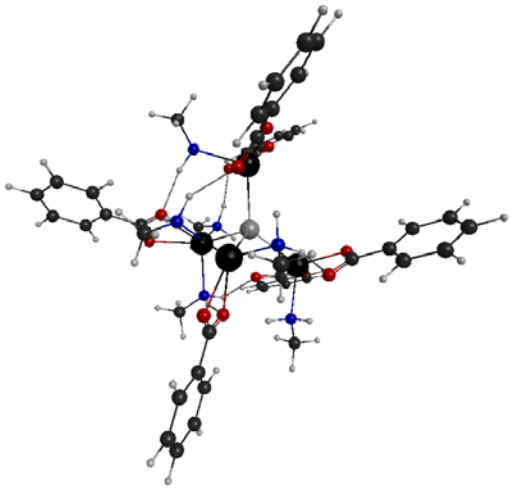
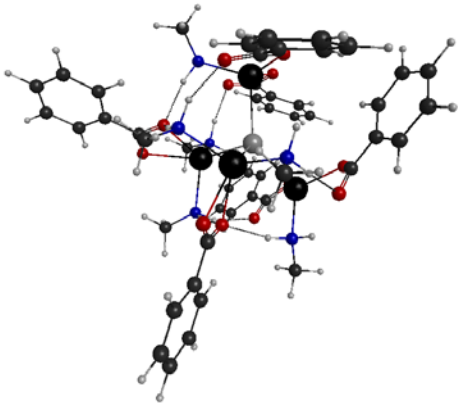
a



b



c

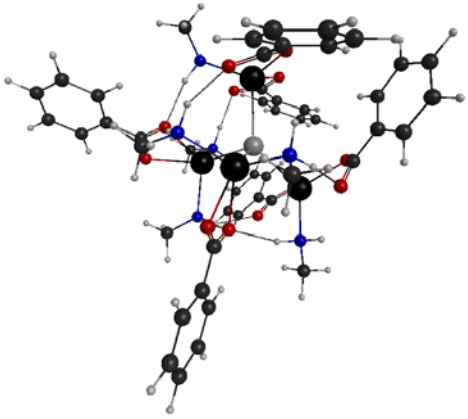
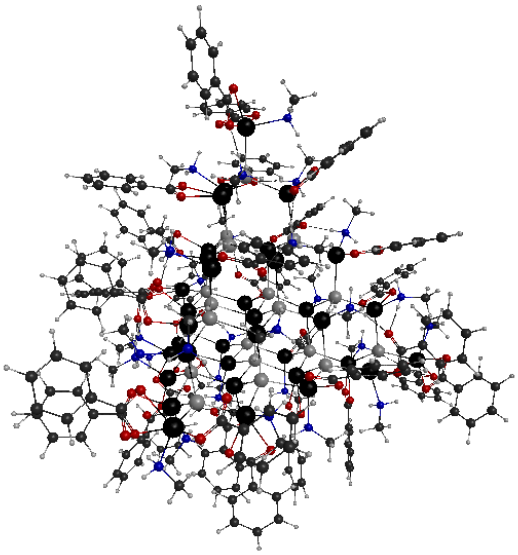


Figure 1S. $Cd_4SeX_6L_6$ (X = benzoate, L = methylamine) structures predicted with PBE0 (**a**), PBE0-D3 (**b**), and MP2 (**c**) methods.

a



b

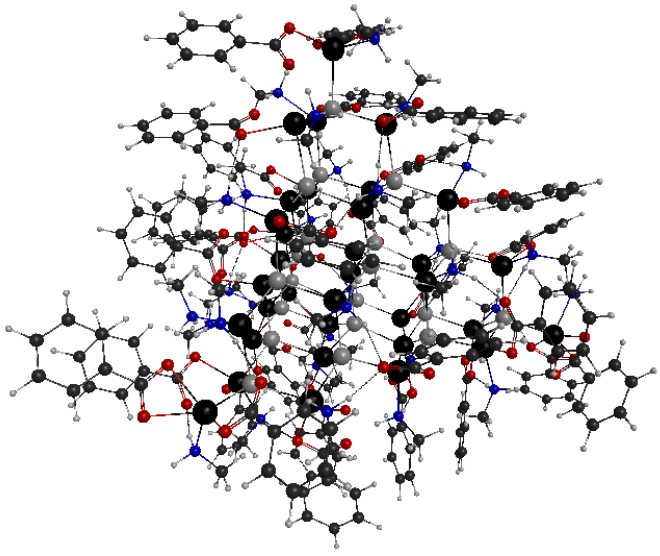


Figure 2S. $Cd_{35}Se_{20}X_{30}L_{30}$ (X = benzoate, L = methylamine) structures predicted with PBE0 (**a**), PBE0-D3 (**b**) methods.

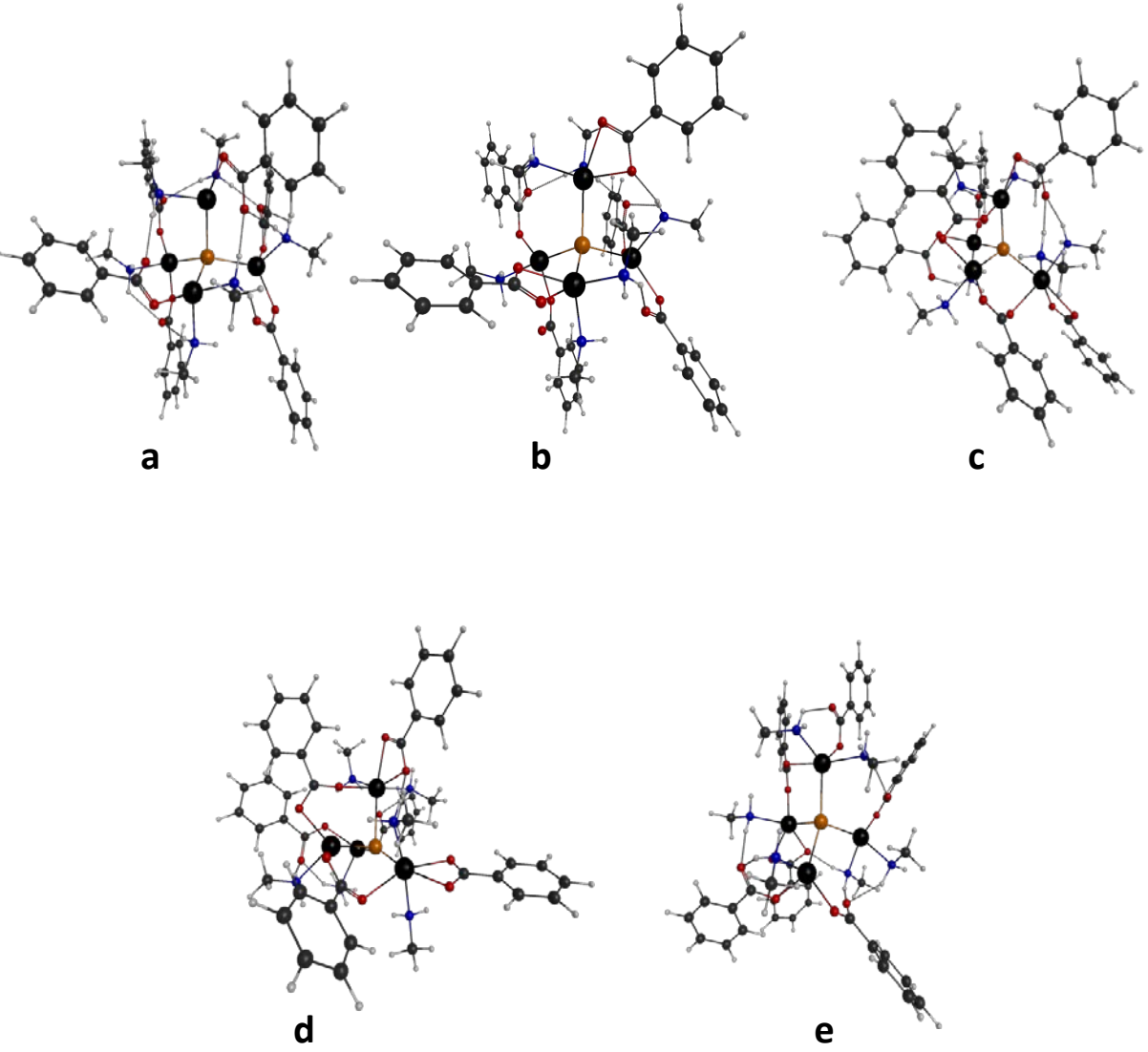


Figure 3S. Structures of the T1 isomers of $Cd_4SeX_6L_6$ (X = benzoates, L = methylamine).

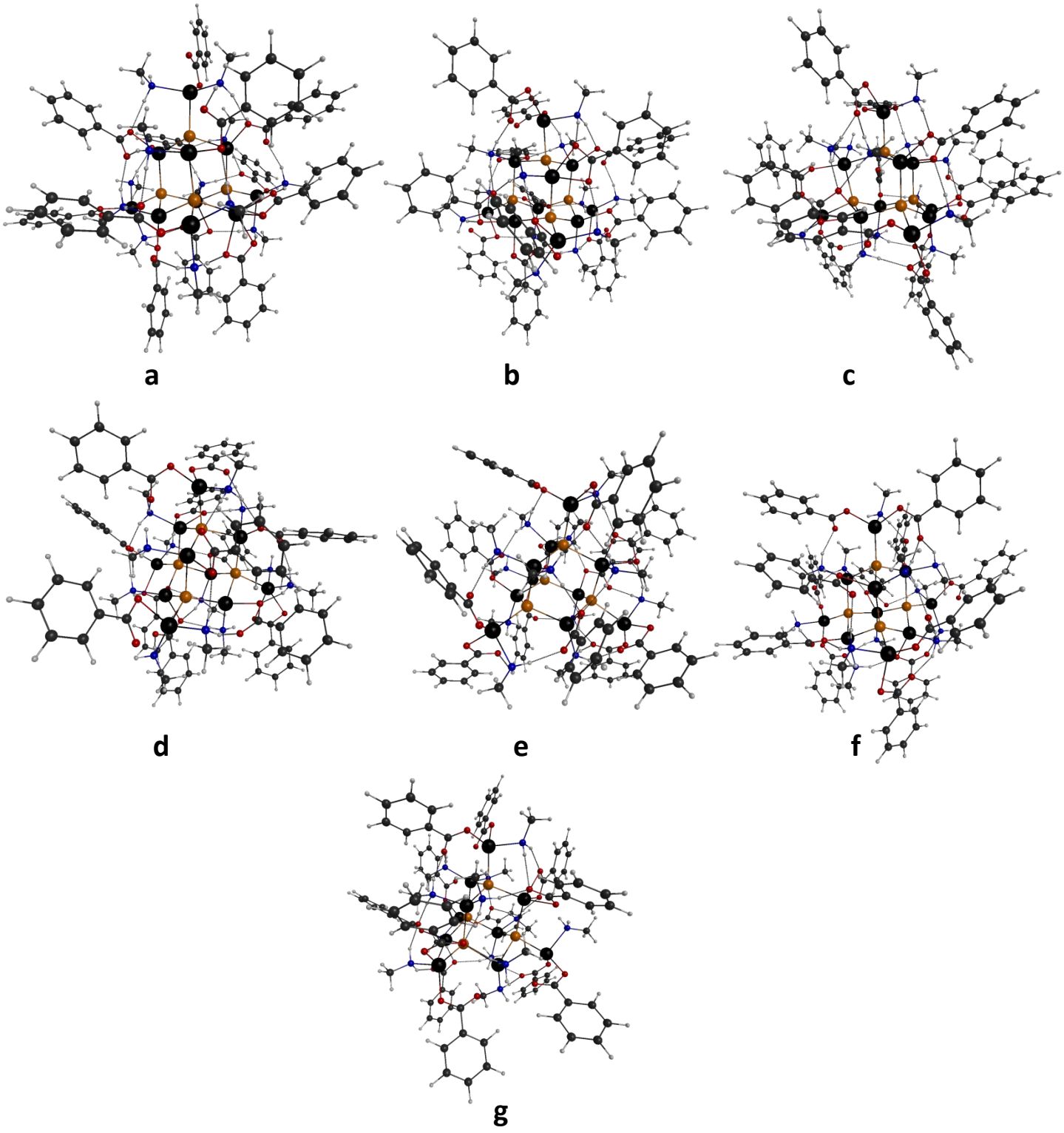


Figure 4S. Structures of the T2 isomers of $Cd_{10}Se_4X_{12}L_{12}$ (X = benzoate, L = methylamine), $4A_{X,2L}2E_{2X}4E_{X,L}$ (**a**), $3A_{X,2L}A_{2X,L}E_{2X}5E_{X,L}$ (**b**), ($4A_{2X,L}2E_{2X}4E_{2L}$ (**c**), $2A_{X,2L}2A_{2X,L}6E_{X,L}$ (**d**), $4A_{2X,L}2E_{2L}4E_{X,L}$ (**e**), $3A_{2X,L}A_{2X,L}2E_{2L}4E_{X,L}$ (**f**), $4A_{2XI}4E_{2L}2E_{2X}$ (**g**).

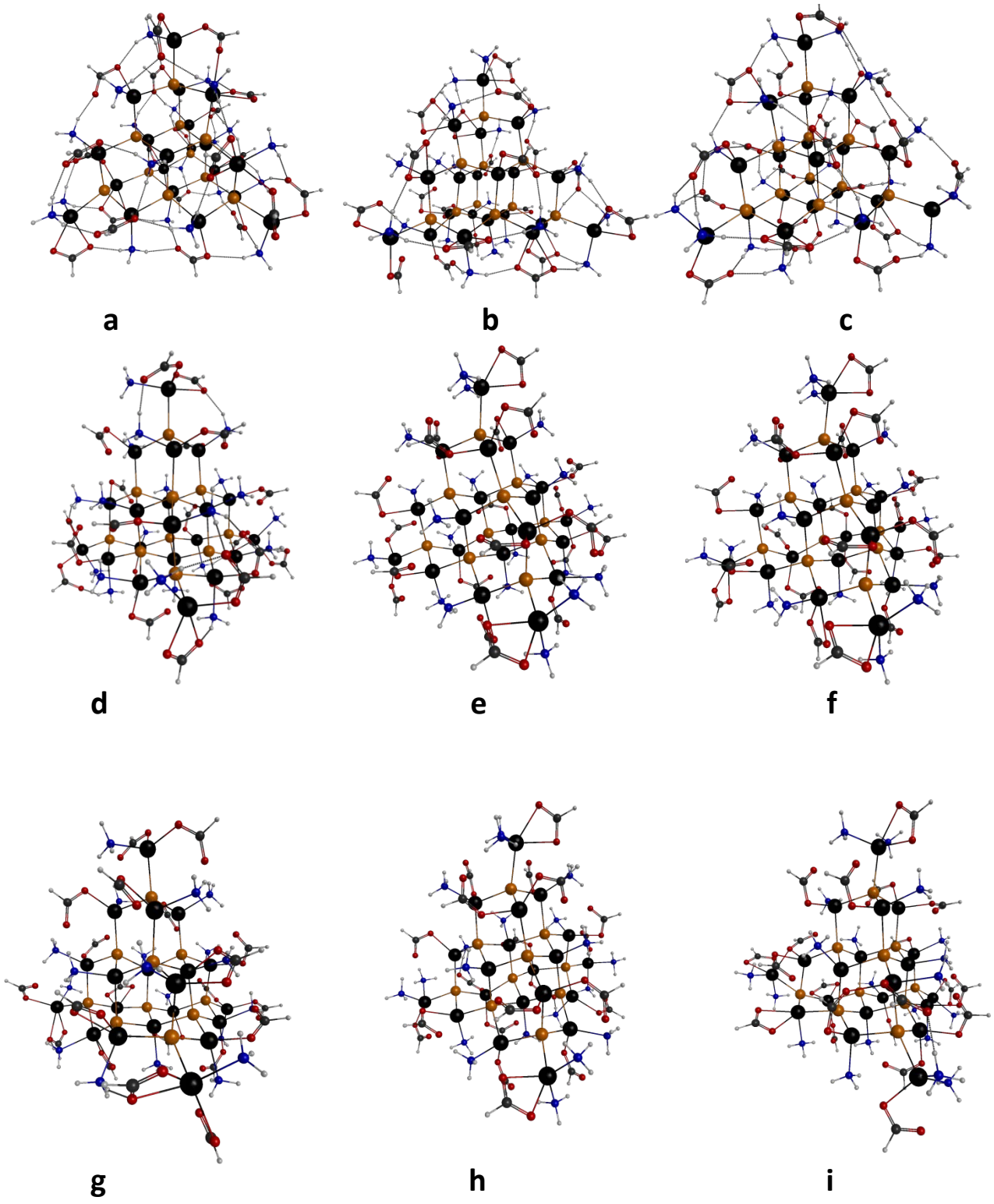


Figure 5S. Structures of the T3 isomers of $Cd_{20}Se_{10}$ (X = formate, L = ammonia), $2A_{2x,L}2A_{X,2L}5E_{2X,2L}E_{4X}$ $4F_L$ (**a**), $2A_{2X,L}2A_{X,2L}6E_{2X,2L}$ $2F_X2F_L$ (**b**), $4A_{X,2L}6E_{2X,2L}$ $4F_X$ (**c**), $4A_{2X,L}6E_{2X,2L}4F_L$ (**d**), $2A_{2x,L}2A_{X,2L}5E_{2X,2L}$ $E_{4X}4F_L$ (**e**), $4A_{X,2L}5E_{2X,2L}E_{4X}$ $4F_L$ (**f**), $4A_{2X,L}6E_{2X,2L}4F_L$ with C_2 symmetry (**g**), $4A_{2X,L}4E_{2X,2L}2E_{4X}4F_L$ (**h**), $4A_{X,2L}4E_{3X,L}E_{2X,2L}4F_L$ (**i**)

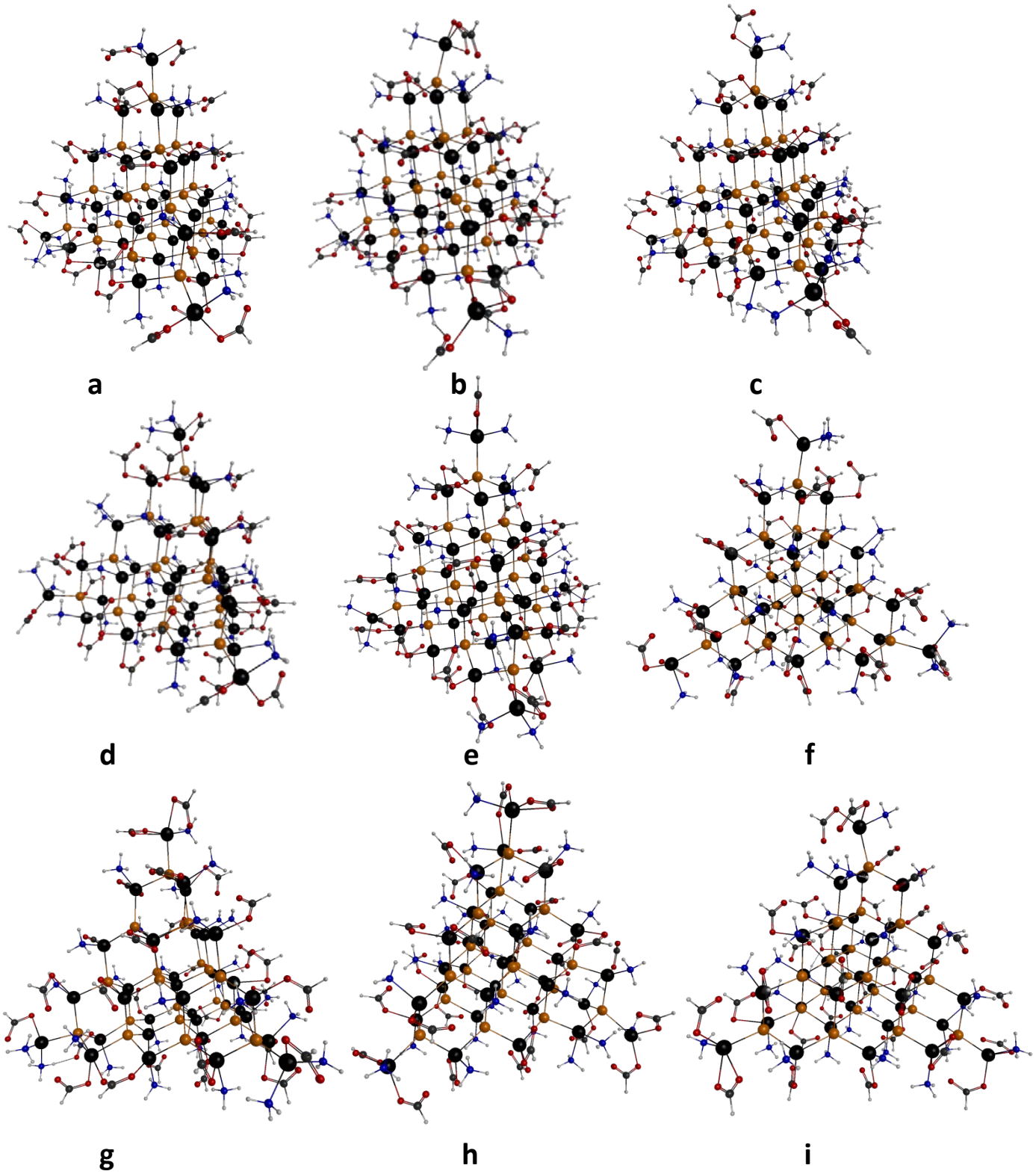


Figure 6S. Structures of the T4 isomers of $Cd_{35}Se_{20}$ (X = formate, L = ammonia), $4A_{2x,L}4E_{4X,2L}2E_{3X,3L}$ $4F_{3L}$ (**a**), $2A_{2X,L}2A_{X,2L}6E_{4X,2L}$ $2F_X$ $4F_{3L}$ (**b**), $2A_{2X,L}2A_{X,2L}6E_{4X,2L}$ $4F_{2L}$ with C_2 symmetry (**c**), $4A_{X,2L}6E_{4X,2L}4F_L$ (**d**), $2A_{2x,L}2A_{X,2L}5E_{2X,2L}$ $E_{4X}4F_I$ (**e**), $2A_{2X,L}2A_{X,2L}6E_{4X,2L}6F_{3L}$ (**f**), $2A_{2X,L}2A_{X,2L}6E_{3X,3L3}F2_{X,L}F_{3L}$ (**g**), $4A_{2X,L}3E4_{X,2L}E_{2X,4L}$,$2E_{3X,3L}F_{2X,L3}F_{3L}$ (**h**),. $4A_{2X,L}4E_{3X,3L}2E_{2X,4L}3F_{2X,L}F_{3L}$ (**i**)