

K. D. M. HARRIS: LIST OF PUBLICATIONS

398. Elucidating the crystal structure of DL-arginine by combined powder X-ray diffraction data analysis and periodic DFT-D calculations.
C. E. Hughes, I. Boughdiri, C. Bouakkaz, P. A. Williams, K. D. M. Harris.
Crystal Growth & Design, **2018**, *18*, 42–46.
397. Assessing the detection limit of a minority solid-state form of a pharmaceutical by ¹H double-quantum magic-angle spinning nuclear magnetic resonance spectroscopy.
K. Maruyoshi, D. Iuga, A. E. Watts, C. E. Hughes, K. D. M. Harris, S. P. Brown.
Journal of Pharmaceutical Sciences, **2017**, *106*, 3372–3377.
396. *Ab initio* random structure searching of organic molecular solids: assessment and validation against experimental data.
M. Zilka, D. V. Dudenko, C. E. Hughes, P. A. Williams, S. Sturniolo, W. T. Franks, C. J. Pickard, J. R. Yates, K. D. M. Harris, S. P. Brown.
Physical Chemistry Chemical Physics, **2017**, *19*, 25949–25960.
[Assigned as a "Hot Paper"]
395. Sir John Meurig Thomas, FRS: inspirational supervisor, mentor and friend.
K. D. M. Harris.
The Selected Papers of Sir John Meurig Thomas (Editors: J. M. Thomas, K. D. M. Harris), World Scientific Publishing Europe Ltd., London, **2017**, pp. 547–552.
394. Determination of a complex crystal structure in the absence of single crystals: analysis of powder X-ray diffraction data, guided by solid-state NMR and periodic DFT calculations, reveals a new 2'-deoxyguanosine structural motif.
C. E. Hughes, G. N. M. Reddy, S. Masiero, S. P. Brown, P. A. Williams, K. D. M. Harris.
Chemical Science, **2017**, *8*, 3971–3979.
393. "NMR Crystallization": *in-situ* NMR techniques for time-resolved monitoring of crystallization processes.
K. D. M. Harris, C. E. Hughes, P. A. Williams, G. R. Edwards-Gau.
Acta Crystallographica, **2017**, *C73*, 137–148.
392. Structural diversity of solid solutions formed between 3-chloro-*trans*-cinnamic acid and 3-bromo-*trans*-cinnamic acid.
M. A. Khoj, C. E. Hughes, K. D. M. Harris, B. M. Kariuki.
Crystal Growth & Design, **2017**, *17*, 1276–1284.
391. Explorations in the dynamics of crystalline solids and the evolution of crystal formation processes.
K. D. M. Harris.
Israel Journal of Chemistry, **2017**, *57*, 154–170.
390. Complexes of thiourea with alkali metal bromides and iodides: structural properties, mixed-halide and mixed-metal materials, and halide exchange processes.
V. G. Charalamopoulos, B. M. Kariuki, K. D. M. Harris.
Crystal Growth & Design, **2017**, *17*, 786–793.
389. The true structural periodicities and superspace group descriptions of the prototypical incommensurate composite materials: alkane/urea inclusion compounds.
M. Couzi, F. Guillaume, K. D. M. Harris, B. A. Palmer, K. Christensen, S. P. Collins.
EPL (Europhysics Letters), **2016**, *116*, 56001.
388. Determining molecular orientations in disordered materials from X-ray linear dichroism at the iodine L₁-edge.
B. A. Palmer, S. P. Collins, J. Hulliger, C. E. Hughes, K. D. M. Harris.
Journal of the American Chemical Society, **2016**, *138*, 16188–16191.
387. Calculation of solid-state NMR lineshapes using contour analysis.
C. E. Hughes, K. D. M. Harris.
Solid State Nuclear Magnetic Resonance, **2016**, *80*, 7–13.
386. New in situ solid-state NMR strategies for exploring materials formation and adsorption processes: prospects in heterogeneous catalysis.
K. D. M. Harris.
Applied Petrochemical Research, **2016**, *6*, 295–306.
385. Novel technique for spatially resolved imaging of molecular bond orientations using X-ray birefringence.
J. P. Sutter, I. P. Dolbnya, S. P. Collins, K. D. M. Harris, G. R. Edwards-Gau, B. M. Kariuki, B. A. Palmer.
AIP Conference Proceedings, **2016**, *1741*, 050009/1–050009/4.

384. Understanding the solid-state hydration behavior of a common amino acid: identification, structural characterization, and hydration/dehydration processes of new hydrate phases of L-lysine.
P. A. Williams, C. E. Hughes, J. Martin, E. Courvoisier, A. B. M. Buanz, S. Gaisford, K. D. M. Harris.
Journal of Physical Chemistry C, **2016**, *120*, 9385–9392.
383. Combining the advantages of powder X-ray diffraction and NMR crystallography in structure determination of the pharmaceutical material cimetidine hydrochloride.
A. E. Watts, K. Maruyoshi, C. E. Hughes, S. P. Brown, K. D. M. Harris.
Crystal Growth & Design, **2016**, *16*, 1798–1804.
382. Some of tomorrow's catalysts for processing renewable and non-renewable feedstocks, diminishing anthropogenic carbon dioxide and increasing the production of energy.
J. M. Thomas, K. D. M. Harris.
Energy & Environmental Science, **2016**, *9*, 687–708.
381. Structure determination of organic molecular solids from powder X-ray diffraction data: current opportunities and state-of-the-art.
K. D. M. Harris, P. A. Williams.
Advances in Organic Crystal Chemistry (Editors: R. Tamura, M. Miyata), Springer Japan, **2015**, pp. 141–166 (Chapter 8).
380. In situ solid-state NMR studies of crystallization processes.
K. D. M. Harris, C. E. Hughes, P. A. Williams.
Advances in Organic Crystal Chemistry (Editors: R. Tamura, M. Miyata), Springer Japan, **2015**, pp. 31–53 (Chapter 3).
379. New *in-situ* solid-state NMR techniques for probing the evolution of crystallization processes: pre-nucleation, nucleation and growth.
C. E. Hughes, P. A. Williams, V. L. Keast, V. G. Charalampopoulos, G. R. Edwards-Gau, K. D. M. Harris.
Faraday Discussions, **2015**, *179*, 115–140.
378. Discovery of new meta-stable polymorphs in a family of urea co-crystals by solid-state mechanochemistry.
Y. Zhou, F. Guo, C. E. Hughes, D. L. Browne, T. R. Peskett, K. D. M. Harris.
Crystal Growth & Design, **2015**, *15*, 2901–2907.
377. Theoretical analysis of the background intensity distribution in X-ray Birefringence Imaging using synchrotron bending-magnet radiation.
J. P. Sutter, I. P. Dolbnya, S. P. Collins, K. D. M. Harris, G. R. Edwards-Gau, B. A. Palmer.
Journal of Applied Physics, **2015**, *117*, 164902/1–164902/10.
376. Exploiting powder X-ray diffraction to establish the solvent-assisted solid-state supramolecular assembly of pillar[5]quinone.
K. I. Shivakumar, Y. Yan, C. E. Hughes, D. C. Apperley, K. D. M. Harris, G. J. Sanjayan.
Crystal Growth & Design, **2015**, *15*, 1583–1587.
375. L-Lysine: exploiting powder X-ray diffraction to complete the set of crystal structures of the 20 directly-encoded proteinogenic amino acids.
P. A. Williams, C. E. Hughes, K. D. M. Harris.
Angewandte Chemie, International Edition, **2015**, *54*, 3973–3977.
Angewandte Chemie, **2015**, *127*, 4045–4049.
374. Monitoring the evolution of crystallization processes by *in-situ* solid-state NMR spectroscopy.
K. D. M. Harris, C. E. Hughes, P. A. Williams.
Solid State Nuclear Magnetic Resonance, **2015**, *65*, 107–113.
373. X-ray birefringence imaging of materials with anisotropic molecular dynamics.
B. A. Palmer, G. R. Edwards-Gau, B. M. Kariuki, K. D. M. Harris, I. P. Dolbnya, S. P. Collins, J. P. Sutter.
Journal of Physical Chemistry Letters, **2015**, *6*, 561–567.
372. "CLASSIC NMR": An *in-situ* NMR strategy for mapping the time-evolution of crystallization processes by combined liquid-state and solid-state measurements.
C. E. Hughes, P. A. Williams, K. D. M. Harris.
Angewandte Chemie, International Edition, **2014**, *53*, 8939–8943.
Angewandte Chemie, **2014**, *126*, 9085–9089.
[Assigned as a "Hot Paper"]

This paper was highlighted in the following:

Chemical and Engineering News, 28 July 2014, p. 33.

371. Highly efficient chiral resolution of DL-arginine by co-crystal formation followed by recrystallization under preferential enrichment conditions.
S. Iwama, K. Kuyama, Y. Mori, K. Manoj, R. G. Gonnade, K. Suzuki, C. E. Hughes, P. A. Williams, K. D. M. Harris, S. Veessler, H. Takahashi, H. Tsue, R. Tamura.
Chemistry – A European Journal, **2014**, *20*, 10343–10350.
370. Powder diffraction.
K. D. M. Harris, P. A. Williams.
Structure from Diffraction Methods (Inorganic Materials Series) (Editors: D. W. Bruce, D. O'Hare, R. I. Walton), John Wiley & Sons, Chichester, **2014**, pp. 1–81 (Chapter 1).
369. X-ray Birefringence Imaging.
B. A. Palmer, G. R. Edwards-Gau, B. M. Kariuki, K. D. M. Harris, I. P. Dolbnya, S. P. Collins.
Science, **2014**, *344*, 1013–1016.
- This paper was highlighted in the following:
(1) Mapping bond orientations with polarized x-rays, S. Lidin, *Science*, **2014**, *344*, 969–970.
(2) *Chemical and Engineering News*, 2 June 2014, p. 25.
368. An adaptable and dynamically porous organic salt traps unique tetrahalide dianions.
J. Martí-Rujas, L. Meazza, G. K. Lim, G. Terraneo, T. Pilati, K. D. M. Harris, P. Metrangolo, G. Resnati.
Angewandte Chemie, International Edition, **2013**, *52*, 13444–13448.
Angewandte Chemie, **2013**, *125*, 13686–13690.
[Assigned as a "Very Important Paper"]
367. An NMR crystallography DFT-D approach to analyse the role of intermolecular hydrogen bonding and π - π interactions in driving co-crystallisation of indomethacin and nicotinamide.
D. V. Dudenko, J. R. Yates, K. D. M. Harris, S. P. Brown.
CrystEngComm, **2013**, *15*, 8797–8807.
366. Controlling spatial distributions of molecules in multicomponent organic crystals, with quantitative mapping by confocal Raman microspectrometry.
B. A. Palmer, A. Le Comte, K. D. M. Harris, F. Guillaume.
Journal of the American Chemical Society, **2013**, *135*, 14512–14515.
365. Polymorphism in a *trans*-cinnamic acid derivative exhibiting two distinct β -type phases: structural properties, [2+2] photodimerization reactions and polymorphic phase transition behaviour.
M. A. Khoj, C. E. Hughes, K. D. M. Harris, B. M. Kariuki.
Crystal Growth & Design, **2013**, *13*, 4110–4117.
364. An ENDOR and DFT analysis of hindered methyl group rotations in frozen solutions of bis(acetylacetonato)-copper(II).
K. M. Sharples, E. Carter, C. E. Hughes, K. D. M. Harris, J. A. Platts, D. M. Murphy.
Physical Chemistry Chemical Physics, **2013**, *15*, 15214–15222.
363. Exploiting the synergy of powder X-ray diffraction and solid-state NMR spectroscopy in structure determination of organic molecular solids.
D. V. Dudenko, P. A. Williams, C. E. Hughes, O. N. Antzutkin, S. P. Velaga, S. P. Brown, K. D. M. Harris.
Journal of Physical Chemistry C, **2013**, *117*, 12258–12265.
362. Expanding the solid-state landscape of L-phenylalanine: discovery of polymorphism and new hydrate phases, with rationalization of hydration/dehydration processes.
P. A. Williams, C. E. Hughes, A. B. M. Buanz, S. Gaisford, K. D. M. Harris.
Journal of Physical Chemistry C, **2013**, *117*, 12136–12145.
361. A drifting Markov process on the circle, with physical applications.
S.-Y. Yeh, K. D. M. Harris, P. E. Jupp.
Proceedings of the Royal Society A, **2013**, *469*, 20130092.
360. X-ray birefringence in highly anisotropic materials.
S. P. Collins, I. Dolbnya, B. A. Palmer, G. R. Edwards-Gau, A. Morte-Ródenas, B. M. Kariuki, G. K. Lim, K. D. M. Harris, Y. Joly.
Journal of Physics: Conference Series, **2013**, *425*, 132015.
359. A rare case of polymorphism in a three-component co-crystal system, with each polymorph having ten independent molecules in the asymmetric unit.
Y. Yan, C. E. Hughes, B. M. Kariuki, K. D. M. Harris.
Crystal Growth & Design, **2013**, *13*, 27–30.

358. Mechanochemical synthesis: how grinding evolves.
K. D. M. Harris.
Nature Chemistry, **2013**, *5*, 12–14.
357. Crystal structure determination by the combined analysis of NMR and powder diffraction data.
K. D. M. Harris, M. Xu.
Encyclopedia of NMR (Editors: R. K. Harris, R. E. Wasylshen), John Wiley & Sons, Chichester, **2012**, Volume 2, pp. 848–857 (ISBN: 978-0-470-05821-3).
356. New strategies for exploring crystallization processes of organic materials.
K. D. M. Harris, C. E. Hughes, B. A. Palmer, F. Guillaume.
Transactions of the American Crystallographic Association, **2012**, *43*, 97–112.
355. Efficient, scalable and solvent-free mechanochemical synthesis of the OLED material Alq₃ (q = 8-hydroxyquinolate).
X. Ma, G. K. Lim, K. D. M. Harris, D. C. Apperley, P. N. Horton, M. B. Hursthouse, S. L. James.
Crystal Growth & Design, **2012**, *12*, 5869–5872.
354. New insights into the preparation of the low-melting polymorph of racemic ibuprofen.
P. A. Williams, C. E. Hughes, K. D. M. Harris.
Crystal Growth & Design, **2012**, *12*, 5839–5845.
353. X-ray birefringence: a new strategy for determining molecular orientation in materials.
B. A. Palmer, G. R. Edwards-Gau, A. Morte-Ródenas, B. M. Kariuki, G. K. Lim, K. D. M. Harris, I. P. Dolbnya, S. P. Collins.
Journal of Physical Chemistry Letters, **2012**, *3*, 3216–3222.
352. Exploiting in situ solid-state NMR for the discovery of new polymorphs during crystallization processes.
C. E. Hughes, P. A. Williams, T. R. Peskett, K. D. M. Harris.
Journal of Physical Chemistry Letters, **2012**, *3*, 3176–3181.
351. The effect of intermolecular hydrogen bonding on the planarity of amides.
J. A. Platts, H. Maarof, K. D. M. Harris, G. K. Lim, D. J. Willock.
Physical Chemistry Chemical Physics, **2012**, *14*, 11944–11952.
350. Discovery of a new system exhibiting abundant polymorphism: *m*-aminobenzoic acid.
P. A. Williams, C. E. Hughes, G. K. Lim, B. M. Kariuki, K. D. M. Harris.
Crystal Growth & Design, **2012**, *12*, 3104–3113.
349. The crystal structure of L-arginine.
E. Courvoisier, P. A. Williams, G. K. Lim, C. E. Hughes, K. D. M. Harris.
Chemical Communications, **2012**, *48*, 2761–2763.
- This paper was highlighted in the following:
Determining the structure of L-arginine and other organic molecules, J. M. Thomas, *ChemPhysChem*, **2012**, *13*, 2637–2638.
348. Reactions in solid-state inclusion compounds.
K. D. M. Harris, B. A. Palmer, G. R. Edwards-Gau.
Supramolecular Chemistry: From Molecules to Nanomaterials, (Editors: J. W. Steed and P. A. Gale), John Wiley & Sons, Chichester, **2012**, Volume 4, pp. 1589–1612.
347. Structural rationalization of the phase transition behavior in a solid organic inclusion compound: bromocyclohexane/thiourea.
B. A. Palmer, B. M. Kariuki, A. Morte-Ródenas, K. D. M. Harris.
Crystal Growth & Design, **2012**, *12*, 577–582.
346. A new route to aerogels: monolithic silica cryogels.
A. Pons, L. Casas, E. Estop, E. Molins, K. D. M. Harris, M. Xu.
Journal of Non-Crystalline Solids, **2012**, *358*, 461–469.
345. Powder diffraction crystallography of molecular solids.
K. D. M. Harris.
Topics in Current Chemistry, **2012**, *315*, 133–178.
344. Mechanochemistry: opportunities for new and cleaner synthesis.
S. L. James, C. J. Adams, C. Bolm, D. Braga, P. Collier, T. Friščić, F. Grepioni, K. D. M. Harris, G. Hyett, W. Jones, A. Krebs, J. Mack, L. Maini, A. G. Orpen, I. P. Parkin, W. C. Shearouse, J. W. Steed, D. C. Waddell.
Chemical Society Reviews, **2012**, *41*, 413–447.

343. Structure determination from powder X-ray diffraction data of a new polymorph of a high-density organic hydrate material, with an assessment of hydrogen-bond disorder by Rietveld refinement.
G. K. Lim, K. Fujii, K. D. M. Harris, D. C. Apperley.
Crystal Growth & Design, **2011**, *11*, 5192–5199.
342. High-resolution solid-state ^2H NMR spectroscopy of polymorphs of glycine.
A. E. Aliev, S. E. Mann, A. S. Rahman, P. F. McMillan, F. Corà, D. Iuga, C. E. Hughes, K. D. M. Harris.
Journal of Physical Chemistry A, **2011**, *115*, 12201–12211.
341. Cooperativity in solid-state squaramides.
R. Prohens, A. Portell, C. Puigjaner, S. Tomàs, K. Fujii, K. D. M. Harris, X. Alcobé, M. Font-Bardia, R. Barbas.
Crystal Growth & Design, **2011**, *11*, 3725–3730.
340. X-ray birefringence from a model anisotropic crystal.
B. A. Palmer, A. Morte-Ródenas, B. M. Kariuki, K. D. M. Harris, S. P. Collins.
Journal of Physical Chemistry Letters, **2011**, *2*, 2346–2351.
339. Structural chemistry of a new chiral anhydrous phase of $\text{Ru}(\text{bipy})_3(\text{ClO}_4)_2$ established from powder X-ray diffraction analysis.
E. Y. Cheung, K. Fujii, F. Guo, K. D. M. Harris, S. Hasebe, R. Kuroda.
Crystal Growth & Design, **2011**, *11*, 3313–3317.
338. Structural diversity, but no polymorphism, in a homologous family of co-crystals of urea and α,ω -dihydroxyalkanes.
J. Martí-Rujas, B. M. Kariuki, C. E. Hughes, A. Morte-Ródenas, F. Guo, Z. Glavcheva-Laleva, K. Taştēmür, L. Ooi, L. Yeo, K. D. M. Harris.
New Journal of Chemistry, **2011**, *35*, 1515–1521.
337. Natural-abundance solid-state ^2H NMR spectroscopy at high magnetic field.
A. E. Aliev, S. E. Mann, D. Iuga, C. E. Hughes, K. D. M. Harris.
Journal of Physical Chemistry A, **2011**, *115*, 5568–5578.
336. Exploiting powder X-ray diffraction for direct structure determination in structural biology: the P2X4 receptor trafficking motif YEQGL.
K. Fujii, M. T. Young, K. D. M. Harris.
Journal of Structural Biology, **2011**, *174*, 461–467.
335. Structural properties of carboxylic acid dimers confined within the urea tunnel structure: an MD simulation study.
A. J. Illott, S. Palucha, A. S. Batsanov, K. D. M. Harris, P. Hodgkinson, M. R. Wilson.
Journal of Physical Chemistry B, **2011**, *115*, 2791–2800.
334. An incommensurate thiourea inclusion compound.
B. A. Palmer, B. M. Kariuki, V. K. Muppidi, C. E. Hughes, K. D. M. Harris.
Chemical Communications, **2011**, *47*, 3760–3762.
333. Direct structure elucidation by powder X-ray diffraction of a metal-organic framework material prepared by solvent-free grinding.
K. Fujii, A. Lazuen Garay, J. Hill, E. Sbircea, Z. Pan, M. Xu, D. C. Apperley, S. L. James, K. D. M. Harris.
Chemical Communications, **2010**, *46*, 7572–7574.
332. Arrays of P=O dipoles as a recurrent structural motif in *bis*-diphenylphosphine oxides, established from powder X-ray diffraction.
G. K. Lim, Z. Zhou, K. Fujii, P. Calcagno, E. Tedesco, S. J. Kitchin, B. M. Kariuki, D. Philp, K. D. M. Harris.
Crystal Growth & Design, **2010**, *10*, 3814–3818.
331. A strategy for retrospectively mapping the growth history of a crystal.
B. A. Palmer, K. D. M. Harris, F. Guillaume.
Angewandte Chemie, International Edition, **2010**, *49*, 5096–5100.
Angewandte Chemie, **2010**, *122*, 5222–5226.
- This paper was highlighted in the following:
Chemical and Engineering News, 28 June 2010, p. 39
330. A solid-state dehydration process in an organic material associated with substantial hydrogen-bond reorganization, investigated by powder X-ray diffraction.
J. Martí-Rujas, A. Morte-Ródenas, F. Guo, N. Thomas, K. Fujii, B. M. Kariuki, K. D. M. Harris.
Crystal Growth & Design, **2010**, *10*, 3176–3181.

329. Direct observation of a transient polymorph during crystallization.
C. E. Hughes, K. D. M. Harris.
Chemical Communications, **2010**, *46*, 4982–4984.
328. Triptycene-based polymers of intrinsic microporosity: organic materials that can be tailored for gas adsorption.
B. S. Ghanem, M. Hashem, K. D. M. Harris, K. J. Msayib, M. Xu, P. M. Budd, N. Chaukura, D. Book, S. Tedds, A. Walton, N. B. McKeown.
Macromolecules, **2010**, *43*, 5287–5294.
327. Selective transformation pathways between crystalline forms of an organic material established from powder X-ray diffraction analysis.
K. Fujii, Y. Ashida, H. Uekusa, F. Guo, K. D. M. Harris.
Chemical Communications, **2010**, *46*, 4264–4266.
326. Physico-chemical understanding of polymorphism and solid-state dehydration/rehydration processes for the pharmaceutical material acrinol, by *ab initio* powder X-ray diffraction analysis and other techniques.
K. Fujii, H. Uekusa, N. Itoda, G. Hasegawa, E. Yonemochi, K. Terada, Z. Pan, K. D. M. Harris.
Journal of Physical Chemistry C, **2010**, *114*, 580–586.
325. "Amorphous nickel sulfide" is hydrated nanocrystalline NiS with a core-shell structure.
S. Huang, K. D. M. Harris, E. Lopez-Capel, D. A. C. Manning, D. Rickard.
Inorganic Chemistry, **2009**, *48*, 11486–11488.
324. Pathways for hydrogen bond switching in a tetrameric methanol cluster.
M. Mella, K. D. M. Harris.
Physical Chemistry Chemical Physics, **2009**, *11*, 11340–11346.
323. Probing the evolution of water clusters during hydration of the solid acid catalyst H-ZSM-5.
K. D. M. Harris, M. Xu, J. M. Thomas.
Philosophical Magazine, **2009**, *89*, 3001–3012.
322. Combined analysis of NMR and powder diffraction data.
K. D. M. Harris, M. Xu.
NMR Crystallography (Editors: R. K. Harris, R. Wasylishen, M. J. Duer), John Wiley & Sons, Chichester, **2009**, pp. 275–287 (Chapter 19).
321. Selected thoughts on chiral crystals, chiral surfaces, and asymmetric heterogeneous catalysis.
K. D. M. Harris, J. M. Thomas.
ChemCatChem, **2009**, *1*, 223–231.
320. Preferential clustering of water molecules during hydration of the ammonium form of the solid acid catalyst ZSM-5.
M. Xu, K. D. M. Harris, J. M. Thomas.
Catalysis Letters, **2009**, *131*, 16–20.
319. Nitrogen and hydrogen adsorption by an organic microporous crystal.
K. J. Msayib, D. Book, P. M. Budd, N. Chaukura, K. D. M. Harris, M. Helliwell, S. Tedds, A. Walton, J. E. Warren, M. Xu, N. B. McKeown.
Angewandte Chemie, International Edition, **2009**, *48*, 3273–3277.
Angewandte Chemie, **2009**, *121*, 3323–3327.
318. Crystal structure determination by the combined analysis of NMR and powder diffraction data.
K. D. M. Harris, M. Xu.
Encyclopedia of Magnetic Resonance (Editors: R. K. Harris, R. Wasylishen), John Wiley & Sons, Chichester, **2009**, DOI: 10.1002/9780470034590.emrstm1004. [on-line version]
317. *In situ* solid-state ¹H NMR studies of hydration of the solid acid catalyst ZSM-5 in its ammonium form.
M. Xu, K. D. M. Harris, J. M. Thomas.
Solid State Nuclear Magnetic Resonance, **2009**, *35*, 93–99.
316. The effect of deuteration on polymorphic outcome in the crystallization of glycine from aqueous solution.
C. E. Hughes, K. D. M. Harris.
New Journal of Chemistry, **2009**, *33*, 713–716.
315. Structure solution from powder X-ray diffraction data by Genetic Algorithm techniques, applied to organic materials generated as polycrystalline products from solid state processes.
K. D. M. Harris.
Materials and Manufacturing Processes, **2009**, *24*, 293–302.

314. Multiple-fragment representations of molecular geometry in direct-space structure solution from powder X-ray diffraction data using genetic algorithms.
Z. Zhou, K. D. M. Harris.
Computational Materials Science, **2009**, *45*, 118–121.
313. Fundamentals and applications of genetic algorithms for structure solution from powder X-ray diffraction data.
K. D. M. Harris.
Computational Materials Science, **2009**, *45*, 16–20.
312. Vapour induced crystalline transformation investigated by *ab initio* powder X-ray diffraction analysis.
K. Fujii, Y. Ashida, H. Uekusa, S. Hirano, S. Toyota, F. Toda, Z. Pan, K. D. M. Harris.
Crystal Growth & Design, **2009**, *9*, 1201–1207.
311. Lessons on the assignment of polymorphs, highlighted by the case of the latent pigment DPP-Boc.
E. J. MacLean, M. Tremayne, B. M. Kariuki, J. R. A. Cameron, M. A. Roberts, K. D. M. Harris.
Crystal Growth & Design, **2009**, *9*, 853–857.
310. Bidirectional transport of guest molecules through the nanoporous tunnel structure of a solid inclusion compound.
J. Martí-Rujas, A. Desmedt, K. D. M. Harris, F. Guillaume.
Journal of Physical Chemistry C, **2009**, *113*, 736–743.
309. Direct structural understanding of a topochemical solid state photopolymerization reaction.
F. Guo, J. Martí-Rujas, Z. Pan, C. E. Hughes, K. D. M. Harris.
Journal of Physical Chemistry C, **2008**, *112*, 19793–19796.
308. Counteracting stagnation in genetic algorithm calculations by implementation of a micro genetic algorithm strategy.
Z. Zhou, K. D. M. Harris.
Physical Chemistry Chemical Physics, **2008**, *10*, 7262–7269.
307. Optimizing the number of components in a molecular quasicrystal: a three-component material based on the Penrose tiling.
Z. Zhou, K. D. M. Harris.
Journal of Physical Chemistry C, **2008**, *112*, 16186–16188.
306. A solid state dehydration process associated with a significant change in the topology of dihydrogen phosphate chains, established from powder X-ray diffraction.
D. Albesa-Jové, Z. Pan, K. D. M. Harris, H. Uekusa.
Crystal Growth & Design, **2008**, *8*, 3641–3645.
305. Dynamic properties of solid ammonium cyanate.
A. Desmedt, S. J. Kitchin, K. D. M. Harris, F. Guillaume, R. R. Tykwinski, M. Xu, M. A. Gonzalez.
Journal of Physical Chemistry C, **2008**, *112*, 15870–15879.
304. Optical phonons in millerite (NiS) from single-crystal polarized Raman spectroscopy.
F. Guillaume, S. Huang, K. D. M. Harris, M. Couzi, D. Talaga.
Journal of Raman Spectroscopy, **2008**, *39*, 1419–1422.
303. Predictable disorder *versus* polymorphism in the rationalization of structural diversity: a multi-disciplinary study of eniluracil.
R. C. B. Copley, S. A. Barnett, P. G. Karamertzanis, K. D. M. Harris, B. M. Kariuki, M. Xu, E. A. Nickels, R. W. Lancaster, S. L. Price.
Crystal Growth & Design, **2008**, *8*, 3474–3481.
302. Characterization of a polymorphic system exhibiting a substantial variation of solubility in fluorinated solvent.
M. Côte, C. E. Hughes, T. K. Austin, P. G. A. Rogueda, Z. Pan, K. D. M. Harris, P. C. Griffiths.
Journal of Physical Chemistry C, **2008**, *112*, 14570–14578.
301. A technique for *in situ* monitoring of crystallization from solution by solid-state ¹³C CPMAS NMR spectroscopy.
C. E. Hughes, K. D. M. Harris.
Journal of Physical Chemistry A, **2008**, *112*, 6808–6810.
300. Clustering of glycine molecules in aqueous solution studied by molecular dynamics simulation.
S. Hamad, C. E. Hughes, C. R. A. Catlow, K. D. M. Harris.
Journal of Physical Chemistry B, **2008**, *112*, 7280–7288.

299. Residue-based charge flipping: a new variant of an emerging algorithm for structure solution from X-ray diffraction data.
Z. Zhou, K. D. M. Harris.
Journal of Physical Chemistry A, **2008**, *112*, 4863–4868.
298. Mapping the evolution of adsorption of water in nanoporous silica by *in situ* solid-state ^1H NMR spectroscopy.
M. Xu, K. D. M. Harris, J. M. Thomas.
Journal of the American Chemical Society, **2008**, *130*, 5880–5882.
297. Structural properties of low-temperature phase transitions in the prototypical thiourea inclusion compound: cyclohexane/thiourea.
Z. Pan, A. Desmedt, E. J. MacLean, F. Guillaume, K. D. M. Harris.
Journal of Physical Chemistry C, **2008**, *112*, 839–847.
296. Triple-quantum ^{23}Na MAS NMR spectroscopy as a technique for probing polymorphism in sodium salts.
M. Xu, K. D. M. Harris.
Crystal Growth & Design, **2008**, *8*, 6–10.
295. Aperiodicity in organic materials.
K. D. M. Harris.
Turning Points in Solid-State, Materials and Surface Science (Editors: K. D. M. Harris, P. P. Edwards), Royal Society of Chemistry, Cambridge, **2008**, pp. 302–333 (Chapter 19).
294. Aspects of validation in the structure determination of organic materials from powder X-ray diffraction data.
K. D. M. Harris.
Zeitschrift für Kristallographie, **2007**, *S26*, 45–51.
293. Kinetics of molecular transport in a nanoporous crystal studied by confocal Raman microspectrometry: single file diffusion in a densely filled tunnel.
J. Martí-Rujas, A. Desmedt, K. D. M. Harris, F. Guillaume.
Journal of Physical Chemistry B, **2007**, *111*, 12339–12344.
292. A multi-technique approach for probing the evolution of structural properties during crystallization of organic materials from solution.
C. E. Hughes, S. Hamad, K. D. M. Harris, C. R. A. Catlow, P. C. Griffiths.
Faraday Discussions, **2007**, *136*, 71–89.
291. Alteration of polymorphic selectivity through different crystallization mechanisms occurring in the same crystallization solution.
M. Xu, K. D. M. Harris.
Journal of Physical Chemistry B, **2007**, *111*, 8705–8707.
290. Probing the evolution of adsorption on nanoporous solids by *in situ* solid-state NMR spectroscopy.
M. Xu, K. D. M. Harris, J. M. Thomas, D. E. W. Vaughan.
ChemPhysChem, **2007**, *8*, 1311–1313.
289. Enhanced efficiency of direct-space structure solution from powder diffraction data in the case of conformationally flexible molecules.
A. J. Hanson, E. Y. Cheung, K. D. M. Harris.
Journal of Physical Chemistry B, **2007**, *111*, 6349–6356.
288. Fundamental and applied aspects of urea and thiourea inclusion compounds.
K. D. M. Harris.
Supramolecular Chemistry, **2007**, *19*, 47–53.
287. Mechanistic aspects of the solid-state transformation of ammonium cyanate to urea at high pressure.
R. Méreau, A. Desmedt, K. D. M. Harris.
Journal of Physical Chemistry B, **2007**, *111*, 3960–3968.
286. Advantages of a redefinition of variable-space in direct-space structure solution from powder X-ray diffraction data.
Z. Zhou, V. Siegler, E. Y. Cheung, S. Habershon, K. D. M. Harris, R. L. Johnston.
ChemPhysChem, **2007**, *8*, 650–653.
285. Structural properties of a family of hydrogen-bonded co-crystals formed between gemfibrozil and hydroxy derivatives of *t*-butylamine, determined directly from powder X-ray diffraction data.
E. Y. Cheung, S. E. David, K. D. M. Harris, B. R. Conway, P. Timmins.
Journal of Solid State Chemistry, **2007**, *180*, 1068–1075.

284. A triptycene-based polymer of intrinsic microporosity that displays enhanced surface area and hydrogen adsorption. B. S. Ghanem, K. J. Msayib, N. B. McKeown, K. D. M. Harris, Z. Pan, P. M. Budd, J. Selbie, A. Butler, D. Book, A. Walton. *Chemical Communications*, **2007**, 67–69.
283. Dichroic filters for astronomical X-ray polarimetry. N. P. Bannister, K. D. M. Harris, S. P. Collins, A. Martindale, P. S. Monks, G. Solan, G. W. Fraser. *Experimental Astronomy*, **2006**, *21*, 1–12.
282. Structure-reactivity correlations for solid state enantioselective photochemical reactions, established directly from powder X-ray diffraction. E. Y. Cheung, K. D. M. Harris, T. Kang, J. R. Scheffer, J. Trotter. *Journal of the American Chemical Society*, **2006**, *128*, 15554–15555.
281. *In-situ* monitoring of alkane-alkane guest exchange in urea inclusion compounds using confocal Raman microspectrometry. J. Martí-Rujas, K. D. M. Harris, A. Desmedt, F. Guillaume. *Molecular Crystals and Liquid Crystals*, **2006**, *456*, 139–147.
280. Solid state structural properties of 2,4,6-trimethoxybenzene derivatives, determined directly from powder X-ray diffraction data in conjunction with other techniques. Z. Pan, M. Xu, E. Y. Cheung, J. A. Platts, K. D. M. Harris, E. C. Constable, C. E. Housecroft. *Journal of Solid State Chemistry*, **2006**, *179*, 3214–3223.
279. Design of a molecular quasicrystal. Z. Zhou, K. D. M. Harris. *ChemPhysChem*, **2006**, *7*, 1649–1653.
- This paper was highlighted in the following:
Chemical and Engineering News, 14 August 2006, p. 49
278. Abundant polymorphism in a system with multiple hydrogen-bonding opportunities: oxalyl dihydrazide. S. Ahn, F. Guo, B. M. Kariuki, K. D. M. Harris. *Journal of the American Chemical Society*, **2006**, *128*, 8441–8452.
277. Molecular crystal structures from powder X-ray diffraction techniques. E. Y. Cheung, K. D. M. Harris. *Zeitschrift für Kristallographie*, **2006**, *S23*, 15–20.
276. Understanding structural properties of a dendrimeric material directly from powder X-ray diffraction data. Z. Pan, M. Xu, E. Y. Cheung, K. D. M. Harris, E. C. Constable, C. E. Housecroft. *Journal of Physical Chemistry B*, **2006**, *110*, 11620–11623.
275. Significant conformational changes associated with molecular transport in a crystalline solid. J. Martí-Rujas, K. D. M. Harris, A. Desmedt, F. Guillaume. *Journal of Physical Chemistry B*, **2006**, *110*, 10708–10713.
274. Solid triphenylmethanol: a molecular material that undergoes multiple internal reorientational processes on different timescales. S. J. Kitchin, M. Xu, H. Serrano-González, L. J. Coates, S. Z. Ahmed, C. Glidewell, K. D. M. Harris. *Journal of Solid State Chemistry*, **2006**, *179*, 1335–1338.
273. On the spontaneous induction of chirality in the preparation of Werner's complex *cis*-[CoBr(NH₃)(en)₂]Br₂. F. Guo, M. Casadesus, E. Y. Cheung, M. P. Coogan, K. D. M. Harris. *Chemical Communications*, **2006**, 1854–1856.
272. Contrasting solid state structures of trithiocyanuric acid and cyanuric acid. F. Guo, E. Y. Cheung, K. D. M. Harris, V. R. Pedireddi. *Crystal Growth & Design*, **2006**, *6*, 846–848.
271. Alternative hydrogen bonding modes employed by a helical tubular diol host molecule. W. Yue, K. Nakano, R. Bishop, D. C. Craig, K. D. M. Harris, M. L. Scudder. *CrystEngComm*, **2006**, *8*, 250–256.
270. Highly efficient one-step conversion of cyclohexane to adipic acid using single-site heterogeneous catalysts. R. Raja, J. M. Thomas, M. Xu, K. D. M. Harris, M. Greenhill-Hooper, K. Quill. *Chemical Communications*, **2006**, 448–450.

269. Structural properties of methoxy derivatives of benzyl bromide, determined directly from powder X-ray diffraction data.
Z. Pan, E. Y. Cheung, K. D. M. Harris, E. C. Constable, C. E. Housecroft.
Powder Diffraction, **2005**, *20*, 345–352.
268. Structural and dynamic aspects of hydrogen bonded complexes and inclusion compounds containing α,ω -dicyanoalkanes and urea, investigated by solid state ^{13}C and ^2H NMR techniques.
A. E. Aliev, K. D. M. Harris, P. H. Champkin.
Journal of Physical Chemistry B, **2005**, *109*, 23342–23350.
267. Significantly contrasting solid state dynamics of the racemic and enantiomerically pure crystalline forms of an amino acid.
S. J. Kitchin, G. Tutoveanu, M. R. Steele, E. L. Porter, K. D. M. Harris.
Journal of Physical Chemistry B, **2005**, *109*, 22808–22813.
266. On the prospects for exploiting 4D ultrafast electron microscopy in solid-state organic and biological chemistry.
K. D. M. Harris, J. M. Thomas.
Crystal Growth & Design, **2005**, *5*, 2124–2130.
265. A case study in direct-space structure determination from powder X-ray diffraction data: finding the hydrate structure of an organic molecule with significant conformational flexibility.
Z. Pan, E. Y. Cheung, K. D. M. Harris, E. C. Constable, C. E. Housecroft.
Crystal Growth & Design, **2005**, *5*, 2084–2090.
264. Hydrogen-bonded chains of α,ω -diaminoalkane and α,ω -dihydroxyalkane guest molecules lead to disrupted tunnel structures in urea inclusion compounds.
S.-O. Lee, B. M. Kariuki, K. D. M. Harris.
New Journal of Chemistry, **2005**, *29*, 1266–1271.
263. Altering the polymorphic product distribution in a solid-state dehydration process by rapid sample rotation in a solid-state NMR probe.
M. Xu, K. D. M. Harris.
Journal of the American Chemical Society, **2005**, *127*, 10832–10833.
262. Structural understanding of a molecular material that is accessed only by a solid state desolvation process: the scope of modern powder X-ray diffraction techniques.
F. Guo, K. D. M. Harris.
Journal of the American Chemical Society, **2005**, *127*, 7314–7315.
261. Structural rationalisation of co-crystals formed between trithiocyanuric acid and molecules containing hydrogen bonding functionality.
S. Ahn, J. PrakashaReddy, B. M. Kariuki, S. Chatterjee, A. Ranganathan, V. R. Pedireddi, C. N. R. Rao, K. D. M. Harris.
Chemistry – A European Journal, **2005**, *11*, 2433–2439.
260. Host-guest chiral discrimination in incommensurate 2-hydroxyalkane/urea inclusion compounds: a computational study.
L. Yeo, K. D. M. Harris.
Mendeleev Communications, **2004**, *14*, 263–266.
259. Developments in genetic algorithm techniques for structure solution from powder diffraction data.
K. D. M. Harris, S. Habershon, E. Y. Cheung, R. L. Johnston.
Zeitschrift für Kristallographie, **2004**, *219*, 838–846.
258. How to determine structures when single crystals cannot be grown: opportunities for structure determination of molecular materials using powder diffraction data.
K. D. M. Harris, E. Y. Cheung.
Chemical Society Reviews, **2004**, *33*, 526–538.
257. Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum.
A. Alavi, R. J. C. Brown, S. Habershon, K. D. M. Harris, R. L. Johnston.
Molecular Physics, **2004**, *102*, 869–876.
256. Direct time-resolved and spatially resolved monitoring of molecular transport in a crystalline nanochannel system.
J. Marti-Rujas, A. Desmedt, K. D. M. Harris, F. Guillaume.
Journal of the American Chemical Society, **2004**, *126*, 11124–11125.

255. An efficient algorithm for calculating whole-profile functions in crystal structure solution from powder diffraction data. S. Habershon, E. Y. Cheung, K. D. M. Harris, R. L. Johnston. *Chemical Physics Letters*, **2004**, *390*, 394–398.
254. Urea inclusion compounds. K. D. M. Harris. *Encyclopedia of Supramolecular Chemistry* (Editors: J. L. Atwood, J. W. Steed), Marcel Dekker, New York, **2004**, Volume 2, pp. 1538–1549.
253. Thiourea inclusion compounds. K. D. M. Harris. *Encyclopedia of Supramolecular Chemistry* (Editors: J. L. Atwood, J. W. Steed), Marcel Dekker, New York, **2004**, Volume 2, pp. 1501–1507.
252. Incommensurate and commensurate structures. K. D. M. Harris. *Encyclopedia of Supramolecular Chemistry* (Editors: J. L. Atwood, J. W. Steed), Marcel Dekker, New York, **2004**, Volume 1, pp. 712–716.
251. Structural aspects of a dendrimer precursor determined directly from powder X-ray diffraction data. Z. Pan, E. Y. Cheung, K. D. M. Harris, E. C. Constable, C. E. Housecroft. *Crystal Growth & Design*, **2004**, *4*, 451–455.
250. Modern applications of powder X-ray diffraction in pharmaceutical sciences. K. D. M. Harris. *American Pharmaceutical Review*, **2004**, *7*, 86–91.
249. Applications of evolutionary computation in structure determination from diffraction data. K. D. M. Harris, R. L. Johnston, S. Habershon. *Structure and Bonding*, **2004**, *110*, 55–94.
248. Challenges in direct-space structure determination from powder diffraction data: a molecular material with four independent molecules in the asymmetric unit. D. Albesa-Jové, B. M. Kariuki, S. J. Kitchin, L. Grice, E. Y. Cheung, K. D. M. Harris. *ChemPhysChem*, **2004**, *5*, 414–418.
247. Rationalizing the structural properties of bupivacaine base – a local anaesthetic – directly from powder diffraction data. E. Y. Cheung, K. D. M. Harris, R. L. Johnston, S. J. Kitchin, K. L. Hadden, M. Zakrzewski. *Journal of Pharmaceutical Sciences*, **2004**, *93*, 667–674.
246. Comment on "A deuteron NMR study of the tetrahydrofuran clathrate hydrate. Part II: Coupling of rotational and translational dynamics of water". M. Bach-Vergés, S. J. Kitchin, K. D. M. Harris, M. Zugic, C. A. Koh. *Physical Chemistry Chemical Physics*, **2004**, *6*, 871–872.
245. Powder diffraction indexing as a pattern recognition problem: a new approach for determining unit cell parameters based on an artificial neural network. S. Habershon, E. Y. Cheung, K. D. M. Harris, R. L. Johnston. *Journal of Physical Chemistry A*, **2004**, *108*, 711–716.
244. Probing hydrogen bonding in solids using solid state NMR spectroscopy. A. E. Aliev, K. D. M. Harris. *Structure and Bonding*, **2004**, *108*, 1–53.
243. Co-crystalline hydrogen bonded solids based on the alcohol–carboxylic acid–alcohol supramolecular motif. S. F. Alshahateet, K. Nakano, R. Bishop, D. C. Craig, K. D. M. Harris, M. L. Scudder. *CrystEngComm*, **2004**, *6*, 5–10.
242. Fundamental developments in direct-space techniques for structure solution from powder diffraction data. S. Habershon, D. Albesa-Jové, E. Y. Cheung, G. W. Turner, R. L. Johnston, K. D. M. Harris. *Materials Science Forum*, **2004**, *443–444*, 11–21.
241. Crystallization and preliminary X-ray diffraction data of *Mycobacterium tuberculosis* FbpC1 (Rv3803c). R. A. Wilson, S. Rai, W. N. Maughan, L. Kremer, B. M. Kariuki, K. D. M. Harris, T. Wagner, G. S. Besra, K. Fütterer. *Acta Crystallographica, Section D*, **2003**, *59*, 2303–2305.

240. Direct structure determination of a multi-component molecular crystal prepared by a solid state grinding procedure. E. Y. Cheung, S. J. Kitchin, K. D. M. Harris, Y. Imai, N. Tajima, R. Kuroda. *Journal of the American Chemical Society*, **2003**, *125*, 14658–14659.
239. Structural characterization of industrially relevant polymorphic materials from powder diffraction data. K. D. M. Harris, E. Y. Cheung. *Organic Process Research and Development*, **2003**, *7*, 970–976.
238. Ammonium cyanate shows N–H···N hydrogen bonding, not N–H···O. E. J. MacLean, K. D. M. Harris, B. M. Kariuki, S. J. Kitchin, R. R. Tykwinski, I. P. Swainson, J. D. Dunitz. *Journal of the American Chemical Society*, **2003**, *125*, 14449–14451.
237. Molecular motion in solid ammonia trimethylalane. G. Tutoveanu, S. J. Kitchin, K. D. M. Harris, J. Müller. *Journal of Solid State Chemistry*, **2003**, *176*, 120–126.
236. New opportunities for structure determination of molecular materials directly from powder diffraction data. K. D. M. Harris. *Crystal Growth & Design*, **2003**, *3*, 887–895.
235. Solid-state supramolecular organization, established directly from powder diffraction data, and photoluminescence efficiency of rigid-core oligothiophene-S,S-dioxides. E. Tedesco, F. Della Sala, L. Favaretto, G. Barbarella, D. Albesa-Jové, D. Pisignano, G. Gigli, R. Cingolani, K. D. M. Harris. *Journal of the American Chemical Society*, **2003**, *125*, 12277–12283.
234. Enhancing the enantioselectivity of novel homogeneous organometallic hydrogenation catalysts. M. D. Jones, R. Raja, J. M. Thomas, B. F. G. Johnson, D. W. Lewis, J. Rouzaud, K. D. M. Harris. *Angewandte Chemie, International Edition*, **2003**, *42*, 4326–4331. *Angewandte Chemie*, **2003**, *115*, 4462–4467.
233. A straightforward and effective procedure to test for preferred orientation in polycrystalline samples prior to structure determination from powder diffraction data. E. Y. Cheung, K. D. M. Harris, B. M. Foxman. *Crystal Growth & Design*, **2003**, *3*, 705–710.
232. Development of a multi-population parallel genetic algorithm for structure solution from powder diffraction data. S. Habershon, K. D. M. Harris, R. L. Johnston. *Journal of Computational Chemistry*, **2003**, *24*, 1766–1774.
231. Polymorphism of a novel sodium ion channel blocker. E. Y. Cheung, K. D. M. Harris, R. L. Johnston, K. L. Hadden, M. Zakrzewski. *Journal of Pharmaceutical Sciences*, **2003**, *92*, 2017–2026.
230. The interplay of aryl-perfluoroaryl stacking interactions and inter-stack hydrogen bonding in controlling the structure of a molecular cocrystal. S. Meejoo, B. M. Kariuki, K. D. M. Harris. *ChemPhysChem*, **2003**, *4*, 766–769.
229. Design of a solid inclusion compound with optimal properties as a linear dichroic filter for X-ray polarization analysis. M.-H. Chao, B. M. Kariuki, K. D. M. Harris, S. P. Collins, D. Laundry. *Angewandte Chemie, International Edition*, **2003**, *42*, 2982–2985. *Angewandte Chemie*, **2003**, *115*, 3090–3093.
228. Structural aspects of the β polymorph of (E)-4-formylcinnamic acid: structure determination directly from powder diffraction data and elucidation of structural disorder from solid state NMR. S. Meejoo, B. M. Kariuki, S. J. Kitchin, E. Y. Cheung, D. Albesa-Jové, K. D. M. Harris. *Helvetica Chimica Acta*, **2003**, *86*, 1467–1477.
227. Mechanistic insights into the conversion of cyclohexene to adipic acid by H₂O₂ in the presence of a TAPO-5 catalyst. S.-O. Lee, R. Raja, K. D. M. Harris, J. M. Thomas, B. F. G. Johnson, G. Sankar. *Angewandte Chemie, International Edition*, **2003**, *42*, 1520–1523. *Angewandte Chemie*, **2003**, *115*, 1558–1561.
226. Local structural aspects of one-dimensional solid inclusion compounds. K. D. M. Harris. *Phase Transitions*, **2003**, *76*, 205–218.

225. Recent advances in the opportunities for solving molecular crystal structures directly from powder diffraction data. K. D. M. Harris, R. L. Johnston, G. W. Turner, E. Tedesco, E. Y. Cheung, B. M. Kariuki. *Molecular Crystals and Liquid Crystals*, **2002**, 389, 123–129.
224. Structure determination of molecular materials from powder diffraction data. K. D. M. Harris. *Current Opinion in Solid State and Materials Science*, **2002**, 6, 125–130.
223. Hydrogen bond dynamics in solid triphenylsilanol. A. E. Aliev, C. E. Atkinson, K. D. M. Harris. *Journal of Physical Chemistry B*, **2002**, 106, 9013–9018.
222. Recent advances in the opportunities for solving molecular crystal structures directly from powder diffraction data: new insights in crystal engineering contexts. K. D. M. Harris, R. L. Johnston, E. Y. Cheung, G. W. Turner, S. Habershon, D. Albesa-Jové, E. Tedesco, B. M. Kariuki. *CrystEngComm*, **2002**, 4, 356–367.
221. Towards an environmentally acceptable heterogeneous catalytic method of producing adipic acid by the oxidation of hydrocarbons in air. R. Raja, S.-O. Lee, M. Sanchez-Sanchez, G. Sankar, K. D. M. Harris, B. F. G. Johnson, J. M. Thomas. *Topics in Catalysis*, **2002**, 20, 85–88.
220. Effects of polymorphism on functional group dynamics: solid state ^2H NMR studies of the dynamic properties of the α and β phases of L-glutamic acid. S. J. Kitchin, S. Ahn, K. D. M. Harris. *Journal of Physical Chemistry A*, **2002**, 106, 7228–7234.
219. Structural rationalization of a highly selective ammonium ionophore. B. M. Kariuki, S.-O. Lee, K. D. M. Harris, H.-S. Kim, K.-S. Do, K.-I. Kim. *Crystal Growth & Design*, **2002**, 2, 309–311.
218. Dynamic properties of the guest molecules in the pyrazine/ α -zirconium phosphate intercalation compound: a multi-nuclear solid state NMR study. M. Bach-Vergés, S. J. Kitchin, A. E. Aliev, G. B. Hix, K. D. M. Harris. *Chemistry of Materials*, **2002**, 14, 2656–2663.
217. Design of a bilayer structure in an organic inclusion compound. S.-O. Lee, B. M. Kariuki, K. D. M. Harris. *Angewandte Chemie, International Edition*, **2002**, 41, 2181–2184. *Angewandte Chemie*, **2002**, 114, 2285–2288.
216. Solid-state and solution phase reactivity of 10-hydroxy-10,9-boroxophenanthrene: a model building block for self-assembly processes. L. M. Greig, B. M. Kariuki, S. Habershon, N. Spencer, R. L. Johnston, K. D. M. Harris, D. Philp. *New Journal of Chemistry*, **2002**, 26, 701–710.
215. Characterization of intermolecular interactions in a disordered solid *via* a one-dimensional Patterson synthesis. M.-H. Chao, K. D. M. Harris, B. M. Kariuki, C. L. Bauer, B. M. Foxman. *Journal of Physical Chemistry B*, **2002**, 106, 4032–4035.
214. Gaining insights into the evolutionary behaviour in genetic algorithm calculations, with applications to structure solution from powder diffraction data. S. Habershon, G. W. Turner, K. D. M. Harris, R. L. Johnston, J. M. Johnston. *Chemical Physics Letters*, **2002**, 353, 185–194.
213. Acid-catalyzed trimerization of acetaldehyde: a highly selective and reversible transformation at ambient temperature in a zeolitic solid. S.-O. Lee, S. J. Kitchin, K. D. M. Harris, G. Sankar, M. Dugal, J. M. Thomas. *Journal of Physical Chemistry B*, **2002**, 106, 1322–1326.
212. C–H \cdots O hydrogen bond mediated chain reversal in a peptide containing a γ -amino acid residue, determined directly from powder X-ray diffraction data. E. Y. Cheung, E. E. McCabe, K. D. M. Harris, R. L. Johnston, E. Tedesco, K. M. P. Raja, P. Balaram. *Angewandte Chemie, International Edition*, **2002**, 41, 494–496. *Angewandte Chemie*, **2002**, 114, 512–514.

211. X-ray linear dichroism in an α,ω -dibromoalkane/urea inclusion compound and its application to polarization analysis of magnetic diffraction.
S. P. Collins, D. Laundy, K. D. M. Harris, B. M. Kariuki, C. L. Bauer, S. D. Brown, P. Thompson.
Journal of Physics: Condensed Matter, **2002**, *14*, 123–134.
210. Experimental determination of interaction energies in a porous molecular solid.
S.-O. Lee, K. D. M. Harris, P. E. Jupp, L. Yeo.
Journal of the American Chemical Society, **2001**, *123*, 12913–12914.
209. A new type of layered structure for urea inclusion compounds containing local segments of tunnels.
S.-O. Lee, B. M. Kariuki, A. L. Richardson, K. D. M. Harris.
Journal of the American Chemical Society, **2001**, *123*, 12684–12685.
208. Fine-tuning the crystal morphology of tunnel inclusion compounds: a general strategy.
N. E. Kelly, S.-O. Lee, K. D. M. Harris.
Journal of the American Chemical Society, **2001**, *123*, 12682–12683.
207. Structure determination of molecular crystals directly from powder diffraction data.
K. D. M. Harris.
The Rigaku Journal, **2001**, *18*, 23–32.
206. Structural rationalization directly from powder diffraction data: intermolecular aggregation in 2-(methylsulfonyl)ethyl succinimidyl carbonate.
D. Albesa-Jové, E. Tedesco, K. D. M. Harris, R. L. Johnston, E. Y. Cheung.
Crystal Growth & Design, **2001**, *1*, 425–428.
205. A borazaaromatic analogue of isophthalic acid.
P. R. Ashton, K. D. M. Harris, B. M. Kariuki, D. Philp, J. M. A. Robinson, N. Spencer.
Journal of the Chemical Society, Perkin Transactions 2, **2001**, 2166–2173.
204. Porous poly(D,L-lactide) and poly(D,L-lactide-co-glycolide) by thermal salt elimination from halogenocarboxylates.
M. Siedler, S. J. Kitchin, K. D. M. Harris, A. L. C. Lagoa, H. P. Diogo, M. E. Minas da Piedade, M. Epple.
Journal of the Chemical Society, Dalton Transactions, **2001**, 3140–3148.
203. Structural aspects of high-efficiency blue-emitting 2,5-bis(trimethylsilyl)thiophene-S,S-dioxide and related materials.
E. Tedesco, B. M. Kariuki, K. D. M. Harris, R. L. Johnston, O. Pudova, G. Barbarella, E. A. Marseglia, G. Gigli, R. Cingolani.
Journal of Solid State Chemistry, **2001**, *161*, 121–128.
202. Structure determination of 4,4'-trimethylenedipyridine from powder diffraction data.
E. Tedesco, S. S. Dhillon, K. D. M. Harris, R. L. Johnston, G. W. Turner, B. M. Kariuki.
Materials Science Forum, **2001**, *378–381*, 784–788.
201. Structure solution of molecular crystals from powder diffraction data using genetic algorithms: opportunities in academic and industrial research.
K. D. M. Harris, R. L. Johnston, B. M. Kariuki, E. Tedesco, G. W. Turner.
Materials Science Forum, **2001**, *378–381*, 38–46.
200. Phase transitions and molecular dynamics in the cyclohexane/thiourea inclusion compound.
A. Desmedt, S. J. Kitchin, F. Guillaume, M. Couzi, K. D. M. Harris, E. H. Bocanegra.
Physical Review B, **2001**, *64*, 054106-1–054106-21 [Paper Number: 054106].
199. Substituent effects on aromatic interactions in the solid state.
H. Adams, P. L. Bernad, D. S. Eggleston, R. C. Haltiwanger, K. D. M. Harris, G. A. Hembury, C. A. Hunter, D. J. Livingstone, B. M. Kariuki, J. F. McCabe.
Chemical Communications, **2001**, 1500–1501.
198. *Ab initio* structure determination of a peptide β -turn from powder X-ray diffraction data.
E. Tedesco, K. D. M. Harris, R. L. Johnston, G. W. Turner, K. M. P. Raja, P. Balaram.
Chemical Communications, **2001**, 1460–1461.
197. Towards molecular sieve inorganic catalysts that are akin to enzymes: studies of a selective cyclo-dimerization over ferrierite at ambient temperature.
S.-O. Lee, G. Sankar, S. J. Kitchin, M. Dugal, J. M. Thomas, K. D. M. Harris.
Catalysis Letters, **2001**, *73*, 91–94.

196. Contemporary advances in the use of powder X-ray diffraction for structure determination.
K. D. M. Harris, M. Tremayne, B. M. Kariuki.
Angewandte Chemie, International Edition, **2001**, *40*, 1626–1651.
Angewandte Chemie, **2001**, *113*, 1674–1700.
195. Dynamic properties of the tetrahydrofuran clathrate hydrate, investigated by solid state ^2H NMR spectroscopy.
M. Bach-Vergés, S. J. Kitchin, K. D. M. Harris, M. Zugic, C. A. Koh.
Journal of Physical Chemistry B, **2001**, *105*, 2699–2706.
194. A method for understanding characteristics of multi-dimensional hypersurfaces, illustrated by energy and powder profile R-factor hypersurfaces for molecular crystals.
G. W. Turner, E. Tedesco, K. D. M. Harris, R. L. Johnston, B. M. Kariuki.
Zeitschrift für Kristallographie, **2001**, *216*, 187–189.
193. Polymorphs of a 1:1 co-crystal with tunnel and layer structures: *p,p'*-biphenol/dimethyl sulfoxide.
S. Ahn, B. M. Kariuki, K. D. M. Harris.
Crystal Growth & Design, **2001**, *1*, 107–111.
192. Probing host-guest interaction energies in solid inclusion compounds from experimental studies of competitive inclusion.
S.-O. Lee, K. D. M. Harris, P. E. Jupp, L. Elizabé, S. Swinburn.
Molecular Crystals and Liquid Crystals, **2001**, *356*, 517–525.
191. Solving crystal structures from powder diffraction data using genetic algorithms.
B. M. Kariuki, K. D. M. Harris, R. L. Johnston.
Molecular Crystals and Liquid Crystals, **2001**, *356*, 469–481.
190. A simulated annealing approach for crystal structure solution from powder diffraction data.
G. E. Engel, S. Wilke, K. D. M. Harris, B. M. Kariuki, S. Ahn, F. J. J. Leusen, M. A. Neumann.
Molecular Crystals and Liquid Crystals, **2001**, *356*, 355–364.
189. Structural aspects of the solid state polycondensation reaction in alkali 4-halogenomethylbenzoates.
O. Herzberg, H. Ehrenberg, S. J. Kitchin, K. D. M. Harris, M. Epple.
Journal of Solid State Chemistry, **2001**, *156*, 61–67.
188. Temperature-dependent structural properties and crystal twinning in the fluorocyclohexane/thiourea inclusion compound.
L. Yeo, K. D. M. Harris, B. M. Kariuki.
Journal of Solid State Chemistry, **2001**, *156*, 16–25.
187. Polymorphic phase transformation in the 3-bromo-*trans*-cinnamic acid system.
S. Ahn, K. D. M. Harris, B. M. Kariuki, D. M. S. Zin.
Journal of Solid State Chemistry, **2001**, *156*, 10–15.
186. Intermolecular organisation of triphenylene-based discotic mesogens by interdigitation of alkyl chains.
M. T. Allen, S. Diele, K. D. M. Harris, T. Hegmann, B. M. Kariuki, J. A. Preece, D. Lose, C. Tschierske.
Journal of Materials Chemistry, **2001**, *11*, 302–311.
185. Solving crystal structures from powder diffraction data in direct space – progress in the application of genetic algorithms.
K. D. M. Harris, B. M. Kariuki, R. L. Johnston.
Advances in Structure Analysis (Editors: R. Kuzel, J. Jasek), Czech and Slovak Crystallographic Association, Prague, **2001**, pp. 190–204.
184. Structure determination of an oligopeptide directly from powder diffraction data.
E. Tedesco, G. W. Turner, K. D. M. Harris, R. L. Johnston, B. M. Kariuki.
Angewandte Chemie, International Edition, **2000**, *39*, 4488–4491.
Angewandte Chemie, **2000**, *112*, 4662–4665.
183. Polymorphism in *p*-hydroxybenzoic acid: the effect of intermolecular hydrogen bonding in controlling proton order versus disorder in the carboxylic acid dimer motif.
B. M. Kariuki, C. L. Bauer, K. D. M. Harris, S. J. Teat.
Angewandte Chemie, International Edition, **2000**, *39*, 4485–4488.
Angewandte Chemie, **2000**, *112*, 4659–4662.
182. Polysubstituted derivatives of triphenylene as high resolution electron beam resists for nanolithography.
A. P. G. Robinson, R. E. Palmer, T. Tada, T. Kanayama, M. T. Allen, J. A. Preece, K. D. M. Harris.
Journal of Vacuum Science and Technology B, **2000**, *18*, 2730–2736.

181. Molecular dynamics simulation study of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound. J.-C. Soetens, A. Desmedt, F. Guillaume, K. D. M. Harris. *Chemical Physics*, **2000**, *261*, 125–135.
180. Weak interactions in crystal engineering – understanding the recognition properties of the nitro group. J. M. A. Robinson, D. Philp, K. D. M. Harris, B. M. Kariuki. *New Journal of Chemistry*, **2000**, *24*, 799–806.
179. A triphenylene derivative as a novel negative/positive tone resist at 10 nanometer resolution. T. Tada, T. Kanayama, A. P. G. Robinson, R. E. Palmer, M. T. Allen, J. A. Preece, K. D. M. Harris. *Microelectronic Engineering*, **2000**, *53*, 425–428.
178. Evolutionary algorithms in crystallographic applications. K. D. M. Harris, R. L. Johnston, B. M. Kariuki. *Evolutionary Algorithms in Computer-Aided Molecular Design* (Editor: D. E. Clark), Wiley-VCH, **2000**, pp. 159–194 (Chapter 9).
177. Understanding the structural properties of a homologous series of bis-diphenylphosphine oxides. P. Calcagno, B. M. Kariuki, S. J. Kitchin, J. M. A. Robinson, D. Philp, K. D. M. Harris. *Chemistry – A European Journal*, **2000**, *6*, 2338–2349.
176. Structural understanding of a polymorphic system by structure solution and refinement from powder X-ray diffraction data: the α and β phases of the latent pigment DPP-Boc. E. J. MacLean, M. Tremayne, B. M. Kariuki, K. D. M. Harris, A. F. M. Iqbal, Z. Hao. *Journal of the Chemical Society, Perkin Transactions 2*, **2000**, 1513–1519.
175. Rotary resonance recoupling of ^{13}C - ^1H dipolar interactions in magic angle spinning ^{13}C NMR of dynamic solids. S. J. Kitchin, K. D. M. Harris, A. E. Aliev, D. C. Apperley. *Chemical Physics Letters*, **2000**, *323*, 490–497.
174. Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $\text{O}=\text{H}\cdots\text{O}=\text{C}$ hydrogen bonded system. G. W. Turner, R. L. Johnston, K. D. M. Harris. *Chemical Physics*, **2000**, *256*, 159–168.
173. Using polarisation effects to alter chemical reactivity – a simple host which enhances amine nucleophilicity. P. R. Ashton, P. Calcagno, N. Spencer, K. D. M. Harris, D. Philp. *Organic Letters*, **2000**, *2*, 1365–1368.
172. Intermolecular organization of triphenylene-based discotic mesogens by interdigitation of alkyl chains. M. T. Allen, K. D. M. Harris, B. M. Kariuki, N. Kumari, J. A. Preece, S. Diele, D. Lose, T. Hegmann, C. Tschierske. *Liquid Crystals*, **2000**, *27*, 689–692.
171. Electronic and local structural properties of the $\text{Bi}_2\text{Sr}_2(\text{Ca}_{1-x}\text{Y}_x)\text{Cu}_2\text{O}_{8+\delta}$ family of materials, studied by X-ray absorption spectroscopy. I.-J. Hsu, R.-S. Liu, J.-M. Chen, R.-G. Liu, L.-Y. Jang, J.-F. Lee, K. D. M. Harris. *Chemistry of Materials*, **2000**, *12*, 1115–1121.
170. Polymerization of aniline on copper phosphonate materials. G. B. Hix, V. C. Maddocks, K. D. M. Harris. *Polyhedron*, **2000**, *19*, 765–770.
169. Implementation of Lamarckian concepts in a Genetic Algorithm for structure solution from powder diffraction data. G. W. Turner, E. Tedesco, K. D. M. Harris, R. L. Johnston, B. M. Kariuki. *Chemical Physics Letters*, **2000**, *321*, 183–190.
168. *In-situ* monitoring of solid state polymerization reactions in sodium chloroacetate and sodium bromoacetate by ^{23}Na and ^{13}C solid-state NMR spectroscopy. A. E. Aliev, L. Elizabé, B. M. Kariuki, H. Kirschnick, J. M. Thomas, M. Epple, K. D. M. Harris. *Chemistry – A European Journal*, **2000**, *6*, 1120–1126.
167. Structural aspects of a commensurate tunnel inclusion compound of tri-*ortho*-thymotide containing 1,8-dibromooctane guest molecules. H. Serrano-González, K. D. M. Harris. *Journal of Molecular Structure*, **2000**, *519*, 41–54.

166. Structural properties of self-organised organo-silicon macromolecular films investigated by scanning tunnelling microscopy and X-ray diffraction.
P. Miao, A. W. Robinson, R. E. Palmer, B. M. Kariuki, K. D. M. Harris.
Journal of Physical Chemistry B, **2000**, *104*, 1285–1291.
165. Definition of a "guiding function" in global optimization: a hybrid approach combining energy and R-factor in structure solution from powder diffraction data.
O. J. Lanning, S. Habershon, K. D. M. Harris, R. L. Johnston, B. M. Kariuki, E. Tedesco, G. W. Turner.
Chemical Physics Letters, **2000**, *317*, 296–303.
164. Temperature-dependent structural properties of a solid urea inclusion compound containing chiral guest molecules: 2-bromotetradecane/urea.
L. Yeo, K. D. M. Harris.
Canadian Journal of Chemistry, **1999**, *77*, 2105–2118.
163. Powder Solve – a complete package for crystal structure solution from powder diffraction patterns.
G. E. Engel, S. Wilke, O. König, K. D. M. Harris, F. J. J. Leusen.
Journal of Applied Crystallography, **1999**, *32*, 1169–1179.
162. Structural and diffraction properties of incommensurate solid inclusion compounds formed between α,ω -dihalogenoalkanes and tri-*ortho*-thymotide.
H. Serrano-González, K. D. M. Harris.
Journal of Solid State Chemistry, **1999**, *148*, 63–74.
161. A theoretical framework for the experimental determination of host-guest interaction energies in solid inclusion compounds.
K. D. M. Harris, P. E. Jupp, S.-O. Lee.
Journal of Chemical Physics, **1999**, *111*, 9784–9790.
160. Covalent self-assembly of a dimeric borazaaromatic macrocycle.
P. J. Comina, D. Philp, B. M. Kariuki, K. D. M. Harris.
Chemical Communications, **1999**, 2279–2280.
159. Spring-loading at the molecular level: relaxation of guest-induced strain in channel inclusion compounds.
M. D. Hollingsworth, U. Werner-Zwanziger, M. E. Brown, J. D. Chaney, J. C. Huffman, K. D. M. Harris, S. P. Smart.
Journal of the American Chemical Society, **1999**, *121*, 9732–9733.
158. Recognition-mediated facilitation of a disfavoured Diels-Alder reaction.
R. Bennes, D. Philp, N. Spencer, B. M. Kariuki, K. D. M. Harris.
Organic Letters, **1999**, *1*, 1087–1090.
157. An evolving technique for powder structure solution – fundamentals and applications of the genetic algorithm.
K. D. M. Harris, R. L. Johnston, B. M. Kariuki.
Anales de Química, International Edition, **1999**, *94*, 410–416.
156. 10 nm electron beam lithography using a triphenylene derivative as a negative/positive tone resist.
A. P. G. Robinson, R. E. Palmer, T. Tada, T. Kanayama, M. T. Allen, J. A. Preece, K. D. M. Harris.
Journal of Physics D: Applied Physics, **1999**, *32*, L75–L78.
155. Structure determination of a steroid directly from powder diffraction data.
B. M. Kariuki, K. Psallidas, K. D. M. Harris, R. L. Johnston, R. W. Lancaster, S. E. Staniforth, S. M. Cooper.
Chemical Communications, **1999**, 1677–1678.
154. Unravelling the disordered hydrogen bonding arrangement in solid triphenylmethanol.
H. Serrano-González, K. D. M. Harris, C. C. Wilson, A. E. Aliev, S. J. Kitchin, B. M. Kariuki, M. Bach-Vergés, C. Glidewell, E. J. MacLean, W. W. Kagunya.
Journal of Physical Chemistry B, **1999**, *103*, 6215–6223.
153. Controlling the crystal morphology of one-dimensional tunnel structures – induced crystallization of alkane/urea inclusion compounds as hexagonal flat plates.
S.-O. Lee, K. D. M. Harris.
Chemical Physics Letters, **1999**, *307*, 327–332.
152. The design of a molecularly selective capillary based on an incommensurate intergrowth structure.
A. A. Khan, S. T. Bramwell, K. D. M. Harris, B. M. Kariuki, M. R. Truter.
Chemical Physics Letters, **1999**, *307*, 320–326.

151. Structural and magnetic characterisation of the frustrated triangular lattice antiferromagnets CsFe(SO₄)₂ and RbFe(SO₄)₂.
H. Serrano-González, S. T. Bramwell, K. D. M. Harris, B. M. Kariuki, L. Nixon, I. P. Parkin, C. Ritter.
Physical Review B, **1999**, *59*, 14451–14460.
150. Effects of fluorination on the properties of organic pigments.
G. Chisholm, B. Hay, S. J. Kitchin, K. D. M. Harris, K. M. Morgan.
Dyes and Pigments, **1999**, *42*, 159–172.
149. Structural disorder in solid *p*-iodotoluene.
H. Serrano-González, K. D. M. Harris, S. J. Kitchin, A. Alvarez-Larena, E. Estop, X. Alcobé, E. Tauler, M. Labrador, D. C. Apperley.
Journal of Solid State Chemistry, **1999**, *143*, 285–295.
148. New approaches for solving crystal structures from powder diffraction data.
K. D. M. Harris.
Journal of the Chinese Chemical Society, **1999**, *46*, 23–34.
147. Towards a fundamental understanding of urea and thiourea inclusion compounds.
K. D. M. Harris.
Journal of the Chinese Chemical Society, **1999**, *46*, 5–22.
146. Evolving opportunities in structure solution from powder diffraction data – crystal structure determination of a molecular system with 12 variable torsion angles.
B. M. Kariuki, P. Calcagno, K. D. M. Harris, D. Philp, R. L. Johnston.
Angewandte Chemie, International Edition, **1999**, *38*, 831–835.
Angewandte Chemie, **1999**, *111*, 860–864.
145. A new approach for indexing powder diffraction data based on whole-profile fitting and global optimization using a genetic algorithm.
B. M. Kariuki, S. A. Belmonte, M. I. McMahon, R. L. Johnston, K. D. M. Harris, R. J. Nelmes.
Journal of Synchrotron Radiation, **1999**, *6*, 87–92.
144. Predictable solid state structures incorporating the C≡C–H···O₂N supramolecular synthon.
J. M. A. Robinson, D. Philp, B. M. Kariuki, K. D. M. Harris.
Chemical Communications, **1999**, 329–330.
143. Ring inversion of fluorocyclohexane in its solid thiourea inclusion compound.
R. K. Harris, A. Nordon, K. D. M. Harris.
Magnetic Resonance in Chemistry, **1999**, *37*, 15–24.
142. New light on an old story: the solid state transformation of ammonium cyanate into urea.
J. D. Dunitz, K. D. M. Harris, R. L. Johnston, B. M. Kariuki, E. J. MacLean, K. Psallidas, W. B. Schweizer, R. R. Tykwinski.
Journal of the American Chemical Society, **1998**, *120*, 13274–13275.
141. Application of a genetic algorithm in crystal structure determination from powder diffraction data.
B. M. Kariuki, R. L. Johnston, K. D. M. Harris, K. Psallidas, S. Ahn, H. Serrano-González.
Communications in Mathematical and Computer Chemistry (MATCH), **1998**, *38*, 123–135.
140. Precision in estimating the frequency separation between spectral lines.
P. E. Jupp, K. D. M. Harris, A. E. Aliev.
Journal of Magnetic Resonance, **1998**, *135*, 23–29.
139. Interchangeability of halogen and ethyne substituents in the solid state structures of di- and tri-substituted benzenes.
J. M. A. Robinson, B. M. Kariuki, K. D. M. Harris, D. Philp.
Journal of the Chemical Society, Perkin Transactions 2, **1998**, 2459–2469.
138. ²H NMR lineshape analysis using automated fitting procedures based on local and quasi-global optimization techniques.
A. E. Aliev, K. D. M. Harris.
Magnetic Resonance in Chemistry, **1998**, *36*, 855–868.
137. Magnetic structures of the triangular lattice magnets AFe(SO₄)₂ (A = K, Rb, Cs).
H. Serrano-González, S. T. Bramwell, K. D. M. Harris, B. M. Kariuki, L. Nixon, I. P. Parkin, C. Ritter.
Journal of Applied Physics, **1998**, *83*, 6314–6316.

136. Dynamic properties of dioctanoyl peroxide guest molecules constrained within the urea tunnel structure: a combined incoherent quasielastic neutron scattering and solid state ^2H nuclear magnetic resonance investigation. P. Girard, A. E. Aliev, F. Guillaume, K. D. M. Harris, M. D. Hollingsworth, A.-J. Dianoux, P. Jonsen. *Journal of Chemical Physics*, **1998**, *109*, 4078–4089.
135. The genetic algorithm: foundations and applications in structure solution from powder diffraction data. K. D. M. Harris, R. L. Johnston, B. M. Kariuki. *Acta Crystallographica, Section A*, **1998**, *54*, 632–645.
134. Molecular dynamics of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound: a combined MD-IQNS study. M. J. Jones, S. Camus, F. Guillaume, K. D. M. Harris, A.-J. Dianoux. *Physica B*, **1998**, *241–243*, 472–474.
133. Topotactic synthesis of α -zirconium phenylphosphonate from α -zirconium phosphate. G. B. Hix, S. J. Kitchin, K. D. M. Harris. *Journal of the Chemical Society, Dalton Transactions*, **1998**, 2315–2319.
132. New methodologies for solving crystal structures from powder diffraction data. K. D. M. Harris, B. M. Kariuki, M. Tremayne, R. L. Johnston. *Molecular Crystals and Liquid Crystals*, **1998**, *313*, 1–14.
131. A genetic algorithm for crystal structure solution from powder diffraction data. K. D. M. Harris, R. L. Johnston, B. M. Kariuki, M. Tremayne. *Journal of Chemical Research (S)*, **1998**, 390–391.
130. Crystal structure solution from powder diffraction data by the Monte Carlo method. K. D. M. Harris, B. M. Kariuki, M. Tremayne. *Materials Science Forum*, **1998**, *278–291*, 32–37.
129. Direct measurement of the distance between adjacent guest molecules in a disordered solid inclusion compound using solid-state ^{19}F - $\{^1\text{H}\}$ NMR spectroscopy. A. Nordon, E. Hughes, R. K. Harris, L. Yeo, K. D. M. Harris. *Chemical Physics Letters*, **1998**, *289*, 25–29.
128. Conformational properties of guest molecules in constrained solid state environments: bromine K-edge X-ray absorption spectroscopy of 2-bromoalkane/urea inclusion compounds. L. Elizabé, L. Yeo, K. D. M. Harris, G. Sankar, J. M. Thomas. *Chemistry of Materials*, **1998**, *10*, 1220–1226.
127. Crystal structure solution as an optimization problem: a genetic algorithm for direct space structure solution from powder diffraction data. R. L. Johnston, B. M. Kariuki, K. D. M. Harris. *Fashioning a Model: Optimization Methods in Chemical Physics* (Editors: A. Ernesti, J. M. Hutson, M. Meuwly, N. J. Wright), CCP6, Daresbury, **1998**, pp. 41–47.
126. A computational investigation of host-guest chiral recognition in incommensurate 2-bromoalkane/urea inclusion compounds. L. Yeo, K. D. M. Harris. *Journal of the Chemical Society, Faraday Transactions*, **1998**, *94*, 1633–1639.
125. Dynamic properties of the hydrogen bonding arrangement in solid triphenylmethanol: an investigation by solid state ^2H NMR spectroscopy. A. E. Aliev, E. J. MacLean, K. D. M. Harris, B. M. Kariuki, C. Glidewell. *Journal of Physical Chemistry B*, **1998**, *102*, 2165–2175.
124. Molecular dynamics of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound: an incoherent quasielastic neutron scattering investigation. M. J. Jones, F. Guillaume, K. D. M. Harris, A. E. Aliev, P. Girard, A.-J. Dianoux. *Molecular Physics*, **1998**, *93*, 545–554.
123. Synthesis of layered nickel phosphonate materials based on a topotactic approach. G. B. Hix, K. D. M. Harris. *Journal of Materials Chemistry*, **1998**, *8*, 579–584.

122. Non-ideality and ion association in aqueous electrolyte solutions, and a simple experimental approach for their investigation.
M. R. Wright, I. L. J. Patterson, K. D. M. Harris.
Journal of Chemical Education, **1998**, *75*, 352–357.
121. Crystal structure solution from neutron powder diffraction data by a new Monte Carlo approach incorporating restrained relaxation of the molecular geometry.
M. Tremayne, B. M. Kariuki, K. D. M. Harris, K. Shankland, K. S. Knight.
Journal of Applied Crystallography, **1997**, *30*, 968–974.
120. A triphenylphosphine oxide–water aggregate facilitates an exceptionally short C–H \cdots O hydrogen bond.
B. M. Kariuki, K. D. M. Harris, D. Philp, J. M. A. Robinson.
Journal of the American Chemical Society, **1997**, *119*, 12679–12680.
119. Preferential formation of C \equiv C–H $\cdots\pi$ (C \equiv C) interactions in the solid state.
J. M. A. Robinson, B. M. Kariuki, R. J. Gough, K. D. M. Harris, D. Philp.
Journal of Solid State Chemistry, **1997**, *134*, 203–206.
118. The application of a genetic algorithm for solving crystal structures from powder diffraction data.
B. M. Kariuki, H. Serrano-González, R. L. Johnston, K. D. M. Harris.
Chemical Physics Letters, **1997**, *280*, 189–195.
117. Structural properties of the low-temperature phase of the hexadecane/urea inclusion compound, investigated by synchrotron X-ray powder diffraction.
L. Yeo, B. M. Kariuki, H. Serrano-González, K. D. M. Harris.
Journal of Physical Chemistry B, **1997**, *101*, 9926–9931.
116. A new method for intercalation of basic guest molecules in the layered host material α -zirconium phosphate.
G. B. Hix, K. D. M. Harris.
European Journal of Inorganic and Solid State Chemistry, **1997**, *34*, 589–598.
115. Application of triple-channel ^{13}C – $\{^1\text{H}, ^{19}\text{F}\}$ NMR techniques to probe structural properties of disordered solids.
A. Nordon, R. K. Harris, L. Yeo, K. D. M. Harris.
Chemical Communications, **1997**, 2045–2046.
114. Topochemical rationalization of the solid state polymerization reaction of sodium chloroacetate: crystal structure determination from powder diffraction data by the Monte Carlo method.
L. Elizabé, B. M. Kariuki, K. D. M. Harris, M. Tremayne, M. Epple, J. M. Thomas.
Journal of Physical Chemistry B, **1997**, *101*, 8827–8831.
113. Definitive structural characterization of the conventional low-temperature host structure in urea inclusion compounds.
L. Yeo, K. D. M. Harris.
Acta Crystallographica, Section B, **1997**, *53*, 822–830.
112. The Meldola Lecture: understanding the properties of urea and thiourea inclusion compounds.
K. D. M. Harris.
Chemical Society Reviews, **1997**, *26*, 279–289.
111. *Ab initio* calculation of ^2H quadrupole coupling constants in molecular crystals: application to polymorphs of oxalic acid dihydrate.
S. Camus, K. D. M. Harris, R. L. Johnston.
Chemical Physics Letters, **1997**, *276*, 186–195.
110. Crystal engineering based on nitro derivatives of 10-hydroxy-10,9-borazarophenanthrene.
J. M. A. Robinson, B. M. Kariuki, D. Philp, K. D. M. Harris.
Tetrahedron Letters, **1997**, *38*, 6281–6284.
109. Interfacial science of solid host-guest systems.
K. D. M. Harris.
Interfacial Science: A "Chemistry for the 21st Century" Monograph (Editor: M. W. Roberts), International Union for Pure and Applied Chemistry, Blackwell Science, **1997**, pp. 21–55 (Chapter 2).
108. Mathematical analysis of the alignment of guest molecules in solid one-dimensional inclusion compounds: the design of materials for applications in non-linear optics.
K. D. M. Harris, P. E. Jupp.
Chemical Physics Letters, **1997**, *274*, 525–534.

107. Reorientational motions of dioctanoyl peroxide guest molecules within the urea tunnel structure: assessment of 2-site jump models.
P. Girard, A. E. Aliev, F. Guillaume, K. D. M. Harris, M. D. Hollingsworth, A.-J. Dianoux, P. Jonsen.
Physica B, **1997**, 234–236, 112–114.
106. Dynamic properties of cyclohexane guest molecules constrained within the zeolite H-ZSM-5 host structure: a wide-line solid state ^2H NMR investigation.
A. E. Aliev, K. D. M. Harris.
Journal of Physical Chemistry A, **1997**, 101, 4541–4547.
105. A new hydrogen bonding motif based on 10-hydroxy-10,9-borazaro-phenanthrene.
K. D. M. Harris, B. M. Kariuki, C. Lambropoulos, D. Philp, J. M. A. Robinson.
Tetrahedron, **1997**, 53, 8599–8612.
104. Fluorocyclohexane ring inversion in a thiourea inclusion compound, studied by solid state fluorine-19 NMR with high-power proton decoupling.
A. Nordon, R. K. Harris, L. Yeo, K. D. M. Harris.
Chemical Communications, **1997**, 961–962.
103. Temperature-dependent structural properties of the 1,10-decanedicarboxylic acid/urea inclusion compound.
L. Yeo, K. D. M. Harris, F. Guillaume.
Journal of Solid State Chemistry, **1997**, 128, 273–281.
102. Structure determination of a complex organic solid from X-ray powder diffraction data by a generalized Monte Carlo method: the crystal structure of red fluorescein.
M. Tremayne, B. M. Kariuki, K. D. M. Harris.
Angewandte Chemie, International Edition in English, **1997**, 36, 770–772.
Angewandte Chemie, **1997**, 109, 788–791.
101. Stochastic models for guest-guest interactions in one-dimensional inclusion compounds.
K. D. M. Harris, P. E. Jupp.
Proceedings of the Royal Society A, **1997**, 453, 333–352.
100. A computational investigation of the dynamics of urea molecules in solids.
S. Camus, K. D. M. Harris, S. L. Price.
Molecular Simulation, **1996**, 18, 303–323.
99. Crystal structure determination from powder diffraction data.
K. D. M. Harris, M. Tremayne.
Chemistry of Materials, **1996**, 8, 2554–2570.
98. How strong is a π -facial hydrogen bond ?
H. Adams, K. D. M. Harris, G. A. Hembury, C. A. Hunter, D. Livingstone, J. F. McCabe.
Chemical Communications, **1996**, 2531–2532.
97. Urea, thiourea and selenourea inclusion compounds.
M. D. Hollingsworth, K. D. M. Harris.
Comprehensive Supramolecular Chemistry, Volume 6 (Solid-State Supramolecular Chemistry: Crystal Engineering), (Editors: D. D. MacNicol, F. Toda, R. Bishop), Elsevier, Oxford, **1996**, pp. 177–237 (Chapter 7).
96. Solution of an organic crystal structure from X-ray powder diffraction data by a generalized Monte Carlo method: crystal structure determination of 1-methylfluorene.
M. Tremayne, B. M. Kariuki, K. D. M. Harris.
Journal of Materials Chemistry, **1996**, 6, 1601–1604.
95. Chiral recognition in incommensurate one-dimensional inclusion compounds: a computational investigation.
L. Yeo, K. D. M. Harris.
Tetrahedron: Asymmetry, **1996**, 7, 1891–1894.
94. Structural and dynamic properties of the 1,10-dibromodecane/urea inclusion compound, investigated by variable-temperature powder X-ray diffraction, solid-state ^2H NMR lineshape analysis and solid-state ^2H NMR spin-lattice relaxation time measurements.
A. E. Aliev, S. P. Smart, I. J. Shannon, K. D. M. Harris.
Journal of the Chemical Society, Faraday Transactions, **1996**, 92, 2179–2185.

93. The development of Monte Carlo methods for crystal structure solution from powder diffraction data: simultaneous translation and rotation of a structural fragment within the unit cell.
M. Tremayne, B. M. Kariuki, K. D. M. Harris.
Journal of Applied Crystallography, **1996**, *29*, 211–214.
92. Application of EXAFS spectroscopy to probe structural properties of solid inclusion compounds containing halogenoalkane guest molecules within the *catena*-[(1,2-diaminopropane)cadmium(II) tetra- μ -cyanonickelate(II)] host structure.
M. J. Jones, K. D. M. Harris, G. Sankar, T. Maschmeyer, J. M. Thomas.
Journal of the Chemical Society, Faraday Transactions, **1996**, *92*, 1043–1050.
91. Molecular dynamics of tetrakis(trimethylsilyl)silane in the solid state: an incoherent quasielastic neutron scattering investigation.
M. J. Jones, F. Guillaume, K. D. M. Harris, A.-J. Dianoux.
Proceedings of the Royal Society A, **1996**, *452*, 701–714.
90. Superspace group descriptions of the symmetries of incommensurate urea inclusion compounds.
S. van Smaalen, K. D. M. Harris.
Proceedings of the Royal Society A, **1996**, *452*, 677–700.
89. Crystal structure solution from powder X-ray diffraction data: the development of Monte Carlo methods to solve the crystal structure of the γ phase of 3-chloro-*trans*-cinnamic acid.
B. M. Kariuki, D. M. S. Zin, M. Tremayne, K. D. M. Harris.
Chemistry of Materials, **1996**, *8*, 565–569.
88. Structural and dynamic properties of urea and thiourea inclusion compounds.
K. D. M. Harris.
Journal of Molecular Structure, **1996**, *374*, 241–250.
87. The anhydrous alums as model triangular lattice magnets.
S. T. Bramwell, S. G. Carling, C. J. Harding, K. D. M. Harris, B. M. Kariuki, L. Nixon, I. P. Parkin.
Journal of Physics: Condensed Matter, **1996**, *8*, L123–L129.
86. Temperature-dependent structural properties of the chlorocyclohexane/thiourea inclusion compound investigated by synchrotron X-ray powder diffraction.
M. J. Jones, I. J. Shannon, K. D. M. Harris.
Journal of the Chemical Society, Faraday Transactions, **1996**, *92*, 273–279.
85. Characterization of gauche end-groups in α,ω -dibromoalkanes: vibrational properties of the 1,6-dibromohexane/urea inclusion compound.
L. Elizabe, S. P. Smart, A. El Baghdadi, F. Guillaume, K. D. M. Harris.
Journal of the Chemical Society, Faraday Transactions, **1996**, *92*, 267–272.
84. Crystallography of incommensurate intergrowth compounds.
S. van Smaalen, D. Schmicker, J. L. de Boer, C. Haas, K. D. M. Harris.
Aperiodic '94 (Editors: G. Chapuis, W. Paciorek), World Scientific, **1995**, pp. 102–111.
83. Phase transitions involving re-ordering of the guest molecules in a solid organic inclusion compound: heptanoic anhydride/urea.
I. J. Shannon, K. D. M. Harris, F. Guillaume, E. H. Bocanegra, E. J. MacLean.
Journal of the Chemical Society, Chemical Communications, **1995**, 2341–2342.
82. Surface structural properties of crystalline *s*-triazine: a computational investigation.
A. R. George, P. A. Schofield, K. D. M. Harris.
Molecular Simulation, **1995**, *15*, 65–78.
81. Second-order quadrupolar effects for directly bonded and remote ^{13}C – $^{79/81}\text{Br}$ spin pairs in high-resolution ^{13}C NMR spectra of solids.
A. E. Aliev, K. D. M. Harris, R. K. Harris, S. A. Carss, A. C. Olivieri.
Journal of the Chemical Society, Faraday Transactions, **1995**, *91*, 3167–3176.
80. The synthesis, structural characterization and Raman spectroscopy of the inorganic pigments lead tin yellow types I and II and lead antimonate yellow: their identification on medieval paintings and manuscripts.
R. J. H. Clark, L. Cridland, B. M. Kariuki, K. D. M. Harris, R. Withnall.
Journal of the Chemical Society, Dalton Transactions, **1995**, 2577–2582.

79. Solid state ^2H and ^{13}C NMR studies of hydrogen-bond dynamics in crystalline ferrocene-1,1'-diylbis(diphenylmethanol).
A. E. Aliev, K. D. M. Harris, I. J. Shannon, C. Glidewell, C. M. Zakaria, P. A. Schofield.
Journal of Physical Chemistry, **1995**, *99*, 12008–12015.
78. Representing and understanding geometric features of one-dimensional tunnel structures in solid inclusion compounds.
A. R. George, K. D. M. Harris.
Journal of Molecular Graphics, **1995**, *13*, 138–141.
77. Solid state ^2H NMR studies of guest molecular dynamics in the benzenetricarbonylchromium/thiourea inclusion compound.
A. E. Aliev, K. D. M. Harris, F. Guillaume.
Journal of Chemical Research (S), **1995**, 294–295.
76. Dynamics of benzene and pyridine guest molecules in their tri-*ortho*-thymotide inclusion compounds. Solid state ^2H NMR studies.
A. E. Aliev, K. D. M. Harris, A. Mahdyarfar.
Journal of the Chemical Society, Faraday Transactions, **1995**, *91*, 2017–2026.
75. Probing the conformational properties of guest molecules in solid inclusion compounds *via* EXAFS spectroscopy: bromine K-edge EXAFS studies of the bromocyclohexane/thiourea and *trans*-1-bromo-2-chlorocyclohexane/thiourea inclusion compounds.
I. J. Shannon, M. J. Jones, K. D. M. Harris, M. R. H. Siddiqui, R. W. Joyner.
Journal of the Chemical Society, Faraday Transactions, **1995**, *91*, 1497–1501.
74. Dynamics of the benzene moiety in crystalline benzenetricarbonylchromium: potential and limitations of ^2H NMR lineshape analysis and ^2H NMR spin-lattice relaxation time measurements.
A. E. Aliev, K. D. M. Harris, F. Guillaume.
Journal of Physical Chemistry, **1995**, *99*, 1156–1165.
73. Solid dynamics.
K. D. M. Harris, A. E. Aliev.
Chemistry in Britain, **1995**, *31*, 132–136.
72. Observation of the sliding mode in incommensurate intergrowth compounds: Brillouin scattering from the inclusion compound of urea and heptadecane.
D. Schmicker, S. van Smaalen, J. L. de Boer, C. Haas, K. D. M. Harris.
Physical Review Letters, **1995**, *74*, 734–737.
71. Computational investigation of surface structural relaxation in crystalline urea.
A. R. George, K. D. M. Harris, A. L. Rohl, D. H. Gay.
Journal of Materials Chemistry, **1995**, *5*, 133–140.
70. Carbon-halogen second-order quadrupolar and indirect spin-spin coupling effects in high-resolution solid state ^{13}C NMR spectra of halobenzenes.
A. E. Aliev, K. D. M. Harris, P. J. Barrie, S. Camus.
Journal of the Chemical Society, Faraday Transactions, **1994**, *90*, 3729–3730.
69. Probing chemical transformations in organic solids *via* NMR techniques: the solid state photodimerization reaction of 7-methoxy-4-methylcoumarin.
S. G. Stitchell, K. D. M. Harris, A. E. Aliev.
Structural Chemistry, **1994**, *5*, 327–333.
68. Solid-state ^{13}C nuclear magnetic resonance investigations of molecular dynamics in crystalline benzenetricarbonylchromium.
A. E. Aliev, K. D. M. Harris, F. Guillaume, P. J. Barrie.
Journal of the Chemical Society, Dalton Transactions, **1994**, 3193–3195.
67. Properties of the guest molecules in the 1,10-dibromodecane/urea inclusion compound: a molecular dynamics simulation study.
A. R. George, K. D. M. Harris.
Journal of Materials Chemistry, **1994**, *4*, 1731–1735.
66. Natural abundance high-resolution solid state ^2H NMR spectroscopy.
A. E. Aliev, K. D. M. Harris, D. C. Apperley.
Chemical Physics Letters, **1994**, *226*, 193–198.

65. Structural and dynamic properties of hydrogen bonding in a tetrahedral arrangement of methanol molecules. A theoretical investigation.
E. J. MacLean, K. D. M. Harris, S. L. Price.
Chemical Physics Letters, **1994**, 225, 273–279.
64. Physico-chemical properties of solid one-dimensional inclusion compounds.
K. D. M. Harris.
Materials Science Forum, **1994**, 152–153, 155–162.
63. Simple technique for temperature calibration of a MAS probe for solid-state NMR spectroscopy.
A. E. Aliev, K. D. M. Harris.
Magnetic Resonance in Chemistry, **1994**, 32, 366–369.
62. The rôle of powder diffraction in establishing structure-property relationships for crystalline solids: a new structural assignment of the photoreactive and photostable phases of *p*-formyl-*trans*-cinnamic acid.
K. D. M. Harris, I. L. J. Patterson.
Journal of the Chemical Society, Perkin Transactions 2, **1994**, 1201–1203.
61. Solid state dynamic properties of tetrakis(trimethylsilyl)methane: high-resolution solid state ^{13}C and ^{29}Si NMR investigations.
A. E. Aliev, K. D. M. Harris, D. C. Apperley, R. K. Harris.
Journal of Solid State Chemistry, **1994**, 110, 314–320.
60. Elastic constants of the dioctanoyl peroxide/urea inclusion compound determined by Brillouin scattering.
D. Schmicker, S. van Smaalen, C. Haas, K. D. M. Harris.
Physical Review B, **1994**, 49, 11572–11579.
59. Conformational properties of monosubstituted cyclohexane guest molecules constrained within zeolitic host materials: a multinuclear solid state NMR investigation.
A. E. Aliev, K. D. M. Harris, R. C. Mordi.
Journal of the Chemical Society, Faraday Transactions, **1994**, 90, 1323–1328.
58. Conformational and vibrational properties of α,ω -dihalogenoalkane/urea inclusion compounds: Raman scattering investigations.
S. P. Smart, A. El Baghdadi, F. Guillaume, K. D. M. Harris.
Journal of the Chemical Society, Faraday Transactions, **1994**, 90, 1313–1322.
57. Temperature dependent structural properties of *p*-diiodobenzene: neutron diffraction and high-resolution solid state ^{13}C NMR investigations.
X. Alcobé, E. Estop, A. E. Aliev, K. D. M. Harris, J. Rodriguez-Carvajal, J. Rius.
Journal of Solid State Chemistry, **1994**, 110, 20–27.
56. Crystal structure determination from powder diffraction data by Monte Carlo methods.
K. D. M. Harris, M. Tremayne, P. Lightfoot, P. G. Bruce.
Journal of the American Chemical Society, **1994**, 116, 3543–3547.
55. Zig-zag channels in the structure of sebaconitrile/urea.
M. D. Hollingsworth, B. D. Santarsiero, K. D. M. Harris.
Angewandte Chemie, International Edition in English, **1994**, 33, 649–652.
Angewandte Chemie, **1994**, 106, 698–701.
54. Neutron scattering investigations of guest molecular dynamics in α,ω -dibromoalkane/urea inclusion compounds.
F. Guillaume, S. P. Smart, K. D. M. Harris, A. J. Dianoux.
Journal of Physics: Condensed Matter, **1994**, 6, 2169–2184.
53. Solid state NMR.
K. D. M. Harris, A. E. Aliev.
Nuclear Magnetic Resonance, **1994**, 23, 206–244.
52. Dynamic properties of the urea molecules in α,ω -dibromoalkane/urea inclusion compounds investigated by ^2H NMR spectroscopy.
A. E. Aliev, S. P. Smart, K. D. M. Harris.
Journal of Materials Chemistry, **1994**, 4, 35–39.
51. Aspects of the characterization of cloverite by solid-state n.m.r. techniques.
B. Zibrowius, M. W. Anderson, W. Schmidt, F.-F. Schüth, A. E. Aliev, K. D. M. Harris.
Zeolites, **1993**, 13, 607–610.

50. Structural and dynamic properties of the C₆₀/*n*-pentane inclusion compound: solid state ¹³C NMR investigations. A. E. Aliev, K. D. M. Harris, M. Tegze, S. Pekker. *Journal of Materials Chemistry*, **1993**, 3, 1091–1094.
49. Structural properties of urea inclusion compounds containing carboxylic acid anhydride guest molecules: anomalous modes of guest-molecule ordering. I. J. Shannon, N. M. Stainton, K. D. M. Harris. *Journal of Materials Chemistry*, **1993**, 3, 1085–1090.
48. Dynamic properties of *p*-diiodobenzene investigated by solid state ²H and ¹³C NMR spectroscopy. A. E. Aliev, K. D. M. Harris, X. Alcobé, E. Estop. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 3797–3800.
47. (¹³C, ²H) residual dipolar interaction and spin-spin coupling effects in high-resolution ¹³C NMR spectra of solids. A. E. Aliev, K. D. M. Harris, D. C. Apperley, R. K. Harris, M. M. Sünnetçioğlu. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 3791–3796.
46. Investigating the structure and dynamics of a family of organic solids: the alkane/urea inclusion compounds. K. D. M. Harris. *Journal of Solid State Chemistry*, **1993**, 106, 83–98.
45. Natural abundance solid state ²H NMR studies of phase transitions in rotator phase solids. A. E. Aliev, K. D. M. Harris. *Mendeleev Communications*, **1993**, 153–155.
44. Crystal engineering of hydrogen-bonded co-crystals between cyanuric acid and "diamide" molecules. Investigations on the formation and structure of hydrogen-bonded co-crystals containing cyanuric acid and oxalyl dihydrazide. K. D. M. Harris, N. M. Stainton, A. M. Callan, R. A. Howie. *Journal of Materials Chemistry*, **1993**, 3, 947–952.
43. Investigation and rationalization of hydrogen bonding patterns in sulfonyl amino compounds and related materials: crystal structure determination of microcrystalline solids from powder X-ray diffraction data. P. Lightfoot, M. Tremayne, C. Glidewell, K. D. M. Harris, P. G. Bruce. *Journal of the Chemical Society, Perkin Transactions 2*, **1993**, 1625–1630.
42. Unusual conformational behaviour in the chlorocyclohexane/thiourea inclusion compound: a theoretical rationalization. P. A. Schofield, K. D. M. Harris, I. J. Shannon, A. J. O. Rennie. *Journal of the Chemical Society, Chemical Communications*, **1993**, 1293–1295.
41. EXAFS spectroscopic studies of the bromine environment in the crystalline inclusion compounds formed between urea and α,ω -dibromoalkanes. I. J. Shannon, K. D. M. Harris, A. Mahdyarfar, P. Johnston, R. W. Joyner. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 3099–3104.
40. Conformational properties of monosubstituted cyclohexanes in their thiourea inclusion compounds and in solution: variable temperature one-dimensional and two-dimensional ¹³C NMR investigations. A. E. Aliev, K. D. M. Harris. *Journal of the American Chemical Society*, **1993**, 115, 6369–6377.
39. Ab initio determination of molecular crystal structures using powder diffraction data from a laboratory X-ray source. P. Lightfoot, M. Tremayne, K. D. M. Harris, C. Glidewell, K. Shankland, C. J. Gilmore, P. G. Bruce. *Materials Science Forum*, **1993**, 133–136, 207–212.
38. Theoretical prediction of the guest periodicity of alkane/urea inclusion compounds. I. J. Shannon, K. D. M. Harris, A. J. O. Rennie, M. B. Webster. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 2023–2029.
37. Predicting X-ray diffraction intensity distributions for one-dimensional inclusion compounds via local density functional calculations. K. D. M. Harris, A. R. George, J. M. Thomas. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 2017–2021.
36. Solid state NMR. K. D. M. Harris. *Nuclear Magnetic Resonance*, **1993**, 22, 230–260.

35. A ^{13}C CP/MAS NMR study of a double *tert*-butyl group rotation in the solid state using $T_{1\rho}$ and line shape measurements.
F. G. Riddell, S. Arumugam, K. D. M. Harris, M. Rogerson, J. H. Strange.
Journal of the American Chemical Society, **1993**, *115*, 1881–1885.
34. High-resolution solid state ^{13}C and ^{29}Si NMR investigations of the dynamic properties of tetrakis(trimethylsilyl)silane.
A. E. Aliev, K. D. M. Harris, D. C. Apperley.
Journal of the Chemical Society, Chemical Communications, **1993**, 251–253.
33. Molecular confinement.
K. D. M. Harris.
Chemistry in Britain, **1993**, *29*, 132–136.
32. Evidence for migration of guest molecules into the tunnel structure of urea inclusion compounds.
A. Mahdyarfar, K. D. M. Harris.
Journal of the Chemical Society, Chemical Communications, **1993**, 51–53.
31. $^{37}\text{Cl}/^{35}\text{Cl}$ isotope effects in ^{13}C NMR spectroscopy of chlorohydrocarbons.
A. E. Aliev, K. D. M. Harris.
Magnetic Resonance in Chemistry, **1993**, *31*, 54–57.
30. Variation of ^{13}C NMR linewidths of metallocenes as a function of magic angle sample spinning frequency.
I. J. Shannon, K. D. M. Harris, S. Arumugam.
Bulletin of Magnetic Resonance, **1992**, *14*, 273–277.
29. Application of the combined maximum entropy and likelihood method to the *ab initio* determination of an organic crystal structure from X-ray powder diffraction data.
M. Tremayne, P. Lightfoot, C. Glidewell, K. D. M. Harris, K. Shankland, C. J. Gilmore, G. Bricogne, P. G. Bruce.
Journal of Materials Chemistry, **1992**, *2*, 1301–1302.
28. *Ab initio* structure determination of LiCF_3SO_3 from X-ray powder diffraction data using entropy maximization and likelihood ranking.
M. Tremayne, P. Lightfoot, M. A. Mehta, P. G. Bruce, K. D. M. Harris, K. Shankland, C. J. Gilmore, G. Bricogne.
Journal of Solid State Chemistry, **1992**, *100*, 191–196.
27. High-resolution solid state ^{13}C NMR studies of ferrocene as a function of magic angle sample spinning frequency.
I. J. Shannon, K. D. M. Harris, S. Arumugam.
Chemical Physics Letters, **1992**, *196*, 588–596.
26. Neutron scattering investigation of host molecular motion in the hexadecane/urea inclusion compound.
K. D. M. Harris, F. Guillaume, S. P. Smart, C. Sourisseau, A. J. Dianoux.
Journal of Chemical Research (S), **1992**, 276–277.
25. Dynamic properties of α,ω -dibromoalkane guest molecules constrained within urea inclusion compounds: a neutron scattering study.
S. P. Smart, F. Guillaume, K. D. M. Harris, C. Sourisseau, A. J. Dianoux.
Physica B, **1992**, *180&181*, 687–690.
24. Determination of a molecular crystal structure by X-ray powder diffraction on a conventional laboratory instrument.
P. Lightfoot, M. Tremayne, K. D. M. Harris, P. G. Bruce.
Journal of the Chemical Society, Chemical Communications, **1992**, 1012–1013.
23. Probing hydrogen-bonding patterns in co-crystals of amides and triarylphosphine oxides using high-resolution solid state ^{31}P NMR spectroscopy.
S. Arumugam, C. Glidewell, K. D. M. Harris.
Journal of the Chemical Society, Chemical Communications, **1992**, 724–726.
22. A quantitative analysis of guest periodicity in one-dimensional inclusion compounds.
A. J. O. Rennie, K. D. M. Harris.
Journal of Chemical Physics, **1992**, *96*, 7117–7124.
21. The structural response of the host framework following removal of the guest molecules from a urea inclusion compound: a Monte Carlo simulation study.
K. D. M. Harris.
Journal of Physics and Chemistry of Solids, **1992**, *53*, 529–537.

20. Raman spectroscopic studies of urea inclusion compounds containing α,ω -dibromoalkane guests.
S. P. Smart, K. D. M. Harris, F. Guillaume, A. El Baghdadi.
Molecular Crystals and Liquid Crystals, **1992**, 211, 157–166.
19. Is the guest periodicity of $\text{CH}_3(\text{CH}_2)_n\text{CH}_3$ /urea inclusion compounds linearly dependent on n ? A mathematical analysis.
A. J. O. Rennie, K. D. M. Harris.
Chemical Physics Letters, **1992**, 188, 1–4.
18. The cyanuric acid/biuret co-crystal: a new type of hydrogen-bonded system formed between a molecule and its solution-phase decomposition product.
N. M. Stainton, K. D. M. Harris, R. A. Howie.
Journal of the Chemical Society, Chemical Communications, **1991**, 1781–1784.
17. Structural properties of α,ω -dibromoalkane/urea inclusion compounds: a new type of interchannel guest molecule ordering.
K. D. M. Harris, S. P. Smart, M. D. Hollingsworth.
Journal of the Chemical Society, Faraday Transactions, **1991**, 87, 3423–3429.
16. Probing polymorphism and reactivity in the organic solid state using ^{13}C NMR spectroscopy: studies of *p*-formyl-*trans*-cinnamic acid.
K. D. M. Harris, J. M. Thomas.
Journal of Solid State Chemistry, **1991**, 94, 197–205.
15. Mathematical analysis of intra-stack dimerizations in reactive crystalline solids.
K. D. M. Harris, J. M. Thomas, D. Williams.
Journal of the Chemical Society, Faraday Transactions, **1991**, 87, 325–331.
14. Structural properties of the guest species in diacyl peroxide/urea inclusion compounds: an X-ray diffraction investigation.
K. D. M. Harris, M. D. Hollingsworth.
Proceedings of the Royal Society A, **1990**, 431, 245–269.
13. Probing the properties of urea inclusion compounds.
K. D. M. Harris, J. M. Thomas.
Molecular Crystals and Liquid Crystals, **1990**, 186, 177–184.
12. Powder X-ray diffraction studies of a low-temperature phase transition in the *n*-hexadecane/urea inclusion compound.
K. D. M. Harris, I. Gameson, J. M. Thomas.
Journal of the Chemical Society, Faraday Transactions, **1990**, 86, 3135–3143.
11. A mathematical model of one-dimensional inclusion compounds: a new approach towards understanding commensurate and incommensurate behaviour.
A. J. O. Rennie, K. D. M. Harris.
Proceedings of the Royal Society A, **1990**, 430, 615–640.
10. Structural aspects of urea inclusion compounds and their investigation by X-ray diffraction: a general discussion.
K. D. M. Harris, J. M. Thomas.
Journal of the Chemical Society, Faraday Transactions, **1990**, 86, 2985–2996.
9. Structural aspects of the chlorocyclohexane/thiourea inclusion system.
K. D. M. Harris, J. M. Thomas.
Journal of the Chemical Society, Faraday Transactions, **1990**, 86, 1095–1101.
8. Investigation of a time-dependent 'non-discrete' component of X-ray scattering from monohalocyclohexane/thiourea inclusion compounds.
K. D. M. Harris.
Journal of Solid State Chemistry, **1990**, 84, 280–288.
7. New families of catalysts for the selective oxidation of methane.
J. M. Thomas, W. Ueda, J. Williams, K. D. M. Harris.
Faraday Discussions of the Chemical Society, **1989**, 87, 33–45.
6. Organic crystals: Losing symmetry by design.
K. D. M. Harris, M. D. Hollingsworth.
Nature, **1989**, 341, 19.

5. ^2H NMR investigation of the dynamic behaviour of *n*-hexadecane in its urea inclusion compound.
K. D. M. Harris, P. Jonsen.
Chemical Physics Letters, **1989**, *154*, 593–598.
4. $\text{Cs}_2\text{Bi}_{10}\text{Ca}_6\text{Cl}_{12}\text{O}_{16}$: a new type of catalyst for selective oxidation derived from bismuth oxychloride.
K. D. M. Harris, W. Ueda, J. M. Thomas, G. W. Smith.
Angewandte Chemie, International Edition in English, **1988**, *27*, 1364–1365.
Angewandte Chemie, **1988**, *100*, 1415–1416.
3. Organic molecules in constrained environments.
J. M. Thomas, K. D. M. Harris.
Organic Solid State Chemistry (Editor: G. R. Desiraju), Elsevier, **1987**, pp. 179–206 (Chapter 6).
2. ESR and X-ray diffraction studies of diacyl peroxides in urea and aluminosilicate hosts.
M. D. Hollingsworth, K. D. M. Harris, W. Jones, J. M. Thomas.
Journal of Inclusion Phenomena, **1987**, *5*, 273–277.
1. A comparison between "mixed phase electrode" and percolation models for composite electrodes in solid state cells.
K. D. M. Harris, M. D. Rogers, C. A. Vincent.
Solid State Ionics, **1986**, *18&19*, 833–837.

Books

2. *The Selected Papers of Sir John Meurig Thomas*.
J. M. Thomas, K. D. M. Harris (Editors).
World Scientific Publishing Europe Ltd., London, **2017**.
1. *Turning Points in Solid-State, Materials and Surface Science*.
K. D. M. Harris, P. P. Edwards (Editors).
Royal Society of Chemistry, Cambridge, **2008**.