Malonaldehyde-like systems:BeF_2 clusters. A subtle balance between hydrogen bonds, beryllium bonds and resonance.

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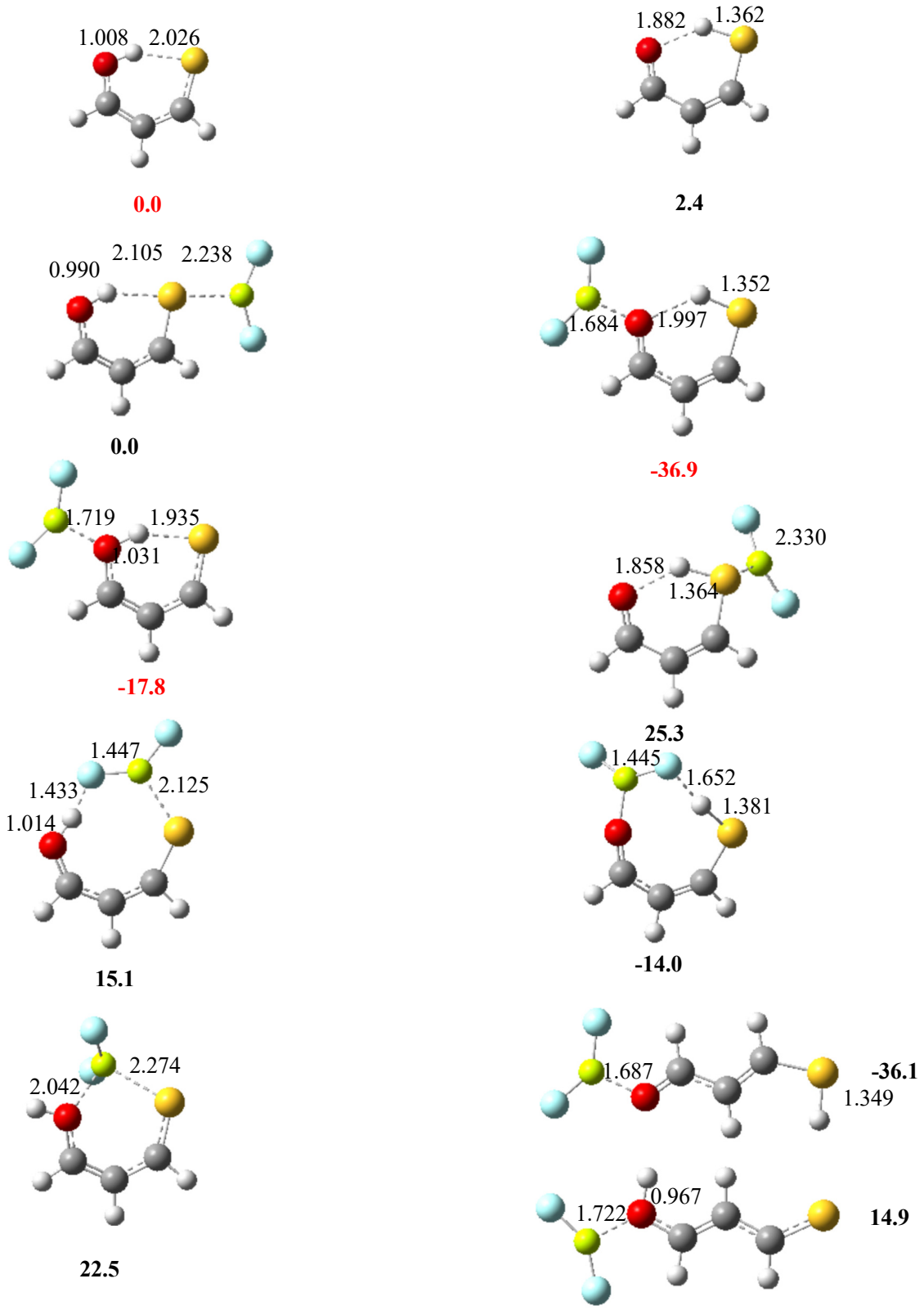
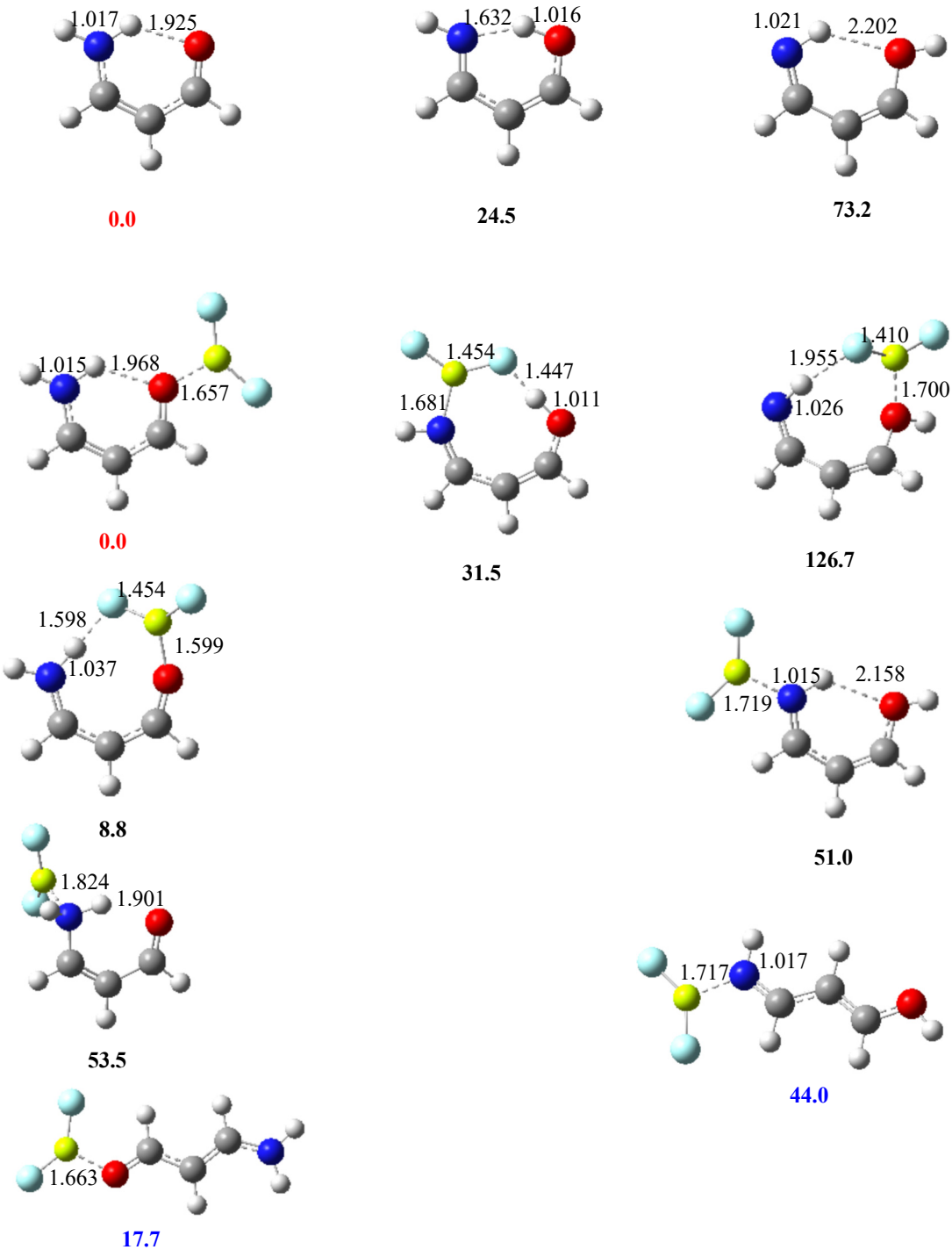


Figure S1. Optimized structures of the complexes between malonaldehyde-like (X = O, Y = S) with BeF_2, showing the relative enthalpies (in $kJ \cdot mol^{-1}$) with respect to the global minimum (in red). Bond lengths are in Å. Atom color code: C, grey; H: white; O: red; S: mustard yellow; Be: lemon yellow; F: light blue.



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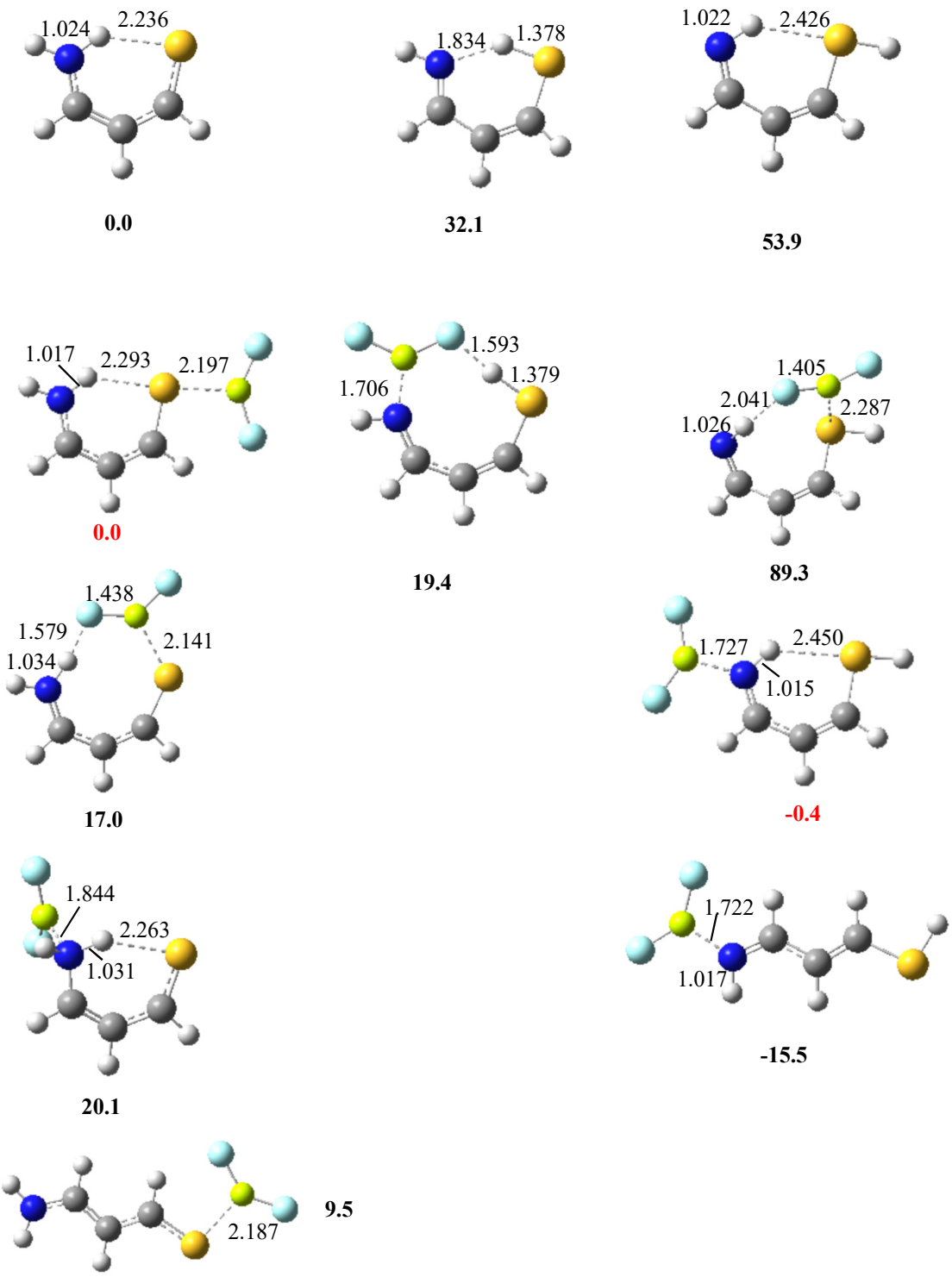

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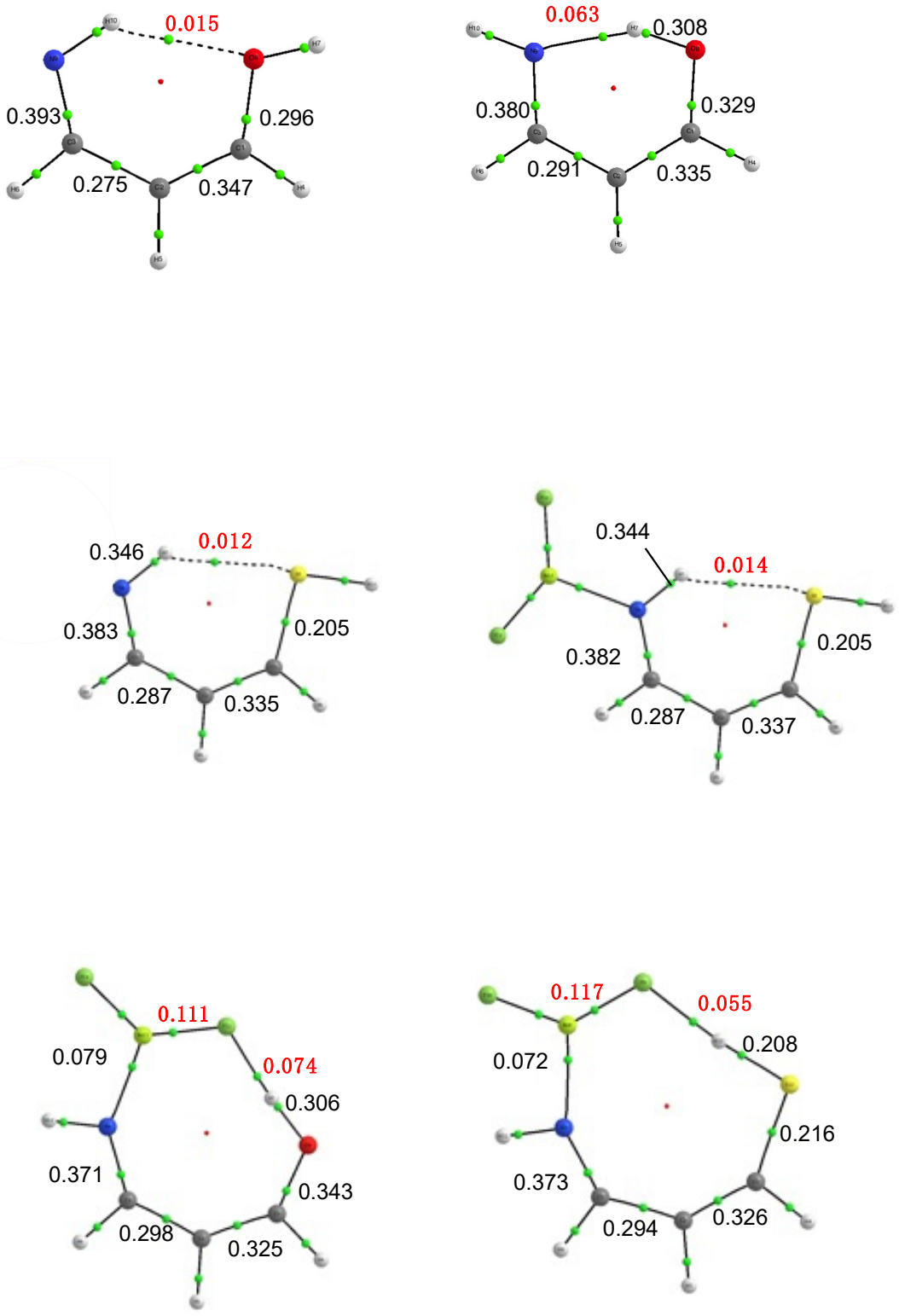

Figure S4. Molecular graphs of the malonaldehyde-like complexes in which X = O, S and Y = NH with BeF_2 molecule. Electron densities at the bond critical points in a.u.