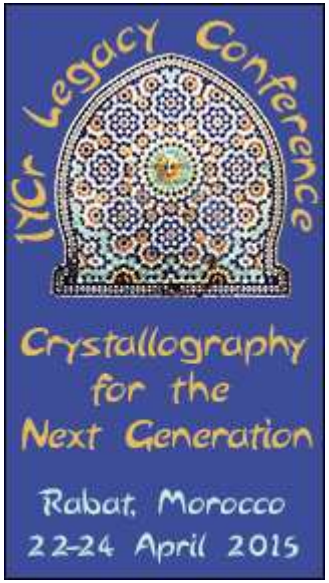


Crystallographic education and research in the developing world: Experiences in DR Congo

Juliette Pradon and Colin Groom

Cambridge Crystallographic Data Centre

The Cambridge Crystallographic Data Centre

International Data Repository
Archive of crystal structure data
High quality scientific database

Scientific Software Provider
Search/analysis/visualisation tools
Scientific applications

Collaborative Research Organisation
New methodologies
Fundamental research

Around 60 permanent staff

Cambridge UK and Rutgers NJ
Scientific editors
Software developers
Applications scientists

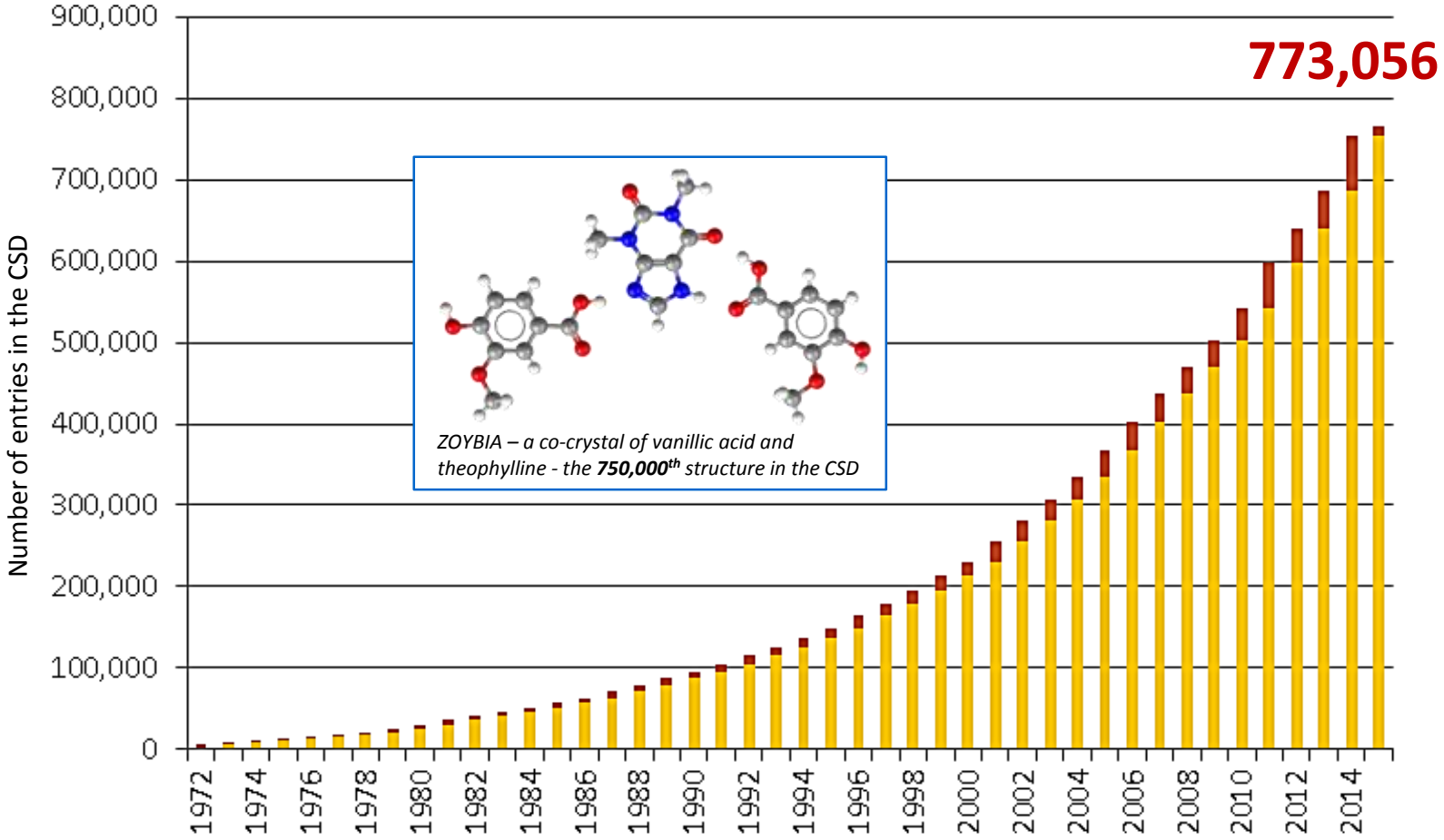
Established in 1965, UK Registered Charity

Community funded and governed

Financially self-supporting, not-for-profit

University Partner Institute

The Cambridge Structural Database



CSD Growth 1970-2015

Sharing crystal structures

- Cambridge Structural Database
  - Web access from 169 countries
  - System installed in 80 countries
  - Over 1,500 institutions
- Performing and supporting fundamental research
  - 60 PhD students helped since 1991
  - Over 700 publications

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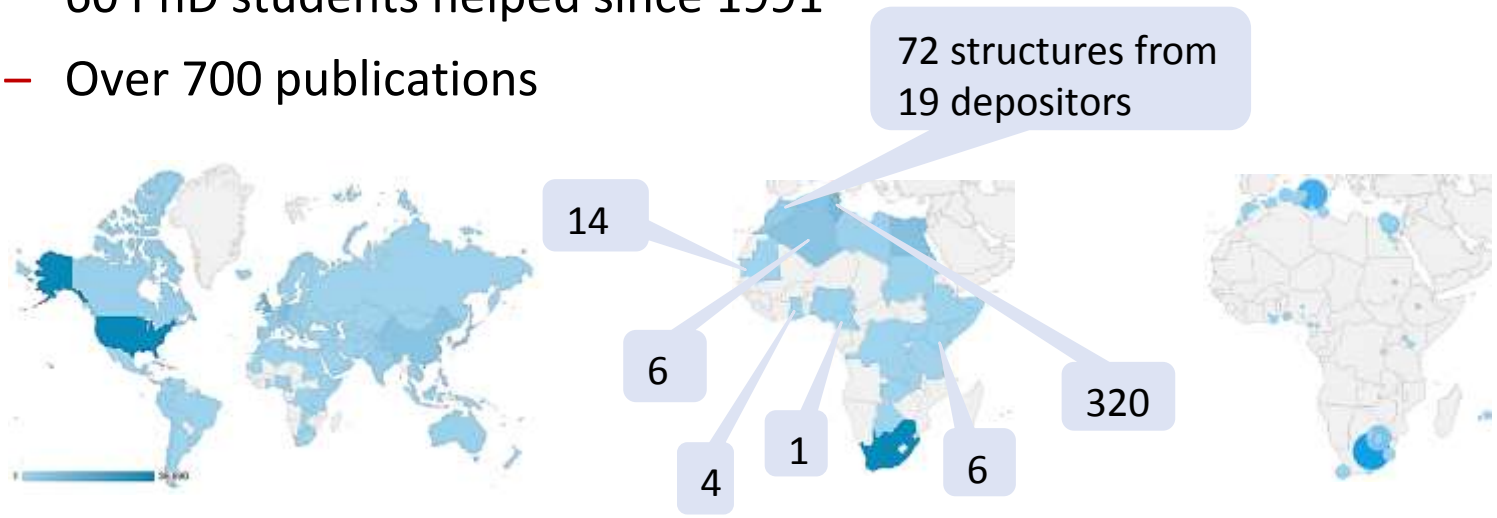


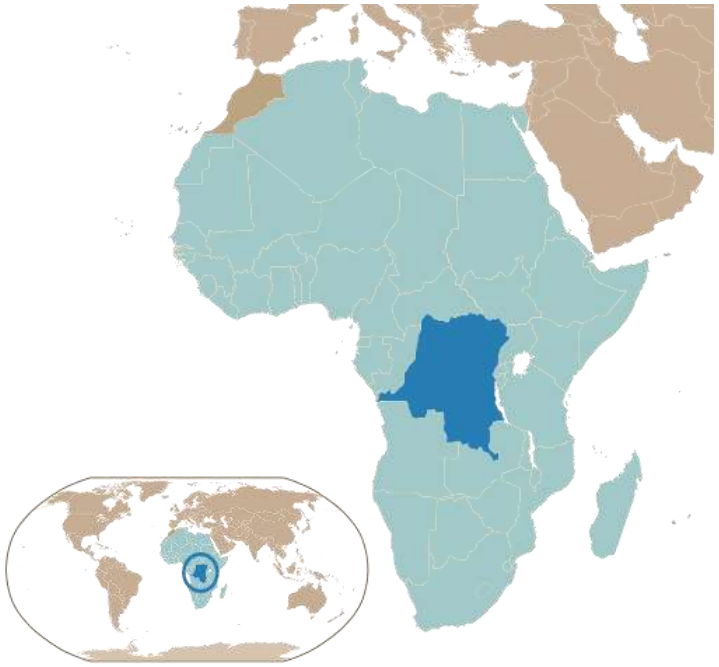
Crystal structures in chemistry education

- Experimental
  - error and statistical variation provides an opportunity to deal with the uncertainties of chemistry
- 3D Conformation, stereochemistry, chirality, metal coordination, molecular symmetry, molecular interactions (such as H-bonds, aromatic interactions, lone pairs), molecular arrays…
- Used to teach chemistry not just crystallography
  - Subsets of structures available (733/770,000)
- Essential resource in US institutions
  - Recommended by American Chemical Society

"Because basic 3D spatial relationships in molecules have systematic and profound causal significance, chemistry is an extraordinary fertile field for visual learning"

Williamson, V. M. *J. Chem. Educ*. (2008) 85, 718-723 Wu, H. K. *Sci. Educ. Res. Pract*. (2004) 8, 61-72
Bodner, G. M. *The Chemical Educator (*1997), 2 2001 NSF Workshop: Molecular Visualisation in Science Education

The Democratic Republic of Congo



- 2nd largest African country
- 2nd largest rainforest in the world, most biodiversity in Africa
- Population over 75 million
- 186 out of 187 countries in the UN's Human Development Index
- 176 out of 178 countries according to Failed State Index

Why crystallography in the DRC?

- Stable university structure in Kinshasa
- Blessed with natural resources
  - Mineral ores
  - Natural products

- Both require crystallographic and structural chemistry expertise to fully exploit

The University of Kinshasa

- First Congolese university, established in 1954, as University of Lovanium
  - affiliated with the University of Leuven in Belgium
- 1971 cut ties with Belgium universities
- 1981 became

- Very limited government budget attributed to the university, over 90% of resources come from university fees charged to students
- Currently:
  - over 24,000 students
  - 2,137 academic and research staff (including 868 PhD qualified professors)
  - 10 faculties
  - 1 nuclear reactor (on standby).

Initial involvement of the CCDC

- 2007: Professor Zéphirin G. Yav (Chemistry Department, UNIKIN, D.R.C
    - Ongoing collaboration Luc van Meervelt (K. U. Leuven, Belgium).
    - Science Training Laboratory project - “Using New Information and Communication Technologies”.
- Achievements:
    - Use of ICT for science teaching and learning as part curriculum in the Science Faculty of Kinshasa University and of two secondary schools in Kinshasa.
    - Development of a website for sharing knowledge in computer use and ICT-based science teaching and learning: www.education-africa.com

BRITISH COUNCIL

DelPHE

Member of:

the humanitarian centre

Collaboration between CCDC & University of Kinshasa to 2013

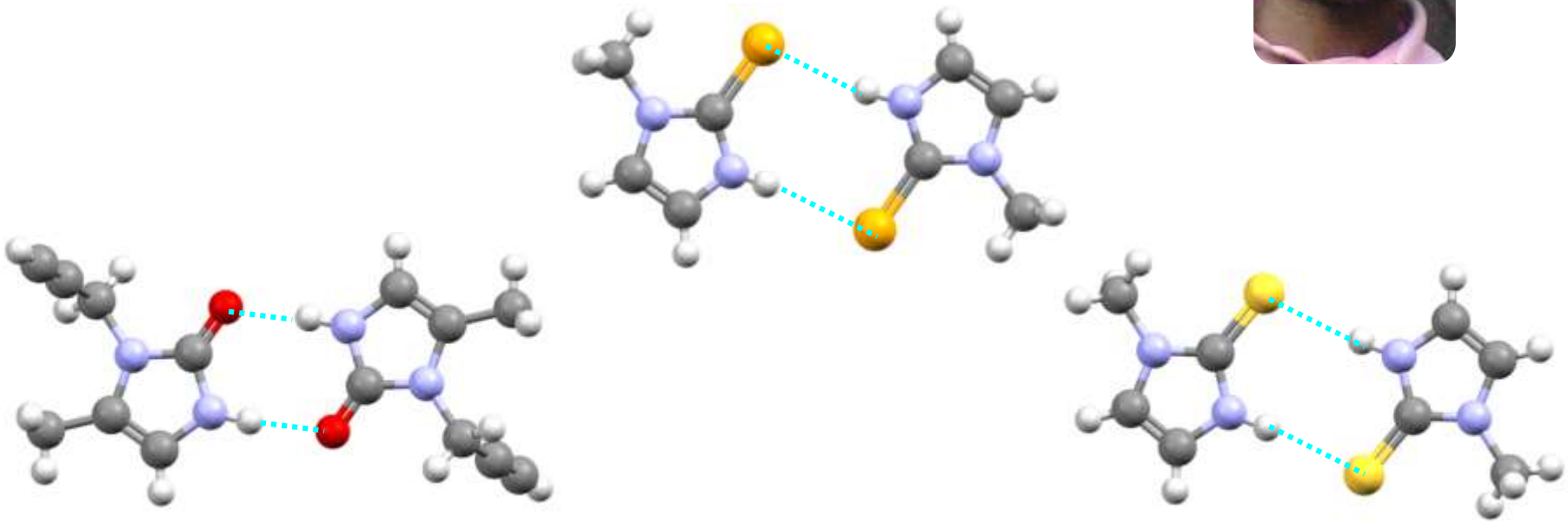
- CCDC seminars and workshops at University of Kinshasa
  - Cambridge Structural Database for both research and teaching purposes
  - Electronic structure theory workshop
  - Drug discovery course
- Attendees: academic and research staff of the Chemistry Department of the University of Kinshasa

- Established the CCDC Scholarship Program in Kinshasa
  - 1 MSc student in Kinshasa
  - 1 PhD student in Kinshasa
  - Visits to CCDC for research
    - Students co-supervised by CCDC scientists
    - Attendance at overseas schools and conferences
- Sabbatical visits of other DRC university scientists to CCDC
- Annual visits of CCDC staff to Kinshasa
  - Workshops, training and lectures
- Scholarship Program to continue

Challenges (for everyone!)

The CCDC Scholarship Program in Kinshasa: The First MSc student

- Albert Lundemba Singa:
  - 2nd (final) year MSc student
  - MSc research project: The interaction geometries and energies of selenium



Albert's results

- Sigma hole interaction energies of divalent Se interacting with the N of HCN or NH_3, compared to those involving S – calculated at B3PW91/6-311++G(3df,2p) and MP2-FC/6-311++G(3df,2p)

σ-hole interaction energy (kcal/mol)	B3PW91	MP2-FC
H_3N--Se(F)F	-13.18 -13.2*	-12.24 -12.2*
H_3N--Se(Cl)Cl	-9.42	-8.61
H_3N--Se(Br)Br	-8.12	-7.68
H_3N--S(F)F	-8.47 -8.4*	-7.77 -7.7*
H_3N--S(Cl)Cl	-6.26	-5.86
H_3N--S(Br)Br	-5.36	

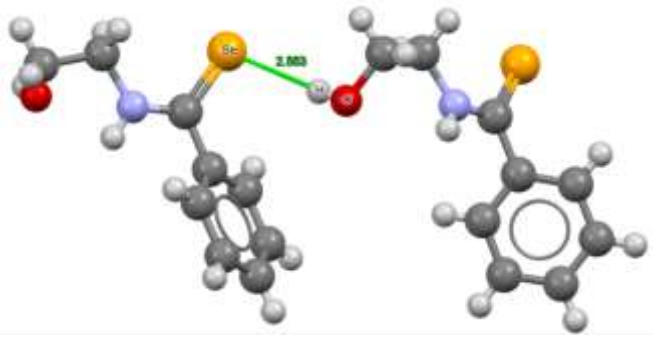
σ-hole interaction energy (kcal/mol)	B3PW91	MP2-FC
HCN--Se(F)F	-4.69 -4.7*	-6.46 -6.4*
HCN---Se(Cl)Cl	-2.84	-5.12
HCN---Se(Br)Br	-2.15	-4.43
HCN--S(F)F	-2.40	-4.43
HCN--S(Cl)Cl	-1.69	-4.07
HCN---S(Br)Br	-1.44	-3.55

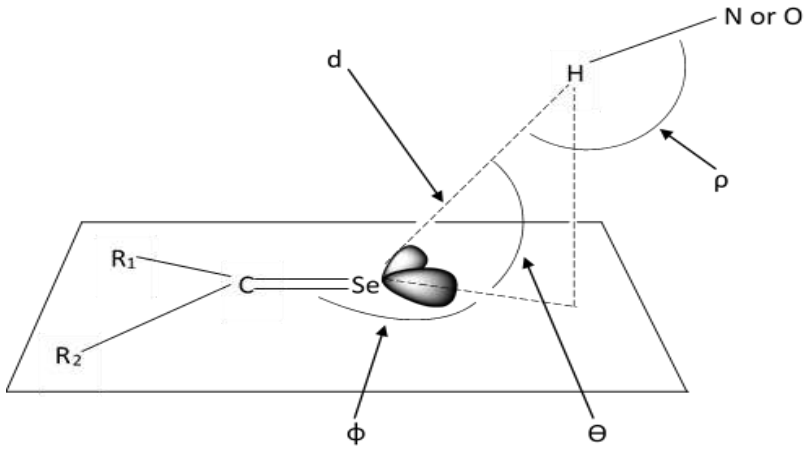
* Indicates literature value

Publication In preparation

The CCDC Student Scholarship Program in Kinshasa: The First PhD student

- Didi Bibelayi Dikima:
  - PhD student now in his second year
  - Research project: The use of the CSD and QM calculations to investigate sigma-hole and hydrogen-bond interactions made by selenium

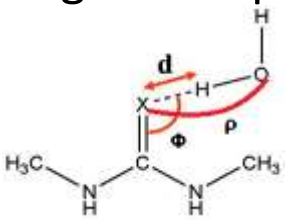




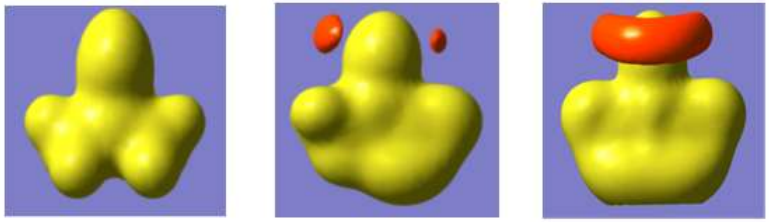
Didi's results

- Analysed H-bonding at monovalent selenium in X_2-C=Se systems found in crystal structures in the CSD
- Calculated B3LYP/6-311++G(3df,2p) H-bond interaction energies and partial charge on the acceptor for $NH(CH_3)$ $NH(CH_3)C=X\cdots H–O$

X	E_t (kJ/mol)	d (Å)	Φ (°)	Partial charge
O	-28.49	1.87	137	-0.763
S	-21.54	2.41	101	-0.443
Se	-21.33	2.50	95	-0.414



- Calculated HF/6-311++G(3df,2p) MEPs for selone, selenoamide & selenourea



$(CH_3)(CH_3)–C=Se$ $(NH_2)(CH_3)–C=Se$ $(NH_2)(NH_2)–C=Se$

- Also:
  - Undertaken his first two research periods at the CCDC
  - Applied for admission to the European School of Quantum Chemistry

- Ongoing CCDC Scholarship Program in Kinshasa established
  - Demonstrated success of advanced structural chemistry research in DRC
- Structural chemistry training now part of the undergraduate curriculum at the University of Kinshasa
  - “Training the trainers” achieved
- Valuable experience for DRC and CCDC scientists
- Modest financial costs
- Opportunity for further investments from other organisations into other nations

Acknowledgements

- Luc van Meervelt, Zephirin Yav, Didi Dikima, Albert Ludemba
- Juliette Pradon, Frank Allen, Peter Galek, Anthony Reilly