

PERSONAL INFORMATION **Rosanna Rizzi**

WORK EXPERIENCE

- February 2001 – Present **Staff scientist (full time/permanent position)**
Institute of Crystallography (IC) - National Research Council (CNR)
Via G. Amendola 122/o, 70126 Bari, Italy
- Development and implementation in crystallographic software of new and efficient methodologies for qualitative phase analysis and structure solution process using X ray diffraction data from powder compounds.
 - X-ray powder diffraction data collection with laboratory diffractometers or at Synchrotron light source .
 - Powder data analysis for qualitative phase characterization and crystal structure solution.
 - Co-author of the crystallographic software: 1) EXPO; 2) QualX; 3) OChemDb (Open Chemistry Database)
- Business or sector** Research
- January 2011 – Present **Head of X-ray powder diffraction laboratory**
Business or sector Research

EDUCATION AND TRAINING

- September 2005 **CNR short-term mobility project**
Project: The development of strategies on Direct-space technique to solve crystal structures from powder diffraction data
University of Geneva, Laboratory of Crystallography
Business or sector Research
- March - May 2004 **CNR short-term mobility project**
Project: Determining low-resolution crystal structures from powder diffraction data
ISIS Facility Rutherford Appleton Laboratory (Oxford). United Kingdom
Business or sector Research
- May 2003 **CNR short-term mobility project**
Project: Natural and synthetic Zeolites
University of Ferrara, Italy
Business or sector Research
- 1999-2002 **PhD in Earth Science**
Title of thesis: Development of crystallographic methodologies for powder structure analysis with particular emphasis for zeolite compounds
University of Bari, Italy
- 1995-1998 **Fellowship in Crystallography**
Fellowship in Crystallography at 'Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche', IRMEC-CNR, Bari, Italy. Tutor: Professor C. Giacovazzo, University of Bari, Italy
- 1988-1994 **Bachelor in Physic**
Title of the Thesis: Processi di assorbimento a due fotoni nei semiconduttori a filo quantico di GaAs-AlxGa1-xAs.

University of Bari

RESEARCH ACTIVITIES

- Main scientist developer for package EXPO [Altomare et al., Crystal Research and Technology (2015), 737-742]
- Main scientist developer for package QUALX [Altomare et al., J. Appl. Cryst. (2015), 48, 598-603]
- Main scientist developer for package OChemDB [Altomare et al., J. Appl. Cryst. (2018), 51, 1229-1236]
- Development of new and innovative algorithms to indexing a powder diffraction pattern
- Development of new and innovative algorithms for the Space Group determination
- Development of new and innovative algorithms to decompose the experimental powder X ray diffraction pattern into single integrated intensities
- Development of the phasing techniques above all Direct Methods to solve small and medium polycrystalline compounds
- Development of new and innovative algorithms for structure model optimization
- Development of new and innovative algorithms to solve polycrystalline materials in the direct space: Simulated Annealing and Big Bang-Big Crunch method
- Development of Machine Learning approaches to unit cell parameters determination

TEACHING AND LECTURES

2022

- Member of the Steering Committee of the fourth Joint Conference of the Italian Crystallographic Association (AIC) and the Italian Society of Synchrotron Light (SILS). (12-15 September, Trieste, Italy).
- Teaching at workshop: Hands-on Software. (28-29 June, Modena, Italy).

2021

- Oral communication at 1st Conference on Crystallography, structural chemistry and biosystem. Title of oral presentation: Solving polycrystalline structures: from data collection to the development of innovative crystallographic methods. (4-6 October, Catania, Italy).
- Teaching at 'International school of crystallography: Molecular crystal engineering'. Title of lessons: 1) Qualitative analysis by using X-ray diffraction: theory, database and software; 2) Polycrystalline materials: crystal structure solution in reciprocal and/or direct space?. (31 Maggio – 4 Giugno, Erice, Italy).
- Member of the scientific committee of the International Crystallography school. (31 August – 4 September, Parma, Italy).

2020

- Conference Committee member of the 2nd International Online Conference on Crystals. 10-20 November.
- Keynote at 2nd International Online Conference on Crystals. Titolo presentazione: Physico-chemical characterization of new rare earths doped calcium phosphates'. 10-20 November 2020.
- Member of the 'Commissione Strumentazione e Calcolo' of Associazione Italiana di Cristallografia (AIC) (2018-2020)

2019

- Guest Editor of the Special issue "Crystal Structure Characterization by Powder Diffraction". Crystals. ISSN 2073-4352
- Member of the Editorial Board of the Crystals International Journal, 'Crystalline Materials' section.

- Organization of EXPO&more International Workshop. Politecnico of Bari, Italy (29 September-3 October).
- Organization of 'Microscopi Giganti: introduzione alle applicazioni delle grandi sorgenti' national workshop. University of Milan, Italy (13 May).
- Oral communication at department of chemical sciences and materials technologies (CNR) conference. Title: Innovative Methodologies and challenging applications of Software for the Characterization of Polycrystalline Compounds. Brixen, Italy, (28-30 September).
- Oral communication at EXPO&more International Workshop. Title of oral presentations: 1) Full pattern decomposition; 2) Reciprocal space methods solution. Politecnico of Bari, Bari-Italy (30 September-03 October).
- Tutor of the computer session at International Workshop: EXPO&more. 3 Politecnico of Bari, Bari-Italy (30 September-03 October).

2018

- Organization of AIC International School: Powder diffraction: theory, software and applications. Bari, Italy (29 August -2 September).
- Organization of 3rd joint AIC-SILS Conference. Rome, Italy (25-28 June).
- Organization of Analisi quantitativa di fasi cristalline: metodi tradizionali e chemiometria a confronto national workshop. University of Bologna, Italy (6 February).
- Oral Communication at International Congress EPDIC16. Title of oral presentation: New algorithms for structure solution of polycrystalline materials in EXPO software. Edinburgh, Scotland, (1-4 July).
- Chair of the MS4 'Methods: Methodological and experimental developments in crystallography and synchrotron techniques' at the 3rd joint AIC-SILS Conference. Rome, Italy, (25-28 June).

2017

- Organization of 'L'esperimento flessibile: studi di diffrazione in condizioni non ambientali' national Workshop. University of Bari, Italy (22 February).

2016

- Organization of 'Analisi di fase qualitativa e quantitativa per applicazioni industriali e ambientali' national Workshop. University of Milano, Italy (16 February).
- Organization of 15th European Powder Diffraction Conference. Bari, Italy (12-15 June).
- Invited lecture at 3rd European Crystallography School (ECS3). Bol, Croatia, (25 September - 02 October).

2015

- Chair of MS39 'Recent advances in diffraction instruments, detectors and data processing' to the 29th European Crystallographic Meeting (ECM29). Rovigno, Croatia (23-28 August).

2014 and older: selected

- Organization of the International EXPO/SIR workshop. Bari, Italy (10-13 June).
- Oral Communication at International EXPO/SIR workshop. Title of presentation: 1) Crystal structure solution by powder diffraction data; 2) Phasing via Direct Methods. University of Bari, Italy (10-13 June).

2013

- Invited lecture at International Workshop on 'Powder and Electron Crystallography'. Patras, Grece (8-12 July).
- Oral Communication at Twenty-second Croatian-Slovenian Crystallographic Meeting (CSCM22). Title of presentation: The Hybrid BigBang-Big Crunch in the EXPO2013 program. Biograd, Croatia (12-16 June).

2012

- Organization of 'Synthesis and characterization of novel Nano-Sized inorganic materials' International school. University of Bari, Italy (17-22 June).
- Invited lecture at 'Structure, microstructure, nanostructure' AIC International School. Trento, Italy (15-20 September).

2011

- Invited lecture at 2011 ICDD (International Centre for Diffraction Data) spring Meetings. Title of presentation: 'From X-ray powder diffraction pattern to structure solution through new algorithms, strategies and tips: the EXPO program'. ICDD Headquarters, Philadelphia, USA (14-18 March).
- Chair at MS95 'Automated Data Processing and Structural Solution for Powder Crystallography'. XXII IUCr congress Madrid, Spain (22-30 August).

2010

- Invited lecture at MISCAII-2nd Meeting of the Italian and Spanish Crystallographic Associations. Title of presentation: 'EXPO2010: algorithms and tips for a successful powder structure solution'. Oviedo, Spain (30 June-3 July).
- Chair at MS6 'Structure Solution'. 26th European Powder Diffraction Conference (EPDIC12), Darmstadt, Germany (27-30 August).

2009

- Invited lecture at 25th European Crystallographic Meeting (ECM25). Title of presentation: 'New strategies in EXPO2009: applications to pharmaceutical compounds. Istanbul, Turkey (16-21 August).

2008

- Teaching at International summer school on structure determination from powder diffraction data on 'Structure solution by powder diffraction with the EXPO program'. Paul Sherrer Institut, Villigen, Switzerland (18-22 June).

2007

- Editor of the Newsletter N. 35 of the Commission on Powder Diffraction (CPD), International Union of Crystallography (IUCr). ISSN 1591-9552.

2006

- Teaching at 'dDffrazione da materiali policristallini' national school. Martina Franca, Italy (26-30 June).

2004

- Teaching activity for the research project entitled: "TECSIS: Diagnostic Technologies and intelligent systems for the development of archeological parks in the south of Italy". 10h. Bari, Italy (17 May- 17 June).

2001

- Oral Communication at 20th European Crystallographic Meeting (ECM20). Title of presentation: 'EXPO: new performances'. Warsaw, Poland (25-31 August).

2000

- Oral Communication at XXX National Congress of Associazione Italiana di Cristallografia (AIC). Title of presentation: 'EXPO2000: new performances for ab initio solution of powder structures'. Martina Franca, Italy (19-22 September).

- Organization of XXX National AIC Congress AIC. Martina Franca, Italy (19-22 September).

1998

- Teaching 'Diffrattometria da materiali policristallini: recenti sviluppi delle tecniche di risoluzione e di raaffinamento strutturale' national AIC school. Perugia, Italy (08-12 September).

1996

- Organization of V SIR workshop: SIRWARE96 Single Crystal and Powder Data X-rays, Neutrons and Electrons. Bari, Italy (17-20 December).

1994-2007

- Teaching assistance for the Crystallography Course (75h) within the III-years Diploma Joint Course in Chemistry and Material Science.

AWARDS

2003 'Alessandro Vaciago' Award

Prize winner 'Alessandro Vaciago', of the Accademia Nazionale dei Lincei

PROJECTS LEADER

2012 - 2013

Fondazione cassa di Risparmio di Puglia (FCRP)

Title of project: Studio cristallografico di radiotraccianti PET in valutazione clinica per la diagnosi precoce dell'Alzheimer.

PROJECTS PARTICIPATION (LAST 5 YEARS)

2019 - 2022

'IDF SHARID' – Program PON

Title: Innovative devices for shaping the risk of diabetes

2108-2020

Bilateral agreement CNR/MOES (Albania)

Title: "New nanomaterials for applications in conservation and consolidation of stony materials part of Culture Heritage in Albania"

2012-2016

FIRB

Title: Integrated network for Nano Medicine (RINAME)

2015-2018

'Software and know how license' contract

between CNR 'Department of chemical sciences and materials technologies' and RIGAKU Corporation for the payment of royalty from RIGAKU to CNR for each non-exclusive license per each sale by RIGAKU, of the software EXPO2015

2005-present

Commercial license agreement

between the Institute of Crystallography (IC)-CNR and the companies interested in the EXPO package

PERSONAL SKILLS

Mother tongue

English, French

WHOLE PUBLICATIONS

Publications

- [1] Corrado Cuocci, Nicola Corriero, Francesco Baldassarre, Marzia Dell'Aera, Aurelia Falcicchio, Rosanna Rizzi, and Angela Altomare. Advanced perspectives in the expo software for solving crystal structures from powder diffraction data. *Journal of Applied Crystallography*, 55(2), 2022.
- [2] Corrado Cuocci, Nicola Corriero, Marzia Dell'Aera, Aurelia Falcicchio, Rosanna Rizzi, and Angela Altomare. Direct space approach in action: Challenging structure solution of microcrystalline materials using the expo software. *Computational Materials Science*, 210:111465, 2022.
- [3] Rosanna Rizzi, Francesco Capitelli, Bogdan I Lazoryak, Vladimir A Morozov, Fabio Piccinelli, and Angela Altomare. A comprehensive study of $\text{Ca}_9\text{Tb}(\text{PO}_4)_7$ and $\text{Ca}_9\text{Ho}(\text{PO}_4)_7$ doped β -tricalcium phosphates: Ab initio crystal structure solution, rietveld analysis, and dielectric properties. *Crystal Growth & Design*, 21(4):2263–2276, 2021.
- [4] Davide Gnocchi, Maria M Cavalluzzi, Giuseppe F Mangiatordi, Rosanna Rizzi, Cosimo Tortorella, Mauro Spennacchio, Giovanni Lentini, Angela Altomare, Carlo Sabbà, and Antonio Mazzocca. Xanthenylacetic acid derivatives effectively target lysophosphatidic acid receptor 6 to inhibit hepatocellular carcinoma cell growth. *ChemMedChem*, 16(13):2121–2129, 2021.
- [5] Benny Danilo Belviso, Francesco Marin, Sara Fuertes, Violeta Sicilia, Rosanna Rizzi, Fulvio Ciriaco, Chiara Cappuccino, Eric Dooryhee, Aurelia Falcicchio, Lucia Maini, et al. Structural insights into the vapochromic behavior of pt-and pd-based compounds. *Inorganic Chemistry*, 60(9):6349–6366, 2021.
- [6] Martina Vrankic, Ankica Saric, Sanja Bosnar, Dario Barisic, Damir Pajic, Dirk Lutzenkirchen-Hecht, Ivana Jelovica Badovinac, Mladen Petravic, Angela Altomare, Rosanna Rizzi, et al. Structural behavior and spin-state features of BaAl_2O_4 scaled through tuned Co^{3+} doping. *Inorganic Chemistry*, 60(12):8475–8488, 2021.
- [7] Monica Pistone, Giuseppe Francesco Racaniello, Ilaria Arduino, Valentino Laquintana, Antonio Lopalco, Annalisa Cutrignelli, Rosanna Rizzi, Massimo Franco, Angela Lopodota, and Nunzio Denora. Direct cyclodextrin based powder extrusion 3d printing for one-step production of the bcs class ii model drug niclosamide. 2021.
- [8] Joseba Orive, Roberto Fernández de Luis, Edurne S Larrea, Ana Martínez-Amesti, Angela Altomare, Rosanna Rizzi, Luis Lezama, María I Arriortua, Juan Luis Gómez-Cámer, María Jauregui, et al. Exploring new hydrated delta type vanadium oxides for lithium intercalation. *Dalton Transactions*, 49(12):3856–3868, 2020.
- [9] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, and Rosanna Rizzi. Solving a structure in the reciprocal space, real space and both by using the expo software. *Crystals*, 10(1):16, 2020.
- [10] Veronica Paterlini, Marco Bettinelli, Rosanna Rizzi, Asmaa El Khouri, Manuela Rossi, Giancarlo Della Ventura, and Francesco Capitelli. Characterization and luminescence of Eu^{3+} -and Gd^{3+} -doped hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$. *Crystals*, 10(9):806, 2020.
- [11] Rosanna Rizzi, Francesco Capitelli, Giancarlo Della Ventura, Wafa Hami, Nicola Corriero, Manuela Rossi, and Angela Altomare. Preparation, structural and spectroscopical properties of silver terbium diphosphate AgTb_2O_7 . *Zeitschrift für Kristallographie-Crystalline Materials*, 234(6):363–369, 2019.
- [12] Nour El Houda Belkafouf, Fayssal Triki Baara, Angela Altomare, Rosanna Rizzi, Abdelkader Chouaih, Ayada Djafri, and Fodil Hamzaoui. Synthesis, pxrd structural determination, hirshfeld surface analysis and dft/td-dft investigation of $3n$ -ethyl- $2n'$ -(2-ethylphenylimino) thiazolidin-4-one. *Journal of Molecular Structure*, 1189:8–20, 2019.
- [13] Angela Altomare, Rosanna Rizzi, Manuela Rossi, Asmaa El Khouri, Mohammed Elaammani, Veronica Paterlini, Giancarlo Della Ventura, and Francesco Capitelli. New $\text{Ca}_2.90(\text{Me}^{2+})_0.10(\text{PO}_4)_2$ β -tricalcium phosphates with $\text{Me}^{2+} = \text{Mn}, \text{Ni}, \text{Cu}$: Synthesis, crystal-chemistry, and luminescence properties. *Crystals*, 9(6):288, 2019.
- [14] Filippo M Perna, Aurelia Falcicchio, Antonio Salomone, Anne Milet, Rosanna Rizzi, Ghanem Hamdoun, Gabriella Barozzino-Consiglio, Dietmar Stalke, Hassan Oulyadi, and Vito Capriati. First direct evidence of an ortho-lithiated aryloxetane: Solid and solution structure, and dynamics. *European Journal of Organic Chemistry*, 2019(31-32):5549–5556, 2019.
- [15] A Altomare, C Cuocci, A Moliterni, and R Rizzi. International tables for crystallography (2019). vol. h, ch. 4.2, p. 395.

- [16] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. Direct-space solution in the expo package: the combination of the hbb-bc algorithm with grasp. *Journal of Applied Crystallography*, 51(2):505–513, 2018.
- [17] Angela Altomare, Francesco Capitelli, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. The rietveld refinement in the expo software: A powerful tool at the end of the elaborate crystal structure solution pathway. *Crystals*, 8(5):203, 2018.
- [18] Wafa Hami, Abdelouahed Zegzouti, Mohamed Daoud, Daniel Zambon, Manuela Rossi, Alessandro Vergara, Francesco Capitelli, Angela Altomare, and Rosanna Rizzi. Synthesis, structural characterization and luminescent properties of tb3+-doped aglap2o7 phosphors. *Ceramics International*, 44(16):19184–19190, 2018.
- [19] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. Ochemdb: the free online open chemistry database portal for searching and analysing crystal structure information. *Journal of Applied Crystallography*, 51(4):1229–1236, 2018.
- [20] Asmaa El Khouri, Mohammed Elaotmani, Giancarlo Della Ventura, Armida Sodo, Rosanna Rizzi, Manuela Rossi, and Francesco Capitelli. Synthesis, structure refinement and vibrational spectroscopy of new rare-earth tricalcium phosphates ca9re (po4) 7 (re= la, pr, nd, eu, gd, dy, tm, yb). *Ceramics International*, 43(17):15645–15653, 2017.
- [21] Manuela Rossi, Rosanna Rizzi, Alessandro Vergara, Francesco Capitelli, Angela Altomare, Fabio Bellatreccia, Michele Saviano, and Rosaria M Ghiara. Compositional variation of turquoise-group minerals from the historical collection of the real museo mineralogico of the university of naples. *Mineralogical Magazine*, 81(6):1405–1429, 2017.
- [22] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. Main features of qualx2. 0 software for qualitative phase analysis. *Powder Diffraction*, 32(S1):S129–S134, 2017.
- [23] Rachida Rahmani, Ahmed Djafri, Abdelkader Chouaih, Ayada Djafri, Fodil Hamzaoui, Rosanna Rizzi, and Angela Altomare. Synthesis, molecular and solid state structure of 5-(5-nitro furan-2-ylmetylen), 3-n-(2-methoxy phenyl), 2-n-(2-methoxyphenyl) imino thiazolidin-4-one: X-ray powder diffraction and dft studies. *Journal of Molecular Structure*, 1143:259–264, 2017.
- [24] Svetoslava Vankova, Daniele Versaci, Julia Amici, Anna Ferrari, Rosanna Rizzi, Angela Altomare, Salvatore Guastella, Carlotta Francia, Silvia Bodoardo, and Nerino Penazzi. A high-capacity cathode based on silicates material for advanced lithium batteries. *Journal of Solid State Electrochemistry*, 21(12):3381–3388, 2017.
- [25] Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi, and Angela Altomare. Computational methodologies for the characterization of polycrystalline materials in software developed by the institute of crystallography. In *CONFERENZA DI DIPARTIMENTO 2017*, page 147, 2017.
- [26] Angela Altomare, Corrado Cuocci, Anna Moliterni, Rosanna Rizzi, Nicola Corriero, and Aurelia Falcicchio. The shift_and_fix procedure in expo: advances for solving ab initio crystal structures by powder diffraction data. *Journal of Applied Crystallography*, 50(6):1812–1820, 2017.
- [27] Giuseppina Balassone, Fabio Bellatreccia, Luisa Ottolini, Angela Mormone, Carmela Petti, Maria Rosaria Ghiara, Angela Altomare, Michele Saviano, Rosanna Rizzi, and Loredana D’orazio. Sodalite-group minerals from the somma-vesuvius volcano (naples, italy): A combined epma, sims, and ftir crystal-chemical study. *The Canadian Mineralogist*, 54(3):583–604, 2016.
- [28] Lucia Veltri, Giuseppe Grasso, Rosanna Rizzi, Raffaella Mancuso, and Bartolo Gabriele. Palladium-catalyzed carbonylative multicomponent synthesis of functionalized benzimidazothiazoles. *Asian Journal of Organic Chemistry*, 5(4):560–567, 2016.
- [29] Lucia Veltri, Giuseppe Grasso, Rosanna Rizzi, Raffaella Mancuso, and Bartolo Gabriele. Cover picture: Palladium-catalyzed carbonylative multicomponent synthesis of functionalized benzimidazothiazoles (asian j. org. chem. 4/2016). *Asian Journal of Organic Chemistry*, 5(4):434–434, 2016.
- [30] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. Qualx2. 0: a qualitative phase analysis software using the freely available database pow_cod. *Journal of Applied Crystallography*, 48(2):598–603, 2015.

- [31] A Altomare, N Corriero, C Cuocci, A Falcicchio, A Moliterni, and R Rizzi. Caratterizzazione di materiali cristallini di interesse per i beni culturali mediante diffrazione di raggi x da polveri. *Preservation and enhancement of Cultural Heritage*, page 127, 2015.
- [32] Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, and Rosanna Rizzi. Expo software for solving crystal structures by powder diffraction data: methods and application. *Crystal Research and Technology*, 50(9-10):737–742, 2015.
- [33] Marina Zenzola, Leonardo Degennaro, Piera Trincherà, Laura Carroccia, Arianna Giovine, Giuseppe Romanazzi, Piero Mastrorilli, Rosanna Rizzi, Luisa Pisano, and Renzo Luisi. Harnessing the ortho-directing ability of the azetidine ring for the regioselective and exhaustive functionalization of arenes. *Chemistry–A European Journal*, 20(38):12190–12200, 2014.
- [34] Angela Altomare, Elena Capparelli, Antonio Carrieri, Nicola A Colabufo, Anna Moliterni, Rosanna Rizzi, and Dritan Siliqi. Crystallographic study of pet radiotracers in clinical evaluation for early diagnosis of alzheimers. *Acta Crystallographica Section E: Structure Reports Online*, 70(11):o1149–o1150, 2014.
- [35] Giuseppina Balassone, Volker Kahlenberg, Angela Altomare, Angela Mormone, Rosanna Rizzi, Michele Saviano, and Nicola Mondillo. Nephelines from the somma-vesuvius volcanic complex (southern italy): crystal-chemical, structural and genetic investigations. *Mineralogy and Petrology*, 108(1):71–90, 2014.
- [36] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Moliterni, Rosanna Rizzi, Nicola Corriero, and Aurelia Falcicchio. Expo2013: a kit of tools for phasing crystal structures from powder data. *Journal of Applied Crystallography*, 46(4):1231–1235, 2013.
- [37] Angela Altomare, Corrado Cuocci, Anna Moliterni, and Rosanna Rizzi. Ramm: a new random-model-based method for solving ab initio crystal structure using the expo package. *Journal of Applied Crystallography*, 46(2):476–482, 2013.
- [38] Angela Altomare, Nicola Corriero, Corrado Cuocci, Anna Moliterni, and Rosanna Rizzi. The hybrid big bang–big crunch method for solving crystal structure from powder diffraction data. *Journal of Applied Crystallography*, 46(3):779–787, 2013.
- [39] Maria Grazia Perrone, Paola Vitale, Paola Malerba, Angela Altomare, Rosanna Rizzi, Antonio Lavecchia, Carmen Di Giovanni, Ettore Novellino, and Antonio Scilimati. Diarylheterocycle core ring features effect in selective cox-1 inhibition. *ChemMedChem*, 7(4):629–641, 2012.
- [40] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Moliterni, and Rosanna Rizzi. Covmap: a new algorithm for structure model optimization in the expo package. *Journal of Applied Crystallography*, 45(4):789–797, 2012.
- [41] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Moliterni, and Rosanna Rizzi. Covariance and correlation estimation in electron-density maps. *Acta Crystallographica Section A: Foundations of Crystallography*, 68(2):244–255, 2012.
- [42] Leonardo Degennaro, Rosmara Mansueto, Elisa Carenza, Rosanna Rizzi, Saverio Florio, Lawrence M Pratt, and Renzo Luisi. Nitrogen dynamics and reactivity of chiral aziridines: generation of configurationally stable aziridinyl-lithium compounds. *Chemistry–A European Journal*, 17(18):4992–5003, 2011.
- [43] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Moliterni, and Rosanna Rizzi. Expo2011: a new package for powder crystallography. *Powder Diffraction*, 26(S1):S2–S12, 2011.
- [44] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Moliterni, and Rosanna Rizzi. Advances in the expo2009 systematic decomposition procedure: an atom-matching-based figure of merit. *Journal of Applied Crystallography*, 44(3):448–453, 2011.
- [45] Angela Altomare, Corrado Cuocci, Carmelo Giacobazzo, Anna Grazia Giuseppina Moliterni, and Rosanna Rizzi. Obtaining models suitable for rietveld refinement: the expo2011 techniques. *Zeitschrift für Kristallographie Crystalline Materials*, 226(12):869–881, 2011.

- [46] Aurelia Falcicchio, Angela Altomare, Corrado Cuocci, Renzo Luisi, Anna Moliterni, and Rosanna Rizzi. Structural analysis of aziridine-2-methanol derivatives. In *ACTA CRYSTALLOGRAPHICA A-FOUNDATION AND ADVANCES*, volume 67, pages C666–C666. INT UNION CRYSTALLOGRAPHY 2 ABBEY SQ, CHESTER, CH1 2HU, ENGLAND, 2011.
- [47] Angela Altomare, Corrado Cuocci, Carmelo Giocovazzo, Anna Moliterni, and Rosanna Rizzi. Automation and efficiency in the powder structure solution by expo package. In *ACTA CRYSTALLOGRAPHICA A-FOUNDATION AND ADVANCES*, volume 67, pages C204–C205. INT UNION CRYSTALLOGRAPHY 2 ABBEY SQ, CHESTER, CH1 2HU, ENGLAND, 2011.
- [48] Angela Altomare, Corrado Cuocci, Carmelo Giocovazzo, Anna Moliterni, and Rosanna Rizzi. The dual-space resolution bias correction algorithm: applications to powder data. *Journal of Applied Crystallography*, 43(4):798–804, 2010.
- [49] Angela Altomare, Corrado Cuocci, Carmelo Giocovazzo, Anna Grazia Giuseppina Moliterni, and Rosanna Rizzi. The main strategies and tools in expo2009. In *Solid State Phenomena*, volume 163, pages 1–8. Trans Tech Publications Ltd, 2010.
- [50] Anna Moliterni, Angela Altomare, Corrado Cuocci, Carmelo Giocovazzo, and Rosanna Rizzi. Ab-initio structure determination by powders: recent developments in expo2010. In *ACTA CRYSTALLOGRAPHICA A-FOUNDATION AND ADVANCES*, volume 66, pages S110–S110. INT UNION CRYSTALLOGRAPHY 2 ABBEY SQ, CHESTER, CH1 2HU, ENGLAND, 2010.
- [51] Angela Altomare, Mercedes Camalli, Corrado Cuocci, Carmelo Giocovazzo, Anna Moliterni, and Rosanna Rizzi. Expo2009: structure solution by powder data in direct and reciprocal space. *Journal of Applied Crystallography*, 42(6):1197–1202, 2009.
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