Supporting Information

CO Activation on the Late Lanthanide Dimers: Matrix Infrared Spectra of the $Ln_2[\eta^2(\mu_2-C, O)]_x$ (Ln = Tb, Dy, Ho, Er, Lu; x = 1, 2) Molecules

Ling Jiang,[†] Xi Jin,[‡] Mingfei Zhou,^{*,‡} and Qiang Xu^{*,†}

National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan, and Department of Chemistry & Laser Chemistry Institute, Shanghai Key Laboratory of Molecular Catalysts and Innovative Materials, Fudan University, Shanghai 200433, P. R. China

E-mail: q.xu@aist.go.jp (Xu), mfzhou@fudan.edu.cn (Zhou). [†] National Institute of Advanced Industrial Science and Technology. [‡] Fudan University.



Figure S1. IR spectra in the $1300-1100 \text{ cm}^{-1}$ region for laser-ablated Dy atoms co-deposited with 0.06% CO in argon at 4 K. (a) 50 min of sample deposition, (b) after annealing to 30 K, (c) after annealing to 34 K, (d) after 15 min of broad-band irradiation, and (e) after annealing to 38 K.



Figure S2. Infrared spectra in the 1300–1100 cm⁻¹ region for laser-ablated Dy atoms co-deposited with isotopic CO in Ar for 50 min at 4 K, followed by annealing to 34 K. (a) $0.06\% \ ^{12}C^{16}O$, (b) $0.06\% \ ^{13}C^{16}O$, (c) $0.05\% \ ^{12}C^{16}O + 0.05\% \ ^{13}C^{16}O$, (d) $0.06\% \ ^{12}C^{18}O$, and (e) $0.05\% \ ^{12}C^{16}O + 0.05\% \ ^{12}C^{18}O$.



Figure S3. IR spectra in the $1300-1100 \text{ cm}^{-1}$ region for laser-ablated Ho atoms co-deposited with 0.1% CO in argon at 4 K. (a) 50 min of sample deposition, (b) after annealing to 30 K, (c) after annealing to 34 K, (d) after 15 min of broad-band irradiation, and (e) after annealing to 38 K.



Figure S4. Infrared spectra in the 1300–1100 cm⁻¹ region for laser-ablated Ho atoms co-deposited with isotopic CO in Ar for 50 min at 4 K, followed by annealing to 34 K. (a) $0.1\% {}^{12}C^{16}O$, (b) $0.1\% {}^{13}C^{16}O$, (c) $0.08\% {}^{12}C^{16}O + 0.08\% {}^{13}C^{16}O$, (d) $0.1\% {}^{12}C^{18}O$, and (e) $0.08\% {}^{12}C^{16}O + 0.08\% {}^{12}C^{18}O$.



Figure S5. IR spectra in the $1300-1100 \text{ cm}^{-1}$ region for laser-ablated Er atoms co-deposited with 0.1% CO in argon at 4 K. (a) 50 min of sample deposition, (b) after annealing to 30 K, (c) after annealing to 34 K, (d) after 15 min of broad-band irradiation, and (e) after annealing to 38 K.



Figure S6. Infrared spectra in the 1300–1100 cm⁻¹ region for laser-ablated Er atoms co-deposited with isotopic CO in Ar for 50 min at 4 K, followed by annealing to 34 K. (a) $0.1\% \ {}^{12}C^{16}O$, (b) $0.1\% \ {}^{13}C^{16}O$, (c) $0.08\% \ {}^{12}C^{16}O + 0.08\% \ {}^{13}C^{16}O$, (d) $0.1\% \ {}^{12}C^{18}O$, and (e) $0.08\% \ {}^{12}C^{16}O + 0.08\% \ {}^{12}C^{16}O$.



Figure S7. IR spectra in the $1300-1050 \text{ cm}^{-1}$ region for laser-ablated Lu atoms co-deposited with 0.15% CO in argon at 4 K. (a) 50 min of sample deposition, (b) after annealing to 30 K, (c) after annealing to 34 K, (d) after 15 min of broad-band irradiation, and (e) after annealing to 38 K.



Figure S8. Infrared spectra in the 1300–1050 cm⁻¹ region for laser-ablated Lu atoms co-deposited with isotopic CO in Ar for 50 min at 4 K, followed by annealing to 34 K. (a) $0.15\% {}^{12}C^{16}O$, (b) $0.15\% {}^{13}C^{16}O$, (c) $0.1\% {}^{12}C^{16}O + 0.1\% {}^{13}C^{16}O$, (d) $0.15\% {}^{12}C^{18}O$, and (e) $0.1\% {}^{12}C^{16}O + 0.1\% {}^{12}C^{18}O$.