

Supporting information for

**«Molecular Structure, thermodynamic and spectral characteristics of metal-free and nickel complex of tetrakis(1,2,5-thiadiazole)porphyrazine»**

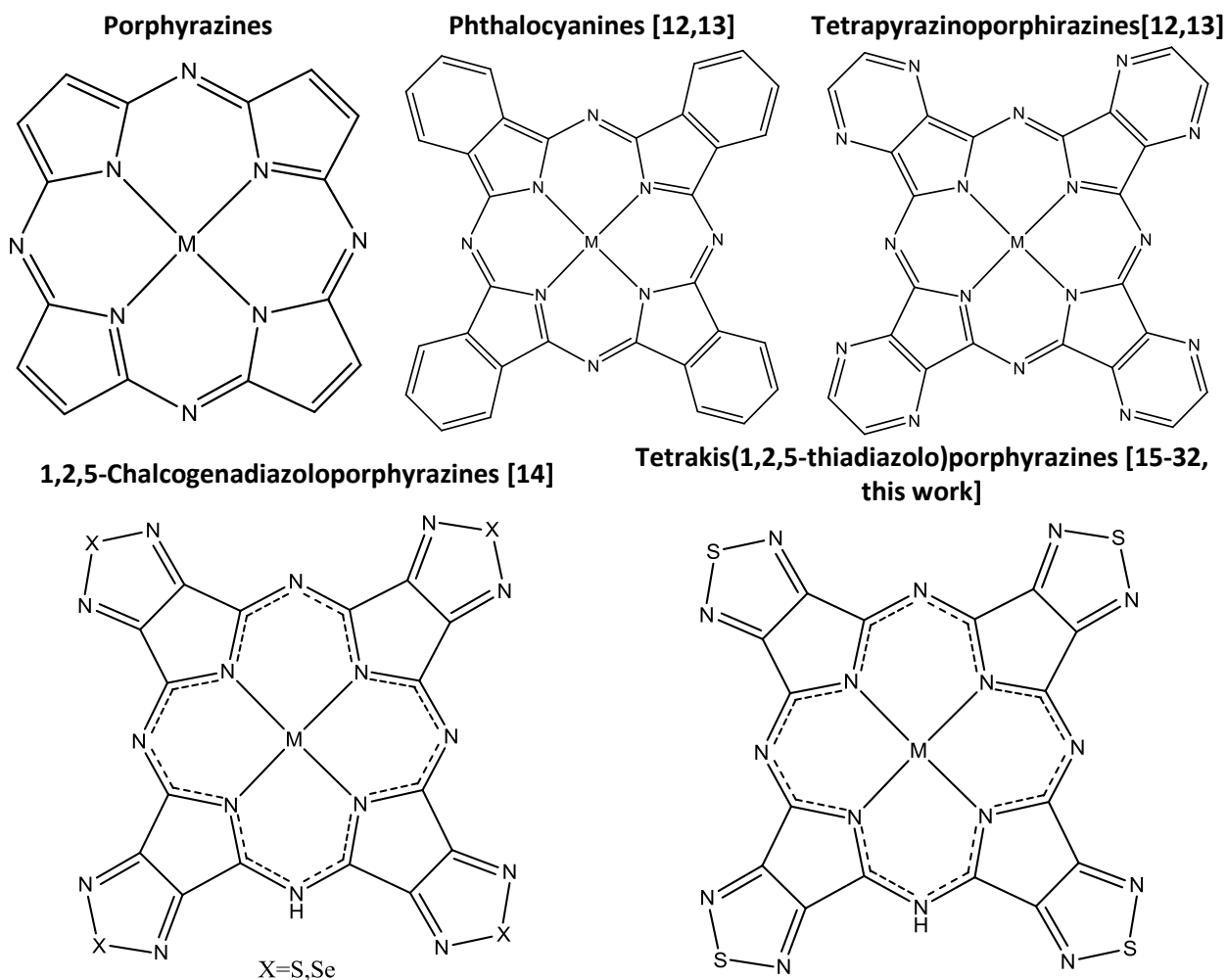
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**Figure S1. Structural formulas of porphyrazines and their derivatives**



**Cartesian coordinates of H<sub>2</sub>TTDPz optimized PBE0/pcseg-2 level of theory:**

N	0.000000000000	1.978811454900	0.000000000000
N	0.000000000000	-1.978811454900	0.000000000000
N	0.000000000000	0.000000000000	-2.046203960200
N	0.000000000000	0.000000000000	2.046203960200
N	0.000000000000	2.391099841400	2.374326410800
N	0.000000000000	-2.391099841400	-2.374326410800
N	0.000000000000	2.391099841400	-2.374326410800
N	0.000000000000	-2.391099841400	2.374326410800
C	0.000000000000	2.765234052400	-1.108498685100
C	0.000000000000	-2.765234052400	1.108498685100
C	0.000000000000	2.765234052400	1.108498685100
C	0.000000000000	-2.765234052400	-1.108498685100
C	0.000000000000	1.157254383600	2.788162570600
C	0.000000000000	-1.157254383600	-2.788162570600
C	0.000000000000	1.157254383600	-2.788162570600
C	0.000000000000	-1.157254383600	2.788162570600
C	0.000000000000	4.167134266100	-0.704184322900
C	0.000000000000	-4.167134266100	0.704184322900
C	0.000000000000	4.167134266100	0.704184322900
C	0.000000000000	-4.167134266100	-0.704184322900

C	0.000000000000	0.708060907000	4.163310557100
C	0.000000000000	-0.708060907000	-4.163310557100
C	0.000000000000	0.708060907000	-4.163310557100
C	0.000000000000	-0.708060907000	4.163310557100
H	0.000000000000	0.000000000000	1.035206320600
H	0.000000000000	0.000000000000	-1.035206320600
N	0.000000000000	1.253933505300	-5.362124418600
N	0.000000000000	-1.253933505300	5.362124418600
N	0.000000000000	1.253933505300	5.362124418600
N	0.000000000000	-1.253933505300	-5.362124418600
N	0.000000000000	5.358525045700	1.255864591700
N	0.000000000000	-5.358525045700	-1.255864591700
N	0.000000000000	5.358525045700	-1.255864591700
N	0.000000000000	-5.358525045700	1.255864591700
S	0.000000000000	0.000000000000	6.390694983900
S	0.000000000000	0.000000000000	-6.390694983900
S	0.000000000000	6.398911216700	0.000000000000
S	0.000000000000	-6.398911216700	0.000000000000

**Cartesian coordinates of singlet NiTTDPz optimized PBE0/pcseg-2 level of theory:**

N	0.000000000000	-1.926902693800	0.000000000000
N	1.926902693800	0.000000000000	0.000000000000
N	0.000000000000	1.926902693800	0.000000000000
N	-1.926902693800	0.000000000000	0.000000000000
N	-2.369204795700	-2.369204795700	0.000000000000
N	2.369204795700	-2.369204795700	0.000000000000
N	2.369204795700	2.369204795700	0.000000000000
N	-2.369204795700	2.369204795700	0.000000000000
C	1.116591026000	-2.727954576300	0.000000000000
C	2.727954576300	1.116591026000	0.000000000000
C	-1.116591026000	2.727954576300	0.000000000000
C	-2.727954576300	1.116591026000	0.000000000000
C	-1.116591026000	-2.727954576300	0.000000000000
C	2.727954576300	-1.116591026000	0.000000000000
C	1.116591026000	2.727954576300	0.000000000000
C	-2.727954576300	-1.116591026000	0.000000000000
C	0.700585082700	-4.113020594100	0.000000000000
C	4.113020594100	0.700585082700	0.000000000000
C	-0.700585082700	4.113020594100	0.000000000000
C	-4.113020594100	0.700585082700	0.000000000000
C	-0.700585082700	-4.113020594100	0.000000000000
C	4.113020594100	-0.700585082700	0.000000000000
C	0.700585082700	4.113020594100	0.000000000000
C	-4.113020594100	-0.700585082700	0.000000000000
N	1.255902817200	-5.307216104300	0.000000000000
N	5.307216104300	1.255902817200	0.000000000000
N	-1.255902817200	5.307216104300	0.000000000000
N	-5.307216104300	1.255902817200	0.000000000000
N	-1.255902817200	-5.307216104300	0.000000000000
N	5.307216104300	-1.255902817200	0.000000000000
N	1.255902817200	5.307216104300	0.000000000000
N	-5.307216104300	-1.255902817200	0.000000000000
S	0.000000000000	-6.339895711100	0.000000000000
S	6.339895711100	0.000000000000	0.000000000000
S	0.000000000000	6.339895711100	0.000000000000

S	-6.339895711100	0.000000000000	0.000000000000
Ni	0.000000000000	0.000000000000	0.000000000000

**Cartesian coordinates of triplet NiTTDPz optimized PBE0/pcseg-2 level of theory:**

N	-1.975864229200	0.000000000000	0.000000000000
N	0.000000000000	-1.975864229200	0.000000000000
N	1.975864229200	0.000000000000	0.000000000000
N	0.000000000000	1.975864229200	0.000000000000
N	-2.375158493000	2.375158493000	0.000000000000
N	-2.375158493000	-2.375158493000	0.000000000000
N	2.375158493000	-2.375158493000	0.000000000000
N	2.375158493000	2.375158493000	0.000000000000
C	-2.756436416700	1.118901536000	0.000000000000
C	-1.118901536000	-2.756436416700	0.000000000000
C	2.756436416700	-1.118901536000	0.000000000000
C	1.118901536000	-2.756436416700	0.000000000000
C	2.756436416700	1.118901536000	0.000000000000
C	-1.118901536000	2.756436416700	0.000000000000
C	-2.756436416700	-1.118901536000	0.000000000000
C	1.118901536000	2.756436416700	0.000000000000
C	-4.159830369900	0.703633342600	0.000000000000
C	-0.703633342600	-4.159830369900	0.000000000000
C	4.159830369900	-0.703633342600	0.000000000000
C	0.703633342600	-4.159830369900	0.000000000000
C	4.159830369900	0.703633342600	0.000000000000
C	-0.703633342600	4.159830369900	0.000000000000
C	-4.159830369900	-0.703633342600	0.000000000000
C	0.703633342600	4.159830369900	0.000000000000
N	-5.347384719300	1.255773280000	0.000000000000
N	-1.255773280000	-5.347384719300	0.000000000000
N	5.347384719300	-1.255773280000	0.000000000000
N	1.255773280000	-5.347384719300	0.000000000000
N	5.347384719300	1.255773280000	0.000000000000
N	-1.255773280000	5.347384719300	0.000000000000
N	-5.347384719300	-1.255773280000	0.000000000000
N	1.255773280000	5.347384719300	0.000000000000
S	-6.393555437300	0.000000000000	0.000000000000
S	0.000000000000	-6.393555437300	0.000000000000
S	6.393555437300	0.000000000000	0.000000000000
S	0.000000000000	6.393555437300	0.000000000000
Ni	0.000000000000	0.000000000000	0.000000000000