Electronic supplementary information

Specific Circularly Polarized Luminescence of Eu(III), Sm(III), and Er(III) Induced by N-Acetylneuraminic acid

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Experimental

Spectral Measurement. Neu5Ac, $EuCl_3$, $Sm(NO_3)_3$, and $ErCl_3$ were purchased from Sigma Aldrich, distilled mill-Q water was used as solvent.

Backscattering Raman and scattered circular polarization (SCP) ROA spectra were acquired on a BioTools ROA spectrometer operating with laser excitation at 532 nm and resolution of 7 cm^{-1}. The laser power was 900 mW, accumulation times were one (Eu sample), four (Sm , and Er) and 12 (plain Neu5Ac) hours. The spectra are presented after subtraction of water background and minor polynomial correction for fluorescence impurities.

Computations. Equilibrium geometries of the anomers were obtained using the Gaussian09 program,[1] adopting the B3LYP functional, 6-31G(d) basis set, and the conductor-like polarizable continuum solvent model (CPCM).[2]. For Eu : Neu5Ac complexes, 6-31G(d) basis set was employed for C, H, and O, and MWB28 pseudopotential basis set for Eu. Free energy (*ΔG*) was calculated in the harmonic oscillator/rigid rotor approximation.

References

1. M. J. T. Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. , *Journal*, 2013, **Revision D.01**.
2. A. Klamt, *J. Phys. Chem.*, 1995, **99**, 2224-2235.

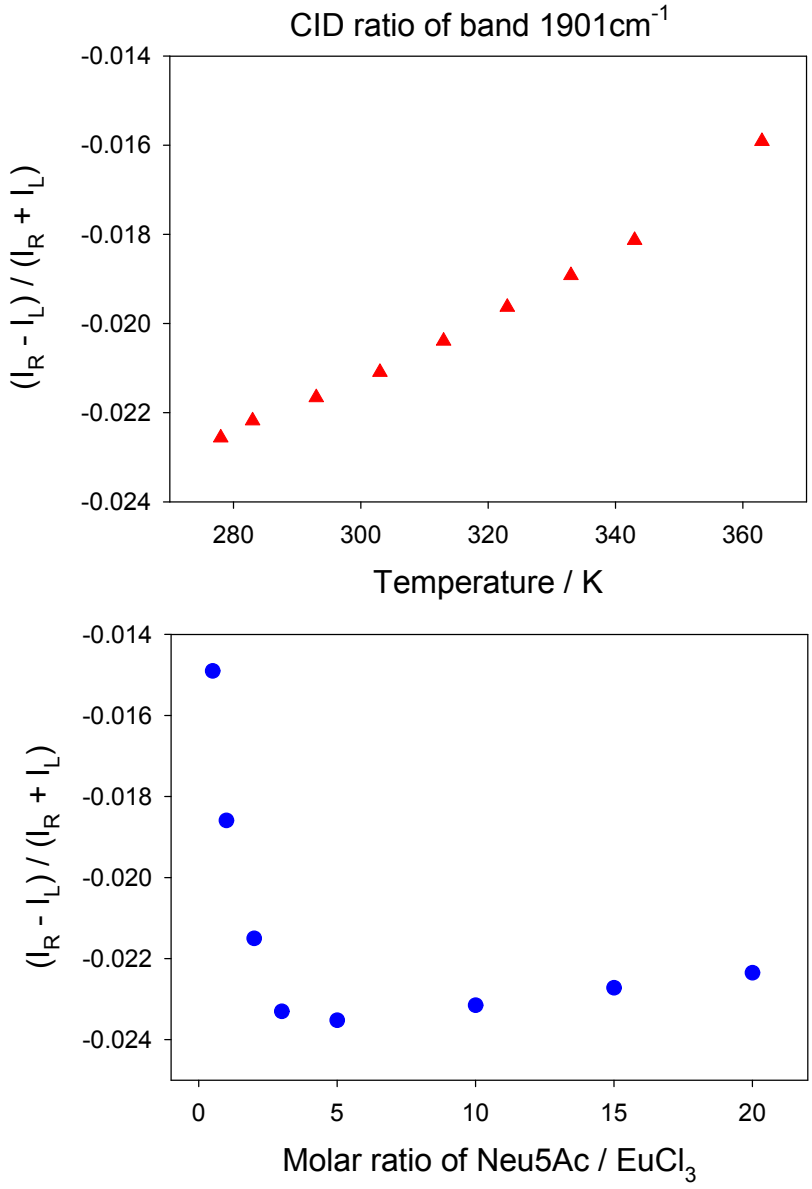

Figure S1. Temperature dependent CID ratio of band 1901cm^{-1} of Neu5Ac : $EuCl_3$ (4mM : 4mM, top); and concentration dependent CID ratio of band 1901cm^{-1} of Neu5Ac : $EuCl_3$ (with $EuCl_3$ = 4mM constant, bottom) in aqueous solution. Although we estimate the error of the y-scale to be about 10 % (given mainly by the concentration variations) the decent CID increase for high molar ratios of Ne5Ac/$EuCl_3$ appears real.

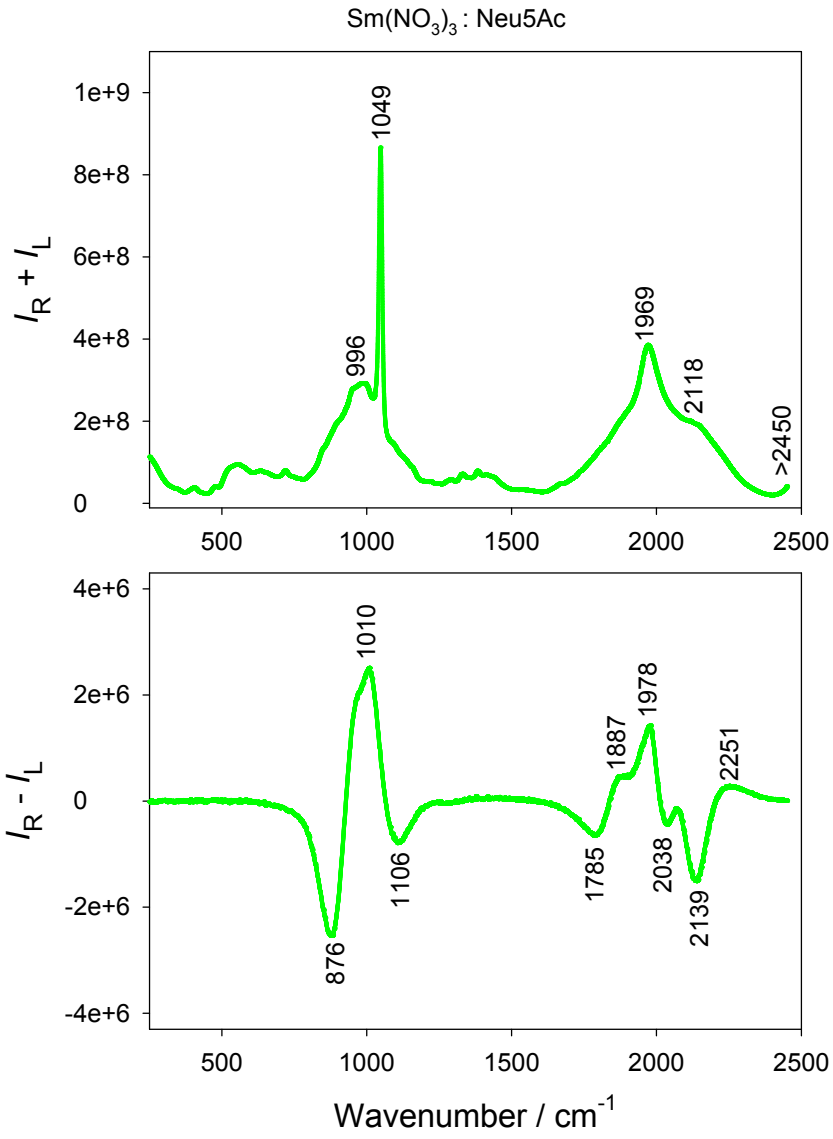

Figure S2. Raman/TL (top) and ROA/CPL (bottom) spectra of Neu5Ac complexes with $Sm(NO_3)_3$ (30mM : 30mM).