Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Further Investigations of Linear Trirhodium complexes: Experimental and Theoretical Studies of $[Rh_3(dpa)_4Cl_2]$ and $[Rh_3(dpa)_4Cl_2](BF_4)$ [dpa = bis(2-pyridyl)amido anion]

Gin-Chen Huang, Isiah Po-Chun Liu, Jau-Huei Kuo, Yi-Lin Huang, Chen-Yu Yeh, Gene-Hsiang Lee, Shie-Ming Peng

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
$Rh_{termial}$-N	2.110	2.090	2.076	2.104	2.084
energy	0	0.231			
$<S^2>$	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
$Rh_{termial}$-N	2.110	2.084	2.076	2.098	2.084
energy	0	0.196			
$<S^2>$	0.753	0.752		2.004	