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Electronic Supplementary Information

Influence of water on the formation of O_2-reactive divalent metal enolate complexes of relevance to acireductone dioxygenases

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Table S1. ^{1}H NMR chemical shifts for **3-6** in CD_3CN at 298 K

assignment	shift (ppm)[a]	$\Delta\nu_{1/2}$(Hz)[b]	rel area
	[(6-PhTPA)Ni(PhC(O)C(OH)C(O)Ph)]ClO_4 (**3**)		
α	150.0	*c*	*c*
β	41.6, 34.8	183, 172	1, 1
β'	44.5, 13.3	450, 179	2, 2
γ	*c*	c	*c*
γ'	10.6	91.6	*c*
CH_2	57.7, 23.3, *c*	*c, c, c*	*c, c, c*
	[(6-PhTPA)Ni(PhC(O)CHC(O)Ph)]ClO_4 (**4**)		
α	148.6	*c*	*c*
β	43.8, *c*	355	*c, c*
β'	41.1, 34.8	183, 214	1, 1
γ	13.2	175	2
γ'	*c*	*c*	*c*
CH_2	138.2, 51.0, 50.5	*c, c, c*	*c, c, c*
CH (dbm)	-13.1	256	1
	[(6-PhTPA)Ni(CH_3CN)(CH_3OH)]$(ClO_4)_2$ (**5**)		
α	150.0	*c*	*c*
β	52.8, c	543, *c*	*c, c*
β'	49.2, 40.8	484, 324	*c*, 1
γ	14.6	126	*c*
γ'	10.1	107	*c*
	[(6-PhTPA)Ni(O_2CPh)]ClO_4 (**6**)		
α	150.9	2922	1
β	46.3, 36.2	*c*, 328	*c*, 1
β'	49.3, 45.1	362, 244	2, *c*
γ	13.5	72	2
γ'	10.0	84	1
CH_2	77.5, *c, c*	*c, c, c*	*c, c, c*

[a]Chemical shifts in ppm relative to the residual solvent peak of C*H*D_2CN (^{1}H, 1.94 (quintet) ppm). [b]Line widths are full width at a half-maximum. [c]Could not be determined.