

# Full Geometry Optimizations of Bond-Stretch Isomers of $C_{20}^{2+}$ Fullerene Dication by the Hybrid Density Functional B3LYP Methods

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**Table S1.** Geometrical isomers with the lowest energy of neutral  $C_{20}$  by using various theoretical methods

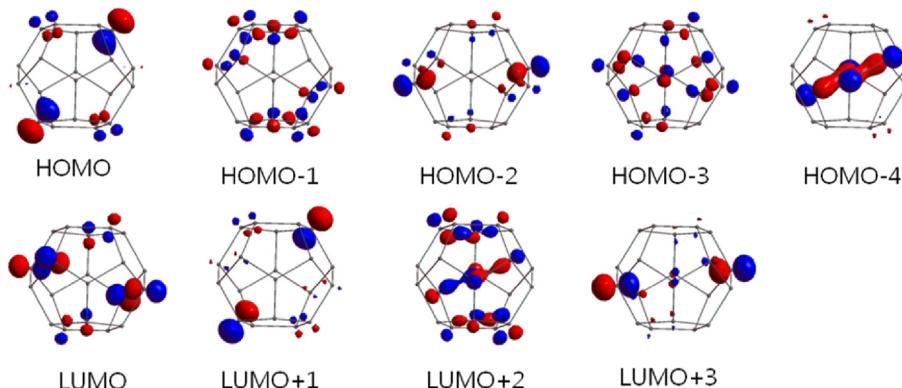
Geometrical isomers	Theoretical methods
Ring	HF-SCF, <sup>13a</sup> BLYP, <sup>16</sup> B3LYP <sup>18</sup>
Bowl	MP2, <sup>14</sup> valence-only pseudopotential QMC, <sup>14</sup> CCSD, <sup>15</sup> B3PW91 <sup>18</sup>
Cage	MP2, <sup>13a,14,18</sup> CCSD(T) <sup>15,16,18</sup>

**Table S2.** The energies (a.u.) of the HOMO and LUMO of  $C_{20}^{2+}$  isomers

Isomers	$C_2$	$C_{2h}$	$D_{2h}$	$T_h$	$I_h$
LUMO energy	-0.47792 (a)	-0.47796 (a <sub>u</sub> )	-0.47798 (b <sub>1u</sub> )	-0.47797 (t <sub>u</sub> )	-0.47788 (g <sub>u</sub> )
HOMO energy	-0.62147 (a)	-0.62143 (a <sub>g</sub> )	-0.62145 (a <sub>g</sub> )	-0.62143 (t <sub>g</sub> )	-0.62149 (h <sub>g</sub> )

Figure for Table S2 is the degenerate HOMOs and LUMOs of  $C_{20}^{2+}$  with the  $I_h$  and  $T_h$  symmetries.

1. The fivefold HOMOs and fourfold LUMOs for  $I_h$  symmetry



2. The threefold HOMOs and LUMOs for  $T_h$  symmetry

