

A Robust Pyridyl-NHC Ligated Rhenium Photocatalyst for CO₂ Reduction in the Presence of Water and Oxygen

Casey A. Carpenter, Phillip Brogdon, Louis E. McNamara, Gregory S. Tschumper, Nathan I. Hammer, and Jared H. Delcamp*

University of Mississippi, Department of Chemistry and Biochemistry, 322 Coulter Hall,
University, MS 38677, USA

*Correspondence: delcamp@olemiss.edu; Tel.: +1-662-915-5332

Table of Contents

Page S2	DFT Cartesian Coordinates for neutral $\text{Re}(\text{pyNHC-PhCF}_3)(\text{CO})_3\text{Br}$.
Page S3	DFT Cartesian Coordinates for anionic $\text{Re}(\text{pyNHC-PhCF}_3)(\text{CO})_3\text{Br}$.

DFT Cartesian Coordinates for neutral $\text{Re}(\text{pyNHC-PhCF}_3)(\text{CO})_3\text{Br}$

C	4.25522550	1.39304798	0.90826189
N	-1.46500546	2.16620920	0.15942125
C	0.53606061	-1.77713693	0.41583250
C	1.99078289	1.40829424	0.11460083
C	-2.80303509	1.76647035	0.10738240
C	-5.14557126	2.15732660	-0.09821562
C	-4.23211384	-0.04125196	0.11540359
C	4.56171685	0.40980458	-0.03572488
N	0.66994085	1.94673506	0.17465893
C	2.28811540	0.44074920	-0.83926870
C	-0.94520688	3.44942709	0.04862707
C	2.96398800	1.89454895	0.98828260
C	-3.85603360	2.66503726	-0.03045735
C	-2.08320096	-2.52155307	0.21827587
C	-5.33888456	0.77933876	-0.02765846
C	-1.20180499	-0.87338694	2.26543752
C	0.39847944	3.30828424	0.06297325
C	3.58279109	-0.06538643	-0.90416286
H	-1.55734678	4.33138254	-0.04009704
H	3.82562723	-0.83318357	-1.63040950
H	-5.98851943	2.83177850	-0.21022133
H	-3.66957189	3.73111697	-0.09153042
H	1.18847817	4.03721929	-0.02369653
H	1.50787650	0.09136421	-1.51414310
H	2.70320942	2.64061253	1.73367328
H	5.02357918	1.75186506	1.58655012
H	-4.32870666	-1.12064205	0.17127009
H	-6.32874680	0.34206330	-0.08499869
O	-2.70999470	-3.49736129	0.11980686
O	1.54110756	-2.36804513	0.45479218
O	-1.25189844	-0.89003622	3.43472272
Br	-1.11323696	-0.54680797	-2.30969136
Re	-1.12600426	-0.82752678	0.36222797
C	-0.47098507	1.21353819	0.24437744
N	-2.97543845	0.43382532	0.19033333
F	6.84640486	0.87256131	-0.41085506
F	6.36486045	-0.59949449	1.10537097
F	6.12157777	-1.09142853	-0.99915913
C	5.96666859	-0.11038208	-0.09196325

DFT Cartesian Coordinates for anionic $\text{Re}(\text{pyNHC-PhCF}_3)(\text{CO})_3\text{Br}$

C	4.38614567	1.53696571	0.70049487
N	-1.40247618	2.20368091	0.03396614
C	0.37544087	-1.82528837	0.65741323
C	2.04612175	1.38644622	0.12066800
C	-2.73826963	1.86861604	-0.06435014
C	-5.06497920	2.36029263	-0.37537408
C	-4.25175342	0.10969268	-0.11593658
C	4.64364829	0.37771005	-0.04510538
N	0.74894081	1.92535855	0.18391610
C	2.29951061	0.23326108	-0.63277958
C	-0.82893156	3.46799364	-0.01348742
C	3.09881237	2.03587054	0.78961335
C	-3.75893817	2.80066052	-0.24827312
C	-2.25566216	-2.42880573	0.38961087
C	-5.31160584	0.96533151	-0.31416162
C	-1.39888842	-0.64270780	2.29899745
C	0.50736978	3.29067190	0.08683235
C	3.59042363	-0.26663099	-0.70637666
H	-1.40653089	4.36972298	-0.13543216
H	3.78184888	-1.16052592	-1.29076885
H	-5.87251187	3.06888497	-0.53103596
H	-3.51985901	3.85888079	-0.30467294
H	1.31320738	4.00575466	0.03404680
H	1.48292721	-0.23928411	-1.17611512
H	2.89271552	2.91354194	1.39662706
H	5.19844245	2.03393809	1.22467662
H	-4.40260418	-0.96504507	-0.06447555
H	-6.31219191	0.56130626	-0.42304494
O	-2.92459925	-3.39058092	0.36825099
O	1.33828052	-2.47790155	0.80720486
O	-1.51106842	-0.54910201	3.46691152
Br	-0.97103463	-0.87521430	-2.32731758
Re	-1.21676204	-0.78966606	0.42538983
C	-0.43929368	1.21169936	0.18255020
N	-2.96651136	0.51375289	0.02865990
F	6.90199710	0.79725641	-0.63427963
F	6.55358061	-0.43484887	1.10979194
F	6.16551880	-1.23686316	-0.87621247
C	6.03709520	-0.12819385	-0.11639557