

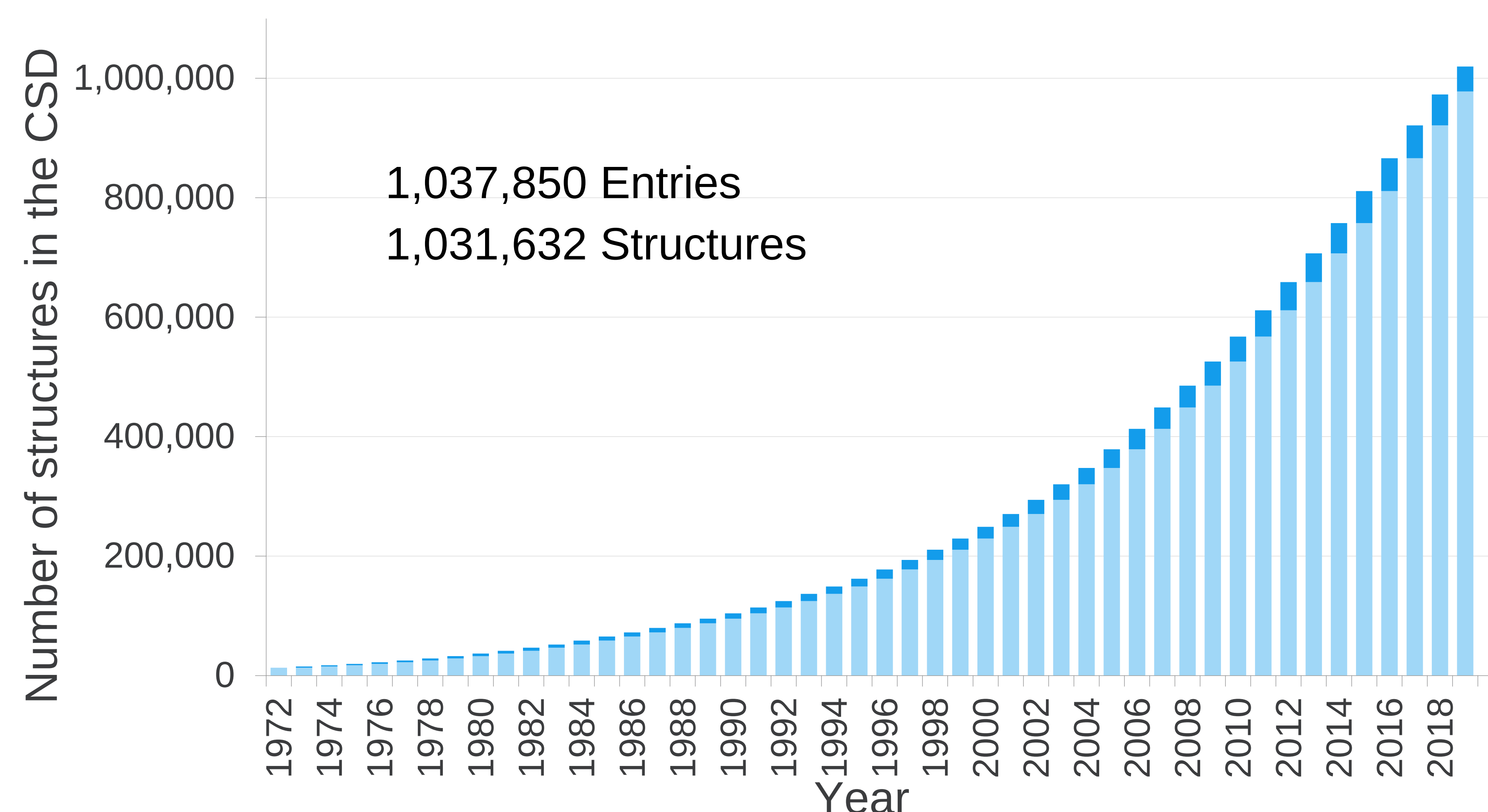
The Cambridge Structural Database (CSD) in Numbers

Yu Gan, Suzanna Ward, Matthew Lightfoot, Clare Tovee, Philip Andrews
The Database Team, The Cambridge Crystallographic Data Centre (CCDC)

Last updated: December 2019 for AsCA2019

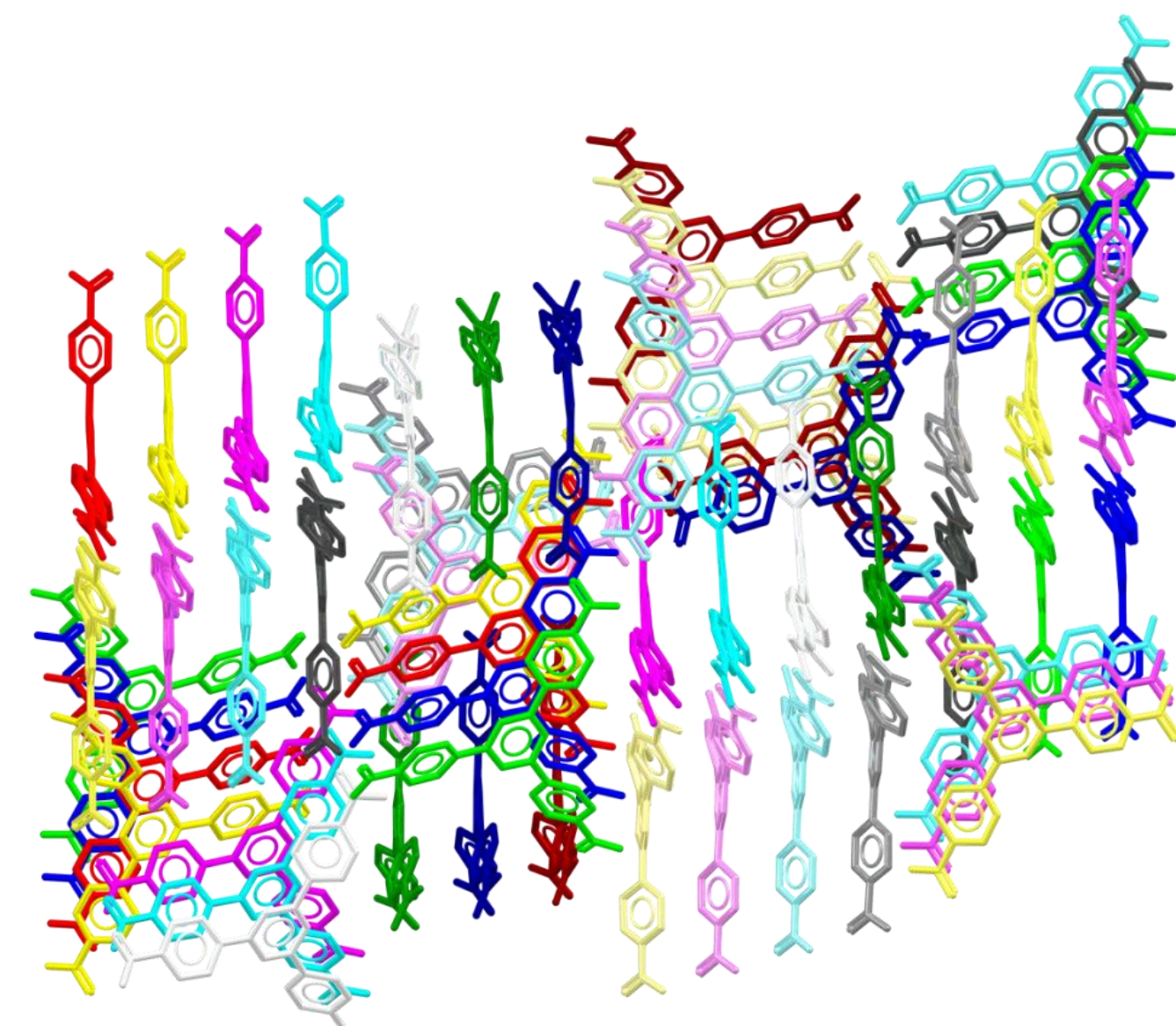
DATABASE

A database of organic and metal-organic experimental structures

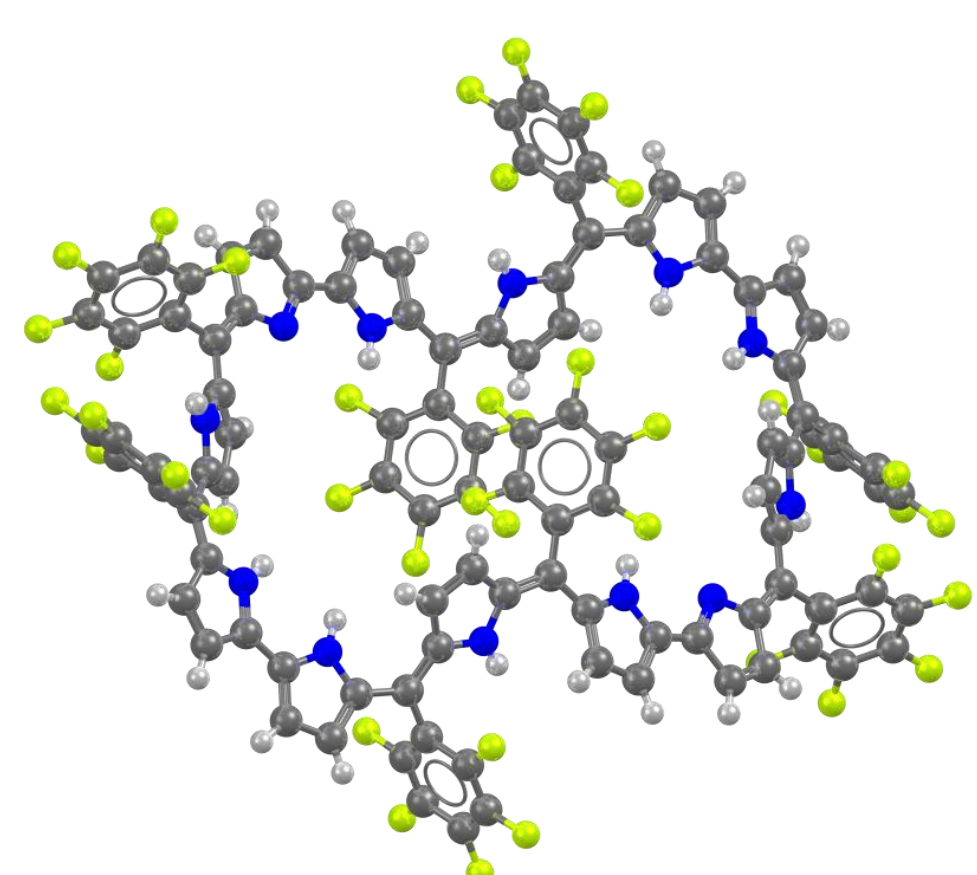


STRUCTURES

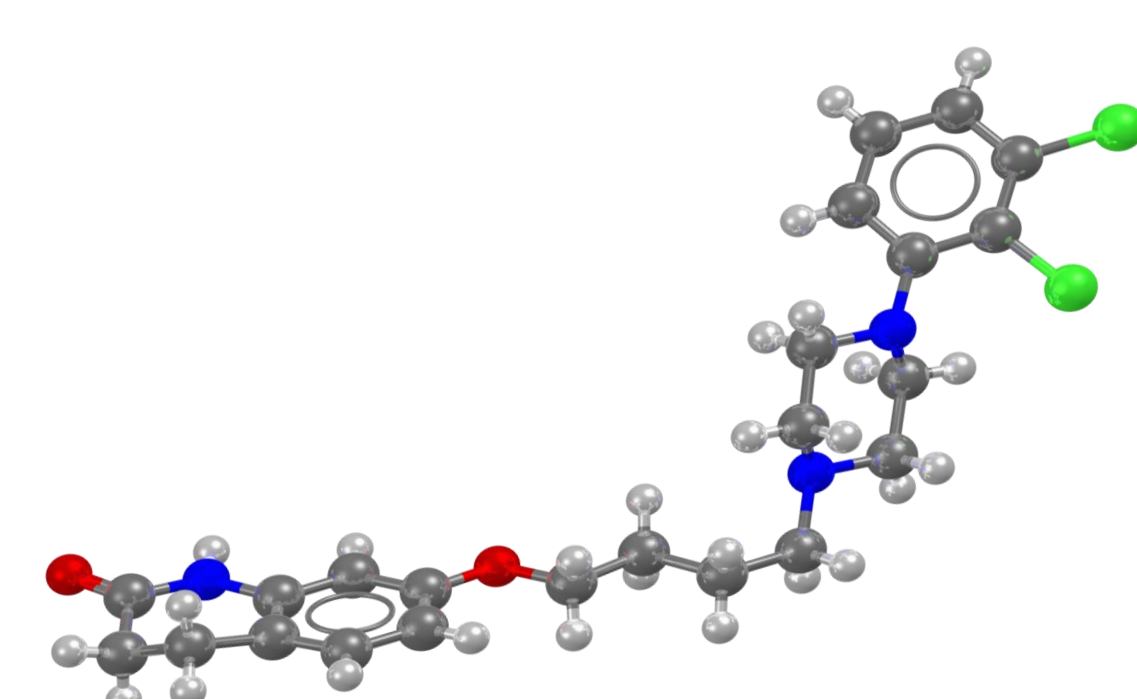
- 940,410 Refcode families
- 11,054 Polymorph families
- 169,968 Melting points
- 865,982 Crystal colours
- 734,175 Crystal habits
- 23,871 Bioactivity data



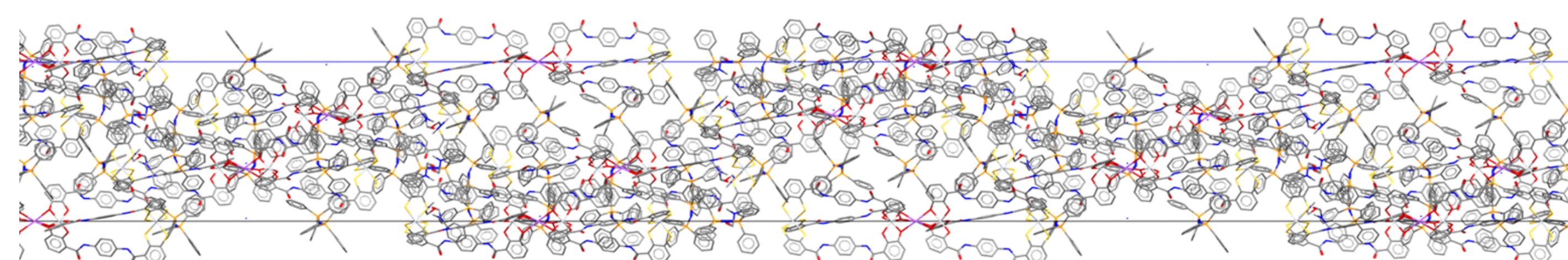
56: Highest Z' value OGUROZ



50π: Most aromatic structure KUHUS



Aripiprazole: The most polymorphic drug MELFIT19



Longest cell axis - $a = 24.236(1)$ $b = 24.236(1)$ $c = 225.276(6)$ Å VIBJAS

SCIENCE

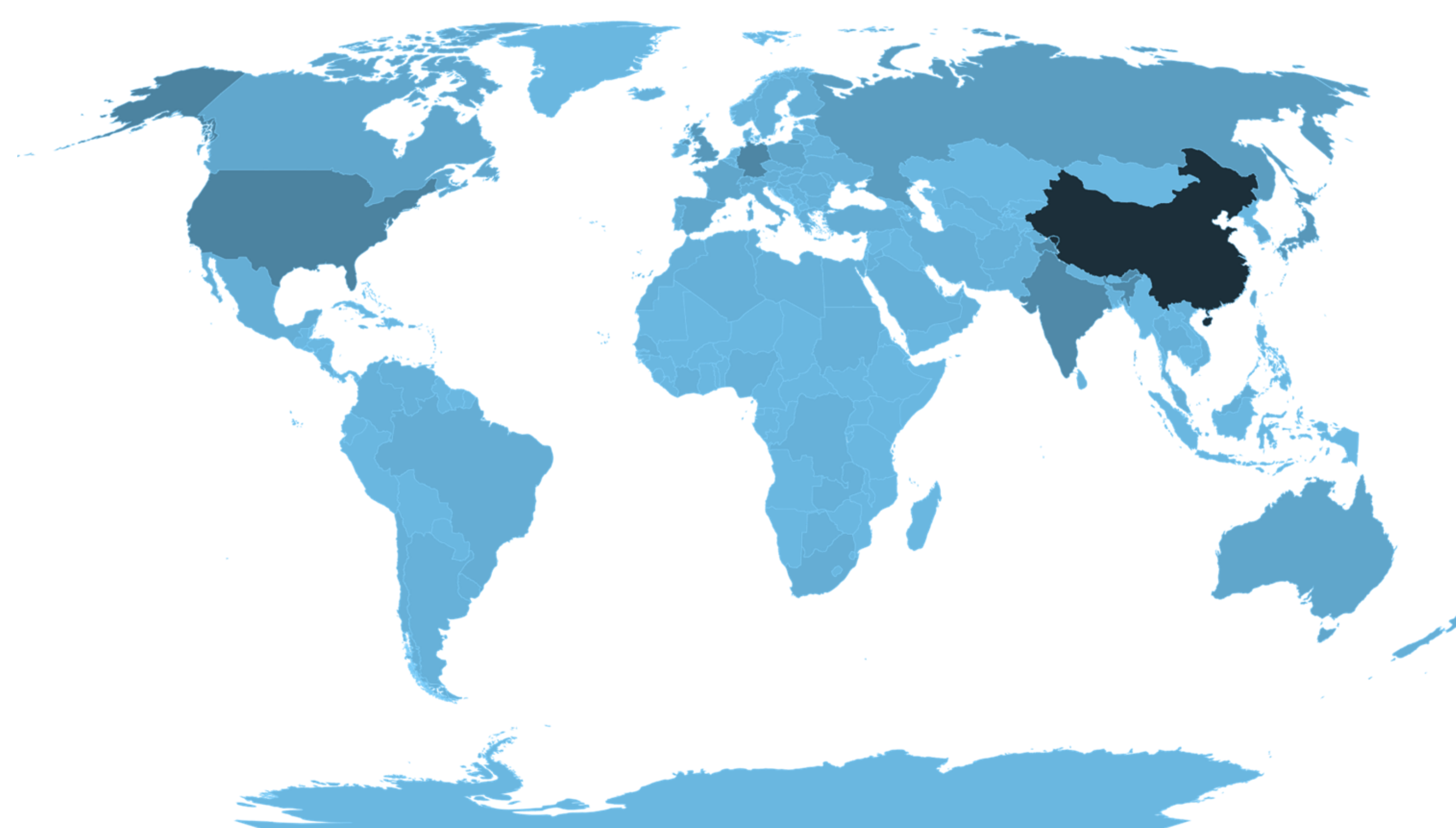
The diagram below shows a breakdown of the fields of research citing the latest CSD paper.

1,232 Chemistry multidisciplinary	373 Chemistry physical	135 Physics atomic molecular chemical	62 Computer science information systems	47 Pharmacology Pharmacy	42 Biochemical research methods
1,002 Crystallography	261 Materials science multidisciplinary	113 Computer science interdisciplinary applications	17 Chemistry Applied	15 Spectroscopy	14 Physics applied
437 Chemistry inorganic nuclear	198 Chemistry organic	110 Chemistry medicinal	17 Mathematical computational biology	13 Chemistry analytical	13 Physics condensed matter
	165 Biochemistry molecular biology	74 Biophysics	17 Multidisciplinary sciences	12 Educational scientific discipline	
			15 Nanoscience nanotechnology	9 Engineering Chemical	7 Materials science

The Cambridge Structural Database. Colin R. Groom, Ian J. Bruno, Matthew P. Lightfoot, Suzanna C. Ward, *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. and Mat.*, 2016, **72**, 171-179, DOI: 10.1107/S2052520616003954

PEOPLE AND PLACES

- > 10,000 Different depositors a year
- 402,180 Unique authors in the CSD
- 498,004 Publications in the CSD



Map showing the country of the crystallographer for structures deposited with the CCDC in 2019

2019 Global leaderboard

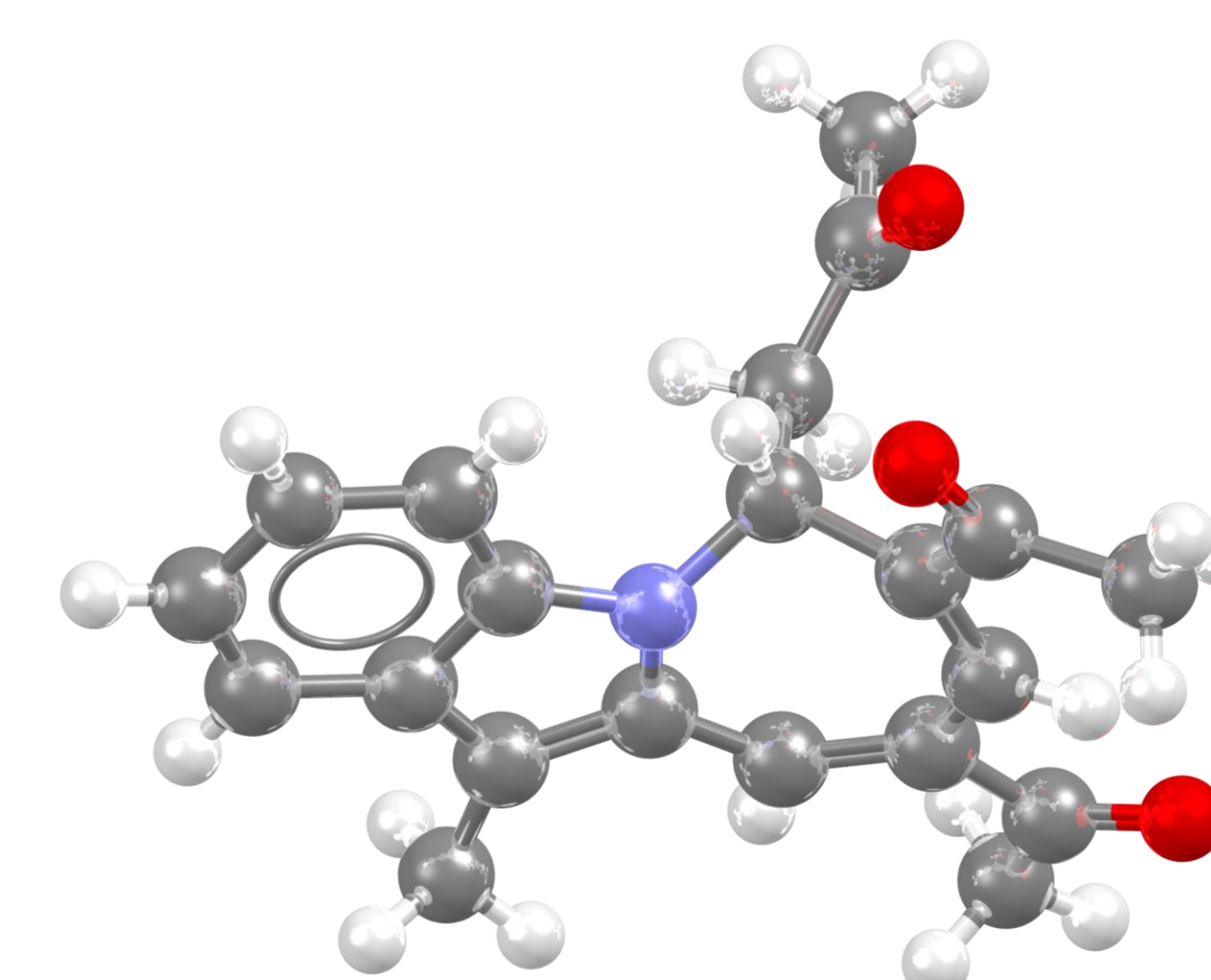
China
United States
Germany
Japan
UK
India
France
Russia
Spain
Australia

There are over 750 authors with over 500 structures in the CSD

CSD's top contributors

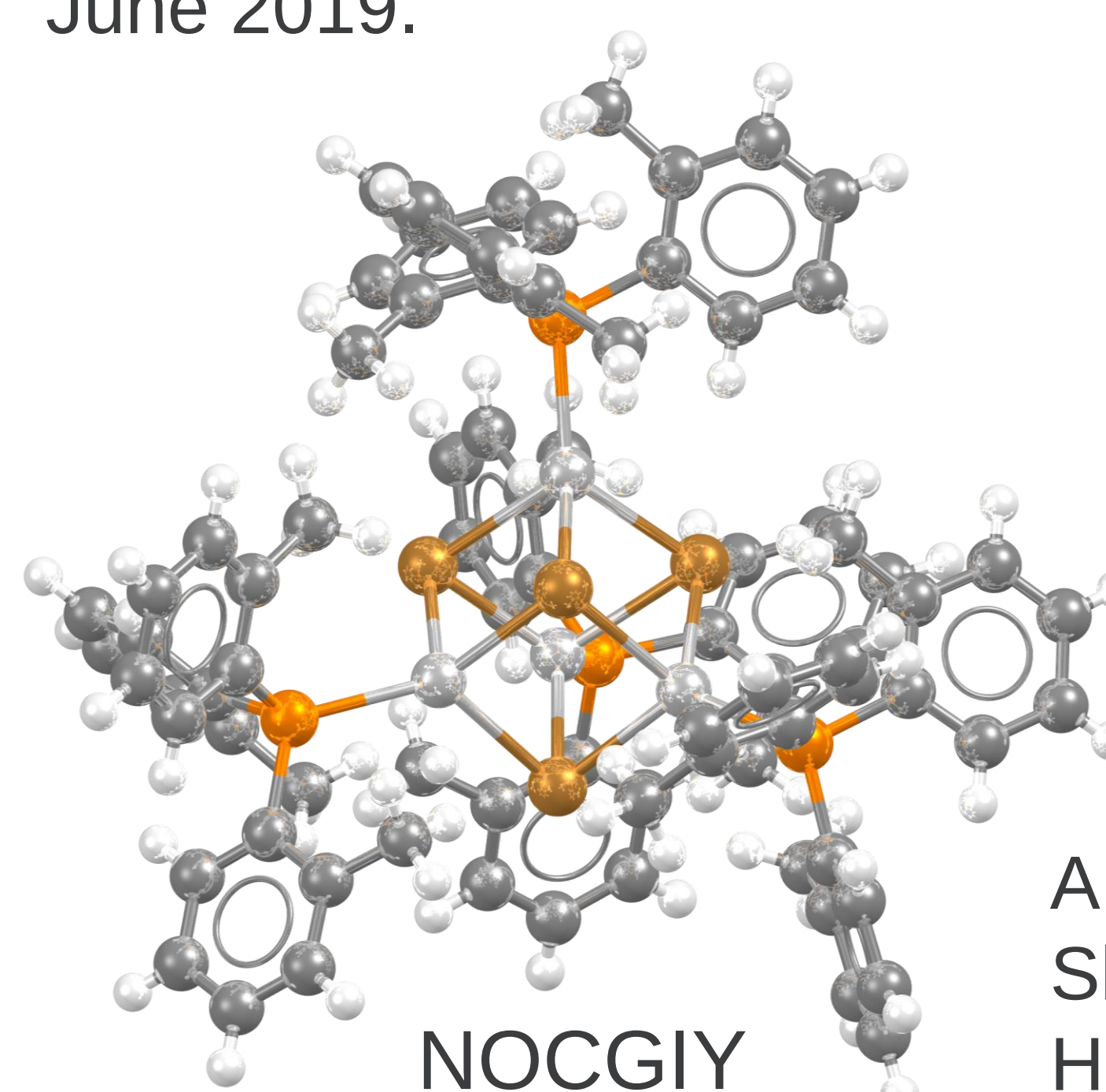
B.W.Skelton
A.H.White
A.L.Rheingold
P.G.Jones
M.B.Hursthouse
A.M.Z.Slawin
F.R.Fronczek
J.A.K.Howard
H.-K.Fun
S.W.Ng

Over a third of depositions are currently from China. Fittingly, we celebrated the one millionth structure with Yao Wang and co-workers from Shandong University in China in June 2019.



XOPCAJ
The millionth structure

Brian Skelton and Allan White from the University of Western Australia have co-authored well over 4,000 structures since 1975.



NOCGIY

A structure by Brian Skelton, Effendy and Allan H. White

Visit www.ccdc.cam.ac.uk/structures and enter the refcode to find out more details about the structures mentioned here
Visit www.ccdc.cam.ac.uk/CCDCStats/ or use the QR code to see the latest statistics and insights on the CSD

