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Polynuclear sandwich derivatives of [10]annulene: a quantum chemical study

Tatyana N. Gribanova, Ruslan M. Minyaev and Vladimir I. Minkin

Table of contents: Atomic coordinates of optimized structures 4, 7, 8 calculated by B3LYP/6-311+G(df,p) and M06/6-311+G(df,p) methods and diagram of the formation of the main stabilizing orbitals of complexes from fragment orbitals (Fig. S1).

4 (M=Cu) [B3LYP/6-311+G(df,p)]
D_{5h}

Cu	0.000000000000	2.435520000000	0.000000000000
Cu	-2.316317000000	0.752617000000	0.000000000000
Cu	2.316317000000	0.752617000000	0.000000000000
Cu	1.431563000000	-1.970377000000	0.000000000000
Cu	-1.431563000000	-1.970377000000	0.000000000000
C	-1.876620000000	-1.373888000000	1.961934000000
C	-0.726738000000	-2.209326000000	1.961934000000
C	0.726738000000	-2.209326000000	1.961934000000
C	1.876620000000	-1.373888000000	1.961934000000
C	2.325769000000	0.008449000000	1.961934000000
C	1.886553000000	1.360217000000	1.961934000000
C	0.710666000000	2.214548000000	1.961934000000
C	-0.710666000000	2.214548000000	1.961934000000
C	-1.886553000000	1.360217000000	1.961934000000
C	-2.325769000000	0.008449000000	1.961934000000
H	-1.047493000000	-3.228356000000	2.164920000000
H	1.047493000000	-3.228356000000	2.164920000000
H	2.746656000000	-1.993842000000	2.164920000000
H	3.394042000000	-0.001392000000	2.164920000000
H	2.745020000000	1.996094000000	2.164920000000
H	1.050140000000	3.227496000000	2.164920000000
H	-1.050140000000	3.227496000000	2.164920000000
H	-2.745020000000	1.996094000000	2.164920000000
H	-3.394042000000	-0.001392000000	2.164920000000
H	-2.746656000000	-1.993842000000	2.164920000000
C	-1.876620000000	-1.373888000000	-1.961934000000
C	-0.726738000000	-2.209326000000	-1.961934000000
C	0.726738000000	-2.209326000000	-1.961934000000
C	1.876620000000	-1.373888000000	-1.961934000000
C	2.325769000000	0.008449000000	-1.961934000000
C	1.886553000000	1.360217000000	-1.961934000000
C	0.710666000000	2.214548000000	-1.961934000000
C	-0.710666000000	2.214548000000	-1.961934000000
C	-1.886553000000	1.360217000000	-1.961934000000
C	-2.325769000000	0.008449000000	-1.961934000000
H	1.047493000000	-3.228356000000	-2.164920000000
H	2.746656000000	-1.993842000000	-2.164920000000
H	3.394042000000	-0.001392000000	-2.164920000000
H	2.745020000000	1.996094000000	-2.164920000000
H	1.050140000000	3.227496000000	-2.164920000000
H	-1.050140000000	3.227496000000	-2.164920000000
H	-2.745020000000	1.996094000000	-2.164920000000
H	-3.394042000000	-0.001392000000	-2.164920000000
H	-2.746656000000	-1.993842000000	-2.164920000000
H	-1.047493000000	-3.228356000000	-2.164920000000

4 (M=Cu) [M06/6-311+G(df,p)]
D_{5h}

Cu	0.000000000000	2.353254000000	0.000000000000
Cu	-2.238077000000	0.727195000000	0.000000000000
Cu	2.238077000000	0.727195000000	0.000000000000
Cu	1.383208000000	-1.903822000000	0.000000000000
Cu	-1.383208000000	-1.903822000000	0.000000000000
C	-1.868610000000	-1.368532000000	1.932592000000
C	-0.724119000000	-2.200053000000	1.932592000000
C	0.724119000000	-2.200053000000	1.932592000000
C	1.868610000000	-1.368532000000	1.932592000000
C	2.316140000000	0.008824000000	1.932592000000
C	1.878983000000	1.354254000000	1.932592000000
C	0.707334000000	2.205507000000	1.932592000000
C	-0.707334000000	2.205507000000	1.932592000000
C	-1.878983000000	1.354254000000	1.932592000000
C	-2.316140000000	0.008824000000	1.932592000000
H	-1.048587000000	-3.227464000000	2.104616000000
H	1.048587000000	-3.227464000000	2.104616000000
H	2.745470000000	-1.994607000000	2.104616000000
H	3.393532000000	-0.000075000000	2.104616000000
H	2.745381000000	1.994729000000	2.104616000000
H	1.048731000000	3.227418000000	2.104616000000
H	-1.048731000000	3.227418000000	2.104616000000
H	-2.745381000000	1.994729000000	2.104616000000
H	-3.393532000000	-0.000075000000	2.104616000000
H	-2.745470000000	-1.994607000000	2.104616000000
C	-1.868610000000	-1.368532000000	-1.932592000000
C	-0.724119000000	-2.200053000000	-1.932592000000
C	0.724119000000	-2.200053000000	-1.932592000000
C	1.868610000000	-1.368532000000	-1.932592000000
C	2.316140000000	0.008824000000	-1.932592000000
C	1.878983000000	1.354254000000	-1.932592000000
C	0.707334000000	2.205507000000	-1.932592000000
C	-0.707334000000	2.205507000000	-1.932592000000
C	-1.878983000000	1.354254000000	-1.932592000000
C	-2.316140000000	0.008824000000	-1.932592000000
H	1.048587000000	-3.227464000000	-2.104616000000
H	2.745470000000	-1.994607000000	-2.104616000000
H	3.393532000000	-0.000075000000	-2.104616000000
H	2.745381000000	1.994729000000	-2.104616000000
H	1.048731000000	3.227418000000	-2.104616000000
H	-1.048731000000	3.227418000000	-2.104616000000
H	-2.745381000000	1.994729000000	-2.104616000000
H	-3.393532000000	-0.000075000000	-2.104616000000
H	-2.745470000000	-1.994607000000	-2.104616000000
H	-1.048587000000	-3.227464000000	-2.104616000000

4 (M=Ni) [B3LYP/6-311+G(df,p)]
D_{5h}

Ni	0.000000000000	2.170898000000	0.000000000000
Ni	-2.064646000000	0.670844000000	0.000000000000
Ni	2.064646000000	0.670844000000	0.000000000000
Ni	1.276022000000	-1.756293000000	0.000000000000
Ni	-1.276022000000	-1.756293000000	0.000000000000
C	-1.863268000000	-1.362354000000	1.926050000000
C	-0.719894000000	-2.193064000000	1.926050000000
C	0.719894000000	-2.193064000000	1.926050000000
C	1.863268000000	-1.362354000000	1.926050000000
C	2.308187000000	0.006966000000	1.926050000000
C	1.871457000000	1.351083000000	1.926050000000
C	0.706644000000	2.197369000000	1.926050000000
C	-0.706644000000	2.197369000000	1.926050000000
C	-1.871457000000	1.351083000000	1.926050000000
C	-2.308187000000	0.006966000000	1.926050000000
H	-1.043105000000	-3.226304000000	2.047137000000
H	1.043105000000	-3.226304000000	2.047137000000
H	2.746061000000	-1.989035000000	2.047137000000
H	3.390735000000	-0.004931000000	2.047137000000
H	2.740264000000	1.997013000000	2.047137000000
H	1.052485000000	3.223257000000	2.047137000000
H	-1.052485000000	3.223257000000	2.047137000000
H	-2.740264000000	1.997013000000	2.047137000000
H	-3.390735000000	-0.004931000000	2.047137000000
H	-2.746061000000	-1.989035000000	2.047137000000
C	-1.863268000000	-1.362354000000	-1.926050000000
C	-0.719894000000	-2.193064000000	-1.926050000000
C	0.719894000000	-2.193064000000	-1.926050000000
C	1.863268000000	-1.362354000000	-1.926050000000
C	2.308187000000	0.006966000000	-1.926050000000
C	1.871457000000	1.351083000000	-1.926050000000
C	0.706644000000	2.197369000000	-1.926050000000
C	-0.706644000000	2.197369000000	-1.926050000000
C	-1.871457000000	1.351083000000	-1.926050000000
C	-2.308187000000	0.006966000000	-1.926050000000
H	1.043105000000	-3.226304000000	-2.047137000000
H	2.746061000000	-1.989035000000	-2.047137000000
H	3.390735000000	-0.004931000000	-2.047137000000
H	2.740264000000	1.997013000000	-2.047137000000
H	1.052485000000	3.223257000000	-2.047137000000
H	-1.052485000000	3.223257000000	-2.047137000000
H	-2.740264000000	1.997013000000	-2.047137000000
H	-3.390735000000	-0.004931000000	-2.047137000000
H	-2.746061000000	-1.989035000000	-2.047137000000
H	-1.043105000000	-3.226304000000	-2.047137000000

4 (M=Ni) [M06/6-311+G(df,p)]
D_{5h}

Ni	0.000000000000	2.142267000000	0.000000000000
Ni	-2.037417000000	0.661997000000	0.000000000000
Ni	2.037417000000	0.661997000000	0.000000000000
Ni	1.259193000000	-1.733131000000	0.000000000000
Ni	-1.259193000000	-1.733131000000	0.000000000000
C	-1.855915000000	-1.357013000000	1.898092000000
C	-0.717087000000	-2.184420000000	1.898092000000
C	0.717087000000	-2.184420000000	1.898092000000
C	1.855915000000	-1.357013000000	1.898092000000
C	2.299099000000	0.006967000000	1.898092000000
C	1.864106000000	1.345740000000	1.898092000000
C	0.703835000000	2.188726000000	1.898092000000
C	-0.703835000000	2.188726000000	1.898092000000
C	-1.864106000000	1.345740000000	1.898092000000
C	-2.299099000000	0.006967000000	1.898092000000
H	-1.042974000000	-3.223572000000	1.994481000000
H	1.042974000000	-3.223572000000	1.994481000000
H	2.743502000000	-1.988066000000	1.994481000000
H	3.388095000000	-0.004211000000	1.994481000000
H	2.738552000000	1.994879000000	1.994481000000
H	1.050984000000	3.220969000000	1.994481000000
H	-1.050984000000	3.220969000000	1.994481000000
H	-2.738552000000	1.994879000000	1.994481000000
H	-3.388095000000	-0.004211000000	1.994481000000
H	-2.743502000000	-1.988066000000	1.994481000000
C	-1.855915000000	-1.357013000000	-1.898092000000
C	-0.717087000000	-2.184420000000	-1.898092000000
C	0.717087000000	-2.184420000000	-1.898092000000
C	1.855915000000	-1.357013000000	-1.898092000000
C	2.299099000000	0.006967000000	-1.898092000000
C	1.864106000000	1.345740000000	-1.898092000000
C	0.703835000000	2.188726000000	-1.898092000000
C	-0.703835000000	2.188726000000	-1.898092000000
C	-1.864106000000	1.345740000000	-1.898092000000
C	-2.299099000000	0.006967000000	-1.898092000000
H	1.042974000000	-3.223572000000	-1.994481000000
H	2.743502000000	-1.988066000000	-1.994481000000
H	3.388095000000	-0.004211000000	-1.994481000000
H	2.738552000000	1.994879000000	-1.994481000000
H	1.050984000000	3.220969000000	-1.994481000000
H	-1.050984000000	3.220969000000	-1.994481000000
H	-2.738552000000	1.994879000000	-1.994481000000
H	-3.388095000000	-0.004211000000	-1.994481000000
H	-2.743502000000	-1.988066000000	-1.994481000000
H	-1.042974000000	-3.223572000000	-1.994481000000

7 (M=Cu) [B3LYP/6-311+G(df,p)]
C_1

C	-3.134555000000	-0.727643000000	-1.540919000000
C	-2.907734000000	-1.879963000000	-0.733783000000
C	-2.531742000000	-2.328593000000	0.595185000000
C	-2.167024000000	-1.886491000000	1.900324000000
C	-1.937207000000	-0.712343000000	2.721112000000
C	-1.937272000000	0.713424000000	2.720681000000
C	-2.167333000000	1.887053000000	1.899150000000
C	-2.532081000000	2.328217000000	0.593732000000
C	-2.908904000000	1.878531000000	-0.734703000000
C	-3.134937000000	0.725659000000	-1.541249000000
H	-3.268674000000	-2.750087000000	-1.277414000000
H	-2.725052000000	-3.397830000000	0.641238000000
H	-2.184976000000	-2.746531000000	2.565876000000
H	-1.852471000000	-1.050432000000	3.751302000000
H	-1.852695000000	1.052172000000	3.750670000000
H	-2.185126000000	2.747555000000	2.564115000000
H	-2.725360000000	3.397488000000	0.638983000000
H	-3.270572000000	2.748136000000	-1.278684000000
H	-3.605568000000	1.047169000000	-2.467513000000
H	-3.604948000000	-1.049892000000	-2.467053000000
C	0.646408000000	-0.726264000000	-2.598423000000
C	0.871034000000	-1.870874000000	-1.796510000000
C	1.249733000000	-2.317825000000	-0.467458000000
C	1.613947000000	-1.880045000000	0.825290000000
C	1.841828000000	-0.705061000000	1.646987000000
C	1.841864000000	0.706385000000	1.646411000000
C	1.613969000000	1.880918000000	0.824006000000
C	1.249421000000	2.318227000000	-0.468842000000
C	0.870176000000	1.870806000000	-1.797567000000
C	0.645469000000	0.725664000000	-2.598765000000
H	1.451468000000	-3.384407000000	-0.534661000000
H	2.002722000000	-2.732570000000	1.375699000000
H	2.331830000000	-1.043774000000	2.555553000000
H	2.331868000000	1.045747000000	2.554737000000
H	2.002920000000	2.733669000000	1.373919000000
H	1.451191000000	3.384768000000	-0.536496000000
H	0.898802000000	2.741207000000	-2.449343000000
H	0.564459000000	1.045643000000	-3.635282000000
H	0.566254000000	-1.046835000000	-3.634823000000
H	0.900503000000	-2.741495000000	-2.447960000000
Cu	-0.440006000000	2.309218000000	0.780393000000
Cu	-1.180150000000	1.426874000000	-1.836353000000
Cu	0.010891000000	0.000981000000	2.391473000000
Cu	-0.439853000000	-2.309433000000	0.781445000000
Cu	-1.179532000000	-1.427415000000	-1.836434000000
B	4.508481000000	-0.000099000000	-0.389431000000
F	5.573883000000	0.000637000000	-1.280445000000
F	3.276282000000	-0.002569000000	-1.111438000000
F	4.537317000000	1.151840000000	0.428270000000
F	4.540467000000	-1.150400000000	0.430409000000

7 (M=Cu) [M06/6-311+G(df,p)]
C_1

C	-3.080190000000	-0.737691000000	-1.525568000000
C	-2.850225000000	-1.878969000000	-0.715184000000
C	-2.469585000000	-2.317073000000	0.609833000000
C	-2.100775000000	-1.869253000000	1.905070000000
C	-1.869495000000	-0.695287000000	2.715316000000
C	-1.871914000000	0.724149000000	2.706475000000
C	-2.107053000000	1.887208000000	1.881601000000
C	-2.477304000000	2.317764000000	0.580950000000
C	-2.856086000000	1.862050000000	-0.738805000000
C	-3.082462000000	0.709911000000	-1.534691000000
H	-3.183540000000	-2.759971000000	-1.266306000000
H	-2.632167000000	-3.395180000000	0.655776000000
H	-2.083839000000	-2.733646000000	2.571096000000
H	-1.748509000000	-1.029216000000	3.747176000000
H	-1.751938000000	1.071347000000	3.734050000000
H	-2.093374000000	2.759817000000	2.536929000000
H	-2.643205000000	3.395839000000	0.613427000000
H	-3.192220000000	2.735064000000	-1.300834000000
H	-3.528554000000	1.029259000000	-2.478030000000
H	-3.525778000000	-1.070350000000	-2.464542000000
C	0.641215000000	-0.737564000000	-2.582402000000
C	0.870146000000	-1.871061000000	-1.778179000000
C	1.254980000000	-2.307168000000	-0.452649000000
C	1.620290000000	-1.863911000000	0.829872000000
C	1.851551000000	-0.688145000000	1.640761000000
C	1.849254000000	0.715649000000	1.632180000000
C	1.614184000000	1.880689000000	0.807100000000
C	1.247347000000	2.306874000000	-0.480820000000
C	0.864399000000	1.853456000000	-1.801078000000
C	0.638746000000	0.709431000000	-2.591282000000
H	1.420732000000	-3.384942000000	-0.502688000000
H	1.979742000000	-2.722215000000	1.399134000000
H	2.316565000000	-1.024116000000	2.568371000000
H	2.312979000000	1.064406000000	2.555693000000
H	1.970527000000	2.747113000000	1.365957000000
H	1.408756000000	3.384644000000	-0.543793000000
H	0.849814000000	2.728681000000	-2.453520000000
H	0.512680000000	1.027446000000	-3.628075000000
H	0.515896000000	-1.068724000000	-3.615171000000
H	0.857961000000	-2.754266000000	-2.419830000000
Cu	-0.420623000000	2.236369000000	0.741692000000
Cu	-1.142473000000	1.366792000000	-1.776450000000
Cu	0.027502000000	0.014373000000	2.314241000000
Cu	-0.413546000000	-2.227367000000	0.767953000000
Cu	-1.138408000000	-1.390086000000	-1.760009000000
B	4.312523000000	-0.000302000000	-0.396750000000
F	5.277230000000	-0.001658000000	-1.377366000000
F	3.021994000000	0.000143000000	-1.000602000000
F	4.411771000000	1.143486000000	0.405991000000
F	4.410296000000	-1.142881000000	0.407815000000

8 (M=Ni) [B3LYP/6-311+G(df,p)]
C_{5h}

C	1.095698000000	2.030510000000	1.910914000000
C	-0.293283000000	2.291581000000	1.932641000000
C	-1.592540000000	1.669533000000	1.910914000000
C	-2.270052000000	0.429208000000	1.932641000000
C	-2.079942000000	-0.998682000000	1.910914000000
C	-1.109686000000	-2.026315000000	1.932641000000
C	0.307066000000	-2.286752000000	1.910914000000
C	1.584229000000	-1.681540000000	1.932641000000
C	2.269719000000	-0.414609000000	1.910914000000
C	2.088793000000	0.987066000000	1.932641000000
H	-0.445125000000	3.362793000000	2.068522000000
H	-2.328792000000	2.462521000000	2.027337000000
H	-3.335758000000	0.615821000000	2.068522000000
H	-3.061632000000	-1.453852000000	2.027337000000
H	-1.616487000000	-2.982195000000	2.068522000000
H	0.436599000000	-3.361050000000	2.027337000000
H	2.336714000000	-2.458919000000	2.068522000000
H	3.331465000000	-0.623392000000	2.027337000000
H	3.060655000000	1.462500000000	2.068522000000
H	1.622360000000	2.975773000000	2.027337000000
C	1.095698000000	2.030510000000	-1.910914000000
C	-0.293283000000	2.291581000000	-1.932641000000
C	-1.592540000000	1.669533000000	-1.910914000000
C	-2.270052000000	0.429208000000	-1.932641000000
C	-2.079942000000	-0.998682000000	-1.910914000000
C	-1.109686000000	-2.026315000000	-1.932641000000
C	0.307066000000	-2.286752000000	-1.910914000000
C	1.584229000000	-1.681540000000	-1.932641000000
C	2.269719000000	-0.414609000000	-1.910914000000
C	2.088793000000	0.987066000000	-1.932641000000
H	-2.328792000000	2.462521000000	-2.027337000000
H	-3.335758000000	0.615821000000	-2.068522000000
H	-3.061632000000	-1.453852000000	-2.027337000000
H	-1.616487000000	-2.982195000000	-2.068522000000
H	0.436599000000	-3.361050000000	-2.027337000000
H	2.336714000000	-2.458919000000	-2.068522000000
H	3.331465000000	-0.623392000000	-2.027337000000
H	3.060655000000	1.462500000000	-2.068522000000
H	1.622360000000	2.975773000000	-2.027337000000
H	-0.445125000000	3.362793000000	-2.068522000000
Ni	1.083780000000	-1.888875000000	0.000000000000
Ni	2.131333000000	0.447042000000	0.000000000000
Ni	-1.461520000000	-1.614431000000	0.000000000000
Ni	-1.987049000000	0.891102000000	0.000000000000
Ni	0.233456000000	2.165162000000	0.000000000000

8 (M=Ni) [M06/6-311+G(df,p)]
C_{5h}

C	-2.186527000000	-0.706843000000	1.884520000000
C	-1.366628000000	-1.851009000000	1.905325000000
C	-0.003426000000	-2.297938000000	1.884520000000
C	1.338103000000	-1.871734000000	1.905325000000
C	2.184410000000	-0.713360000000	1.884520000000
C	2.193621000000	0.694214000000	1.905325000000
C	1.353466000000	1.857057000000	1.884520000000
C	0.017630000000	2.300782000000	1.905325000000
C	-1.347922000000	1.861084000000	1.884520000000
C	-2.182726000000	0.727748000000	1.905325000000
H	-2.001848000000	-2.735534000000	2.012486000000
H	-0.019334000000	-3.386134000000	1.978744000000
H	1.983043000000	-2.749197000000	2.012486000000
H	3.214430000000	-1.064761000000	1.978744000000
H	3.227436000000	1.036437000000	2.012486000000
H	2.005961000000	2.728076000000	1.978744000000
H	0.011622000000	3.389751000000	2.012486000000
H	-1.974678000000	2.750804000000	1.978744000000
H	-3.220253000000	1.058544000000	2.012486000000
H	-3.226379000000	-1.027985000000	1.978744000000
C	-2.186527000000	-0.706843000000	-1.884520000000
C	-1.366628000000	-1.851009000000	-1.905325000000
C	-0.003426000000	-2.297938000000	-1.884520000000
C	1.338103000000	-1.871734000000	-1.905325000000
C	2.184410000000	-0.713360000000	-1.884520000000
C	2.193621000000	0.694214000000	-1.905325000000
C	1.353466000000	1.857057000000	-1.884520000000
C	0.017630000000	2.300782000000	-1.905325000000
C	-1.347922000000	1.861084000000	-1.884520000000
C	-2.182726000000	0.727748000000	-1.905325000000
H	-0.019334000000	-3.386134000000	-1.978744000000
H	1.983043000000	-2.749197000000	-2.012486000000
H	3.214430000000	-1.064761000000	-1.978744000000
H	3.227436000000	1.036437000000	-2.012486000000
H	2.005961000000	2.728076000000	-1.978744000000
H	0.011622000000	3.389751000000	-2.012486000000
H	-1.974678000000	2.750804000000	-1.978744000000
H	-3.220253000000	1.058544000000	-2.012486000000
H	-3.226379000000	-1.027985000000	-1.978744000000
H	-2.001848000000	-2.735534000000	-2.012486000000
Ni	0.545058000000	2.075854000000	0.000000000000
Ni	-1.805823000000	1.159856000000	0.000000000000
Ni	2.142687000000	0.123093000000	0.000000000000
Ni	0.779195000000	-1.999779000000	0.000000000000
Ni	-1.661118000000	-1.359024000000	0.000000000000

Figure S1 Diagram of the formation of the main stabilizing orbitals of complexes $M_5(C_{10}H_{10})_2$ from fragment orbitals