Supporting information for:

Intercluster B-H and B-B Aggregation in *iso*- and *trans*-$[B_{20}H_{18}]^{2-}$. Spherical Aromaticity in Borane Dimers

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Content

Table S1. Energy decomposition analysis of the overall formation energy for both *iso*- and *trans*-$[B_{20}H_{18}]^{2-}$, and the respective energy differences. Values in kcal/mol. Relative energy differences in both kcal/mol and kJ/mol.

	iso-$[B_{20}H_{18}]^{2-}$	*trans*-$[B_{20}H_{18}]^{2-}$		kcal/mol	kJ/mol
ΔE_{Pauli}	19679.5	19625.6	$\Delta\Delta E_{\text{Pauli}}$	53.9	225.5
ΔE_{elstat}	-4336.8	-4302.7	$\Delta\Delta E_{\text{elstat}}$	-34.1	-142.5
ΔE_{orb}	-19851.4	-19836.7	$\Delta\Delta E_{\text{orb}}$	-14.7	-61.3
ΔE_{disp}	-70.6	-70.9	$\Delta\Delta E_{\text{disp}}$	0.4	1.6
ΔE_{int}	-4579.2	-4584.7	$\Delta\Delta E_{\text{int}}$	5.6	23.3

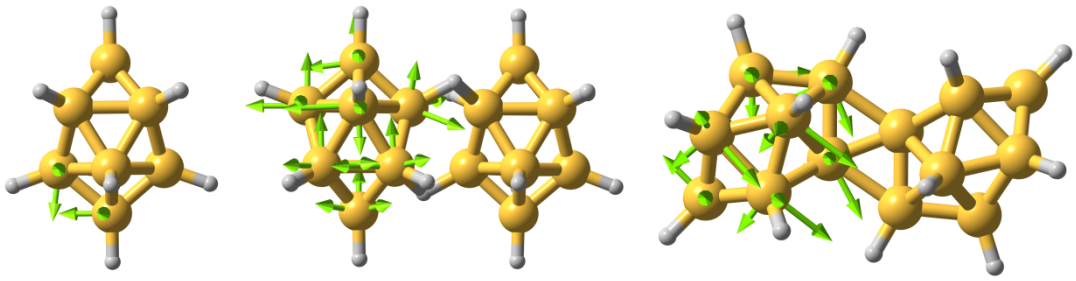

Figure S1. Orientation of the ^{11}B-NMR tensors according to their individual principal axis system (PAS), with the most shielding component denoted as longer arrows

Table S2. Calculated and experimental ^{11}B-NMR parameters, and the related chemical shift anisotropy (CSA) in terms of the absolute shielding tensor (σ_{ij}). Values in ppm. For details of calculation for ^{11}B-NMR chemical shifts, see main text.

closo-$[B_{10}H_{10}]^{2-}$	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	δ^{calc}	δ^{exp}
B	112.93	141.54	170.27	141.58	-28.46	-27.41
B	97.36	119.34	119.44	112.05	1.07	1.56
iso-$[B_{20}H_{18}]^{2-}$						
B	115.97	139.22	162.69	139.30	-26.18	-26.01
B	106.42	144.11	162.70	137.75	-24.63	-24.64
B	107.72	130.44	172.37	136.84	-23.72	-22.63
B	102.42	118.06	121.33	113.94	-0.82	-1.48
trans-$[B_{20}H_{18}]^{2-}$						
B	113.13	126.72	172.22	137.36	-24.24	-24.26
B	106.00	126.63	158.89	130.50	-17.38	-17.99
B	97.27	118.35	168.87	128.17	-15.05	-14.49
B	95.64	100.58	175.16	123.79	-10.67	-10.99
B	94.64	129.06	130.18	117.96	-4.84	-5.54
B	69.63	82.28	136.08	96.00	17.12	17.41
B	45.62	79.48	116.34	80.48	32.64	31.74

Experimental values for *closo*-$[B_{10}H_{10}]^{2-}$ from reference [1]. Experimental values for both *iso*- and *trans*-$[B_{20}H_{18}]^{2-}$ isomers from reference [2].

References

1 S. Kapuściński, M. B. Abdulmojeed, T. E. Schafer, A. Pietrzak, O. Hietsoi, A. C. Friedli and P. Kaszyński, *Inorg. Chem. Front.*, 2021, **8**, 1066–1082.

2 V. V. Avdeeva, V. I. Privalov, A. S. Kubasov, S. E. Nikiforova, E. A. Malinina and N. T. Kuznetsov, *Inorganica Chim. Acta*, 2023, **555**, 121564.