

## Supporting Information

### Ligand Noninnocence in FeNO Corroles: Insights from $\beta$ -Octabromocorrole Complexes

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#### Optimized B3LYP/TZ2P coordinates

Ir [Br <sub>8</sub> TPFPC] (NMe <sub>3</sub> ) <sub>2</sub>			
Ir	0.000000	0.000000	0.371041
Br	0.000000	1.803893	5.931520
Br	0.000000	3.126075	-4.758459
Br	0.000000	4.728286	4.048207
Br	0.000000	5.393266	-2.259063
Br	0.000000	-1.803893	5.931520
Br	0.000000	-3.126075	-4.758459
Br	0.000000	-4.728286	4.048207
Br	0.000000	-5.393266	-2.259063
F	0.000000	0.000000	-8.577467
F	0.000000	8.932149	1.246416
F	0.000000	-8.932149	1.246416
F	2.357237	0.000000	-4.513608
F	2.357639	4.889388	0.832561
F	2.357639	-4.889388	0.832561
F	2.357701	7.584611	1.114994
F	2.357701	-7.584611	1.114994
F	2.358102	0.000000	-7.223091
F	-2.357237	0.000000	-4.513608
F	-2.357639	4.889388	0.832561
F	-2.357639	-4.889388	0.832561
F	-2.357701	7.584611	1.114994
F	-2.357701	-7.584611	1.114994
F	-2.358102	0.000000	-7.223091
N	0.000000	1.256851	1.897363
N	0.000000	1.479065	-0.985788
N	0.000000	-1.256851	1.897363
N	0.000000	-1.479065	-0.985788
N	2.229427	0.000000	0.354815
N	-2.229427	0.000000	0.354815
C	0.000000	0.000000	-2.961577
C	0.000000	0.000000	-4.450192
C	0.000000	0.000000	-7.244274
C	0.000000	0.719030	3.155055
C	0.000000	1.277482	-2.340467
C	0.000000	1.837014	4.048891
C	0.000000	2.608303	-2.935766

C	0.000000	2.614979	1.887662
C	0.000000	2.821616	-0.648841
C	0.000000	2.996451	3.285683
C	0.000000	3.346824	0.671055
C	0.000000	3.529977	-1.921214
C	0.000000	4.827395	0.820654
C	0.000000	7.605775	1.114806
C	0.000000	-0.719030	3.155055
C	0.000000	-1.277482	-2.340467
C	0.000000	-1.837014	4.048891
C	0.000000	-2.608303	-2.935766
C	0.000000	-2.614979	1.887662
C	0.000000	-2.821616	-0.648841
C	0.000000	-2.996451	3.285683
C	0.000000	-3.346824	0.671055
C	0.000000	-3.529977	-1.921214
C	0.000000	-4.827395	0.820654
C	0.000000	-7.605775	1.114806
C	1.186216	0.000000	-5.168578
C	1.186781	5.540537	0.903971
C	1.186781	-5.540537	0.903971
C	1.203156	6.916668	1.046907
C	1.203156	-6.916668	1.046907
C	1.203182	0.000000	-6.551777
C	2.764484	0.000000	-1.035567
C	2.781858	1.203440	1.037169
C	2.781858	-1.203440	1.037169
C	-1.186216	0.000000	-5.168578
C	-1.186781	5.540537	0.903971
C	-1.186781	-5.540537	0.903971
C	-1.203156	6.916668	1.046907
C	-1.203156	-6.916668	1.046907
C	-1.203182	0.000000	-6.551777
C	-2.764484	0.000000	-1.035567
C	-2.781858	1.203440	1.037169
C	-2.781858	-1.203440	1.037169
H	2.412217	2.101921	0.555171
H	2.412217	-2.101921	0.555171
H	2.427297	0.884403	-1.561650
H	2.427297	-0.884403	-1.561650
H	2.487145	1.205396	2.080556
H	2.487145	-1.205396	2.080556
H	3.855750	0.000000	-1.001778
H	3.871857	1.184684	0.973002
H	3.871857	-1.184684	0.973002
H	-2.412217	2.101921	0.555171
H	-2.412217	-2.101921	0.555171
H	-2.427297	0.884403	-1.561650
H	-2.427297	-0.884403	-1.561650
H	-2.487145	1.205396	2.080556
H	-2.487145	-1.205396	2.080556
H	-3.855750	0.000000	-1.001778

H	-3.871857	1.184684	0.973002
H	-3.871857	-1.184684	0.973002

Fe[Br<sub>8</sub>TPFPC] (NO)

Br	-5.615886	-0.236620	-1.760926
Br	-3.780430	-0.028639	-4.685414
Br	2.480812	-0.034028	-5.353710
Br	4.948801	-0.268372	-3.093012
Br	4.948801	-0.268372	3.093012
Br	2.480812	-0.034028	5.353710
Br	-3.780430	-0.028639	4.685414
Br	-5.615886	-0.236620	1.760926
Fe	-0.120284	0.380955	0.000000
F	-0.626629	-2.256624	-4.987166
F	-0.922018	-2.135999	-7.678448
F	-1.028025	0.280369	-8.920049
F	-0.857209	2.574519	-7.471374
F	-0.562961	2.450784	-4.778888
F	4.787953	2.131894	0.000000
F	7.497504	2.033646	0.000000
F	8.762532	-0.372854	0.000000
F	7.323218	-2.678459	0.000000
F	4.613711	-2.576854	0.000000
F	-0.562961	2.450784	4.778888
F	-0.857209	2.574519	7.471374
F	-1.028025	0.280369	8.920049
F	-0.922018	-2.135999	7.678448
F	-0.626629	-2.256624	4.987166
O	0.293967	3.189892	0.000000
N	-1.560414	-0.029045	-1.220912
N	1.152526	-0.049163	-1.433920
N	1.152526	-0.049163	1.433920
N	-1.560414	-0.029045	1.220912
N	0.004927	2.069644	0.000000
C	-3.000612	-0.044373	-2.967826
C	-1.602785	0.000934	-2.593590
C	-0.434189	0.031364	-3.345357
C	0.872620	-0.011778	-2.783044
C	2.128786	-0.062975	-3.495113
C	3.134472	-0.145741	-2.568968
C	2.521024	-0.125592	-1.258144
C	3.154185	-0.157726	0.000000
C	2.521024	-0.125592	1.258144
C	3.134472	-0.145741	2.568968
C	2.128786	-0.062975	3.495113
C	0.872620	-0.011778	2.783044
C	-0.434189	0.031364	3.345357
C	-1.602785	0.000934	2.593590
C	-3.000612	-0.044373	2.967826
C	-3.741633	-0.113488	1.807270
C	-2.814944	-0.094320	0.713581
C	-2.814944	-0.094320	-0.713581

C	-3.741633	-0.113488	-1.807270
C	-0.581334	0.093723	-4.824999
C	-0.682347	-1.062420	-5.586745
C	-0.832402	-1.014045	-6.961680
C	-0.887736	0.220301	-7.597031
C	-0.800122	1.391857	-6.856039
C	-0.650810	1.314612	-5.481309
C	4.643360	-0.220391	0.000000
C	5.401044	0.942039	0.000000
C	6.784707	0.905641	0.000000
C	7.431642	-0.323475	0.000000
C	6.694957	-1.501169	0.000000
C	5.312148	-1.436071	0.000000
C	-0.581334	0.093723	4.824999
C	-0.650810	1.314612	5.481309
C	-0.800122	1.391857	6.856039
C	-0.887736	0.220301	7.597031
C	-0.832402	-1.014045	6.961680
C	-0.682347	-1.062420	5.586745