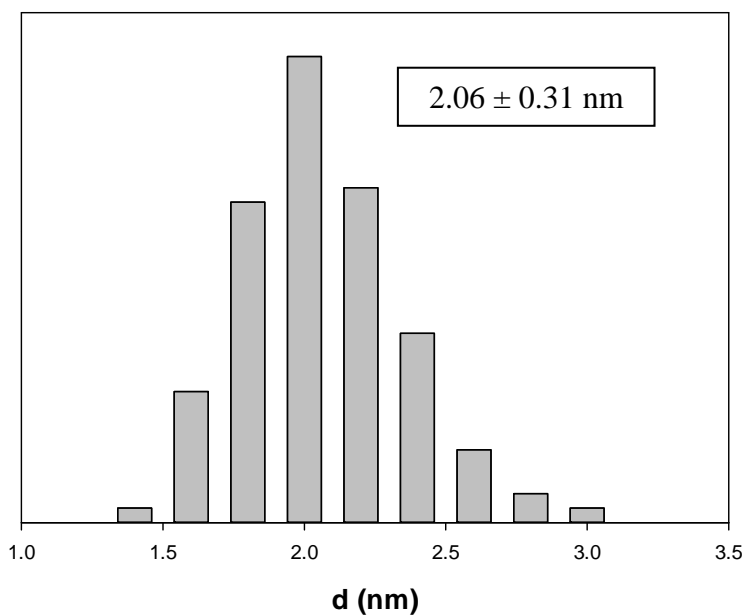
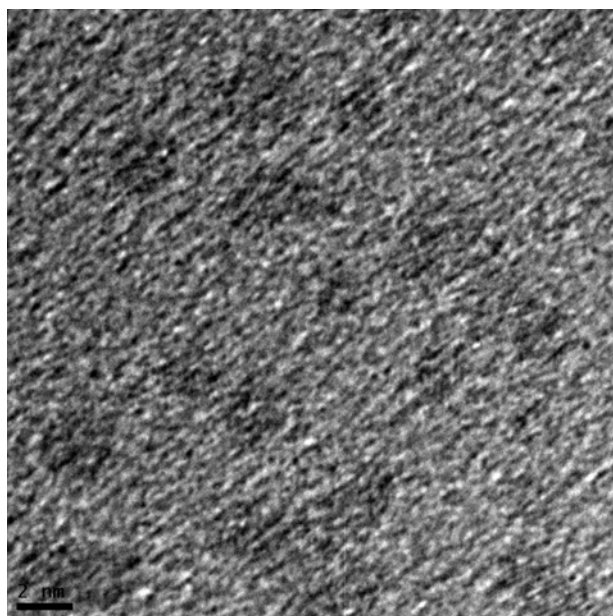


*Electronic Supplementary Information*

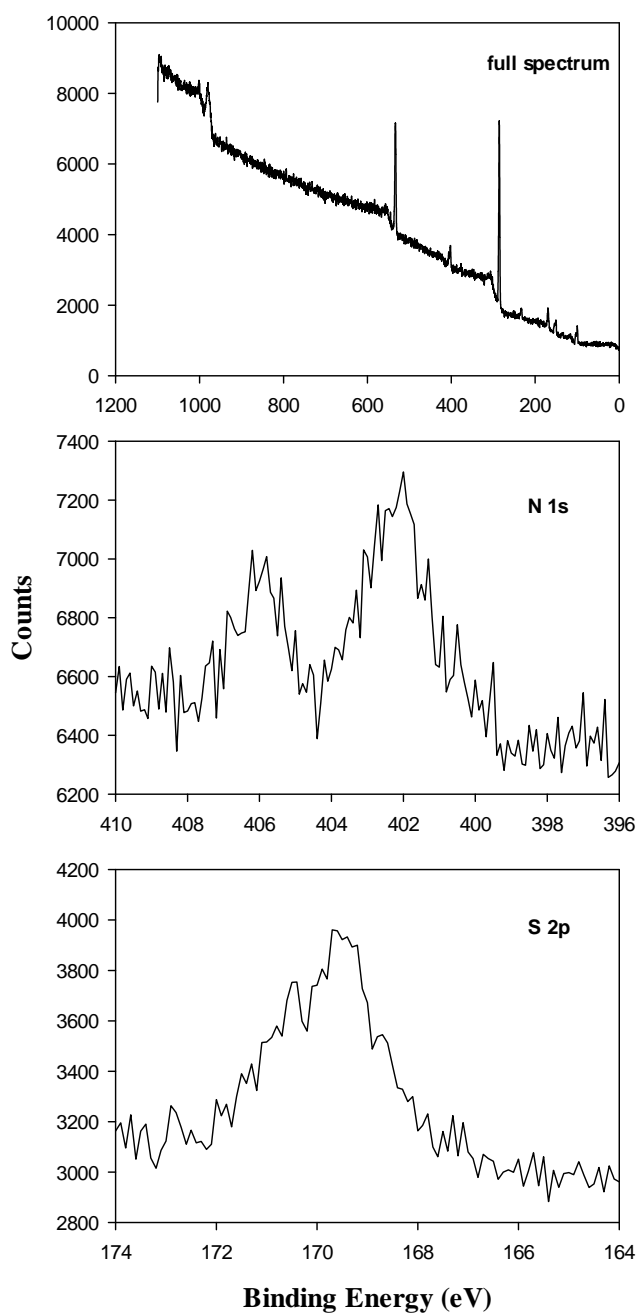
**Nitrene-Functionalized Ruthenium Nanoparticles**

Xiongwu Kang, Yang Song, and Shaowei Chen\*

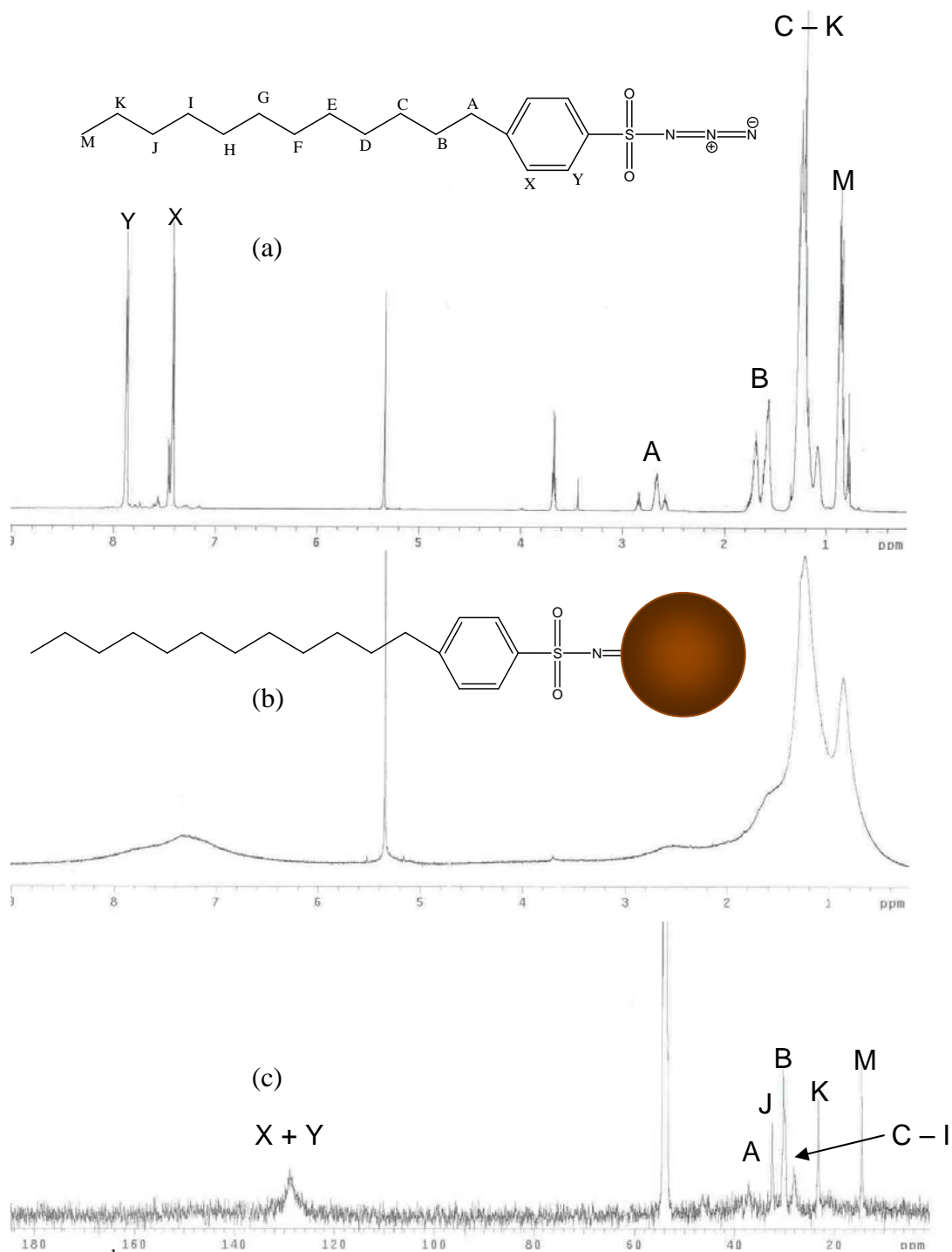
*Department of Chemistry and Biochemistry, University of California, 1156 High Street, Santa Cruz, California 95064*



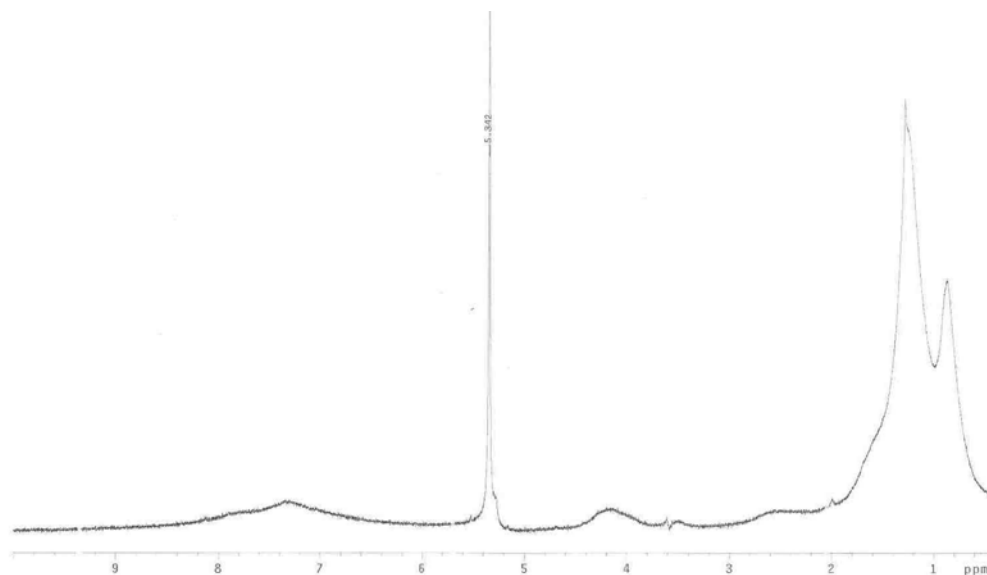
**Figure S1.** (top) Representative TEM micrograph and (bottom) core size histogram of Ru=N nanoparticles. Scale bar 2 nm.



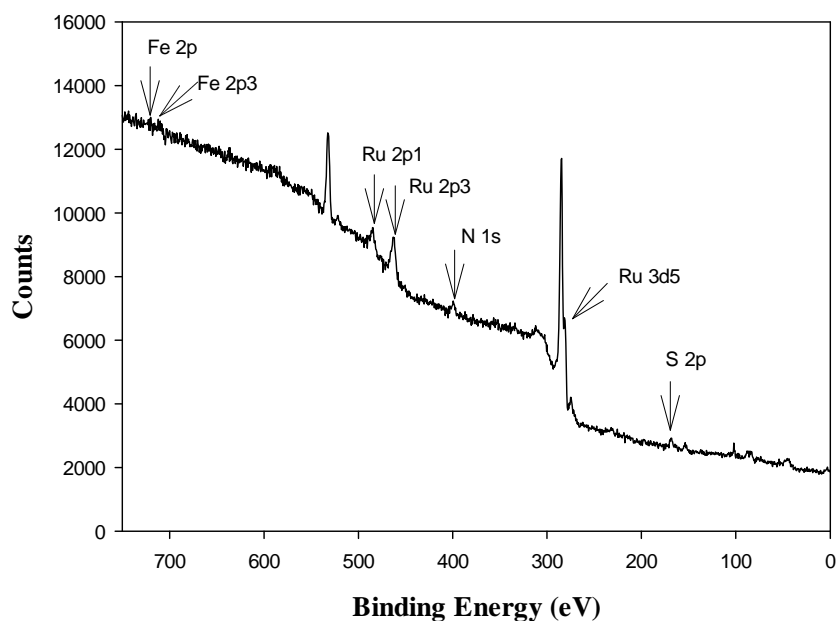
**Figure S2.** (top) XPS survey spectrum of 4-dodecylbenzenesulfonyl azide, and high-resolution scans of the (middle) N1s and (bottom) S2p electrons of the sample. The N1s peaks can be identified at 405.9 eV and 402.1 eV (middle panel), with an atomic ratio of ca. 1:2. S2p electrons appear at 169.5 eV, with the atomic ratio between S and N at approximately 1:3.



**Figure S3.**  $^1\text{H}$  NMR spectra in  $\text{CD}_2\text{Cl}_2$  of (a) 4-dodecylbenzenesulfonyl azide and (b) Ru=NTs nanoparticles. The corresponding  $^{13}\text{C}$  NMR spectrum of Ru=NTs nanoparticles is included in panel (c). Insets depict the structures of the azide ligand as well as the nanoparticle. Letters show the peak assignments of the ligands. Notably, the spectral features of the nanoparticles were all markedly broadened, as compared with those of the monomeric ligands, indicating that the ligands were indeed bound onto the nanoparticle surface and there were no excessive free ligands. In panels (a) and (b), the peak at ca. 3.7 ppm might be assigned to trace water in the sample and the peak at 3.4 ppm to a tiny amount of methanol in (a), whereas the origin of the peak at ~0.8 ppm in (a) was not clear at this moment.



**Figure S4.** <sup>1</sup>H NMR spectrum of Ru=N(Fc) nanoparticles in CD<sub>2</sub>Cl<sub>2</sub>. In comparison with that of Ru=N nanoparticles (Figure S1), there appears a new peak between 3.8 and 4.5 ppm, which may be assigned to the ferrocenyl protons. Also, the absence of any sharp features indicates that the nanoparticles were free of excessive ligands and the spectral responses were all due to nanoparticle-bound ligands.



**Figure S5.** XPS survey spectrum of Ru=N(Fc) nanoparticles. In addition to those of the Ru=N nanoparticles (Figure 1), a pair of new peaks appear at 708.6 eV and 720.7 eV, which may be assigned to the Fe2p electrons, as observed previously (*Nanoscale* **2011**, 3, 1984). Yet the peak intensities are too low to have a reliable evaluation of the ferrocene concentration on the nanoparticle surface.