

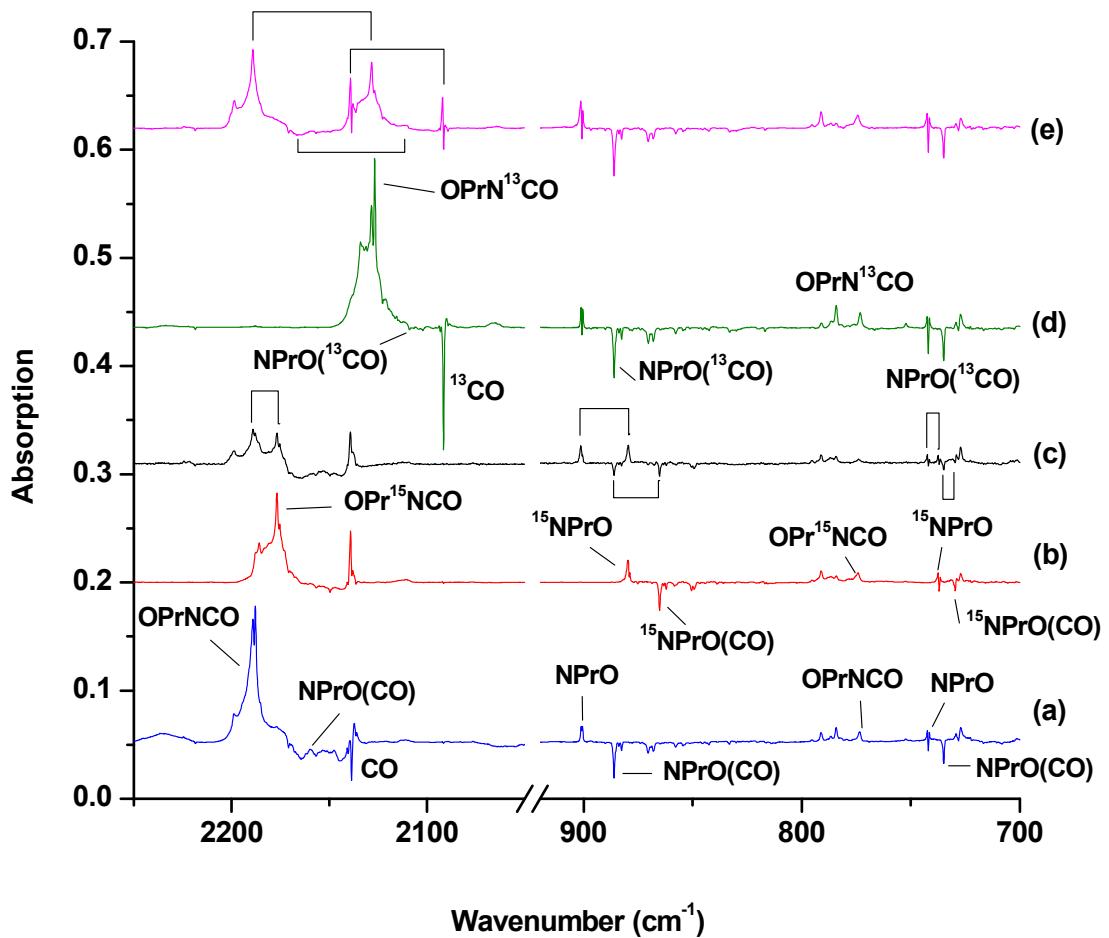
## **Supporting Information**

### **Isocyanate Formation from Reactions of Early Lanthanide Metal Atoms with NO and CO in Solid Argon**

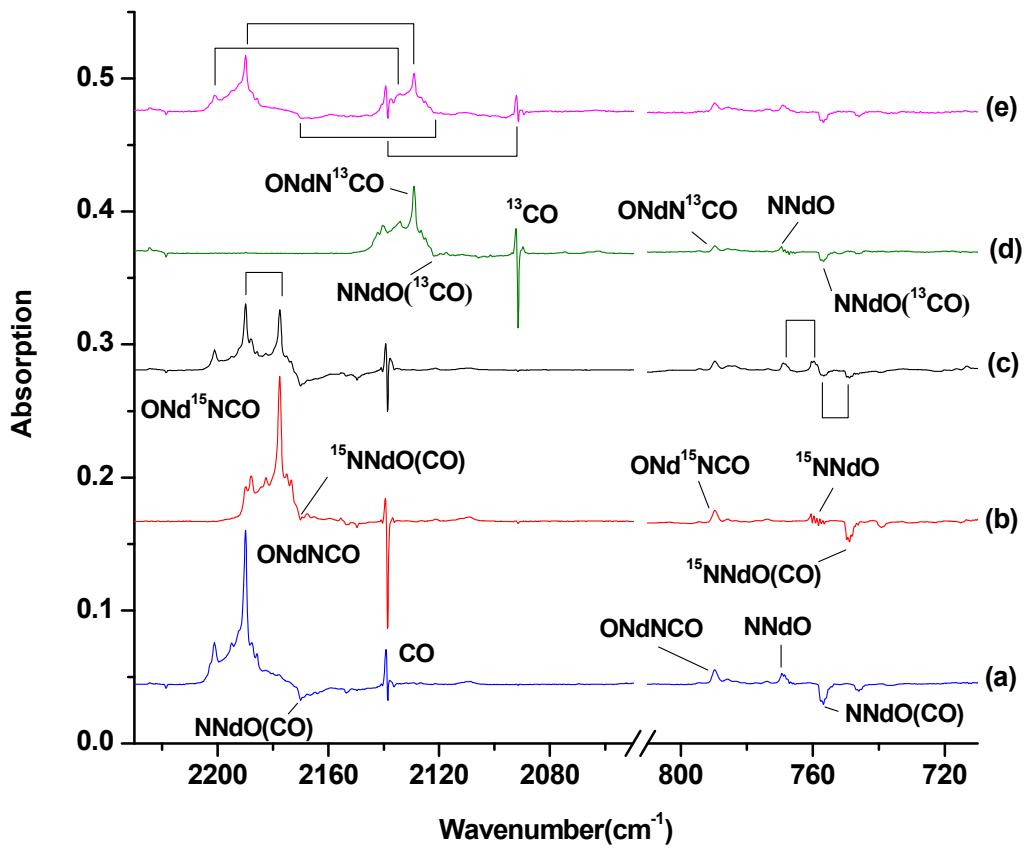
Jiwen Jian, Qingnan Zhang, Xuan Wu, Mingfei Zhou\*

Department of Chemistry, Shanghai Key Laboratory of Molecular Catalysis and Innovative materials, Collaborative Innovation Center of Chemistry for Energy Materials, Fudan University, Shanghai, 200433, China. Tel: (+86) 21-6564-3532, Email: mfzhou@fudan.edu.cn

*Complete Ref. (35): Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.*



**Fig S1.** Difference infrared spectra in the 2250-2150 and 920-700 cm<sup>-1</sup> regions from co-deposition of Pr atoms with isotopic-labeled NO and CO in excess argon (spectrum recorded after 15 min of UV light irradiation minus spectrum recorded after 30 K annealing). (a) 0.05 % NO + 0.05 % CO, (b) 0.05 % <sup>15</sup>NO + 0.05 % CO, (c) 0.05 % NO + 0.05 % <sup>15</sup>NO + 0.05 % CO, (d) 0.05 % NO + 0.05 % <sup>13</sup>CO, and (e) 0.05 % NO + 0.05 % <sup>12</sup>CO + 0.05 % <sup>13</sup>CO.



**Figure S2.** Difference infrared spectra in the 2230-2050 and 810-710  $\text{cm}^{-1}$  regions from co-deposition of Nd atoms with isotopic-labeled NO and CO in excess argon (spectrum recorded after 15 min of UV light irradiation minus spectrum recorded after 30 K annealing). (a) 0.05 % NO + 0.05 % CO, (b) 0.05 %  $^{15}\text{NO}$  + 0.05 % CO, (c) 0.05 % NO + 0.05 %  $^{15}\text{NO}$  + 0.05 % CO, (d) 0.05 % NO + 0.05 %  $^{13}\text{CO}$ , and (e) 0.05 % NO + 0.05 %  $^{12}\text{CO}$  + 0.05 %  $^{13}\text{CO}$ .