Supplementary Material (ESI) for Chemical Science

Dinitrogen Complexation With Main Group Radicals

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Supporting Information

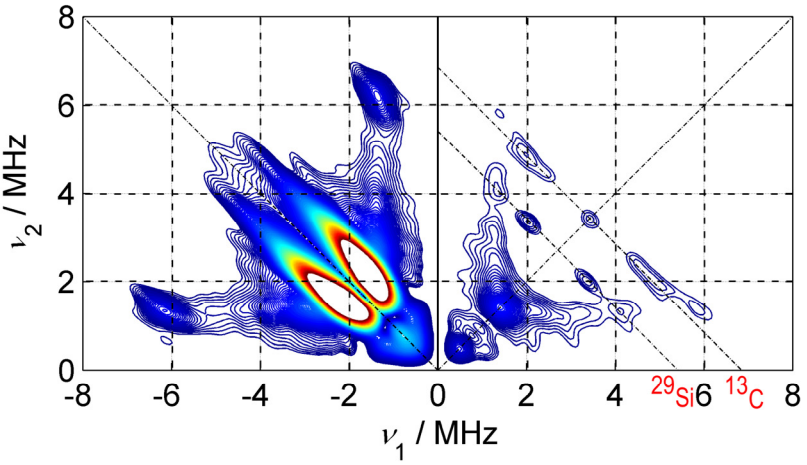

Figure S1: Full spectrum of $SnHyp_3$ in pentane saturated with Ar (x/y direction).

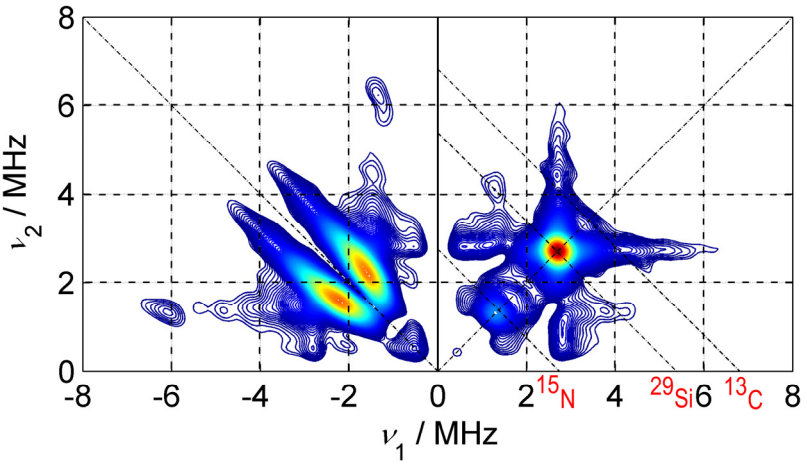

Figure S2: Spectrum of $SnHyp_3$ in pentane saturated with $^{15}N_2$ (x/y direction). Please note the strong ^{15}N matrix peak due to statistically distributed $^{15}N_2$ in the solution at 1.46 MHz as well as the coupled nitrogen nuclei at approx. 1.8 MHz. At 2.8 MHz a strong ^{29}Si (superimposed by quadrupolar couplings in the ^{14}N case) signal is visible, due to the silicon based ligands in the x/y plane.

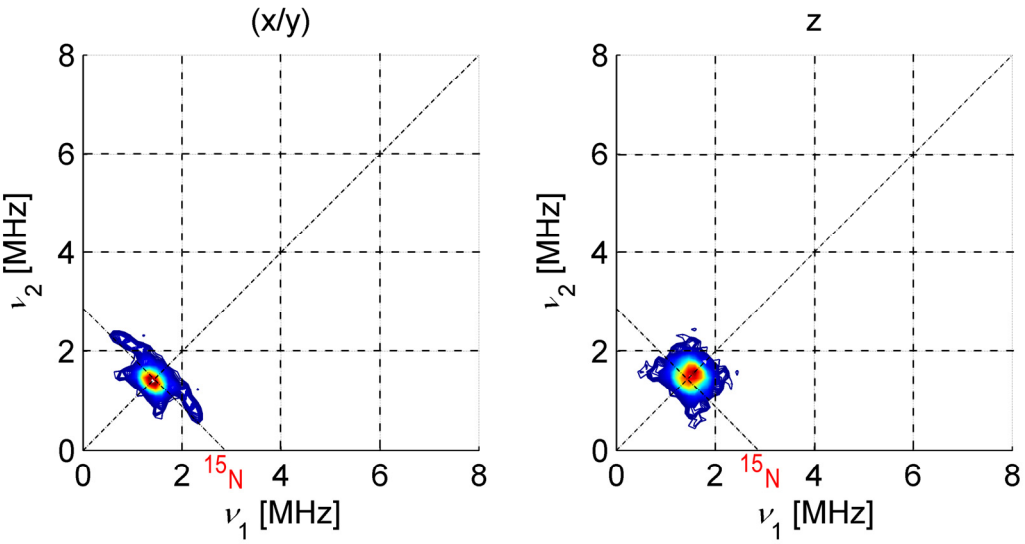

Figure S3: Simulated $^{15}N_2$ coupling in x/y- and z-direction, superimposed with a $^{15}N_2$ matrix peak. According to the stronger coupling in z-direction the relative intensity of the matrix peak is weaker in z and stronger in x/y.

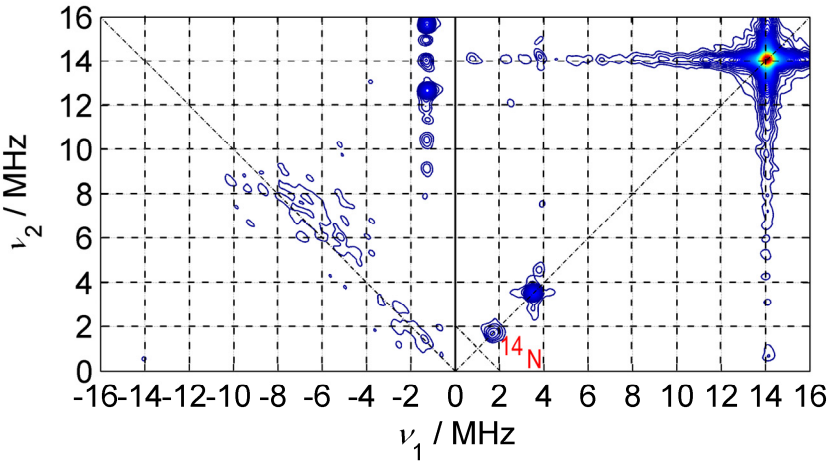

Figure S4. Full spectrum of TAM in methanol saturated with N_2. The hydrogen signals are located at 14 MHz.

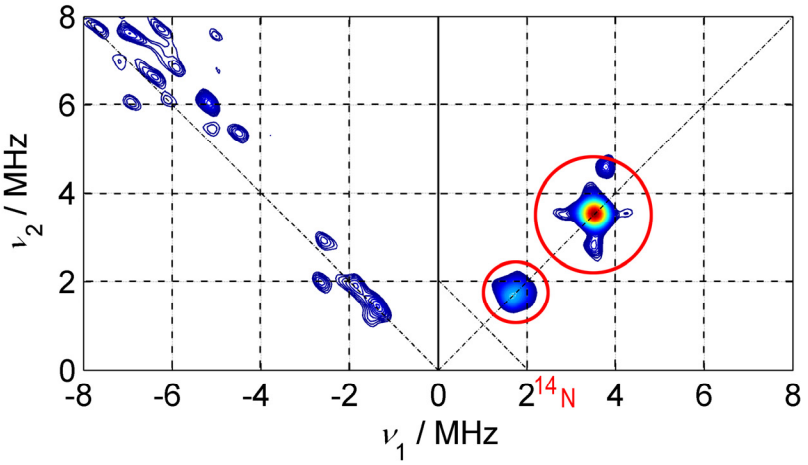

Figure S5. Close-up view of the spectrum of TAM in methanol saturated with N_2. Nitrogen couplings are marked with the red circle. The signals on the left are artifacts.

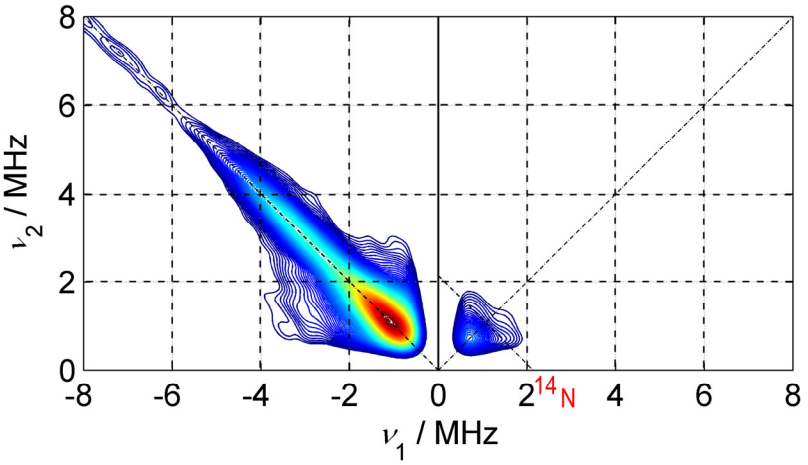

Figure S6. Close-up view of the spectrum of TAM in methanol saturated with argon. All visible signals are artifacts.

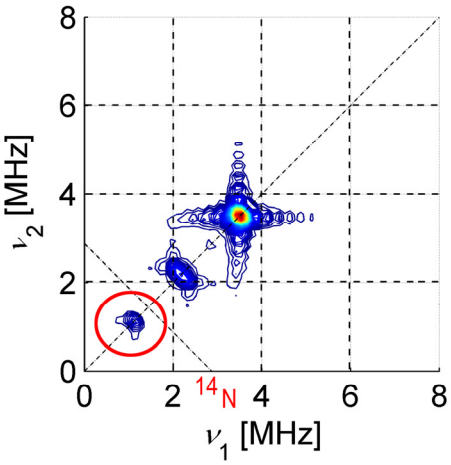

Figure S7. Simulation of the HYSCORE-detected dinitrogen coupling to TAM. Please notice the additional ridge marked, with the red circle. It is not visible in Figure 2. This can be explained by the perfect S/N-ratio of the simulated spectrum.

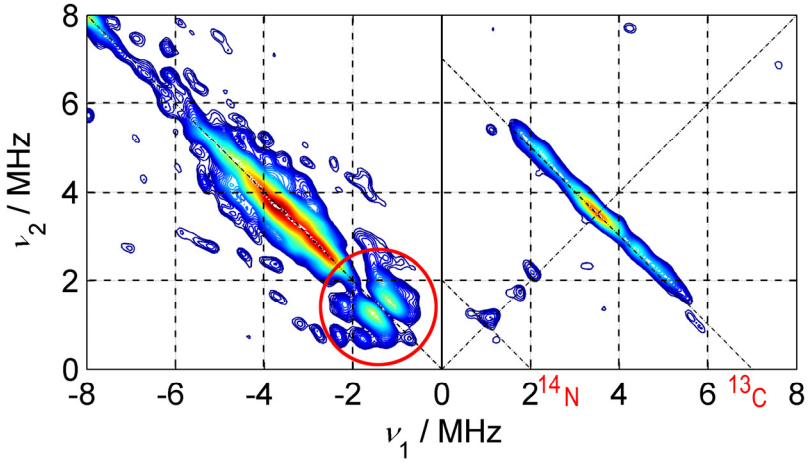

Figure S8. Spectrum of Tempol in methanol saturated with N_2. The dinitrogen coupling is marked with the red circle.

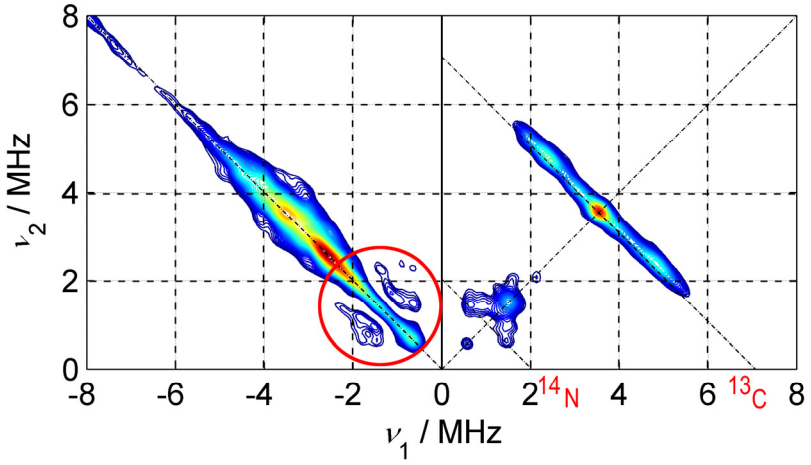

Figure S9. Spectrum of Tempol in methanol saturated with Ar. Please notice that a dinitrogen coupling with a very weak intensity is still visible (marked red), due to residual N_2 in solution.

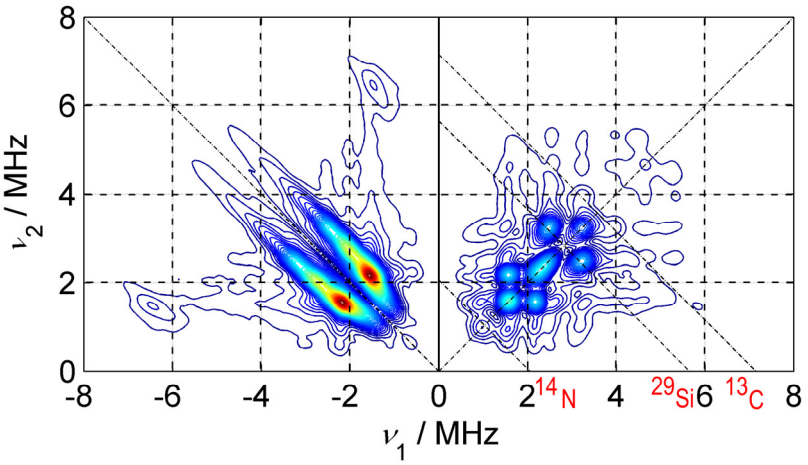

Figure S10. Spectrum of $SnHyp_3$ in pentane saturated with a mix of Ar and N_2 (x/y direction). Please notice the changes in intensity of the dinitrogen coupling pattern, compared to the spectrum of $SnHyp_3$ in N_2 saturated pentane.

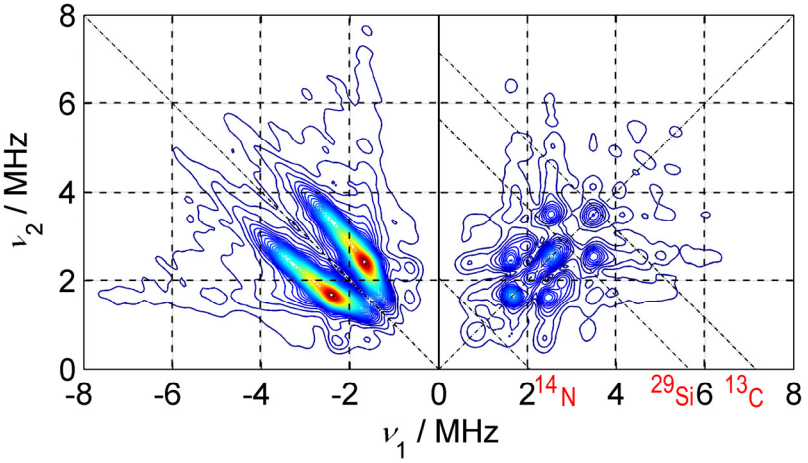

Figure S11. HYSCORE spectrum of $SnHyp_3$ in pentane saturated with a mix of Ar and N_2 (z direction).

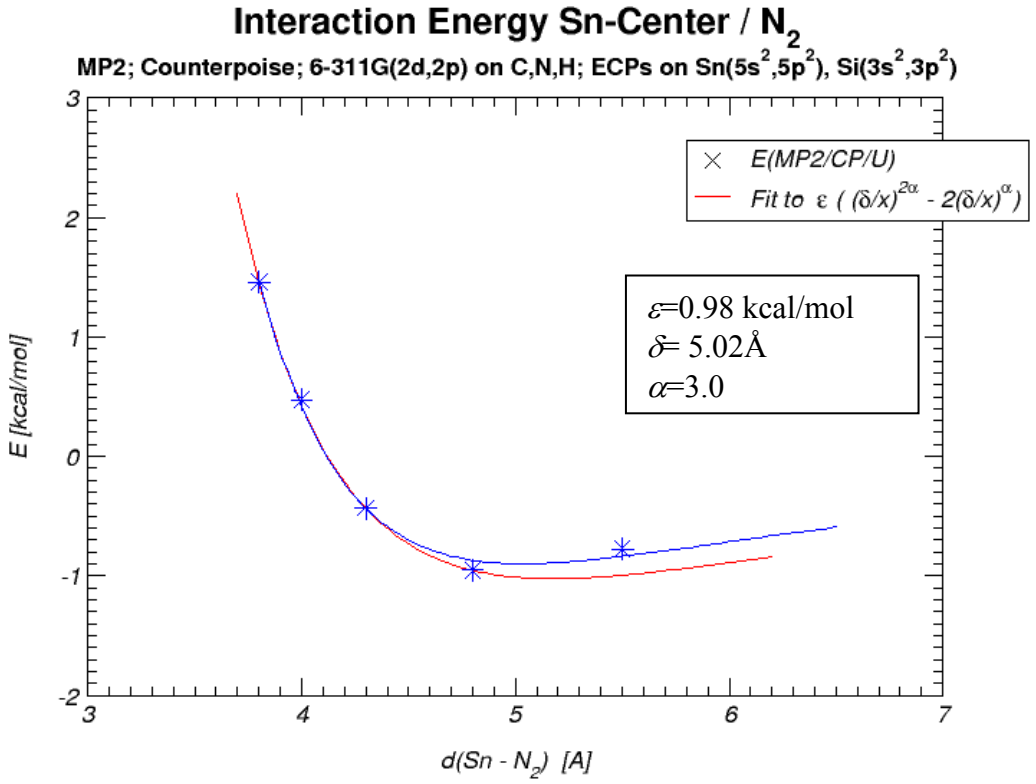

Figure S12. MP2 interaction energies of $SnHyp_3$ and N_2. The red curve is a fit (as shown in the upper inset) to the points between 4.0 and 4.8Å, the blue curve to the points between 4.0 and 5.5Å. The extracted fit parameters from the blue curve are shown in the lower inset.