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Supporting Information

Rotating Iron and Titanium Sandwich Complexes

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chem_201704829_sm_miscellaneous_information.pdf

Table S1. Structural parameters **Fc** and **TdP** in staggered (D_{5d}) and eclipsed (D_{5h}) conformation obtained on OPBE/TZP level of theory

	Fc		TdP	
	D_{5d}	D_{5h}	D_{5d}	D_{5h}
M-ring	1.596 Å	1.593 Å	1.775 Å	1.742 Å
M-C / M-P	2.007 Å	2.004 Å	2.547 Å	2.528 Å
C-C / P-P	1.429 Å	1.430 Å	2.147 Å	2.154 Å
C-H	1.086 Å	1.086 Å	-	-

Table S2. Spin state energetics of **Fc** and **TdP** in eclipsed (D_{5h}) and staggered (D_{5d}) conformation relative to ground low spin state

	Fc			TdP		
	LS*	IS*	HS*	LS*	IS*	HS*
D_{5d} conformation	0.0	48.3	50.3	0.0	31.4	57.3
D_{5h} conformation	0.0	48.9	51.6	0.0	34.4	65.1

*LS- low spin, IS- intermediate spin, HS- high spin

S3: Energy decomposition analysis

Table S3. Energy decomposition analysis of D_{5d} structure obtained by rotation by 180° and optimized D_{5d} structure of **Fc**

Fc			
	D_{5d} (rot.) kcal/mol	Δ ($D_{5d}(\text{opt.}) - D_{5d}(\text{rot.})$)	D_{5d} (opt.) kcal/mol
E	-3118.07	-0.05	-3118.12
ΔE_{prep}	240.62	-0.72	239.90
ΔE_{deform}	1.62	-0.22	1.40
$\Delta E_{\text{cyc-cyc}}$	103.29	-0.50	102.79
ΔE_{valexc}	135.71	0.00	135.71
ΔE_{elstat}	-620.47	0.74	-619.73
ΔE_{Pauli}	348.46	-2.83	345.63
ΔE_{orbint}	-634.45	2.79	-631.66
E_{total}	-665.84	-0.02	-665.86