

(1,3,5-C₃P₃H₃)M 与(1,3,5-C₃P₃H₃)₂M (M=Ti, V, Cr)

配合物的结构与芳香性

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Structures and Aromaticities of Complexes (1,3,5-C₃P₃H₃)M and (1,3,5-C₃P₃H₃)₂M (M=Ti, V, Cr)

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表 S1 (1,3,5-C₃P₃H₃)M (M=Ti, V, Cr)解离为不同自旋态金属解离反应的解离能(*E*)

Table S1 The dissociation reactions energies (*E*) of (1,3,5-C₃P₃H₃)M (M=Ti, V, Cr) dissociate into metal with different spin multiplicity

Reaction	<i>E</i> /(kJ/mol)		
	(C ₃ P ₃ H ₃)Ti	(C ₃ P ₃ H ₃)V	(C ₃ P ₃ H ₃)Cr
(C ₃ P ₃ H ₃)M(*,C _{3v})→C ₃ P ₃ H ₃ (¹ A ₁ ' ,D _{3h})+M(¹ G/ ² G)	294.58	417.99	105.82
(C ₃ P ₃ H ₃)M(*,C _{3v})→C ₃ P ₃ H ₃ (¹ A ₁ ' ,D _{3h})+M(³ G/ ⁴ G)	163.30	-109.74	-153.93
(C ₃ P ₃ H ₃)M(*,C _{3v})→C ₃ P ₃ H ₃ (¹ A ₁ ' ,D _{3h})+M(⁵ G/ ⁶ G)	-12.61	-304.03	-319.79

The electronic state: (1,3,5-C₃P₃H₃)Ti (C_{3v}) is ⁵A₁; (1,3,5-C₃P₃H₃)Cr is ¹A₁; (1,3,5-C₃P₃H₃)V is ²A₁; Ti and Cr are ¹G, ³G and ⁵G; V is ²G, ⁴G, ⁶G.