

Electronic Supplementary Information for:

Heterometallic complexes with cube-type [MTi₃N₄] cores containing

Group 10 metals in a variety of oxidation states

Noelia Martínez-Espada, Miguel Mena, Adrián Pérez-Redondo, Víctor Varela-Izquierdo

and Carlos Yélamos*

Departamento de Química Orgánica y Química Inorgánica, Universidad de Alcalá. 28871

Alcalá de Henares-Madrid (Spain). FAX: (+34) 91-8854683. E-mail:

carlos.yelamos@uah.es

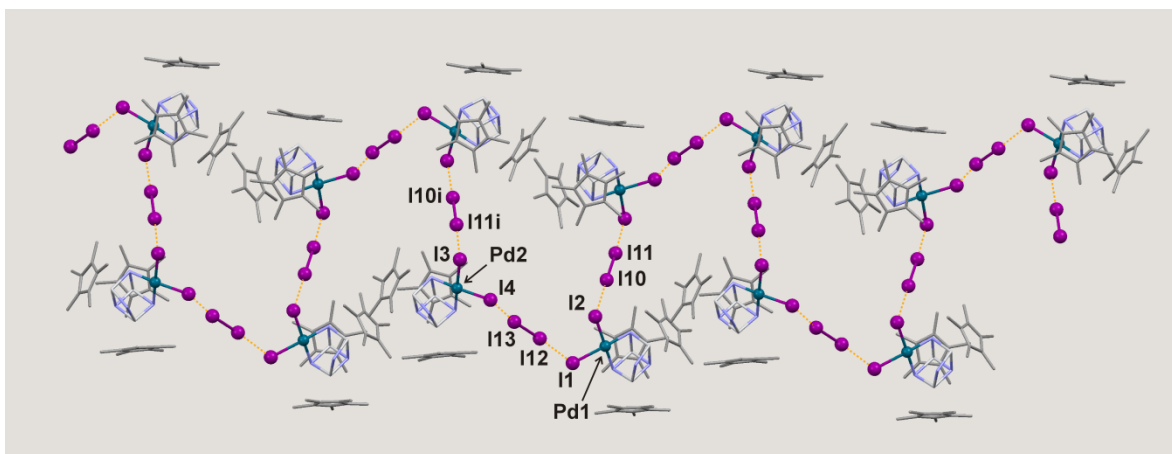


Fig. S1. Intermolecular halogen bonds in complex **8**.

Table S1. Halogen bonds in compound **8**.

Halogen bond	I \cdots I/ \AA	Pd-I \cdots I/ $^\circ$	I \cdots I-I/ $^\circ$	R _{II} ^a
Pd(1)-I(1) \cdots I(12)-I(13)	3.411(1)	116.5(1)	172.4(1)	0.861
Pd(1)-I(2) \cdots I(10)-I(11)	3.375(1)	102.6(1)	172.1(1)	0.852
Pd(2)-I(3) \cdots I(11)i-I(10)i ^b	3.374(1)	97.3(1)	176.0(1)	0.852
Pd(2)-I(4) \cdots I(13)-I(12)	3.391(1)	112.5(1)	169.1(1)	0.856

^a The normalized distance R_{II} involves normalization relative to the sum of van der Waals radii of the two iodine atoms, R_{II} = $d(\text{I}\cdots\text{I})/2r_{\text{I}}$, where r_{I} is the van der Waals radius of iodine (1.98 \AA).^b Symmetry code: (i) $1 - x, -1/2 + y, 1/2 - z$.

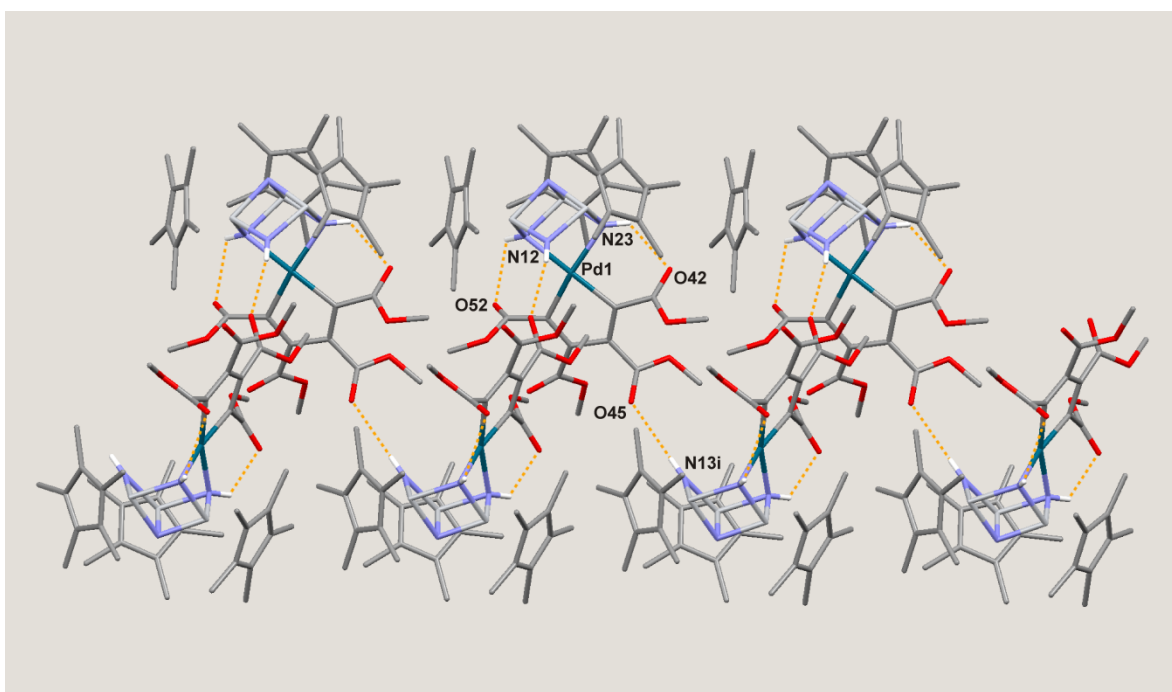


Fig. S2. Intra- and intermolecular hydrogen bonds in complex **9**. Lengths (Å) N(23)⋯O(42) 2.920(1), N(12)⋯O(52) 3.335(1), N(13)⋯O(45)i 3.423(1). Symmetry transformation: (i) $3/2 - x, -1/2 + y, 1/2 - z$.