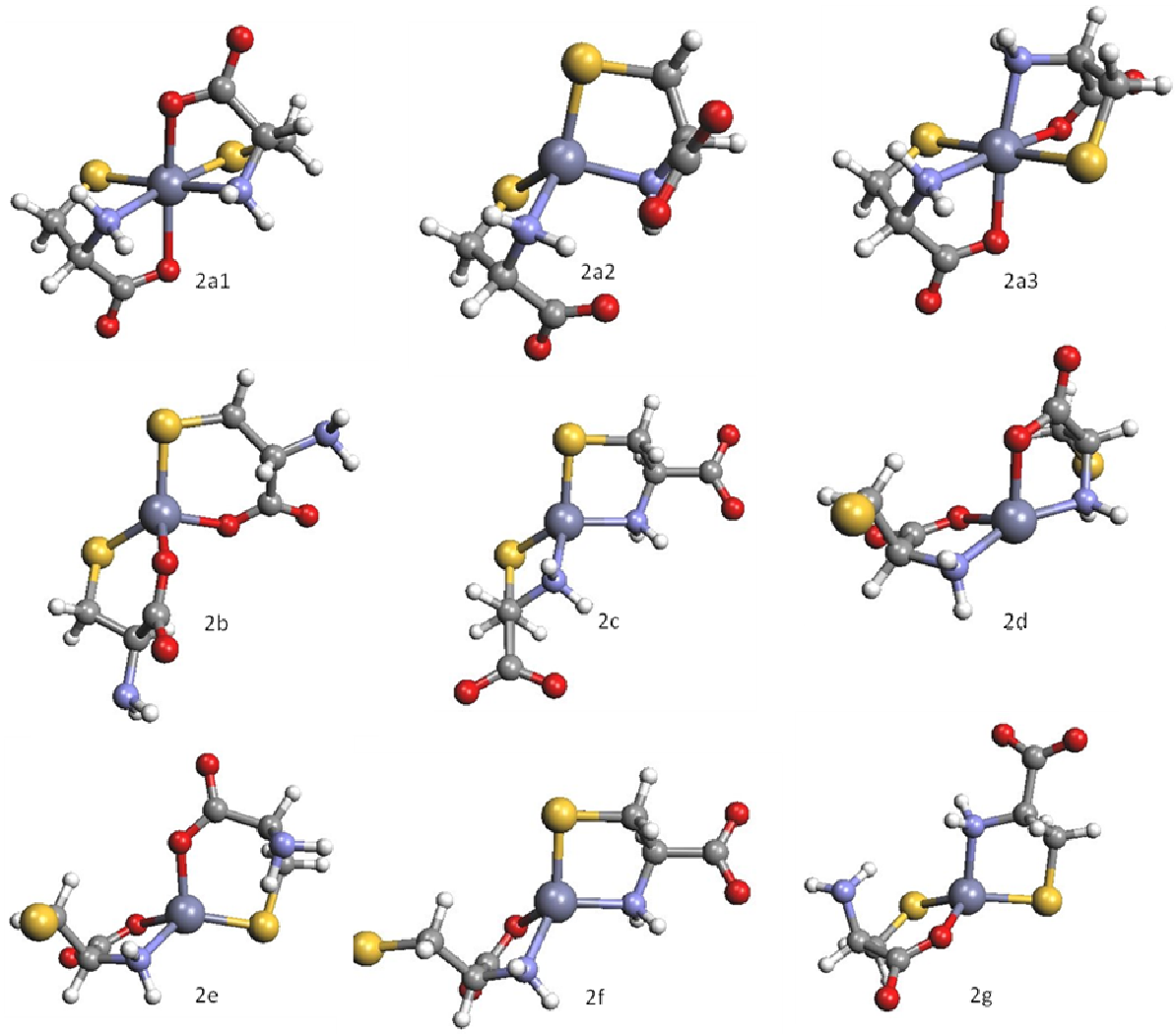

Figure S1. Optimized (BP86/TZVP+COSMO) structures for the studied $ZnCys_2$ complexes. If the initial binding mode differs from the final one, the previous is shown in parentheses.

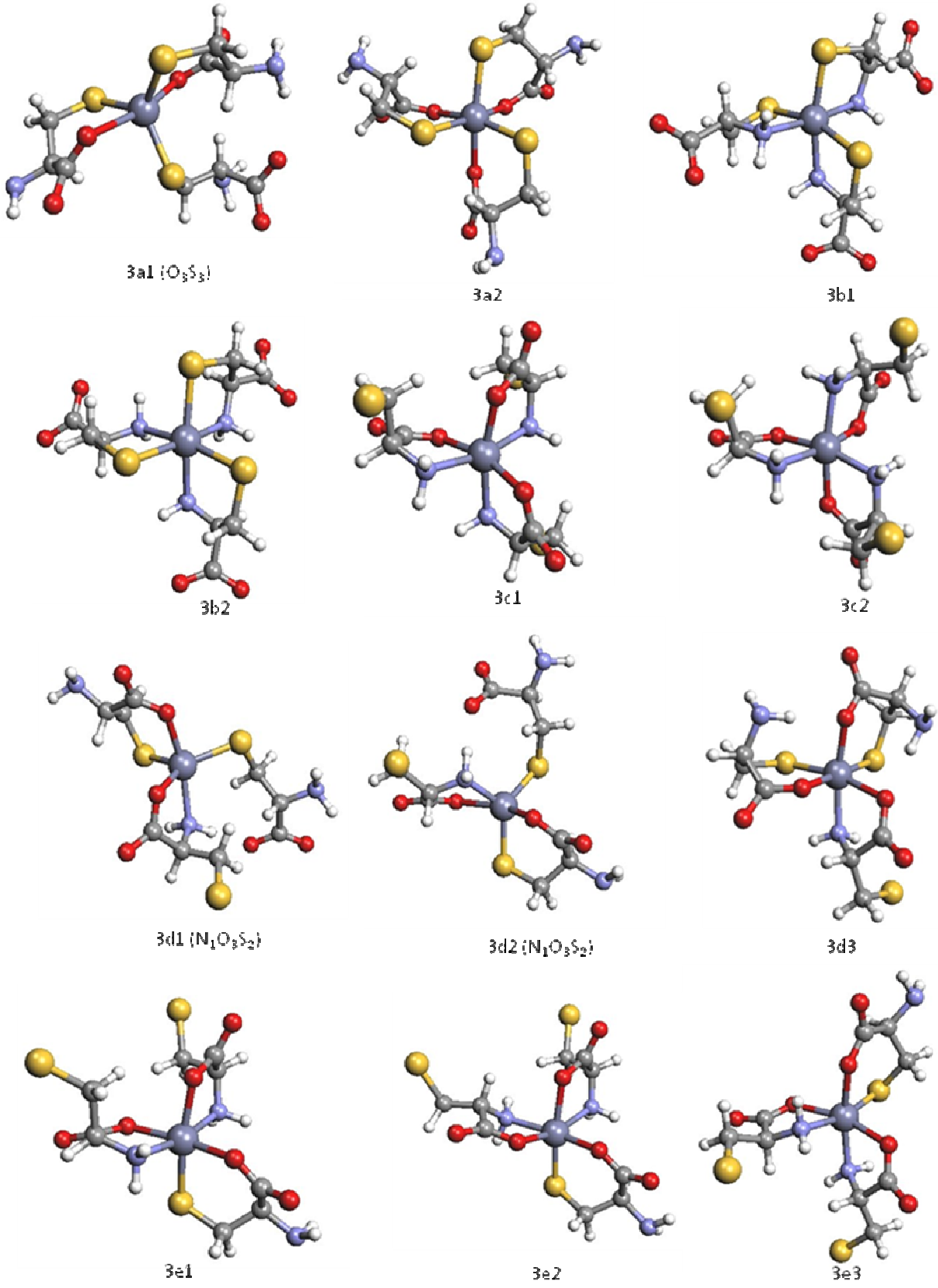

Figure S2. Optimized (BP86/TZVP+COSMO) structures for the studied $ZnCys_3$ complexes. If the initial binding mode differs from the final one, the previous is shown in parentheses.

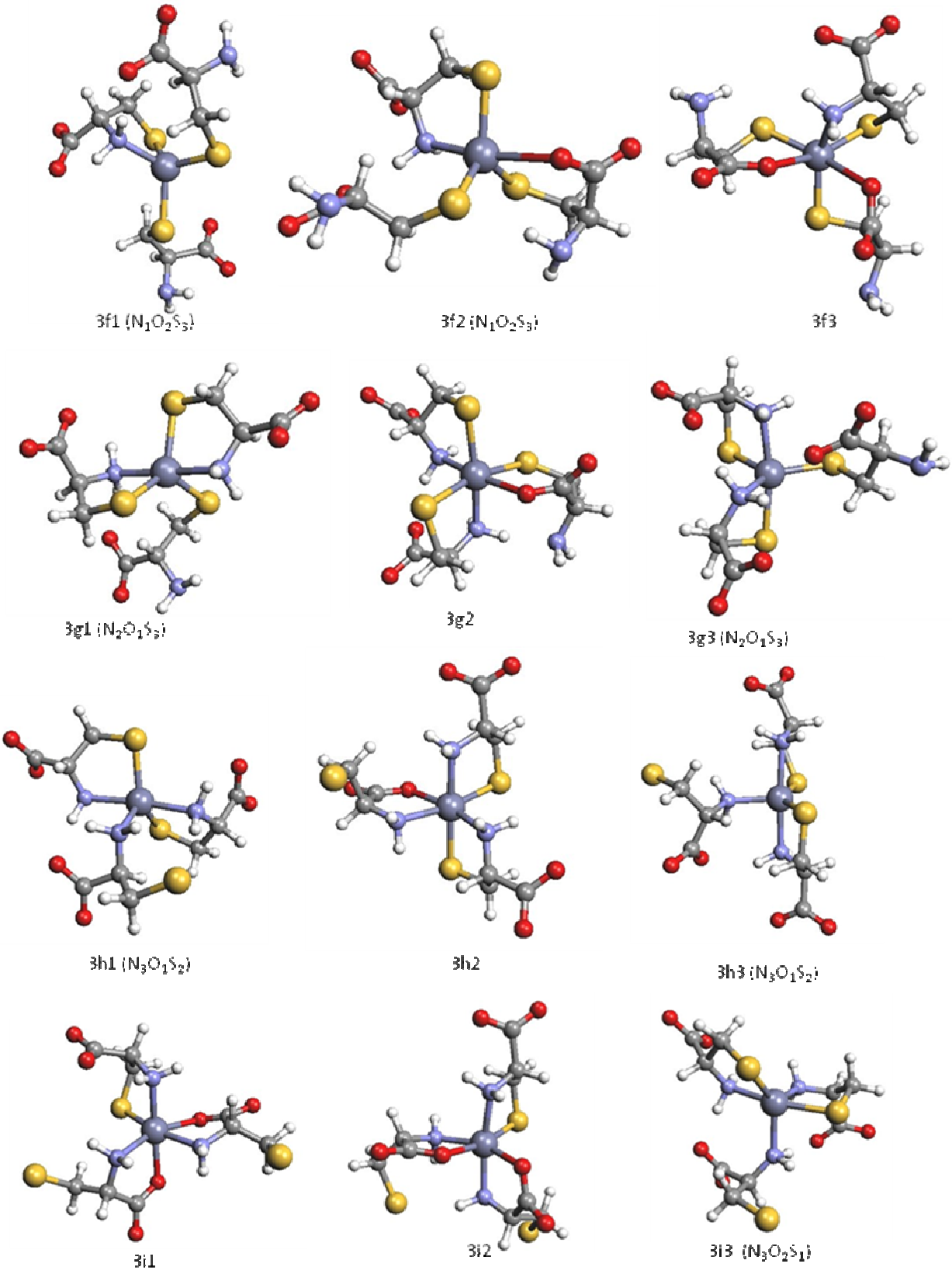

Figure 2. Continuing

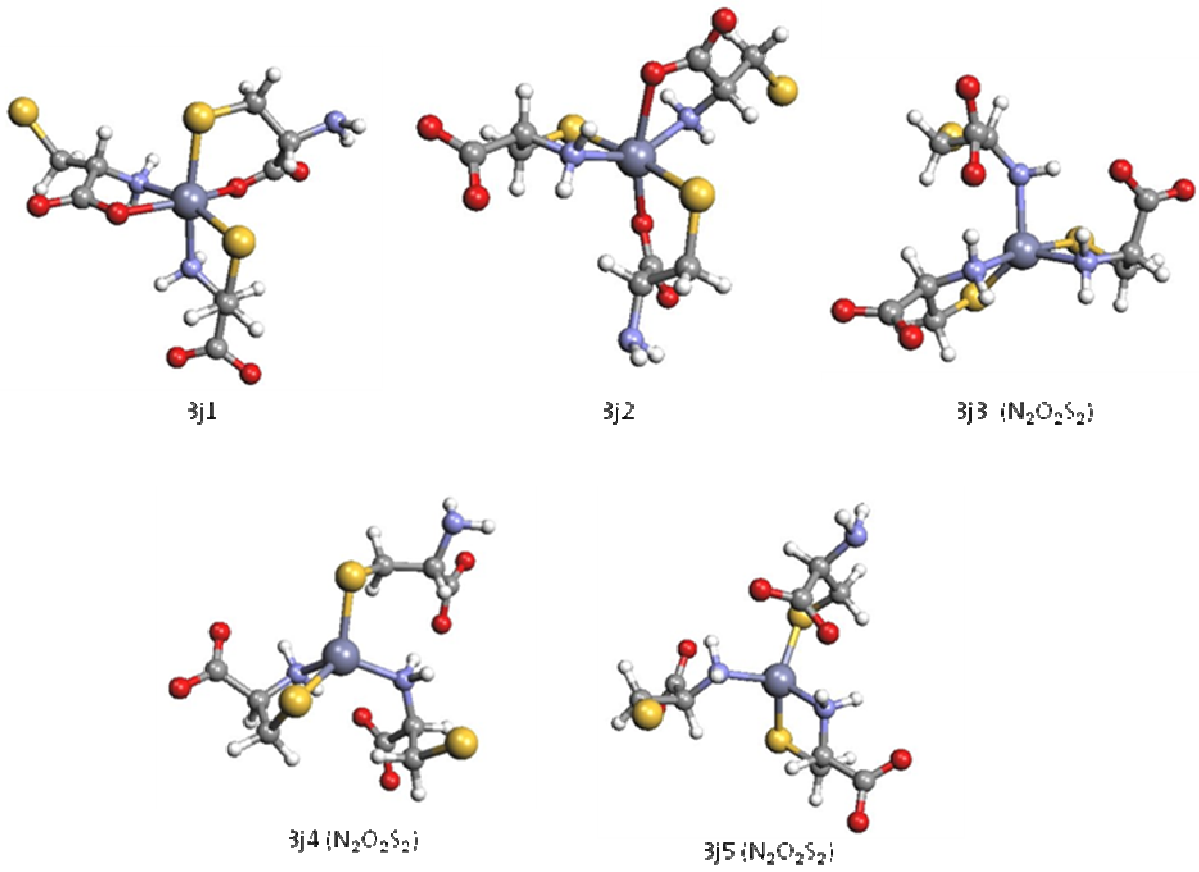

Figure 2. Continuing