

Supporting Information:

Trimetallic Nitride Cluster Dynamics Inside Icosahedral C₈₀ Cage

Wujun Fu, Xuelei Wang, Hugo Azuremendi, Jianyuan Zhang and Harry C. Dorn*

Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061,
USA

* To whom correspondence should be addressed: email: hdorn@vt.edu, Tel: 540-231-5953.

Table of Contents:

Figure 1 HPLC Chromatography of purified M₃N@C₈₀ (M = Lu, Y and Sc) samples in PYE column (a 4 x 250 mm 5PYE column; λ =390 nm; flow rate 2.0 mL/min; toluene as eluent; 25 °C)

Figure 2 Positive ionization LD-TOF mass spectra of M₃N@C₈₀ (M = Lu, Y and Sc) samples.

Figure 3 The ⁴⁵Sc NMR of Sc₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Table 1 The Line width and chemical shift of ⁴⁵Sc signal of Sc₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Figure 4 Line-fitting plot (ln(line width) and 1/T (K⁻¹)) for ⁴⁵Sc NMR of Sc₃N@I_h-C₈₀

Table 2 The Line width and chemical shift of ¹⁴N signal of Sc₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Figure 5 Line-fitting plot (ln(line width) and 1/T (K⁻¹)) for ¹⁴N NMR of Sc₃N@I_h-C₈₀

Figure 6 The ¹⁴N NMR of Y₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Table 3 The Line width and chemical shift of ¹⁴N signal of Y₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Figure 7 Line-fitting plot (ln(line width) and 1/T (K⁻¹)) for ¹⁴N NMR of Y₃N@I_h-C₈₀

Figure 8 The ¹⁴N NMR of Lu₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Table 4 The Line width and chemical shift of ¹⁴N signal of Lu₃N@I_h-C₈₀ in 1,2-dichlorobenzene-*d*₄ at various temperatures

Figure 9 Line-fitting plot (ln(line width) and 1/T (K⁻¹)) for ¹⁴N NMR of Lu₃N@I_h-C₈₀

Figure 1

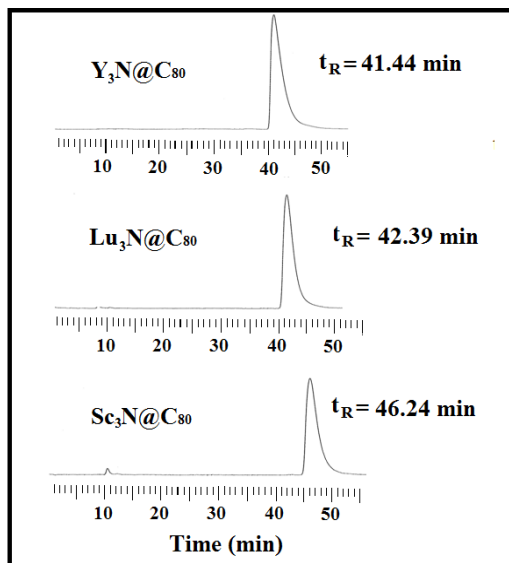


Figure 2

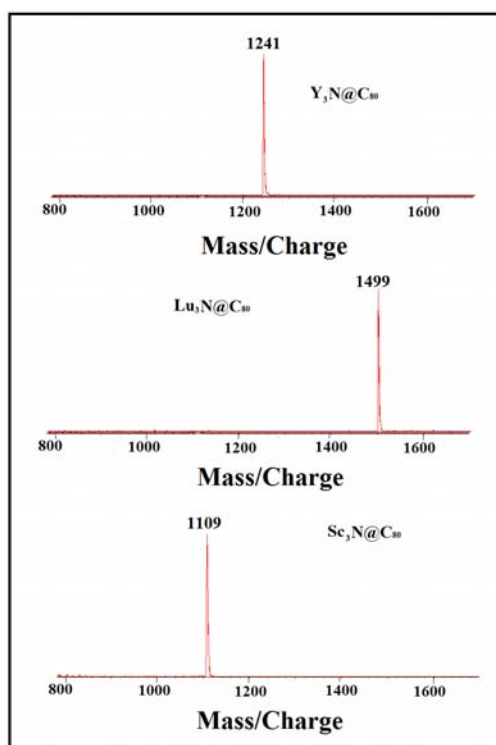


Figure 3

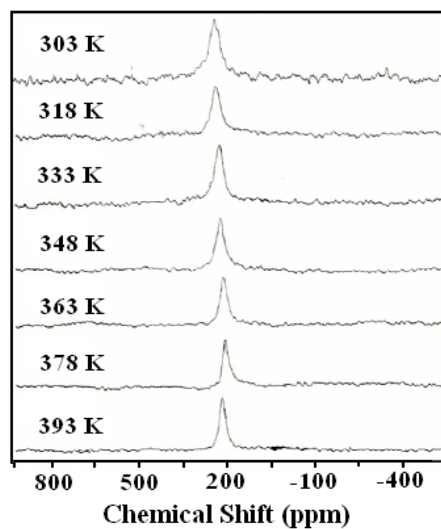


Table 1

Temperature (K)	1/T (K ⁻¹)	ln(Line width)	Chemical shift (ppm)
303	0.00330	8.38	196.6
318	0.00314	8.24	196.9
333	0.00300	8.18	194.4
348	0.00287	8.03	194.1
363	0.00275	7.89	196.2
378	0.00264	7.81	194.4
393	0.00254	7.74	194.7

Figure 4

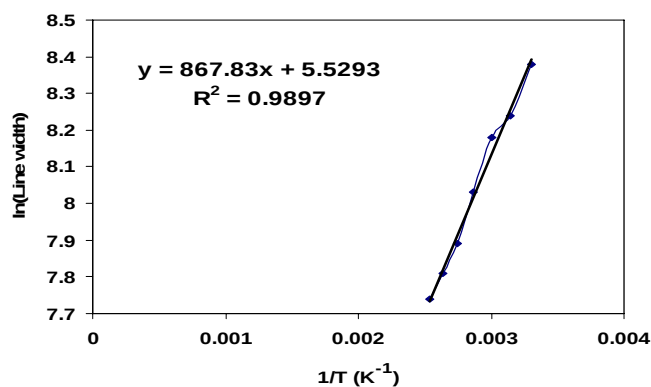


Table 2

Temperature (K)	1/T (K ⁻¹)	ln(Line width)	Chemical shift (ppm)
268	0.00373	4.51	394.1
298	0.00336	4.20	395.9
328	0.00305	3.95	396.6
358	0.00279	3.71	397.3
388	0.00263	4.23	397.9

Figure 5

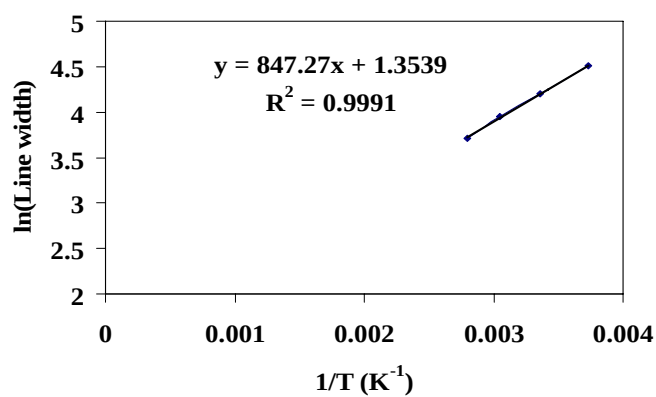
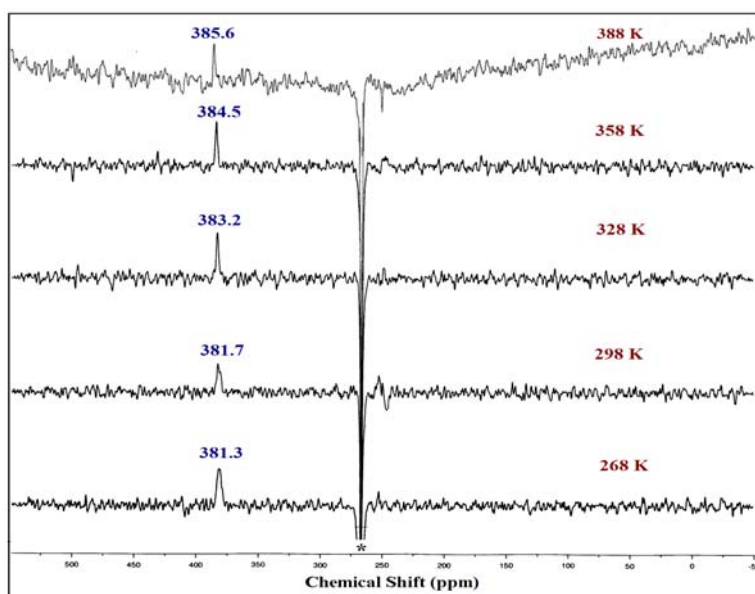


Figure 6



The * corresponds to signals which came from NMR probe.

Table 3

Temperature (K)	1/T (K ⁻¹)	ln(Line width)	Chemical shift (ppm)
268	0.00373	4.69	381.3
298	0.00336	4.48	381.7
328	0.00305	3.78	383.2
358	0.00279	3.53	384.5
388	0.00263	3.18	385.6

Figure 7

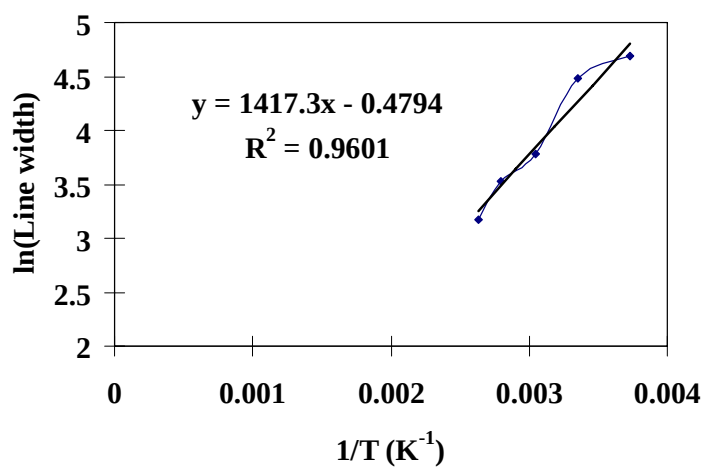
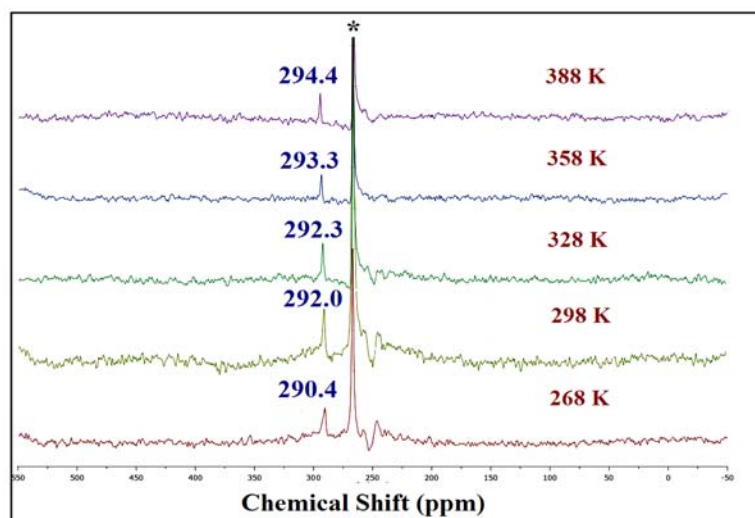


Figure 8



The * corresponds to signals which came from NMR probe.

Table 4

Temperature (K)	1/T (K ⁻¹)	ln(Line width)	Chemical shift (ppm)
268	0.00373	4.77	290.4
298	0.00336	4.03	292.0
328	0.00305	3.50	292.3
358	0.00279	3.04	293.3
388	0.00263	2.56	294.4

Figure 9

