

1:

Identification and Quantification of Local Antiaromaticity in Polycyclic Aromatic Hydrocarbons (PAHs) on the magnetic criterion.

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E-mail: ekleinp@uni-potsdam.de

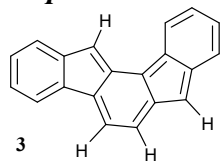
Supporting Information

Schemes: Compounds studied S2

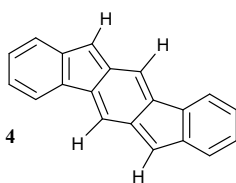
Figures: Spatial magnetic properties (TSNMRS) of the studied compounds [top and side view(s)] by different ICSS of -0.5 ppm (*orange*), -0.1 ppm (red) *deshielding* and 5 ppm (blue), 2 ppm (cyan), 0.5 ppm (green) and 0.1 ppm (yellow) *shielding* S3 – S19

2:

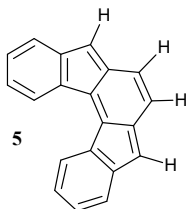
Compounds studied:



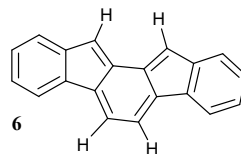
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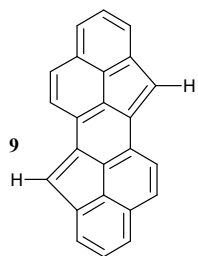
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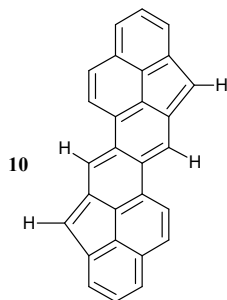
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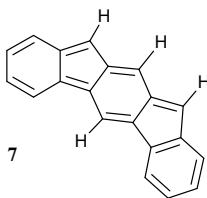
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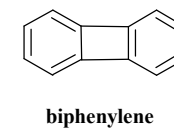
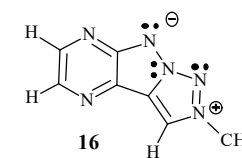
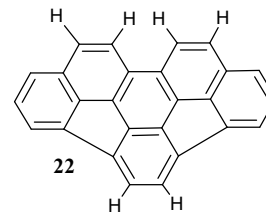
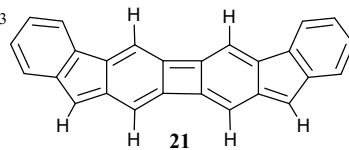
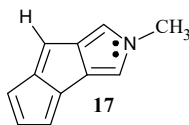
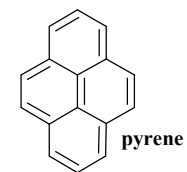
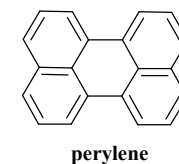
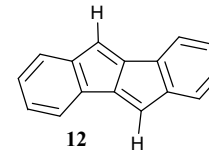
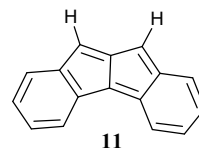
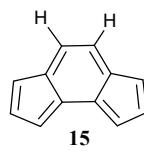
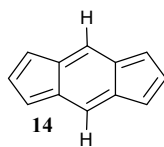
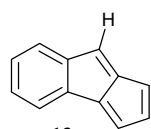
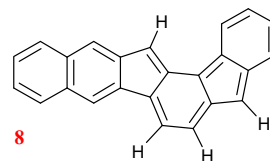
cyclopenta[qr]indeno[2,1,7-ijk]tetraphen



cyclopenta[qr]indeno[7,2,1-cde]picene



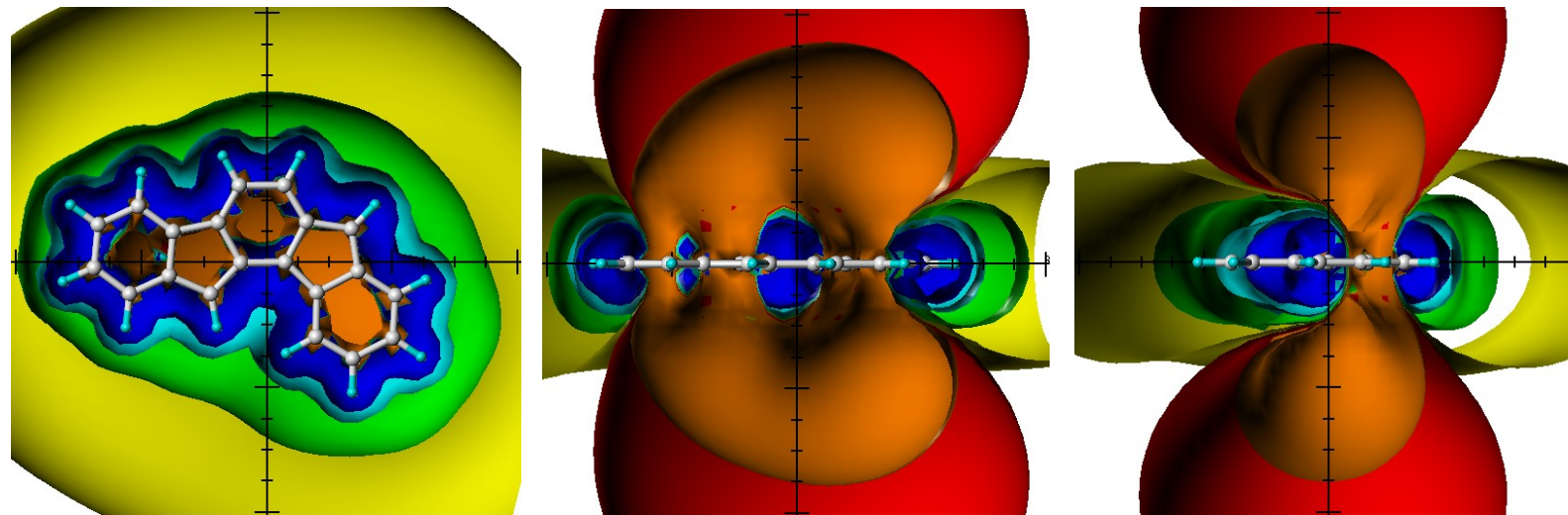
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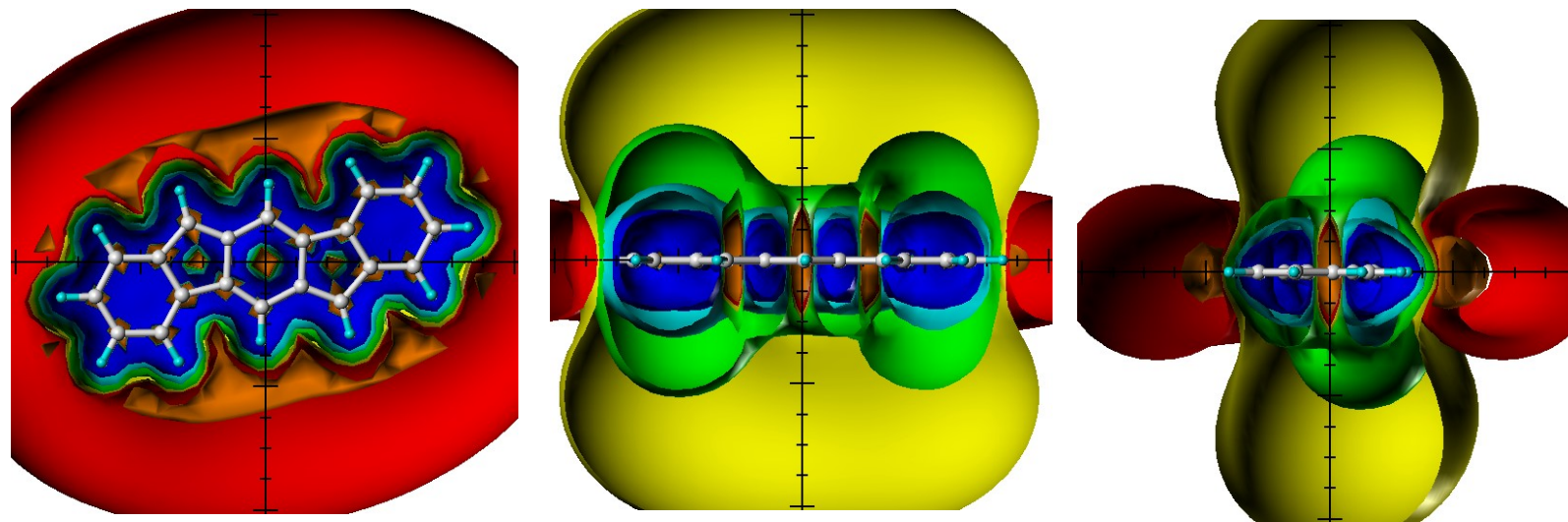
3:

Figure S1. Spatial magnetic properties (TSNMRS) of the studied compounds [top and side view(s)] by different ICSS of -0.5 ppm (*orange*), -0.1 ppm (*red*) *deshielding* and 5 ppm (*blue*), 2 ppm (*cyan*), 0.5 ppm (*green*) and 0.1 ppm (*yellow*) *shielding*.

3

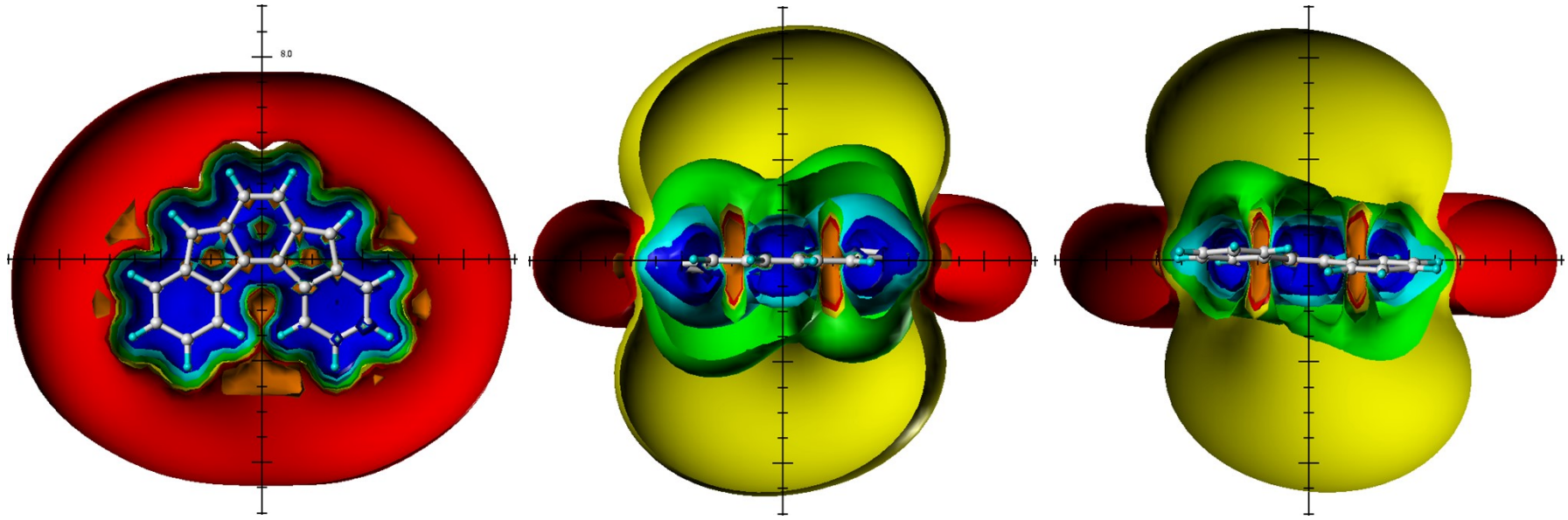


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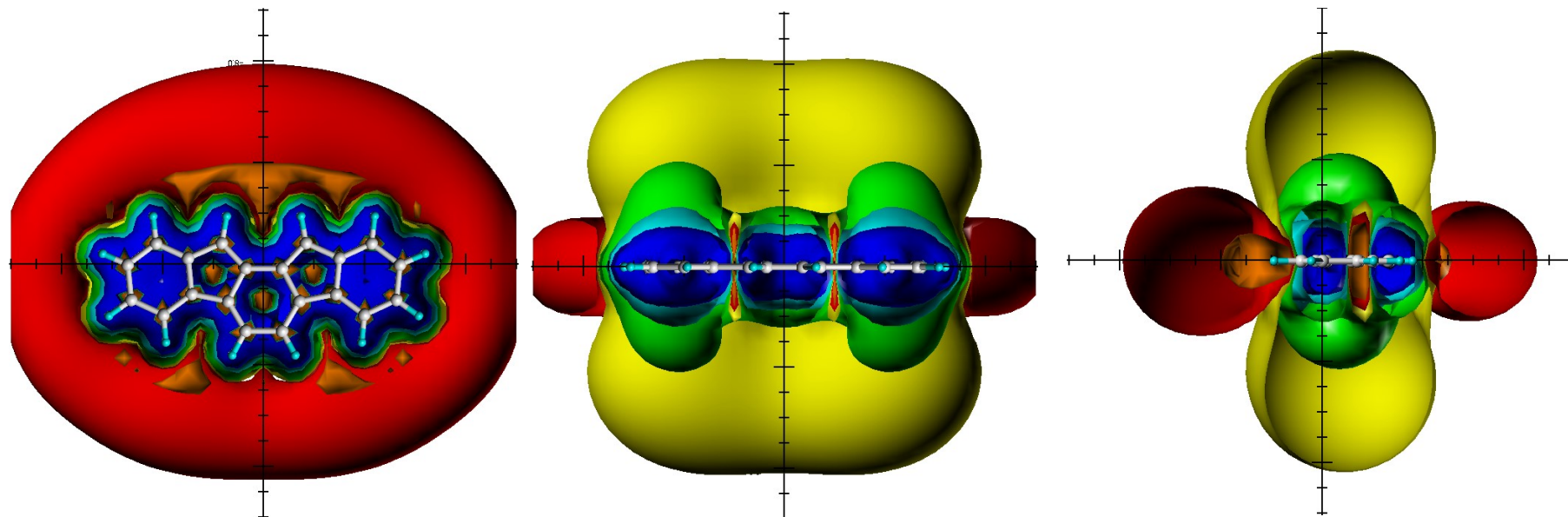
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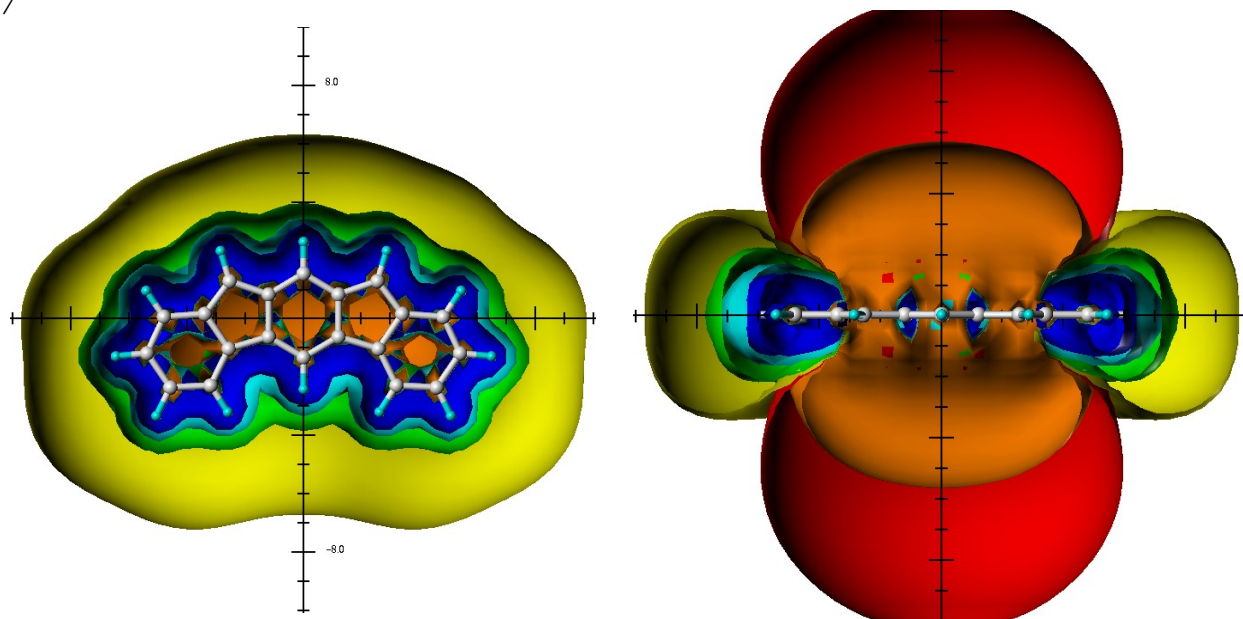


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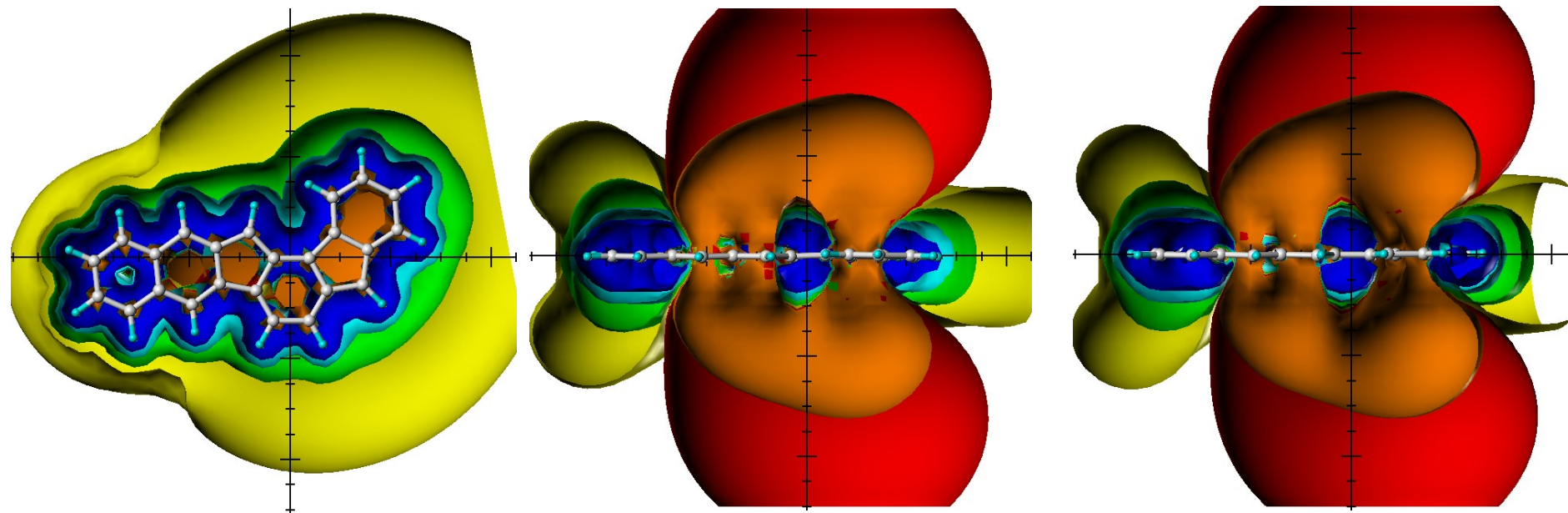


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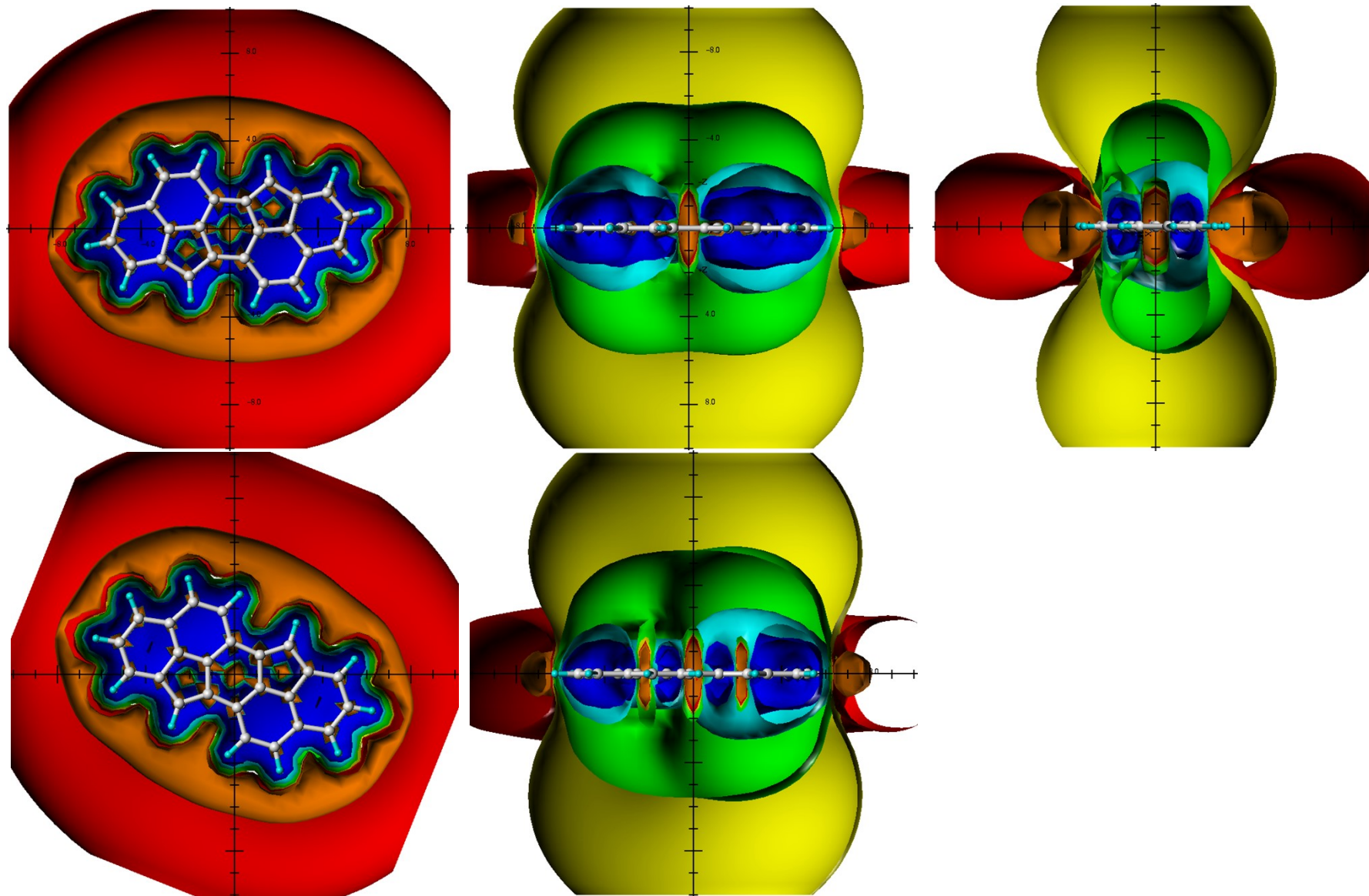
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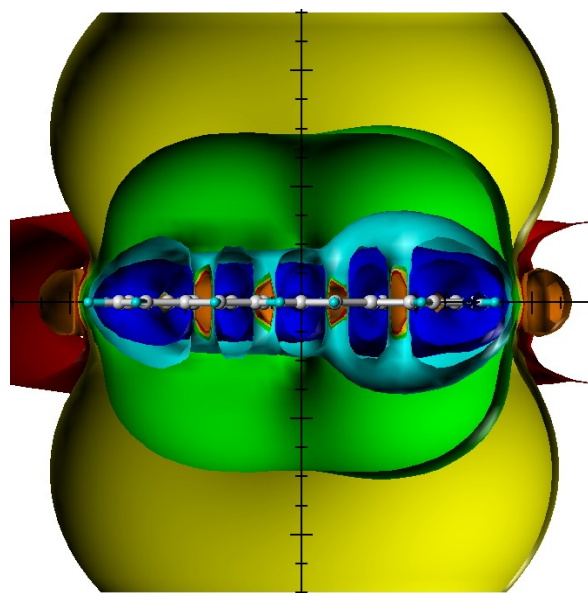
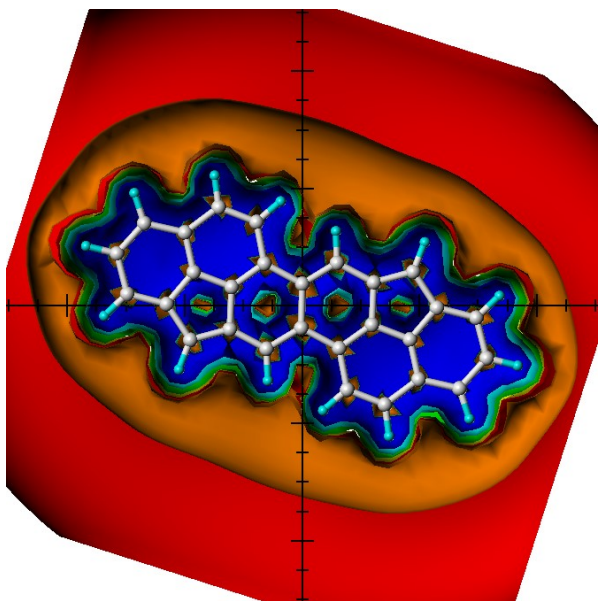
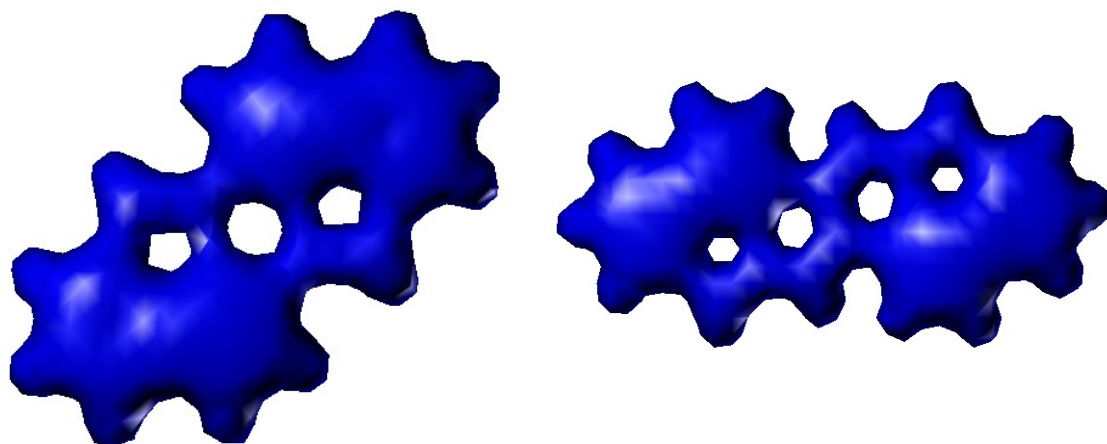
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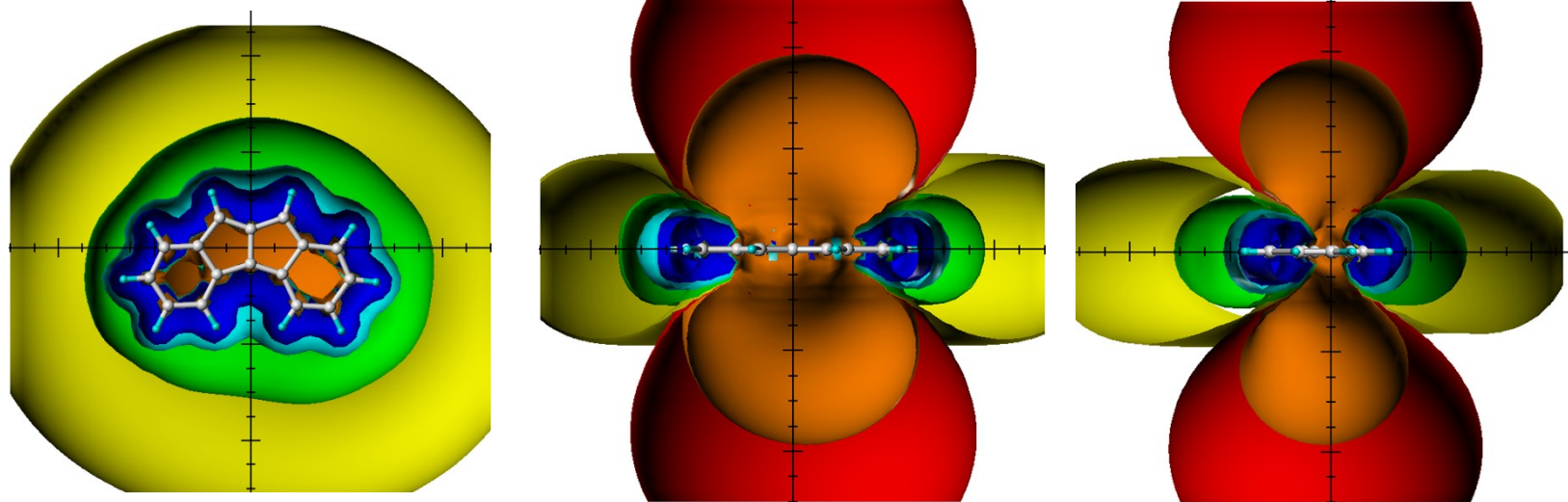
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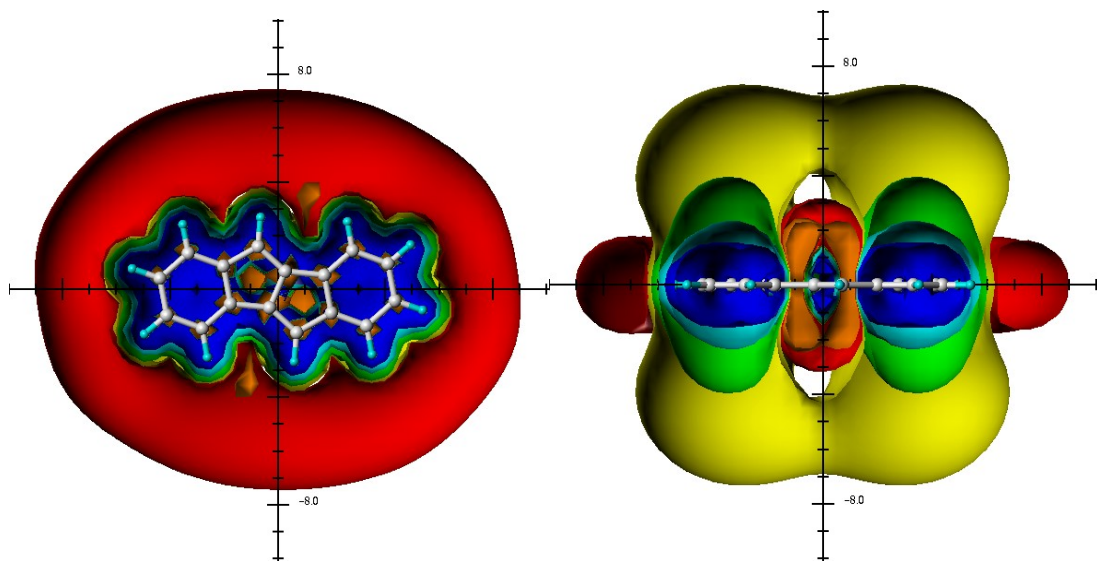


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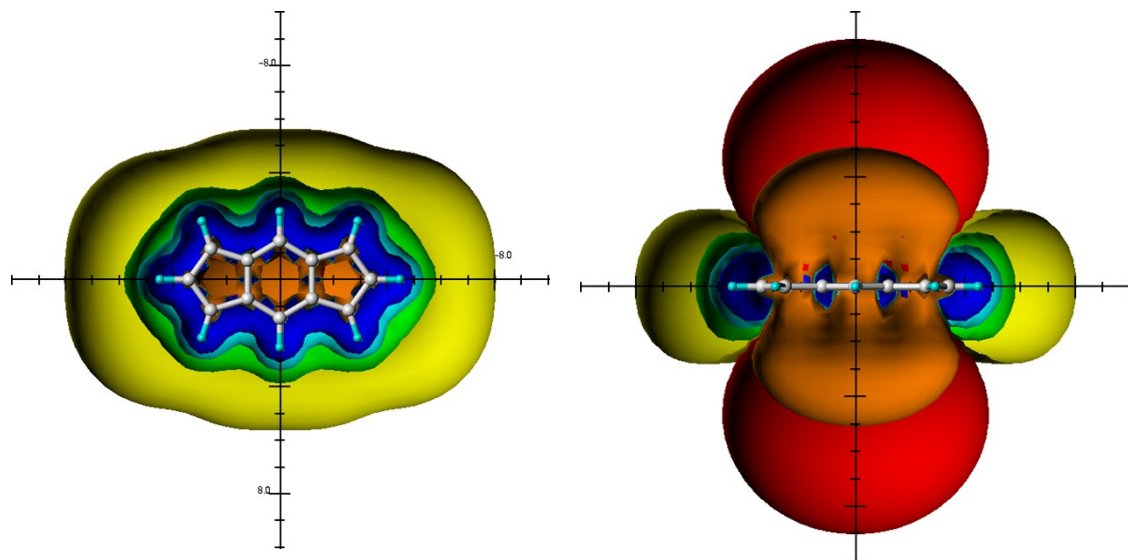


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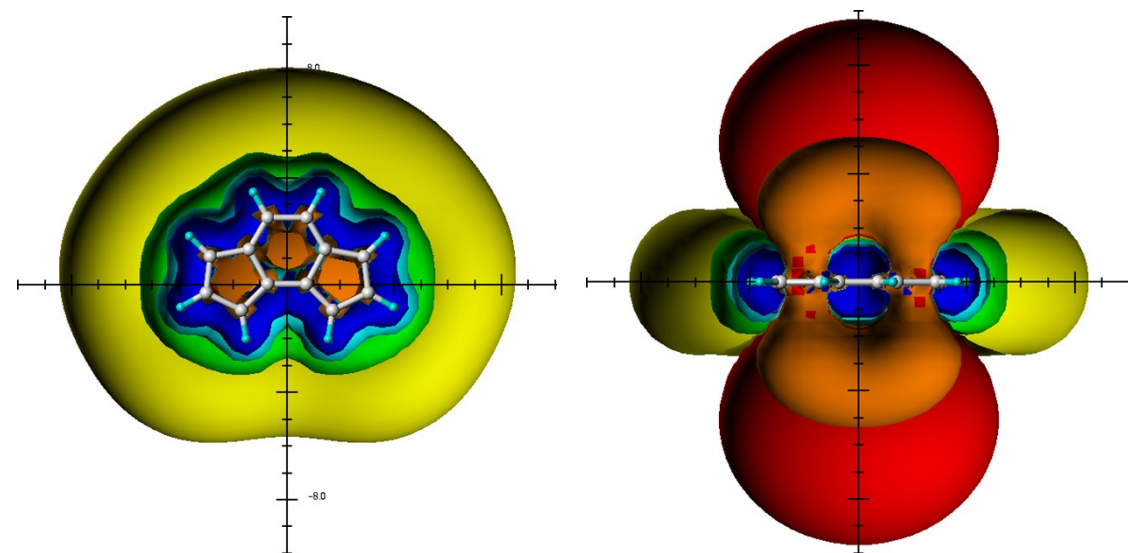


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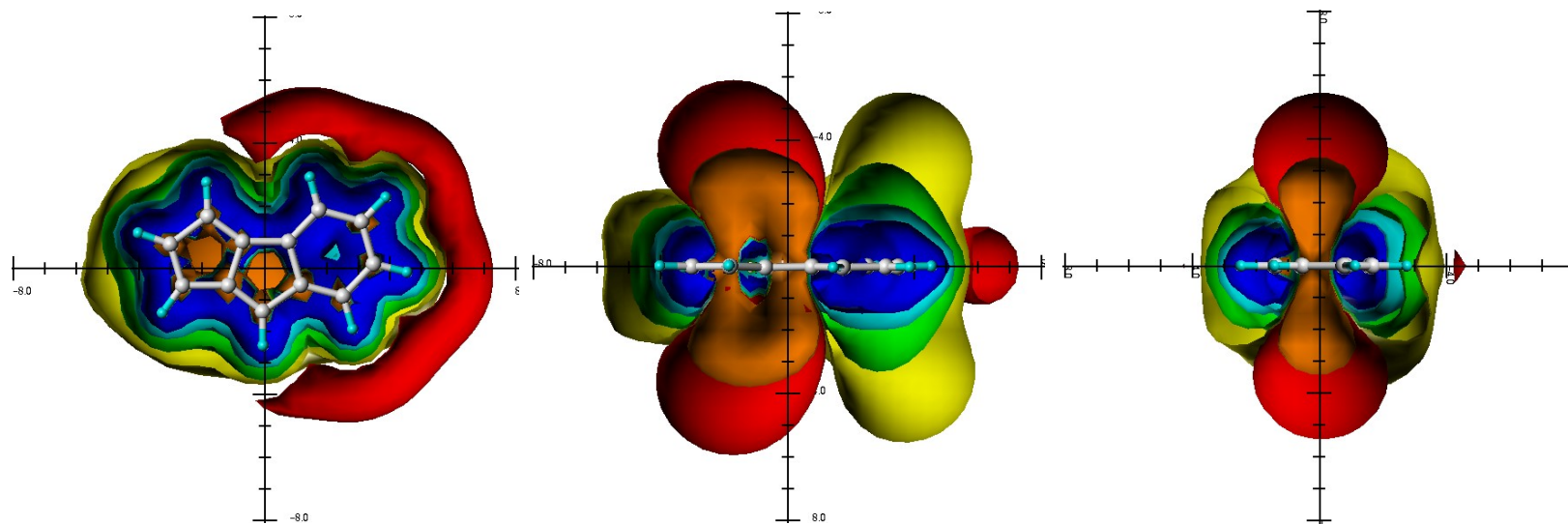


14



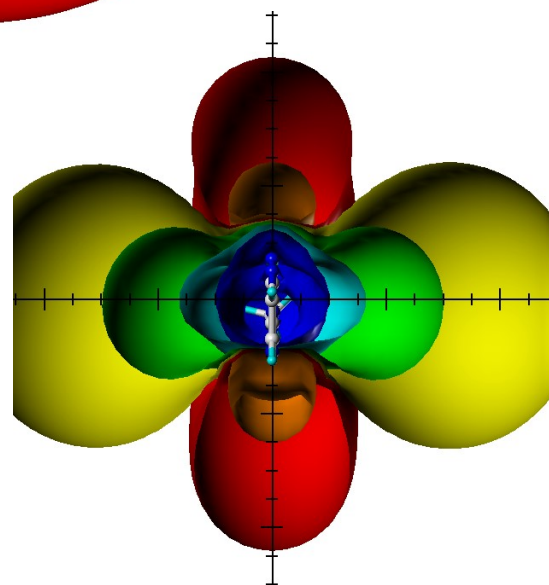
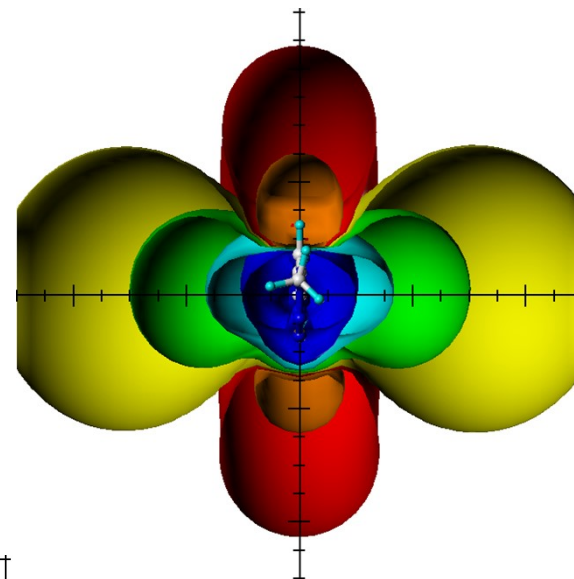
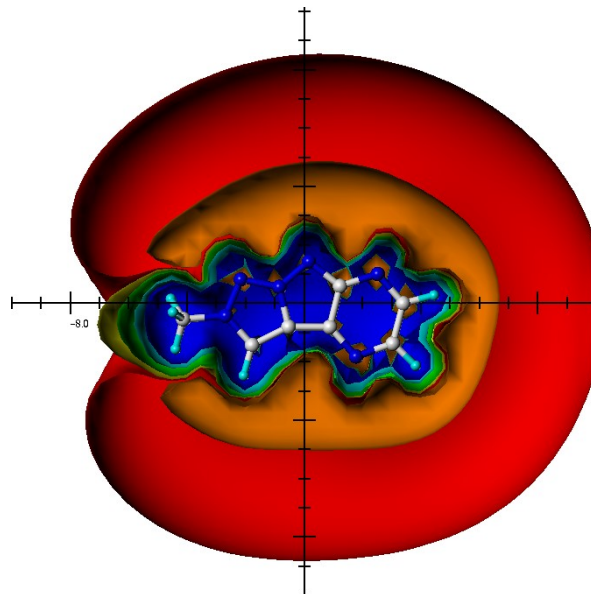
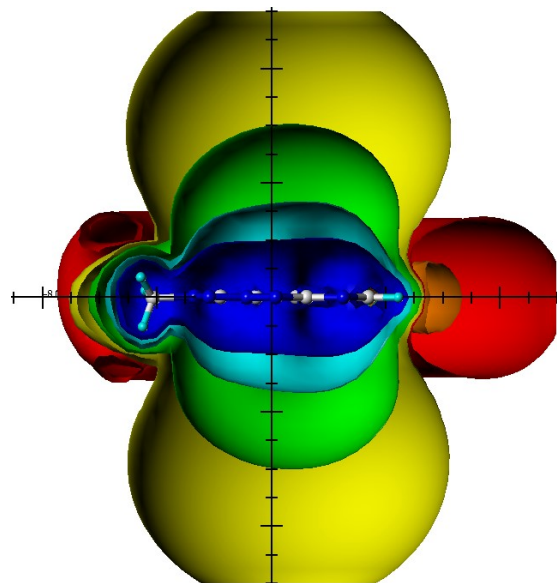
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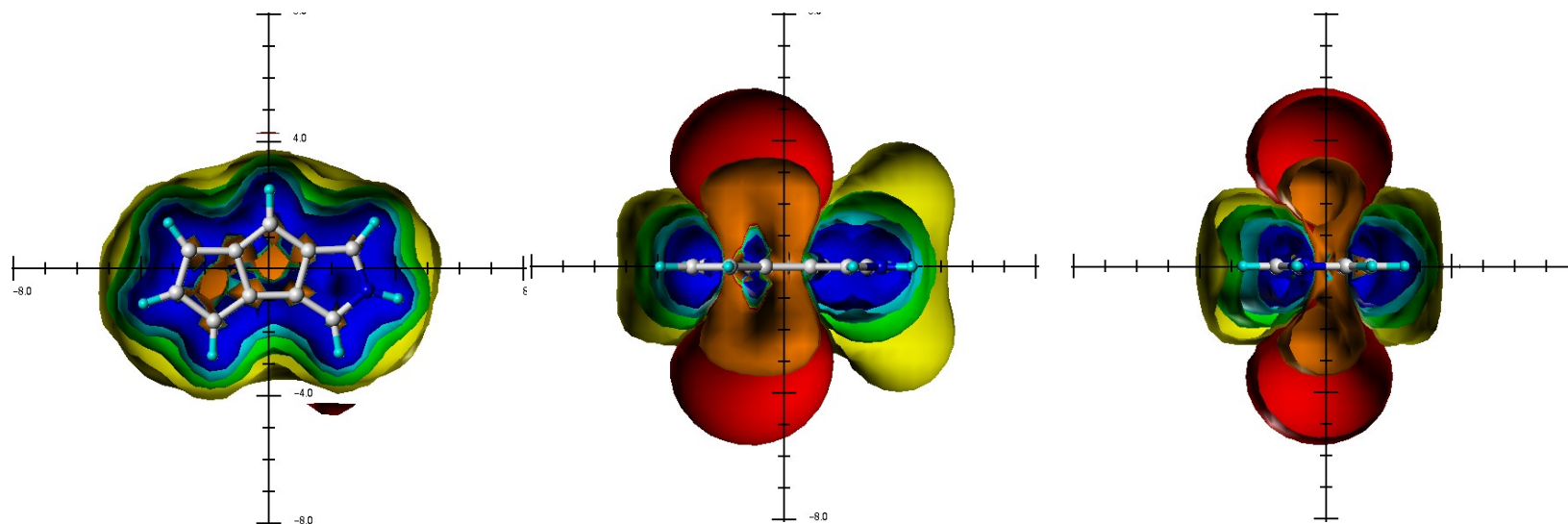
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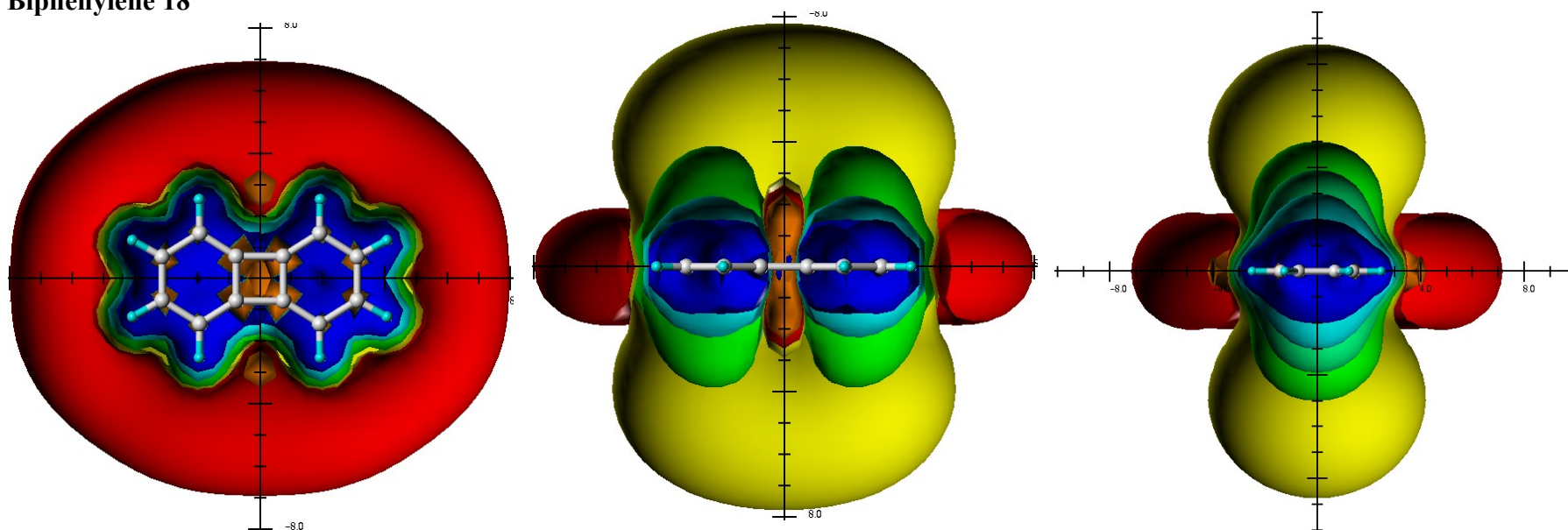


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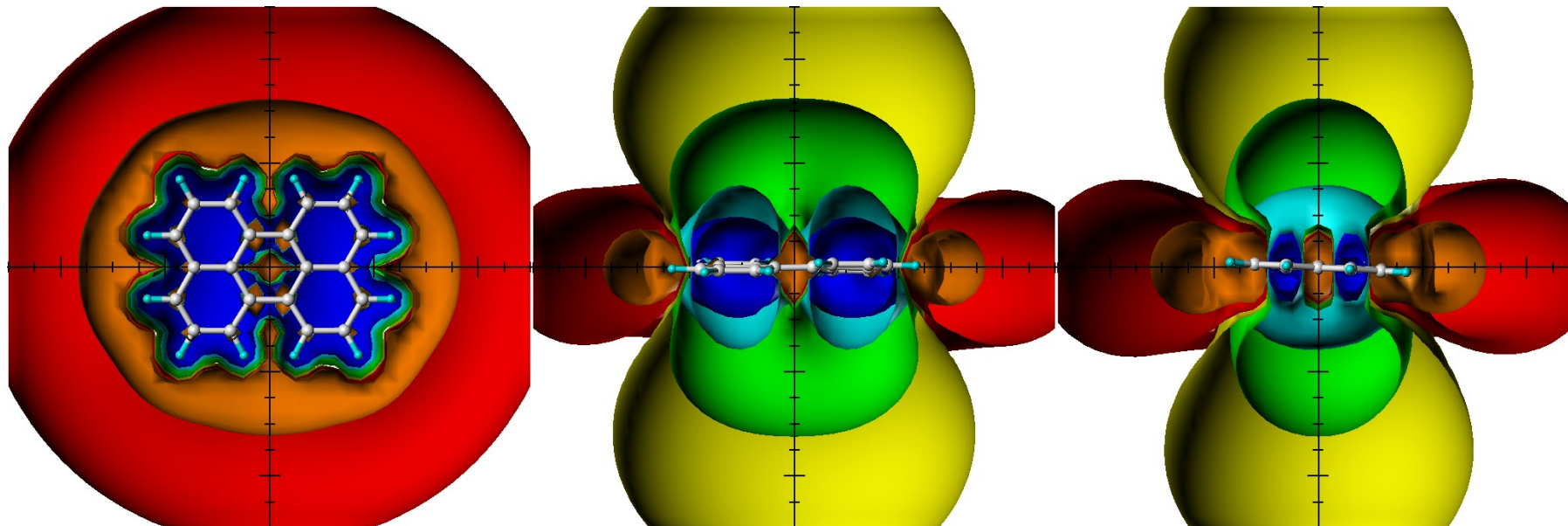


Biphenylene 18

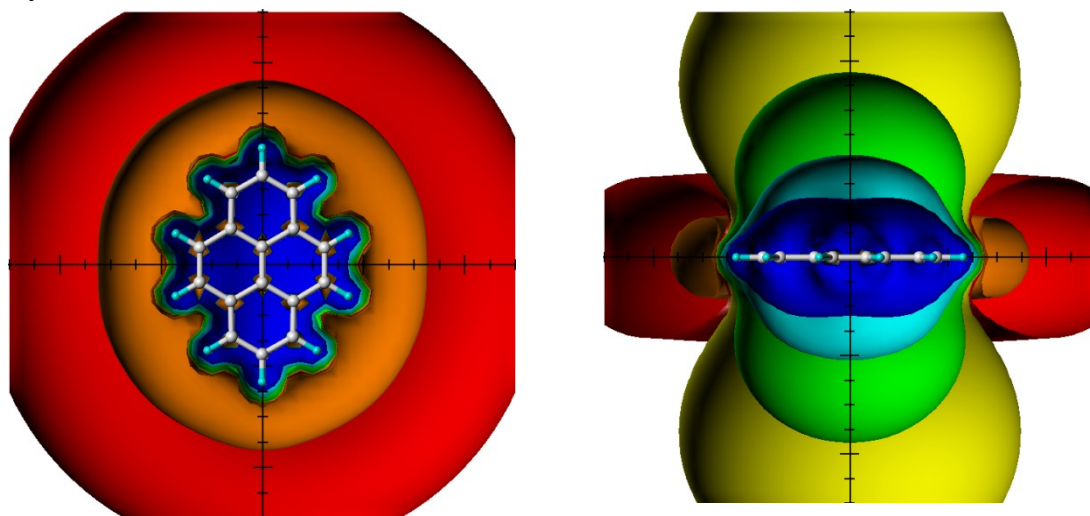


14:

Perylene 19

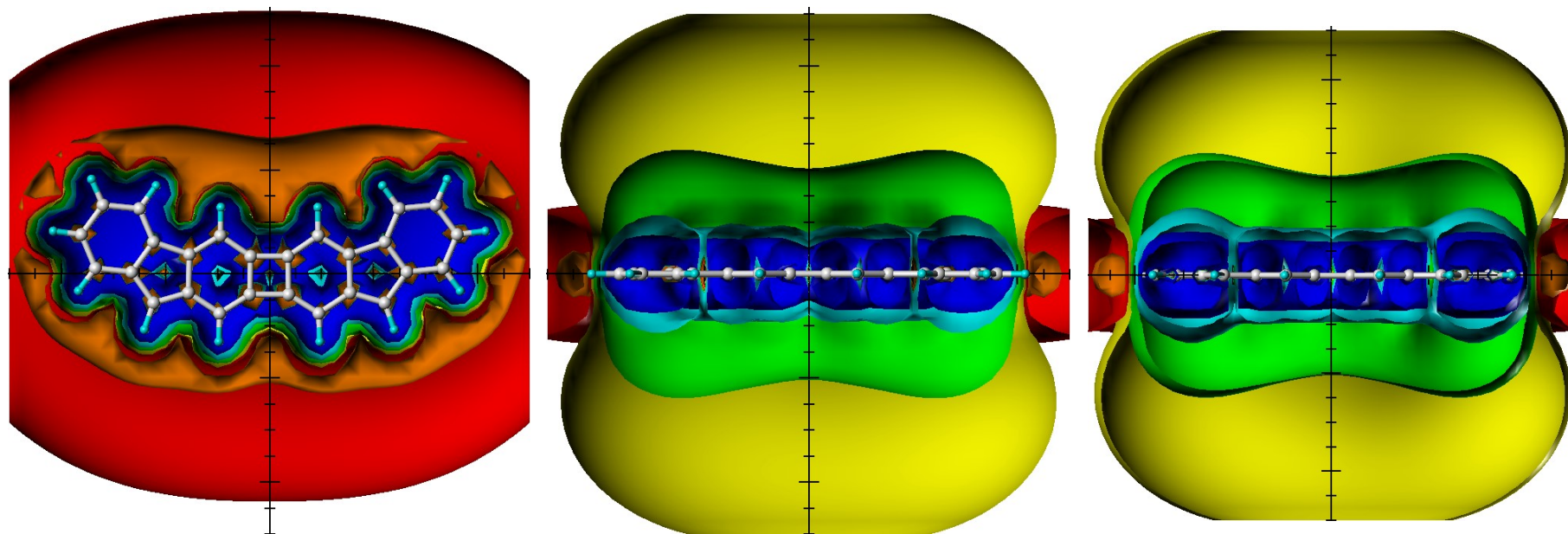


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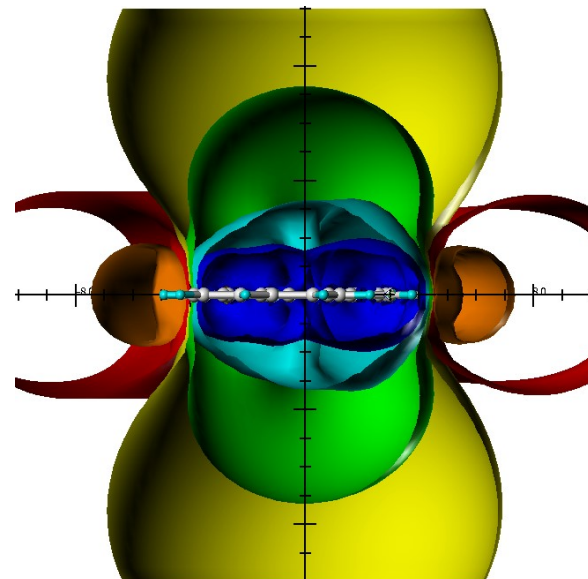
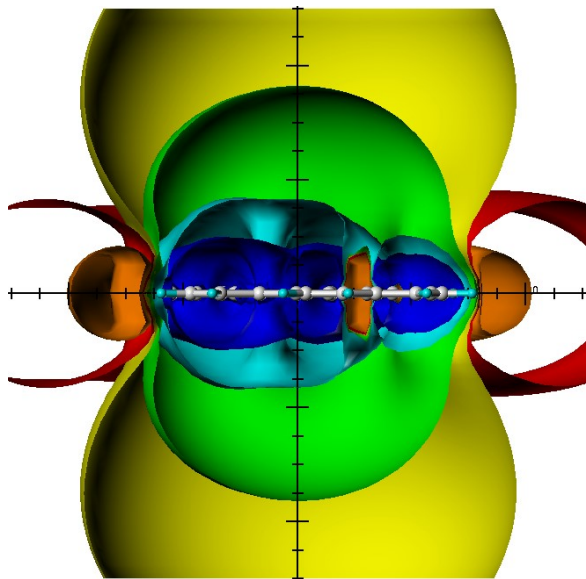
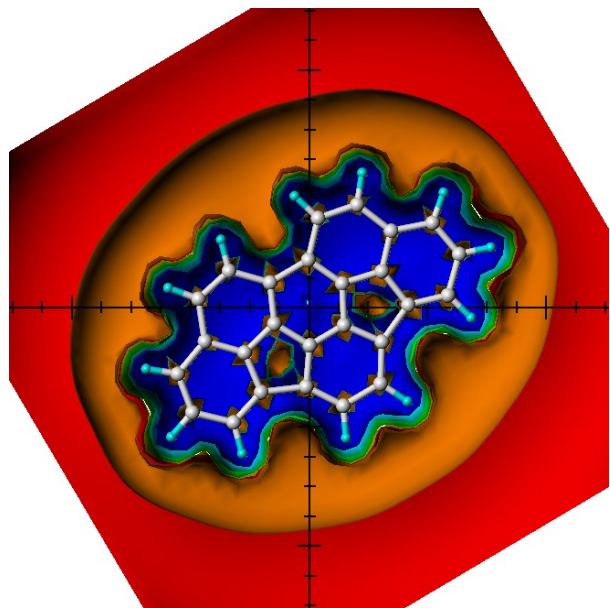
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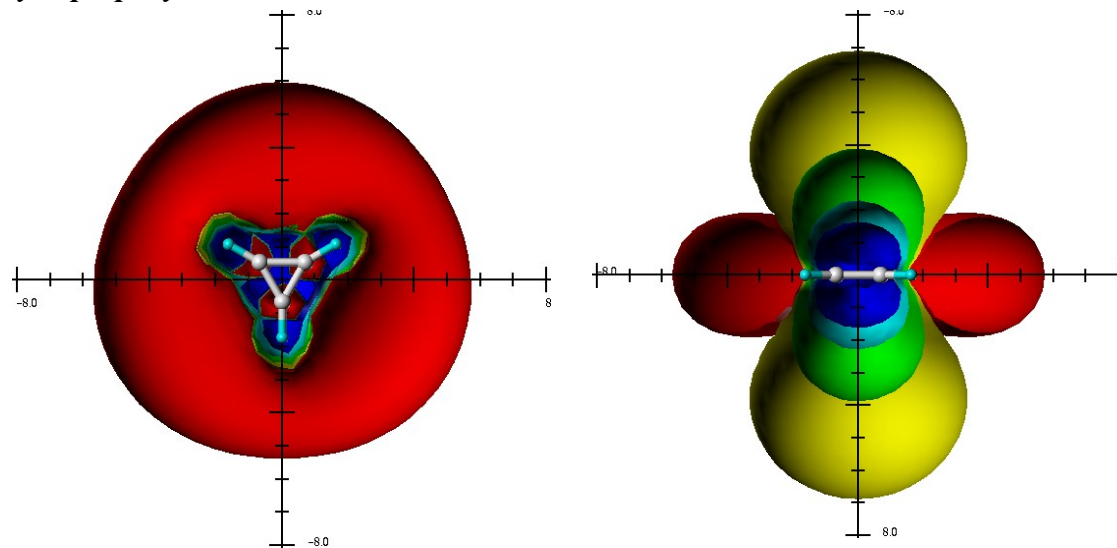
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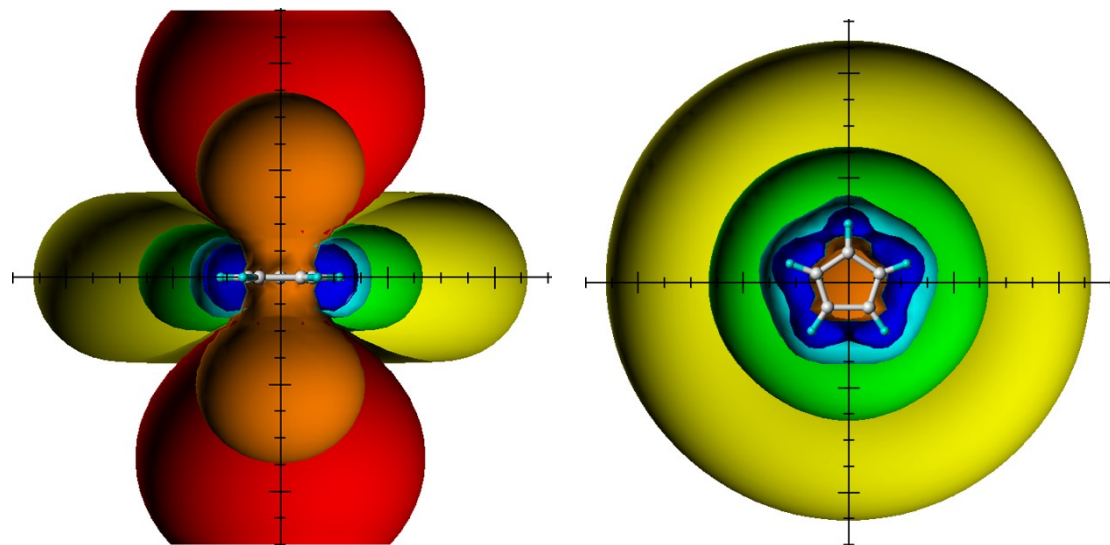


17:

Cyclopropenylum cation

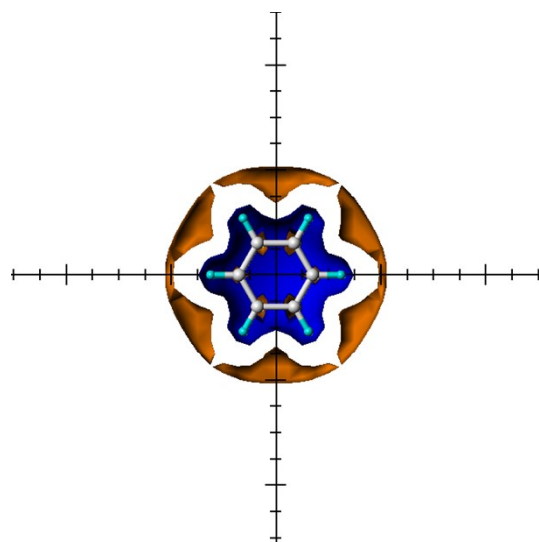
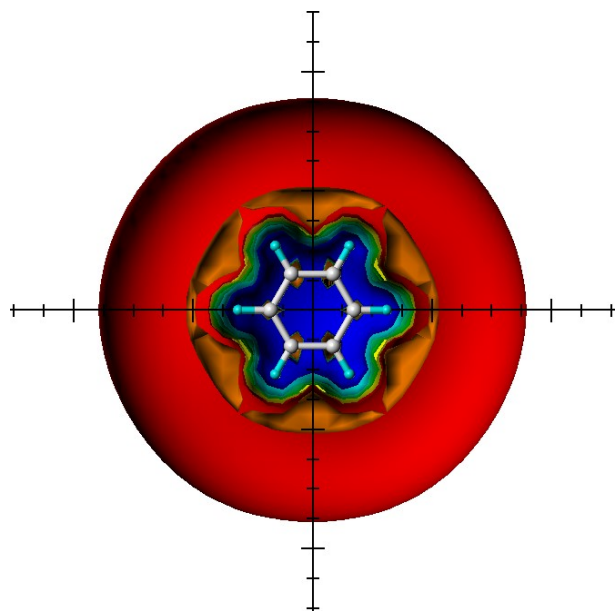
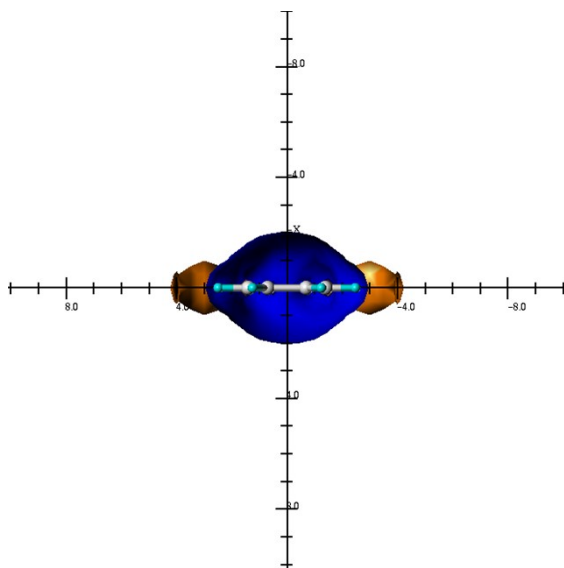
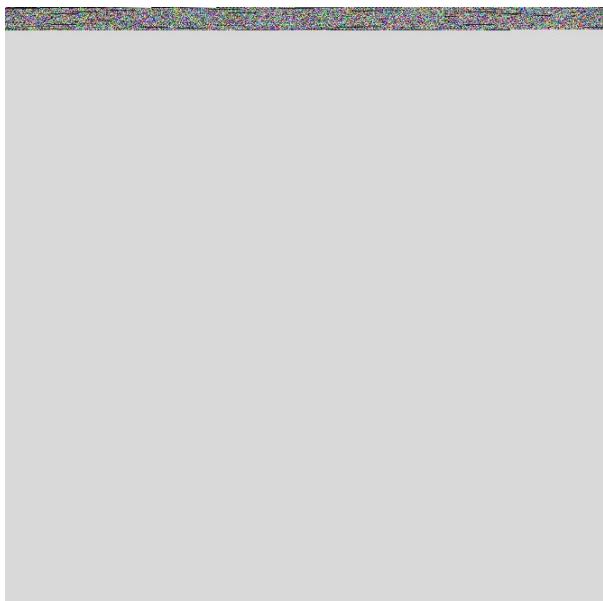


Cyclopentadienylum cation

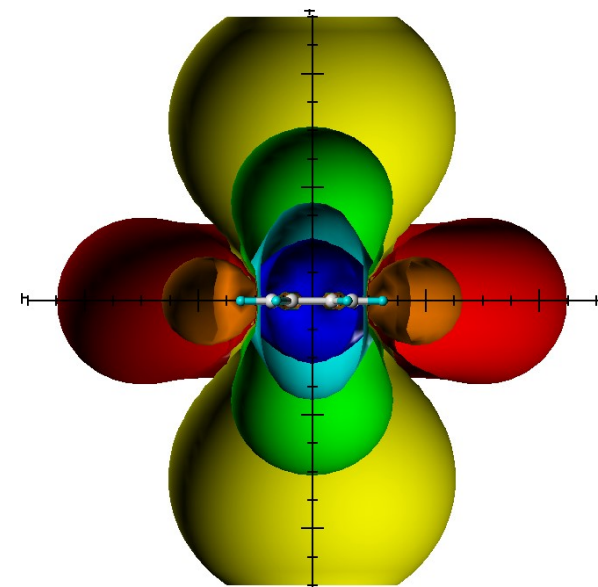


18:

Benzene



Naphthalene



19:

