

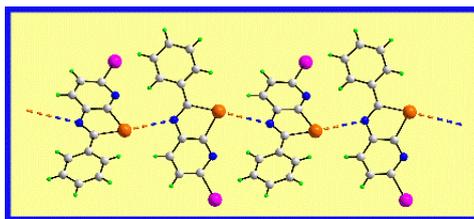
Research Centre of Crystallography

Annual Review for 2022

After many of the covid-19-inspired restrictions were lifted, the year 2022 saw Research Centre of Crystallography (RCCM) staff return to campus to enable access to equipment and the possibility of experimental work, as opposed to a focus upon data mining and the writing of review papers.

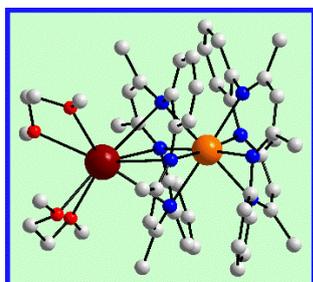
Publications

As per normal, the focus of the Centre was upon publication and two papers were published in the number one ranked *Journal* for Inorganic and Nuclear Chemistry, namely *Coordination Chemistry Reviews* (IF: 24.833). The first of these entitled “*Te···N secondary-bonding interactions in tellurium crystals: Supramolecular aggregation patterns and a comparison with their lighter congeners* ([10.1016/j.ccr.2021.214397](https://doi.org/10.1016/j.ccr.2021.214397))” complemented two articles in the same *Journal* published in 2021 focussing on similar chalcogen-bonding interactions in crystals but involving selenium. These articles evaluate crystallographic data deposited in the Cambridge Structural Database for key intermolecular contacts, often overlooked by authors.



As these contacts pertain to drug-protein interactions, natural biochemical processes in the case of selenium, catalysis, materials chemistry, etc., such output relates to Sustainable Development Goals (SDG's) such as GOAL 3: Good Health and Well-being, reflecting the continuing change of emphasis in the RCCM's research to align with SDG's.

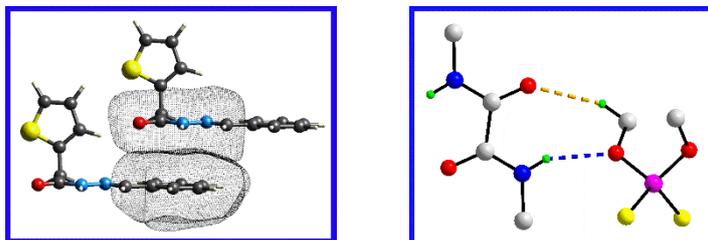
Another article was published in *Coordination Chemistry Reviews* with colleague Dr Abdul Qaiyum Bin Ram, now at Universiti Sains Malaysia. The focus of this review was upon the synthesis, spectroscopic characteristics and crystal structures of dibenzotetraaza[14]annulenes. The paper entitled “*Synthesis, functionalization and coordination chemistry of dibenzotetraaza[14]annulenes* ([10.1016/j.ccr.2022.214672](https://doi.org/10.1016/j.ccr.2022.214672))”



Having a core smaller than that of porphyrins, a different chemistry is noted for these molecules which have applications as electronic devices (*e.g.* illustrated is a potassium salt of

a dysprosium complex, a molecular magnet) and in drug development, e.g. as anti-cancer agents. With the lifting of restrictions, Qaiyum was able to visit us at SunU.

Several primary research papers were published during the year related to SGD Goal #3, e.g. home-grown “*Synthesis, characterisation and biological activity of diorganotin compounds of (E)-N'-(5-nitro-2-hydroxybenzylidene)-3-hydroxy-2-naphthohydrazide* (10.1016/j.poly.2022.115955)” by Lee See Mun *et al.*, and with collaborators throughout the World, e.g. “*Designing, physiochemical confirmation, evaluation of biological and in-silico potential of triorganotin(IV) complexes* (10.1016/j.molstruc.2022.132814)” with B. Hanifa, M. Sirajuddin (Pakistan) *et al.*, and “*Cadmium(II) compounds of the bis-cyanoethyl derivative (L_{CX}) of Mes[14]aneC (L_C): characterization and antibacterial studies* (10.1016/j.heliyon.2022.e09678)” with a collaborator of approaching 30 years, Tapashi Roy (Bangladesh) *et al.*



The theme of ascertaining the nature of intermolecular interactions in crystals, two papers in *CrystEngComm* stand out in 2022, namely “*Experimental and computational evidence for stabilising parallel, offset $\pi[C(=O)N(H)N=C] \cdots \pi(\text{phenyl})$ interactions in acetohydrazide derivatives* (10.1039/d1ce01492g)” with another long-term collaborator Jim Wardell (Brazil) *et al.*, exploiting the considerable expertise of RCCM’s Tan Sang Loon (Alan), and the entirely SunU-based work: “*Unusual $\{\cdots HNC_2O \cdots HC_nO\}$, $n = 1$ or 2 , synthons predominate in the molecular packing of one-dimensional coordination polymers, $\{Cd[S_2P(OR)_2]_2(^3LH_2)\}_n$, for $R = Me$ and Et , but are precluded when $R = i-Pr$; $^3LH_2 = N,N'$ -bis(3-pyridylmethyl)oxalamide* (10.1039/d2ce00208f)”. With stabilising, first time to be recognised interactions between an extended, non-aromatic π -system and a phenyl ring (left-hand image) and $\{\cdots HNC_2O \cdots HC_nO\}$, $n = 1$ or 2 , synthons, these clearly relate to supramolecular association in biologically-relevant systems.

Regrettably, Huey Chong Kwong, aka Stone, left the RCCM in May to pursue opportunities in Singapore as a Research & Development chemist at EMK Technologies. We all wish Stone well and look forward to finalising other papers with him in 2023.

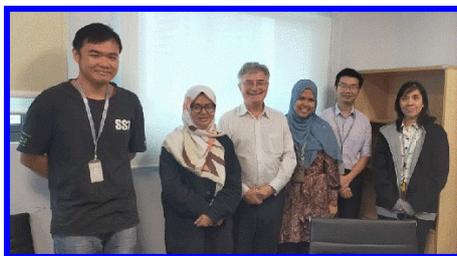
For a full listing of RCCM’s publications in 2022, see <https://scholar.google.com/citations?user=q2vxxGsAAAAJ>

Teaching Engagement

Staff in the RCCM were once again heavily engaged in supervising/co-supervising Final Year Project students from the Department of Biology. Thus, **Yeo Chien Ing** (Ally; Senior Research Fellow) mentored Tan Zing Hern, Kam Xin Xuan, Teng Zhen An, Teo Yuan Hui, Leow Jing Yan Meredith, Emilia A/P Kasi, Lim Jing Yu, Ng Pei Ying and Soong Wei Si. **Lee See Mun**

(Annie) took care of Natelie Lam Rou Yi, Wong Chi Chen, Tiwa Wei Tian, Sheikh Danial Irfan bin Ahmad Kamal, Shirlyn Lu Shiau Shean, Willian Ngan Shi Wee and Fong Carlson Bernard. **Tan Sang Loon** (Alan; ; Senior Research Fellow) taught Deranya Manahari Amarasinghe Kodippuli Arachchige and Tey Wei Xin. Finally, **Tan Yee Seng** (Senior Research Fellow) engaged Wong Yan Bin and Farhan Rehman Sherief in the 2022 FYP programme.

Graduate students also joined RCCM during 2022. Tan Sang Loon (Alan) welcomed Aileen Wee Shu Yeen (a First Class Honours degree graduate in Biotechnology from UCSI University) as a Research Assistant investigating the anti-dengue potential of synthetic organic molecules. In the same way, Yeo Chien Ing (Ally) introduced intern Thow Jing Wen (Monash University Malaysia) to the Centre. Jing Wen's research will focus upon the synthesis, characterisation and the evaluation of the neuroprotective effects of phosphanegold(I) O-methyl-N-phenyl thiocarbamate on the BV-2 cell line. While not formally a member of the Centre Ms Nurul Amalina Binti Abd Aziz is a welcome guest researcher accessing a broad range of equipment in support of a jointly funded FRGS grant in anti-cancer organotin compounds, as detailed in the next section.



Over and above these teaching duties, the Centre organised two Workshops in 2022. The first of these was a Nuclear Magnetic Resonance (NMR) Metabonomics Workshop held during June with Yeo Chien Ing (Ally) being the chief protagonist. The Centre is humble in acknowledging the generous sponsorship from Kinematic Resources Sdn Bhd, Alpha Gas Solution Sdn Bhd and the Royal Society of Chemistry's Researcher Development Grant. In October, a Chemical Crystallography Workshop, chaired by Tan Yee Seng, was conducted. Again, generous sponsorship from Crest Nanosolutions Sdn Bhd, RGS Corporation Sdn Bhd, Cambridge Crystallographic Data Centre and the Royal Society of Chemistry's Researcher Development Grant are gratefully acknowledged.

Making sure everything went to plan was our own Ainnul Hamidah Syahadah Azizan whose primary responsibility was taking care of the NMR lab. It is rather unfortunate that Ainnul is no longer with the Centre – she is greatly missed by those of us who remain.

The formal and informal teaching and mentoring involving RCCM staff obviously relate to **SDG #4 Quality Education**.

Research Funding

Securing research funding, especially external research funding, is a focus of the Centre. Complimenting other FRGS grants (*i.e.* "Apoptosis induction by potential anti-cancer agent, novel organotin(IV) ethylbenzylthiocarbamate derivatives in A549 human lung adenocarcinoma cells (PI: Normah Binti Awang; UKM)" and " QSAR-guided, molecular diversity oriented synthesis and

evaluation of 1,3,5-triazine derivatives as potent and selective anticancer agents (PI: Anton V. Dolzhenko; Monash University Malaysia)” was a new FRGS grant “*Mechanistic understanding of rapid disintegrant action by visualization and the design of better disintegrants for orally disintegrating tablets prepared by direct compression*”; (PI: Celine Valeria Liew; Monash University Malaysia)”.



The latter represents an excursion to pharmacy-orientated research with Tan Yee Seng and Yeo Chien Ing (Ally) providing expertise in PXRD and solid-state NMR, respectively. All grants involving RCCM reflect the Centre’s commitment to SunU’s SDG’s.

It was a singular accomplishment for RCCM when Tan Yee Seng secured a FRGS grant in his own right – a first for the Centre! The proposal “*Tailoring supramolecular isomerism for efficient carbon dioxide adsorption*”, as the title suggests, relates to the targeted synthesis of Metal-Organic Framework (MOF) materials and their utility to absorb the greenhouse gas CO₂, all work conducted in the Centre and relates to **SDG #13 Climate Action**.

The Centre also most gratefully acknowledges the receipt of internal funding “*Unprecedented structural and polymorphism study of cocrystals of trialkyl/arylphosphane gold(I) n-mercaptobenzoates (for n = 2, 3 and 4) and bipyridyl molecules*: PI: Yeo Chien Ing (Ally)” and “*Evaluation of thiourea derivatives as potential anti-dengue therapeutics by in vitro assays and molecular dynamics simulation*”; PI: Tan Sang Loon (Alan)” which will kick-start projects ahead of applying for external support in 2023.

Consultancy

From its inception, RCCM has been engaged with external parties to provide expertise and experimental support for colleagues in other Universities and in Industry and in so doing, provide revenue to support the maintenance of the equipment housed in the Centre’s labs. The primary activities relate to X-ray diffraction methods (single crystal and powder) and NMR (solid-state). The Centre is always open to pursuing new external relationships.

Conclusions

In alignment with SunU’s ambitions, the Centre has just about completed its realignment of all research activities towards topics directly related to SDG’s and has secured external funding in these areas. Further, the emphasis of publication has been towards more impactful papers rather than crystallographic reports.

Inevitably, as one year concludes and another starts, staffing changes. The contributions to SunU/RCCM of Huey Chong Kwong and Ainnul Hamidah Syahadah Azizan have already been mentioned. We also note the departure of Lee See Mun (Annie) from the Centre at the conclusion of 2022. We wish all former staff well in their future endeavours!