Armel Le Bail **Juin 2004**
DR2 - Matricule 51892 - Section 15
Laboratoire des Oxydes et Fluorures - UMR 6010
Université du Maine, Faculté des Sciences
Avenue Olivier Messiaen
72085 LE MANS Cedex 9
☎ (33) 02 43 83 33 47
Fax (33) 02 43 83 35 06
E-mail alb@cristal.org
Web http://www.cristal.org/

LISTE COMPLETE
des
PRODUCTIONS SCIENTIFIQUES
1976-2004

PLAN

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 2003 ainsi qu'il peut être obtenu dans le **Science Citation Index** (ISI) par consultation du **Web of Science**.

- 135 "Renewed interest in powder diffraction data indexing," J. Bergmann, A. Le Bail, R. Shirley and V. Zlokazov, Z. Kristallogr., Submitted.

- 134 "Monte Carlo indexing with McMaille," A. Le Bail, *Powder Diffraction*, Accepted.

- 133 "Size-strain line-broadening analysis of the ceria round-robin sample. II. The results of the Round Robin" D. Balzar, N. Audebrand, M.R. Daymond, A. Fitch, A. Hewat, J.I. Langford, A. Le Bail, D. Louër, O. Masson, N.C. Popa, P.W. Stephens, B. Toby, *J. Appl. Cryst.*, submitted.

- 132 "Geometrically restrained inorganic structure prediction : GRINSP," A. Le Bail, IUCr Computing Commission Newsletter, submitted.

- 131 "Unindexed powder pattern of the week (UPPW)," A. Le Bail, CPD Newsletter 31 (2004) 63-64.

- 130 "PPP - Powder Pattern Prediction," A. Le Bail, CPD Newsletter 31 (2004) 51-53.

- 129 "Characterization and structure determination of ammonium bismuth oxalate $Bi(NH_4)(C_2O_4)_2.xH_2O$," G. Vanhoyland, A. Le Bail, J. Mullens, L.C. Van Poucke, *Inorg. Chem*. 43 (2004) 785-789.

- 128 "How easy/hard is to convert raw data into a Web database," A. Le Bail, IUCr Computing Commission Newsletter 2 (2003) 39-41.

- 127 "Reverse Monte Carlo and Rietveld modelling of $BaMn(Fe,V)F_7$ glass structures from neutron data," A. Le Bail, Chemistry Preprint Server http://preprint.chemweb.com/inorgchem/0310001 (2003).

- 126 "Results and conclusions of the internet based Search/Match Round Robin 2002", J-M. Le Meins, L.M.D. Cranswick, A. Le Bail, *Powder Diffraction*, 18 (2003) 106-113.

- 125 "SDPD Round Robin 2002 Results," A. Le Bail & L. Cranswick, *CPD Newsletter* 29 (2003) 31-34.

- 124 "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.

- 123 "Distorted chiolite crystal structures of α-$Na_5M_3F_{14}$ (M=Cr, Fe, Ga) studied by X-ray powder diffraction," A. Le Bail & A.-M. Mercier, *Powder Diffraction*, 18 (2003) 128-134.

- **122** "Size-strain line-broadening analysis of the ceria round-robin sample. I. Methodology and the comparative analysis of the measurements" D. Balzar, N. Audebrand, M.R. Daymond, A. Fitch, A. Hewat, J.I. Langford, A. Le Bail, D. Louër, O. Masson, C.N. McCowan, N.C. Popa, P.W. Stephens, B. Toby, *J. Appl. Cryst.*, submitted.

- **121** "Order through random numbers : Indexing and solving crystal structures from powder diffraction data using Monte Carlo methods." A. Le Bail, IUCr Computing Commission Newsletter 1 (2003) 84-87.

- **120** " Methods for integrated intensities extraction in powder diffractometry - Out of prehistory." A. Le Bail, *Z. Kristallogr*. **217** (2002) 338-340.

- **119** "Rietveld microstructural study of $BaCO_3$ from natural carbonation of $Ba(OH)_2.8H_20$," A. Le Bail & Y. Laligant, *Chemistry Preprint Server*: http://preprint.chemweb.com/inorgchem/0202001 (2002).

- **118** "*Ab initio* structure determination of lanthanum cyclo-tetratungstate α-$La_2W_2O_9$ from X-ray and neutron powder diffraction." Y. Laligant, A. Le Bail and F. Goutenoire, *J. Solid State Chem*. **159** (2001) 223-227.

- **117** "Revisiting the 1998 SDPD Round Robin." A. Le Bail and L.M.D. Cranswick, IUCr CPD Newsletter 25 (2001) 7-9.

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

- **115** "Structure Determination by Powder Diffractometry : Internet Course." A. Le Bail, Y. Laligant and A. Jouanneaux, *Mat. Sci. Forum*, **378-381** (2001) 47-52.

- **114** "Trends in structure determination by powder diffractometry." A. Le Bail, in : *Advances in Structure Analysis*, Edited by R. Kuzel and J. Hasek, published by the Czech and Slovak Crystallographic Association (2001) 166-189.

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

- **112 (22)** "The room-temperature crystallisation of a one-dimensional gallium fluorophosphate, $Ga(HPO_4)_2F.H_3N(CH_2)_3NH_3\bullet 2H_2O$, a precursor to three-dimensional microporous gallium fluorophosphates." R.I. Walton, F. Millange, D. O'Hare, A. Le Bail, T. Loiseau, C. Serre, G. Férey, Chem. Comm. 3, 203-204 (2000).

- **111** "Reverse Monte Carlo and Rietveld Modelling of the $NaPbM_2F_9$ (M = Fe, V) Fluoride Glass Structures." A. Le Bail, *J. Non -Cryst. Solids* **271**, 249-259 (2000).

- **110** "New developments in microstructure analysis via Rietveld refinements." A. Le Bail, *Advances in X-ray Analysis*, Vol. **42**., 191-203 (2000).

- **109** "Investigation of mixed divalent cation phosphates: synthesis and X-ray powder structure determination of $CdBa_2(P_2O_7)(HPO_4)$. L. Ben Taher, L. Smiri, Y. Laligant and A. Le Bail, *Solid State Sciences* **2**, 285-292 (2000).

- **108** "The powder diffraction handicap." A. Le Bail, *IUCr Newsletter* **7, N°4**, p. 4.

- **107** “Solving structures by reverse Monte Carlo from scratch.” A. Le Bail, *CPD Newsletter* **21**, 13-14 (1999).

- **106** “Accounting for size and microstrain in whole-powder pattern fitting.” A. Le Bail, in : Defect and Microstructure Analysis by Diffraction, R. Snyder, J. Fiala & H. Bunge Editors, Oxford Science Publications, Chapter 22, 535-555 (1999).

- **105** "Structure of $[Co(NH_3)_5CO_3]NO_3 \bullet H_2O$." J.H. Zhu, H.X. Wu and A. Le Bail, *Solid State Science* **1**, 55-62 (1999).

- **104** "Structure of α-$NaCaAlF_6$ determined *ab initio* from conventional powder diffracton data." A. Le Bail, A. Hemon-Ribaud and G. Courbion, *Eur. J. Solid State Inorg. Chem*. **35**, 265-272 (1998).

- **103** "$Li_6P_6O_{18}$: X-ray powder structure determination of lithium cyclohexaphosphate." T. Ben-Chaabane, L. Smiri-Dogguy, Y. Laligant and A. Le Bail, *Eur. J. Solid State Inorg. Chem*. **35**, 255-264 (1998).

- **102** "Synthesis and crystal structure of alpha-Ba_2ZrF_8 and Pb_2ZrF_8 determined ab initio from synchrotron and neutron powder diffraction data." A. Le Bail and J.P. Laval, *Eur. J. Solid State Inorg. Chem*. **35**, 357-372 (1998).

- **101** "Structure of $Na_2Ca(HPO_4)_2$ Determined ab initio from Conventional Powder Diffraction Data." T. Ben Chaabane, L. Smiri-Dogouy, Y. Laligant and A. Le Bail, *Eur. J. Solid State Inorg. Chem*. 34, 937-946 (1997).

- **100** "Structure of $BaGaF_5.2H_2O$ from Conventional and Synchrotron Powder Diffraction Data." A. Jouanneaux and A. Le Bail, *Eur. J. Solid State Inorg. Chem*. 34, 925-936 (1997).

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

- **98 (17)** "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).

- **97** "Structure of $Sr_5Zr_3F_{22}$ Determined from an Inversion Twinned Crystal." A. LE BAIL, *Eur. J. Solid State Inorg. Chem*., **33**, 1211-1222 (1996).

- **96** "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).

- **95** "Structure of $FeVMoO_7$." A. LE BAIL, L. PERMER and Y. LALIGANT, *Eur. J. Solid State Inorg. Chem*. **32**, 883-892 (1995).

- **94** "Synthesis and Structure Approach of Barium Oxomercurato(II)-Oxoruthenate(VI) $BaRuHgO_5$," T. HANSEN, A. LE BAIL and Y. LALIGANT, *J. Solid State Chem*. **120**, 223-230 (1995).

- 93 "Crystal Structure of $Fe_4V_2Mo_3O_{20}$ determined from Conventional X-ray Powder Diffraction Data," Y. LALIGANT, L. PERMER and A. LE BAIL, *Eur. J. Solid State Inorg. Chem.*, 32, 325-334 (1995).

- 92 (14) "Modelling the Silica Glass Structure by the Rietveld Method." A. LE BAIL, *J. Non-Cryst. Solids*, **183**, 39-42 (1995).

- 91 "Helical Octahedral *cis* Chains in α'-$BaFeF_5$." A. LE BAIL and A.M. MERCIER, *Eur. J. Solid State Inorg. Chem.*, **32**, 15-24 (1995).

- 90 "Structure of $[Pd(NH_3)_4]Cr_2O_7$." Y. LALIGANT and A. LE BAIL, *Powder Diffraction*, **10**, 159-164 (1995).

- 89 "*Ab initio* Crystal Structure Determination of $VO(H_2PO_2)_2.H_2O$ 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).

- 88 "Synthesis and Crystal Structure of $Li_8Bi_2PdO_{10}$ Determined *Ab Initio* from X-ray Powder Diffraction Data", Y. LALIGANT and A. LE BAIL, *Eur. J. Solid State Inorg. Chem*. **30**, 689-698 (1993).

- 87 (13) "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).

- 86 "Synthesis and Structure Approach of $K_3Ba_7Al_6F_{33}Cl_2$", A. LE BAIL, A. HEMON-RIBAUD and G. COURBION, *J. Solid State Chem*., **107**, 234-244 (1993).

- 85 (19) "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).

- 84 "Crystal Structure Approach of $KCaAl_2F_9$. A New Hexagonal-Tungsten-Bronze Related Structure", A. HEMON, A. LE BAIL and G. COURBION, *Eur. J. Solid State Inorg. Chem*., **30**, 415-426 (1993).

- 83 "The Structure of $Li_3Cu_2O_4$, a Compound With Formal Mixed Valence" R BERGER, P. ONNERUD, Y. LALIGANT and A. LE BAIL, *J. of Alloys and Compounds*, **190**, 295-299 (1993).

- 82 "On the Structure of $Na_5V_2P_3O_{14}.H_2O$", A. LE BAIL, *J. Solid State Chem*., **102**, 281-282 (1993).

- 81 "Modelling Anisotropic Crystallite Size/Microstrain in Rietveld Analysis", A. LE BAIL, *N.I.S.T. Special Publication* **846**, 142-153 (1992).

- 80 (10) "Synthesis and crystal structure of γ-$BaZrF_6$", A. LE BAIL and A.M. MERCIER, *J. Solid State Chem*. **101**, 229-236 (1992).

- 79 "*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).

- 78 (14) "Crystal structure and thermal behaviour of $H_2Ti_3O_7$: a new defective ramsdellite form from Li^+/H^+ exchange on $Li_2Ti_3O_7$", A. LE BAIL and J.L. FOURQUET, *Mat. Res. Bull.* **27**, 75-85 (1992).

- 77 (17) "Synthesis and crystal structure of α-$NH_4(VO_2)(HPO_4)$", P. AMOROS and A. LE BAIL, *J. Solid State Chem.* **97**, 283-291 (1992).

- 76 "Crystal structure and thermolysis of $K_2(H_5O_2)Al_2F_9$", A. LE BAIL, H. DUROY and J.L. FOURQUET, *J. Solid State Chem*. **98**, 151-158 (1992).

- 75 "Polymorphism of $CsAlF_4$. Synthesis and structure of two new crystalline forms". U. BENTRUP, A. LE BAIL, H. DUROY and J.L. FOURQUET, *Eur. J. Solid State Inorg. Chem*. **29**, 371-381 (1992).

- 74 "Synthesis, X-ray single crystal structure determination and dehydration study of $BaZr_2F_{10}.2H_2O$ by X-ray powder Thermodiffractometry", Y. GAO, J. GUERY, A. LE BAIL and C. JACOBONI, *J. Solid State Chem.* **98**, 11-24 (1992).

- 73 "Structure and phase transitions of low-dimensional Thallium Vanadium Bronze $Tl_xV_2O_5$ ($0.44<x<0.48$)", M. GANNE, A. JOUANNEAUX, M. TOURNOUX and A. LE BAIL, *J. Solid State Chem*. **97**, 186-198 (1992).

- 72 "Crystal structure of $Pb_2MnFe_2F_{12}.3H_2O$, A. LE BAIL and A.M. MERCIER, *Acta Cryst.* **C48**, 239-241 (1992).

- 71 "Crystal structure of $Pb_8MnFe_2F_{24}$", A. LE BAIL and A.M. MERCIER, *Eur. J. Solid State Inorg. Chem.*. **29**, 183-190 (1992).

- 70 "Crystalline phases related to the icosahedral Al-Li-Cu phase: a single crystal X-ray diffraction study of the tetragonal tau-$Al5_6(Cu,Zn)_{11}Li_{33}$ phase". M. LEBLANC, A. LE BAIL and M. AUDIER, *Physica B* 173, 329-355 (1991).

- 69 "Crystalline phases related to the icosahedral Al-Li-Cu phase: A single crystal X-ray diffraction study of the hexagonal Z-$Al_{59}Cu_5Li_{26}Mg_{10}$ phase". A. LE BAIL, M. LEBLANC and M. AUDIER, *Acta Cryst*. B47, 451-457 (1991).

- 68 "Structure of the decahydrated octaacetate of dineodyme (III) and cobalt (II), $Nd_2Co(CH_3COO)_8.10H_2O$". A. GONZALEZ, A. BELTRAN and A. LE BAIL, *Acta Cryst*. C47, 1624-1627 (1991).

- 67 (11) "Layer structure of $[CoCl(H_2PO_2)].H_2O$". M.D. MARCOS, R. IBANEZ, P. AMOROS and A. LE BAIL, *Acta Cryst*. C47, 1152-1155 (1991).

- 66 "Synthesis, crystal structure and magnetic properties of $Co_3(HPO_4)_2(OH)_2$ related to the mineral Lazulite". J.L. PIZARRO, G. VILLENEUVE, P. HAGENMULLER and A. LE BAIL**,** *J. Solid State Chem*. 92, 273-285 (1991).

- 65 "Crystal structure of $Pd(NO_3)_2(H_2O)_2$". Y. LALIGANT, G. FEREY and A. LE BAIL, *Mat. Res. Bull.* 26, 269-275 (1991).

- 64 (42) "Recent advances in the chemistry and properties of oxovanadium phosphates". D. BELTRAN-PORTER, A. BELTRAN-PORTER, P. AMOROS, R.

IBANEZ, E. MARTINEZ, A. LE BAIL, G. FEREY, G. VILLENEUVE. *Eur. J. Solid State Inorg. Chem*. 28, 131-161 (1991).

- 63 "Synthesis and crystal structure of $NaSrAlF_6$". A. HEMON, A. LE BAIL and G. COURBION, *Eur. J. Solid State Inorg. Chem*. 27, 905-912 (1990).

- 62 (11) "Defect structure of the anion-excess fluorite-related $SmF_{1.60}O_{0.70}$ phase". J.P. LAVAL, A. ABAOUZ, B. FRIT AND A. LE BAIL, *Eur. J. Solid State Inorg. Chem*. 27, 545-555 (1990).

- 61 "Structure determination of NiV_2O_6 from X-ray powder diffraction: a rutile-ramsdellite intergrowth". A. LE BAIL and M.A. LAFONTAINE, *Eur. J. Solid State Inorg. Chem*. 27, 671-680 (1990).

- 60 (16) "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. SAMOUEL, *J. Solid State Chem*. 89, 282-291 (1990).

- 59 "The crystal and molecular structures of $[Cr(NH_3)_6].[Ni(H_2O)_6].Cl_5.(NH_4Cl)_{0.5}$". M.C. MORON, A. LE BAIL and J. PONS, *J. Solid State Chem*. 88, 498-504 (1990).

- 58 (10) "NH_4CdF_3 : Structure of the low temperature phase."A. LE BAIL, J.L. FOURQUET, J. RUBIN, E. PALACIOS and J. BARTOLOME, *Physica B* 162, 231-236 (1990).

- 57 (11) "Synthesis and crystal structure of $Na_{1+x}V_4P_4O_{17}(OH)$ (x = 1.44)" A. LE BAIL, M. LEBLANC and P. AMOROS, *J. Solid State Chem*. 87, 178-185 (1990).

- 56 (22) "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).

- 55 "A new structure type in mixed valence fluorinated compounds: $K_5Cr^{2+}{}_4Cr^{3+}{}_6F_{31}$." Y. LALIGANT, A. LE BAIL, M. LEBLANC and G. FEREY, *J. Solid State Chem*. 85, 151-158 (1990).

- 54 "Structure determination of $A_2NaAl_3F_{12}$ (A = K,Rb)." A. LE BAIL, Y. GAO, J.L. FOURQUET and C. JACOBONI, *Mat. res. Bull*. 25, 831-839 (1990).

- 53 "Mossbauer study of a new crystalline fluoride: $NaPbFe_2F_9$." J.M. GRENECHE, A. LE BAIL, M. LEBLANC, *Hyperfine Interactions* 54, 545-550 (1990).

- 52 "Reinvestigation of the structure of K_2FeF_5." A. LE BAIL, A. DESERT and J.L. FOURQUET, *J. Solid State Chem*. 84, 408-412 (1990).

- 51 (12) "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. FEREY, *J. Solid State Chem*. 85, 220-227 (1990).

- 50 (19) "Structure determination of $NaPbFe_2F_9$ by X-ray powder diffraction." A. LE BAIL, *J. Solid State Chem*. 83, 267-271 (1989).

- 49 (39) "Structure of vanadyl hydrogenphosphate dihydrate α-$VO(HPO_4).2H_2O$ solved from X-ray and neutron powder diffraction". A. LE BAIL, G. FEREY, P. AMOROS and D. BELTRAN-PORTER, *Eur. J. Solid State Inorg. Chem*. 26, 419-426 (1989).

- 48 (15) "$(NH_4)_2FeF_5$: crystal structures of its α and β forms." J.L. FOURQUET, A. LE BAIL, H. DUROY and M.C. MORON, *Eur. J. Solid State Inorg. Chem*. 26, 435-443 (1989).

- 47 "Crystal structure determination of $Rb_2Cr_5F_{17}$". Y. LALIGANT, A. LE BAIL and G. FEREY, *Eur. J. Solid State Inorg. Chem*. 26, 445-454 (1989).

- 46 "Crystal structure of $Rb_2NaAl_6F_{21}$; a new term of the $A_2Na(Al_xF_{3x+1})_3$ family (A = Rb, Cs). A. LE BAIL, Y. GAO and C. JACOBONI, *Eur. J. Solid State Inorg. Chem*. 26, 281-288 (1989).

- 45 "Crystal structure of $Na_3Sr_4Al_5F_{26}$". A. HEMON, A. LE BAIL and G. COURBION, *J. Solid State Chem*. 81, 299-304 (1989).

- 44 "Li^+/H^+ topotactic exchange on $LiSbO_3$: The series $Li_{1+x}H_xSbO_3$ ($0<x<1$)." J.L. FOURQUET, P.A. GILLET and A. LE BAIL, *Mat. Res. Bull.* 24, 1207-1214 (1989).

- 43 "Complex Palladium Oxides V. Crystal structure of $LiBiPd_2O_4$. An example of three different fourfold coordinations of cations." Y. LALIGANT, A. LE BAIL and G. FEREY, *J. Solid State Chem*., 81, 58-64 (1989).

- 42 "Crystal structure of Li_3ThF_7 solved by X-ray and neutron diffraction". Y. LALIGANT, A. LE BAIL, D. AVIGNANT, J.C. COUSSEINS et G. FEREY, *J. Solid State Chem*., 80, 206-212 (1989).

- 41 (38) "Crystal structure of β-$VO(HPO_4).2H_2O$ solved from X-ray powder diffraction". A. LE BAIL, G. FEREY, P. AMOROS, D. BELTRAN-PORTER and G. VILLENEUVE, *J. Solid State Chem*. 79, 169-176 (1989).

- 40 (56) "Synthetic pathways to vanadyl phosphates". D. BELTRAN-PORTER, P. AMOROS, R. IBANEZ, E. MARTINEZ, A. BELTRAN-PORTER, A. LE BAIL, G. FEREY, G. VILLENEUVE, *Solid state Ionics*, 32/33, 57-69 (1989).

- 39 (10) "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).

- 38 (22) "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. FEREY and G. VILLENEUVE., *Eur. J. Solid State Inorg. Chem*. 25, 599-607 (1988).

- 37 "Determination of the crystal structure of Li_2TbF_6 from X-ray and neutron powder diffraction. An example of Lithium in fivefold coordination". Y. LALIGANT, A. LE BAIL, G. FEREY, D. AVIGNANT and J.C. COUSSEINS, *Eur. J. Solid State Inorg. Chem*. 25, 551-563 (1988).

- 36 "Chemical vapour deposition of fluorides. Molecular dynamic simulation of amorphous systems" B. BOULARD, A. LE BAIL, C. JACOBONI and J.H. SIMMONS, *Materials Science Forum* 32-33, 61-68 (1988).

- 35 (34) "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).

- 34 "Li^+/H^+ topotactic exchange on beta-$Li_{(1-x)}Nb_{(1-x)}W_xO_3$ ($0<x<0.5$). The series $H_{(1-x)}Nb_{(1-x)}W_xO_3$. J.L. FOURQUET, P.A. GILLET and A. LE BAIL, *Mat. Res. Bull*. 23, 1253-1260 (1988).

- 33 (17) "$LiNbWO_6$: crystal structure of its two allotropic forms ". J.L. FOURQUET, A. LE BAIL and P.A. GILLET, *Mat. Res. Bull.* 23, 1163-1170 (1988).

- 32 "Synthesis and ab-initio structure determination from X-ray powder data of Ba_2PdO_3 with sevenfold coordinated Ba^{2+}. Structural correlations with K_2NiF_4 and Ba_2NiF_6". Y. LALIGANT, A. LE BAIL, G. FEREY, M. HERVIEU, B. RAVEAU, A. WILKINSON and A.K. CHEETHAM, *Eur. J. Solid State Inorg. Chem*. 25, 237-247 (1988).

- 31 (22) "Ordered Pd^{2+}-Cu^{2+} substitution in 1.2.3. superconductor : the oxide $YBa_2Cu_{(3-x)}Pd_xO_y$ ($x = 0.5$) with Pd^{2+} in square planar coordination". G. FEREY, A. LE BAIL, Y. LALIGANT, M. HERVIEU, B. RAVEAU, A. SULPICE and R. TOURNIER, *J. Solid State Chem*. 73, 610-614 (1988).

- 30 "Electron microscopy study of the superconductor $Bi_2Sr_2CaCu_2O_{8+}$". M. HERVIEU, C. MICHEL, B. DOMENGES, Y. LALIGANT, A. LE BAIL, G. FEREY and B. RAVEAU, *Modern Physics Letters* B, 2(1), 491-500 (1988).

Republié comme article dans "Chemical and structural aspects of high temperature superconductors" World Scientific-Ed. C.N.R. RAO, F.R.S, *Progress in High Temperature Superconductivity*, Vol 7, p.159-168 (1988).

- 29 (388) "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).

- 28 (15) "Structural aspects of amorphous iron (III) fluorides J.M. GRENECHE, A. LE BAIL, M. LEBLANC, A. MOSSET, F. VARRET, J. GALY and G. FEREY, *J. Phys. C : Solid State Phys*. 21, 1351-1361 (1988).

- 27 "Les variétés bronze de tungstène hexagonal des trifluorures VF_3 et CrF_3" R. DE PAPE, A. LE BAIL, F. LUBIN et G. FEREY, *Revue de Chimie Minérale* 24, 545-551 (1987).

- 26 "Structure of fluorozirconate glasses: a quasi crystalline modelling of $BaZr_2F_{10}$" A. LE BAIL, B. BOULARD and C. JACOBONI, *Materials Science Forum* 19-20 ,127-136 (1987).

- 25 "A premartensitic phase in $KAlF_4$: neutron and X-ray scattering evidences" A. GIBAUD, A. BULOU, A. LE BAIL, J. NOUET and C.M.E. ZEYEN, *J. Physique* 48, 1521-1532 (1987).

- 24 (55) "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. of the Less-Common Metals* 129, 65-76 (1987).

- 23 "Local environment of Zr in baryum fluorozirconate glasses : the EXAFS point of view" B. BOULARD, A. LE BAIL, J.P. LAVAL et C. JACOBONI, *J. de Physique, Colloque* C8, 47, 791-794 (1986).

- 22 (11) "Local environment of tungsten in mixed valence tungsten phosphate glasses : an EXAFS study" F. STUDER, A. LE BAIL and B. RAVEAU, *J. Solid State Chem*. 63, 414-423 (1986).

- 21 "EXAFS of mixed valence iron potassium phosphate glasses" F. STUDER and A. LE BAIL, *J. de Physique, Colloque* C8, 47 , 781-785 (1986).

- 20 (15) "A re-investigation of the room-temperature phase of $KAlF_4$: evidence of antiphase domains" A. GIBAUD, A. LE BAIL and A. BULOU, *J. Phys. C: Solid State Phys*. 19, 4623-4633 (1986).

- 19 (10) "Fluorocomplexes of Niobium IV. Part V : the magnetic structure of $MnNbF_6$" D. BIZOT, J. CHASSAING, J. PANNETIER, M. LEBLANC, A. LE BAIL, G. FEREY, *Solid State Commun*. 58, 71-74 (1986).

- 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 : FeF_3, xHF (0,4 < x < 1)" M. LEBLANC, G. FEREY, 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 "$Pb_2Mt^{II}Mt^{III}F_9$ " 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 "Pb_2MnFeF_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-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 '$Pb_2M_2F_9$' 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 PbF_2-$M^{II}F_2$-$M^{III}F_3$ 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 PbF_2-MF_2-MF_3". C. JACOBONI, A. LE BAIL, R. DE PAPE et J.P. RENARD, *Stud. Inorg. Chem.* 3, 687-690 (1983).

- 7 (32) "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 $PbMnFeF_7$ et Pb_2MnFeF_9". 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 $PbMnFeF_7$ and Pb_2MnFeF_9". 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 stoechiometrique 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://sdpd.univ-lemans.fr/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 vrais 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.

2004

- 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 Diffractometry 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 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-AlF_3, 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. 6éme 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 PbF_2-MF_2-MF_3."

-6. Journées de l'Etat Solide - Bordeaux (1984) "Structure des verres fluorés $Na_6M(ii)_5M(iii)_9F_{43}$ 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 Congrés International de cristallographie - Hambourg (1984) "A quasi-crystalline simulation of $Pb_2M(ii)M(iii)F_9$ 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 "$Pb_2M_2F_9$"

-11. même congrès: "Synthesis, characterization and crystallization of the amorphous iron (III) fluoride FeF_3,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 BaZr2F10 ."

-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: $VO(H_xPO_4)_x.yH_2O$."

-24. IIth International Symposium on the Reactivity of Solids - Princeton - USA (1988) "Synthetic pathways to vanadyl phosphates ".

-25 5éme 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 : $NaPbFe_2F_9$

-27. Workshop on Rietveld Analysis: NERF, Petten, Pays-Bas (1989) "Characterisation of the unusual disordered phase $La_2C_{0.74}O_{4.74}Li_{0.52}$ 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. 32éme IUPAC Congress - Stockholm (1989) "Structures of oxocuprate(II) vanadate(V) hydrates $Cu_3V_2O_{8.3}H_2O$, $Cu_3V_2O_8.H_2O$ and $CuV_2O_6(H_2O)_2$

-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 $Co_3(HPO_4)_2(OH)_2$ 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'_2F_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, 4^{th}-13^{th} 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 $Ba(OH)_2.8H_2O$."
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.”

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. “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 Catlo; indexation de diagramme et solution de structure."

20 - ECM-21, 24-49 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 - Deuxième Congrès Algérien de Cristallographie, Constantine, Algérie, 17-21 Avril 2005. " Prédiction de structures inorganiques par contraintes géométriques."