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Publications traditionnelles

Entre parenthèses, après le numéro d'ordre, est donné, lorsqu'il est supérieur ou égal à 10, le **nombre de citations** dans la période 1975- mars 2001 ainsi qu'il peut être obtenu dans le **Science Citation Index (ISI)** par consultation du **Web of Science**.

- **118** "Ab initio structure determination of lanthanum cyclo-tetrasilicate α - $\text{La}_2\text{W}_2\text{O}_9$ from X-ray and neutron powder diffraction." Y. Laligant, A. Le Bail and F. Goutenoire, *J. Solid State Chem.* In press.

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- **115** "Combining the Reverse Monte Carlo and the Rietveld Glass Structure Modelling Methods." A. Le Bail, The Chemistry Preprint Server, CPS: inorgchem/0008001 (2000), <http://preprint.chemweb.com/>

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- **113** "Structure Determination by Powder Diffractometry : Internet Course." A. Le Bail, Y. Laligant and A. Jouanneaux, *Mat. Sci. Forum*, in press.

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- 18 "Etude EXAFS de la structure pyrochlore type RbNiCrF_6 " A. LE BAIL, C. JACOBONI et R. DE PAPE, *J. Solid State Chem.* 61, 188-196 (1986).

- 17 "Analyse globale des spectres de diffraction des matériaux mal cristallisés". A. LE BAIL, Comptes Rendus- 10ème Colloque Siemens sur les Rayons X, 45-58, Grenoble (1985).

- 16 "Synthesis, characterization and crystallization of the amorphous iron(III) fluoride : $\text{FeF}_3 \cdot x\text{HF}$ ($0,4 < x < 1$)" M. LEBLANC, G. FERREY, J.M. GRENECHE, A. LE BAIL, F. VARRET, R. DE PAPE et J. PANNETIER., *J. de Physique, colloque C8*, 46, 175-179 (1985).

- 15 "Partial structure factors of fluoride glasses " $\text{Pb}_2\text{Mt}^{\text{II}}\text{Mt}^{\text{III}}\text{F}_9$ " by neutron diffraction" A. LE BAIL, C. JACOBONI et R. DE PAPE, *J. Non Crystalline Solids* 74, 213-221 (1985).

- 14 "Neutron magnetic diffraction study of fluoride " $\text{Pb}_2\text{MnFeF}_9$ " spin glass diluted by diamagnetic ions" A. LE BAIL, C. JACOBONI et R. DE PAPE, *J. Non Crystalline Solids* 74, 205-212 (1985).

- 13 "Correlations between magnetic and crystallochemical behaviour in $3d\text{-U}^{4+}$ fluoride glasses " G. COURBION, J. GUERY, A. LE BAIL et C. JACOBONI, *Materials Science Forum* Vol. 6, 739-742 (1985).

- 12 "Actual knowledge of 3d transition metal fluoride glasses structure " A. LE BAIL, C. JACOBONI et R. DE PAPE, *Materials Science Forum* Vol. 6, 441-448 (1985).

- **11** "Refining structural models for glasses: is it possible ? The case of 'Pb₂M₂F₉' A. LE BAIL, C. JACOBONI et R. DE PAPE, *J. de Physique, Colloque C8*, 46, 163-168 (1985).
- **10** "Comparaison de Procédures d'Evaluation des distorsions et de la taille des cristallites par analyse des raies de diffraction des rayons X" D. LOUER, R. COUPE et A. LE BAIL, *J. Appl. Cryst.* 17, 131-133 (1984).
- **9 (21)** "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).
- **8** "Physical properties and structure approach of the 3d transition metal fluoride glasses PbF₂-MF₂-MF₃". C. JACOBONI, A. LE BAIL, R. DE PAPE et J.P. RENARD, *Stud. Inorg. Chem.* 3, 687-690 (1983).
- **7 (31)** "Fluoride glasses of 3d transition metals". C. JACOBONI, A. LE BAIL et R. DE PAPE, *Glass Technology* 24, 164-167 (1983).
- **6 (14)** "Ordre antiferromagnétique dans les verres fluorés PbMnFeF₇ et Pb₂MnFeF₉". A. LE BAIL, C. JACOBONI et R. DE PAPE, *J. Solid State Chem.* 48, 168-175 (1983).
- **5** "Short range antiferromagnetic ordering in fluoride glasses PbMnFeF₇ and Pb₂MnFeF₉". A. LE BAIL, C. JACOBONI and R. DE PAPE, *J. De Physique C9*, 677-680 (1982).
- **4** "Etude par diffraction des rayons X de la transformation d'un hydroxynitrate de nickel non stoechiométrique en hydroxyde". A. LE BAIL et D. LOUER, *Rev. Chim. Miner.* 17, 522 (1980).
- **3 (23)** "Smoothing and validity of crystallite-size distributions from X-ray line-profile analysis". A. LE BAIL et D. LOUER, *J. Appl. Cryst.* 11, 50-55 (1978).
- **2** "Crystallite-size distributions from X-ray line profile analysis : smoothing, validity and application to a chemical reaction". A. LE BAIL et D. LOUER, Proc. Conf. on Applied Crystallography, Kozubnik (Poland), 477-490 (1978)
- **1** "Détermination directe des coefficients de Fourier lors de l'analyse des profils de raies de diffraction des rayons X". A. LE BAIL et D. LOUER, *Bull. Soc. Fr. Miner. Cristallographie* 99, 211-215 (1976).

Publications Electroniques

voir l'équivalent électronique de cette page, avec liens hypertextes à l'URL

<http://www.cristal.org/new.html>

Ces "publications" sont tournées vers l'international, elles sont donc en anglais pour la plupart. Il s'agit ci-dessous de la liste des nouveautés ajoutées au site Web, année après année. On y trouve des didacticiels, des posters, des conférences complètes (texte et transparents), des logiciels avec manuel d'utilisation, de vraies publications dans des journaux purement électroniques, avec referees, des bases de données avec moteur de recherche par mots-clés, des compte-rendus de contribution à des Round Robin en cristallographie.

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 Diffractometry 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

1994

- Powder diffractometers and Rietveld method
- Bréviaire du chercheur (in french)

Communications - Posters

- 1. 6ème 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. 5ème Congrès International de Physique des Solides Non-Cristallins - Montpellier (1982) "Short range antiferromagnetic ordering in fluoride glasses PbMnFeF_7 and PbMnFeF_9 ."
- 5. 2ème 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. XIIIème 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. 3ème 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 $\text{FeF}_3\text{,xHF}$ ($x < 1$)"

- 12. Progress in X-ray Studies by Synchrotron Radiation - Strasbourg (1985) "Local structure in phosphotungstate glasses by EXAFS at tungsten absorption edge"
- 13. même congrès: "Local environment of M in pyrochlores AM_2F_6 by EXAFS"
- 14. 10ème Colloque sur les Rayons X - Siemens - Grenoble (1985) "Analyse globale des spectres de diffraction des matériaux mal cristallisés"
- 15. 3ème 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 $LaNi_5D_{6.7}$ 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. 4ème International Symposium on Halide Glasses - Monterey - USA (1987) "Structure of baryum fluorozirconate glasses. A quasi crystalline modelization of $BaZr_2F_{10}$."
- 22. High-Temperature Superconductors and Materials and Mechanisms of Superconductivity - Interlaken - Suisse (1988) "Ordered Pd^{2+} - Cu^{2+} substitution in 1.2.3. superconductor : The oxyde $YBa_2Cu_{2.5}Pd_{0.5}O_x$."
- 23. First European Inorganic Chemistry Seminar (Euchem) - Dourdan - France (1988) "Structure and magnetic properties of oxovanadium (IV) hydrogénophosphate hydrates: $VO(H_xPO_4)_x \cdot yH_2O$."
- 24. Iith International Symposium on the Reactivity of Solids - Princeton - USA (1988) "Synthetic pathways to vanadyl phosphates ".
- 25 5ème 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 : NaPbFe₂F₉
- 27. Workshop on Rietveld Analysis: NERF, Petten, Pays-Bas (1989) "Characterisation of the unusual disordered phase La₂C_{0.74}O_{4.74}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 Cu₃V₂O_{8.3}H₂O, Cu₃V₂O₈.H₂O and CuV₂O₆(H₂O)₂
- 30. Ninth European Symposium on Fluorine Chemistry - Leicester (1989) "Crystal Structure of Li₂TbF₆ and magnetic study under high magnetic field".
- 31. International Congress on Powder Diffraction - Toulouse - France (1990) "Crystal structure of Co₃(HPO₄)₂(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 AMM'₂F₉: Structural and Magnetic Study" (poster)
- 34. même congrès: "Structures of New CsAlF₄ Polymorphs" (poster)
- 35. même congrès: "Crystal Structure of a new MX₃ 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>

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 Crystallographis Meeting, ECM 20, August 25-31, 2001, Kraków, Poland. "Stucture determination by powder diffractometry : Distance teaching and distance learning."