

Supporting Information

Recyclable and superior selective CO₂ adsorption of C₄B₃₂ and Ca@C₄B₃₂: A new category of perfect cubic heteroborosphenes

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Fig. S1 Low-lying isomers of C-doped heteroborospherene C_4B_{32} with the relative energy less than 1.00 eV.

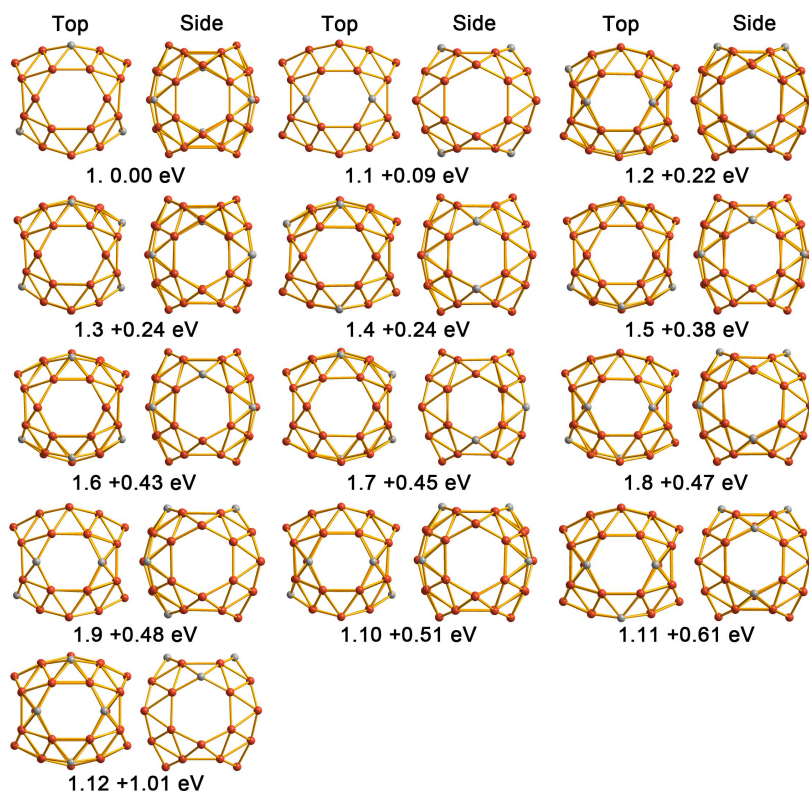


Fig. S2 π -CMOs of C_{2v} C_4B_{32} .

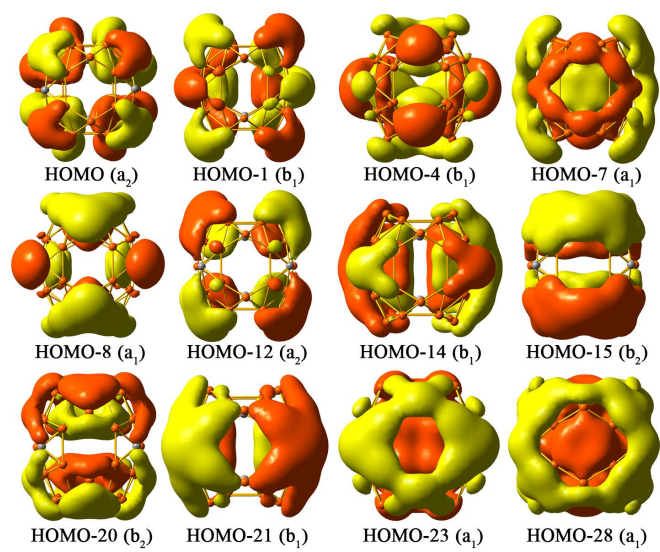
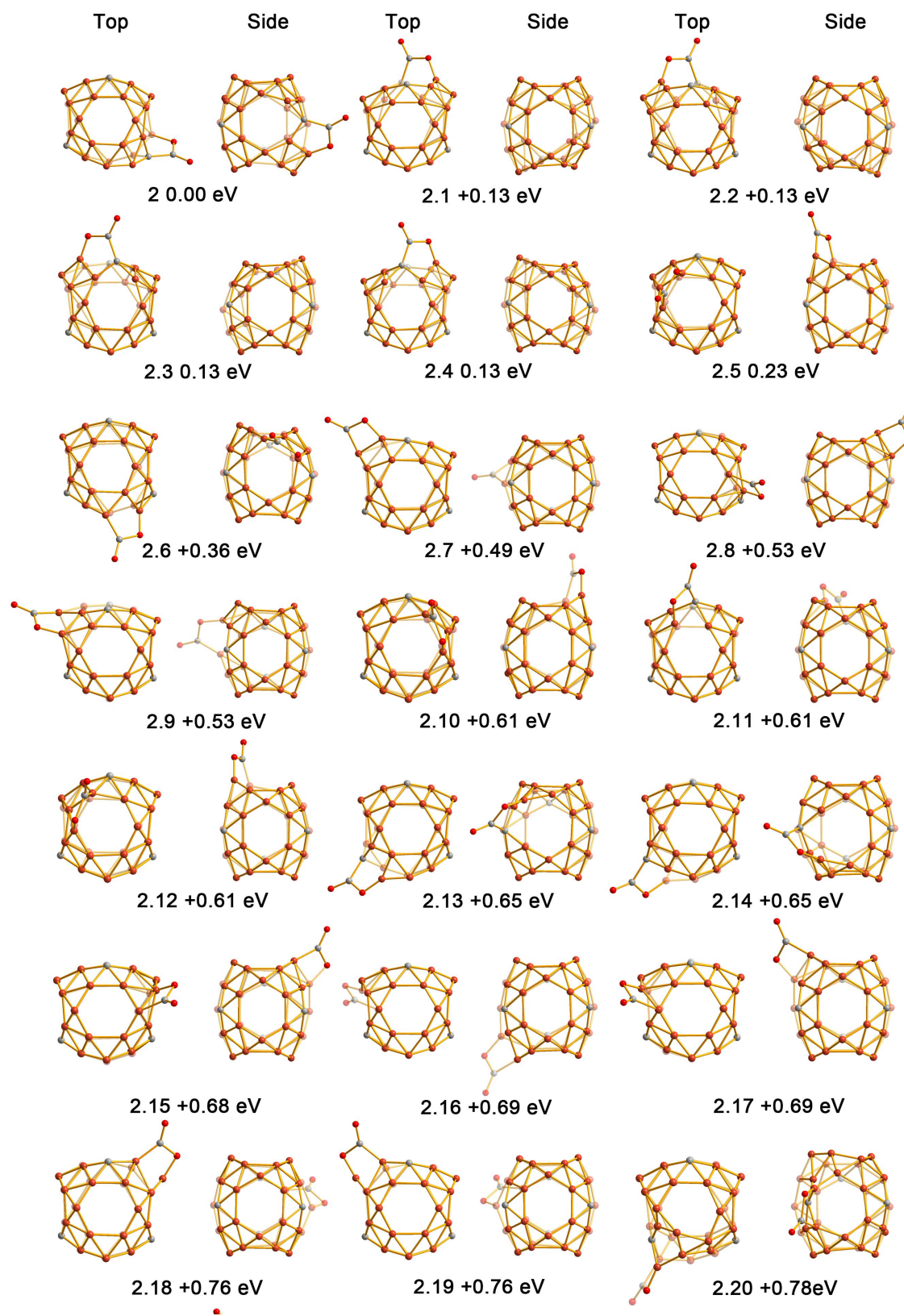


Fig. S3 Low-lying isomers of CO₂&C₄B₃₂ with the relative energy indicated in eV.



(Fig. S3 Continued)

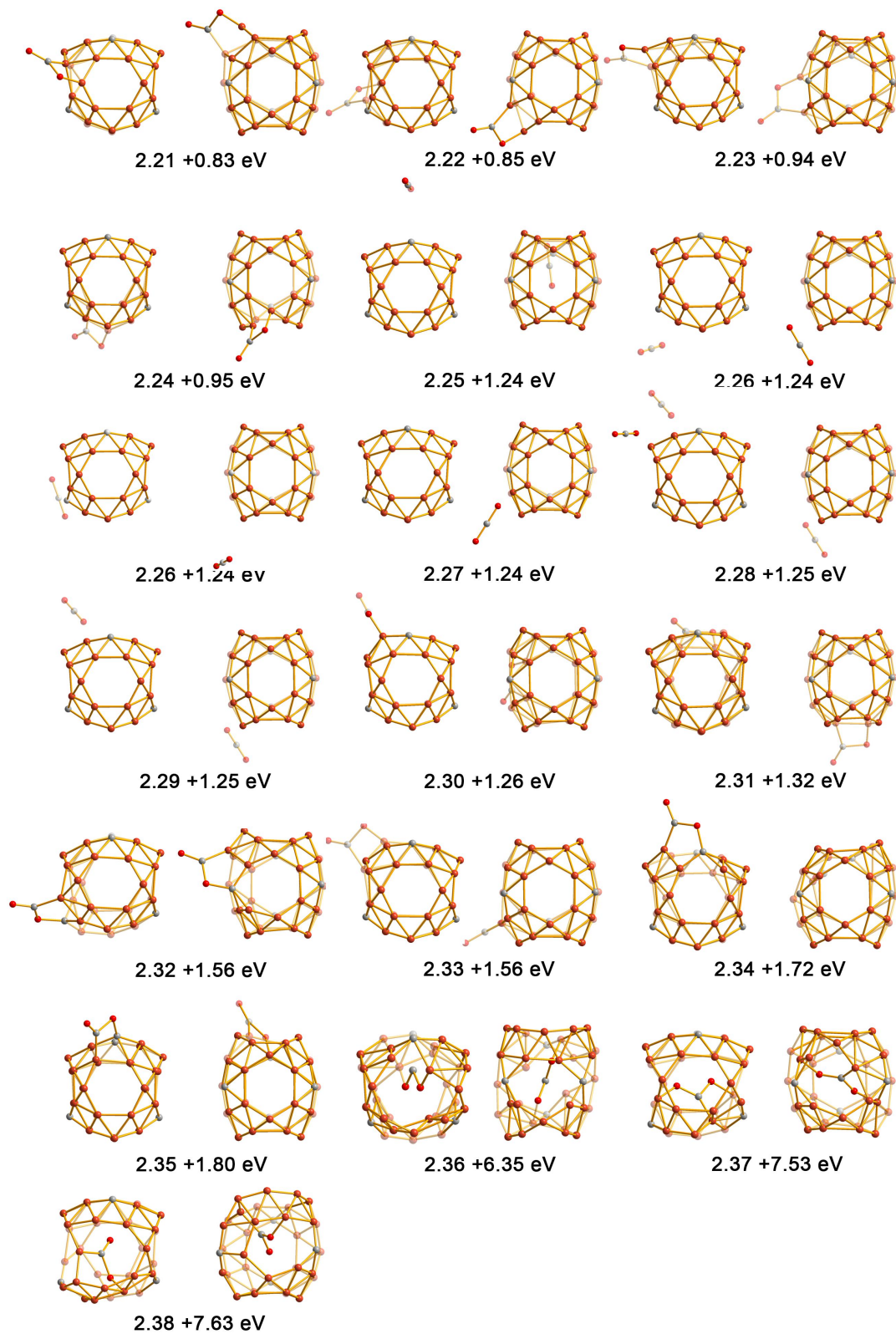
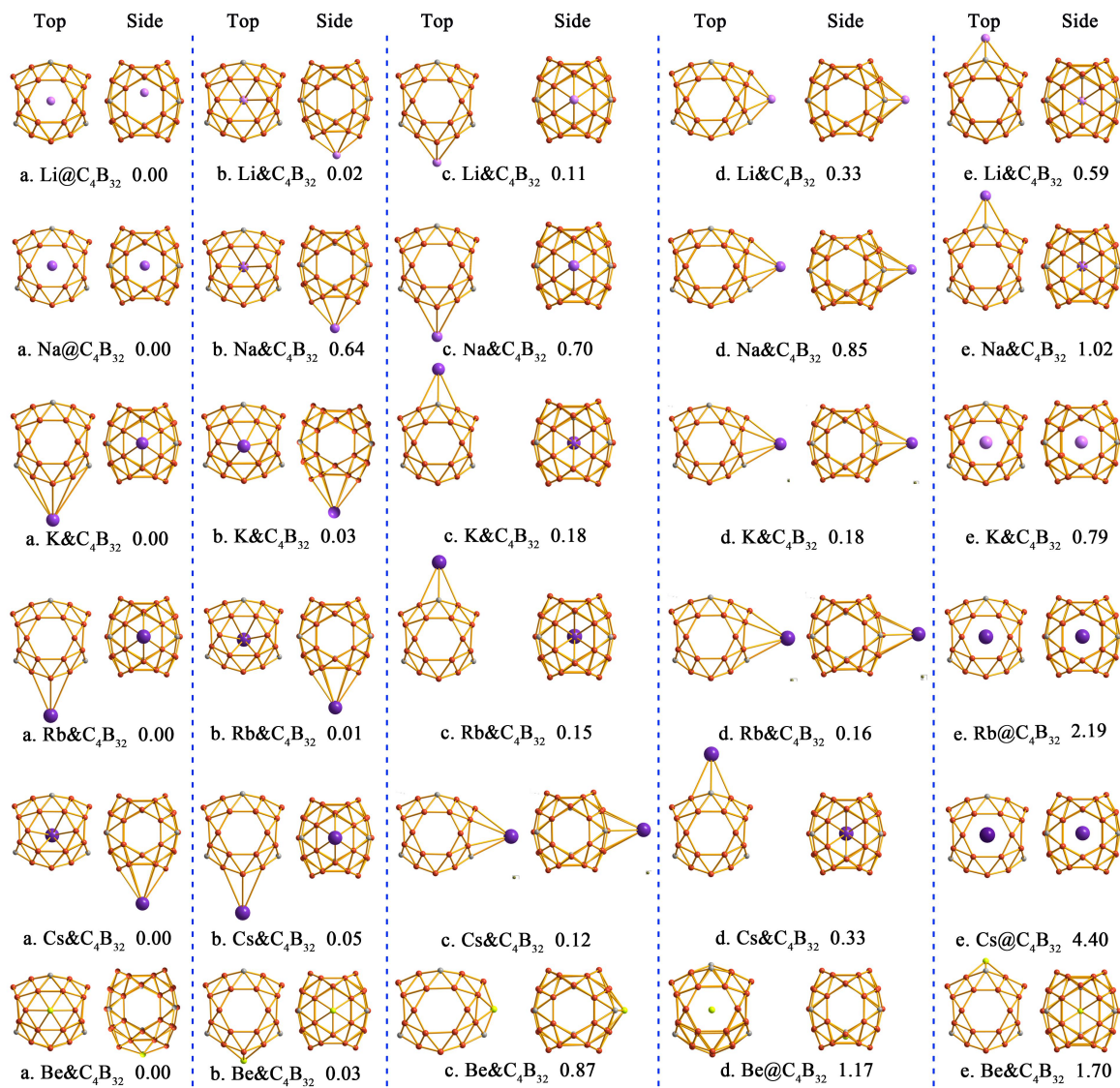


Fig. S4 Low-lying isomers of M-doped C_4B_{32} fullerenes (M=Li, Na, K, Rb, Cs, Be, Mg, Ca, Sr, Ba, Sc, Y, Ti) with their relative energies indicated in eV.



(Fig. S4 Continued)

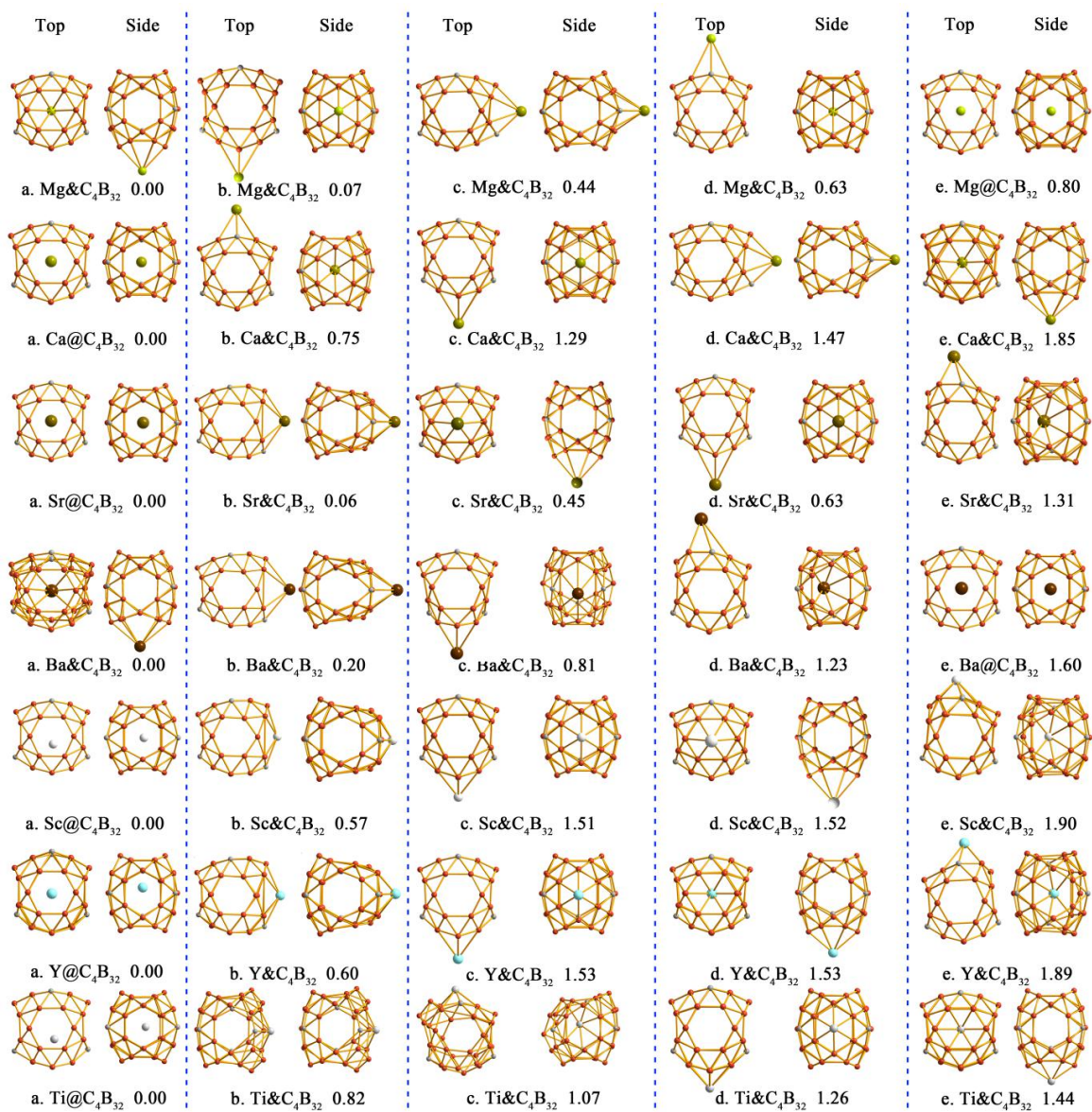


Table S1. Optimized coordinates of the most stable structures of C_4B_{32} and CO_2 & C_4B_{32} at the PBE0/6-311+G* level.

(1) $C_{2v} C_4B_{32}$

B	-0.917877	2.360242	1.407523
B	-1.320725	0.867368	-2.206387
B	-1.314134	-0.910803	2.247994
B	-1.320725	-0.867368	-2.206387
B	-0.881595	2.282943	-1.331580
B	-0.917877	-2.360242	1.407523
B	-0.881595	-2.282943	-1.331580
B	-2.304376	-1.433468	-0.916831
B	-1.679587	2.675186	0.009580
B	-1.314134	0.910803	2.247994
B	-2.177095	-1.323380	0.824561
B	-2.304376	1.433468	-0.916831
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B	-1.679587	-2.675186	0.009580
B	1.679587	-2.675186	0.009580
B	0.000000	1.728626	2.645864
B	0.000000	-1.728626	2.645864
B	1.679587	2.675186	0.009580
B	2.601689	0.000000	-1.641325
B	-2.601689	0.000000	-1.641325
C	0.000000	1.596416	-2.445714
C	0.000000	-1.596416	-2.445714
C	2.383657	0.000000	1.550498
C	-2.383657	0.000000	1.550498

(2) C₁ CO₂&C₄B₃₂

B	1.165649	-1.797125	1.522959
B	-0.237964	-1.813763	-1.903550
B	1.832074	2.142708	0.940988
B	-0.344870	-0.246050	-2.573311
B	-0.164528	-2.896590	-0.528778
B	0.720085	2.777334	-0.171113
B	-0.479864	1.455353	-2.373919
B	1.044397	0.690133	-2.094456
B	1.192297	-2.905041	0.304414
B	1.808627	-0.288651	1.381388
B	1.649070	1.418937	-0.631818
B	1.232852	-2.098853	-1.116773
B	2.292493	-1.612781	0.219794
B	-0.919889	2.886324	0.599546
B	-2.711778	0.078430	-1.570680
B	-0.585236	0.218219	2.562616
B	-2.600184	-1.510603	-0.860032
B	-2.018839	1.667952	-1.583795
B	-0.536751	-1.493241	2.355241
B	-1.745373	-2.495271	0.260054
B	-2.907259	-1.383091	0.829181
B	-0.752871	1.898546	2.005191
B	-2.039260	-0.605762	2.145855
B	-3.082234	1.229096	-0.334387
B	-2.155524	1.777944	1.033341
B	0.717846	2.282819	-1.713442
B	-2.247731	2.672308	-0.345986
B	0.797601	-0.566054	2.568979
B	0.495772	2.815560	1.490765
B	-1.875719	-2.223085	1.832767
B	-3.565693	-0.331690	-0.225726
B	1.120656	-0.925822	-2.211606
C	-1.482967	-2.456182	-1.283707
C	-1.687106	0.496452	-2.621486
C	-1.957072	0.902583	2.272715
C	2.527330	0.816184	0.560934
C	3.796042	0.174784	0.041866
O	3.588122	-1.166270	-0.145293
O	4.828550	0.704535	-0.216014