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LISTE COMPLETE
des
PRODUCTIONS SCIENTIFIQUES
1976-2008

PLAN

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Publications traditionnelles

Liste restreinte des articles les plus cités (index de Hirsch $h = 23$)

116 articles dans le Web au Knowledge (153 au total en incluant chapitres de livres et articles non répertoriés par Thomson-ISI)

2203 citations de ces 116 articles cités dans 1725 articles, hors auto-citations

19 citations en moyenne par article

h -index = 23

article le plus cité : 755 citations

Liste des publications citées 23 fois ou plus (Nombre de citations en début de référence) :

- 755** - *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).
- 84** - A new study of the structure of $\text{LaNi}_5\text{D}_{6.7}$ 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).
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- 60** - 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).
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- 46** - The room-temperature crystallisation of a one-dimensional gallium fluorophosphate, $\text{Ga}(\text{HPO}_4)_2\text{F}\cdot\text{H}_3\text{N}(\text{CH}_2)_3\text{NH}_3\cdot 2\text{H}_2\text{O}$, a precursor to three-dimensional microporous gallium fluorophosphates, Walton, RI, Millange, F, Le Bail, A, Loiseau, T, Serre, C, O'Hare, D, Férey, G, *Chem. Comm.*, 203-204 (2000).
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- 40** - Crystal structure of $\beta\text{-VO}(\text{HPO}_4)\cdot 2\text{H}_2\text{O}$ 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).
- 38** - Extracting structure factors from powder diffraction data by iterating full pattern profile fitting, A. Le Bail, *NIST Special Publication* **846**, 213 (1992).
- 38** - 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.
- 37** - Structure of Zeolitic $\text{K}_2\text{TiSi}_3\text{O}_9\cdot\text{H}_2\text{O}$ Determined ab initio from Powder Diffraction Data. M.S. Dadachov and A. Le Bail, *Eur. J. Solid State Inorg. Chem.* **34**, 381-390 (1997).
- 35** - Modelling the Silica Glass Structure by the Rietveld Method. A. Le Bail, *J. Non-Cryst. Solids*, **183**, 39-42 (1995).
- 34** - Fluoride glasses of 3d transition metals. C. Jacoboni, A. Le Bail et R. De Pape, *Glass Technology* **24**, 164-167 (1983).
- 33** - Short-range order in the anion-excess fluorite-related $\text{Ca}_{0.68}\text{Ln}_{0.32}\text{F}_{2.32}$ 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).
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- 29** - 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).

- 26** - β -Ba₃AlF₉, a Complex Structure Determined from Conventional X-Ray Powder Diffraction, A. Le Bail, *J. Solid State Chem.*, **103**, 287-291 (1993).
- 26** - Copper containing minerals: I. Cu₃V₂O₇(OH)₂.2H₂O: 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).
- 26** - Crystal structure of A(VO₂)(HPO₄) , (A=NH⁴⁺,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).
- 24** - *t*-AlF₃: Crystal structure determination from X-ray powder diffraction data. A new MX₃ corner-sharing octahedra 3D network. A. Le Bail, J.L. Fourquet and U. Bentrup, *J. Solid State Chem.* **100**, 151-159 (1992).
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- 23** - Ordre local dans quelques verres fluorés du système PbF₂-M^{II}F₂-M^{III}F₃ par E.X.A.F.S. A. Le Bail, C. Jacoboni et R. De Pape, *J. Solid State Chem.* **52**, 32-44 (1984).
- 23** - Structure determination of β and γ -BaAlF₅ by X-ray and neutron powder diffraction. A model for the $\alpha \rightarrow \beta \leftrightarrow \gamma$ transitions. A. Le Bail, G. Férey, A.-M. Mercier, A. De Kozak and M. Samouël, *J. Solid State Chem.* **89**, 282-291 (1990).

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CL=Chapitre de livre

IUCr-N = International Union for Crystallography Newsletters

- **153** "The third Structure Determination by Powder Diffractometry Round Robin (SDPDRR-3)." L.M.D Cranswick, A. Le Bail, *Acta Cryst* **A64** (2008) C209-210.
- **152** "The predicted powder diffraction database (P2D2)" A. Le Bail, *Acta Cryst* **A64** (2008) C626.
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- **150** "Frontiers between crystal structure prediction and determination by powder diffractometry" A. Le Bail, *Powder Diffraction*, Suppl. **23** (2008) 5-12.
- **149** **CL** "Structure Solution." A. Le Bail, Chapter 7 in "Principles and Applications of Powder Diffraction, Ed. A. Clearfield, J.H. Reibenspies & N. Bhuvanesh, Wiley-Blackwell, Oxford (2008) 261-309.
- **148** **CL** "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.
- **147** **IUCr-N** "Search-matching inorganics through the PPDF-1 (Predicted Powder Diffraction File)" A. Le Bail, *IUCr CPD Newsletter*, **35** (2007) 27-28.
- **146** "Inorganic structure prediction: too much and not enough", A. Le Bail, *Solid State Phenomena* **130** (2007) 1-6.

- **145** « Predicted corner-sharing titanium silicates » A. Le Bail, *Z. Kristallogr.*, Suppl. **26** (2007) 203-208.
- **144** "New 1D hybrid fluoroaluminate templated by an original tetramine", K. Adil, A. Le Bail, G. Dujardin and V. Maisonneuve, *Polyhedron* **26** (2007) 2493-2497.
- **143** "Hypothetical AlF₃ crystal structures" A. Le Bail, F. Calvayrac, *J. Solid State Chem.*, **179** (2006) 3159-3166.
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- **136 IUCr-N** "Geometrically restrained inorganic structure prediction : GRINSP," A. Le Bail, *IUCr Computing Commission Newsletter* **4** (2004) 37-45.
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- **128** "A crystal structure for the souzalite/gormanite series from synchrotron powder diffraction data," A. Le Bail, P.W. Stephens & F. Hubert, *European Journal of Mineralogy*, **15** (2003) 719-723.
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- **120 (9)** "Ab initio structure determination of lanthanum cyclo-tetrahedral α -La₂W₂O₉ from X-ray and neutron powder diffraction." Y. Laligant, A. Le Bail and F. Goutenoire, *J. Solid State Chem.* **159** (2001) 223-227.
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- **98** "Barium-Oxomercurato(II)-Oxoruthenate(VI) BaHgRuO_5 : A new Oxomercurate with a Cyclic Mercurate-Ruthenate Anion. High Pressure Synthesis and *Ab Initio* Structure Approach by X-Ray Powder Diffraction." Th. Hansen, A. Le Bail and Y. Laligant, *Materials Science Forum*, Vols **228-231**, 729-734 (1996).
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- **92** "Structure of [Pd(NH₃)₄]Cr₂O₇." Y. Laligant and A. Le Bail, *Powder Diffraction*, **10**, 159-164 (1995).
- **91 (7)** "*Ab initio* Crystal Structure Determination of VO(H₂PO₂)₂·H₂O from X-ray and Neutron Powder Diffraction Data. A Monodimensional Vanadium(IV) Hypophosphite." A. Le Bail, M.D. Marcos and P. Amoros, *Inorg. Chem.* **33**, 2607-2613 (1994).
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2008

- [Contributions](#) to the XXI IUCr Meeting, 23-31 August 2008, Osaka, Japan



- Contribution to the CECAM workshop : [Energy Landscape of Solids: from \(hypothetical\) topologies to material properties](#), 22-25 July 2008, Lausanne, Switzerland
- [Contribution to CAC-3](#) (3rd Crystallography Algerian Congress), 20-22 April 2008, Oran, Algeria
- [PCOD](#) (Predicted Crystallography Open Database)
2008 update : > 100 000 entries
- [P2D2](#) (Predicted Powder Diffraction Database)
2008 update : > 100 000 entries
[Files for EVA](#) (Bruker)
- [SDPDRR-3](#) : Structure Determination by Powder Diffractometry Round Robin 3. Starting February 1st, 2008, deadline April 30, 2008 - best wishes.

2007

- Latin American Workshop on Applications of Powder Diffraction, April 16-20, 2007, Campinas, Brazil. [Pictures and contributions](#).
- Search-match is possible by EVA (Bruker) combined with the [PPDF-1](#) : a positive identification of your experimental powder pattern with the calculated pattern of a predicted crystal structure is now equivalent to an ab initio structure solution, even before indexing. [Contact](#).
- Creation of the [PPDF](#) (Predicted Powder Diffraction File) version 1, from > 60.000 PCOD entries.
- PCOD [update](#) with 58.500 [new hypothetical models](#)

2006

- [McMaille version 4](#), parallelized for multi core processors
- New [GRINSP](#) version, parallelized for dual core processors
- [Contributions](#) to XX Conference on Applied Crystallography, Wisla, Poland, 11-14 September 2006
- [Contributions to EPDIC-10](#), 1-4 September 2006, Geneva
- Contribution to [X-EL 2006](#), Antwerp (School on Structure Determination by the Combination of X-ray Powder Diffraction and Electron Crystallography), satellite conference of ECM-23 (23rd European Crystallographic Meeting) ([zipped](#)).
- Contribution to the "Gordon Conference Style" Workshop : "Global Optimisation Techniques Applied to the Prediction of Structures, 5-7 July 2006, University College London ([.ppt](#) or [zipped](#))
- Paper about [hypothetical AlF₃ crystal structures](#)
- Contribution (in French) to EMC3 (Ecole Marocaine de Cristallographie - 3), Agadir, Morocco (8-12 May, 2006). PowerPoint [file](#), MS Word [file](#) and see a few [pictures](#).

- [GRINSP](#) update. The version 2.00 is more user friendly and allows for the modelling of larger structures (up to 192 cations like in faujasite). New satellite software allow for the analysis of the (sometimes) huge lists of predicted inorganic crystal structures.
- Contribution (in French) to the "[Rencontres Scientifiques Soleil/LLB](#) (March 2-3, 2006). Talk about "Progress in Structure Determination by Powder Diffraction" ([.ppt](#) or [zipped](#))
- PCOD [update](#) with > 1000 titanosilicates

2005

- [Contributions](#) to [IUCr XX](#), Florence: talk about GRINSP ([.ppt](#)) and poster about COD and PCOD ([.ppt](#)). See a few [pictures](#)
- Sign the [Petition for Open Data in Crystallography](#)
- Contribution to [CAC2](#)
- Contribution to the Open Access tendency at IUCr (not cheap : 800 USD...) *J. Appl. Cryst.* **38**, 389-395. (about GRINSP).

2004

- [Contributions to ESCA-9](#), Assiut, Egypt, 2 November - 2 December 2004
- Contributions to EMC2 (Ecole Marocaine de Cristallographie), El Jadida, Morocco, 10-14 May 2004 -PowerPoint files : [part 1](#) (or [zipped](#)) and [part 2](#) (or [zipped](#)) - and see a few [pictures](#)
- [Powder Diffraction Indexing Benchmarks](#).
- A subset of the COD stores atomic coordinates of predicted crystal structure : the [PCOD](#)
- New Monte Carlo code for inorganic structure prediction : [GRINSP](#)

2003

- See the new [UPPW](#) service (Unindexed Powder Pattern of the Week).
- Contribution to SSPD03, Stara Lesna, Slovakia, 14-19 September 2003 ([PowerPoint](#) or [zipped](#) PowerPoint file, abstract in [PDF](#)). See also some [pictures](#).
- [Answer](#) from the IUCr to the COD asking for permission to give a link to their CIFs
- Contribution to ECM-21, Durban, South Africa, 24-29 August 2003 ([PowerPoint](#) or [zipped](#) PowerPoint file). See also a few [pictures](#).
- Contribution to CONCIM 2003, Bonn, Germany, 8-12 April 2003 (PowerPoint or zipped PowerPoint).
- The Crystallography Open Database : The COD.

2002

- McMaille : A new powder pattern indexing software by Monte Carlo or grid search in pseudo direct space.
- SDPDRR-2 : The second Structure Determination by Powder Diffraction Round Robin - starting September 9th, 2002.
- Search-Match Round Robin - Deadlines June 15 and June 30, 2002.
- Contribution to SIZE-STRAIN III, Analysis of microstructure and residual stress by diffraction methods, December 2-5, 2001, Trento, Italy. PDF file.

2001

- Contributions to ECM-20, Krakow, Poland, August 25-31, 2001 : Conference 1 about the SDPD Internet Course (html, zipped power-point file), and conference 2 about amorphous structure modelling (html, zipped power-point file) - See also a few pictures
- List of > 300 minerals with unknown crystal structure

- Trends in SDPD activity
- ESPOIR version for parallel computing (Florent Calvayrac)
- Most cited papers from Le Mans (ISI source)
- Most cited papers about Powder Diffraction (ISI source)
- Rapport CNRS "à deux ans" 1999-2001

2000

- Contributions to the chemistry preprints server <http://preprint.chemweb.com/>
- Liste de discussion : REcherche SCientifique Française (RESCIF)
- A new tutorial for speeding up ESPOIR use
- Contribution to the Size/Strain Round Robin with program ARIT
- K-alpha : believe your eyes or trust mathematics
- Contributions to EPDIC-7, Barcelona, 20-23 May 2000 : poster 1 (or preprint) and poster 2 (or preprint)
- ESPOIR 3.50 now driven by a Windows GUI. It can locate up to 6 independent molecules by Monte Carlo from powder diffraction data. Torsion angles are automatically located and possibly varied (recent developments sponsored by the DuPont Company) – GNU Public License
- Contributions to the Sixth International School and Workshop of Crystallography, 22-27 January 2000, Ismailia, Egypt : conference 1 and conference 2

1999

- CrySoCoM : Crystallography Source Code Museum
- PowBase : a free-access database of raw powder patterns
- SDPD Internet Course : learn to determine a crystal structure from powder diffraction data
- Webcam of the University of Maine, Sciences Faculty
- Contributions to IUCr XVIIIth, Glasgow, Scotland : Workshop on structure solution from powder data, computer Fayre, and poster
- Contribution to the Kunming (China) workshop on structure determination and refinement from powder data
- In french : Succès-échecs, des dossiers gagnants, ou perdants, ou même gagnants-perdants ! N'hésitez plus à contribuer.
- New Reverse Monte Carlo code for ab initio structure determination from powder diffraction data : ESPOIR 0.9 and then ESPOIR 1.0, and now ESPOIR 2.0 allowing molecule location
- Personal research report for 1995-99 as MS Word 97 .doc files, zipped, in french, of course
- Birth of the SDPD Mailing List
- Authors versus number of Rietveld-refined structures in ICSD and the sub-populations working with neutrons, conventional X-ray and synchrotron radiation
- Authors versus number of structures in ICSD (first 1000, or all)
- This Web site mirrored in Australia

1998

- The Rietveld Mailing List archives are partly available, searchable by keywords
- Discuss about Structure Determination by Powder Diffractometry using the SDPD Forum
- In french : Comment mettre en ligne une petite base de données
- Search among the Fluoride Lab's ~600 publications
- New web site created in the USA
- Contribution to the First International Conference on Inorganic Materials, Versailles
- Contribution to ECSOC-2
- Preliminary report on the SDPD Round Robin at ECM-18, Prague

- Contribution to ECM-18, Prague
- Contribution to the 47th Annual Denver X-ray Conference, Colorado Springs
- Structure Determination by Powder Diffraction Round Robin (SDPDRR)
- ARIT is available (very old and obsolete Rietveld method software)
- This site mirrored in England
- The Researcher's Breviary : an automatic translation from an hilarious french document, using Altavista ! No correction from the raw translation, expecting it to be more fun (?-)
- HKLGEN : Win95 software for [hkl, d(hkl), 2-theta] generation from cell parameters and space group
- Search the whole site by keywords with Altavista-like user interface
- ARRED : Academic Research Rare Expert Directory, add yourself if you expect external collaboration

1997

- Are you listed by ISI among the 10858 most cited chemists ? See also the most cited french chemists or search by author name. Finally, try the 1120 most cited physicists
- NOCHAOS : Win 95 software building quickly configuration files for Reverse Monte Carlo Modelling
- RMCAW95 : Win 95 executables of RMCA, RandOM, MOVEOUT and CRYSTAL
- Contribution to ACA'97, StLouis
- GLASSVIR : Win 95 software creating VRML files of RMCA output for 3D visualization
- Contribution to the RMC Modelling Internet Conference 1997
- Jeu des caricatures (in french)
- Tutorial for *Ab initio* structure determination from powder diffraction data
- τ -AlF₃, molecule of the month
- TREOR, ITO13 and DICVOL for Win95, with possible zeropoint correction
- ERACEL : Win95 software refining cell parameters

1996

- STRUVIR : Win 95 software creating VRML files for crystal structure 3D visualization
- VRML and crystallography
- Contribution to IUCr XVII, Seattle, 1996
- 6-connected 3D nets
- Université du Maine virtuelle (in french)
- Rapport d'activités (in french)
- SHELX76 for Win95
- libi77.lib and libf77.lib compiled for using f2c under Win95 with MSVC++2.0

1995

- ARITVE : Win95 software for amorphous structure modelling based on the Rietveld method
- SDPD-D : Structure Determination from Powder Diffraction - Database
- OVERLAP : Win95 software selecting reflections during a SDPD
- ICDD and Rietveld method

Communications - Posters

- 1. 6^{ème} Colloque Annuel du Groupe Français de Croissance Cristalline (1977) "Détermination des fonctions de répartition de taille des cristallites à partir du profil des raies de diffraction des rayons X. Croissance des cristallites d'hydroxyde de nickel provenant de la transformation d'un hydroxynitrate."
- 2. Conference on Applied Crystallography - Kozubnik - Pologne (1978) "Crystallite-size distributions from X-ray line profile analysis: smoothing, validity and application to a chemical reaction."
- 3. International Symposium: Order-Disorder in Solids - Paris (1978) "X-ray study of the transformation nickel hydroxynitrate into hydroxyde"
- 4. 5^{ème} Congrès International de Physique des Solides Non-Cristallins - Montpellier (1982) "Short range antiferromagnetic ordering in fluoride glasses PbMnFeF_7 and PbMnFeF_9 ."
- 5. 2^{ème} Conférence Européenne de Chimie de l'Etat Solide - Eindhoven (1982) "Physical properties and structure approach of the 3d transitions metal fluoride glasses $\text{PbF}_2\text{-MF}_2\text{-MF}_3$."
- 6. Journées de l'Etat Solide - Bordeaux (1984) "Structure des verres fluorés $\text{Na}_6\text{M(ii)}_5\text{M(iii)}_9\text{F}_{43}$ par diffraction des rayons X et des neutrons - séparation de six fonctions de paires partielles"
- 7. Workshop on High Resolution Neutron Powder Diffraction - Grenoble (1984) "Fourier analysis in Rietveld method for ideal or imperfect crystallized powder sample".
- 8. XIII^{ème} Congrès International de cristallographie - Hambourg (1984) "A quasi-crystalline simulation of $\text{Pb}_2\text{M(ii)}\text{M(iii)}\text{F}_9$ fluoride glass structure"
- 9. même congrès: "The Rietveld method using an experimental profile convoluted by adjustable analytical function"
- 10. 3^{ème} Int. Conf. on the Structure of Non-Crystalline Materials - Grenoble (1985) "Refining structural models for glasses: is it possible ? The case of $\text{Pb}_2\text{M}_2\text{F}_9$ "
- 11. même congrès: "Synthesis, characterization and crystallization of the amorphous iron (III) fluoride $\text{FeF}_3\cdot x\text{HF}$ ($x < 1$)"
- 12. Progress in X-ray Studies by Synchrotron Radiation - Strasbourg (1985) "Local structure in phosphonate glasses by EXAFS at tungsten absorption edge"
- 13. même congrès: "Local environment of M in pyrochlores AM_2F_6 by EXAFS"
- 14. 10^{ème} Colloque sur les Rayons X - Siemens - Grenoble (1985) "Analyse globale des spectres de diffraction des matériaux mal cristallisés"
- 15. 3^{ème} International Symposium on Halides Glasses - Rennes (1985) "Actual knowledge of 3d transition metal fluoride glasses structure"
- 16. même congrès: "Correlations between magnetic and crystallochemical behaviour in 3d- U^{4+} fluoride glasses"
- 17. 3rd European Meeting of Solid State Chemistry - Regensburg - RFA (1986) "EXAFS study of some Copper Fluorides"
- 18. International Symposium on the Properties and Applications of Metal Hydrides V - Maubuisson - France (1986) "A new study of the structure of $\text{LaNi}_5\text{D}_{6.7}$ using a modified Rietveld method for the refinement of neutron powder data"
- 19. EXAFS and Near-Edge Structure IV - Fontevraud - France (1986) "Local environment of Zr in baryum fluorozirconate glasses : the EXAFS point of view"
- 20. même congrès: "EXAFS of mixed valence iron potassium phosphate glass."
- 21. 4^{ème} International Symposium on Halide Glasses - Monterey - USA (1987) "Structure of baryum fluorozirconate glasses. A quasi crystalline modelization of $\text{BaZr}_2\text{F}_{10}$."
- 22. High-Temperature Superconductors and Materials and Mechanisms of Superconductivity - Interlaken - Suisse (1988) "Ordered $\text{Pd}^{2+}\text{-Cu}^{2+}$ substitution in 1.2.3. superconductor : The oxyde $\text{YBa}_2\text{Cu}_{2.5}\text{Pd}_{0.5}\text{O}_x$."
- 23. First European Inorganic Chemistry Seminar (EuChem) - Dourdan - France (1988) "Structure and magnetic properties of oxovanadium (IV) hydrogénophosphate hydrates: $\text{VO}(\text{H}_x\text{PO}_4)_x\cdot y\text{H}_2\text{O}$."
- 24. 11th International Symposium on the Reactivity of Solids - Princeton - USA (1988) "Synthetic pathways to vanadyl phosphates".
- 25. 5^{ème} International Symposium on Halide Glasses - Japon (1988) "Chemical vapour deposition of fluorides. Dynamic simulation of amorphous systems."
- 26. ICAME'89 - Budapest "Mossbauer study of a new crystalline fluoride : $\text{NaPbFe}_2\text{F}_9$
- 27. Workshop on Rietveld Analysis: NERF, Petten, Pays-Bas (1989) "Characterisation of the unusual disordered phase $\text{La}_2\text{C}_{0.74}\text{O}_{4.74}\text{Li}_{0.52}$ by powder diffraction"

- 28. M.R.S. Spring Meeting - San Diego - USA (1989) "Crystal structure of some by-products of the synthesis of copper and palladium substituted high Tc superconductors."
- 29. 32^{ème} IUPAC Congress - Stockholm (1989) "Structures of oxocuprate(II) vanadate(V) hydrates $\text{Cu}_3\text{V}_2\text{O}_{8.3}\text{H}_2\text{O}$, $\text{Cu}_3\text{V}_2\text{O}_8 \cdot \text{H}_2\text{O}$ and $\text{CuV}_2\text{O}_6(\text{H}_2\text{O})_2$ "
- 30. Ninth European Symposium on Fluorine Chemistry - Leicester (1989) "Crystal Structure of Li_2TbF_6 and magnetic study under high magnetic field".
- 31. International Congress on Powder Diffraction - Toulouse - France (1990) "Crystal structure of $\text{Co}_3(\text{HPO}_4)_2(\text{OH})_2$ related to mineral Lazulite solved by X-ray and neutron powder diffraction"
- 32. Accuracy in Powder Diffraction II (APD-II), Gaithersburg - USA (1992) "Extracting Structure Factors by Iterating Full Profile Pattern Fitting" (poster)
- 33. IVth European Conference on Solid State Chemistry - Dresde (1992) "Crystal Chemistry in Fluoride $\text{AMM}'_2\text{F}_9$: Structural and Magnetic Study" (poster)
- 34. même congrès: "Structures of New CsAlF_4 Polymorphs" (poster)
- 35. même congrès: "Crystal Structure of a new MX_3 Corner-Sharing Octahedra 3D Network" (poster)
- 36. Journées de la Division Chimie du Solide (SFC), Paris, 4-6 Septembre 1996. "Réseaux Tridimensionnels 6-Connectés". Poster en ligne à : <http://www.cristal.org/vrml/6c3d/6c3dnets.html>
- 37. First International Conference on Inorganic materials - Versailles - France (Septembre 1998). "Comparing RMC and RDM glass structure modelling methods". Poster en ligne à : <http://www.cristal.org/glasses/versailles/poster.html>
- 38. XVIIIth IUCr Congress & General Assembly, 4th-13th August 1999, Glasgow, Scotland . "Does conventional powder diffraction beat a synchrotron ?". Poster en ligne à : <http://www.cristal.org/glasgow/poster/glasgowposter.html>
- 39. EPDIC-7 – 7th European Powder Diffraction Conference – Barcelona, 20-23 May 2000. "ESPOIR : A Program for Solving Structures by Monte Carlo from Powder Diffraction Data." Poster en ligne à : <http://www.cristal.org/epdic-7/poster1/index.html>
- 40. EPDIC-7 – 7th European Powder Diffraction Conference – Barcelona, 20-23 May 2000. "Structure Determination by Powder Diffractometry : Internet Course." Poster en ligne à : <http://www.cristal.org/epdic-7/poster2/index.html>
- 41. Size Strain III, Analysis of microstructure and residual stress by diffraction methods, December 2-5, 2001, Trento, Italy. "Rietveld microstructural study of BaCO_3 from natural carbonation of $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$." Proceedings en ligne à : <http://sdpd.univ-lemans.fr/postscript/carbonation.pdf>
- 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 $\text{Al}(\text{OH})_3$ -*guaz*- HF_{aq} -éthanol par voie micro-ondes ; quatre nouveaux fluoroaluminates hybrides à sous-réseau inorganique de dimensionnalité croissante." A. Cadiou, 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 " $\text{La}_{14}\text{W}_8\text{O}_{45}$ "", objet du SDPDRR-3," M.-H. Chambrier, A. Le Bail, F. Goutenoire.
- 51. IUCr XXI, Osaka, Japan, August 23-31. "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. "The predicted powder diffraction database (P2D2)" A. Le Bail.

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, 4th-13th 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. “Structure 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)F₇ 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 - EMC² - 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 - EMC² - 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 - EMC³ - 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 Prédicte)."

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')

- **135 (8)** "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

- **133 (8)** "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

- **116 (16)** "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, ARIT, ARITVE, HKLGEN, OVERLAP, TMACLE, NOCHAOS, GLASSVIR

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

- **29 (755)** "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

<http://www.crystallography.net/>

~70.000 fichiers CIF de structure cristallines avec moteur de recherche par mot-clé, paramètres de maille, volume, formulation chimique.

PCOD : Predicted Crystallography Open Database

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

>110.000 fichiers CIF de structures prédites par le logiciel GRINSP, avec moteur de recherche par mot-clé, paramètres de maille, volume, formulation chimique.

P2D2 : Predicted Powder Diffraction Database

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

>110.000 diagrammes de poudre de composés prédits par le logiciel GRINSP, pour identification, incorporés dans les logiciels EVA (Bruker) et Highscore (Panalytical).