

Forward.

During the course of my graduate career, I have had the opportunity to conduct research in two distinct areas of chemistry. The first area is in the design of molecular devices; the second area incorporates the study of molybdenum carbonyl systems applicable to our chemical education research. I have divided the content of this dissertation into three sections to guide the reader. The first section addresses the investigation of a new supramolecular device for photoinitiated electron collection, $\{[(\text{bpy})_2\text{Ru}(\text{dpp})]_2\text{RhCl}_2\}(\text{PF}_6)_5$, where $\text{bpy} = 2,2'$ -bipyridine, and $\text{dpp} = 2,3$ -bis(2-pyridyl)pyrazine. The second addresses the synthesis and characterization of $[\text{Mo}(\text{CO})_4(\text{N-N})]$ complexes, where N-N is a bidentate nitrogen donor ligand. The final section addresses the design and implementation of integrated molecular modeling, synthesis, and characterization experiments into the undergraduate curriculum.

Elizabeth R. Bullock

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List of Abbreviations.

bpm	2,2'-bipyrimidine
bpy	2,2'-bipyridine
bpz	bipyrazine
5-Cl phen	5-chloro-1,10-phenanthroline
CAChe	Computer aided chemistry software (Oxford Molecular)
CAMD	Computer aided molecular design
CMM	Center for molecular modeling
DPA	2,2'-dipyridylamine
dpb	2,3-bis(2-pyridyl)benzoquinoxaline
dpp	2,3-bis(2-pyridyl)pyrazine
dpq	2,3-bis(2-pyridyl)quinoxaline
ECEC	electrochemical-chemical-electrochemical-chemical
en	ethylenediamine
HOMO	highest occupied molecular orbital
LF	ligand field
LMCT	ligand to metal charge transfer
LUMO	lowest unoccupied molecular orbital
4,7-Me ₂ -phen	4,7-dimethyl-1,10-phenanthroline
2,9-Me ₂ -4,7-Ph ₂ -phen	2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline
MLCT	metal to ligand charge transfer
NHE	normal hydrogen electrode
NIH	National Institutes of Health
NMR	nuclear magnetic resonance
N-N	bidentate nitrogen donor ligand
5-NO ₂ -phen	5-nitro-1,10-phenanthroline
OSWV	Osteryoung square wave voltammetry
PEC	photoinitiated electron collection
phen	1,10-phenanthroline

4,7-Ph ₂ -phen	4,7-diphenyl-1,10-phenanthroline
PMD	photochemical molecular device
TBAH	tetrabutylammonium hexafluorophosphate
TMEDA	N,N,N',N'-tetramethylethylenediamine
tpp	2,3,5,6-tetrakis(2-pyridyl)pyrazine
tpy	2,2',6,2''-terpyridine
ZINDO	Zerner's incomplete neglect of differential overlap

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