

Supplementary data for the article:

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# CHEMISTRY

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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

	<b>Fc</b>		<b>TdP</b>	
	$D_{5d}$	$D_{5h}$	$D_{5d}$	$D_{5h}$
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

	<b>Fc</b>			<b>TdP</b>		
	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  $180^\circ$  and optimized  $D_{5d}$  structure of **Fc**

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