Supporting Information

Crystal structure of $NiFe(CO)_5$(tri(pyridylmethyl)azaphosphatrane): a synthetic mimic of the NiFe hydrogenase active site incorporating a pendant pyridine base

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Table S1. List of NiFe complexes with Ni-Fe bond distances.

CSD refcodes	Ni-Fe distance (Å)	Ref
FANHEK	2.621	1 (Song *et al.*, 2017)
FANHEK01	2.614	1 (Song *et al.*, 2017)
FANGUZ	2.460	1 (Song *et al.*, 2017)
FANHIO	2.650	1 (Song *et al.*, 2017)
FANHUA	2.660	1 (Song *et al.*, 2017)
LAZWEP	2.467	2 (Zhu *et al.*, 2005)
SUQQOL	2.613	3 (Barton *et al.*, 2009)
UCUXOH	2.684	4 (Carroll *et al.*, 2011)
UCUXUN	2.596	4 (Carroll *et al.*, 2011)
UQAJAZ	2.550	5 (Manor & Rauchfuss, 2013)
YOKWIE	2.447	6 (Walther *et al.*, 1995)

Table S2. List of NiFe complexes with Ni-Fe bond distances.

CSD refcodes	Ni-Fe distance (Å)	Ref
EJUSEJ	2.572	7 (Sun *et al.*, 2016)
EJUSUZ	3.164*	7 (Sun *et al.*, 2016)
FOTKOP	3.296	8 (Tanino *et al.*, 2009)
QEKLAT	2.800	9 (Liaw *et al.*, 2000)
FANHUA	2.660	1 (Song *et al.*, 2017)

- Average of two structures in the unit cell.

Reference:

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