Electronic Supplementary Information

Title:

Efficient synthetic method for organometallic radicals: Structures and properties of gold(I)–(nitronyl nitroxide)-2-ide complexes

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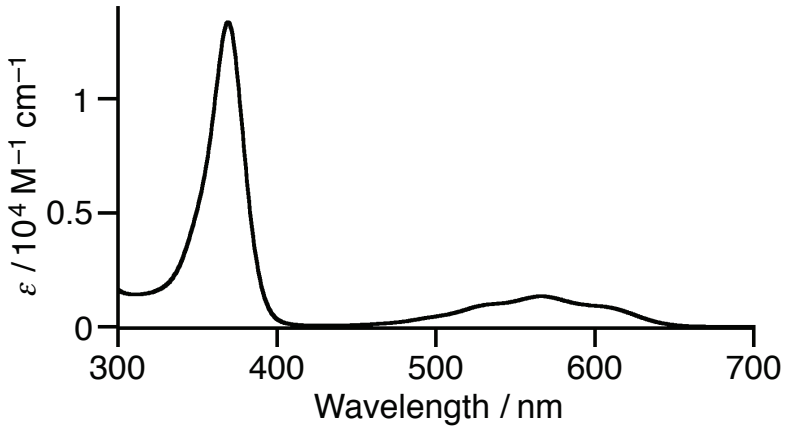

Fig. S1. Absorption spectrum of **NN-Au-2** in CH_2Cl_2.

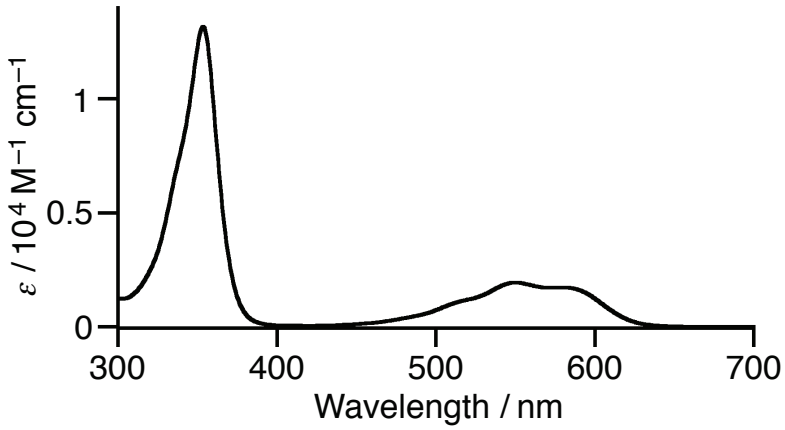

Fig. S2. Absorption spectrum of **NN-Au-3** in CH_2Cl_2.

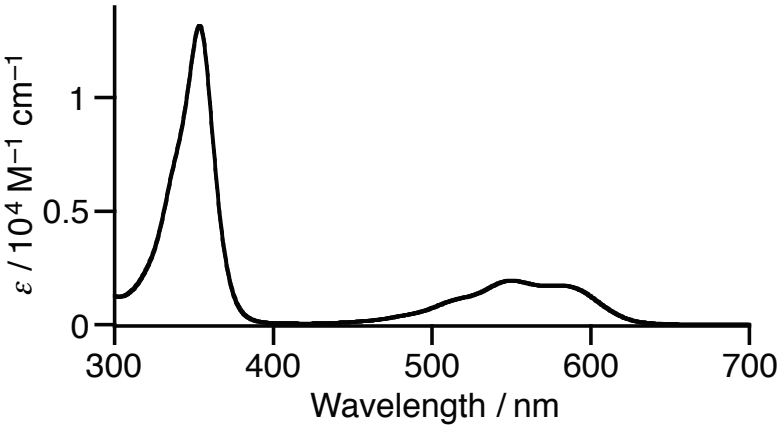

Fig. S3. Absorption spectrum of **NN-Au-5** in CH_2Cl_2.

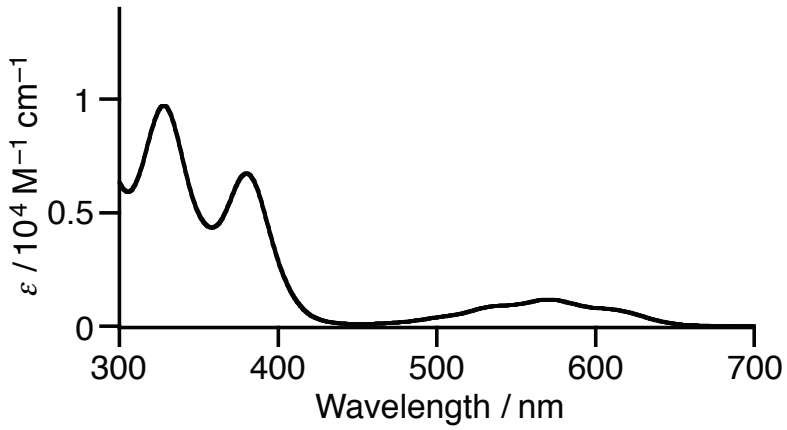

Fig. S4. Absorption spectrum of **NN-Au-6** in CH_2Cl_2.

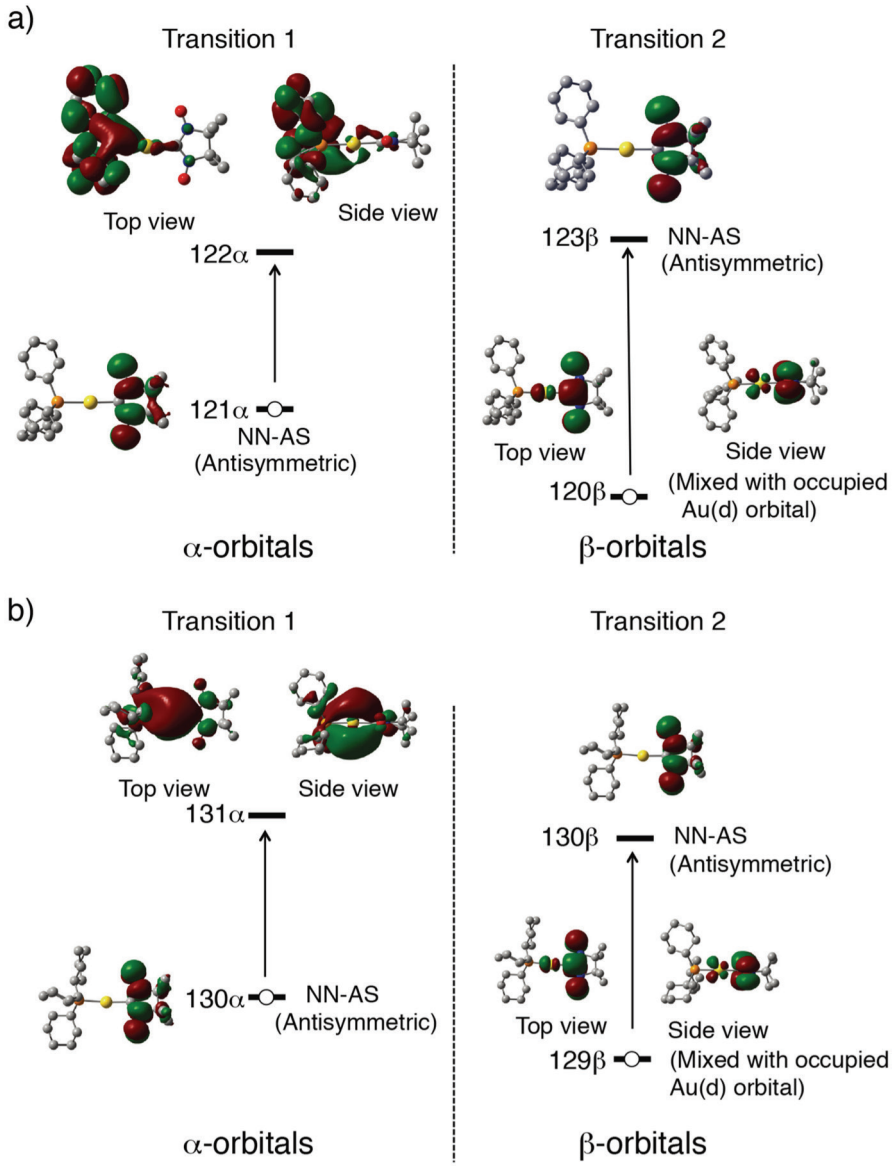

Fig. S5. MO-interaction diagram for **NN-Au-1**.[S1] a) for α-orbitals, b) for β-orbitals.

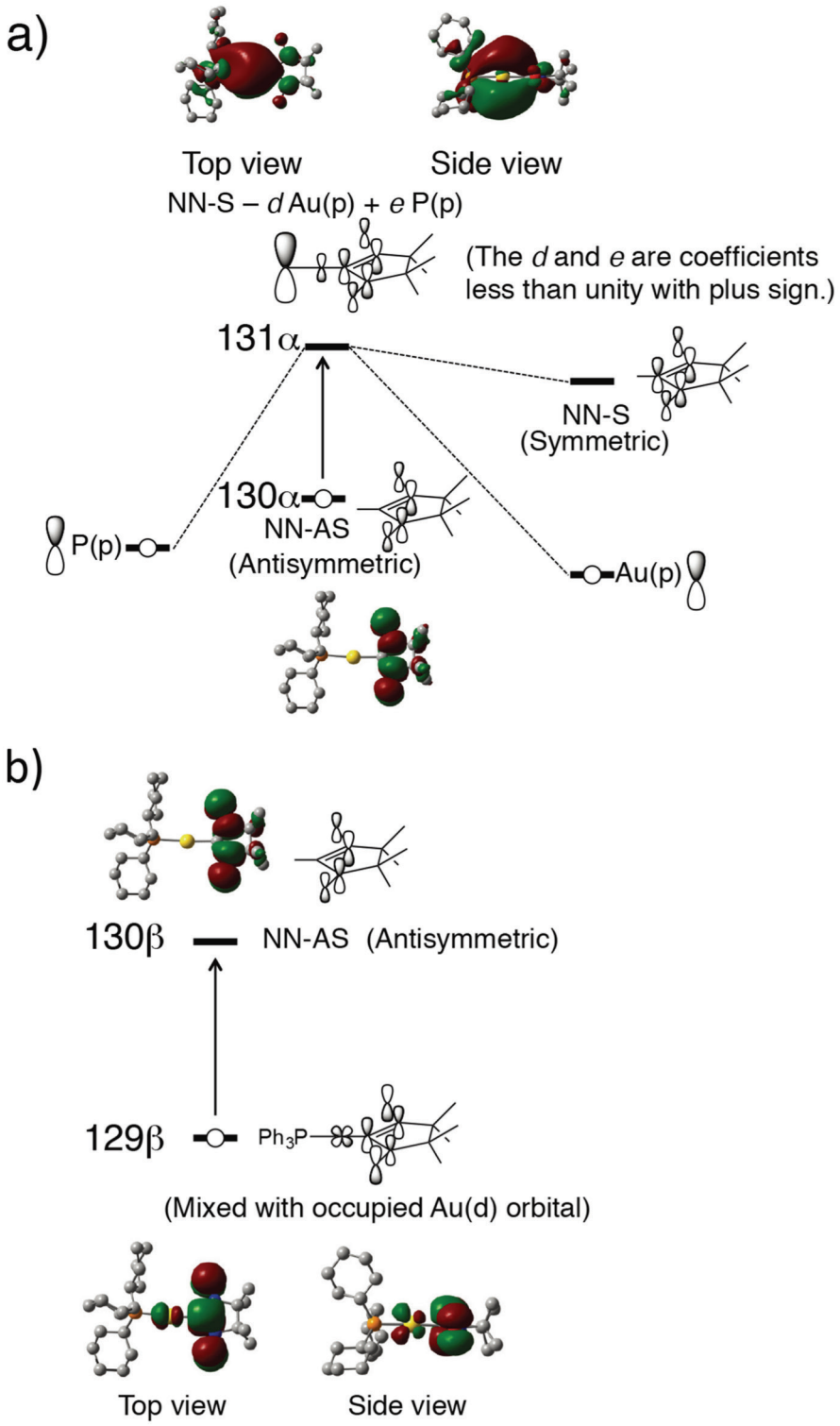

Fig. S6. MO-interaction diagram for **NN-Au-4**.[S1] a) for α-orbitals, b) for β-orbitals.

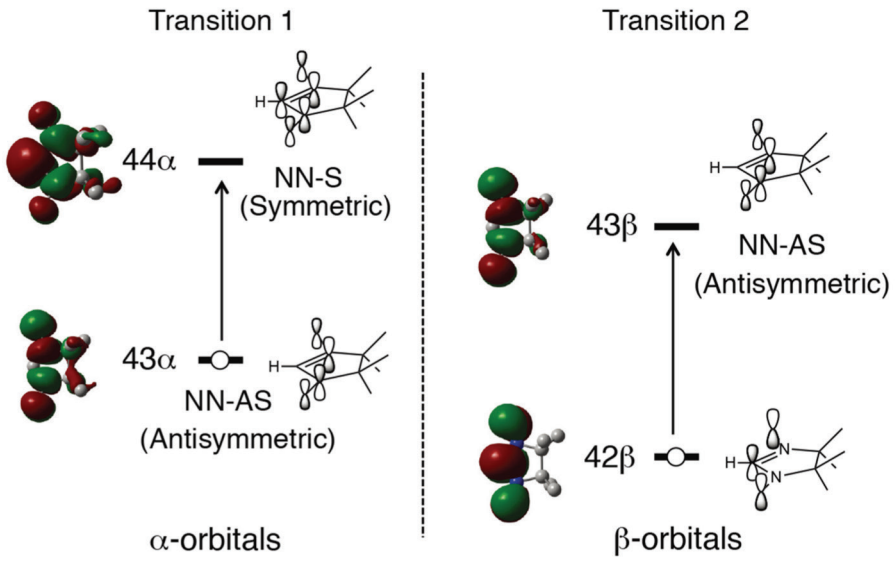

Fig. S7. MO-transitions 1,2 contributing for the longest absorption of **NN-H**.[S1] The calculated longest wavelength and the transition coefficients were as follows: **NN-H** (43 α-orbitals and 42 β-orbitals), 447.2 nm (*f* = 0.01), transition 1: 43α → 44α (*c* = 0.556), 42β → 43β (*c* = 0.669). For the strong absorption around 300 nm was calculated: 283.1 nm (*f* = 0.24), 43α → 44α (c = 0.741), 42β → 43β (c = -0.647).

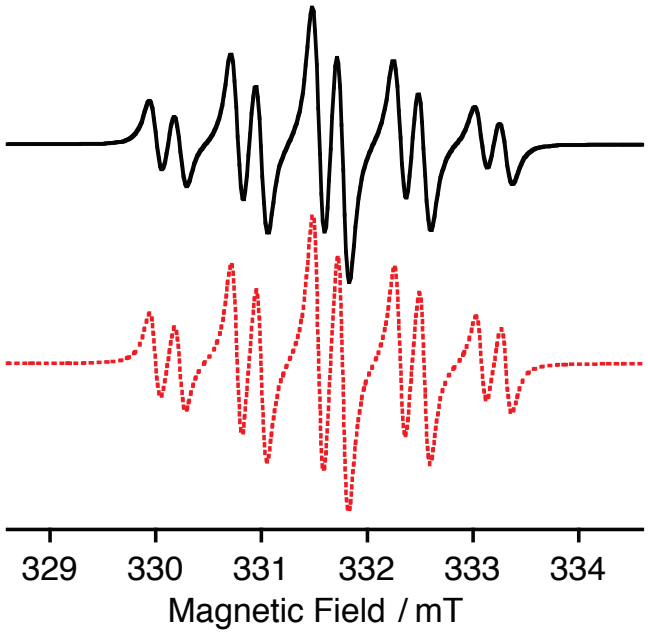

Fig. S8. Observed (in CH_2Cl_2: solid line) and simulated (red dashed line) ESR spectra of **NN-Au-1**.

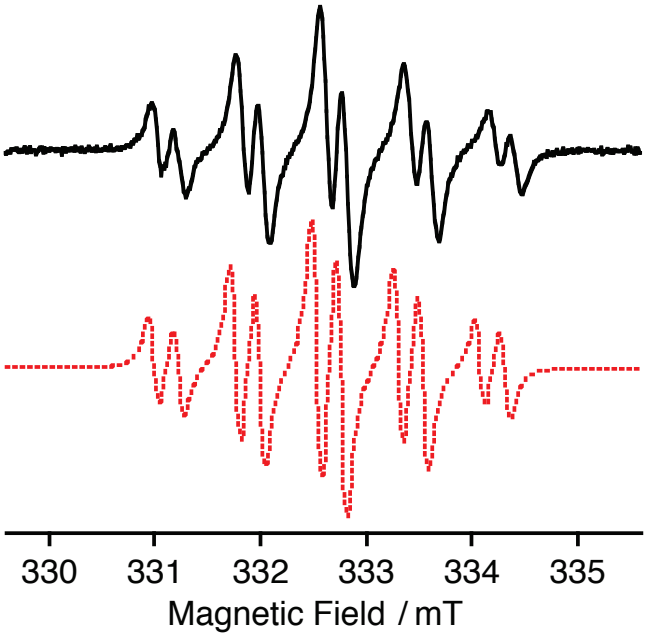

Fig. S9. Observed (in CH_2Cl_2: solid line) and simulated (red dashed line) ESR spectra of **NN-Au-3**.

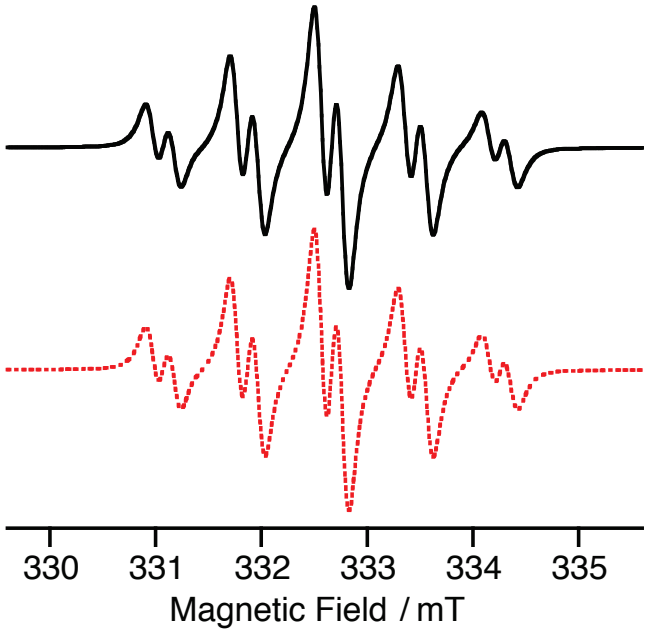

Fig. S10. Observed (in CH_2Cl_2: solid line) and simulated (red dashed line) ESR spectra of **NN-Au-4**.

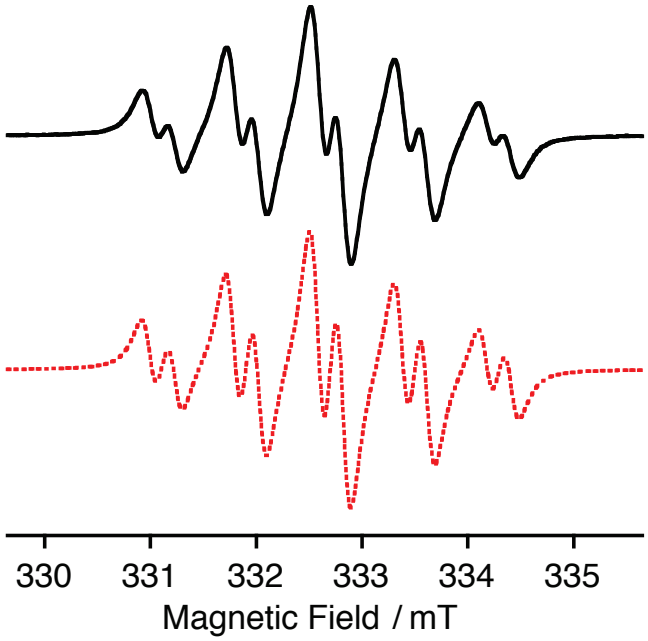

Fig. S11. Observed (in CH_2Cl_2: solid line) and simulated (red dashed line) ESR spectra of **NN-Au-5**.

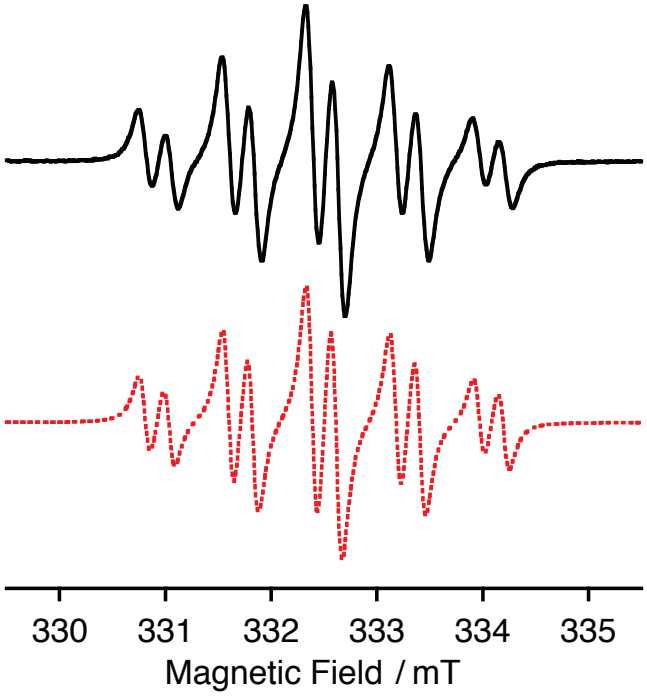

Fig. S12. Observed (in CH_2Cl_2: solid line) and simulated (red dashed line) ESR spectra of **NN-Au-6**.

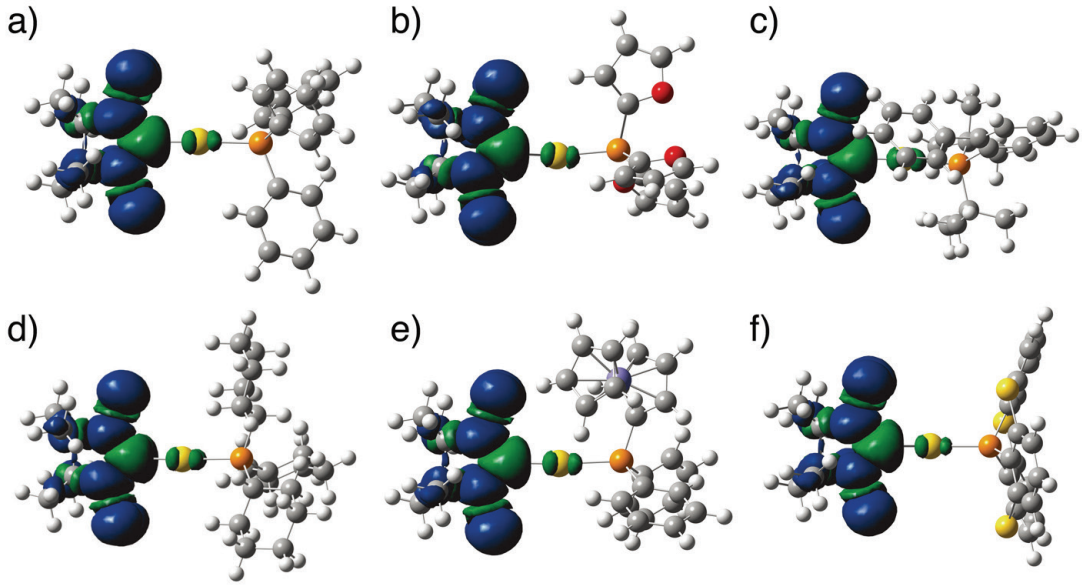

Fig. S13. Spin density distributions of (a) **NN-Au-1** (b) **NN-Au-2** (c) **NN-Au-3**, (d) **NN-Au-4**, (e) **NN-Au-5**, and (f) **NN-Au-6** calculated by *Gaussian 09* using at the UB3PW91 level of theory with 6-31G(d) basis set for C, H, N, O, P, and S atoms, and LANLSDZ basis set for Au atom.[S1]

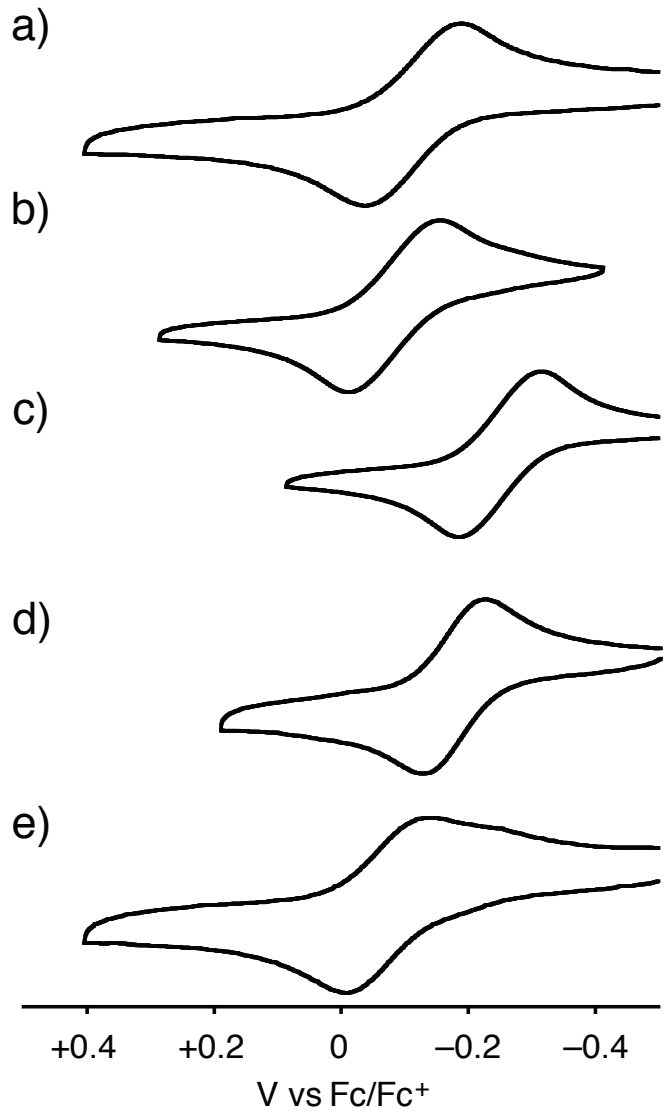

Fig. S14. Cyclic voltammograms of (a) **NN-Au-1**, (b) **NN-Au-2**, (c) **NN-Au-3**, (d) **NN-Au-4**, and (e) **NN-Au-6** in 1,2-dichloroethane.

Reference

(S1) *Gaussian 09*, Revision C.01, 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, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, 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, 2010.