

SUPPLEMENTARY INFORMATION

**Natural Resonance-Theoretic Conceptions  
of Extreme Electronic Delocalization in Soft Materials**

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A ready-to-run *Gaussian-16* input file for the diberyllocene numerical application is given below, showing fully optimized structural coordinates, vibrational frequencies, and keyword input for the NBO/NRT results described in the main text:

```
-----  
%mem=2gb  
%nprocshared=8  
%chk=cp_be_be_cp  
#b3lyp/6-311++G** pop=nbo7read  
  
Cp-Be-Be-Cp (C5h), -416.707779049  
nu: 2,67,69,...  
Vibrational temperatures:      3.02      96.72      99.68      246.70      280.69  
      (Kelvin)      281.08      581.10      581.38      615.72      616.30  
      851.95      881.49      881.63      882.13      882.28  
      1121.75      1195.35      1195.67      1203.21      1203.31  
      1234.61      1257.67      1257.74      1258.73      1258.80  
      1322.92      1323.22      1325.51      1325.64      1375.21  
      1490.39      1490.65      1491.40      1491.63      1562.48  
      1562.84      1564.29      1564.56      1657.03      1658.42  
      1852.47      1852.50      1996.60      1996.65      1998.22  
      1998.27      2115.63      2115.80      2117.79      2117.94  
      4640.02      4640.05      4640.09      4640.11      4660.26  
      4660.37      4660.41      4660.51      4676.82      4676.84  
  
Zero-point correction=                0.172421 (Hartree/Particle)  
Thermal correction to Energy=          0.182740  
Thermal correction to Enthalpy=        0.183684  
Thermal correction to Gibbs Free Energy= 0.132897  
Sum of electronic and zero-point Energies= -416.535358  
Sum of electronic and thermal Energies= -416.525039  
Sum of electronic and thermal Enthalpies= -416.524095  
Sum of electronic and thermal Free Energies= -416.574882  
  
0 1  
6      2.554957      0.254797      1.178829  
6      2.554868      1.199930      0.121857  
6      2.554618      0.486760     -1.103604  
6      2.554532     -0.899196     -0.804000  
6      2.554753     -1.042536      0.606558  
1      2.494895      0.482473      2.232076  
1      2.494699      2.271982      0.230791  
1      2.494127      0.921691     -2.089478  
1      2.494107     -1.702492     -1.522221  
1      2.494453     -1.973893      1.148509  
6     -2.554638      0.250876      1.179784  
6     -2.554886     -1.044453      0.603115  
6     -2.554961     -0.896295     -0.806985  
6     -2.554719      0.490605     -1.101832  
6     -2.554490      1.199582      0.126067
```

1	-2.494251	0.474950	2.233785
1	-2.494712	-1.977670	1.141874
1	-2.494963	-1.697135	-1.527980
1	-2.494413	0.928885	-2.086235
1	-2.494042	2.271240	0.238657
4	1.020479	-0.000023	0.000295
4	-1.020506	-0.000091	0.000077

\$nbo file=cp\_be\_be\_cp archive plot nrt nrtres=40000 memory=50gb \$end

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