Supplementary Material

Theoretical Investigations on the Geometrical Structures, Energies and Electronic Properties of the Heterofullerenes Made of the Smallest Fullerene

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Fig. S1. Framework and the atomic index of $C_{19}X$ ($X = B, N, O, Al, Si, P, S, Ga, Ge, As$ and Se) and C_{20} Cages.

Table S1. Bond lengths of C₂₀ and the doped cages (the atomic index is shown in Fig. S1).

Bond-Index	C ₁₉ B	C ₁₉ Al	C ₁₉ Ga	C ₂₀	C ₁₉ Si	C ₁₉ Ge	C ₁₉ N	C ₁₉ P	C ₁₉ As	C ₁₉ O	C ₁₉ S	C ₁₉ Se
R(1, 2)	1.550	1.923	1.940	1.486	1.847	1.929	1.477	1.887	1.987	1.436	1.839	1.956
R(1, 3)	1.549	1.923	1.940	1.486	1.854	1.945	1.477	1.897	1.987	1.686	1.839	1.956
R(1, 4)	1.550	1.923	1.940	1.400	1.854	1.945	1.477	1.897	1.987	1.686	1.839	1.956
R(2, 6)	1.446	1.447	1.445	1.423	1.439	1.434	1.421	1.430	1.433	1.412	1.430	1.433
R(2, 9)	1.447	1.447	1.445	1.445	1.439	1.434	1.421	1.430	1.433	1.412	1.430	1.433
R(3, 12)	1.446	1.447	1.445	1.422	1.392	1.381	1.421	1.420	1.433	1.428	1.430	1.433
R(3, 13)	1.446	1.447	1.445	1.445	1.521	1.520	1.421	1.458	1.433	1.472	1.430	1.433
R(4, 7)	1.446	1.447	1.445	1.486	1.392	1.381	1.421	1.420	1.433	1.428	1.430	1.433
R(4, 8)	1.447	1.447	1.445	1.486	1.521	1.520	1.421	1.458	1.433	1.424	1.430	1.433
R(5, 8)	1.447	1.436	1.436	1.445	1.452	1.452	1.463	1.463	1.439	1.410	1.414	1.413
R(5, 11)	1.447	1.461	1.462	1.443	1.452	1.452	1.463	1.463	1.457	1.493	1.494	1.493
R(5, 15)	1.447	1.443	1.443	1.445	1.445	1.447	1.463	1.450	1.445	1.401	1.449	1.448
R(6, 8)	1.494	1.523	1.521	1.423	1.518	1.518	1.452	1.473	1.487	1.493	1.510	1.519
R(6, 10)	1.447	1.436	1.436	1.400	1.406	1.403	1.452	1.436	1.439	1.413	1.414	1.413
R(7, 11)	1.432	1.436	1.436	1.443	1.477	1.481	1.451	1.472	1.439	1.405	1.414	1.413
R(7, 12)	1.494	1.523	1.521	1.536	1.521	1.534	1.455	1.454	1.487	1.493	1.510	1.519
R(9, 13)	1.493	1.523	1.521	1.536	1.429	1.430	1.453	1.416	1.487	1.493	1.510	1.519
R(9, 14)	1.432	1.436	1.436	1.445	1.420	1.420	1.451	1.454	1.439	1.446	1.414	1.413
R(10, 14)	1.470	1.461	1.462	1.422	1.435	1.431	1.452	1.445	1.457	1.490	1.494	1.493
R(10, 15)	1.432	1.443	1.443	1.422	1.477	1.481	1.451	1.472	1.445	1.455	1.449	1.448
R(11, 16)	1.470	1.443	1.443	1.445	1.429	1.430	1.453	1.416	1.445	1.405	1.449	1.448
R(12, 17)	1.448	1.436	1.436	1.422	1.435	1.431	1.452	1.445	1.439	1.410	1.414	1.413
R(13, 18)	1.448	1.436	1.436	1.445	1.518	1.518	1.452	1.473	1.439	1.401	1.414	1.413
R(14, 19)	1.448	1.443	1.443	1.486	1.406	1.403	1.452	1.436	1.445	1.472	1.449	1.448
R(15, 20)	1.470	1.448	1.447	1.486	1.485	1.495	1.453	1.426	1.458	1.464	1.456	1.455
R(16, 17)	1.432	1.443	1.443	1.423	1.469	1.468	1.451	1.473	1.445	1.455	1.449	1.448
R(16, 20)	1.447	1.448	1.447	1.486	1.451	1.453	1.455	1.437	1.458	1.470	1.456	1.455
R(17, 18)	1.432	1.461	1.462	1.423	1.420	1.420	1.451	1.454	1.457	1.490	1.494	1.493
R(18, 19)	1.432	1.443	1.443	1.486	1.469	1.468	1.451	1.473	1.445	1.470	1.449	1.448
R(19, 20)	1.448	1.448	1.447	1.445	1.451	1.453	1.455	1.437	1.458	1.446	1.456	1.455

Figure S2. HOMO (left) and LUMO (right) of C_{20} and the doped cages.