Electronic Supplementary Material (ESI) for Dalton Transactions
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Probing the structural and magnetic properties of transition metal-benzene anion complexes

Supplementary Information

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Table S1 Calculated vertical detachment energies (VDEs) for $TiBz^-$ by considering the C_{2v} point symmetry, all units in eV.

System	VDE(α) (triplet)	VDE(β) (quintet)	Expt.[a]
$TiBz^-$ (quartet)	0.68		1.05±0.05
		0.90	
	0.93		
	1.00		
	1.28		

[a] Experimental VDEs from ref. 3.

Table S2 Calculated vertical detachment energies (VDEs) for $TiBz^-$ by considering the C_{6v} point symmetry, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt.[a]
$TiBz^-$ (doublet)		0.77	1.05±0.05
	0.83		
	0.91		

[a] Experimental VDEs from ref. 3.

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Table S3 Calculated vertical detachment energies (VDEs) for $TiBz_2^-$, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt.[a]
$TiBz_2^-$ (doublet)	0.37		0.23±0.05
		1.23	
		1.23	
	1.38		
	1.38		

[a] Experimental VDEs from ref. 3.

Table S4 Calculated vertical detachment energies (VDEs) for $Ti_2Bz_2^-$ by considering D_{2h} point symmetry, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)
$Ti_2Bz_2^-$ (D_{2h})		0.45
	0.49	
	0.58	
		0.77
	0.90	
		2.19
	2.24	
		2.49
	2.57	

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Table S5 Calculated vertical detachment energies (VDEs) for $Ti_2Bz_2^-$ by considering C_{2h} point symmetry, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)
$Ti_2Bz_2^-$ (C_{2h})	0.42	
		0.91
	0.94	
		1.89
		1.90
	1.92	
	1.94	
		1.96
	2.16	

Table S6 Calculated vertical detachment energies (VDEs) for $Ti_2Bz_3^-$ by considering quartet spin state, all units in eV.

System	VDE(α) (triplet)	VDE(β) (quintet)	Expt. [a]
$Ti_2Bz_3^-$ (quartet)	0.81		0.90±0.075
	0.90		
		1.10	
	1.18		
	1.27		
		1.93	
		2.12	
	2.33		
	2.34		

[a] Experimental VDEs from ref. 3.

Table S7 Calculated vertical detachment energies (VDEs) for $Ti_2Bz_3^-$ by

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considering doublet spin state, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt. [a]
$Ti_2Bz_3^-$ (doublt)		0.87	0.90±0.075
		0.90	
		0.90	
	1.02		
	1.02		
		2.21	
		2.21	
	2.32		
	2.32		

[a] Experimental VDEs from ref. 3.

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Table S8 Calculated vertical detachment energies (VDEs) for $CoBz^-$, all units in eV.

System	VDEs (doublet)	VDEs (quartet)
$CoBz^-$ (triplet)		0.26
	0.91	
		1.10
	1.74	
		2.00
	2.01	
		2.03
	2.59	
	2.61	

Table S9 Calculated vertical detachment energies (VDEs) for $CoBz_2^-$, all units in eV.

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System	VDEs (doublet)	Expt. [a]
$CoBz_2^-$ (singlet)	0.75	0.70
	1.37	
	1.43	1.45
	2.27	2.20
	2.33	

[a] Experimental VDEs from ref. 4.

Table S10 Calculated vertical detachment energies (VDEs) for $Co_2Bz_2^-$, all units in

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eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt. [a]
$Co_2Bz_2^-$ (doublet)		0.94	1.11
		1.03	
	1.24		
	1.34		
	1.40		
		1.49	1.50
		1.66	
		1.79	1.79
	1.86		
		0.96	
	2.01		
	2.07		
		2.31	
	2.36		
		2.43	
	2.61		
		2.72	
	2.76		
	3.24		

[a] Experimental VDEs from ref. 4.

Table S11 Calculated vertical detachment energies (VDEs) for $Co_2Bz_3^-$ by

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considering the lowest-energy sandwich structure, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt. [a]
$Co_2Bz_3^-$ (doublet)		0.78	0.95
	1.30		1.30
	1.34		
		1.49	
		1.61	
	1.74		1.75
		1.79	
	1.91		
		2.01	
	2.29		
	2.33		
		2.48	2.45
		2.50	
		2.57	
		2.63	
	2.79		
	2.81		
	2.86		
	2.90		

[a] Experimental VDEs from ref. 4.

Table S12 Calculated vertical detachment energies (VDEs) for $Co_2Bz_3^-$ by

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considering the lowest-energy rice-ball structure, all units in eV.

System	VDE(α) (singlet)	VDE(β) (triplet)	Expt. [a]
$Co_2Bz_3^-$ (doublet)	1.27		1.30
	1.273		
		1.46	
	1.59		
		1.81	1.75
	1.83		
		1.86	
		2.02	
		2.07	
	2.12		
	2.17		
	2.21		2.45
		2.68	
		2.77	
	2.79		
	2.99		
		3.05	
	3.06		
	3.22		

[a] Experimental VDEs from ref. 4.