An Examination of the Silver Colloid Binding Behavior of Disulfide Tethered Bipyridine Ligands and Their *fac* Tricarbonyl Re(I) Complexes.

Heather J. Montgomery, Diane Pelleteret, Steven E. J. Bell, Nicholas C. Fletcher*

Supplementary Figures

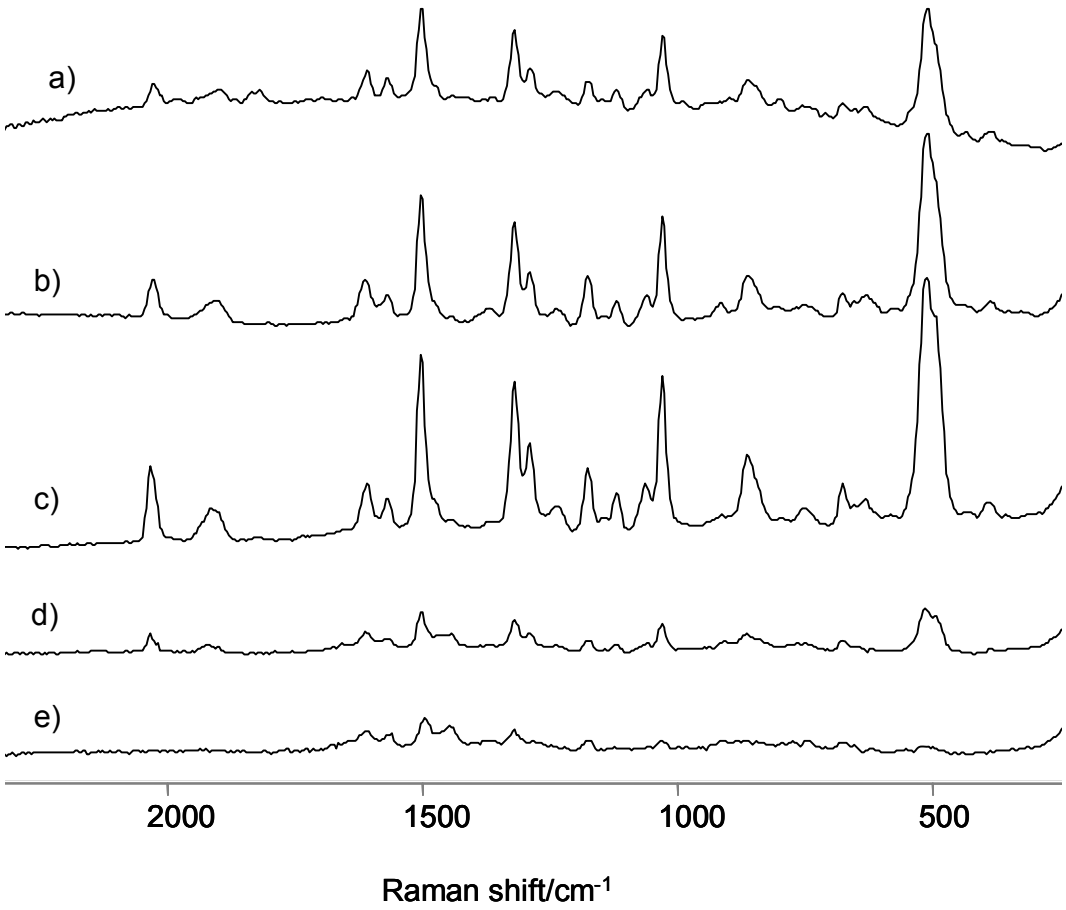

Figure S1. Concentration dependence of the SERRS spectrum of $[Re(CO)_3(\mathbf{L1})Br]$ in the presence of 160 µl silver colloid with 20 µl of 0.01 moldm^{-3} KBr (aq), 40 µl of 0.1 moldm^{-3} $MgSO_4$ (aq) and 40 µl acetone at a concentration of (a) 3.85 x 10^{-5} M b) 7.70 x 10^{-6} M c) 3.85 x 10^{-6} M d) 7.70 x 10^{-7} M e) 3.85 x 10^{-7} M excited at 532 nm.

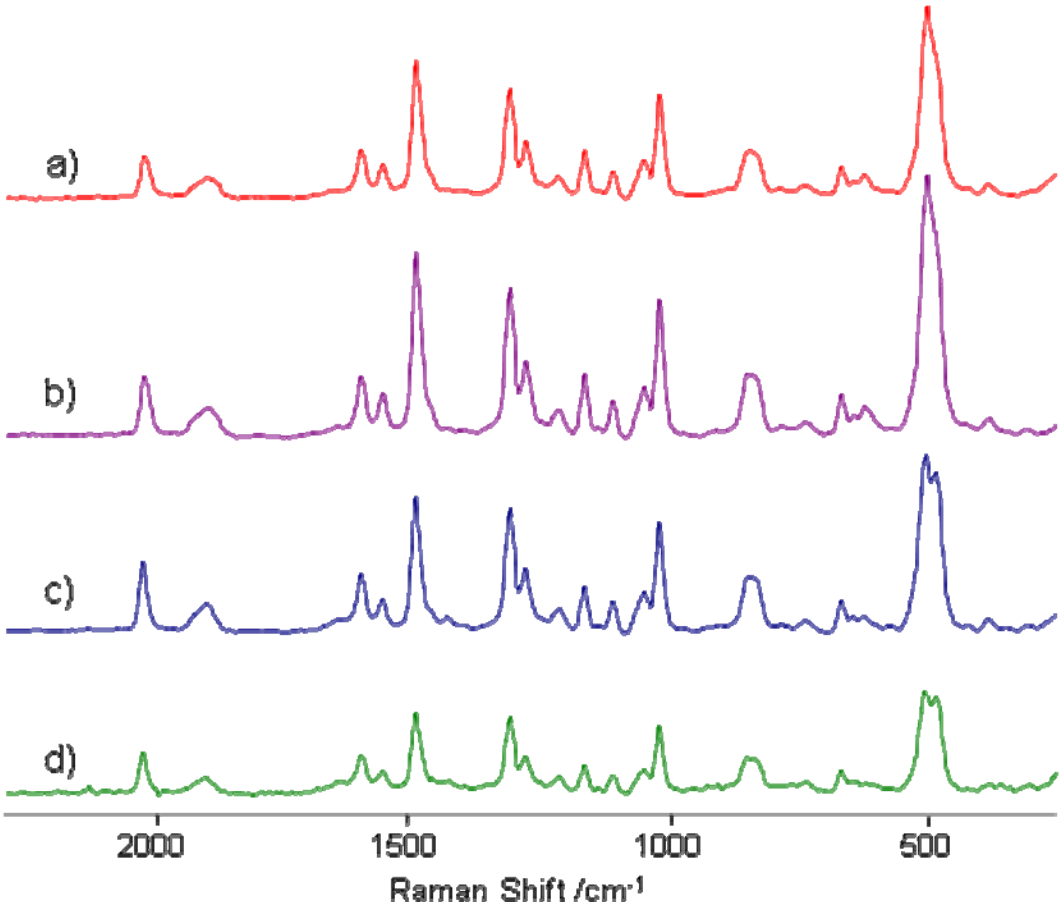

Figure S2. Concentration dependence of the SERRS spectrum of [$Re(CO)_3$(**L2**)Br] in the presence of 160 µl silver colloid with 20 µl of 0.01 $moldm^{-3}$ KBr (aq), 40 µl of 0.1 $moldm^{-3}$ $MgSO_4$ (aq) and 40 µl acetone at a concentration of (a) 3.85 x 10^{-5} M b) 7.70 x 10^{-6} M c) 3.85 x 10^{-6} M d) 7.70 x 10^{-7} M excited at 532 nm.

Cartesian Coordinates of the Optimized Structures

Calculations. These were run using the Gaussian03 program.[1] Geometry optimization and calculation of Raman frequencies was carried out using DFT at the B3LYP level of theory.[2] For C, H, N and O the 6-31G basis set was used while the Los Alamos National Laboratory 2-double-ζ (Lanl2DZ) was used for Re, Br and S atoms;[3] the first five HOMO and LUMO orbitals were calculated.

References

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2. Becke, A. D., *J. Chem. Phys.*, **1993**, *98*, 5648-5652; Lee, C. T.; Yang, W. T.; Parr, R. G., **1988**, *Phys. Rev. B., 37*, 785-789.
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1. [$Re(CO)_3(L1)Br$]

55 Atoms
C:/ReL1_opt.mol

C	-4.777000	1.349000	-0.233000
C	-7.185000	1.444000	-0.352000
C	-7.196000	0.062000	-0.533000
C	-5.984000	-0.617000	-0.556000
C	-3.439000	1.954000	-0.080000
C	-1.932000	3.809000	0.235000
C	-0.854000	2.921000	0.187000
C	-1.140000	1.570000	0.001000
H	-8.111000	2.010000	-0.325000
H	-8.123000	-0.490000	-0.649000
H	-5.944000	-1.691000	-0.685000
H	-1.764000	4.874000	0.375000
H	-0.343000	0.842000	-0.043000
C	0.559000	3.420000	0.360000
H	0.741000	4.304000	-0.263000
H	0.743000	3.720000	1.399000
O	1.469000	2.377000	-0.002000
C	2.792000	2.682000	0.129000
O	3.175000	3.767000	0.502000
C	3.656000	1.499000	-0.250000
C	-5.963000	2.091000	-0.202000
C	-3.226000	3.324000	0.103000
H	-5.936000	3.163000	-0.056000
H	-4.062000	4.012000	0.141000
N	-4.799000	0.003000	-0.413000
N	-2.391000	1.095000	-0.133000
H	3.364000	1.175000	-1.258000
H	3.389000	0.664000	0.413000
C	5.154000	1.806000	-0.175000
C	6.018000	0.599000	-0.563000
H	5.404000	2.133000	0.841000
H	5.381000	2.657000	-0.830000
C	7.519000	0.899000	-0.486000
H	5.785000	-0.247000	0.098000
H	5.762000	0.276000	-1.583000
H	7.752000	1.744000	-1.154000
H	7.786000	1.221000	0.529000
C	8.424000	-0.274000	-0.885000
C	9.916000	0.146000	-0.975000
H	8.094000	-0.679000	-1.849000
C	10.865000	-0.941000	-0.460000
H	10.161000	0.404000	-2.013000
H	10.061000	1.048000	-0.370000
H	11.872000	-0.551000	-0.281000
H	10.926000	-1.792000	-1.145000
S	8.272000	-1.743000	0.274000
S	10.180000	-1.506000	1.147000
Re	-2.865000	-1.044000	-0.324000
C	-2.634000	-1.056000	-2.227000
C	-3.557000	-2.846000	-0.333000
C	-1.079000	-1.721000	-0.042000
O	-2.495000	-1.059000	-3.384000
O	0.010000	-2.075000	0.142000
O	-4.026000	-3.907000	-0.330000
Br	-3.248000	-0.906000	2.363000

2. [$Re(CO)_3(L2)Br$]

56

C:/ReL2_opt.mol

C	-4.497000	0.264000	-0.531000
C	-6.702000	-0.708000	-0.664000
C	-6.115000	-1.969000	-0.581000
C	-4.732000	-2.053000	-0.476000
C	-3.557000	1.400000	-0.495000
C	-3.000000	3.746000	-0.550000
C	-1.648000	3.418000	-0.405000
C	-1.330000	2.064000	-0.318000
H	-7.779000	-0.599000	-0.743000
H	-6.709000	-2.876000	-0.592000
H	-4.231000	-3.011000	-0.399000
H	-3.306000	4.786000	-0.630000
H	-0.301000	1.749000	-0.203000
C	-0.585000	4.496000	-0.312000
H	-0.888000	5.355000	-0.926000
H	-0.501000	4.850000	0.722000
C	1.793000	4.104000	0.227000
O	1.650000	4.529000	1.365000
C	3.119000	3.554000	-0.278000
C	-5.884000	0.416000	-0.639000
C	-3.954000	2.738000	-0.589000
H	-6.324000	1.404000	-0.695000
H	-5.001000	2.995000	-0.697000
N	-3.935000	-0.970000	-0.454000
N	-2.244000	1.080000	-0.371000
H	3.874000	4.335000	-0.127000
H	3.083000	3.337000	-1.354000
C	3.516000	2.291000	0.508000
C	4.888000	1.739000	0.101000
H	2.755000	1.514000	0.359000
H	3.508000	2.535000	1.576000
C	5.214000	0.422000	0.819000
H	4.912000	1.576000	-0.986000
H	5.666000	2.485000	0.320000
H	5.132000	0.577000	1.905000
H	4.468000	-0.338000	0.552000
C	6.615000	-0.129000	0.546000
C	6.899000	-1.436000	1.291000
H	7.374000	0.618000	0.802000
C	8.234000	-2.045000	0.875000
H	6.916000	-1.229000	2.370000
H	6.089000	-2.149000	1.099000
H	8.375000	-3.045000	1.294000
H	9.077000	-1.408000	1.156000
N	0.746000	4.051000	-0.670000
H	0.924000	3.746000	-1.617000
S	6.832000	-0.455000	-1.335000
S	8.259000	-2.271000	-1.006000
Re	-1.752000	-1.056000	-0.177000
C	-1.404000	-1.268000	-2.051000
C	-1.613000	-2.957000	0.135000
C	0.125000	-0.853000	0.210000
O	-1.196000	-1.392000	-3.191000
O	1.249000	-0.681000	0.445000
O	-1.585000	-4.100000	0.327000
Br	-2.354000	-0.678000	2.443000