Electronic Supplementary Information (ESI) for *Chem. Commun.*

Nitric oxide coupling mediated by iron porphyrins: the N-N bond formation step is facilitated by electrons and a proton

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Part A: Complete reference for Gaussian-09

Part B: Coordinates of the Optimized Geometries

i. $[(P)Fe(NONO)]^{0}$
ii. $[(P)Fe(NONO)]^{-1}$
iii. $[(P)Fe(NONO)(Im)]_{//}^{0}$
iv. $[(P)Fe(NONO)(Im)]_{//}^{-1}$
v. $[(P)Fe(NONO)(Im)]_{\perp}^{0}$
vi. $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$
vii. $[(P)Fe(NONOH)(Im)]_{\perp}^{0}$
viii. $[(P)Fe(NONHO)(Im)]_{\perp}^{0}$
ix. $[(P)Fe(NOHNO)(Im)]_{\perp}^{0}$
x. $[(P)Fe(NOHNO)(Im)]_{//}^{0}$

Part C:

i. Fig. S1: Contour plots of α-spin orbitals for complexes $[(P)Fe(NONO)(Im)]_{//}^{0}$ and $[(P)Fe(NONO)(Im)]_{//}^{-1}$
ii. Fig. S2: Contour plots of β-spin orbitals for complexes $[(P)Fe(NONO)(Im)]_{\perp}^{0}$ and $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$.
iii. Fig. S3: Calculated spin densities, using the B3LYP/TZVP method, for selected atoms of $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$ and the products **A**-**C** that result from protonation.
iv. Fig. S4: Variation in the SOMO of $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$ upon protonation to give product **C**.

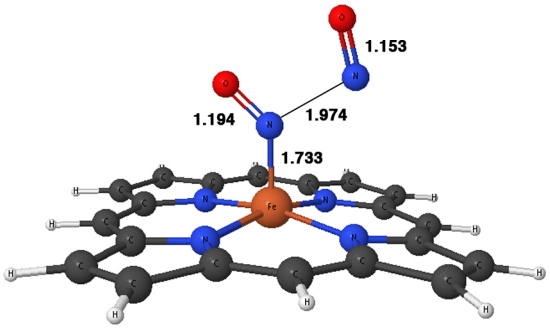
Part A: **Complete reference for Gaussian-09**

Gaussian 09, Revision A.1

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Part B: Coordinates of the Optimized Geometries:

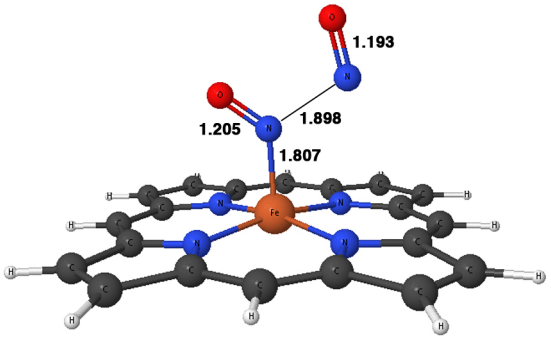
i. $[(P)Fe(NONO)]^0$, E = -2512.670411 Hartree



	X (Å)	Y (Å)	Z (Å)
Fe	-0.073934	0.000408	-0.182056
N	1.574794	-1.12062	-0.47815
C	1.651617	-2.504129	-0.437996
C	3.019222	-2.944087	-0.583562
C	3.781023	-1.820666	-0.728626
C	2.880913	-0.693511	-0.656037
C	3.281331	0.631597	-0.742678
C	2.427421	1.720918	-0.64166
N	1.054823	1.646901	-0.464283
C	0.630296	2.964694	-0.389697
C	1.746743	3.868592	-0.525495
C	2.861129	3.096897	-0.690765
H	3.891063	3.414569	-0.838538
H	1.668901	4.953658	-0.510224
C	-0.691336	3.369828	-0.267089
C	-1.783423	2.513481	-0.263037
N	-1.713656	1.13106	-0.330368
C	-3.033025	0.705733	-0.340424
C	-3.934101	1.832993	-0.299887
C	-3.158373	2.954401	-0.24657
H	-3.472053	3.995482	-0.209022
H	-5.01916	1.757127	-0.313833
C	-3.441809	-0.618791	-0.374556
C	-2.583955	-1.709005	-0.388372
N	-1.199343	-1.632903	-0.38528
C	-0.766253	-2.950059	-0.350672
C	-1.890436	-3.853861	-0.358314
C	-3.018385	-3.084345	-0.38727
H	-4.058081	-3.403761	-0.405314
H	-1.809762	-4.938785	-0.348975
C	0.561157	-3.357736	-0.351349
H	0.758688	-4.431075	-0.329951
H	-4.514811	-0.818462	-0.376924
H	-0.889368	4.442114	-0.217875
H	4.344655	0.832494	-0.884674
H	4.855838	-1.744005	-0.878413
H	3.336467	-3.984773	-0.591746
N	-0.109274	-0.032033	1.550429
O	-0.962137	-0.110746	2.382772
N	1.618477	0.030106	2.502185
O	1.338466	-0.01181	3.619925

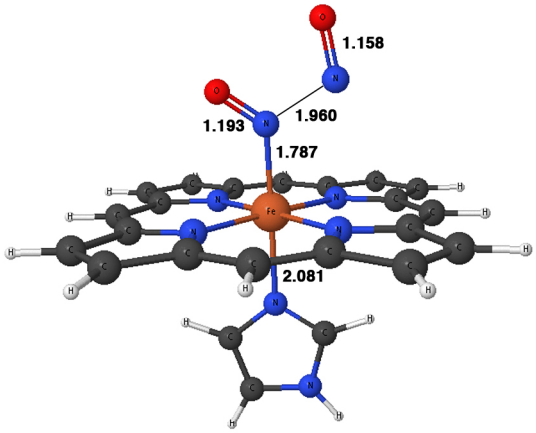
ii. $[(P)Fe(NONO)]^{-1}$: E = -2512.74952 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.07386	0.000003	-0.212198
N	-1.335448	1.409927	-0.476018
C	-1.154787	2.78496	-0.478592
C	-2.419859	3.468619	-0.611071
C	-3.383609	2.501964	-0.689196
C	-2.704646	1.229702	-0.603325
C	-3.345987	0.000449	-0.663461
C	-2.704856	-1.228907	-0.603623
N	-1.335713	-1.409502	-0.476091
C	-1.155433	-2.7846	-0.479056
C	-2.420643	-3.467902	-0.611984
C	-3.384111	-2.500961	-0.69003
H	-4.460786	-2.619911	-0.800722
H	-2.538357	-4.550103	-0.641745
C	0.072624	-3.427803	-0.396476
C	1.303761	-2.785138	-0.347618
N	1.483933	-1.409765	-0.336219
C	2.860255	-1.23079	-0.299238
C	3.543513	-2.502663	-0.298801
C	2.575462	-3.46851	-0.328421
H	2.694654	-4.5509	-0.338764
H	4.625498	-2.623036	-0.279529
C	3.501755	-0.000416	-0.272603
C	2.860559	1.230097	-0.299684
N	1.484302	1.409413	-0.336624
C	1.304456	2.784833	-0.347827
C	2.576329	3.467903	-0.328696
C	3.544129	2.501792	-0.299381
H	4.626155	2.621896	-0.280286
H	2.695766	4.550259	-0.338904
C	0.073449	3.427809	-0.396234
H	0.07393	4.520398	-0.402173
H	4.593944	-0.000553	-0.240649
H	0.0728	-4.520391	-0.402593
H	-4.433801	0.000548	-0.763383
H	-4.460268	2.621244	-0.799628
H	-2.537324	4.550864	-0.640483
N	0.039276	0.000514	1.594844
O	0.982336	0.000244	2.344846
N	-1.617557	-0.00029	2.521468
O	-1.377124	-0.00088	3.689955



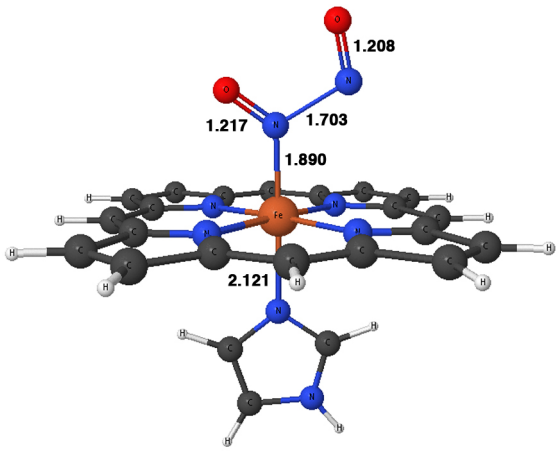
iii. $[(P)Fe(NONO)(Im)]_{//}^{0}$, E = -2738.988492 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.052785	0.000082	-0.175727
N	-1.384652	-1.420189	0.008985
C	-1.187651	-2.786438	0.018425
C	-2.453696	-3.475207	0.148209
C	-3.421602	-2.51369	0.219295
C	-2.747304	-1.235318	0.134699
C	-3.386639	0.000248	0.195821
C	-2.747164	1.23574	0.13473
N	-1.384438	1.420512	0.009555
C	-1.187352	2.786736	0.019227
C	-2.45338	3.475601	0.148644
C	-3.421384	2.514155	0.219285
H	-4.497576	2.641305	0.318079
H	-2.569695	4.557213	0.176509
C	0.047907	3.420712	-0.078937
C	1.277819	2.782955	-0.212611
N	1.472135	1.4169	-0.255109
C	2.828549	1.234561	-0.437036
C	3.503574	2.513056	-0.497507
C	2.542298	3.472397	-0.354064
H	2.65999	4.554174	-0.351983
H	4.575372	2.641581	-0.633547
C	3.465319	0	-0.524354
C	2.828413	-1.234533	-0.437754
N	1.472019	-1.416789	-0.255619
C	1.277506	-2.782819	-0.213839
C	2.541861	-3.472376	-0.355938
C	3.503243	-2.513091	-0.499046
H	4.574986	-2.641711	-0.635429
H	2.659413	-4.554169	-0.354446
C	0.047535	-3.420489	-0.080205
H	0.051364	-4.512251	-0.063317
H	4.546721	-0.000011	-0.673584
H	0.05183	4.512468	-0.061686
H	-4.474177	0.000317	0.29238
H	-4.497771	-2.640774	0.318415
H	-2.570104	-4.556813	0.175928
N	-0.061582	0.000265	-1.958692
O	0.734703	0.000214	-2.846584
N	-1.813305	0.000676	-2.836854
O	-1.548522	0.0008	-3.96436
N	0.231469	-0.000191	1.89795
C	1.401512	-0.000396	2.636781
C	1.097107	-0.001264	3.976146
N	-0.287425	-0.00168	4.040871
C	-0.772559	-0.001037	2.768126
H	-1.828426	-0.001122	2.518004
H	-0.848265	-0.002404	4.886803
H	1.719171	-0.001781	4.863848
H	2.372309	0.000179	2.154298



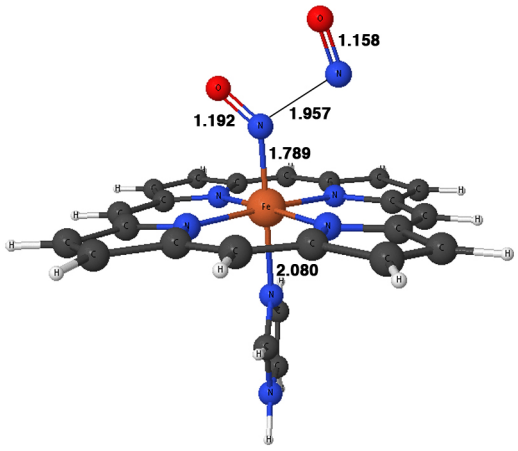
iv. $[(P)Fe(NONO)(Im)]_{//}^{-1}$, E = -2739.052444 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	-0.040701	0.000005	-0.179621
N	1.380995	1.417749	-0.01846
C	1.192748	2.786882	-0.030764
C	2.458967	3.474794	0.096871
C	3.424803	2.51055	0.189195
C	2.745854	1.234554	0.115402
C	3.383862	-0.000008	0.188635
C	2.745836	-1.234563	0.115471
N	1.380978	-1.417746	-0.018403
C	1.192713	-2.786877	-0.030649
C	2.458923	-3.474801	0.097032
C	3.424768	-2.510565	0.189332
H	4.50233	-2.633893	0.288184
H	2.576761	-4.557575	0.104988
C	-0.039209	-3.426057	-0.138565
C	-1.271636	-2.787556	-0.236835
N	-1.460478	-1.417713	-0.249362
C	-2.826968	-1.234808	-0.364789
C	-3.507314	-2.510573	-0.416246
C	-2.540454	-3.475196	-0.338359
H	-2.657888	-4.557892	-0.353101
H	-4.585359	-2.634112	-0.509353
C	-3.466765	0.000023	-0.414089
C	-2.826953	1.234846	-0.364813
N	-1.46046	1.417739	-0.249404
C	-1.271604	2.78758	-0.236915
C	-2.540415	3.475232	-0.338446
C	-3.507286	2.510617	-0.416295
H	-4.585331	2.634164	-0.509393
H	-2.657838	4.557929	-0.353216
C	-0.03917	3.426072	-0.138684
H	-0.038618	4.518948	-0.142858
H	-4.555244	0.000028	-0.511549
H	-0.038669	-4.518934	-0.142702
H	4.472179	-0.000013	0.287787
H	4.502367	2.633869	0.288028
H	2.57682	4.557568	0.10478
N	0.077114	-0.000034	-2.066013
O	-0.859424	0.000048	-2.843186
N	1.605885	-0.000224	-2.817289
O	1.46013	-0.000242	-4.016334
N	-0.196681	0.00004	1.935903
C	-1.346709	-0.000065	2.703968
C	-1.013208	-0.000084	4.038426
N	0.374447	0.000199	4.071457
C	0.825461	0.000173	2.780259
H	1.87455	0.000293	2.498617
H	0.955891	0.000325	4.902426
H	-1.612961	-0.000191	4.942108
H	-2.326469	-0.000179	2.237695



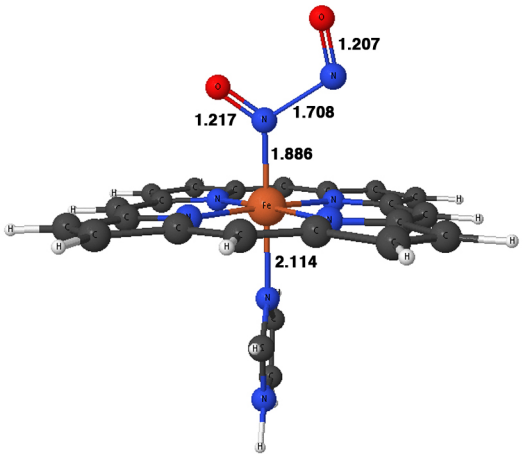
v. $[(P)Fe(NONO)(Im)]_{\perp}^{0}$, E = -2738.988442 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.04454	0.009863	-0.181274
N	1.603318	-1.248102	-0.309461
C	2.938158	-0.910895	-0.410485
C	3.748491	-2.103045	-0.533862
C	2.891275	-3.166469	-0.521757
C	1.555743	-2.626939	-0.383204
C	0.398579	-3.398607	-0.302824
C	-0.888848	-2.903603	-0.106858
N	-1.21595	-1.566635	0.005902
C	-2.572012	-1.529497	0.258091
C	-3.109886	-2.87246	0.3031
C	-2.067666	-3.72456	0.069539
H	-2.07865	-4.811723	0.022475
H	-4.15514	-3.114596	0.484287
C	-3.328553	-0.372557	0.417298
C	-2.841079	0.925502	0.305027
N	-1.526649	1.264576	0.059517
C	-1.498201	2.643271	-0.005431
C	-2.82665	3.182485	0.194393
C	-3.657908	2.117591	0.395149
H	-4.729771	2.120687	0.582389
H	-3.072766	4.242442	0.186
C	-0.350692	3.412845	-0.180616
C	0.946248	2.915261	-0.284221
N	1.293642	1.578778	-0.256206
C	2.668624	1.54335	-0.367661
C	3.199523	2.886671	-0.449391
C	2.131447	3.736792	-0.402904
H	2.128648	4.824131	-0.444588
H	4.256101	3.129996	-0.539933
C	3.439439	0.386574	-0.420731
H	4.520742	0.506872	-0.510629
H	-0.474485	4.497114	-0.216345
H	-4.396035	-0.493298	0.611756
H	0.513391	-4.481899	-0.378267
H	3.125048	-4.226263	-0.601747
H	4.832574	-2.107591	-0.62643
N	-0.107014	0.031965	-1.959391
O	0.661949	0.116342	-2.866911
N	0.257793	-0.006719	1.887636
C	0.263694	1.081195	2.742762
C	0.449003	0.648295	4.033631
N	0.557244	-0.729988	3.94993
C	0.437041	-1.087237	2.639782
H	0.483193	-2.109743	2.280369
H	0.701634	-1.368577	4.725302
H	0.512213	1.179274	4.976494
H	0.135531	2.09147	2.37092
N	-1.876836	-0.093608	-2.784827
O	-1.651165	-0.047639	-3.919788



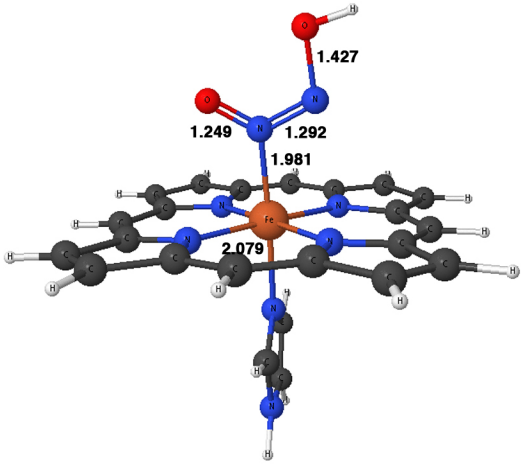
vi. $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$, E = -2739.052594 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.026301	0.01536	-0.182108
N	1.526521	-1.314834	-0.316877
C	2.878463	-1.040447	-0.415968
C	3.637851	-2.266769	-0.51926
C	2.734761	-3.294747	-0.491384
C	1.424572	-2.693969	-0.364817
C	0.234016	-3.411418	-0.272409
C	-1.029548	-2.851324	-0.093925
N	-1.293526	-1.496677	-0.012633
C	-2.655852	-1.398005	0.202507
C	-3.256743	-2.712716	0.25746
C	-2.246831	-3.616512	0.070735
H	-2.304289	-4.703752	0.038665
H	-4.318371	-2.902015	0.409657
C	-3.360941	-0.207874	0.341461
C	-2.809085	1.064931	0.253825
N	-1.46972	1.340743	0.050125
C	-1.377119	2.719356	0.020071
C	-2.68027	3.320127	0.207824
C	-3.569476	2.29175	0.35632
H	-4.646183	2.341158	0.512071
H	-2.87223	4.392192	0.21755
C	-0.1946	3.439046	-0.135613
C	1.075266	2.879997	-0.25393
N	1.348493	1.524175	-0.25666
C	2.723664	1.42443	-0.366782
C	3.323821	2.739275	-0.424079
C	2.299613	3.643981	-0.358711
H	2.350623	4.731712	-0.380214
H	4.392518	2.92828	-0.515141
C	3.438258	0.232887	-0.427279
H	4.525355	0.303118	-0.514854
H	-0.26752	4.529419	-0.149071
H	-4.439523	-0.278383	0.50215
H	0.297769	-4.501073	-0.328638
H	2.921502	-4.365954	-0.55464
H	4.721784	-2.317424	-0.612801
N	-0.140506	0.047104	-2.060799
O	0.771063	0.129066	-2.862584
N	-1.689236	-0.051712	-2.774973
O	-1.574329	-0.018587	-3.976103
N	0.242299	-0.029005	1.920635
C	0.28274	1.038915	2.798044
C	0.455579	0.577844	4.082488
N	0.521087	-0.8041	3.972549
C	0.387739	-1.127135	2.649711
H	0.40084	-2.14178	2.263314
H	0.646273	-1.462323	4.733807
H	0.536411	1.086203	5.037131
H	0.184175	2.057862	2.438029



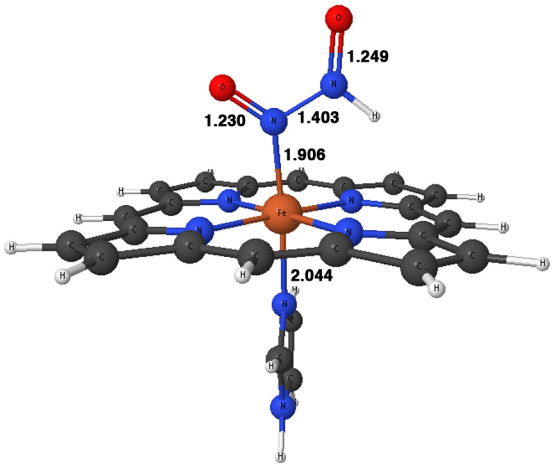
vii. $[(P)Fe(NONOH)(Im)]_{\perp}^{0}$, E = -2379.58364 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.00802	0.019243	-0.128634
N	2.014215	-0.029311	-0.194565
C	2.87412	1.052665	-0.226258
C	4.24257	0.603834	-0.326248
C	4.207708	-0.761689	-0.371724
C	2.817489	-1.148045	-0.288681
C	2.366158	-2.464388	-0.279756
C	1.034479	-2.850545	-0.15635
N	-0.039371	-1.989335	-0.04729
C	-1.151802	-2.795324	0.102929
C	-0.768809	-4.187684	0.092885
C	0.5871	-4.222643	-0.0764
H	1.239847	-5.090763	-0.143029
H	-1.461801	-5.020594	0.19197
C	-2.461447	-2.344496	0.212959
C	-2.851299	-1.012891	0.141504
N	-1.996783	0.063008	-0.004594
C	-2.808411	1.177278	-0.077102
C	-4.198508	0.793398	0.0245
C	-4.224343	-0.56501	0.168945
H	-5.086734	-1.21974	0.275065
H	-5.03535	1.488105	-0.009669
C	-2.363744	2.490904	-0.188088
C	-1.028354	2.880398	-0.214667
N	0.052559	2.024277	-0.155355
C	1.173134	2.833308	-0.191779
C	0.787349	4.222677	-0.258401
C	-0.578741	4.252161	-0.280013
H	-1.237133	5.116356	-0.340569
H	1.484636	5.056658	-0.299987
C	2.48838	2.386894	-0.200231
H	3.276794	3.140704	-0.23603
H	-3.119567	3.276478	-0.243593
H	-3.245957	-3.09478	0.327847
H	3.114027	-3.254869	-0.366265
H	5.038642	-1.458503	-0.46207
H	5.107543	1.261916	-0.373366
N	0.000319	0.044611	-2.109291
O	0.768296	0.773944	-2.771975
N	-0.871995	-0.760682	-2.617874
O	-0.810041	-0.675725	-4.040843
N	0.102122	0.05604	1.948008
C	-0.614944	0.868619	2.808166
C	-0.253292	0.590396	4.104248
N	0.700254	-0.410157	4.017045
C	0.888529	-0.70633	2.700254
H	1.580943	-1.457368	2.335016
H	1.179752	-0.851055	4.795375
H	-0.577401	1.002223	5.053027
H	-1.334449	1.588924	2.435227
H	-1.507537	-1.319849	-4.268683



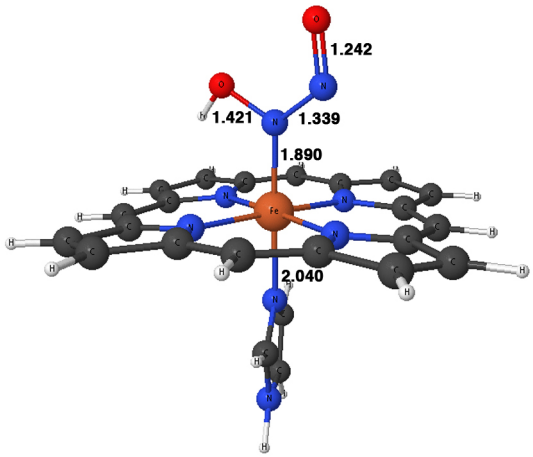
viii. $[(P)Fe(NONHO)(Im)]_{\perp}^{0}$, E = -2379.586474 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.037824	0.015668	-0.152771
N	1.720186	-1.069905	-0.217951
C	3.016366	-0.595076	-0.248307
C	3.952515	-1.693474	-0.341141
C	3.212377	-2.840224	-0.382695
C	1.822527	-2.444153	-0.305376
C	0.751478	-3.333621	-0.286764
C	-0.588036	-2.976686	-0.154235
N	-1.059398	-1.680265	-0.056849
C	-2.426308	-1.793	0.130628
C	-2.818546	-3.184207	0.143849
C	-1.679651	-3.917321	-0.038224
H	-1.572099	-4.998932	-0.088687
H	-3.839683	-3.538258	0.268794
C	-3.309348	-0.721346	0.241694
C	-2.953288	0.623103	0.164519
N	-1.664545	1.094377	-0.017651
C	-1.777394	2.47122	-0.081654
C	-3.16122	2.868289	0.050937
C	-3.889841	1.72362	0.209876
H	-4.964806	1.616473	0.33869
H	-3.514173	3.897261	0.027675
C	-0.710635	3.3573	-0.200341
C	0.633346	2.99668	-0.233183
N	1.113936	1.703841	-0.178885
C	2.489553	1.813703	-0.216576
C	2.881767	3.204343	-0.278278
C	1.730469	3.938103	-0.295275
H	1.615672	5.01883	-0.347759
H	3.910556	3.555974	-0.316827
C	3.379797	0.746277	-0.226346
H	4.445489	0.979915	-0.260724
H	-0.946029	4.422227	-0.248638
H	-4.367511	-0.953891	0.374624
H	0.981761	-4.398034	-0.363621
H	3.559055	-3.868388	-0.464542
H	5.034003	-1.582638	-0.382627
N	0.038981	0.040488	-2.058483
O	0.997693	0.237297	-2.803727
N	-1.189579	-0.196181	-2.693415
O	-1.360424	-0.220071	-3.930417
N	0.138762	0.00371	1.889058
C	-0.05643	1.071572	2.748161
C	0.103726	0.647844	4.045047
N	0.400619	-0.701952	3.960929
C	0.413433	-1.055237	2.64503
H	0.619938	-2.056666	2.283057
H	0.580944	-1.326282	4.740405
H	0.035831	1.169602	4.992608
H	-0.295608	2.060659	2.374789
H	-1.957584	-0.348053	-2.01736



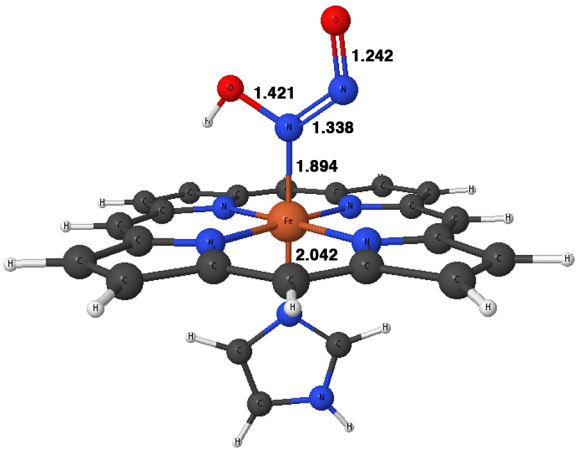
ix. $[(P)Fe(NOHNO)(Im)]_{\perp}^{0}$, E = -2739.581979 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	-0.000598	0.00358	-0.153264
N	-0.04226	-2.005382	-0.165707
C	1.031916	-2.876496	-0.167886
C	0.566555	-4.242949	-0.221522
C	-0.798918	-4.194679	-0.264181
C	-1.171276	-2.799454	-0.220058
C	-2.482732	-2.333632	-0.171466
C	-2.856054	-1.000432	-0.029658
N	-1.986162	0.067333	0.040618
C	-2.77646	1.185712	0.213586
C	-4.172692	0.809942	0.271016
C	-4.223269	-0.544092	0.110377
H	-5.097227	-1.191574	0.082613
H	-4.996056	1.509459	0.398326
C	-2.31431	2.494484	0.275494
C	-0.986739	2.877331	0.11712
N	0.072012	2.012323	-0.060614
C	1.186236	2.80756	-0.233137
C	0.817682	4.205036	-0.159936
C	-0.528451	4.247836	0.067028
H	-1.169679	5.119608	0.177623
H	1.513288	5.034429	-0.269854
C	2.491154	2.347919	-0.392294
C	2.883126	1.012215	-0.372597
N	2.022778	-0.067646	-0.26635
C	2.83605	-1.191288	-0.205563
C	4.225125	-0.805619	-0.281711
C	4.253314	0.557211	-0.394803
H	5.11982	1.209491	-0.481521
H	5.061867	-1.500704	-0.264472
C	2.373239	-2.502728	-0.151147
H	3.118171	-3.300277	-0.139723
H	3.276182	3.098328	-0.503387
H	-3.054676	3.285504	0.407453
H	-3.281547	-3.07577	-0.223898
H	-1.504128	-5.021394	-0.320101
H	1.21415	-5.116919	-0.239942
N	-0.137042	0.072345	-2.036823
O	0.809039	-0.582942	-2.871087
N	-1.19173	0.568712	-2.695752
O	-1.167657	0.49564	-3.935335
N	0.149291	-0.045472	1.880361
C	1.0096	0.684689	2.682086
C	0.794072	0.354116	3.997792
N	-0.21546	-0.593475	3.982631
C	-0.580269	-0.809276	2.688347
H	-1.354723	-1.502352	2.377999
H	-0.619357	-1.052697	4.792549
H	1.254704	0.697811	4.916661
H	1.712481	1.392744	2.258482
H	1.529839	-0.741951	-2.222453



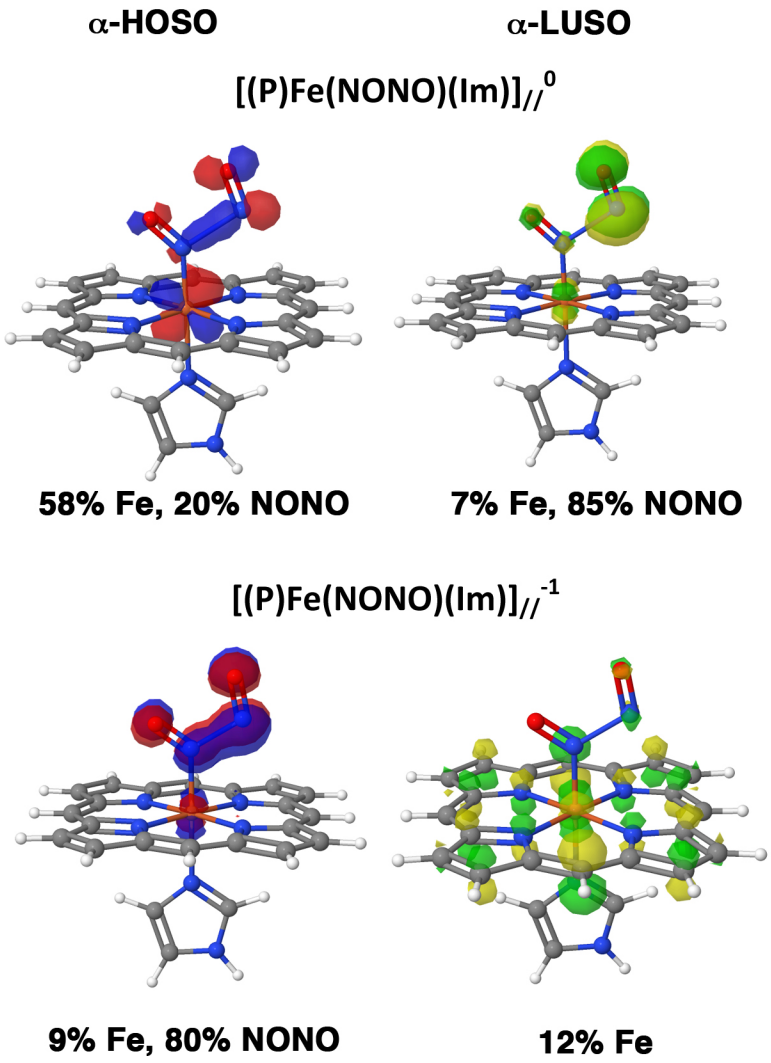
x. $[(P)Fe(NOHNO)(Im)]_{//}^{0}$, E = -2739.581576 Hartree

	X (Å)	Y (Å)	Z (Å)
Fe	0.002929	-0.008413	-0.148733
N	-1.623332	-1.149684	0.070373
C	-1.652801	-2.525899	0.138617
C	-3.018849	-2.995173	0.243223
C	-3.81859	-1.890302	0.228134
C	-2.94248	-0.743802	0.113608
C	-3.379393	0.574992	0.057848
C	-2.54712	1.68417	-0.061522
N	-1.169131	1.636683	-0.117108
C	-0.749874	2.94671	-0.223794
C	-1.889978	3.836996	-0.225045
C	-3.005194	3.054112	-0.125348
H	-4.04908	3.359822	-0.103913
H	-1.828006	4.92049	-0.302871
C	0.572896	3.370971	-0.311023
C	1.690837	2.543843	-0.326564
N	1.662325	1.160076	-0.291557
C	2.991715	0.757968	-0.309398
C	3.861475	1.909022	-0.365989
C	3.055393	3.013623	-0.376728
H	3.346761	4.061188	-0.416817
H	4.947942	1.8628	-0.397403
C	3.417326	-0.567842	-0.286984
C	2.574375	-1.674436	-0.214021
N	1.19576	-1.625847	-0.111308
C	0.778636	-2.939288	-0.033232
C	1.915596	-3.829229	-0.086991
C	3.029455	-3.04569	-0.198339
H	4.070589	-3.352891	-0.270287
H	1.852988	-4.914779	-0.049792
C	-0.541613	-3.359912	0.090132
H	-0.72017	-4.435492	0.142757
H	4.491176	-0.754331	-0.343631
H	0.748114	4.446875	-0.369798
H	-4.455959	0.75206	0.089557
H	-4.904156	-1.836711	0.274283
H	-3.309134	-4.041872	0.305689
N	-0.146996	-0.097753	-2.034888
O	0.997017	-0.007088	-2.873344
N	-1.268531	-0.428105	-2.685785
O	-1.201645	-0.503786	-3.92384
N	0.148956	0.111088	1.884805
C	1.270667	-0.089991	2.671544
C	0.935247	0.079138	3.992022
N	-0.41559	0.388754	3.995435
C	-0.855257	0.3981	2.708463
H	-1.87659	0.610493	2.411335
H	-0.985709	0.577469	4.813761
H	1.517137	0.009574	4.903721
H	2.229793	-0.34464	2.235762
H	1.646134	0.370705	-2.239267

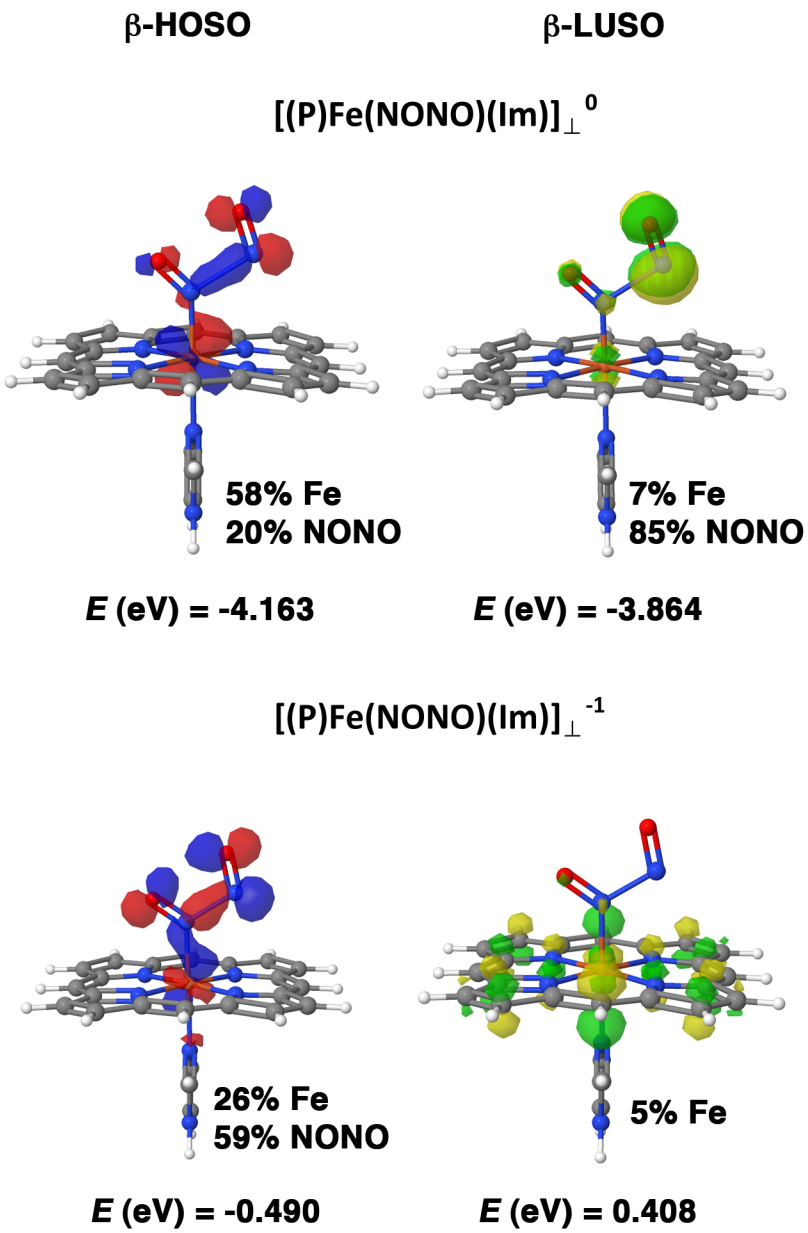


***Part C*:**

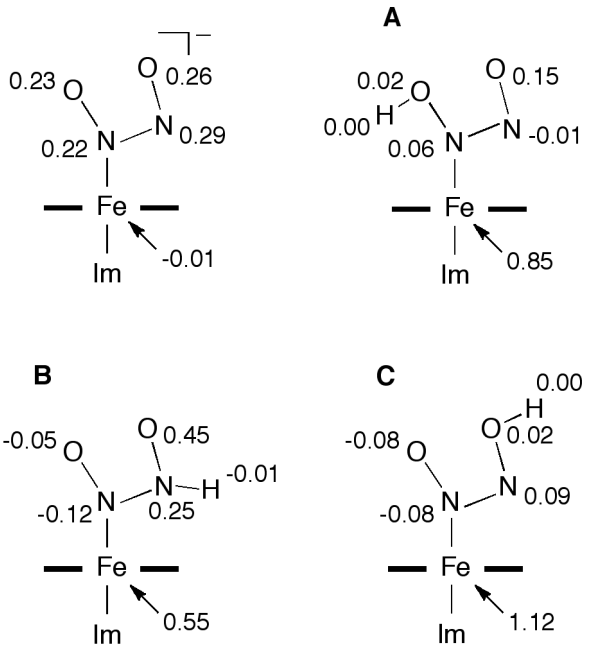
i. Fig. S1: Contour plots of α-spin orbitals for complexes $[(P)Fe(NONO)(Im)]_{//}^{0}$ and $[(P)Fe(NONO)(Im)]_{//}^{-1}$



ii. Fig. S2: Contour plots of β-spin orbitals for complexes $[(P)Fe(NONO)(Im)]_{\perp}^{0}$ and $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$.



iii. Fig. S3: Calculated spin densities, using the B3LYP/TZVP method, for selected atoms of $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$ and the products **A**-**C** that result from protonation.



iv. Fig. S4: Variation in the SOMO of $[(P)Fe(NONO)(Im)]_{\perp}^{-1}$ upon protonation to give product **C**.