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**Supporting information for article:**

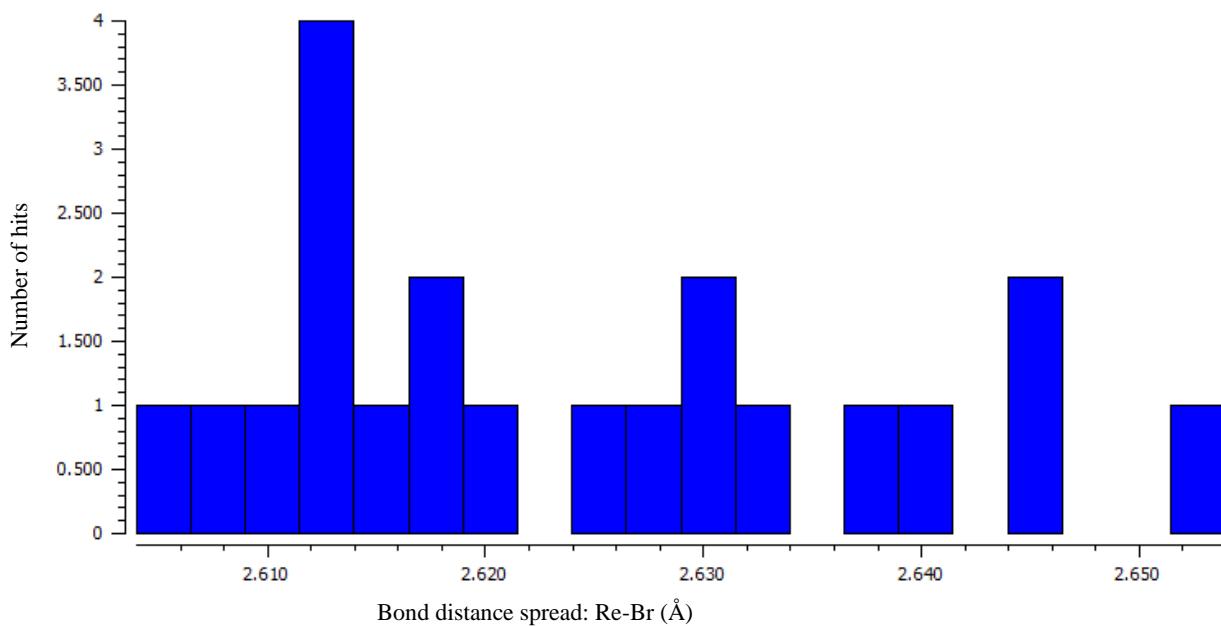
**Formation of a highly dense tetra-rhenium cluster in a protein crystal and its implications in medical imaging**

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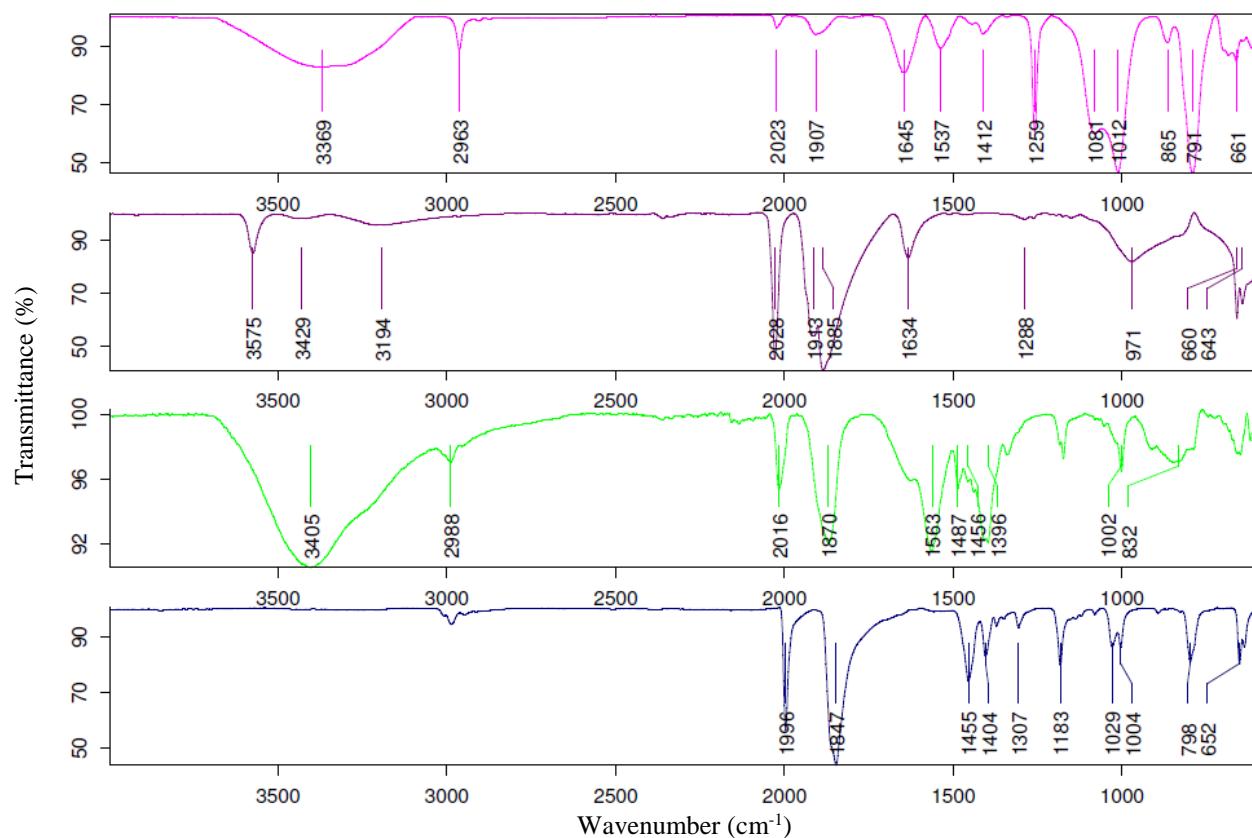
**Table S1** Summary of all rhenium binding in three structures after crystallizations, and time on shelf collections at 1 and 2 years.

<u>IUCrJ 2017</u> <u>Fresh crystallised</u>	<u>1Yr - Y</u>	<u>2Yr - X</u>
Residue (Orthorhombic $P2_12_12_1$ )	(Orthorhombic $P2_12_12_1$ )	(Tetragonal $P4_32_12$ )
His 15 A & B	His 15 A & B	His 15
Asp 119A	Asp 119 A & B	Asp 119
Asp 18 A & B	Asp 18A	
Asp 52 A & B	Asp 52 A & B	
Glu 7B	Glu 7A (non bonded)	Glu 7
Glu 35 A & B	Glu 35 A	
Arg 125 B	Arg 125A	
Arg 61B		
Leu 125 A ??		
Leu 129 B	Leu 129B	
Non-bonded in vicinity of	Non-bonded in vicinity of	Non-bonded in vicinity of
Leu 129 B	Leu 129A	
Pro 70 A and Arg 61A		
Arg 14 B		
	Glu 7A and Lys 1A	
	Trp 63B	
	Asp 101B	

	Ala 107B	
	Gly 71 B	
Cluster Formation	Cluster Formation	Cluster Formation
	Leu 129 A	
	Arg 3A	
		Arg 5
	Trp63 A / Ser 100A	
		Trp 123
	Pro 70A	Pro 70
	Asn 103	
		Lys 33



**Figure S1** Comparison of all possible small molecule Re-Br bond distances. *Mogul* (Bruno et al., 2004)<sup>1</sup>, CSD Data analysis (version update 5.39) of Re-Br bond distances of small molecule hits utilising the Re-Br distance found within the *fac*-[Re(CO)<sub>3</sub>(N)(O)]<sup>+</sup> fragment as search criteria found on the CSD database, with a total of 21 Hits. Colour bars indicate number of structure hit entries with respect to bond length (Å) in data libraries used: CSD version update 5.39. Minimum/maximum bond distances (2.60 / 2.65 Å) with a standard deviation of 0.014 Å and a mean value of 2.62 Å.



**Figure S2** ATR-IR spectra of the rhenium complexes. (A) IR of crystals contain HEWL-rhenium with cluster formation. Crystals remained for two years in sitting drop in the specified buffer solution. (B) Solid state IR of  $[\text{Re}_4(\mu_3\text{-OH})_4(\text{CO})_{12}]$  cluster complex, synthesised according to Egli, et al., 1997. (C) Solid state IR of *fac*- $[\text{Re}(\text{CO})_3(\text{Br})_3]^{2+}$  dissoved in 10% NaCl, NaOAc 0.04 M (pH 4.7) for 3 months. (D) Solid state IR of *fac*- $[\text{Re}(\text{CO})_3(\text{Br})_3]^{2+}$ .

<sup>1</sup> Bruno, I. J., Cole, J. C., Kessler, M., Luo, J., Motherwell, W. D. S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.