Supporting Information for

Aromatic interactions in hydrotris(3-methylindazolyl)borate organometallic complexes: control of an alkyne ligand orientation in the crystal

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Analysis of aromatic interactions in 1-prox

The relevant data for the analysis of aromatic interactions of **1-prox** have been retrieved from the CCSD under VOKSIX. Basically, there are many aromatic interactions present, but based on the analysis of the metric parameters they all are very weak. The results are provided in Table S1 and in Figure S1. An attractive interaction $(Pz\text{-}Pz)_{att}$ (Table S1, entry *A*) is present between two pyrazolyl rings of neighbouring complexes related by an inversion centre. It is thus similar to $(Ind\text{-}Ind)_{att}$ (Table 1, entry *A*) for **2-dist** except that benzo rings interact in **2-dist**. Given the distance and the offset between centroids (Table S1), this interaction is much weaker in **1-prox** than in **2-dist**. For this given pyrazolyl ring, another pyrazolyl ring of these two molecules shows a weak repulsive interaction $(Pz\text{-}Pz)'_{rep}$ (Table S1, entry *B*). A third type of interaction involving pyrazolyl rings that can be identify is slightly attractive $(Pz\text{-}Pz)''_{att}$ (Table S1, entry *C*). It involves one of the two molecules of the previous couple with another molecule related by a C_2 axis. Again, the parameters for this interaction indicate it is relatively weak. Most importantly, the phenyl ring of the co-ordinated phenylpropyne is not involved in any *inter*molecular interaction with either a pyrazolyl ring or a phenyl ring of neighbouring complexes, whether attractive or repulsive. Interestingly, the phenyl ring of the phenyl propyne in **1-prox** is engaged in very weak repulsive *intra*molecular aromatic interactions $(Pz\text{-}Ph)_{rep}$ and $(Pz\text{-}Ph)'_{rep}$ (Table S1, entries *D* and *E*) with the two proximal dimethylpyrazolyl rings. Overall, the compared analysis of aromatic interactions in **2-dist** and **1-prox** strongly suggests that it is the presence of the benzo ring of the indazole involved in the stabilizing interaction $(Ind\text{-}Ph)_{att}$ in **2-dist** that is controlling alkyne orientation in the crystal.

Table S1 Aromatic interactions within a crystal of **1-prox** (see **Figure S1** for a pictorial description)

entry	interaction name	Ctd-Ctd/ Å[a]	Ctd-Plane/Å[b]	Angle/deg[c]	Offset/Å	interaction type
A	$(Pz\text{-}Pz)_{att}$	4.72	3.88	0	2.69	attractive
B	$(Pz\text{-}Pz)'_{rep}$	4.90	1.83	60	4.59	repulsive
C	$(Pz\text{-}Pz)''_{att}$	3.93	3.64	22	1.49	attractive
D	$(Pz\text{-}Ph)_{rep}$	4.80	2.23	51	4.25	repulsive
E	$(Pz\text{-}Ph)'_{rep}$	4.87	1.98	62	4.45	repulsive

[a] Distance between centroids. [b] Distance between a centroid and the interacting plane. [c] Angle between planes.

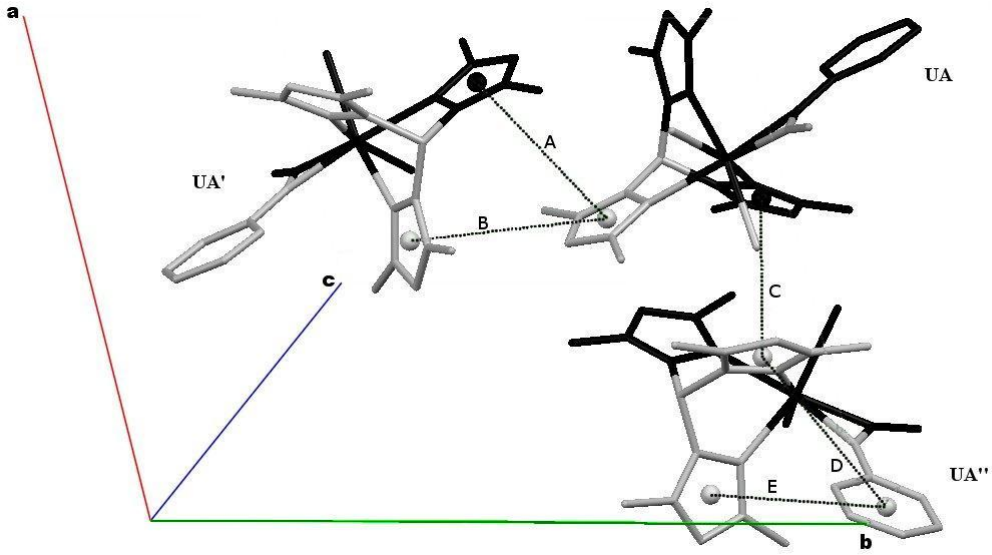

Figure S1: Aromatic interactions within a crystal of **1-prox** as analysed from the CCSD as VOKSIX, see **Table S1** for details.