SUPPORTING INFORMATION

for

Why are Some $(CH)_4X_6$ and $(CH_2)_6X_4$ Polyheteroadamantanes So Stable?

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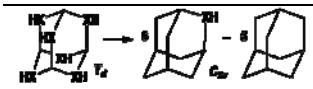
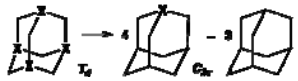
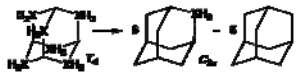
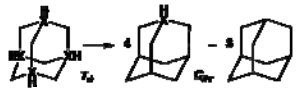
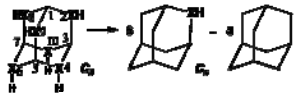
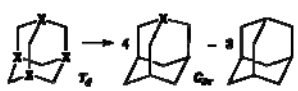
Table S1. Structural data (in Å and deg), NBO Charges (B3LYP/6-311+G**), and NICS (PW91/6-311+G**) at Cage Centers (NICS(0), in ppm) for **1-19**. The B3LYP/6-311+G** optimized geometries were used throughout. All the data for reference mono-substituted compounds are given in the parentheses.

Isodesmic equations	X	C–X	A–C–X[b]	C–X–C	$q_{C(X)}$	q_X	NICS(0)
	**1, B**	1.571	104.1	119.4	–1.24	0.71	5.95
		(1.573)	(107.4)	(112.9)	(–0.60)	(0.79)	(0.85)
	2, Al	1.954	106.4	115.3	–2.00	1.49	2.19
		(1.970)	(106.0)	(98.5)	(–0.79)	(1.59)	(0.34)
	3, Ga	1.983	106.6	115.0	–1.76	1.26	2.01
		(1.997)	(106.1)	(97.1)	(–0.70)	(1.30)	(1.03)
	**4, B**	1.591	91.1	116.9	–1.14	0.98	–5.07
		(1.568)	(98.4)	(116.5)	(–0.78)	(1.01)	(–4.74)
	5, Al	1.978	96.5	115.1	–1.62	1.68	6.89
		(1.958)	(96.2)	(110.1)	(–0.97)	(1.68)	(–0.79)
	6, Ga	2.008	95.6	115.4	–1.43	1.44	11.95
		(1.985)	(96.8)	(109.1)	(–0.87)	(1.41)	(–1.68)
	**7, Si**	1.898	110.5	107.3	–1.62	1.20	–0.50
		(1.895)	(107.8)	(97.8)	(–0.65)	(1.15)	(0.14)
	8, Ge	1.985	110.6	107.2	–1.46	1.03	–0.15
		(1.984)	(107.4)	(95.0)	(–0.58)	(0.95)	(0.38)
	**9, Si**	1.895	111.9	108.2	–1.35	1.43	–0.50
		(1.891)	(106.8)	(103.3)	(–0.83)	(1.37)	(0.11)
	10, Ge	1.981	111.8	108.3	–1.22	1.25	0.33
		(1.976)	(106.4)	(101.7)	(–0.76)	(1.16)	(0.41)
	**11, N**	1–2:1.470 2–3:1.463 3–4:1.474 3–10:1.483	8–1–2:110.0 2–3–10:108.4 2–3–4:107.2 4–3–10:113.8	1–2–3:108.8 3–4–5:108.6 (111.5)	1:0.32 3,5,7:0.32 (–0.03)	2,8,9:–0.69 4,6,10:– 0.71	4.59 (0.65)
		(1.479)	(111.9, 107.8)			(–0.69)	
	12, P	1–2:1.885 2–3:1.891 3–4:1.885 3–10:1.879	8–1–2:113.6 2–3–10:112.5 2–3–4:107.9 4–3–10:120.2	1–2–3:100.2 3–4–5:100.3 (93.9)	1:–1.18 3,5,7:–1.18 (–0.50)	2,8,9:0.65 4,6,10:0.65 (0.56)	3.01 (0.56)
		(1.886)	(112.7,107.1)				
	13, As	1–2:2.007 2–3:2.014 3–4:2.007 3–10:2.000	8–1–2:114.0 2–3–10:112.5 2–3–4:108.6 4–3–10:120.6	1–2–3:99.4 3–4–5:99.4 (89.9)	1: –1.23 3,5,7:–1.22 (–0.49)	2,8,9:0.72 4,6,10:0.71 (0.59)	3.09 (0.74)
		(2.014)	(112.1,106.9)				
	**14, N**	1.477	112.4	108.0	–0.00	–0.58	8.34
		(1.473)	(111.5)	(109.7)	(–0.24)	(–0.56)	(1.61)
		1.476[b]	113.6[b]	107.2[b]			
	15, P	1.871	123.4	101.7	–1.05	0.85	6.15
		(1.875)	(114.0)	(97.5)	(–0.68)	(0.77)	(1.67)
	16, As	1.993	124.7	100.9	–1.07	0.92	4.03
		(2.001)	(113.5)	(94.9)	(–0.68)	(0.81)	(1.42)
	**17, O**	1.412	109.9	108.7	0.67	–0.58	5.62
		(1.442)	(109.9)	(112.7)	(0.13)	(–0.62)	(0.70)
	18, S	1.840	114.1	99.1	–0.71	0.30	4.42
		(1.852)	(110.0)	(94.6)	(–0.33)	(0.17)	(0.76)

		1.84[b]	114.5[b]				
	19, Se	1.983 (2.002)	114.6 (109.5)	97.9 (89.9)	–0.90 (–0.37)	0.43 (0.25)	5.43 (0.79)

[a] A = C or X. [b] Experimental values (crystalline). **14** see [ref] Becka, L. N.; Cruickshank, D. W. J. *Proc. R. Soc. London, Ser. A.* **1963**, *273*, 435-454. **18** see [ref] (a) Fredga, A.; Olsson, K. *Ark. Kemi* **1956**, *9*, 163-168. (b) Andersen, E. K.; Lindqvist, I. *Ark. Kemi* **1956**, *9*, 169-173.

Reference

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