Supporting Information

Dithionite and Sulfinate Complexes from the Reaction of SO$_2$ with Decamethylsamarocene

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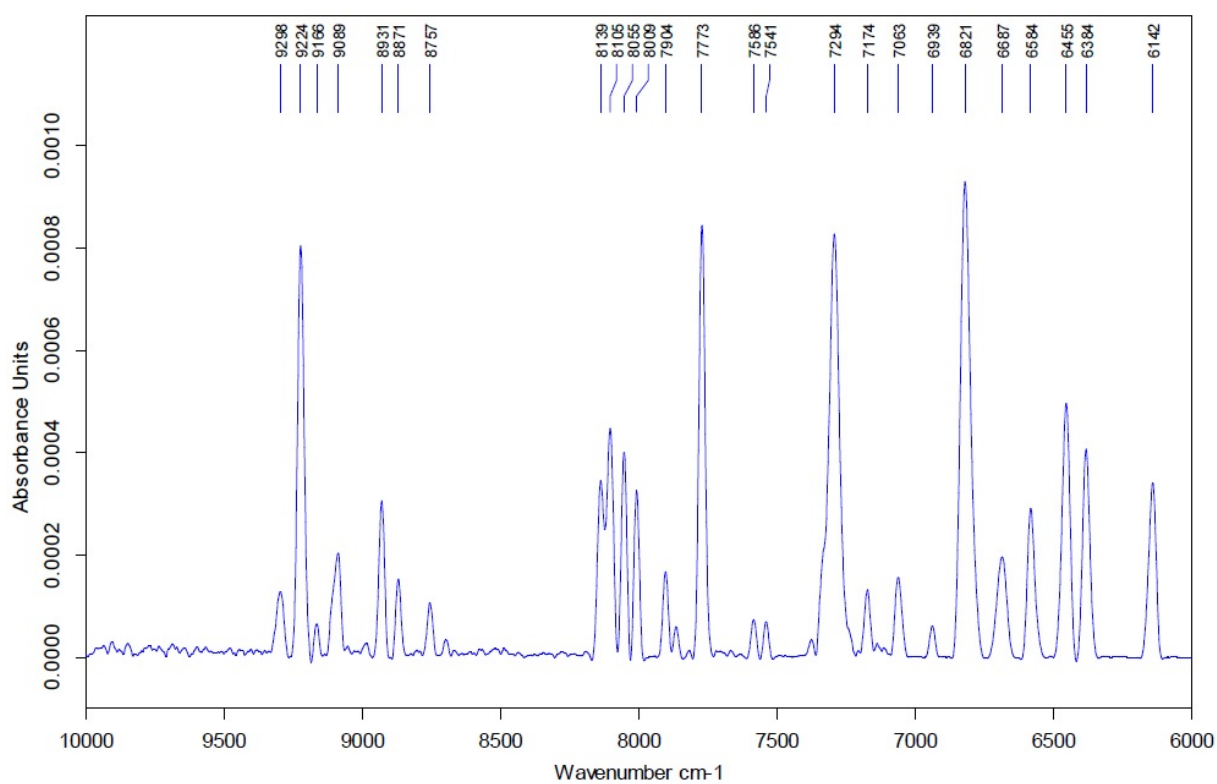
Figure S1. NIR-spectrum of **1**.
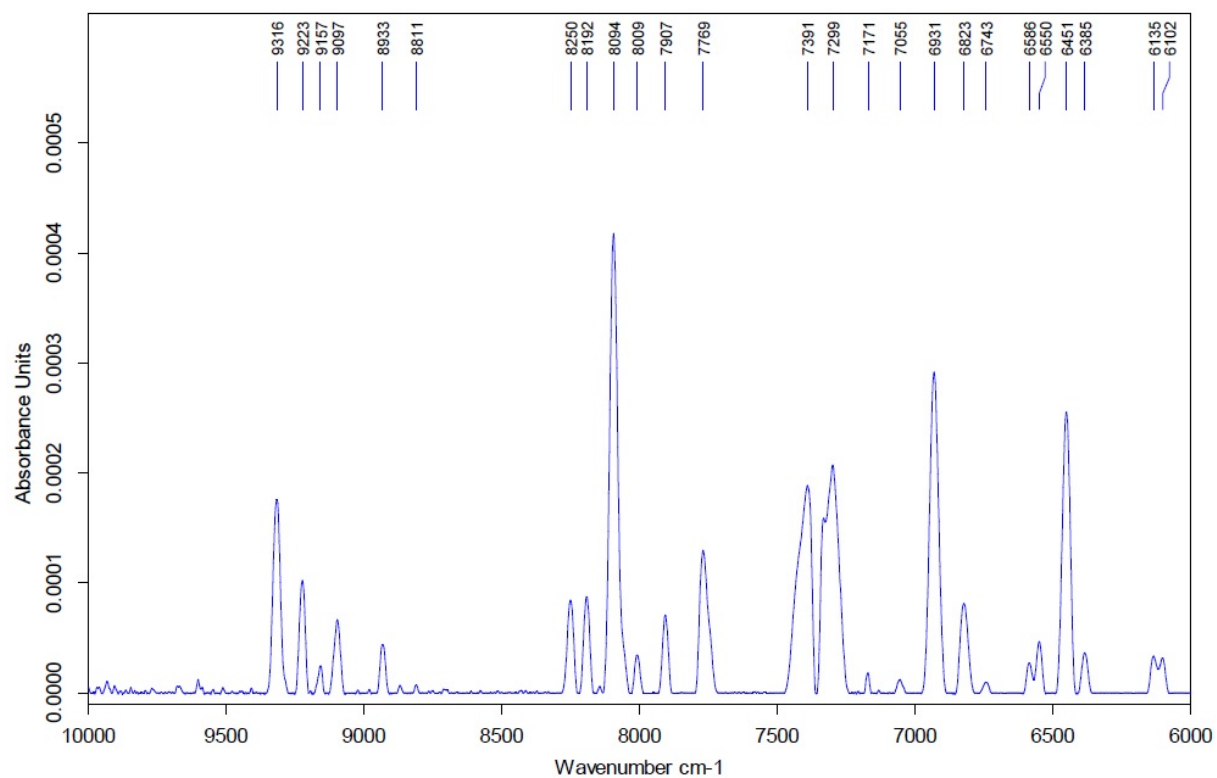

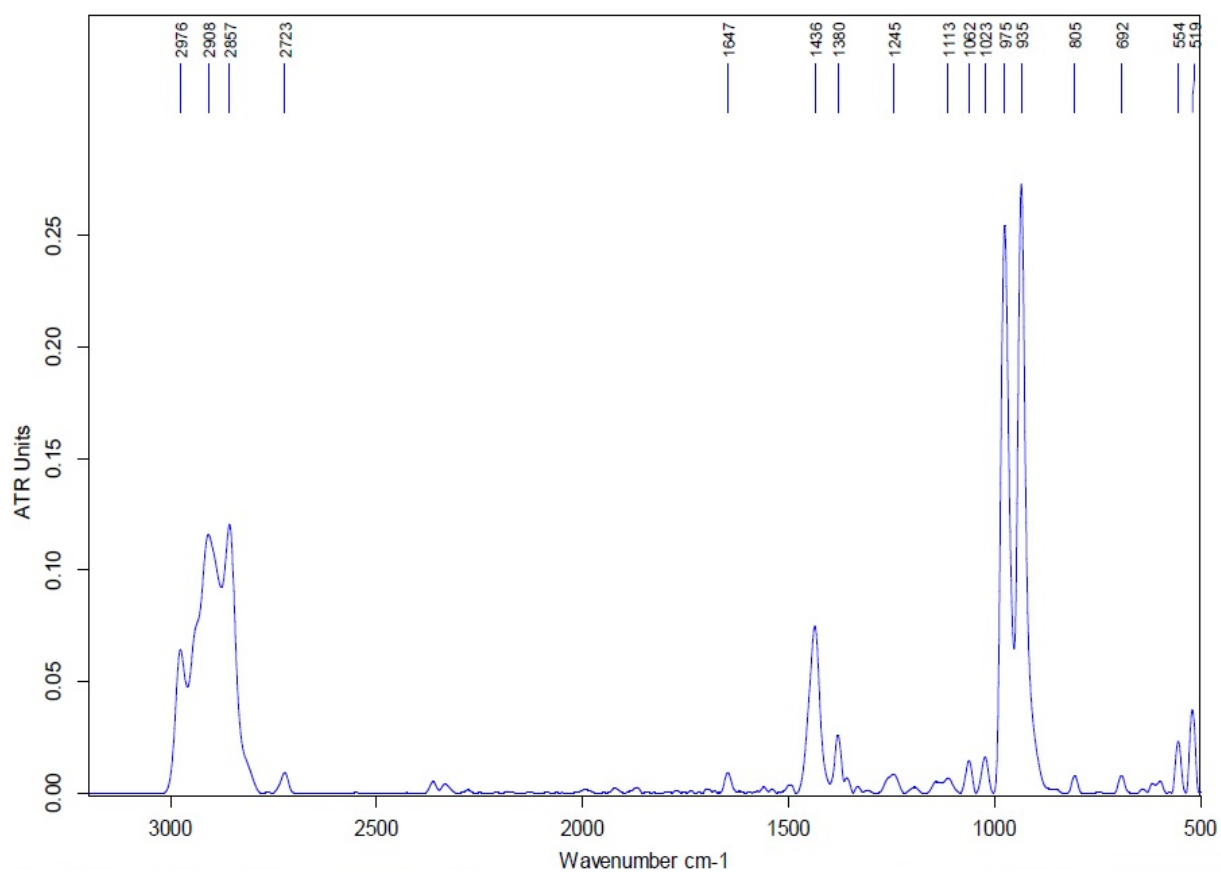**Figure S2.** NIR-spectrum of **2**.

Figure S3. IR-spectrum of **1**.
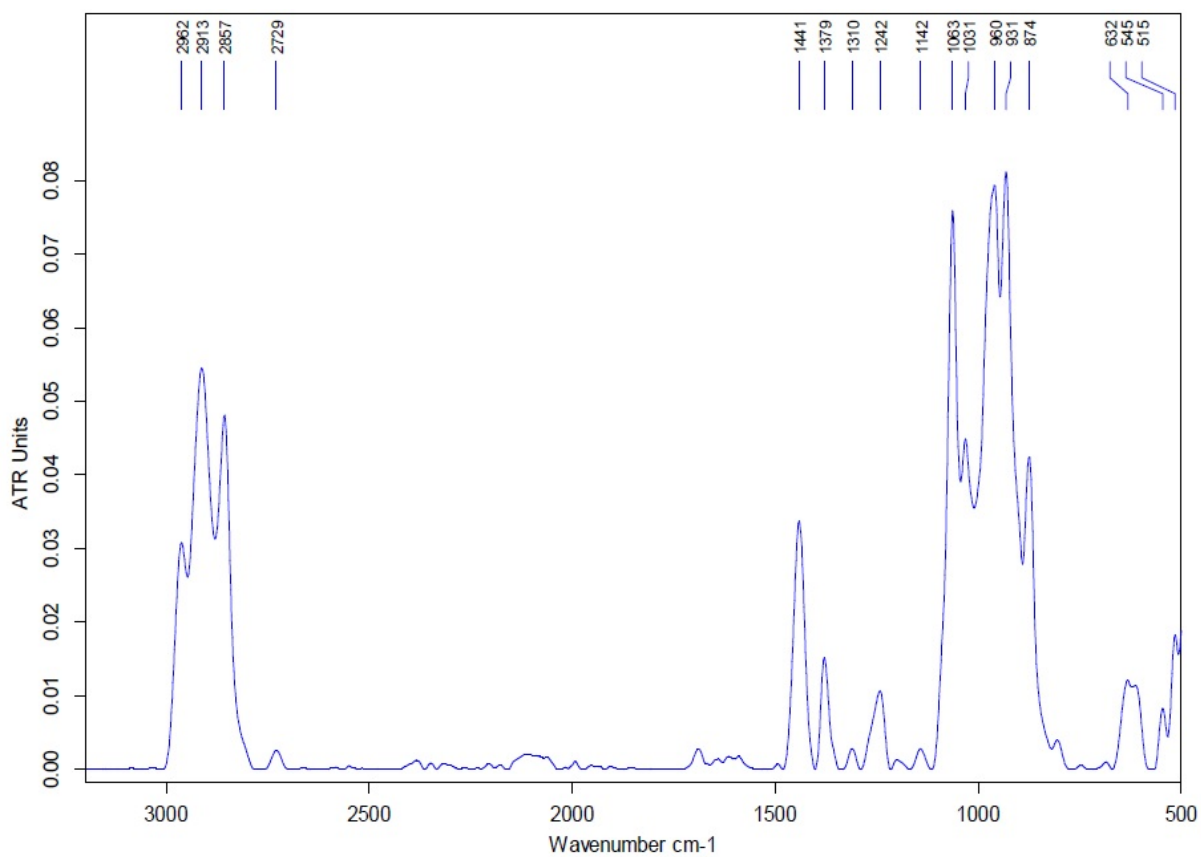

Figure S4. IR-spectrum of **2**.
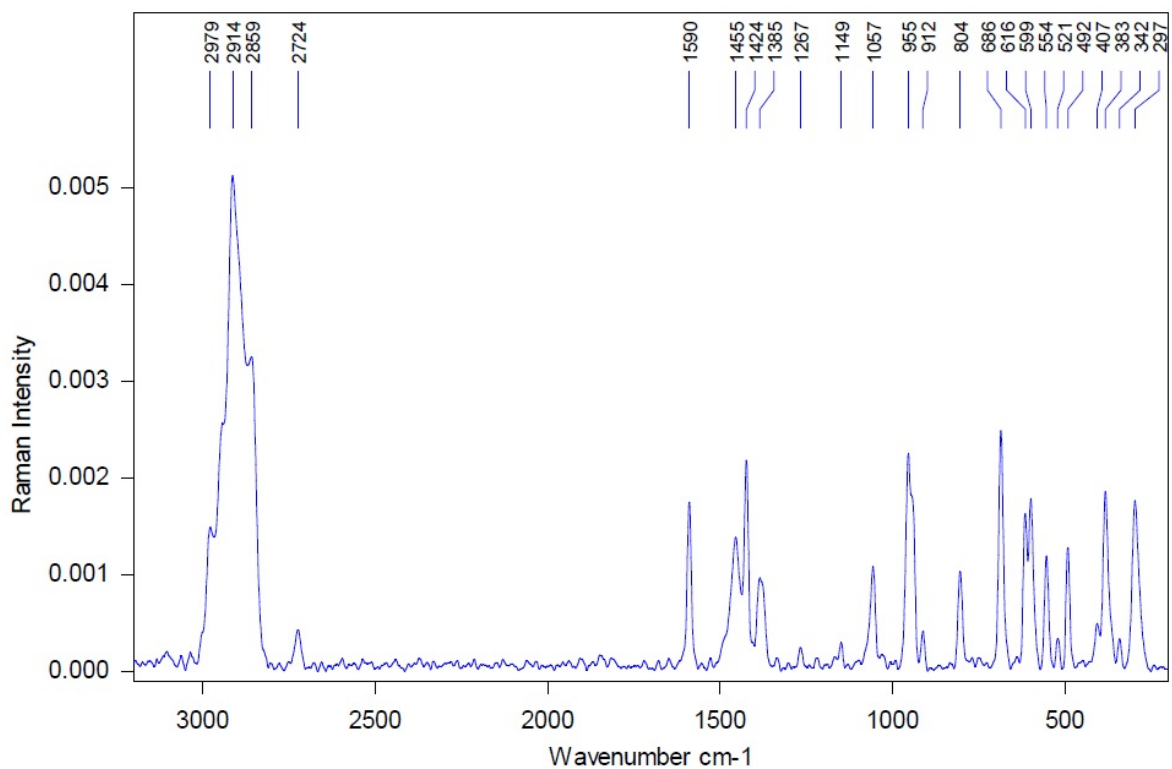
Figure S5. Raman-spectrum of **1**.

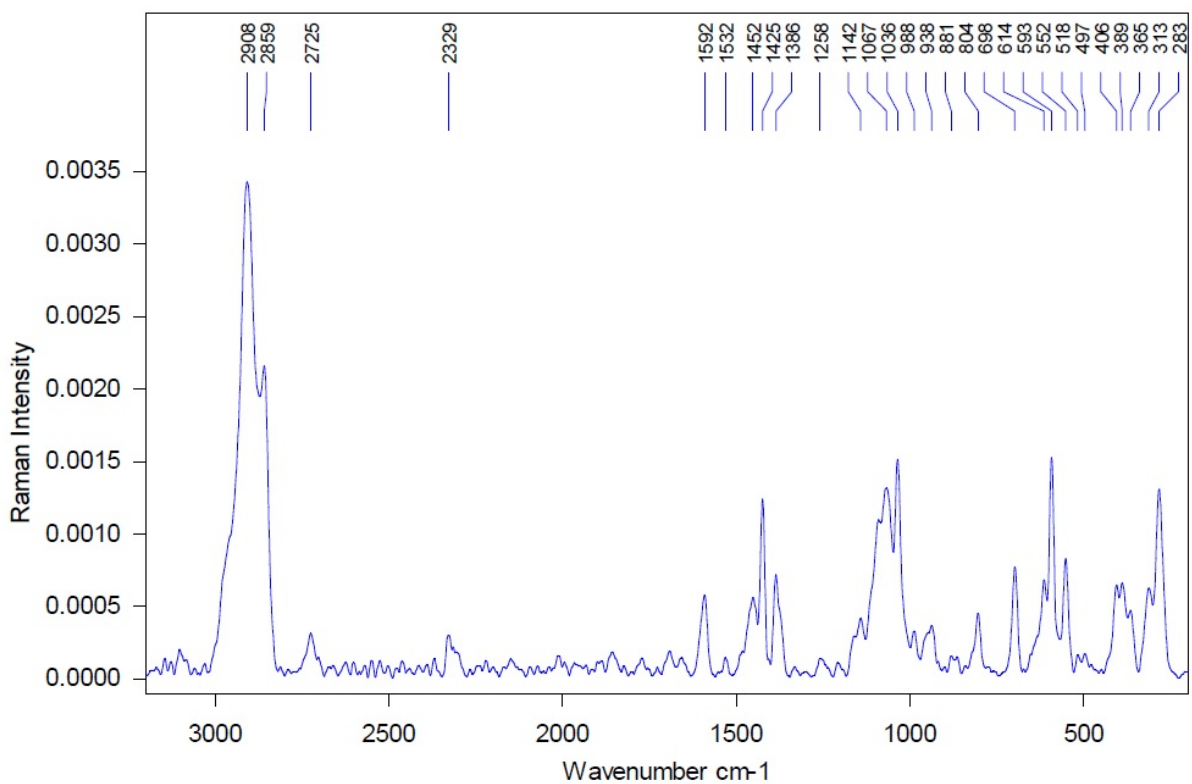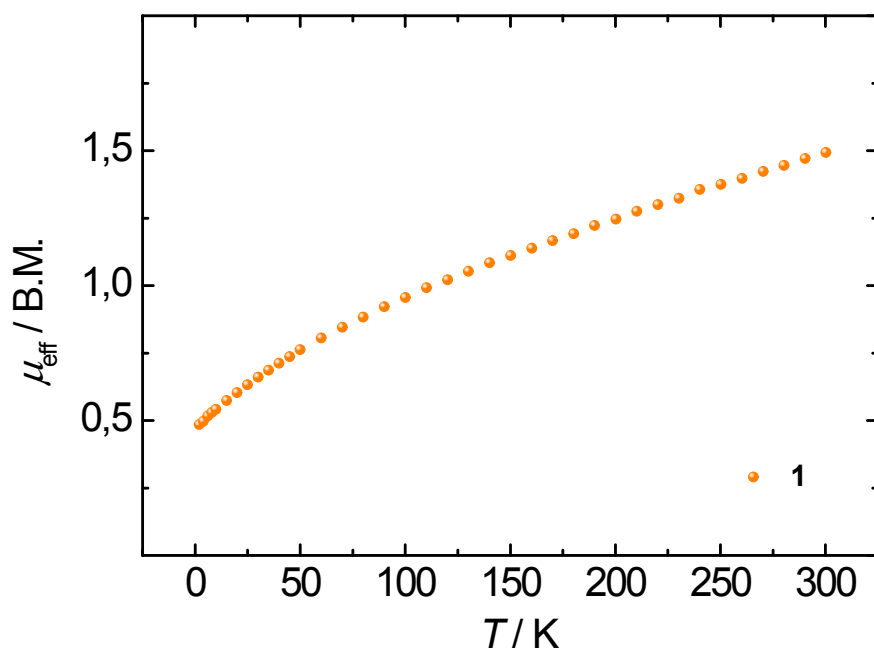**Figure S6.** Raman-spectrum of **2**.

Figure S7. Temperature-dependent SQUID magnetization data for **1** per one metal center.

The ground term for Sm^{3+} (f^5) is $J = 5/2$, therefore, and based on the isolated free ion ground term $^6H_{5/2}$, a magnetic moment of $0.84\mu_B$ is calculated. However, the corresponding experimental value is typically observed around $1.5\mu_B$.[1] The observed significant difference results from nearby (low-lying) excited terms, with separations comparable to kT at room temperature and, consequently, their contributions to the susceptibility cannot be neglected. For Sm^{3+}, the first excited term, $J = 7/2$, is approx. 1000 cm^{-1} above the ground term ($J = 5/2$).

Considering the close separation between the lowest lying terms for Sm^{3+} the dependence of χ_m on T is small. Accordingly, the magnetic moment per Sm^{3+} ion range from $0.69\mu_B$ at 2 K to $1.49\mu_B$ at 300 K.

References

[1] E.A. Boudreaux and L.N. Mulay, "Theory and Application of Molecular Paramagnetism", John Wiley & Sons, 1976. Chapter 5 "Magnetic Behavior of Lanthanide Compounds" by A.T. Casey and S. Mitra.