

Supplementary Material (ESI) for Dalton Transactions
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Electronic Supplementary Information

Further Investigations of Linear Trirhodium complexes: Experimental and Theoretical Studies of $[\text{Rh}_3(\text{dpa})_4\text{Cl}_2]$ and $[\text{Rh}_3(\text{dpa})_4\text{Cl}_2](\text{BF}_4)$ [dpa = bis(2-pyridyl)amido anion]

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Table S1 Relevant geometrical parameters (distances in Å) and results computed for **1** and **2** in D_4 symmetry. (basis set: BSII, functionals: BP86.)

	1			2	
	2A_2	2B_2	exptl.	3B_1	exptl.
Rh-Rh	2.446	2.432	2.392	2.445	2.363
Rh-Cl	2.509	2.678	2.586	2.485	2.411
Rh _{middle} -N	2.016	2.014	2.014	2.004	2.010
Rh _{terminal} -N	2.110	2.090	2.076	2.104	2.084
energy	0	0.231			
$\langle S^2 \rangle$	0.754	0.753		2.028	

Table S2 Relevant geometrical parameters (distances in Å) and results computed for **1** and **2** in D_4 symmetry. (basis set: BSI, functionals: PW91.)

	1			2	
	2A_2	2B_2	exptl.	3B_1	exptl.
Rh-Rh	2.446	2.447	2.392	2.439	2.363
Rh-Cl	2.509	2.681	2.5863	2.486	2.411
Rh _{middle} -N	2.016	2.008	2.014	2.000	2.010
Rh _{terminal} -N	2.110	2.084	2.076	2.098	2.084
energy	0	0.196			
$\langle S^2 \rangle$	0.753	0.752		2.004	