

Formation of a Dynamic κ O,N-Hydroxylaminato
Zirconocene Complex by Nitrosoarene Insertion into a
Zr-C σ -Bond

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Supporting Material

Calculation:

$$\Delta G^\# = RT_c (22.96 + \ln(T_c/\Delta v) J \text{ mol}^{-1}; 1J = 0.2388459 \text{ cal}; R = 8.31451$$

1) $\Delta G^\#_{\text{exchange}} [\Delta v(\text{Cp}, 163K) = 317 \text{ Hz}; T_c = 198K] = 8.8 \pm 0.3 \text{ kcal mol}^{-1}$.

2.0) Average: $\Delta G^\#_{\text{aryl-rot}} = 9.4 \pm 0.3 \text{ kcal mol}^{-1}$.

2.1) $\Delta G^\#_{\text{aryl-rot}} [\Delta v(\text{o-Ph}, 163K) = 196 \text{ Hz}; T_c = 203K] = 9.3 \text{ kcal mol}^{-1}$.

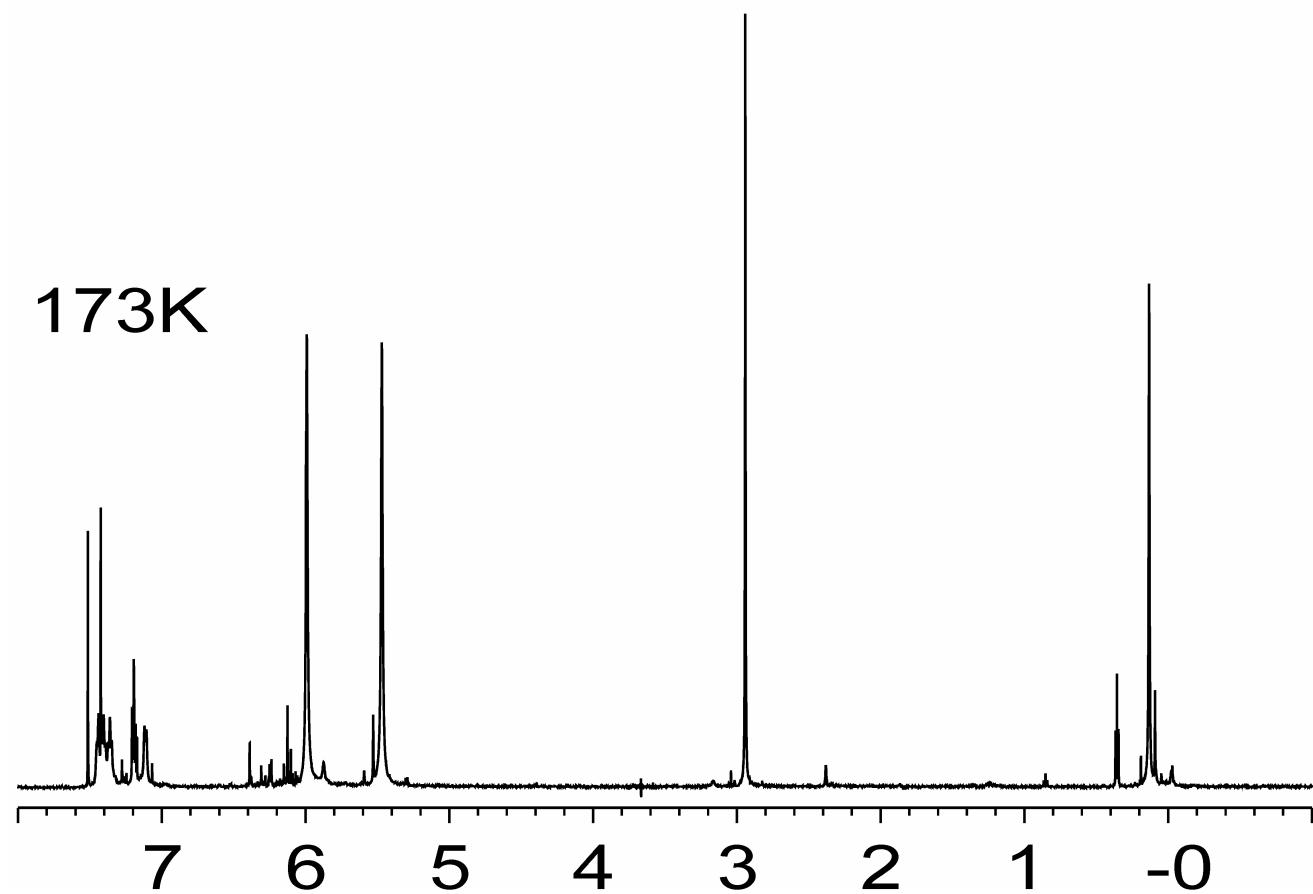
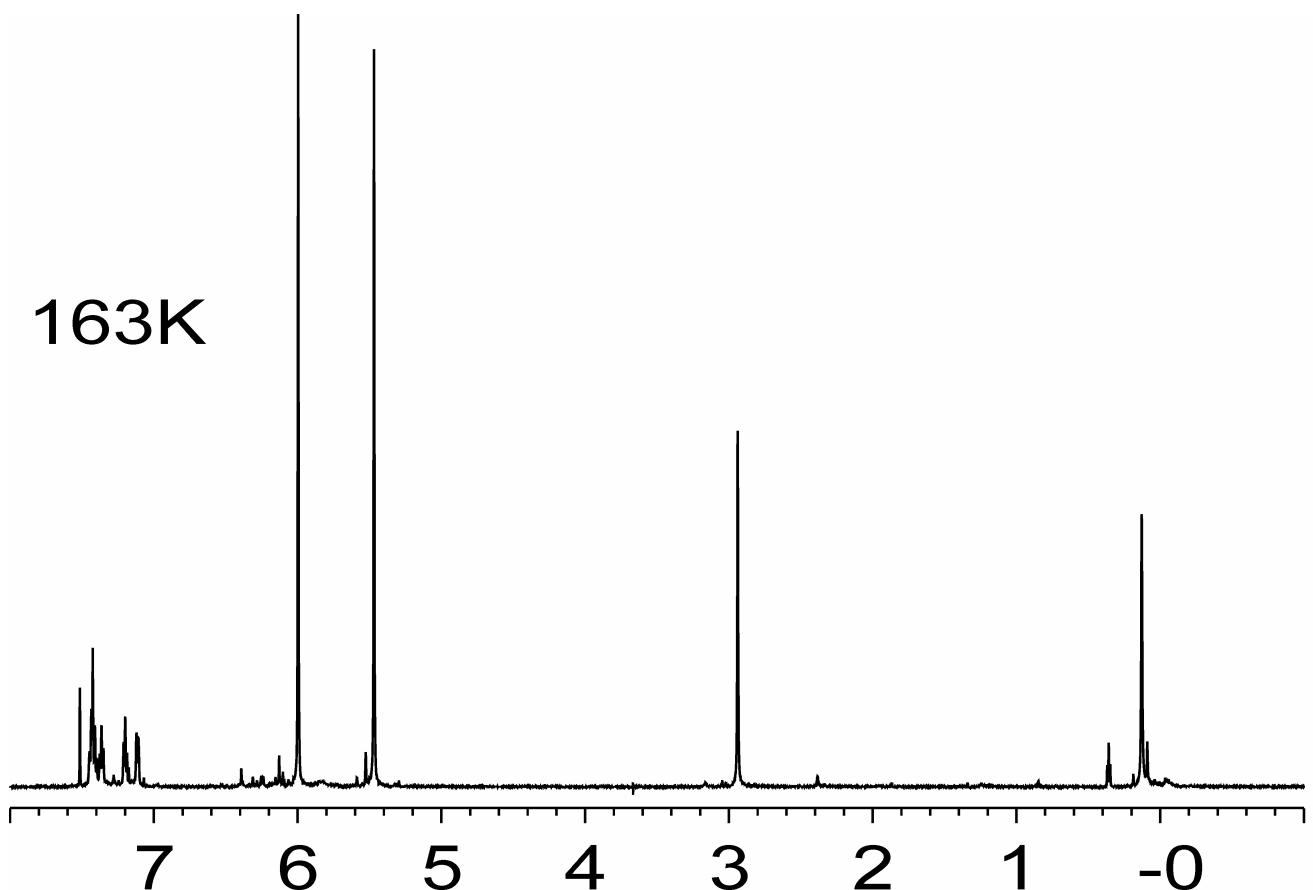
$\Delta G^\#_{\text{aryl-rot}} [\Delta v(\text{o-Ph}, 163K) = 196 \text{ Hz}; T_c = 213K] = 9.8 \text{ kcal mol}^{-1}$.

Average: $\Delta G^\#_{\text{aryl-rot}} [\delta v(\text{o-Ph}, 163K) = 196 \text{ Hz}; T_c = 208K] = 9.5 \pm 0.3 \text{ kcal mol}^{-1}$.

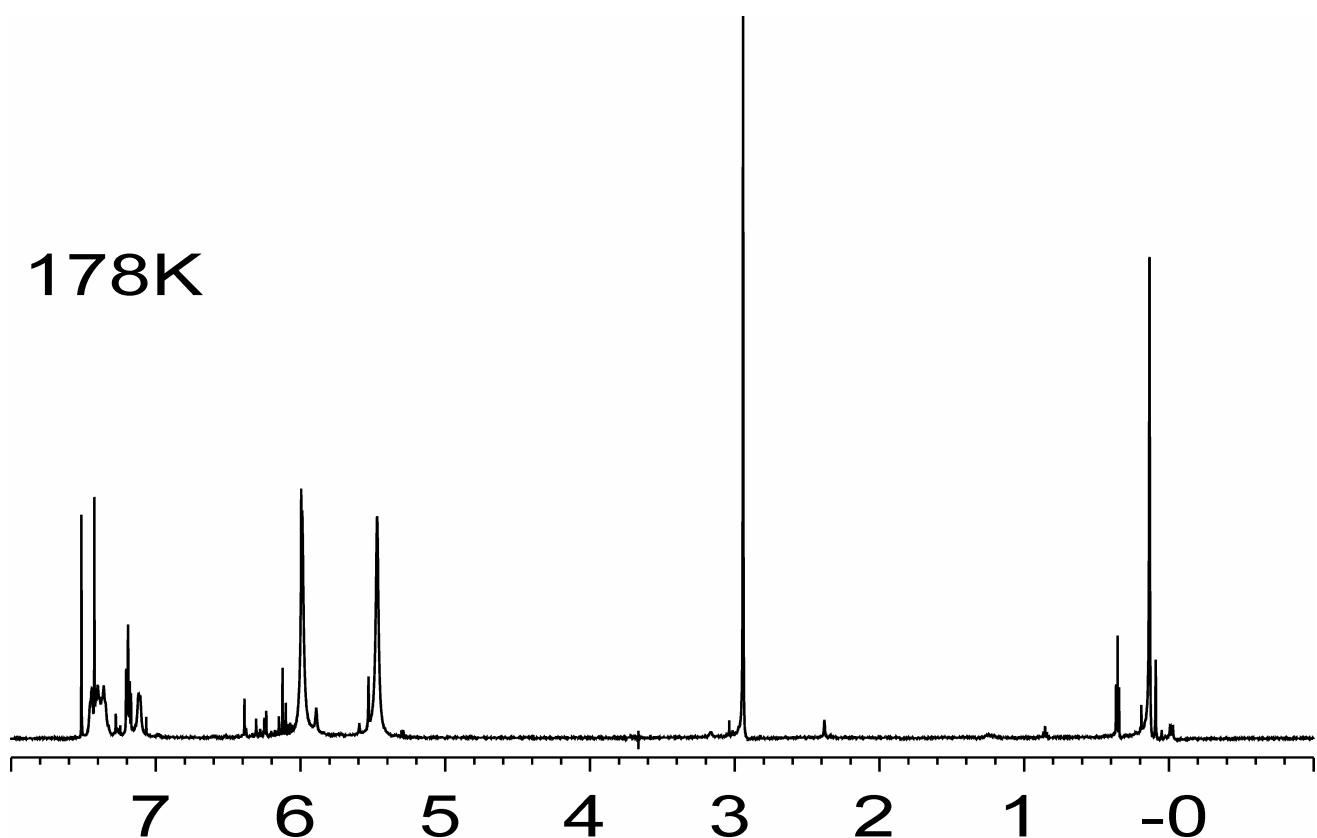
2.2) $\Delta G^\#_{\text{aryl-rot}} [\Delta v(\text{m-Ph}, 163K) = 28 \text{ Hz}; T_c = 183K] = 9.0 \text{ kcal mol}^{-1}$.

$\Delta G^\#_{\text{aryl-rot}} [\Delta v(\text{m-Ph}, 163K) = 28 \text{ Hz}; T_c = 193K] = 9.5 \text{ kcal mol}^{-1}$.

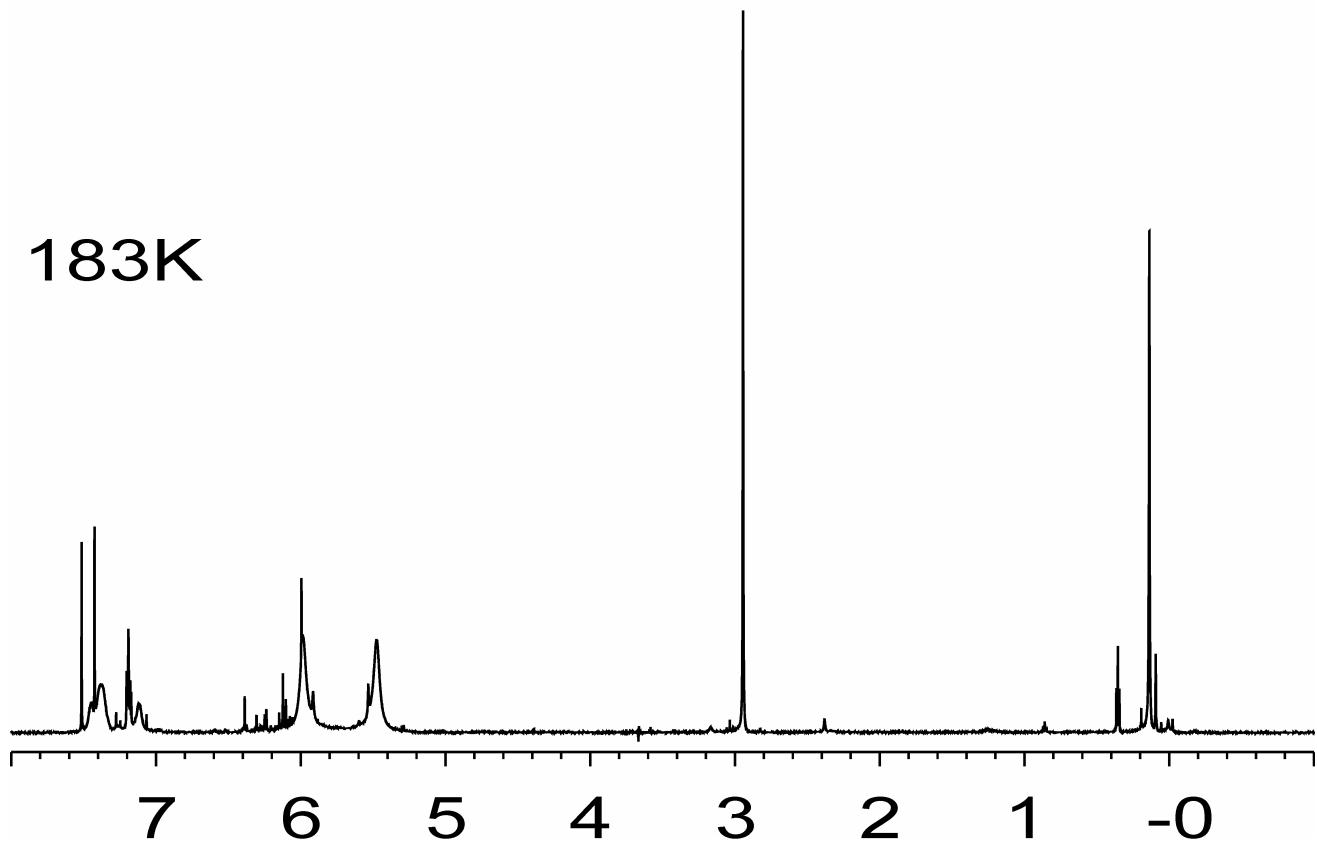
Average: $\Delta G^\#_{\text{aryl-rot}} [\Delta v(\text{m-Ph}, 163K) = 28 \text{ Hz}; T_c = 188K] = 9.3 \pm 0.3 \text{ kcal mol}^{-1}$.



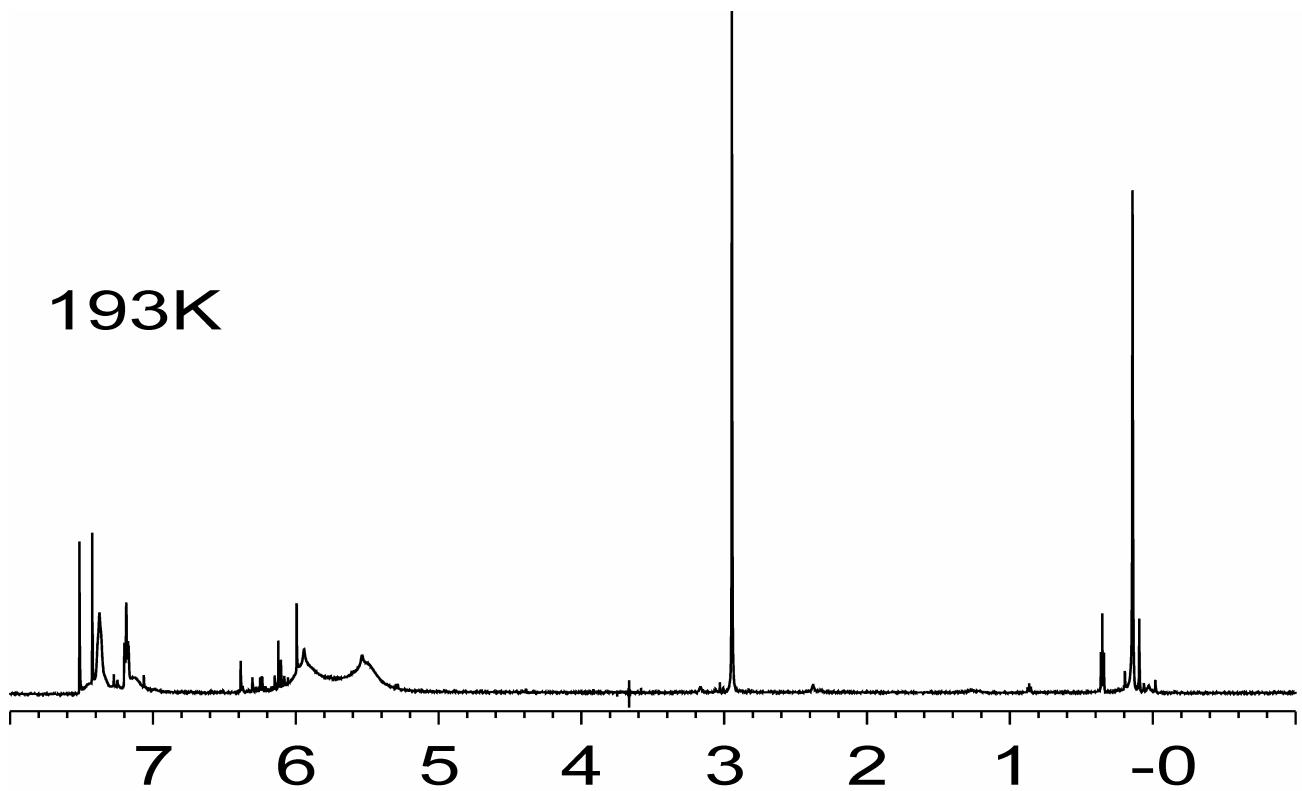
178K



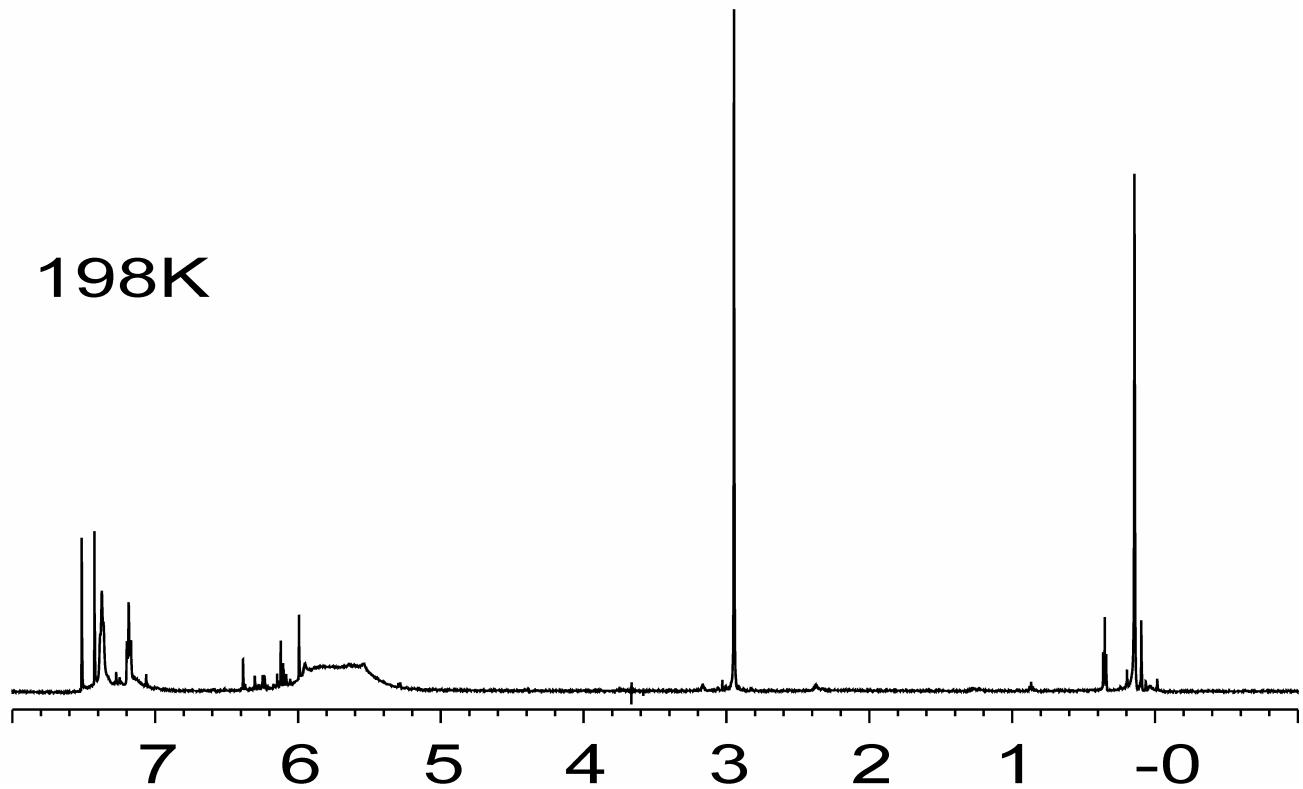
183K



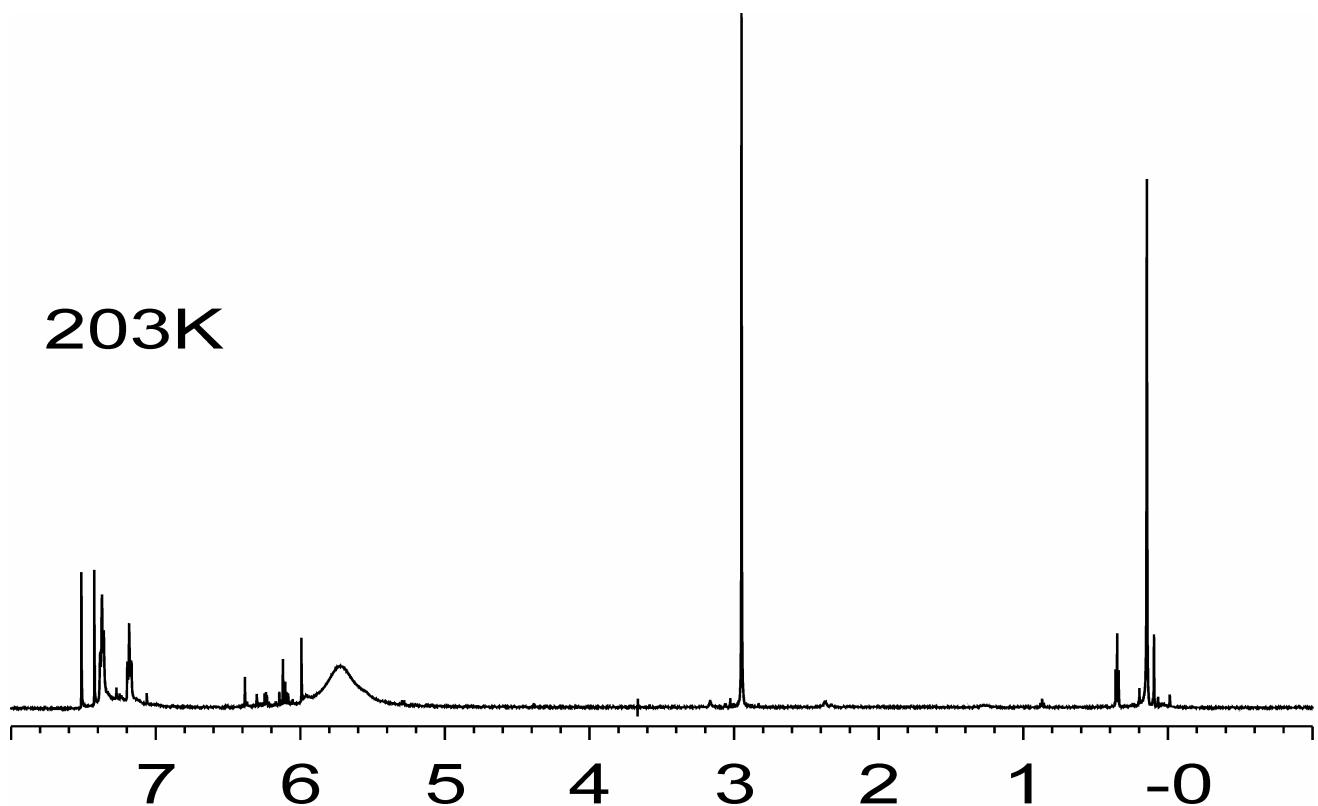
193K



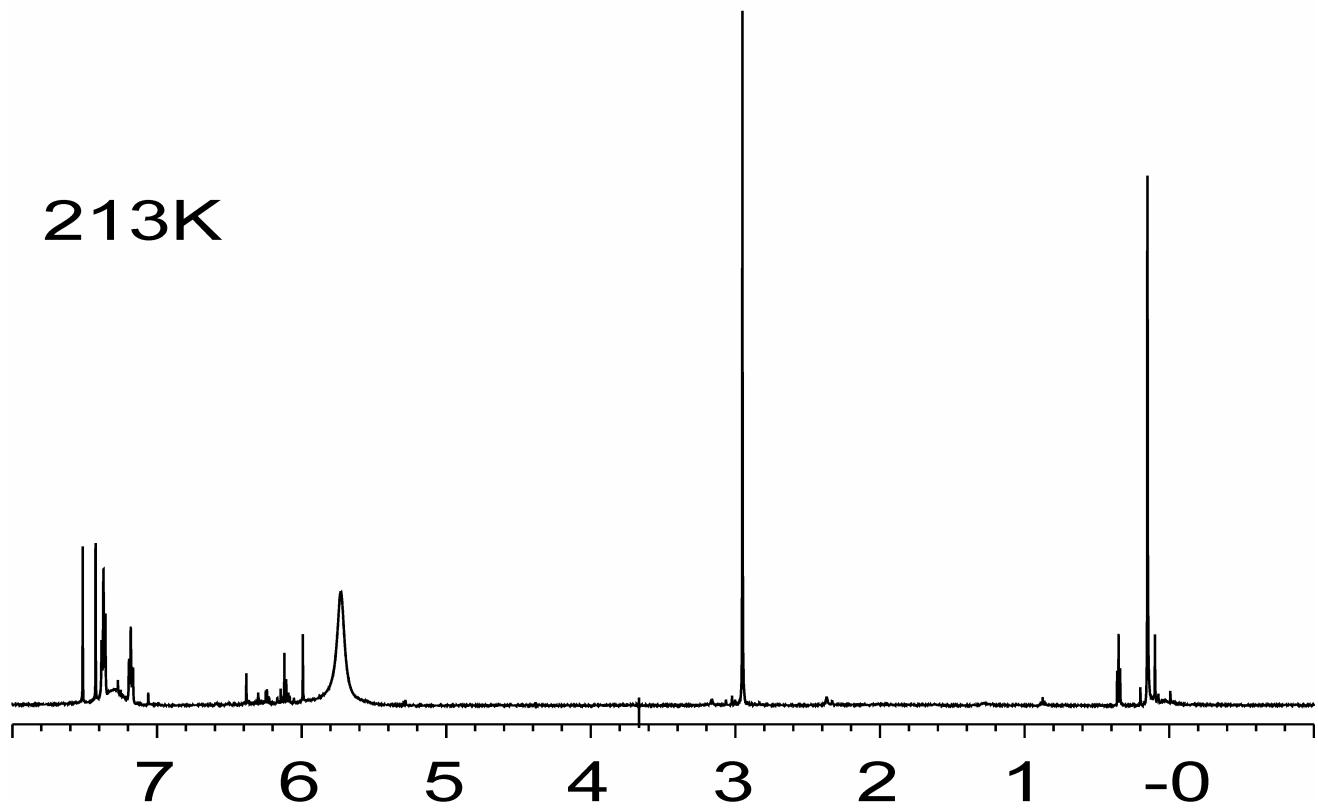
198K



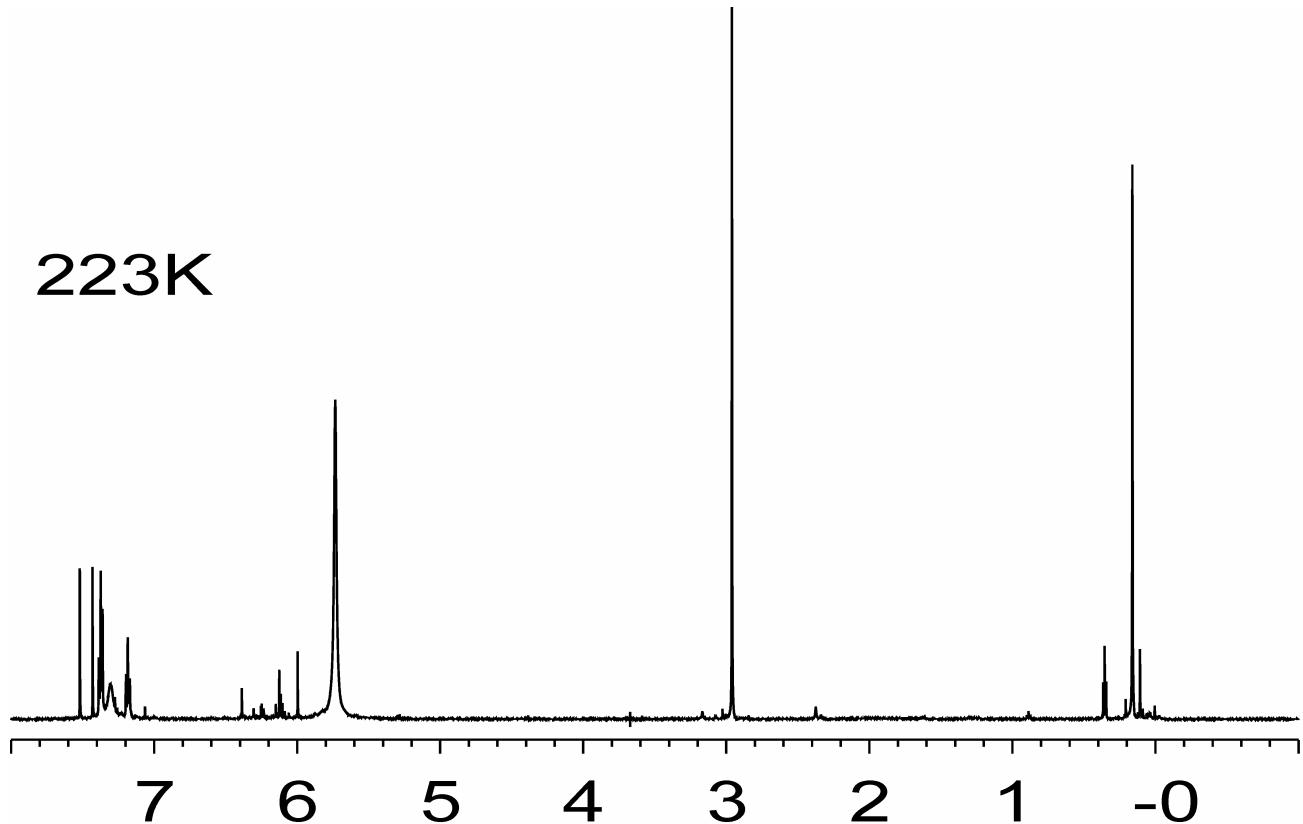
203K



213K



223K



233K

