

# Open Data in the Chemical Sciences

The logo of the Royal Society of Chemistry, featuring a stylized circular emblem with various colored segments (teal, grey, yellow) and the text "ROYAL SOCIETY OF CHEMISTRY" in white capital letters.

ROYAL SOCIETY  
OF CHEMISTRY

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# Royal Society of Chemistry

Knowledge

Voice

Profession





# Our data policy

We publish 44 peer-reviewed journals

We **encourage** researchers to make all data associated with their publications freely available in an accessible and **usable format**, enabling other researchers to replicate and build on that research.

# ESI is the status quo

Issue 22, 2012

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From the journal:  
**Dalton Transactions**

## Co-linear, double-uranyl coordination by an expanded Schiff-base polypyrrole macrocycle

[Polly L. Arnold](#)<sup>\*a</sup> [Guy M. Jones](#)<sup>a</sup> [Qing-Jiang Pan](#)<sup>bc</sup> [Georg Schreckenbach](#)<sup>b</sup> and [Jason B. Love](#)<sup>\*a</sup>

[⊕ Author affiliations](#)

### Abstract

Expansion of a Schiff-base polypyrrolic macrocycle allows the formation of a binuclear uranyl complex with co-linear uranyl ions and a very short oxo–oxo distance.

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PDF format



Article HTML

### Supplementary files

[Supplementary information](#)

PDF (500K)

[Crystal structure data](#)

TXT (41K)

Free to access, easy to read, but less discoverable and less and reusable



## Synthesis and Characterisation

### $^1\text{H}$ NMR Spectrum of $\text{H}_4\text{L}^{\text{A}}$ synthesised by literature methods

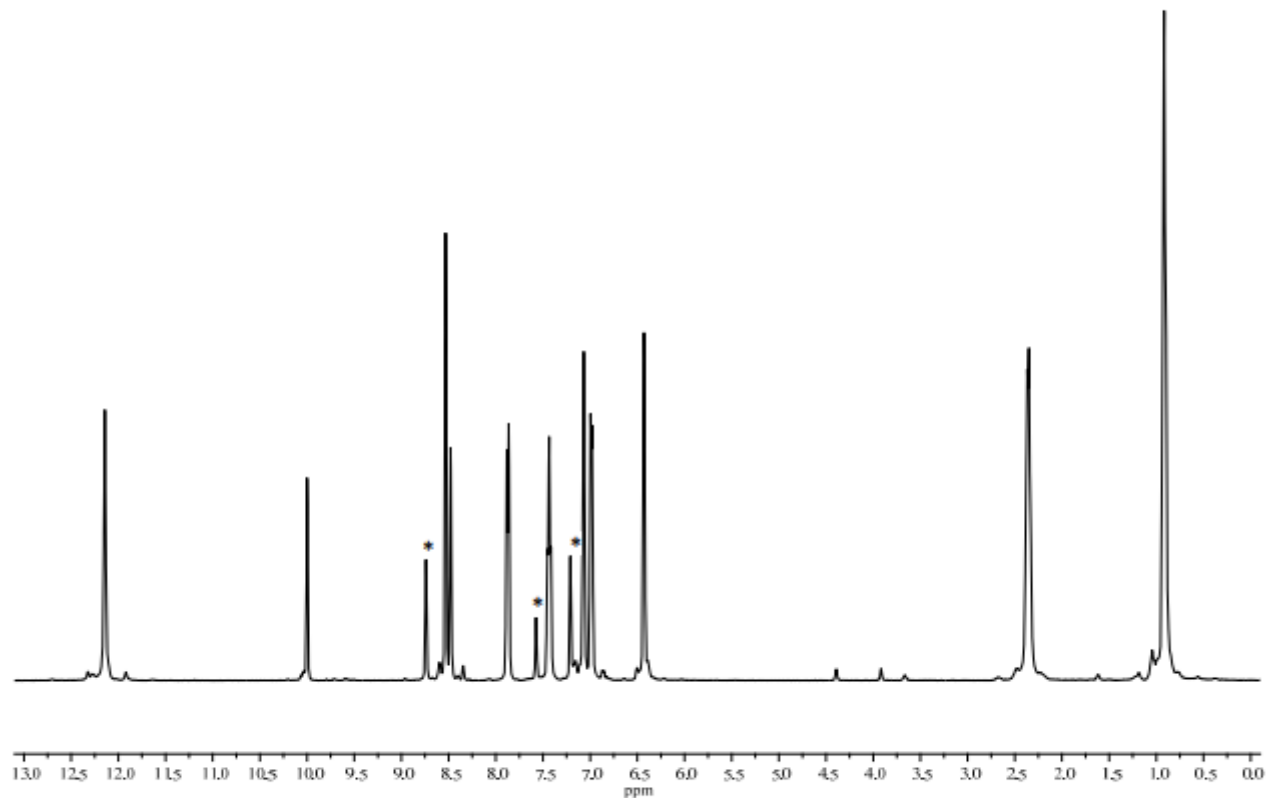


Fig. S1.1:  $^1\text{H}$  NMR spectrum of  $\text{H}_4\text{L}^{\text{A}}$  in  $d_5$ -pyridine, \* = residual  $\text{C}_3\text{D}_4\text{HN}$

### Synthesis of $[(\text{UO}_2)(\text{py})(\text{H}_2\text{L}^{\text{A}})]$ **1** and $\{[\text{UO}_2(\text{py})]_2(\text{L}^{\text{A}})\}$ **2**

To a solution of  $\text{H}_4\text{L}^{\text{A}}$  (100 mg, 0.116 mmol) in pyridine (2 mL) was added a solution of  $[\text{UO}_2\{\text{N}(\text{SiMe}_3)_2\}_2(\text{py})_2]$  (174 mg, 0.232 mmol) in pyridine (2 mL) and the resulting brown solution stirred for four days at room temperature causing



“I never release my data to anyone other than collaborators before publication.”

“Only about 3 people in the world would ever want to reproduce a specific set of detailed results – and they can write to the author and request the data.”

“I’m very careful over the quality of the downloaded material – this strongly depends on where it was downloaded from.”

“I already publish what I want to release and put it in the publication and the SI.” “SI is good enough, especially to fix the length constraints of print.”

“There are enough platforms to share [additional] content already.”

# Mandates, Motivations

**EPSRC**

Pioneering research  
and skills



**erc**

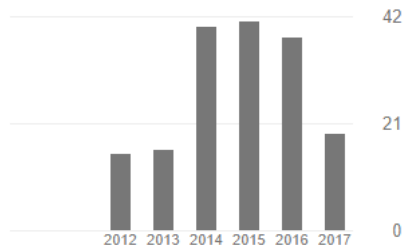
European  
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**DFG**  
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	All	Since 2012
Citations	169	169
h-index	5	5
i10-index	5	5



PDF



*Supplementary Information for*

**3D hole-transporting materials based on coplanar quinolino acridine for highly efficient perovskite solar cells†**

Mingdao Zhang,<sup>\*ab</sup> Gang Wang,<sup>c</sup> Danxia Zhao,<sup>c</sup> Chengyan Huang,<sup>ad</sup> Hui Cao<sup>\*\*</sup> and Mindong Chen<sup>\*\*</sup>



# A voice in the conversation

Standards



Partnership & collaboration



**Open PHACTS**

**ChemRxiv**<sup>TM</sup>

Policy



**Chemistry Research Data  
Interest Group**





# Policy and practice

## UK REF input

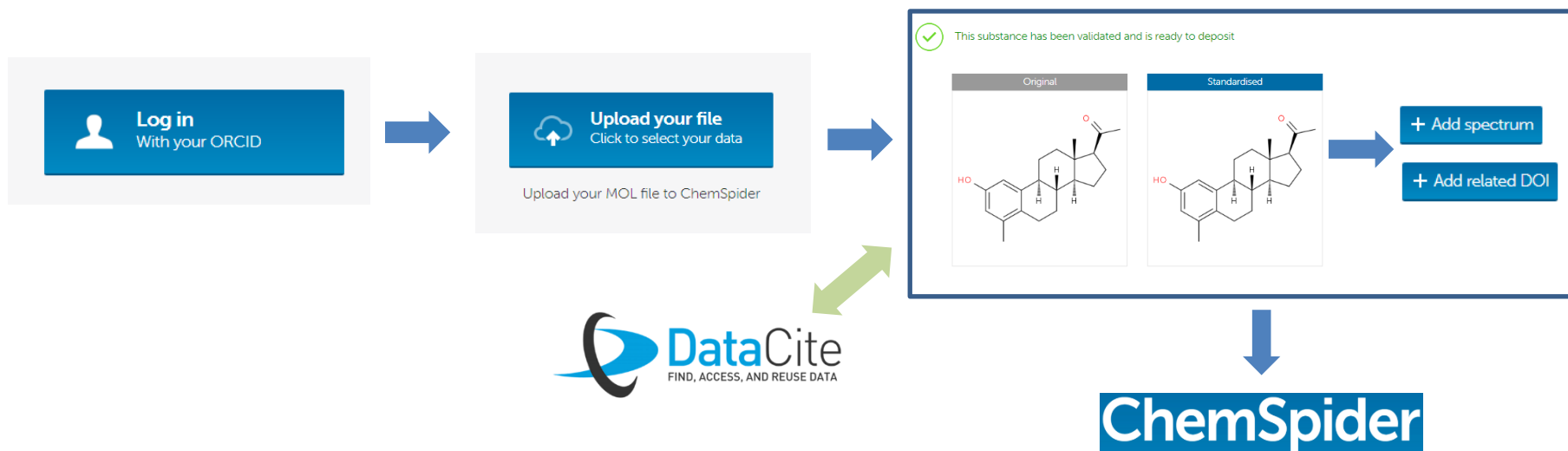
36. Do you agree with the proposals for providing additional credit to units for open access?
37. What comments do you have on ways to incentivise units to share and manage their research data more effectively?

## Open Scholarship Initiative

**OSI2016-25**

[osinitiative.org](http://osinitiative.org)

# Research data publication in ChemSpider



Deposit chemical structures and spectra  
and publish with a DOI -

<https://deposit.chemspider.com/>



# National Compound Collection

Pilot - 800 UK theses, manual curation



From the journal:  
Chemical Science

## The creation and characterisation of a National Compound Collection: the Royal Society of Chemistry pilot



[David M. Andrews](#),<sup>\*a</sup> [Laura M. Broad](#),<sup>b</sup> [Paul J. Edwards](#),<sup>c</sup> [David N. A. Fox](#),<sup>a</sup> [Timothy Gallagher](#),<sup>b</sup>  
[Stephen L. Garland](#),<sup>d</sup> [Richard Kidd](#)<sup>a</sup> and [Joseph B. Sweeney](#)<sup>e</sup>



# As publisher?

validation | reproducibility  
field by field  
standards development

policies

divisions / members (catalyse discussions)

community norms

reflect and return the value



# My takeaways

direct return

structured and interoperable > open

concentrate on the known

complexity

global | community | practice