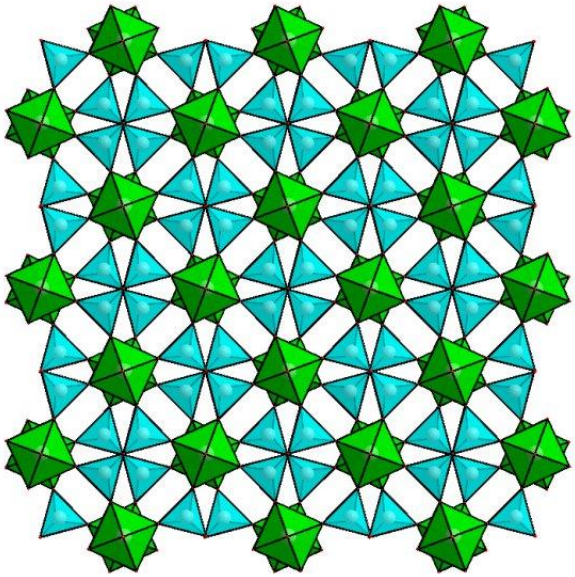


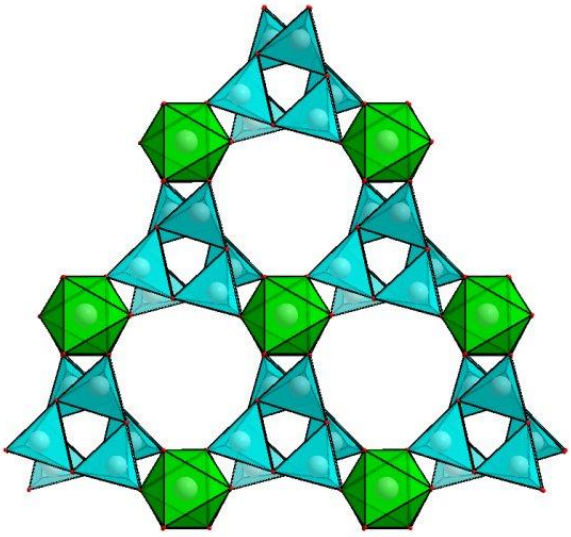


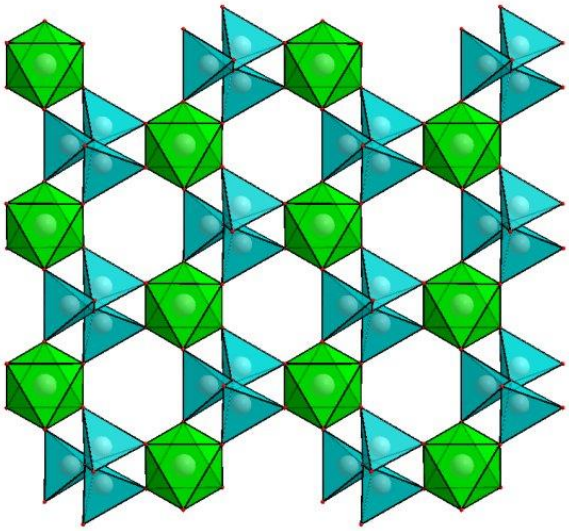


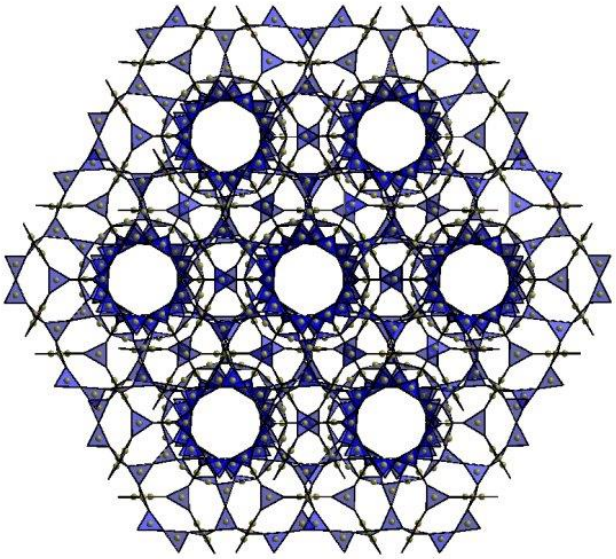


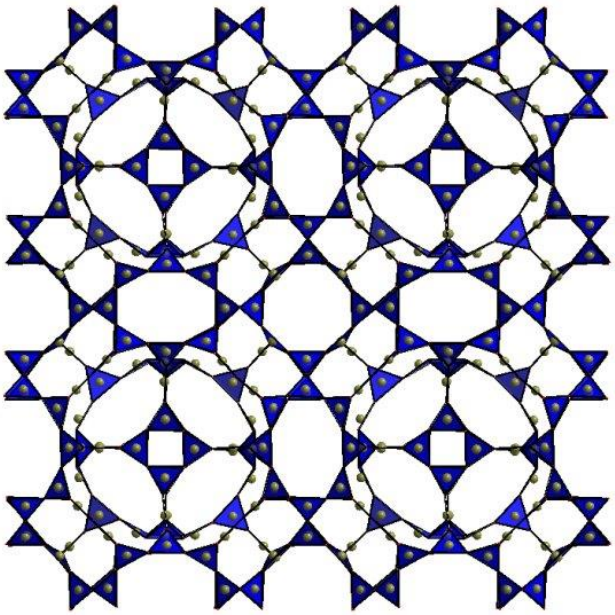


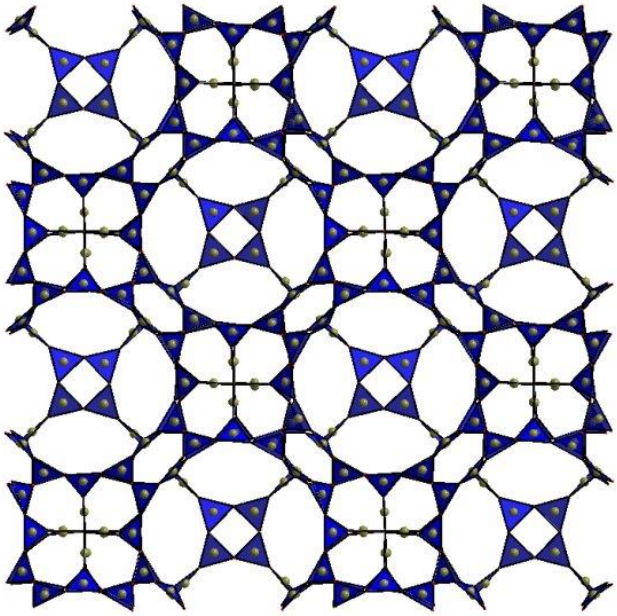
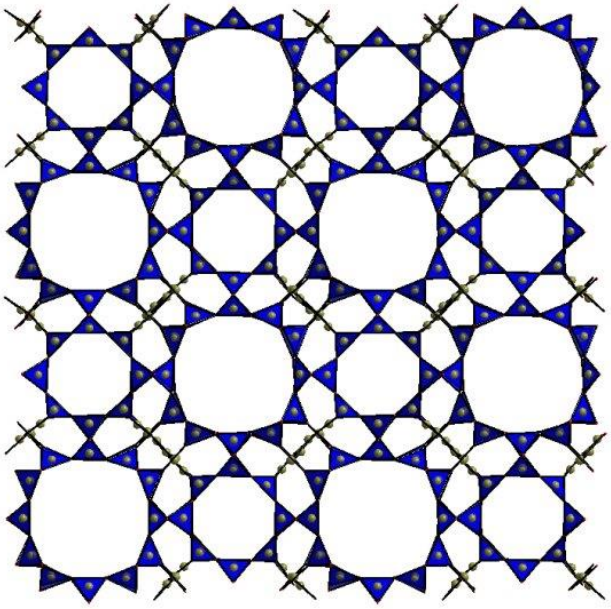
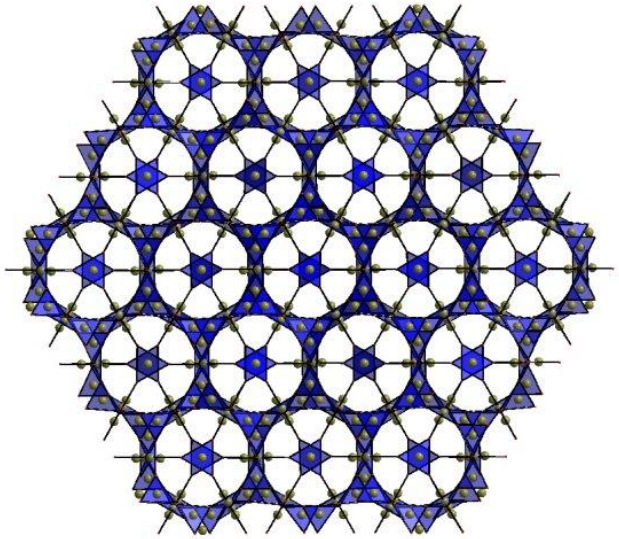
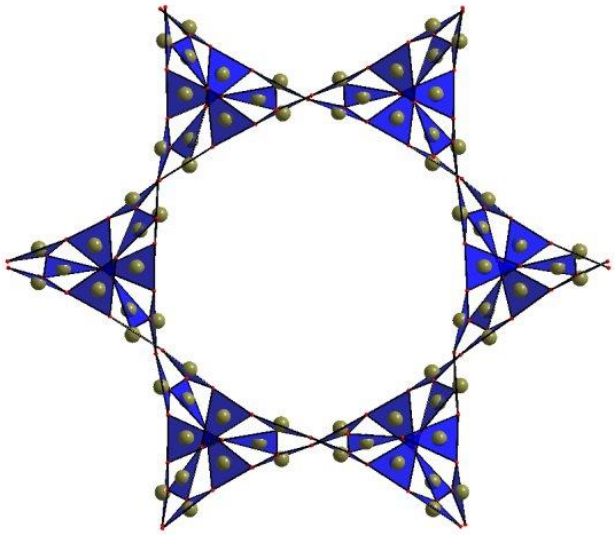
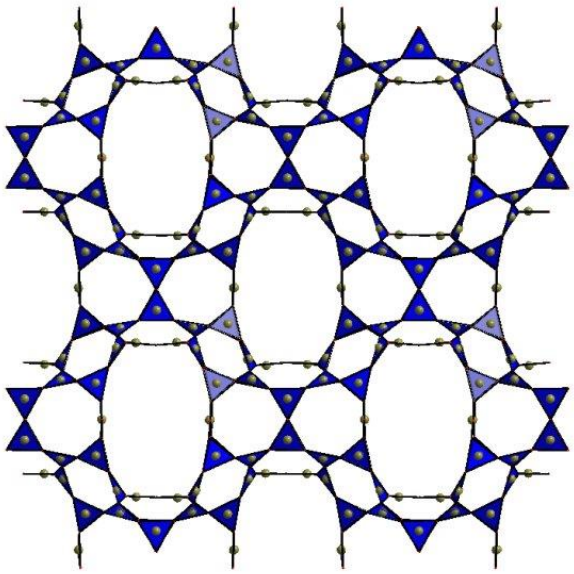
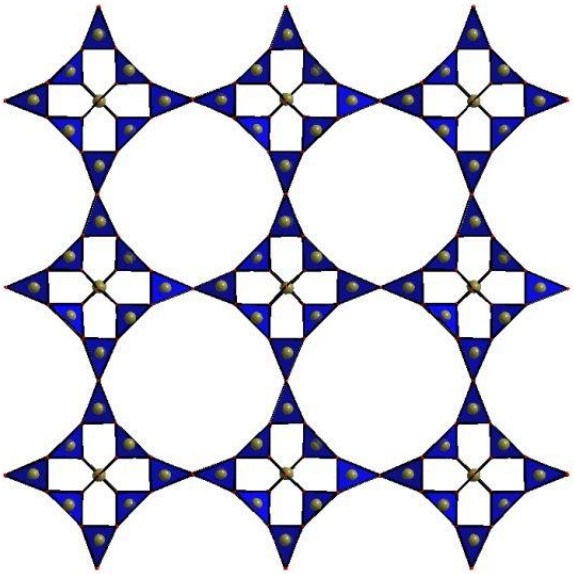


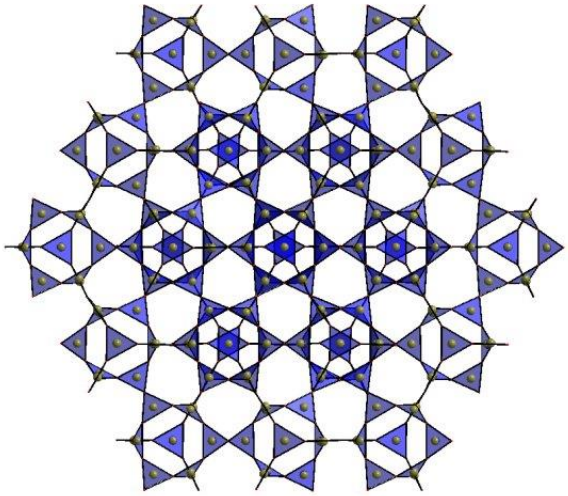


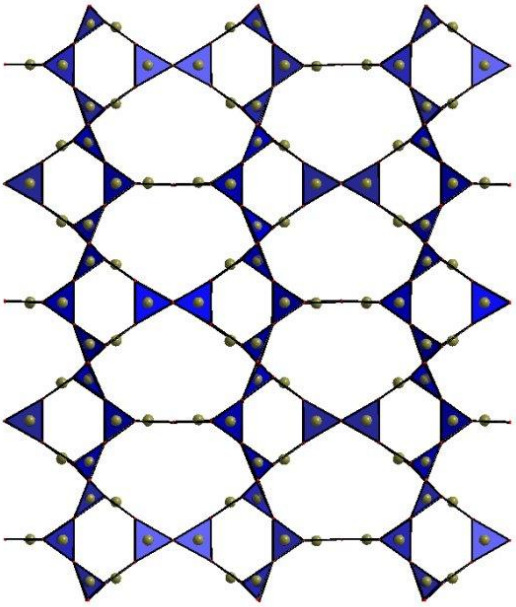


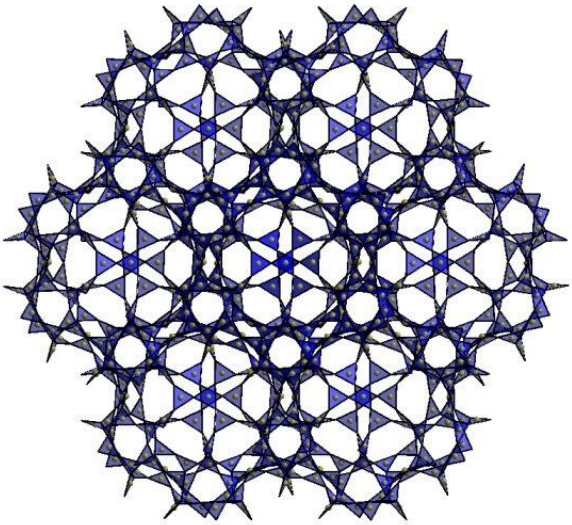


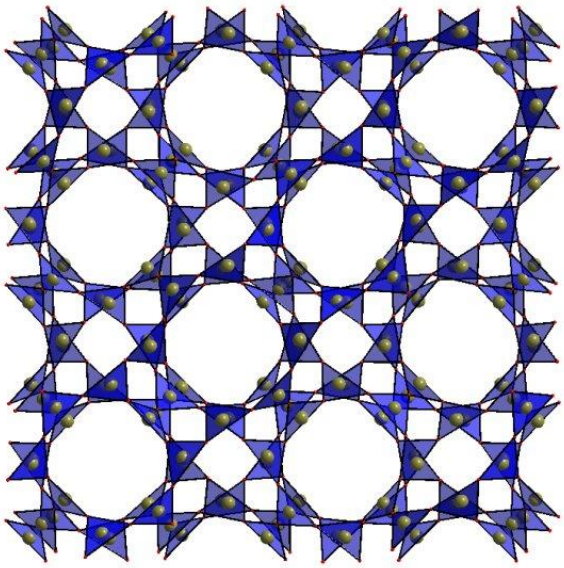


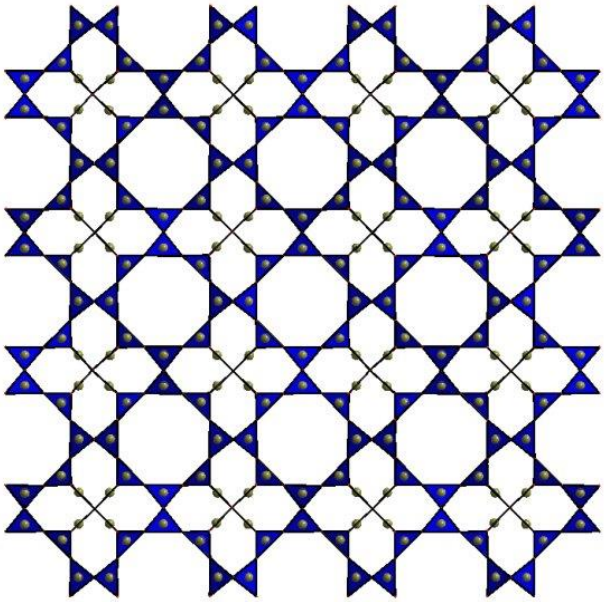







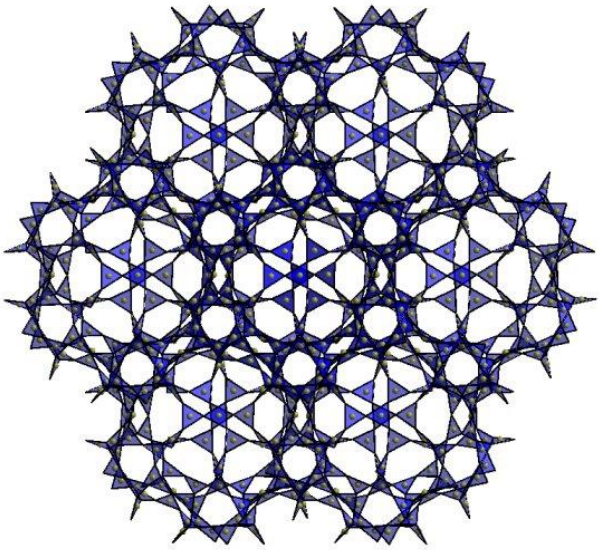


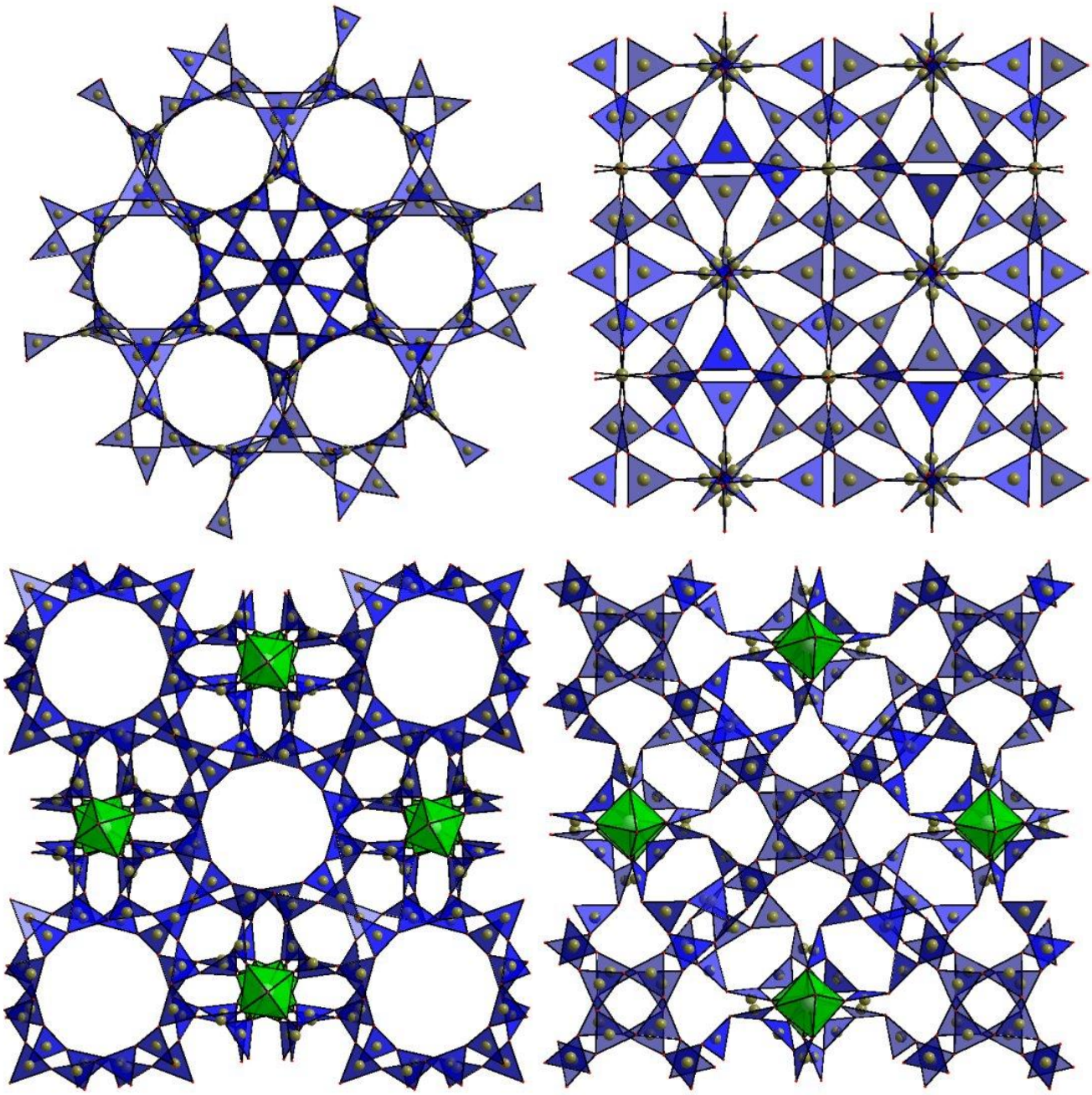




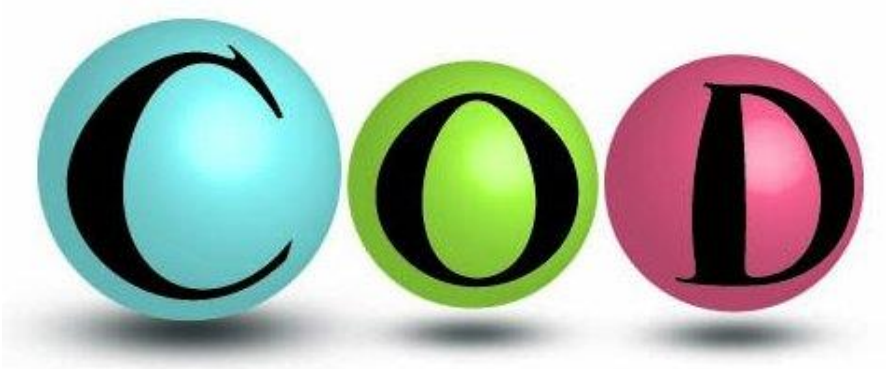








The candidate : Exceptionnal pictures, aren't they ? Thanks again to the CNRS for making this possible ! Retrieve all that in the COD and PCOD crystallography open databases http://www.crystallography.net/ which I co-founded in 2003 and contain now ~300000 and >1 million entries, for existing and predicted structures, respectively, in total free access. A testimony in a few words : full crystal structure prediction will be the simple consequence of the real full mastering of quantum physics and chemistry. We will probably not see that so soon but maybe before the end of this XXIth century. And then...



Devil's advocate : Well, OK, you will be DRCE then... Anyway you clearly don't believed to the possibility to succeed, don't you ? This non-standard report is only for the fun, isn't it ? Any patent with high revenue, commercial applications, CO_2 storage in your compounds, sub-marine data transfer by optical fiber made of fluorinated glasses, supraconducting materials for train levitation, a-centric compounds with exceptional behaviour, compounds with giant pores that will deliver pharmaceutical molecules at the right place in the human body, or even solely "breathing", nanomaterials having giga- or even only mega-properties (...) ? Nothing, I am afraid... You are even not in the recent list of the 3200 most cited authors, including 80 french ones. So I would suggest you to try a reconversion in the automatic prediction of decorative ceramic plaques for bathrooms.

The candidate : Well, properties are there, mostly not applicable because being too weak. So what ? A vast majority of new compounds have properties without any interest because a few present much better performances. Good idea about bathrooms ! But I will probably be occupied with the building of more CIF files to enter into the COD, though this is quite boring. Ooops, I realize that I told nothing about my work on amorphous compounds or size-strain line broadening analysis, and some oldest other details (EXAFS, modelling glass structures, etc...). Never mind, trying to prove by yourself that you are "excellent", internationally shining and so brilliant, this is really weird. Indeed, this report is limited to the description of the pleasure I had. About pleasure, good luck to the next generations of CNRS engineers and researchers, if any true "autonomy" is available for them (Mme Fioraso and many technocrates are working hard in the opposite direction) ! An autonomy to find the money by yourself, being either a slave or a dictator, or a mercenary like I was, there is no other possibility. To the crystallochemists, I would say them to think to powder diffraction as a now quite efficient tool allowing to solve interesting problems that would otherwise sleep forever in drawers (anyway, so many new single crystals are very easily obtained for hybrids compounds that you can be occupied exclusively with them for centuries, if you wish, even keeping only the compounds with largest cell parameters and reserving the others to the dustbin). And finally, the most important advice : do not sell too much bullshit like if it was high-level real science. Politicians will eat it, then you will obtain money, teams working for you, and rewards on your unique name, but when the promises will fail to be honoured... well, you will be retired, after all, so that it will be to your successors, ex younger co-workers, to become sick with your untenable marvelous announced potentialities - unless you are extremely lucky and your production has really met commercial/societal applications up to a high level (indeed, this could happen 20 or 30 years after your seminal work having unexpected consequences).

LISTE DES PUBLICATIONS

1976-2015

Articles les plus cités

147 articles actuellement dans le Web au Knowledge, plus de 150 au total d'ici la fin 2015 (194 en incluant chapitres de livres et articles non répertoriés par Thomson-Reuter-ISI).
> 3680 citations de ces 147 articles cités dans ~3000 articles, hors auto-citations.
> 25 citations en moyenne par article.
h-index = 28
article le plus cité : >1330 citations

Liste des publications citées 28 fois ou plus (Nombre de citations en début de référence - **en bleu** les références absentes (erreur ou journal/livre non-référencé) du Web of Science mais obtenues par l'option "Cited Reference Search" :

1333 (+43) - *Ab-initio* structure determination of $LiSbWO_6$ by X-Ray powder diffraction. A. Le Bail, H. Duroy and J.L. Fourquet, *Mat. Res. Bull*. **23**, 447-452 (1988).

150 "The profile of a Bragg reflection for extracting intensities." A. Le Bail, Chapter 5 in: Powder Diffraction: Theory and Practice, Ed. R.E. Dinnebier & S.J.L. Billinge, Royal Society of Chemistry, Cambridge (2008) 134-165.

140 - Size-strain line broadening analysis of the ceria round-robin sample. D. Balzar, N Audebrand, MR Daymond, A Fitch, A Hewat, JI Langford, A Le Bail, D Louër, O Masson, CN McCowan, NC Popa, PW Stephens, BH Toby, *J. Appl. Cryst*. **37** (2004) 911-924.

109- Whole powder pattern decomposition methods and applications - A retrospection. A. Le Bail, *Powder Diffraction* **20** (2005) 316-326.

107 - A new study of the structure of $LaNi_5D_{6.7}$ using a modified Rietveld method for the refinement of neutron powder diffraction data. C. Lartigue, A. Le Bail and A. Percheron-Guegan, *J. Less-Common Metals* **129**, 65-76 (1987).

86 - Monte Carlo indexing with McMaille. A. Le Bail, *Powder Diffraction*, **19** (2004) 249-254.

85 - Crystal structure of the metastable form of aluminium trifluoride β-AlF_3 and the gallium and indium homologs. A. Le Bail, C. Jacoboni, M. Leblanc, R. De Pape, H. Duroy and J.L. Fourquet, *J. Solid State Chem*. **77**, 96-101 (1988).

68 - Crystallography Open Database – an open access collection of crystal structures. S. Gražulis, D. Chateigner, R.T. Downs, A.F.T. Yokochi, M. Quirós, L. Lutterotti, E. Manakova, J. Butkus, P. Moeck and A. Le Bail, *J. Appl. Cryst*. **42** (2009) 726-729.

63 - Synthetic pathways to vanadyl phosphates. D. Beltran-Porter, P. Amoros, R. Ibanez, E. Martinez, A. Beltran-Porter, A. Le Bail, G. Férey, G. Villeneuve, *Solid state Ionics*, **32/33**, 57-69 (1989).

62 - Modelling the Silica Glass Structure by the Rietveld Method. A. Le Bail, *J. Non-Cryst. Solids*, **183**, 39-42 (1995).

59 - Recent advances in the chemistry and properties of oxovanadium phosphates. D. Beltan-Porter, A. Beltran-Porter, P. Amoros, R. Ibanez, E. Martinez, A. Le Bail, G. Férey, G. Villeneuve. *Eur. J. Solid State Inorg. Chem*. **28**, 131-161 (1991).

56 - The room-temperature crystallisation of a one-dimensional gallium fluorophosphate, $Ga(HPO_4)_2F•H_3N(CH_2)_3NH_3•2H_2O$, a precursor to three-dimensional microporous gallium fluorophosphates, Walton, RI, Millange, F, Le Bail, A, Loiseau, T, Serre, C, O'Hare, D, Ferey, G, *Chem. Comm*., 203-204 (2000).

52 - ESPOIR : A Program for Solving Structures by Monte Carlo from Powder Diffraction Data. A. Le Bail, *Mat. Sci. Forum*, **378-381** (2001) 65-70.

51 - Extracting structure factors from powder diffraction data by iterating full pattern profile fitting, A. Le Bail, *NIST Special Publication* **846** , 213 (1992).

48 - Electron microscopy study of the superconductor $Bi_2Sr_2CaCu_2O_{8+}$. M. Hervieu, C. Michel, B. Domenges, Y. Laligant, A. Le Bail, G. Férey and B. Raveau, *Modern Physics Letters* B, 2(1), 491-500 (1988).

46 - Structure of Zeolitic $K_2TiSi_3O_9•H_2O$ Determined ab initio from Powder Diffraction Data. M.S. Dadachov and A. Le Bail, *Eur. J. Solid State Inorg. Chem*. **34**, 381-390 (1997).

46 - Copper containing minerals: I. $Cu_3V_2O_7(OH)_2.2H_2O$: the synthetic homologue of volborthite; crystal structure determination from X-ray and neutron data; structural correlations. M.A. Lafontaine, A. Le Bail and G. Férey, *J. Solid State Chem*. **85**, 220-227 (1990).

44 - Structure of vanadyl hydrogenphosphate dihydrate α-$VO(HPO_4).2H_2O$ solved from X-ray and neutron powder diffraction. A. Le Bail, G. Férey, P. Amoros and D. Beltran-Porter, *Eur. J. Solid State Inorg. Chem*. **26**, 419-426 (1989).

43 - Crystal structure of β-$VO(HPO_4).2H_2O$ solved from X-ray powder diffraction. A. Le Bail, G. Férey, P. Amoros, D. Beltran-Porter and G. Villeneuve, *J. Solid State Chem*. **79**, 169-176 (1989).

40 - Synthesis and Crystal Structure of a Tubular Hydroxyphosphite: $Zn_{11}(HPO_3)_8(OH)_6$, M.D. Marcos, P. Amoros and A. Le Bail, *J. Solid State Chem.* **107**, 250-257 (1993).

40 - A Qualitative Account for Anisotropic Broadening in Whole Powder Diffraction Pattern Fitting by Second-Rank Tensors. A. Le Bail and A. Jouanneaux, *J. Appl. Cryst*., 30, 265-271 (1997).

37 - *t*-AlF_3: Crystal structure determination from X-ray powder diffraction data. A new MX_3 corner-sharing octahedra 3D network. A. Le Bail, J.L. Fourquet and U. Bentrup, *J. Solid State Chem*. **100**, 151-159 (1992).

36 - Short-range order in the anion-excess fluorite-related $Ca_{0.68}Ln_{0.32}F_{2.32}$ solid solutions: EXAFS study of the Ln^{3+} environment. J.P. Laval, A. Abaouz, B. Frit and A. Le Bail, *J. Solid State Chem.* **85**, 133-143 (1990).

36 - Crystal structure and protonic conductivity of pyrochlore phases $Al_2[(OH)_{1-x}F_x]_6.H_2O$ and $Al_2[(OH)_{1-x}F_x]_6$ (x=0.5). J.L. Fourquet, M. Riviere, A. Le Bail, M. Nygrens and J. Grins, *Eur. J. Solid State Inorg. Chem*. 25, 535-540 (1988).

34 - Fluoride glasses of 3d transition metals. C. Jacoboni, A. Le Bail et R. De Pape, *Glass Technology* **24**, 164-167 (1983).

33 - Smoothing and validity of crystallite-size distributions from X-ray line-profile analysis. A. Le Bail et D. Louër, *J. Appl. Cryst*. **11**, 50-55 (1978).

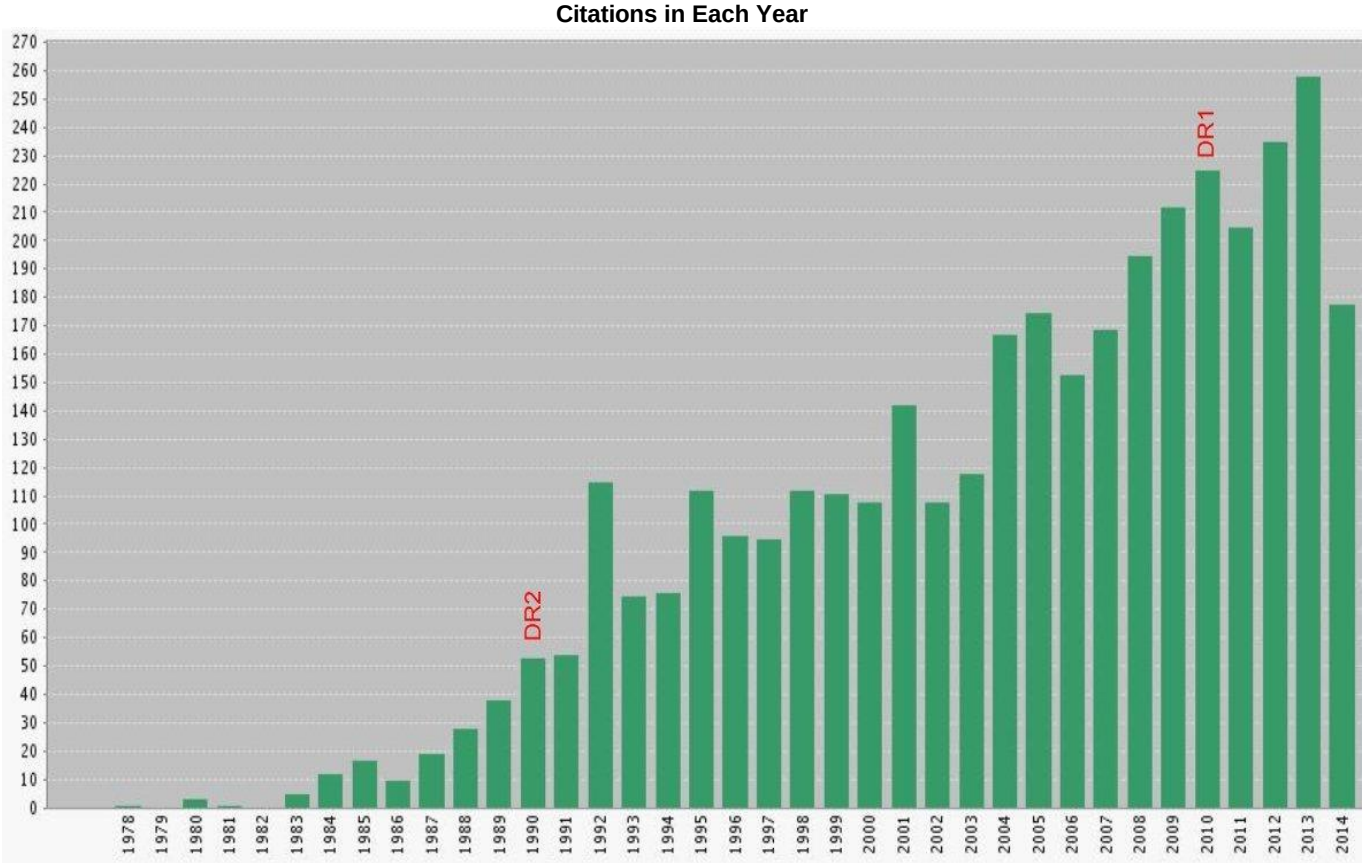
33 - Inorganic structure prediction with GRINSP. A. Le Bail, *J. Appl. Cryst*. **38** (2005) 389-395 - et *Acta Cryst* A**61** (2005) c97.

31- Structure determination of β and γ-$BaAlF_5$ by X-ray and neutron powder diffraction. A model for the α→β↔γ transitions. A. Le Bail, G. Ferey, A.-M. Mercier, A. De Kozak and M. Samouël, *J. Solid State Chem*. **89**, 282-291 (1990).

30 - Crystal structure of $A(VO_2)(HPO_4)$, ($A=NH^{4+},K^+,Rb^+$) solved from X-ray powder diffraction. P. Amoros, D. Beltran-Porter, A. Le Bail, G. Férey and G. Villeneuve, *Eur. J. Solid State Inorg. Chem*. **25**, 599-607 (1988).

28 - β-Ba_3AlF_9, a Complex Structure Determined from Conventional X-Ray Powder Diffraction, A. Le Bail, *J. Solid State Chem*., **103**, 287-291 (1993).

28 - $LiNbWO_6$: crystal structure of its two allotropic forms. J.L. Fourquet, A. Le Bail and P.A. Gillet, *Mat. Res. Bull.* 23, 1163-1170 (1988).



Un peu plus de citations d'après Google Scholar :

Google Scholar

Citations	Toutes	Depuis 2009
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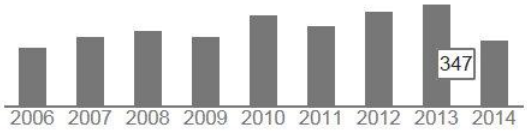
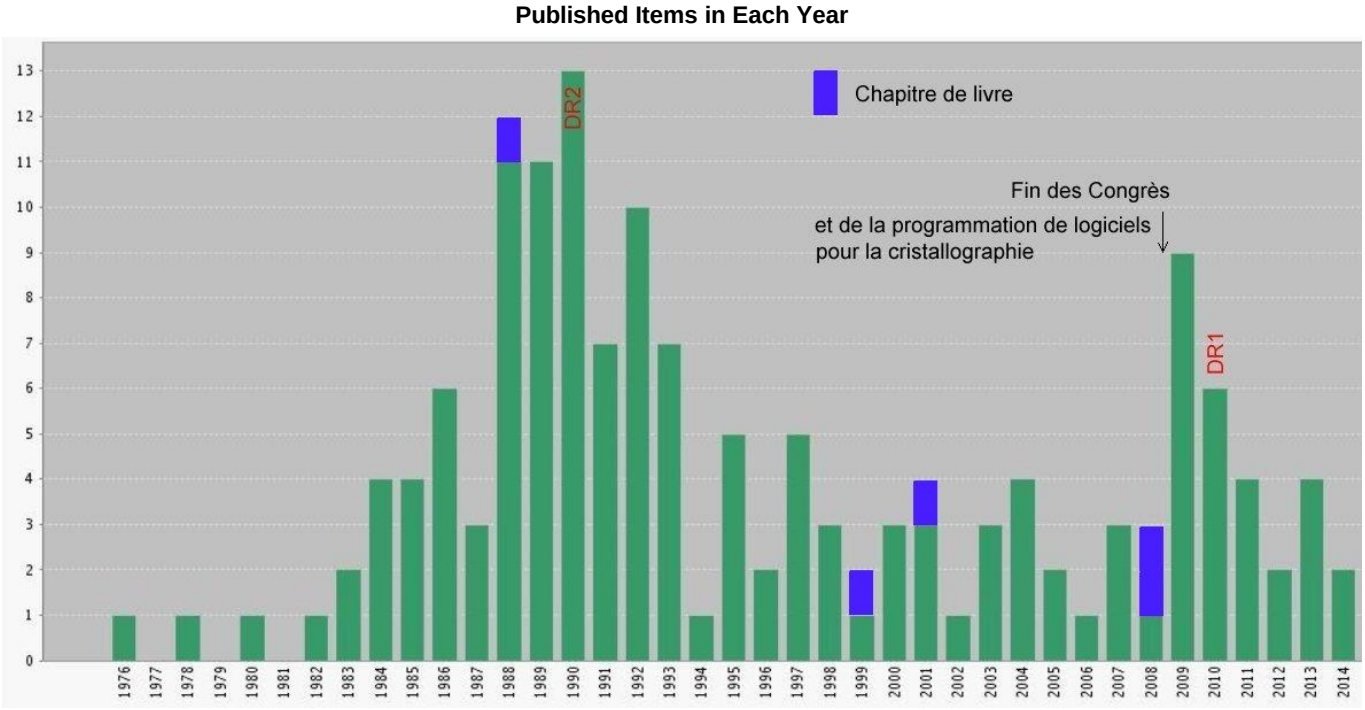
indice i10	69	24



Titre	Citée par	Année
Ab-initio structure determination of LiSbWO< sub> 6</sub> by X-ray powder diffraction A Le Bail, H Duroy, JL Fourquet Materials Research Bulletin 23 (3), 447-452	1614	1988
Size-strain line-broadening analysis of the ceria round-robin sample D Balzar, N Audebrand, MR Daymond, A Fitch, A Hewat, JI Langford, ... Journal of Applied Crystallography 37 (6), 911-924	174	2004
Whole powder pattern decomposition methods and applications: a retrospection A Le Bail Powder Diffraction 20 (04), 316-326	123	2005
A new study of the structure of LaNi< sub> 5</sub> D< sub> 6.7</sub> using a modified Rietveld method for the refinement of neutron powder diffraction data C Lartigue, A Le Bail, A Percheron-Guegan Journal of the Less Common Metals 129, 65-76	123	1987
Modelling the silica glass structure by the Rietveld method A Le Bail Journal of Non-Crystalline Solids 183 (1), 39-42	96	1995
Monte Carlo indexing with McMaille A Le Bail	94	2004
Crystal structure of the metastable form of aluminum trifluoride β-AlF< sub> 3</sub> and the gallium and indium homologs A Le Bail, C Jacoboni, M Leblanc, R De Pape, H Duroy, JL Fourquet Journal of Solid State Chemistry 77 (1), 96-101	89	1988
Crystallography Open Database-an open-access collection of crystal structures S Grazulis, D Chateigner, RT Downs, AFT Yokochi, M Quirós, L Lutterotti, ... Journal of applied crystallography 42 (4), 726-729	84	2009
Extracting structure factors from powder diffraction data by iterating full pattern profile fitting A LeBail Accuracy in powder diffraction II, Special publication 846, 213	76	1992
ESPOIR: A program for solving structures by Monte Carlo from powder diffraction data A Le Bail EPDIC-7, Barcelona	66	2000
Electron Microscopy Study of the Superconductor``Bi2Sr2CaCu2O8+ delta" M Hervieu, C Michel, B Domenges, Y Laligant, A Lebail, G Ferey, ... Modern Physics Letters B 2, 491-500	63	1988

Liste complète par ordre de parution



Sur les 194 articles répertoriés ci-dessous, 147 sont dans par le Web of Science (en vert sur la figure ci-dessus). 5 chapitres de livres sont en bleu, Il manque 34 articles publiés dans des comptes rendus de colloques, newsletters de cristallographie et 7 à paraitre en 2015 dont un chapitre de livre.

Entre parenthèses, après le numéro d'ordre, est donné le **nombre de citations** dans la période 1975 à août 2014 ainsi qu'il peut être obtenu dans le **Science Citation Index** (ISI) par consultation du **Web of Knowledge**.

CL=Chapitre de livre

IUCr-N = International Union for Crystallography Newsletters

Derniers projets à concrétiser : article soumis ou en préparation

- **195 "**A quarter of a century after its synthesis and with >200 papers based on its use, `$Co(CO_3)_{0.5}(OH)\cdot 0.11H_2O$′ proves to be $Co_6(CO_3)_2(OH)_8\cdot H_2O$ from synchrotron powder diffraction data," P. Bhojane, A. Le Bail and P. M. Shirage, Acta Cryst. (2019). C75, 61-64. https://doi.org/10.1107/S2053229618017734
- **194** "$Cu_3AlF_7O[CH_3N_5]_4.H_2O$," ?
- **193** "Thermodiffractometry and crystal structure of $Pb_3FeF_9(H_2O)$ and of its derivatives $Pb_3FeF_9(H_2O)_x$ ($0 < x < 1$), γ-, β- and α-Pb_3FeF_9," A. Le Bail, *Powder Diffraction*
- **192** "Polymorphism of K_2ZrF_6," A. Le Bail, M. Boca and L. Smrcok, *Inorg. Chem*.
- **191** "First microporous class 1 hybrid aluminum fluoride : crystal structures of [H*taz*]$_3$.(Al_3F_{12}).$3H_2O$ and of the dehydrated form," Laurent J. Jouffret, Jérôme Lhoste, Amandine Cadiau, Monique Body, Christophe Legein, Armel Le Bail, Vincent Maisonneuve. *Chem Mat.*
- **190 "***Ab initio* structure determination of kidney stone potassium quadriurate from synchrotron powder diffraction data, a 150 year problem solved," Dominique Bazin, Michel Daudon, Erik El kaim, Armel Le Bail, Ľubomír Smrčok, Comptes Rendus Chimie, Volume 19, Issues 11–12, November–December 2016, Pages 1535-1541. https://doi.org/10.1016/j.crci.2015.02.003
- **189** "Face-sharing octahedra in $Cs_3Al_2F_9$ and Cs_2AlF_5," A. Le Bail and L. Smrcok, *Powder diffraction, Volume 30, Issue 2, June 2015 , pp. 130-138. https://doi.org/10.1017/S0885715614001444*

Article à paraître (chapitre de livre)

- **188** **CL** "Data reduction to $|F_{hkl}|$," A. Le Bail, International Tables for Crystallography, Vol. H, Powder Diffraction, to be published (early 2015).

Articles parus :

2014

- **187** "$La_{10}W_2O_{21}$" an anion deficient fluorite related superstructure with oxide ion conduction," M.-H. Chambrier, A. Le Bail, F. Giovannelli, A. Redjaïmia, P. Florian, D. Massiot, E. Suard, F. Goutenoire, *Inorg. Chem.* **63**, 2014, 147-159. DOI: 10.1021/ic401801u
- **186** "On two new K_2FeF_5 forms," A. Le Bail, *Powder Diffraction* **29**, 2014, 33-41. DOI: 10.1017/s0885715613001334
- **185** "Launching the Theoretical Crystallography Open Database," S. Grazulai, A. Merkys, A. Vaitkus, A. Le Bail, L.Vilciauskas, S. Cottenier, T. Björkman and P. Murray-Rust, *Acta Cryst.* **A70**, C1736 (2014).
- **184** "Chemical information presentation in the Crystallography Open Database," A. Merkys, A. Matuseviciute, A. Vaitkus, A. Le Bail, D. Chateigner, L. Lutterotti , M. Quiros-Olozabal, M. Okulic-Kazarinasa, P. Moeck, P. Murray-Rust, R.T. Downs, S. Girdzijauskaite and S. Grazulis, *Acta Cryst.* **A70**, C1710 (2014).

2013

- **183** "Tetraammine(carbonato-κ^2O,O')cobalt(III) nitrate; a powder X-ray diffraction study,' A. Le Bail, *Acta Cryst.* **E69**, i42-i43 (2013) - doi:10.1107/S1600536813017522
- **182 (2)** "Decafluorocyclohex-1-ene at 4.2K - crystal structure and theoretical analysis of weak interactions," L. Smrcok, P. Mach, A. Le Bail, *Acta Cryst.* **B69**, 395-404 (2013) - doi:10.1107/S2052519213013365
- **181** "A new compound in kidney stones ? Powder X-ray diffraction study of calcium glycinate trihydrate," A. Le Bail, M. Daudon, D. Bazin, *Acta Cryst.* **C69**, 734-737 (2013) - doi:10.1107/S0108270113015709
- **180** "Tetrapotassium pyrophosphates γ- and δ-$K_4P_2O_7$," A. Le Bail, T. Hansen, W.A. Crichton, *Powder Diffraction* **28**, 2-12 (2013). DOI: 10.1017/S0885715612000954

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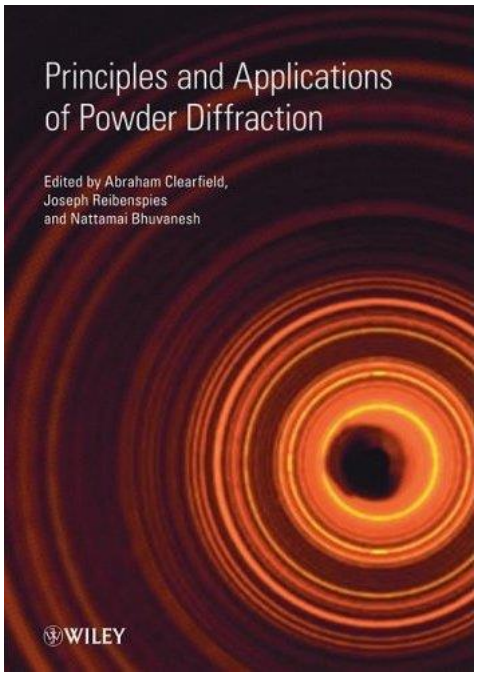

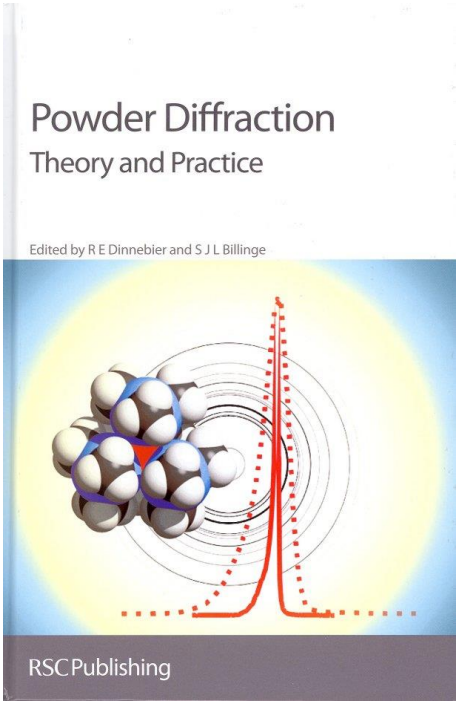

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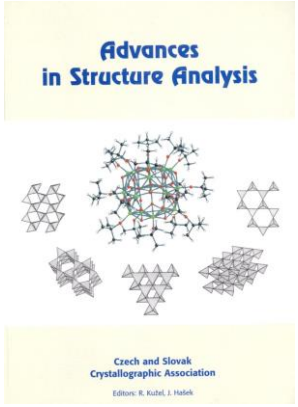

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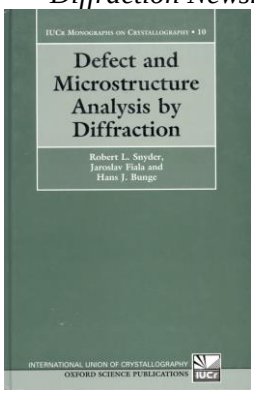

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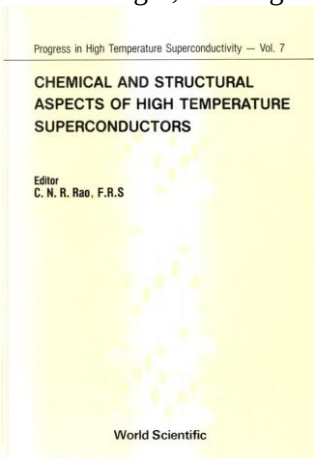

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-42. IUCr XIX, 6-15 August 2002, Geneva. "Size-strain round robin: first results and the comparative analysis of the measurements."
-43. IUCr XIX, 6-15 August 2002, Geneva. "Beyond classical Rietveld analysis using Le Bail fitting."
-44. IUCr XIX, 6-15 August 2002, Geneva. "A crystal structure for the souzalite/gormanite series from synchrotron powder diffraction data."
-45. SFC 2005, 23-25 Mai 2005, Batz sur Mer, "Elaboration de matériaux fluorés construits autour de précurseurs organiques originaux."
-46. IUCr XX, 23-31 August 2005, Florence, Italy "COD (Crystallography Open Database) and PCOD (Predicted)."
-47. EPDIC 10, 1-4 September 2006, Genève, Suisse : « Predicted corner-sharing titanium silicates. »
-48. Congrès Européen du Fluor, Prague, 2007, « New layered organic-inorganic fluorides » K. Adil, A. Ben Ali, A. Le Bail, M. Leblanc, A. Hémon-Ribaud, V. Maisonneuve.
-49. Colloque de l'Association Française de Cristallographie - AFC 2008, Rennes, 7-10 juillet 2008, "Etude du système $Al(OH)_3$-*guaz*-$HF_{aq.}$-éthanol par voie micro-ondes ; quatre nouveaux fluoroaluminates hybrides à sous-réseau inorganique de dimensionnalité croissante." A. Cadiau, A. Hémon-Ribaud, A. Le Bail, M. Leblanc et V. Maisonneuve.
-50. Colloque de l'Association Française de Cristallographie - AFC 2008, Rennes, 7-10 juillet 2008, "Structure cristalline de "$La_{14}W_8O_{45}$", objet du SDPDRR-3," M.-H. Chambrier, A. Le Bail, F. Goutenoire.
-51. IUCr XXI, Osaka, Japan, August 23-31, 2008. "The third Structure Determination by Powder Diffractometry Round Robin (SDPDRR-3)." L.M.D Cranswick, A. Le Bail.
-52. IUCr XXI, Osaka, Japan, August 23-31, 2008. "The predicted powder diffraction database (P2D2)" A. Le Bail.
-53. 26th European Crystallographic Meeting (ECM26), 29 August- 2 September 2010, Darmstadt, Germany, "Software for maintaining and expanding the Crystallography Open Database," S. Gražulis, J. Butkus, R. Downs, M. Quirós Olozábal, A. Le Bail.
-54. 16th European Symposium on Fluorine Chemistry, 18-23 July, 2010, Ljubljana, Slovenia. "Study of $Al(OH)_3$-Am_2TAZ-HF_{aq}-ethanol system by micro-wave heating: four new hybrid fluoroaluminates with increasing dimensionality of the inorganic network," A. Cadiau, A. Hemon-Ribaud, A. Le Bail, M. Leblanc and V. Maisonneuve.

-55. First North African Crystallographic Conference, November 23rd-26th 2010, Casablanca, Morocco. "Elaboration of new fluorinated Metal-Organic-Frameworks," Amandine Cadiau, Armel Le Bail, Annie Hémon-Ribaud, M. Leblanc, V. Maisonneuve, K. Adil.

-56 Congrès de l'Association Française de Cristallographie, Bordeaux, 2-5 juillet 2013. "News in Open structure and property Databases," Daniel Chateigner, Saulius Grazulis, Justas Butkus, Andrius Merkys, Adriana Daškevič, Olivier Pérez, Giancarlo Pepponi, Luca Lutterotti, Miguel Quirós Olozábal, Armel Le Bail, Robert Downs, Peter Moeck, Alexandre F.T. Yokochi.

-57 American Crystallographic Association Annual Meeting, Hawaii 2013, July 20-24, Honolulu. "The Crystallography Open Database in its 11th year," Peter Moeck, Daniel Chateigner, Robert T. Downs, Saulius Gražulis, Armel Le Bail, Luca Lutterotti, Miguel Quirós.

-58 The 28th European Crystallographic Meeting (ECM28) 25th-29th August 2013 The University of Warwick, UK. "C_6F_{10} at 4.2K - Crystal Structure and Theoretical Analysis of Weak Interactions" Lubomir Smrcok, Pavel Mach, Armel Le Bail.

-59 23rd Congress of the International Union of Crystallography, Montréal 2014, August 5-12. "Chemical information presentation in the Crystallography Open Database," A. Merkys, A. Matuseviciute, A. Vaitkus, A. Le Bail, D. Chateigner, L. Lutterotti , M. Quiros-Olozabal, M. Okulic-Kazarinasa, P. Moeck, P. Murray-Rust, R.T. Downs, S. Girdzijauskaite and S. Grazulis.

-60 23rd Congress of the International Union of Crystallography, Montréal 2014, August 5-12. "Launching the Theoretical Crystallography Open Database," S. Grazulai, A. Merkys, A. Vaitkus, A. Le Bail, L.Vilciauskas, S. Cottenier, T. Björkman and P. Murray-Rust.

Conférences invitées

1 - L.U.R.E. - ORSAY (10.03.1986).
"Imperfections cristallines et méthode de RIETVELD: possibilités actuelles"

2 - GALERNE 1986 - CAEN (29/09-03/10/1986).
"Analyse globale des spectres de diffraction de composés mal cristallisés"

3 - UNIVERSITE DE VALENCE (ESPAGNE) - Juillet 1988.
"Ab initio crystal structure determination from powder diffraction data."

4 - UNIVERSITE DE VALENCE (ESPAGNE) - Avril 1990.
"Twinning and superstructures: some recent examples of structure solution from X-Ray diffraction".

5 - CONGRES INTERNATIONAL "POWDER DIFFRACTION", 16-19 Juillet 1990, TOULOUSE.
"The practice of structure determination from powder data: how to succeed".

6 - CONGRES INTERNATIONAL "ACCURACY IN POWDER DIFFRACTION II" (APD-II), 26-29 Mai 1992, Gaithersburg, USA.
"Modelling Anisotropic Size/Microstrain in Rietveld Analysis".

7 - CONGRES INTERNATIONAL "SIZE - STRAIN'95", Août 1995, Slovaquie.
"Accounting for Size/Microstrain in Whole Powder Pattern Fitting".

8 - XVII Congress and General Assembly of the International Union of Crystallography, August 8-17, 1996, Seattle, USA."VRML as a tool for exploring complex structures".
Conférence en ligne à : http://www.cristal.org/vrml/seattle/seattle.html

9 - ACA'97, July 19-25, 1997, St. Louis, Missouri, USA. "Standard and special strategies in structure determination from powder data".

Conférence en ligne à : http://www.cristal.org/iniref/aca97/aca97.html

10- 47th Annual Denver X-ray Conference, August 3-7, 1998, Colorado Springs, Colorado, USA. "New Developments in Microstructure Analysis via Rietveld Refinement".
Conférence en ligne à : http://www.cristal.org/microstruct/denver/index.html

11- ECM-18, August 15-20, 1998, Prague, République Tchèque. "Trends in Structure Determination by Powder Diffractometry".
Conférence en ligne à : http://www.cristal.org/iniref/ecm18/ecm18.html

12 - Kunming IUCr Workshop, China, July 1999. “Structure Determination by Powder Diffractometry”.
Conférence en ligne à : http://sdpd.univ-lemans.fr/kunming/index.html

13 - XVIIIth IUCr Congress & General Assembly, 4^{th}-13^{th} August 1999, Glasgow, Scotland . Structure Solution from Powder Diffraction Data Workshop. “The Practice of "|Fobs|" Extraction from Powder Diffraction Data”.
Conférence en ligne à : http://www.cristal.org/glasgow/index.html

14 – Sixth International School and Workshop of Crystallography, 22-27 January 2000, Ismailia, Egypt. “Combining the Reverse Monte Carlo and the Rietveld Methods for Amorphous Materials Structure Modelling”.
Conférence en ligne à : http://www.cristal.org/egypte/conf1/index.html

15 – Sixth International School and Workshop of Crystallography, 22-27 January 2000, Ismailia, Egypt. “Advances in Microstructure Analysis by the Rietveld Method”.
Conférence en ligne à : http://www.cristal.org/egypte/conf2/index.html

16 – 20th European Crystallographic Meeting, ECM 20, August 25-31, 2001, Kraków, Poland. “Stucture determination by powder diffractometry : Distance teaching and distance learning.”
Conférence en ligne à : http://sdpd.univ-lemans.fr/conf.html

17 – 20th European Crystallographic Meeting, ECM 20 August 25-31, 2001, Kraków, Poland. “Old-style amorphous structure modelling, does it can still bring something ?”
Conférence en ligne à : http://sdpd.univ-lemans.fr/conf.html

2002 : 2 conférences invitées annulées (EPDIC-8, Uppsala, Suède et ACA-2002, San Antonio, USA) en raison d'un grave accident de voiture.

18 - CONCIM 2003 - Conference on Non-Crystalline Inorganic Materials, Bonn, Allemagne, 8-12 avril 2003. "Reverse Monte Carlo and Rietveld modelling of $BaMn(Fe,V)F_7$ glass structures from neutron data."

19 - AFC-2003, 7-10 Juillet 2003, Caen, France, "Diffraction de poudre et Monte Carlo; indexation de diagramme et solution de structure."

20 - ECM-21, 24-29 August 2003, Durban, South Africa. "McMaille v3: indexing via Monte Carlo search, matching against an idealized powder profile."

21 - One day Single Crystal and Powder Diffraction Software Workshop ECM 21 : International Conference Centre, Durban, South Africa, 24th August 2003. "Limits of powder indexing of impure samples using whole profile methods."

22 - SSPD-03, 14-19 September 2003, Stara Lesna, Slovakia. "Monte Carlo indexing with McMaille."

23 - EMC^2 - Deuxième Ecole Marocaine de Cristallographie, El Jadida, Maroc, 10-14 Mai 2004. "Méthode Monte Carlo appliquée à l'indexation des diagrammes de poudre et à la résolution de structure."

24 - EMC^2 - Deuxième Ecole Marocaine de Cristallographie, El Jadida, Maroc, 10-14 Mai 2004. "Bases de données publiques, archives de laboratoires en ligne."

25 - ESCA-9, Recent Advances in X-ray Powder Diffraction, 27 Novembre - 2 Décembre 2004, Assiut, Egypt, "Structure prediction of inorganic compounds."

26 – CAC2 : Deuxième Congrès Algérien de Cristallographie, Constantine, Algérie, 17-21 Avril 2005. " Prédiction de structures inorganiques par contraintes géométriques."

27 - IUCr XX, 23-31 August 2005, Florence "Inorganic Structure Prediction with GRINSP."

28 – Rencontres LLB-SOLEIL, Diffraction de Poudres, 2-3 mars 2006. « Progrès en résolution de structure par diffractométrie de poudres.»

29 - EMC^3 - Troisième Ecole Marocaine de Cristallographie, Agadir, Maroc, Mai 2006. "Composés Inorganiques Virtuels - Structures et Propriétés."

30 – Global Optimization Techniques Applied to the Prediction of Structures, London, 6-7 July 2006 : "Microporous titanium silicates predicted by GRINSP."

31 – X-EL 2006, satellite meeting of ECM23, 1-4 August 2006, Antwerp, Belgique : "Indexing XRD patterns, getting cell parameters."

32 – EPDIC 10, 1-4 September 2006, Genève, Suisse : « McMaille : sous le capot. »

33 – XX Conference on Applied Crystallography, 11-14 September 2006, Wisla, Poland : "Inorganic structure prediction : too much and not enough."

34 – Summer School on Polycrystalline Structure Determination, 14-16 September 2006, Wisla, Poland, "Structure prediction" and "Rietveld refinement."

35 - Latin American Workshop on Applications of Powder Diffraction, April 16-20, 2007, Campinas, Brazil : "Frontiers between crystal structure prediction and determination by powder diffractometry."

36 - Latin American Workshop on Applications of Powder Diffraction, Satellite workshop "Methods of Powder Diffraction", April 16-20, 2007, Campinas, Brazil : "Getting cell parameters from powder diffraction data."

37 - CAC-3 : 3rd Crystallography Algerian Congress, April 20-22, 2008, Oran, Algérie : "Recent activities around the crystallography open databases COD, PCOD and P2D2."

38 - CECAM Workshop Energy Landscape of Solids: from (hypothetical) topologies to material properties, July 23-25, 2008, Lausanne, Suisse : "The PCOD and P2D2 databases (P for Predicted)."

Logiciels / Algorithmes

Encore disponibles en accès ouvert (GPL = GNU Public Licence)

GRINSP (2005)

Prédiction de structures cristallines à réseaux N-connectés
(simple pour N = 3, 4, 5, 6, et mixte N/N')

- 146 (33) "Inorganic structure prediction with GRINSP." A. Le Bail, *J. Appl. Cryst*. **38** (2005) 389-395.

McMaille (2004)

Indexation de diagramme de poudre par méthode Monte Carlo

- 142 (86) "Monte Carlo indexing with McMaille." A. Le Bail, *Powder Diffraction*, **19** (2004) 249-254.

ESPOIR (2001)

Solution de structure sur poudre ou monocristal dans l'espace direct

- 122 (52) "ESPOIR : A Program for Solving Structures by Monte Carlo from Powder Diffraction Data." A. Le Bail, *Mat. Sci. Forum*, **378-381** (2001) 65-70.

STRUVIR (1995)

Reprise de STRUPLO avec production de fichiers en langage VRML

pour affichage sur le Web.

Logiciels plus anciens :

SIZEDIST **(33)**, ARIT **(1333)**, ARITVE **(62)**, HKLGEN, OVERLAP, TMACLE, NOCHAOS, GLASSVIR

Algorithme incorporé dans GSAS, FULLPROF, WinMPROF, RIETAN, EXPO, EXTRA, EXTRACT, etc :

« Méthode Le Bail » (1988)

extraction des intensités d'un diagramme de poudre
par itération de la formule de décomposition de Rietveld

- 31 (1333) "Ab-initio structure determination of $LiSbWO_6$ by X-Ray powder diffraction" A. Le Bail, H. Duroy et J.L. Fourquet, *Mat. Res. Bull*. 23, 447-452 (1988).

Bases de données

COD : Crystallography Open Database (création en 2003)

http://www.crystallography.net/

~300.000 fichiers CIF de structures cristallines distribuées, avec moteur de recherche par mot-clé, paramètres de maille, volume, formulation chimique (etc).

- **159 (68)** "Crystallography Open Database – an open access collection of crystal structures." S. Gražulis, D. Chateigner, R.T. Downs, A.F.T. Yokochi, M. Quirós, L. Lutterotti, E. Manakova, J. Butkus, P. Moeck and A. Le Bail, *J. Appl. Cryst*. **42** (2009) 726-729.

PCOD : Predicted Crystallography Open Database

http://www.crystallography.net/pcod/

>160.000 fichiers CIF de structures prédites par le logiciel GRINSP, avec moteur de recherche par mot-clé, paramètres de maille, volume, formulation chimique.

> 900.000 fichiers CIF de structures de zéolithes prédites par ZEFSA II (M.W. Deem)

TCOD : Theoretical Powder Diffraction Database

Création 2013. But : rassembler les structures cristallines passées à la moulinette DFT et autres approches de type "Quantum Chemistry."

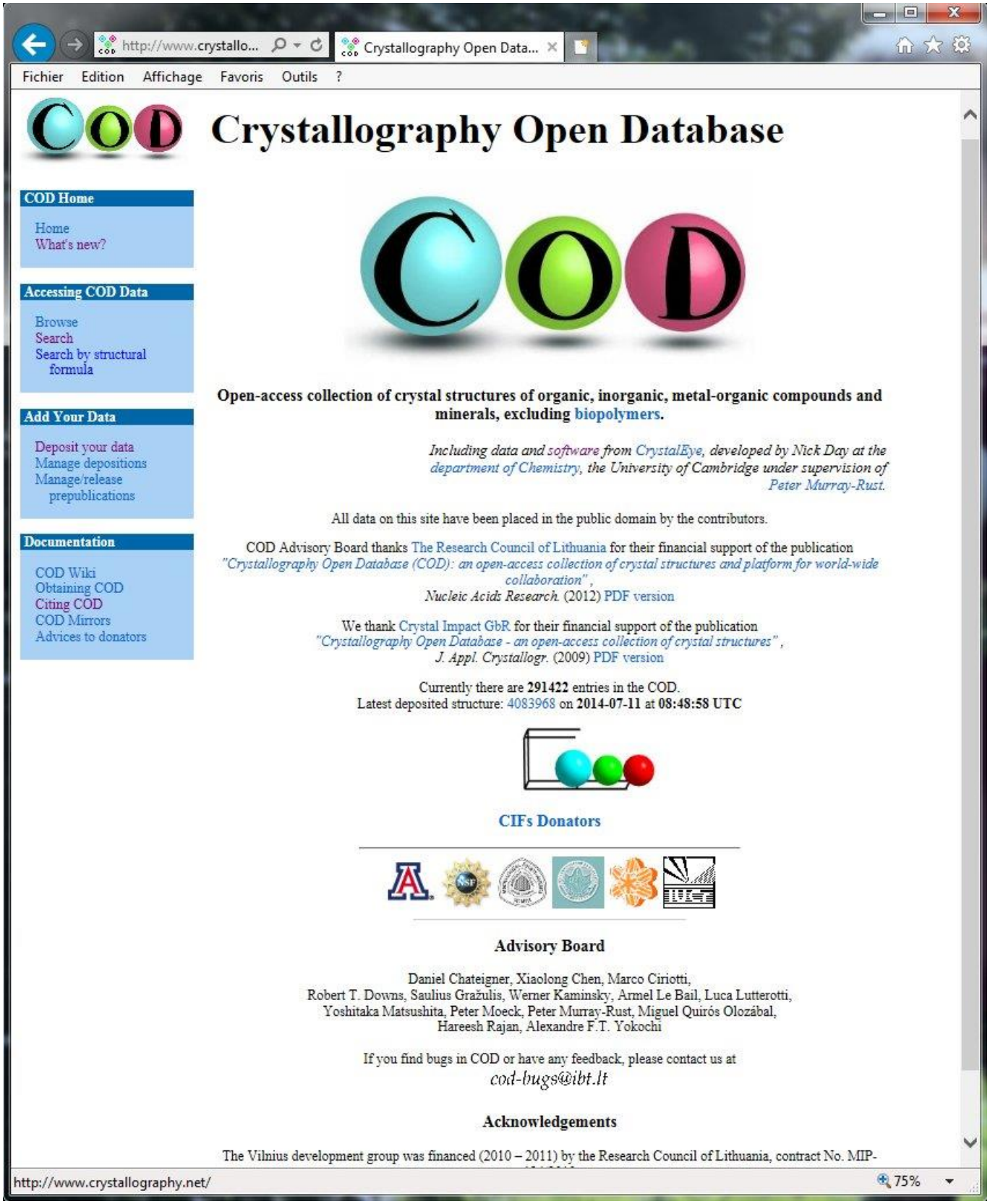
P2D2 : Predicted Powder Diffraction Database

http://www.crystallography.net/pcod/p2d2/

>160.000 diagrammes de poudre de composés prédits par le logiciel GRINSP, pour identification, incorporés dans les logiciels EVA (Bruker) et Highscore (Panalytical).

> 900.000 diagrammes de poudre de structures de zéolites prédites par ZEFSA II (M.W. Deem)

Ces bases de données sont adoptées et distribuées par la plupart des fabriquants de diffractomètres à poudre et/ou des vendeurs de logiciels d'identification de phase par "search-match" (Bruker, Rigaku, PANalytical, Crystal Impact).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