Supporting Information for: The trials and triumphs of modelling X-ray absorption spectra of transition metal phthalocyanines

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1 Experimental spectra in the SI

- The N K-edge experimental data for CoPcF16 was adapted from a previous study by Balle *et al.* with the title "Influence of the Fluorination of CoPc on the Interfacial

Electronic Structure of the Coordinated Metal Ion".[1] Copyright © 2017, American Chemical Society.

- The N K-edge experimental data for FePcF16 was adapted from a previous study by Greulich *et al.* with the title "Influence of the Fluorination of Iron Phthalocyanine on the Electronic Structure of the Central Metal Atom".[2] Copyright © 2021 The Authors. Published by American Chemical Society.

- The K-edge experimental data for CoPc were taken from a study by Uihlein *et al.*, with the title "Influence of Graphene on Charge Transfer between CoPc and Metals: The Role of Graphene–Substrate Coupling".[3] This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/) Copyright © 2011, American Chemical Society.

- The fluorine K-edge experimental spectra of FePcF16 were adapted from a previous study by Belser *et al.* with the title "Interaction Channels Between Perfluorinated Iron Phthalocyanine and Cu(111)"[5] Copyright © 2018 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

2 ASS1ST results

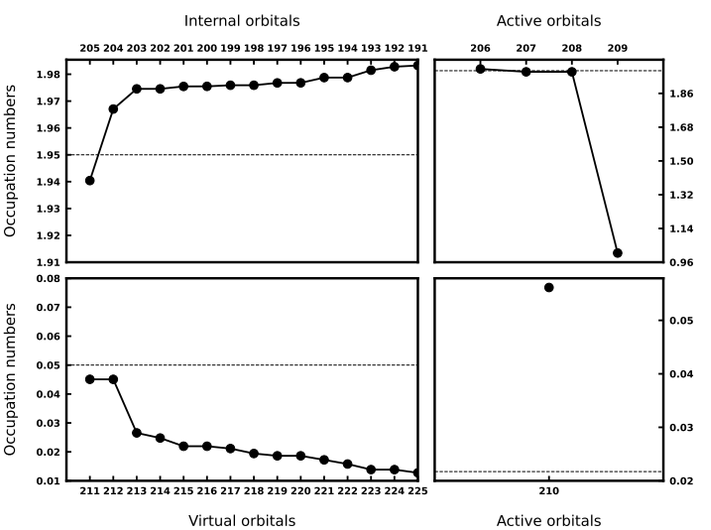

Figure 1 ASS1ST scheme for CoPcF16.

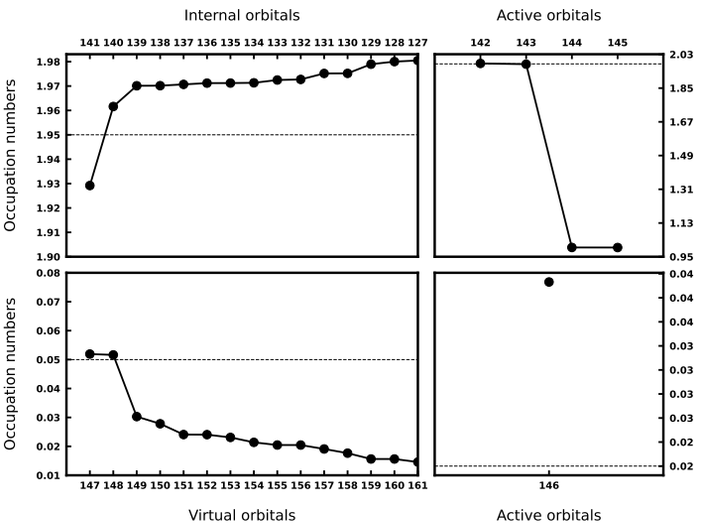

Figure 2 ASS1ST scheme for FePc.

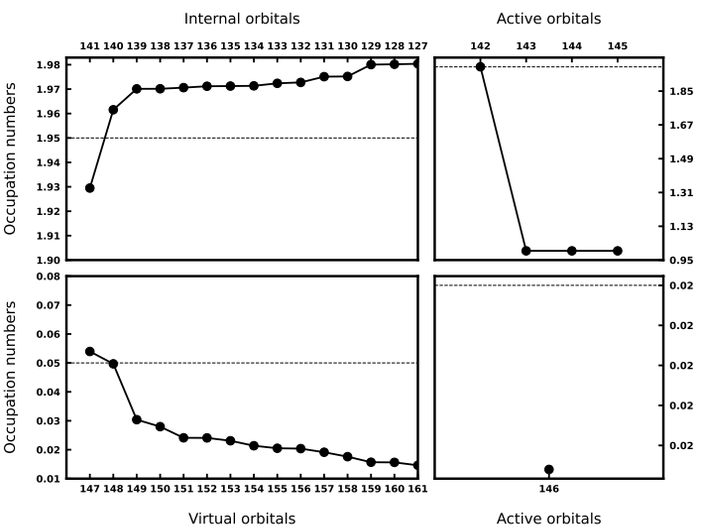

Figure 3 ASS1ST scheme for MnPc.

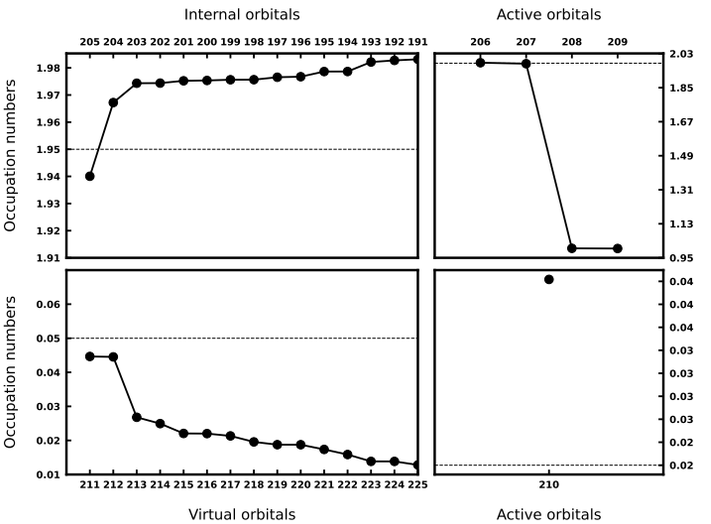

Figure 4 ASS1ST scheme for FePcF16.

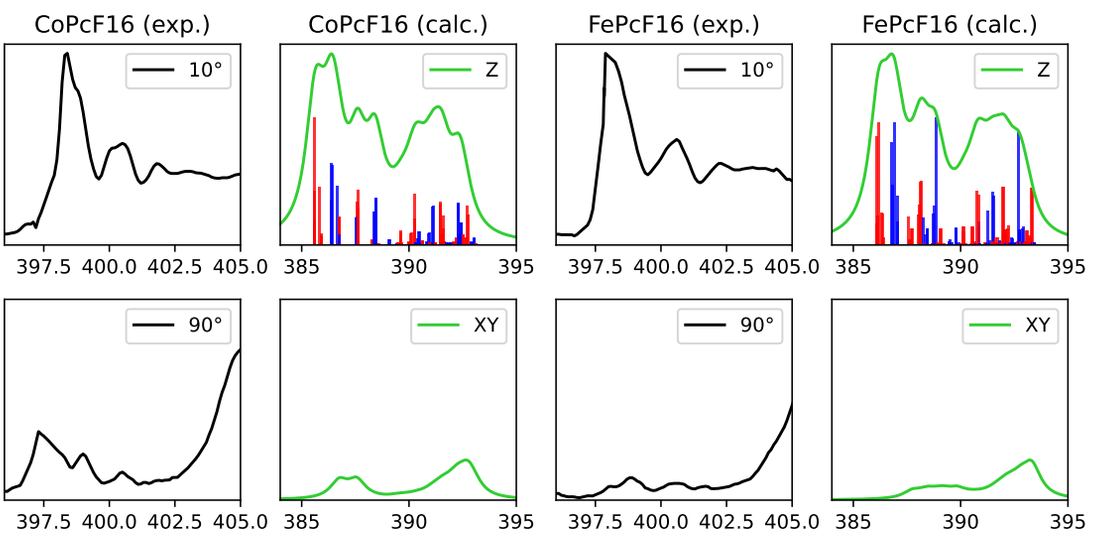

Figure 5 Experimental (black) and calculated (green) nitrogen K-edge XAS for TMPcF16s. Energies are given in eV units, and the intensities are normalized. The experimental spectra for CoPcF16 and FePcF16 were adapted from previous investigations by Balle *et al.*[1] and Greulich *et al.*,[2] respectively.

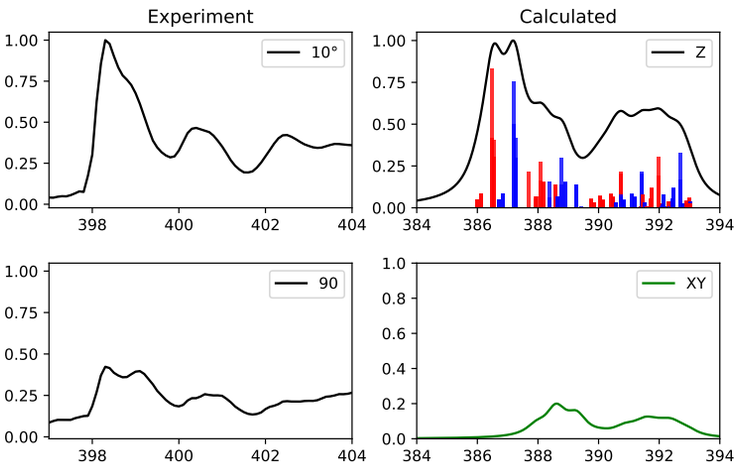

Figure 6 Experimental and calculated N K-edge spectra for CoPc with ${}^2E_g$ symmetry. The transitions originating from $\mathbf{N_{aza}}$ and $\mathbf{N_{pyr}}$ are denoted with red and blue bars, respectively. The experimental data for CoPc on graphene/Pt(111) were taken from a study by Uihlein *et al.*[3]

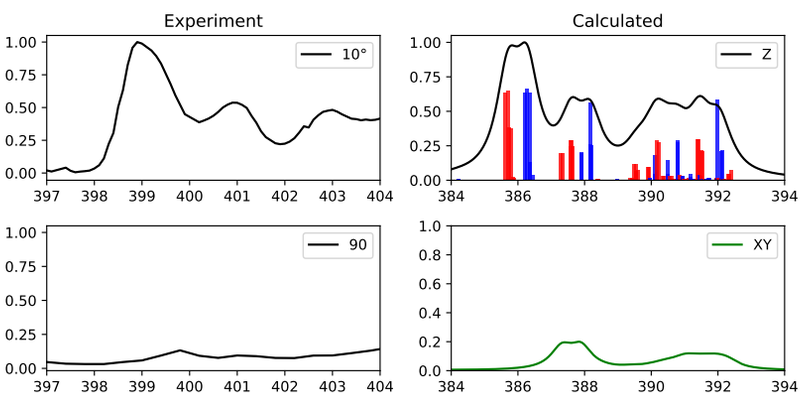

Figure 7 Experimental and calculated N K-edge spectra for FePc with ${}^3A_{1g}$ symmetry. The transitions originating from $\mathbf{N_{aza}}$ and $\mathbf{N_{pyr}}$ are denoted with red and blue bars, respectively. The experimental data for FePc on rutile TiO_2(110) were adapted from a previous study of Karstens *et al.*[4]

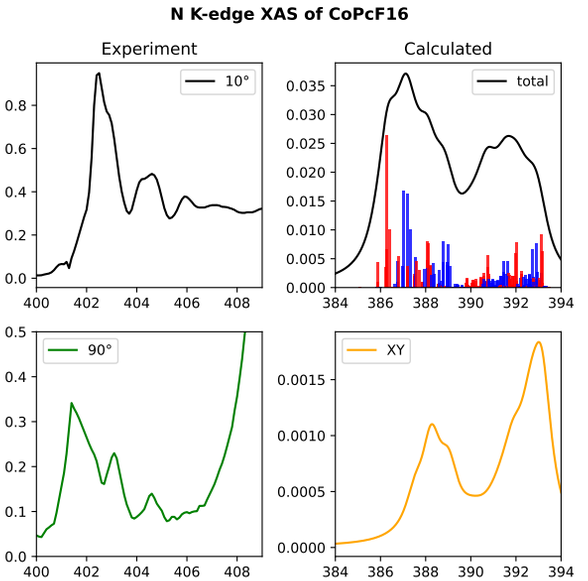

Figure 8 Experimental and calculated N K-edge spectra for CoPcF16 with ${}^2E_g$ symmetry. The transitions originating from $\mathbf{N_{aza}}$ and $\mathbf{N_{pyr}}$ are denoted with red and blue bars, respectively. The experimental curves of CoPcF16 on Ni(111) were taken from a previous study Balle *et al.*[1]

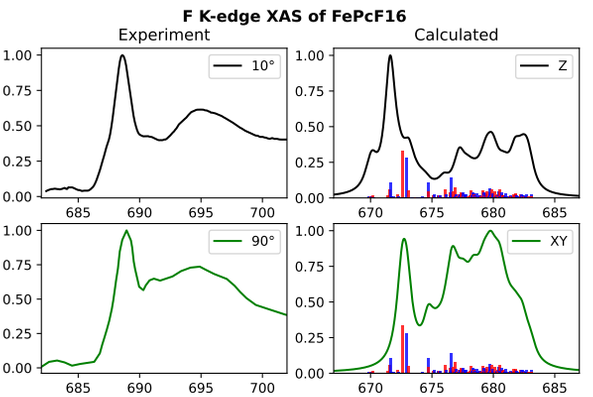

Figure 9 Experimental and calculated F K-edge spectra for FePcF16. Only one 1s orbital per fluorine-type ($\mathbf{F_{inner}}$ and $\mathbf{F_{outer}}$) has been taking into account. The experimental results were taken from a previous study on Cu(111) surfaces.[5]

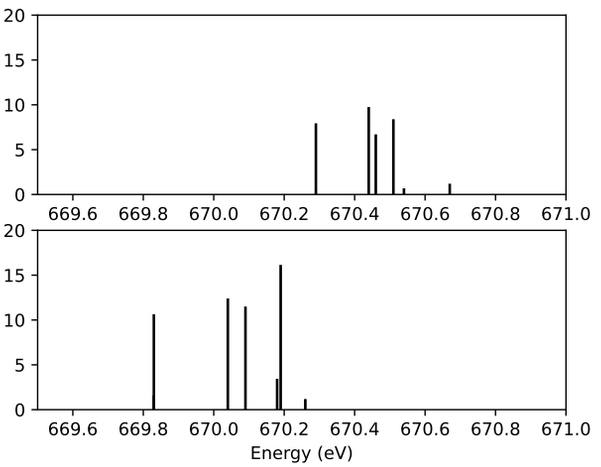

Figure 10 Calculated fluorine K-edge of CoPcF16 (top) and FePcF16 (bottom). Only the lowest energy transitions are shown.

3 Nitrogen K-edge

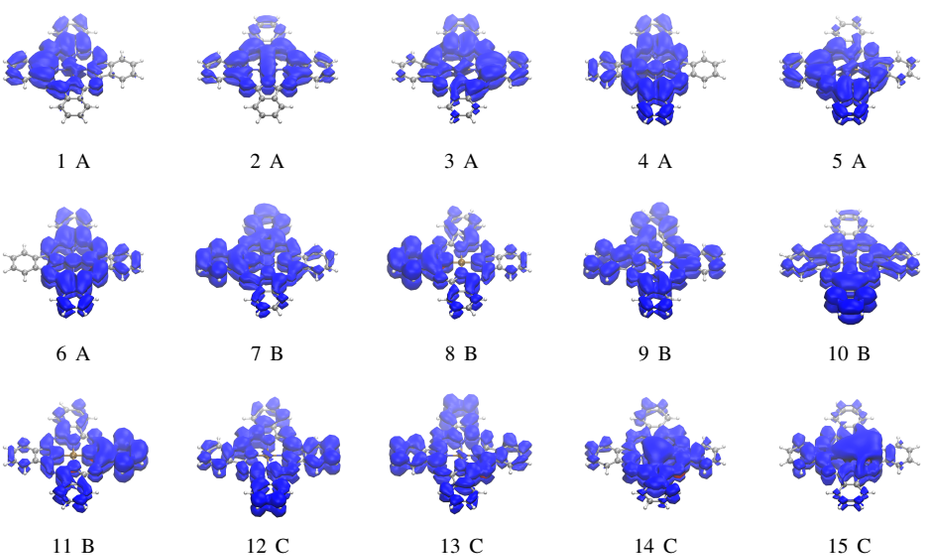

Figure 11 Natural difference orbitals (NDOs) for the nitrogen K-edge of CoPc.

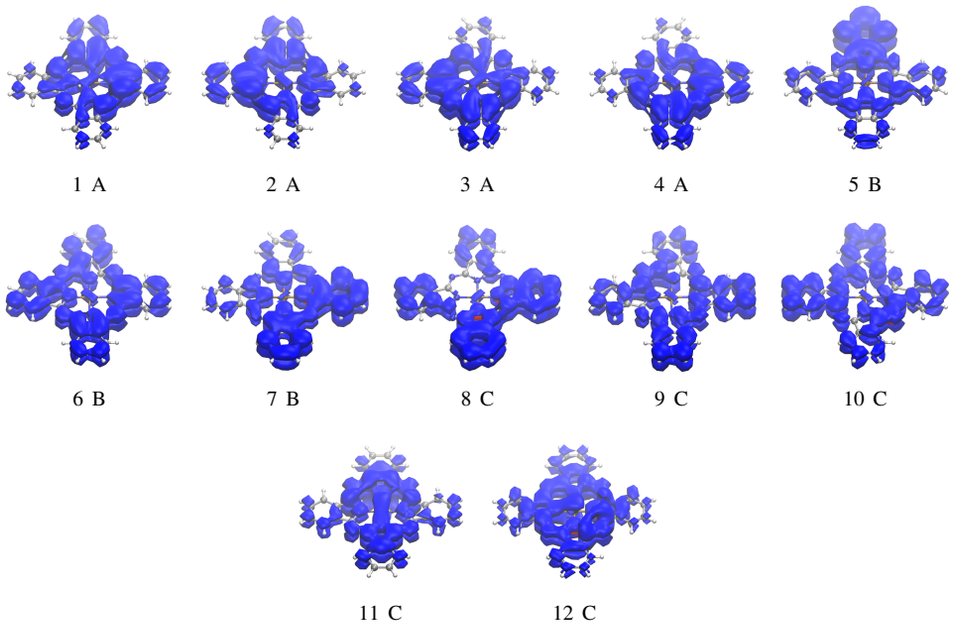

Figure 12 Natural difference orbitals (NDOs) for the nitrogen K-edge of FePc.

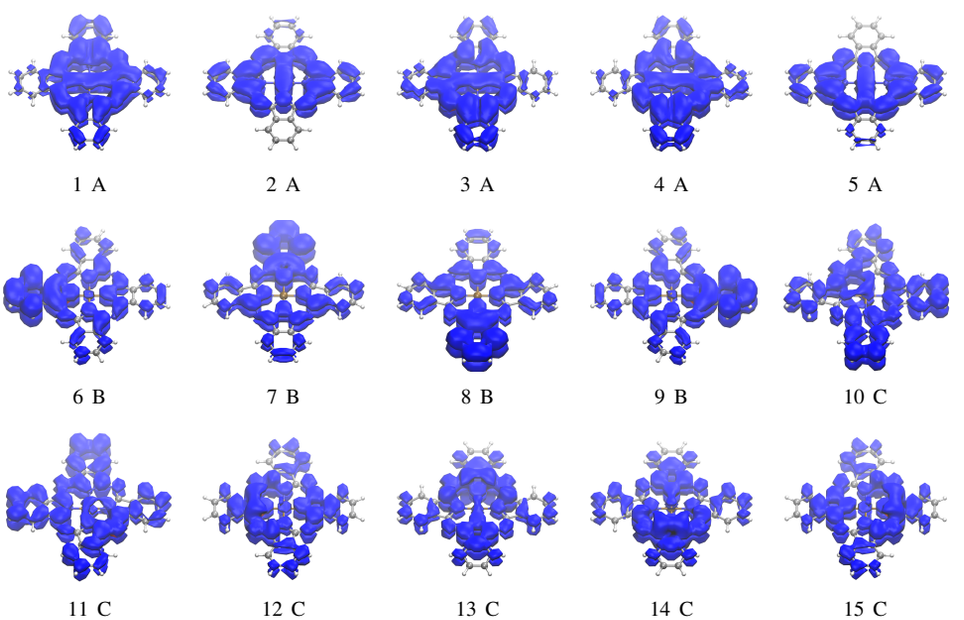

Figure 13 Natural difference orbitals (NDOs) for the nitrogen K-edge of MnPc.

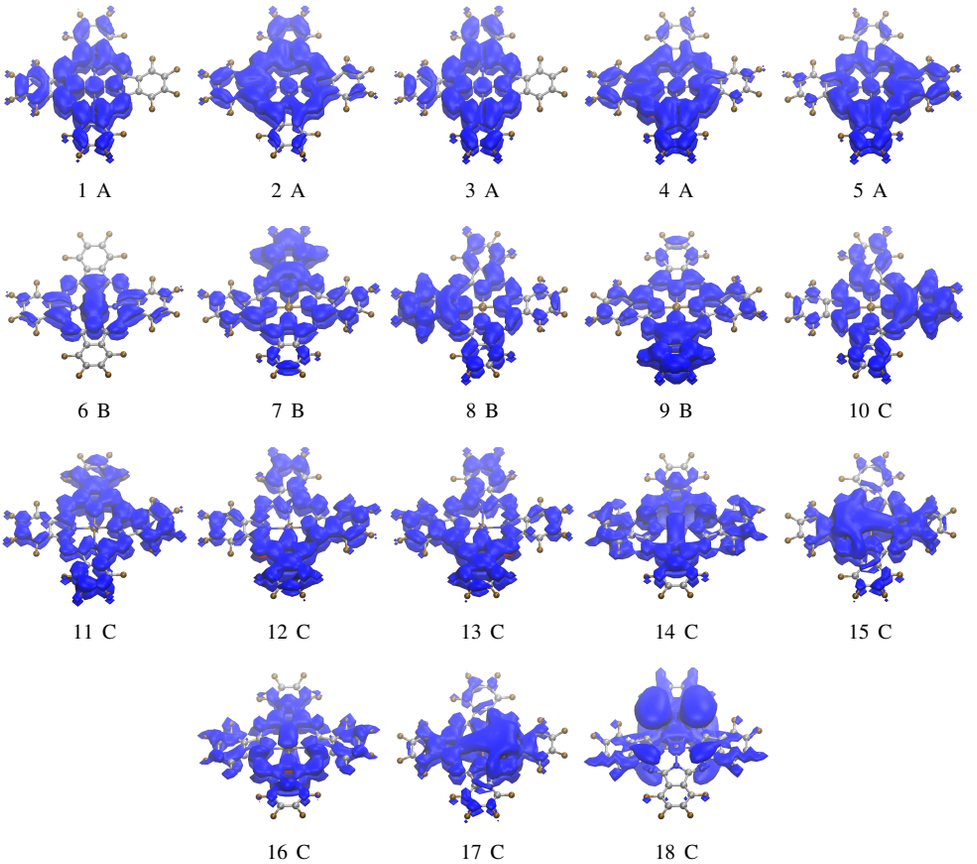

Figure 14 Natural difference orbitals (NDOs) for the nitrogen K-edge of CoPcF16.

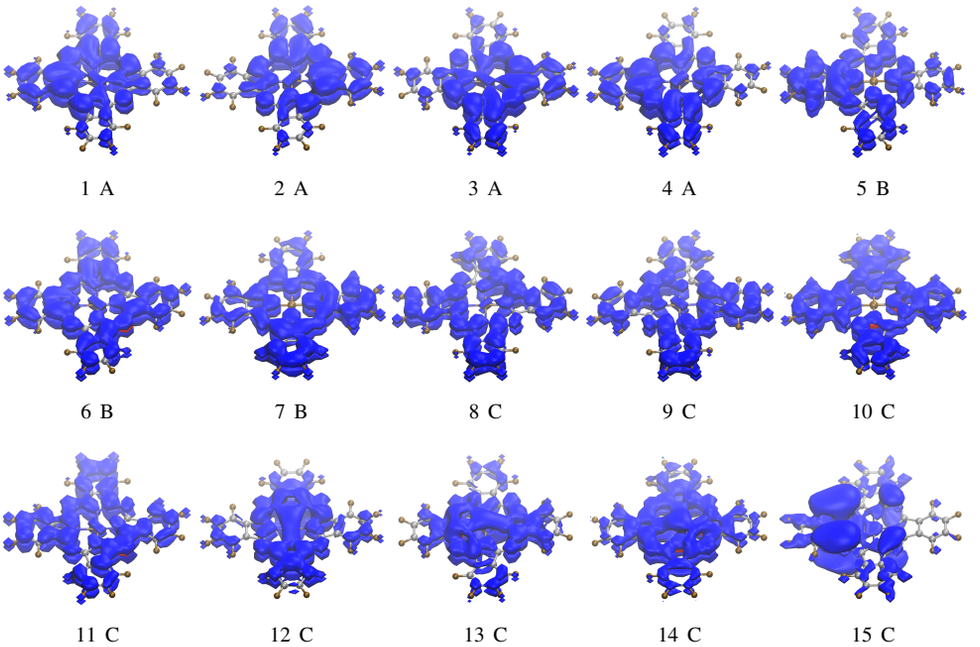

Figure 15 Natural difference orbitals (NDOs) for the nitrogen K-edge of FePcF16.

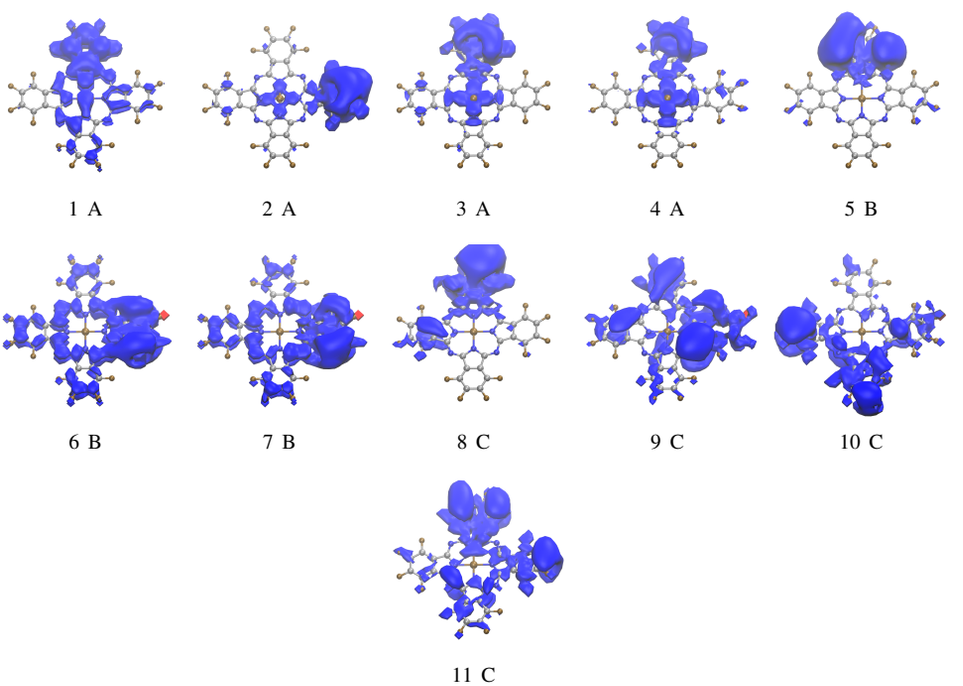

Figure 16 Natural difference orbitals (NDOs) for the fluorine K-edge of CoPcF16.

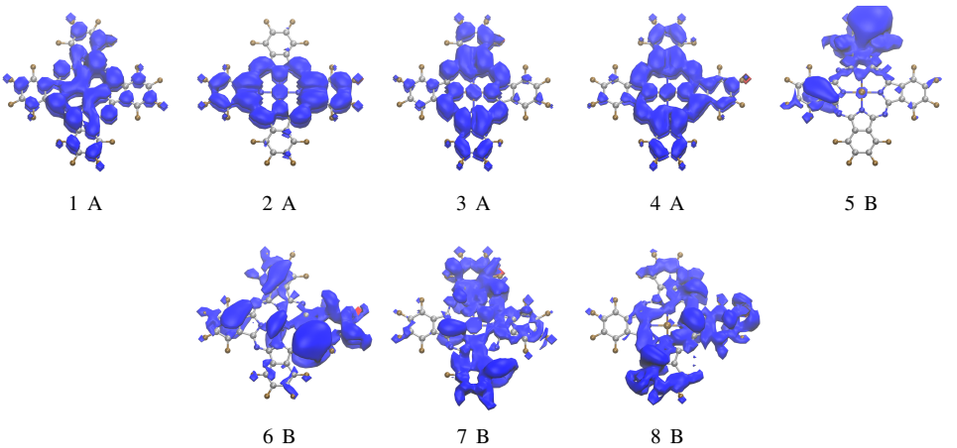

Figure 17 Natural difference orbitals (NDOs) for the fluorine K-edge of FePcF16.

4 Transition metal L-edge

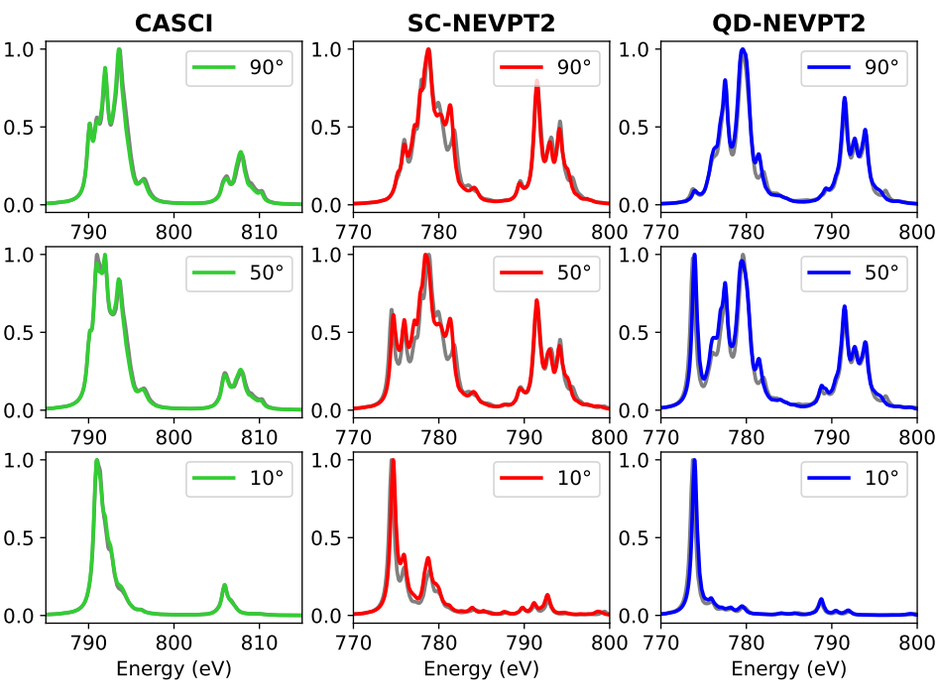

Figure 18 Calculated Co L-edge XAS of CoPcF16 (along with CoPc spectra in grey) for comparison.

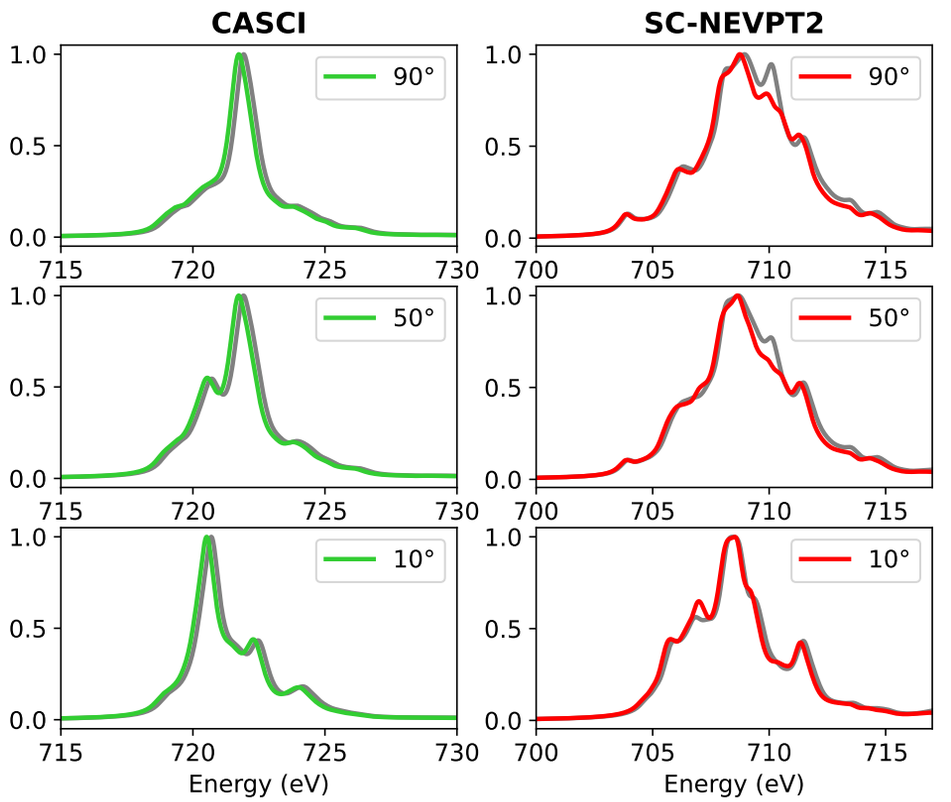

Figure 19 Calculated Fe L-edge XAS of FePcF16 (along with FePc spectra in grey) for comparison.

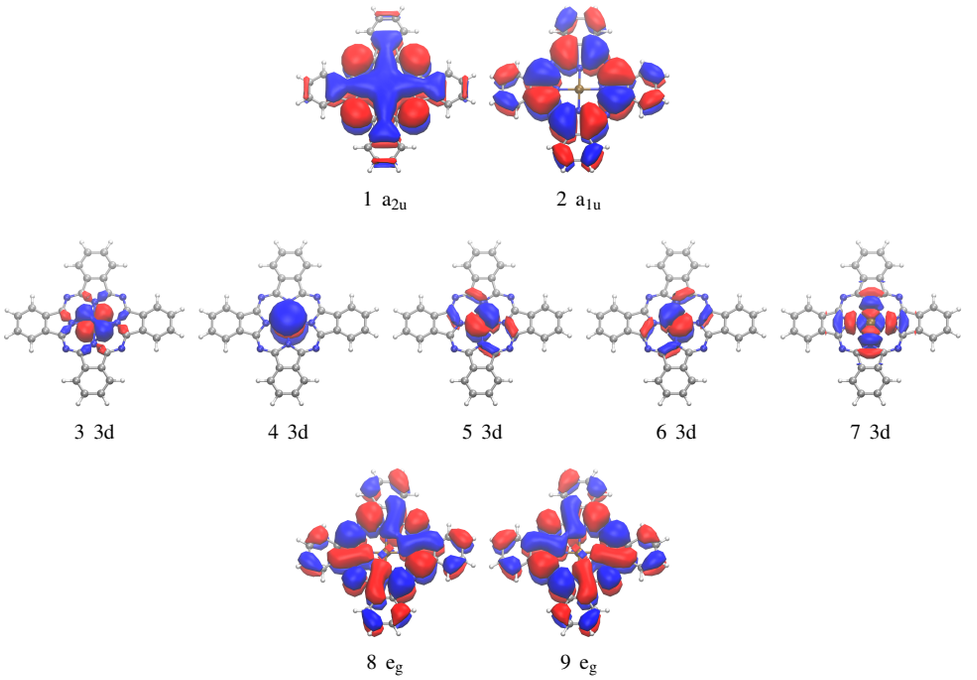

Figure 20 Active orbitals of the extended active space. Gouterman-like ligand orbitals as well as metal based 3d orbitals are included in the active manifold.

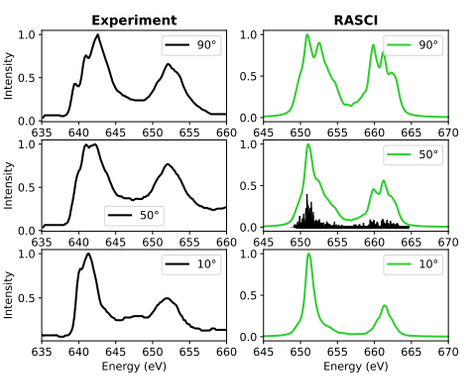

Figure 21 Experimental and calculated Mn L-edge XAS for MnPc. The experimental results were adapted from a previous study on Ag(111) surfaces.[6]

5 Example input block for TDDFT calculations

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%tddft NRoots 500
XASLoc[0] = 5,12
XASLoc[1] = 5,12
OrbWin[0] = 5,12,-1,-1
OrbWin[1] = 5,12,-1,-1
DoQuad True
TDA True
end
```

6 Example input block for CASCI/NEVPT2 calculations

```
%casscf
nel 13
norb 8
mult 4,2
nroots 40,115
TrafoStep RI
MaxIter 1
rel dosoc true end
PTMethod SC_NEVPT2
PTSettings
QDtype 3
end
end
```

7 Example configuration space for RASCI calculations

```
%casscf
nel 16
norb 12
mult 5,3,1
nroots 200,200,200
TrafoStep RI
rel dosoc true
dodtensor false
end
maxiter 1
refs
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8 XYZ coordinates

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C	-2.75252143119075	-1.11310338753599	-0.00031247027121
C	-2.75396440818147	1.11392519998125	-0.00029830766715
C	-1.11421709766337	2.75392058396862	-0.00032659174286
C	1.11277918816089	2.75244004520974	-0.00029020156432
C	4.14653941033955	0.69863298399871	-0.00011758693264
C	4.14645012940469	-0.70223874336906	-0.00013927774573
C	0.70215372453563	-4.14682025104444	-0.00013763703790
C	-0.69872976761546	-4.14691577392334	-0.00011523695788
C	-4.14653626240210	-0.69902195412293	-0.00013004571559

C	−4.14649546024451	0.70184782844038	−0.00010941937679
C	−0.70215208259611	4.14646084575735	−0.00013336361380
C	0.69872536468819	4.14652005379882	−0.00012972186979
C	5.33793658961799	1.41705781618286	0.00012326931358
C	6.52484725802694	0.69712896945764	0.00028923816977
C	6.52477946996587	−0.70659107063644	0.00025060789466
C	5.33681015677643	−1.42374176960539	0.00003653867936
C	1.42357310094969	−5.33726142029200	0.00006116950425
C	0.70635340801399	−6.52518639195252	0.00026184180933
C	−0.69737482154099	−6.52524529943025	0.00028091977727
C	−1.41723539146686	−5.33826207238707	0.00010136506830
C	−5.33790540567545	−1.41749966097557	0.00008271810580
C	−6.52484925314067	−0.69762131710430	0.00026703294923
C	−6.52483135200696	0.70610266138825	0.00025892199020
C	−5.33689331675129	1.42329915746670	0.00007363178023
C	−1.42352351614197	5.33693781803323	0.00006183815473
C	−0.70627066567950	6.52482499639409	0.00024676026168
C	0.69745241099528	6.52484106537977	0.00026803301216
C	1.41726856218086	5.33784255602610	0.00008500753736
H	5.33271973320394	2.49893181375720	0.00014596072185
H	5.32871105459239	−2.50561231518257	0.00003553054890
H	2.50544401616776	−5.32927863489223	0.00005022892286
H	−2.49909943720310	−5.33292449667697	0.00013457671293
H	−5.33262844475115	−2.49936963693981	0.00008137978811
H	−5.32885591818423	2.50517007029015	0.00010116841015
H	−2.50539504694048	5.32901694043139	0.00006283989166
H	2.49913217724629	5.33246248105765	0.00011310995963
H	7.47013997729430	1.22534608656610	0.00048218598043
H	7.46953184246570	−1.23558551023121	0.00042068739535
H	1.23532308220156	−7.46995200970030	0.00041594053531
H	−1.22563259663811	−7.47051587863805	0.00046778635690
H	−7.47012028879009	−1.22587860318798	0.00042617929873
H	−7.46960816900623	1.23505308106409	0.00043097867598
H	−1.23520533970540	7.46960822613967	0.00040637846172
H	1.22574185135611	7.47009395225740	0.00043676469318
Fe	−0.00003263030626	−0.00018798797547	−0.00062500230057

8.3 MnPc

N	1.94885290431288	−0.00013770397919	0.00030956236231
N	2.38780640354127	−2.37744574139792	0.00022051156257
N	0.00005648420359	−1.96215017176507	0.00037821069778

N	−2.38770231460935	−2.37752410533222	0.00022332299341
N	−1.94888054890581	−0.00022485350644	0.00036430270295
N	−2.38784604848528	2.37708145598923	0.00023476198920
N	−0.00010186479127	1.96178461592909	0.00035221940701
N	2.38767736518723	2.37713617385777	0.00015404917376
C	2.76235336341250	1.12184431205517	0.00017617302178
C	2.76241487691730	−1.12212257960997	0.00021995122377
C	1.12023506927749	−2.76566733042193	0.00026618372391
C	−1.12007431235246	−2.76562294787354	0.00026274723336
C	−2.76236294961763	−1.12222640636679	0.00024841986688
C	−2.76245940509173	1.12175887169900	0.00025121030343
C	−1.12027461120560	2.76531646642832	0.00026444070855
C	1.12004284838330	2.76522455245828	0.00021973881715
C	4.15697343097844	0.69939143713648	0.00001800838789
C	4.15696903807769	−0.69955655489039	0.00005197218162
C	0.70341509031201	−4.14672432811008	0.00015384400760
C	−0.70337708047609	−4.14673395646832	0.00015314405596
C	−4.15698000850561	−0.69977716757416	0.00007752849370
C	−4.15699616121263	0.69917480592808	0.00008632365081
C	−0.70343011431184	4.14635679295502	0.00015651215890
C	0.70336633833194	4.14633490064705	0.00013721447025
C	5.34585194315615	1.41876323409019	−0.00018213315105
C	6.53615393082941	0.70035403920185	−0.00030994048730
C	6.53613757539471	−0.70053750164261	−0.00025614715179
C	5.34583336912932	−1.41893208093276	−0.00009375539420
C	1.42194449293582	−5.34368635493051	−0.00000450758058
C	0.70402092686346	−6.52660361995509	−0.00014216104520
C	−0.70433467578411	−6.52658776493423	−0.00014213893055
C	−1.42210358810677	−5.34356136692100	−0.00000004603614
C	−5.34581743216974	−1.41920516050610	−0.00013148392944
C	−6.53614750115444	−0.70084862853474	−0.00032562068794
C	−6.53617504746199	0.70003890540354	−0.00031234652571
C	−5.34590054621605	1.41848186342580	−0.00011362060238
C	−1.42190887254341	5.34335446306405	0.00003380194248
C	−0.70393715557882	6.52624168777465	−0.00011288508577
C	0.70441642789170	6.52617552155803	−0.00012826484443
C	1.42213878803907	5.34312487365252	−0.00001962442265
H	5.33881815158168	2.50063722278337	−0.00021760850122
H	5.33873101216119	−2.50080291289221	−0.00006608303681
H	2.50379651943813	−5.33799445526684	−0.00000505850047
H	−2.50395281613874	−5.33765281285098	−0.00000835957852
H	−5.33874219541903	−2.50108080963917	−0.00014922427475

H	−5.33890545368547	2.50035628955877	−0.00012195385936
H	−2.50376038833766	5.33773033350272	0.00003705022477
H	2.50398686404755	5.33715714629356	−0.00004398579469
H	7.48025405147707	1.23054334194374	−0.00044940200469
H	7.48022615455029	−1.23075047319436	−0.00037081880284
H	1.23109080769132	−7.47250812491849	−0.00026004930498
H	−1.23145143757097	−7.47246640317011	−0.00026023429329
H	−7.48022667966855	−1.23107229651628	−0.00049294108265
H	−7.48027760010111	1.23022392248919	−0.00047954159109
H	−1.23097130090558	7.47216515481220	−0.00020332736008
H	1.23157092417368	7.47203260118240	−0.00024659168833
Mn	−0.00003704188853	−0.00016637171853	0.00059865018714

8.4 CoPcF16

N	1.92841505816256	−0.00030279957971	−0.16638642313408
N	2.36868406088132	−2.38448739916422	−0.13204946960590
N	0.00001217525767	−1.91328070311633	−0.16370690369063
N	−2.36863754290399	−2.38436959499222	−0.13193133381107
N	−1.92843674022866	−0.00015743309321	−0.16629983273148
N	−2.36868626165874	2.38405424140041	−0.13199788887337
N	−0.00004179392645	1.91283635878504	−0.16376010918178
N	2.36861102574798	2.38390703109109	−0.13194273319341
C	2.73727356330004	1.10642703716175	−0.13680662388353
C	2.73733044570195	−1.10700963510001	−0.13645803061048
C	1.11554382642851	−2.73142283621758	−0.13711184159599
C	−1.11551751654463	−2.73134756719060	−0.13666331918158
C	−2.73730612037416	−1.10689101029515	−0.13677913011717
C	−2.73731402705962	1.10657011290545	−0.13637893141192
C	−1.11554940730986	2.73099760233623	−0.13711512607899
C	1.11549901683810	2.73088745232912	−0.13669215089226
C	4.12533740258543	0.70272315325002	−0.07878775485604
C	4.12545787338931	−0.70319893673017	−0.07909362380265
C	0.69915148809078	−4.13383698826185	−0.08392955899863
C	−0.69914119947022	−4.13384965185734	−0.08423540876741
C	−4.12536330250366	−0.70314529999502	−0.07874347792804
C	−4.12543967068509	0.70278449964731	−0.07904558280345
C	−0.69913466136344	4.13340334481943	−0.08397296227466
C	0.69915854673446	4.13340046180889	−0.08423573292117
C	5.31483135128159	1.40825234106195	0.01673142538901
C	6.50620010370781	0.69788324325260	0.12712992128371
C	6.50631000911183	−0.69803578755652	0.12701336024375

C	5.31503571938691	-1.40856644083460	0.01656426336306
C	1.40631252479636	-5.31640311881151	0.00842506302114
C	0.69503190506378	-6.51386113590278	0.11643059595107
C	-0.69511650269095	-6.51381388707565	0.11650173279608
C	-1.40635119193181	-5.31631142624570	0.00852137364961
C	-5.31490825222710	-1.40860493021171	0.01669764841111
C	-6.50624621649807	-0.69818114791056	0.12708601776568
C	-6.50629309270645	0.69773563398395	0.12704532456178
C	-5.31498218399754	1.40820608230817	0.01662074702296
C	-1.40628688292659	5.31598041743527	0.00833665778161
C	-0.69499556006085	6.51342889377372	0.11638082459996
C	0.69515360795221	6.51336167908851	0.11656514549938
C	1.40637922142202	5.31584995794296	0.00861244699456
F	5.36230839309944	2.73750960585600	0.02110401298845
F	5.36269984594574	-2.73781845557393	0.02067661333642
F	2.73422893142659	-5.36587284128574	0.01331710604933
F	-2.73426733323479	-5.36572660312016	0.01343601997204
F	-5.36248851705732	-2.73786339770833	0.02097173549481
F	-5.36257796293413	2.73746276837679	0.02080802837190
F	-2.73420280513160	5.36547603742521	0.01311972696537
F	2.73429558132762	5.36525001932908	0.01362480856722
F	7.66338721569730	1.35105967782632	0.24476272359334
F	7.66358511082836	-1.35107422831948	0.24450088244608
F	1.35240266216110	-7.66741349652608	0.23117695226573
F	-1.35254577763371	-7.66732613417762	0.23128283869641
F	-7.66346037053662	-1.35131966831426	0.24467065531844
F	-7.66353272317084	1.35082643122289	0.24456637475449
F	-1.35235289697330	7.66700021292111	0.23105925789399
F	1.35258643074855	7.66686553414996	0.23140854074002
Co	-0.00004658333515	-0.00023327632114	-0.18102487544278

8.5 FePcF16

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N	2.39667186952585	-2.39687551238573	-0.00032884287411
N	0.00310607681533	-1.94411593735907	-0.00017646164220
N	-2.39000073773558	-2.39020263565171	0.00004337767127
N	-1.94391311433227	0.00290386589616	0.00035067476551
N	-2.39667077556495	2.39646778313845	0.00042188885390
N	-0.00310693124608	1.94370962254697	0.00035072340908
N	2.38999919074555	2.38979652530156	0.00004393080286

C	2.76236772044550	1.12007032694080	0.00003966420687
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C	1.12561561404412	-2.76665241663621	-0.00026299109428
C	-1.12027407472486	-2.76257113539207	0.00003872175438
C	-2.76236733801797	-1.12047529759790	0.00006675901819
C	-2.76644957504488	1.12541412855581	0.00037270998730
C	-1.12561699930510	2.76624602294144	0.00037233830327
C	1.12027235455829	2.76216351801817	0.00006667789737
C	4.16319092383346	0.70716183662350	0.00010624074167
C	4.16462179505192	-0.71320282851445	-0.00012941203991
C	0.71299888214132	-4.16482556799938	-0.00013100542857
C	-0.70736605507465	-4.16339448021233	0.00010441864325
C	-4.16319061835931	-0.70756757638470	-0.00006448822524
C	-4.16462161134580	0.71279651176306	0.00017164615025
C	-0.71299909669485	4.16441788677337	0.00017054630266
C	0.70736475440143	4.16298664706754	-0.00006536864560
C	5.36681420570375	1.42770378032389	0.00027115906376
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C	5.36838493424025	-1.43700473729945	-0.00017195352870
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C	0.71373351378679	-6.57650704561858	-0.00000733274774
C	-0.70201188964730	-6.57484186111287	0.00021063327592
C	-1.42790796279108	-5.36701788915132	0.00026843346923
C	-5.36681404505655	-1.42810888269509	-0.00029619038973
C	-6.57463751390834	-0.70221227864896	-0.00030307073042
C	-6.57630205062342	0.71353291142899	-0.00008433946276
C	-5.36838392302842	1.43659961312048	0.00014818465568
C	-1.43680173380569	5.36818039599370	0.00014624827505
C	-0.71373448812728	6.57609810205140	-0.00008704969515
C	0.70201064752667	6.57443314465468	-0.00030550688059
C	1.42790683675647	5.36660952792689	-0.00029777085504
F	5.41627239646772	2.75915019953073	0.00049387951638
F	5.41326978830010	-2.76816073540622	-0.00038269029513
F	2.76795660018944	-5.41347389239669	-0.00038485261771
F	-2.75935471864547	-5.41647614471042	0.00049088736852
F	-5.41627327912549	-2.75955566510677	-0.00052738745415
F	-5.41326772945803	2.76775426867008	0.00035245247430
F	-2.76795635044867	5.41306490992751	0.00035029185110
F	2.75935330177894	5.41606797979593	-0.00052887319395
F	7.74226636906939	1.34817298632491	0.00037076564576
F	7.74517659696649	-1.35948894731833	-0.00005010180659

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F    1.35928448064144     -7.74538053729203     -0.00005409099290
F   -1.34837749453536      -7.74247003372037      0.00036627643824
F   -7.74226591953191      -1.34857720336371      -0.00052688493350
F   -7.74517540261769       1.35908401188477      -0.00010518952979
F   -1.35928508287653       7.74497174029930      -0.00010882444853
F    1.34837585093753       7.74206133526552     -0.00053003743954
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