Supporting Information

for

# Magnetic structure of $(C_5H_{12}N)CuBr_3$: Origin of the uniform Heisenberg chain behavior and the magnetic anisotropy of the $Cu^{2+}$ (S = 1/2) ions

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Table S1. Values of the coefficients $n_1 – n_7$ of Eq. 2 for the seven ordered spin states FM and AF1 – AF6

| | $n_1$ | $n_2$ | $n_3$ | $n_4$ | $n_5$ | $n_6$ |
|---|---|---|---|---|---|---|
| FM | -4 | -4 | -8 | -4 | -8 | -8 |
| AF1 | +4 | +4 | -8 | +4 | -8 | -8 |
| AF2 | -4 | -4 | -8 | +4 | +8 | 0 |
| AF3 | +4 | -4 | +8 | +4 | -8 | -8 |
| AF4 | +4 | -4 | +8 | -4 | +8 | 0 |
| AF5 | 0 | +4 | 0 | 0 | +8 | 0 |
| AF6 | -4 | -4 | -8 | -4 | -8 | +8 |

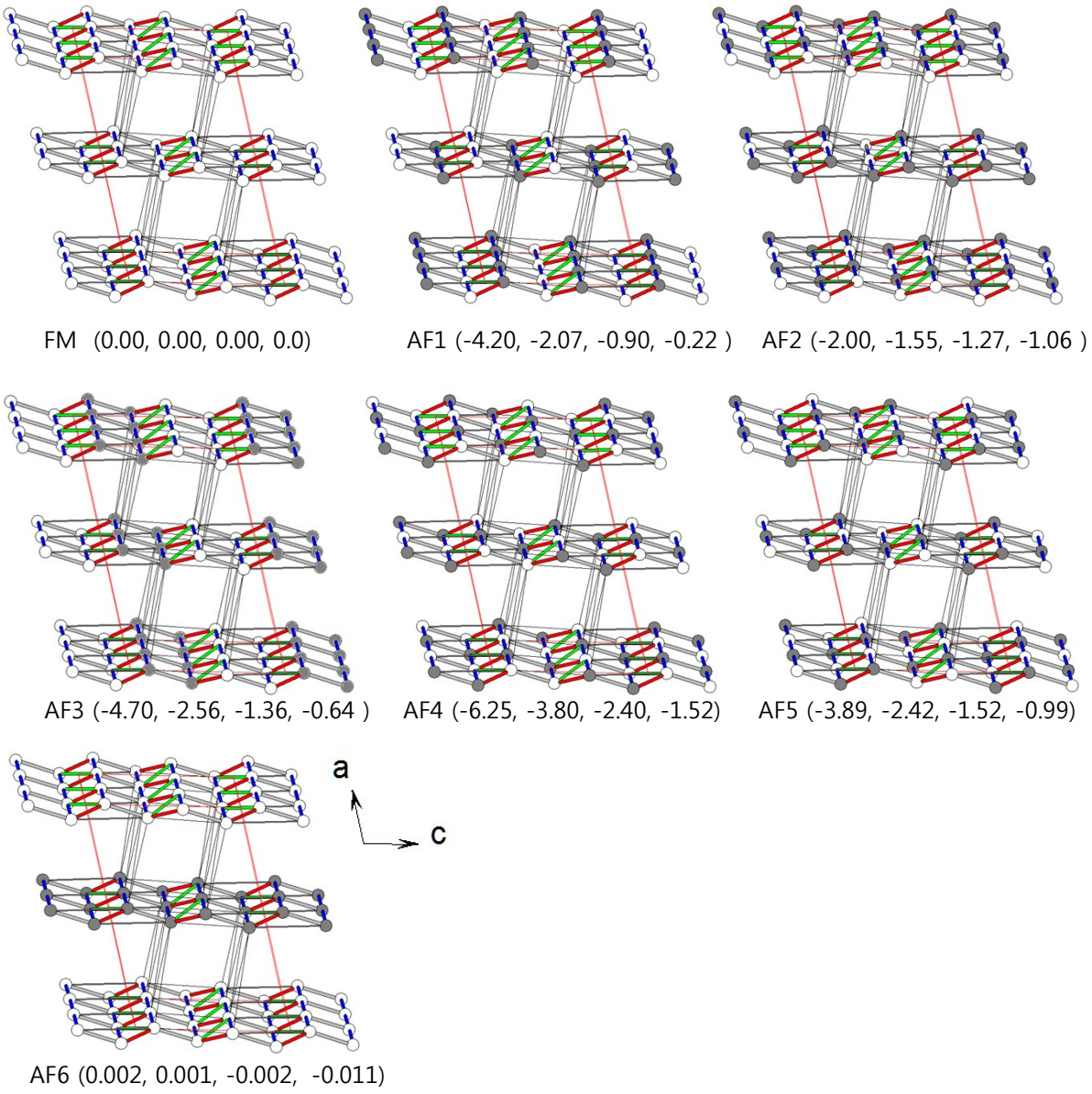


Figure S1. Ordered spin arrangements of $(C_5H_{12}N)CuBr_3$ employed for the extraction of the six spin exchange parameters $J_1 - J_6$. The up-spin and down-spin Cu sites are indicated by open and filled circles, respectively. The numbers in the parentheses for each state are the relative energies (in meV per formula unit) obtained from the DFT+U calculations, where the numbers from left to right refer to the cases of $U^{eff}$ = 2, 4, 6, and 8 eV, respectively.