Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Structures, stabilities and aromatic properties of endohedrally transition metal doped boron clusters $M@B_{22}$, M = Sc and Ti: A theoretical study

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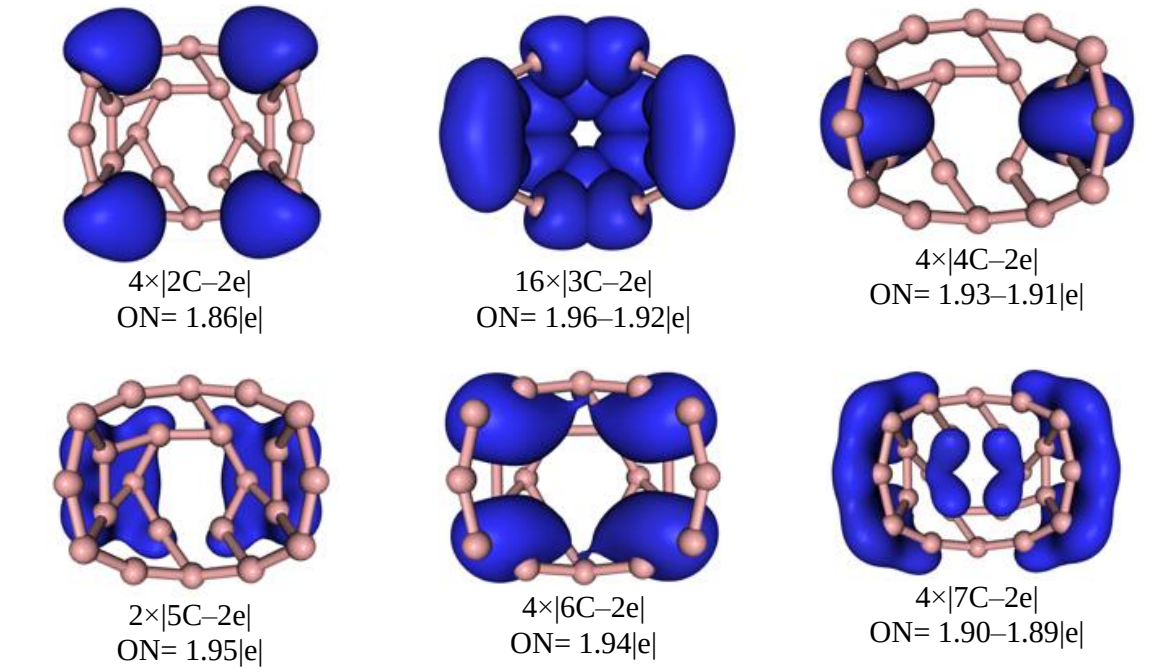

Figure S1. AdNDP analysis for the cage **5** (B_{22}-C_{2v}).

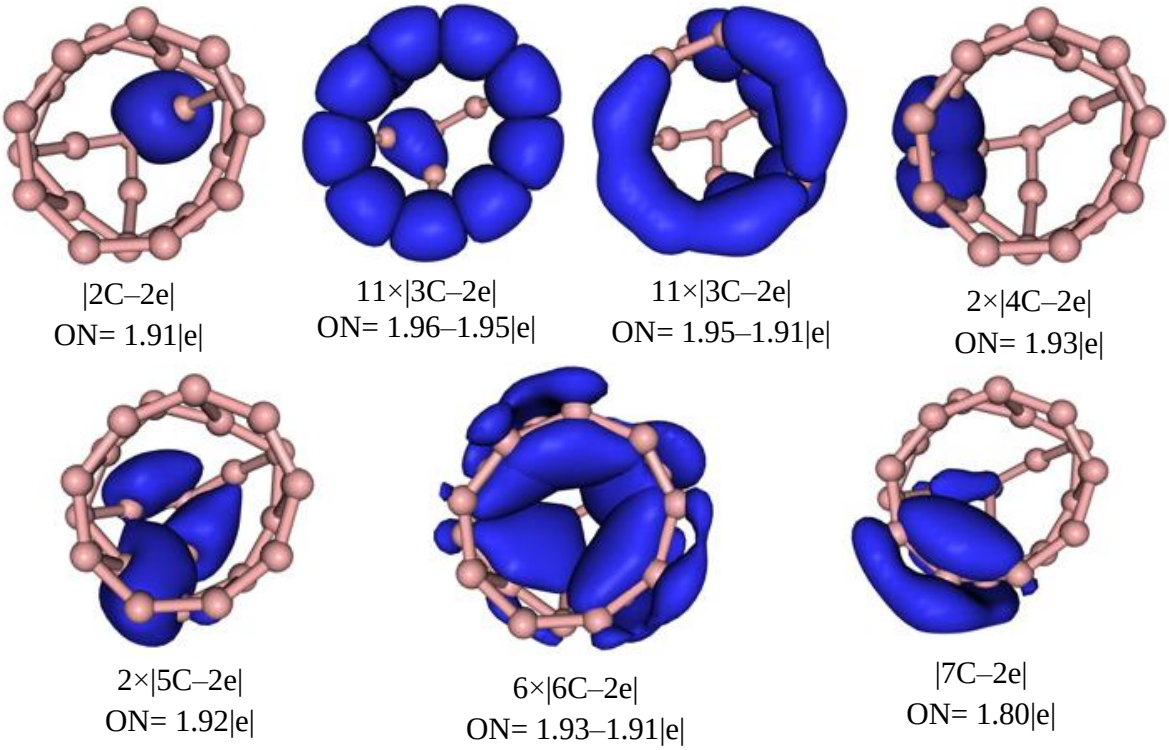

Figure S2. AdNDP analysis for the cage **4**(B_{22}-C_1).

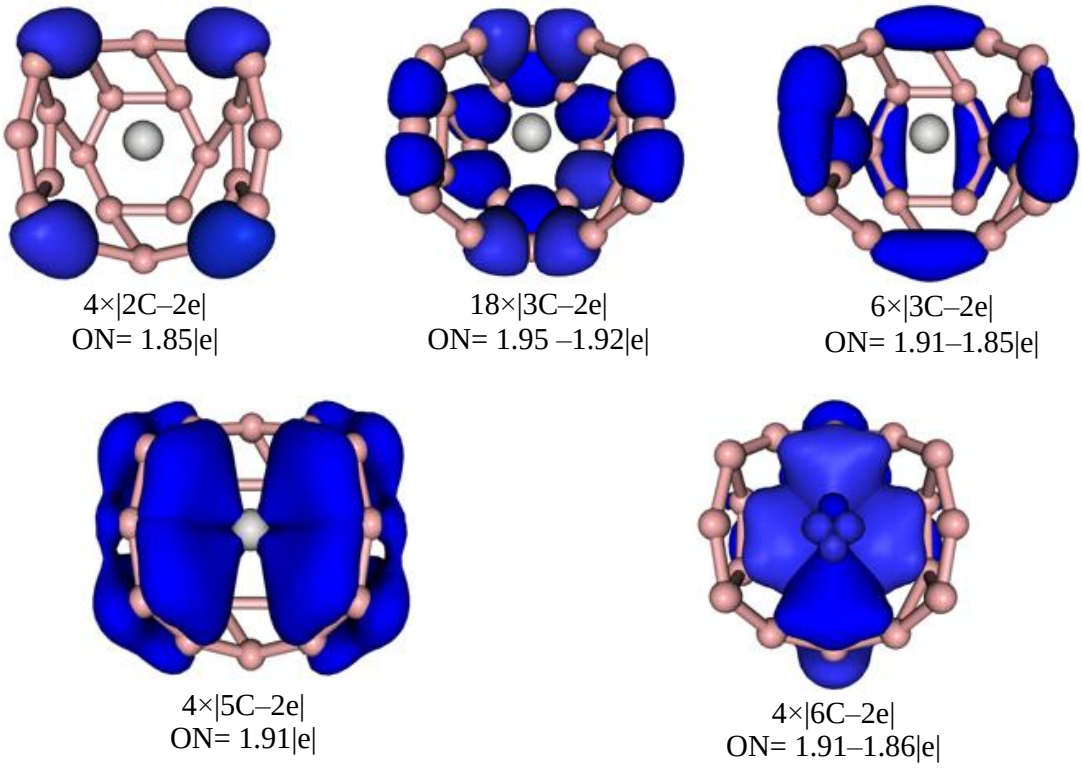

Figure S3. AdNDP analysis for the endohedral ***5-Sc***.

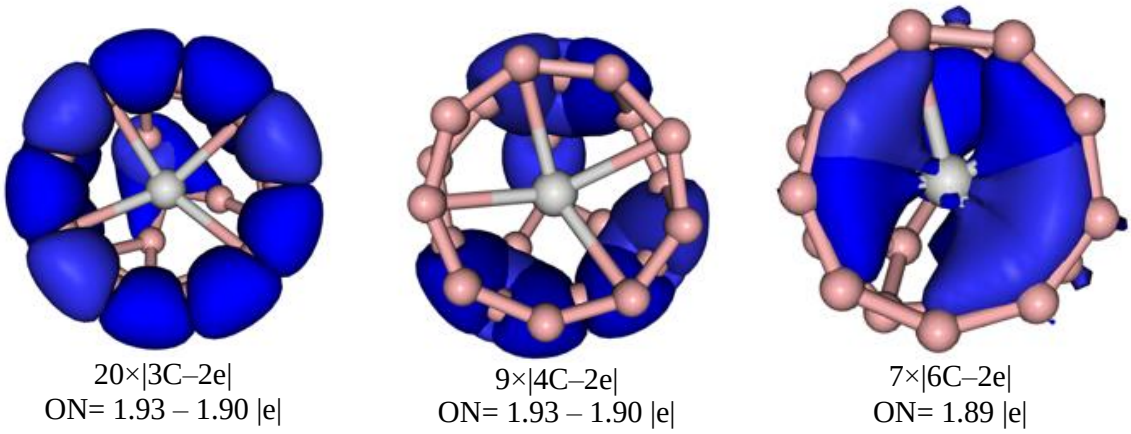

Figure S4. AdNDP analysis for the endohedral ***4-Sc***.

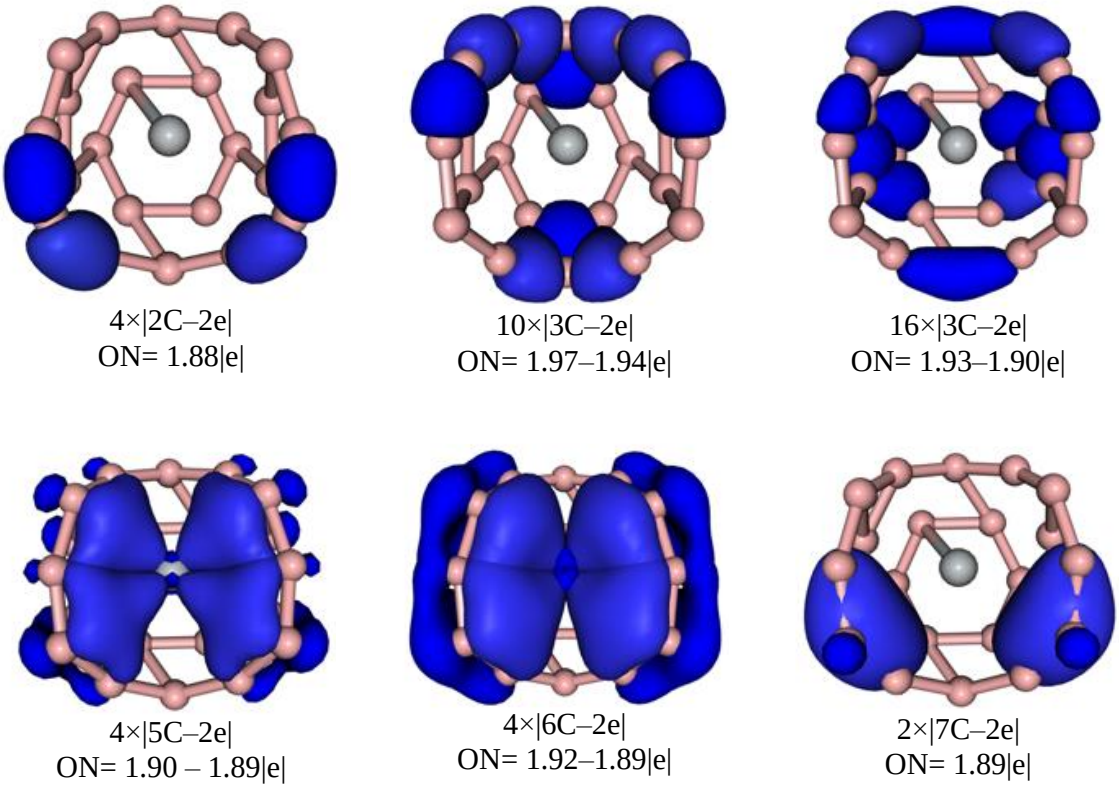

Figure S5. AdNDP analysis for the endohedral ***5-Ti*.**

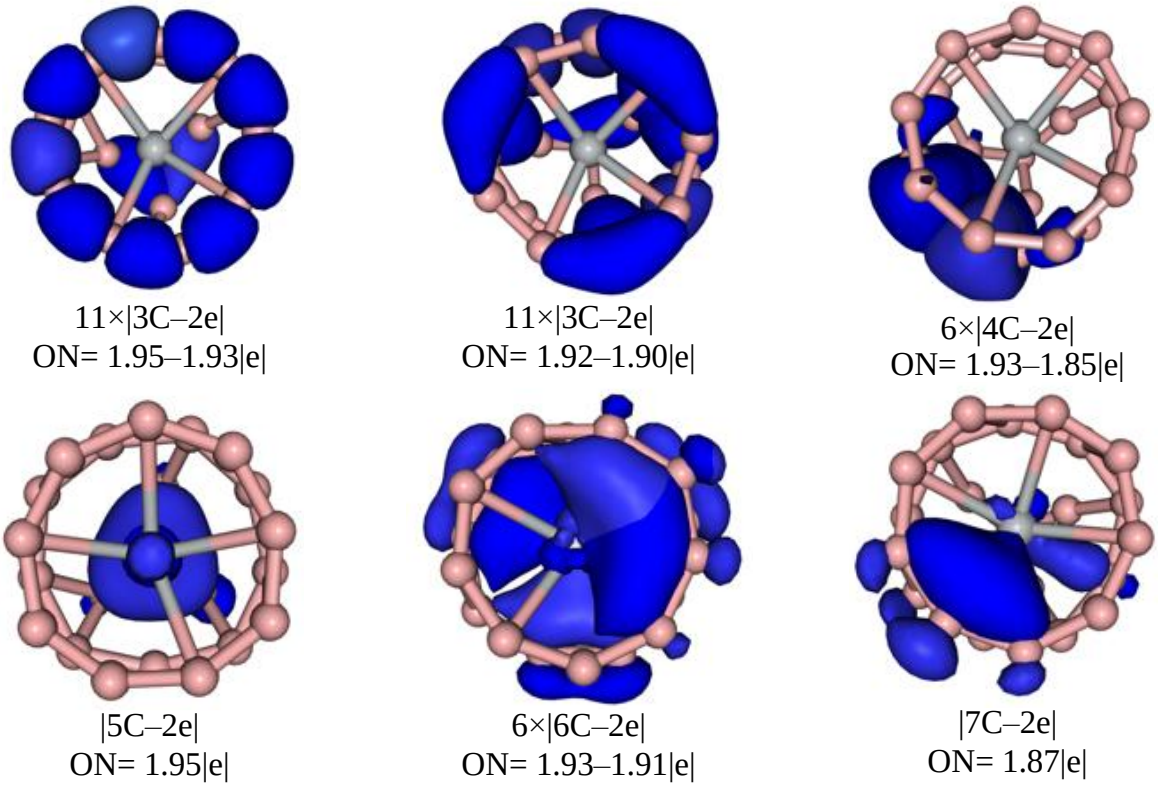

Figure S6. AdNDP analysis for the endohedral **4-*Ti***.

2 Endohedral coordinates XYZ

5-Ti

23

Ti@B22-C_1

B	-0.83268	0.26089	2.16476
B	0.05452	1.56797	1.55818
B	-2.34302	-0.15680	1.39526
B	1.49938	1.33011	-0.87000
B	-1.64062	-1.24436	2.27486
B	-0.07548	-1.37238	2.42967
B	2.68557	0.55505	-0.00000
B	-2.64518	0.61206	-0.00000
B	-0.07549	-1.37239	-2.42966
B	0.85900	0.20842	2.16811
B	-1.38936	1.33501	-0.84561
B	-2.34303	-0.15679	-1.39526
B	2.30310	-0.25515	1.34286
B	0.85900	0.20843	-2.16811
B	0.05452	1.56798	-1.55818
B	2.30310	-0.25516	-1.34286
B	-0.83268	0.26090	-2.16476
B	1.49938	1.33011	0.87001
B	-1.64063	-1.24436	-2.27487
B	1.45671	-1.38309	-2.01248
B	1.45672	-1.38308	2.01251
B	-1.38936	1.33500	0.84561
Ti	0.03882	-0.39787	-0.00000

4-Ti

23

#Ti@B22-C_{2v}

B	-1.87417	-0.42695	-0.78959
B	-0.43700	-1.72384	-1.12123
B	-0.49729	-0.02460	-2.23559
B	-1.21153	-1.26311	1.16672
B	-1.55359	1.02485	-1.58624
B	-2.03037	1.23485	-0.06057
B	2.20950	-0.32991	-1.39918
B	1.22278	0.68594	-2.14461
B	0.10612	1.75456	-1.85557
B	0.75738	-1.03936	-2.09511
B	1.32821	-1.79492	-0.77860
B	1.35227	-1.88389	0.83248
B	-1.71189	0.76045	1.44936
B	0.41461	-1.25595	1.97798
B	-0.84276	2.38160	-0.73970
B	-0.78393	2.26638	0.84546
B	2.47929	-0.68179	0.12039
B	-1.71792	-1.88512	-0.20232
B	-0.74306	-0.16906	2.33785
B	-0.20403	1.50897	2.10489
B	0.93604	0.44065	2.43231
B	1.97679	-0.42774	1.61186
Ti	0.18580	0.19212	0.02837

5-Sc

23

Sc@B_{22}–C_1

B	-0.84254	0.24444	2.22833
B	0.04356	1.50623	1.56760
B	-2.31705	-0.21093	1.41363
B	1.47320	1.19122	-0.85871
B	-1.59312	-1.27009	2.30116
B	-0.03946	-1.36112	2.59047
B	2.64488	0.38471	0.00000
B	-2.61828	0.53766	0.00000
B	-0.03946	-1.36112	-2.59047
B	0.85519	0.19556	2.22856
B	-1.40176	1.27432	-0.85869
B	-2.31705	-0.21093	-1.41363
B	2.30090	-0.34450	1.41403
B	0.85519	0.19556	-2.22856
B	0.04356	1.50623	-1.56760
B	2.30090	-0.34450	-1.41403
B	-0.84254	0.24444	-2.22833

B	1.47320	1.19122	0.85871
B	-1.59312	-1.27009	-2.30116
B	1.51701	-1.35975	-2.30195
B	1.51701	-1.35975	2.30195
B	-1.40176	1.27432	0.85869
Sc	-0.01845	-0.65309	0.00000

4-Sc

23

Sc@B_{22}–C_1

B	-1.87726	-0.41001	-0.85619
B	-0.43462	-1.72674	-1.15698
B	-0.50615	-0.04019	-2.20697
B	-1.23088	-1.25516	1.20639
B	-1.56009	1.04950	-1.59643
B	-2.02039	1.23267	-0.05881
B	2.21230	-0.34121	-1.40881
B	1.20190	0.65930	-2.20468
B	0.05996	1.74319	-1.92285
B	0.77087	-1.05089	-2.10605
B	1.32801	-1.79314	-0.77193
B	1.37923	-1.89326	0.84550
B	-1.70691	0.75052	1.45458
B	0.41608	-1.25929	1.97739
B	-0.83865	2.38820	-0.73609
B	-0.86452	2.28003	0.87754
B	2.50370	-0.73192	0.12137
B	-1.70041	-1.84933	-0.19973
B	-0.73781	-0.17119	2.35979
B	-0.23826	1.50775	2.14221
B	0.93307	0.42935	2.45462
B	1.99057	-0.46602	1.64047
Sc	0.28149	0.29198	0.04503