Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

for

Photo-induced reversible nitric oxide capture by Fe-M$(CO_2H)_4$ (M= Co, Ni, Cu) as building blocks of mixed metal BTC-based MOFs

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Content

Cartesian coordinates of isolated Fe-M$(CO_2H)_4$ systems as well as their complexes with NO molecule.

Table S1. Comparison of the structural parameters and electronic transition wavelengths of $Cu_2(BTC)_4$ obtained by different DFT methods with experimental values.

	Cu-Cu(Å)	Cu-O(Å)	λ(nm)	λ(nm)
Exp.[1, 2]	**2.50**	**1.94**	**333**	**500**
PBE0	2.50	1.96	317	448
TPSSH	2.47	1.96	308	439
MN12-L	2.45	1.94	302	398
M06-2X	2.48	1.97	321	456
HSE06	2.50	1.95	338	490
BP86	2.52	1.98	346	458
B3LYP	2.54	1.98	324	462

1- K. S. Lin, A. K. Adhikari, Ch. N. Ku, Ch. L. Chiang and H. Kuo, International Journal of Hydrogen Energy. 2012, 37, 13865-13871.

2- H. K. Kim, W. S. Yun, M. B. Kim, J. Y. Kim, Y.S. Bae, J. D. Lee and N. Ch. Jeong, J. Am. Chem. Soc. 2015, 137, 10009–10015.

Table S2. Geometric and electronic properties of the Fe-M $(CO_2H)_4$ (M=Co, Ni, Cu) in their possible spin state configurations.

	2S+1	Fe-O (Å)	M-O (Å)	Fe-M (Å)	∠O-Fe-O (deg)	∠O-M-O (deg)	q_{Fe} (e)	q_M (e)	J (cm^{-1})
Fe-Co$(CO_2H)_4$	doublet	1.93	1.92	2.35	89.95	89.97	0.79	0.77	
	quartet	1.92	1.92	2.43	90.96	89.87	0.85	0.77	$J_{4\leftrightarrow2}$ 1557
	sextet	2.02	1.91	2.53	88.76	89.99	1.25	0.74	$J_{6\leftrightarrow4}$ 3898
	octet	2.02	2.02	2.57	88.92	89.95	1.243	1.094	$j_{8\leftrightarrow6}$ 2606
Fe-Ni$(CO_2H)_4$	singlet	1.96	1.86	2.32	89.96	89.98	0.76	0.75	
	triplet	1.95	1.88	2.44	89.85	89.93	0.80	0.75	$J_{3\leftrightarrow1}$ 5248
	quintet	2.09	1.88	2.50	89.21	90.01	1.22	0.70	$J_{5\leftrightarrow3}$ 1267
	septet	2.00	2.01	2.51	89.13	89.99	1.25	1.01	$J_{7\leftrightarrow5}$ 2538
Fe-Cu$(CO_2H)_4$	doublet	1.93	1.97	2.57	89.39	89.90	0.62	0.58	
	quartet	1.93	1.97	2.57	89.26	89.83	0.69	0.44	$J_{4\leftrightarrow2}$ 7497
	sextet	2.05	1.95	2.72	87.89	89.90	0.92	0.42	$J_{6\leftrightarrow4}$ 62

Table S3. Computed HFC tensors (in MHz) and g-tensors for the Fe and M nuclei of the Fe-M$(CO_2H)_4$ systems in their possible spin state configurations.

				Fe				M			
	2S+1	$g_{\parallel}$	$g_{\perp}$	A^{FC}	A^{PC}	A^{iso}	A	A^{FC}	A^{PC}	A^{iso}	A
Fe-Co$(CO_2H)_4$	2	1.90	2.60	501	350	850	1193, 1139, 275	-401	-150	-552	-458, -458, -686
	4	2.01	2.23	114	76	190	118, 118, 386	122	82	205	139, 218, 219
	6	2.00	2.10	32	13	45	80, 80, -26	77	30	107	90, 90, 142
	8	2.00	2.11	10	9	19	44, 44, -29	46	41	87	-14, 138, 138
Fe-Ni$(CO_2H)_4$	3	1.95	3.80	-78	-280	-358	-513, -513, -46	7	8	15	24, 24, -1
	5	2.03	2.10	-18	-9	-27	-51, -48, 13	-0.5	-0.5	-1	34, -33, -3
	7	2.04	2.09	-12	-3	-15	-25, -25, 4	-19	-19	-38	-43, -43, -28
Fe-Cu$(CO_2H)_4$	2	1.27	2.46	-45	-7	-51	-43, -87, -22	1	18	20	-30,43, 46
	4	1.95	2.05	8	3	11	-6, 21, 21	-1	-6	-7	-15, -15, 8
	6	2.04	2.05	6	2	8	-3, 15, 15	1	5	5	11, 11, 8

Table S4. The electronic excitation parameters, wavelengths λ (nm), oscillator strength (f), and the molecular orbital contributions in the dominant electronic transitions for Fe-Ni$(BTC)_4$ and Fe-Ni$(BDC)_4$ systems.

	λ (nm)	*f*	Major contributions	The character of involved MOs*	Type
Fe-Ni$(BTC)_4$	1530	0.0005	H-4→L+4(%92)	H-4 (%0 Ni, %0 Fe) L+4 (%5 Ni, %66 Fe)	LMCT
	808	0.003	H-1→L+4(%82)	H-1 (%82 Ni, %0 Fe) L+4 (%5 Ni, %66 Fe)	MMCT
Fe-Ni$(BDC)_4$	679	0.001	H-2 → L+2 (%61)	H-2(%0 Ni, %0 Fe) L+2 (%69 Ni, %10 Fe)	LMCT
	479	0.003	H-1→L+2(%69)	H-1(%0 Ni, %85 Fe) L+2 (%69 Ni, %10 Fe)	MMCT

* H and L refer to HOMO and LUMO, respectively.

Table S5. Adsorption enthalpies for different adsorption modes of NO molecule over Fe-M$(CO_2H)_4$ (M=Co, Ni, Cu) systems.

Host systems		Host+ Guest systems 2S+1)		ΔH_{ads}(kcal mol^{-1}) **Fe-site**		ΔH_{ads}(kcal mol^{-1}) **M-site**	
Host systems	(2S+1)	HS	LS	HS	LS	HS	LS
Fe-Co$(CO_2H)_4$	2	3	1	-8.39	-4.44	-7.029	27.67
$[Fe\text{-}Co(CO_2H)_4]^-$	3	4	2	-58.86	-30.23	-50.84	-14.49
Fe-Ni$(CO_2H)_4$	3	4	2	-38.58	-31.45	-12.16	0.78
$[Fe\text{-}Ni(CO_2H)_4]^-$	2	3	1	-18.02	-17.05	-10.42	-
Fe-Cu$(CO_2H)_4$	2	3	3	-8.51	-8.2	7.93	-

*The paramagnetic NO having an unpaired electron can form Low spin (LS) or high spin (HS) complexes with the host system.

Table S6. The calculated HFC tensor (MHz) for nitric oxide.

	A^{FC}	A^{PC}	A^{iso}	A^{SD}	A
NO	10	-5	5	-36, -38, 74	-25, -43, 84

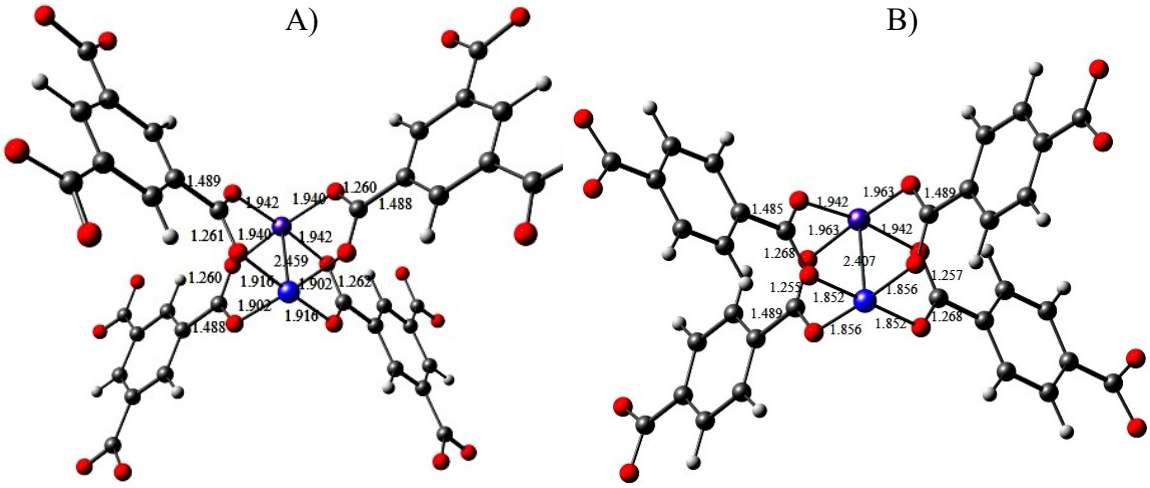

Figure S1. Optimized structure of A) Fe-Ni(BTC)$_4$,B) Fe-Co(BTC)$_4$ and C) Fe-Ni(BDC)$_4$. [color code: violet = Fe, red = O, gray = C, white = H, and dark blue= Ni].

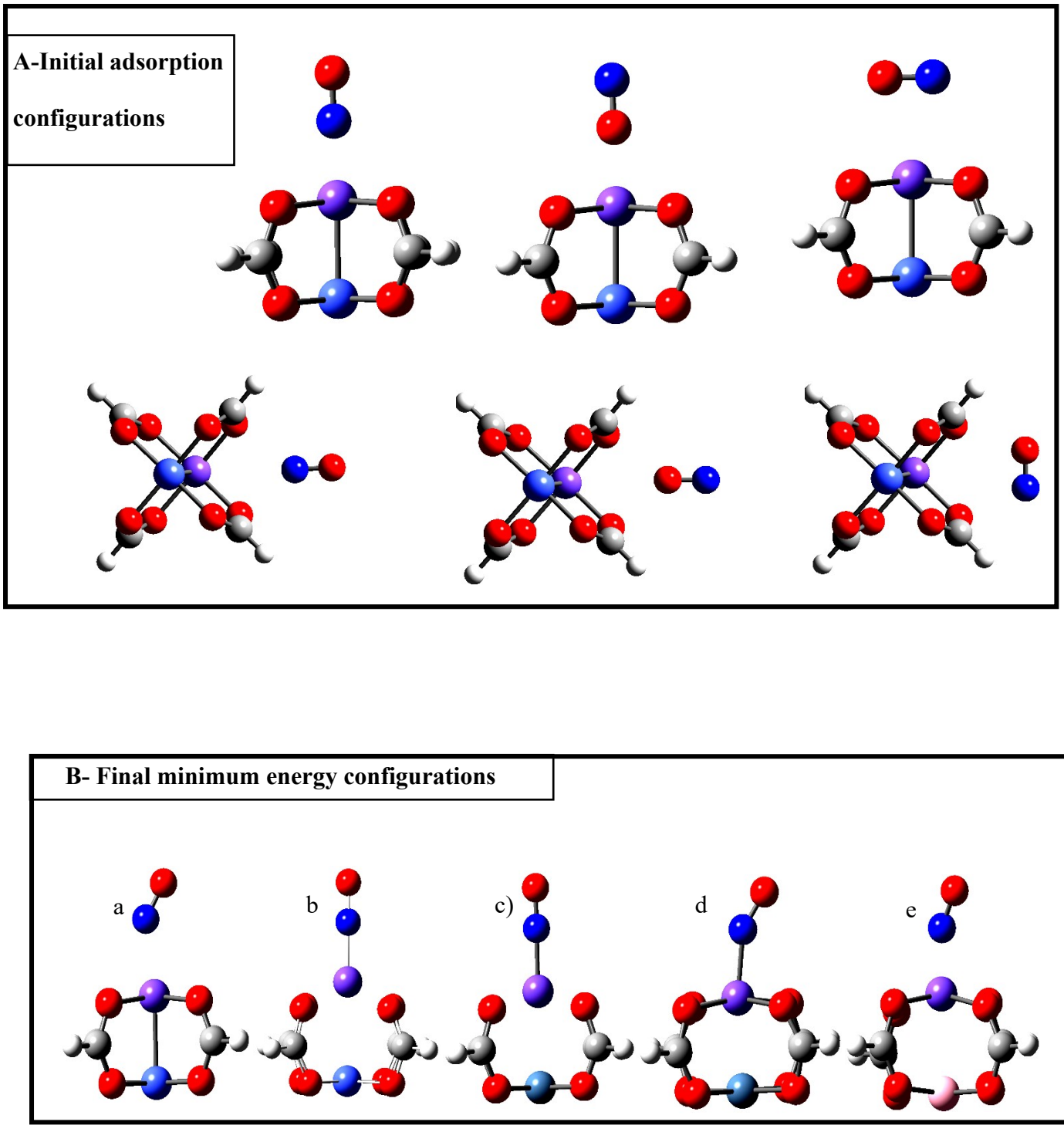

Figure S2. A) Possible orientations for the initial configurations of NO adsorption over Fe-M$(CO_2H)_4$ systems. B) Global minima configurations related to the lowest energy configurations for the adsorption of NO over a) Fe-Co$(CO_2H)_4$, b) [Fe-Co$(CO_2H)_4]^-$, c) Fe-Ni$(CO_2H)_4$, d) [Fe-Ni$(CO_2H)_4]^-$, and e) Fe-Cu$(CO_2H)_4$systems. [color code: red = O, dark blue= N, gray = C, white = H, violet = Fe, blue=Co, pink=Cu and light blue= Ni].

Cartesian coordinates of isolated Fe-M$(CO_2H)_4$ and [Fe-M$(CO_2H)_4$]$^-$ as well as their complexes with NO molecule and also the test systems Fe-Ni$(BTC)_4$ and Fe-Ni$(BDC)_4$.

System	Multiplasity	Energy
Fe-Co$(CO_2H)_4$	Doublet	E= -3402.45 a. u.
Co	0.00000000	0.00000000	1.15655500
Fe	0.00000000	0.00000000	-1.19435500
O	-1.35390600	1.35390500	1.11064100
O	1.35390500	-1.35390600	1.11064100
O	-1.35390600	-1.35390600	1.11064100
O	1.35390500	1.35390600	1.11064100
O	1.36508600	1.36508500	-1.13693900
O	-1.36508500	-1.36508600	-1.13693800
O	1.36508600	-1.36508600	-1.13693900
O	-1.36508500	1.36508600	-1.13693800
C	-1.75629700	1.75629700	-0.00532400
C	1.75629700	-1.75629800	-0.00532400
C	-1.75629700	-1.75629800	-0.00532400
C	1.75629700	1.75629700	-0.00532400
H	2.53168100	-2.53168000	0.00202100
H	-2.53168100	-2.53168000	0.00202100
H	-2.53168100	2.53168000	0.00202100
H	2.53168000	2.53168100	0.00202100
Fe-Ni$(CO_2H)_4$	Triplet	E= -3527.98 a. u.
Ni	0.00003500	-0.06281100	1.90738800
Fe	-0.00003200	2.35388800	1.90745500
O	0.00005300	0.00070000	0.02751100
O	0.00005300	0.00079400	3.78726500
O	1.87991100	0.00070000	1.90736900

O	-1.87984300	0.00079400	1.90736900
O	-1.94821400	2.25456700	1.90747800
O	1.94814800	2.25447600	1.90747800
O	-0.00005400	2.25456700	3.85563700
O	-0.00005400	2.25447500	-0.04072600
C	0.00000200	1.11387600	-0.56040100
C	0.00000200	1.11393700	4.37524300
C	2.46782300	1.11387700	1.90742200
C	-2.46782100	1.11393700	1.90742200
H	-0.00000700	1.06858600	5.47127300
H	3.56385600	1.06859600	1.90742800
H	-0.00000700	1.06859600	-1.65643300
H	-3.56385000	1.06858600	1.90742800

Fe-Cu(CO_2H)$_4$ Doublet E= -3660.16a. u.

Cu	0.00000000	0.00000000	1.22913500
Fe	0.00000000	0.00000000	-1.34430300
O	0.00000000	1.97058300	1.12125900
O	0.00000000	-1.97058300	1.12125900
O	-1.97058300	0.00000000	1.12125900
O	1.97058300	0.00000000	1.12125900
O	1.91345300	0.00000000	-1.12648800
O	-1.91345300	0.00000000	-1.12648800
O	0.00000000	-1.91345300	-1.12648800
O	0.00000000	1.91345300	-1.12648800
C	0.00000000	2.49800000	-0.01395000
C	0.00000000	-2.49800000	-0.01395000
C	-2.49800000	0.00000000	-0.01395000
C	2.49800000	0.00000000	-0.01395000
H	0.00000000	-3.59499000	-0.04772800
H	-3.59499000	0.00000000	-0.04772800
H	0.00000000	3.59499000	-0.04772800
H	3.59499000	0.00000000	-0.04772800

$[Fe\text{-}Co(CO_2H)_4]^-$ Triplet E= -3402.49 a. u.

Co	0.00000000	0.00000000	1.18506500
Fe	0.00000000	0.00000000	-1.18493400
O	0.00000000	1.97370300	1.11350200
O	0.00000000	-1.97370300	1.11350200
O	-1.97370300	0.00000000	1.11350200
O	1.97370300	0.00000000	1.11350200
O	1.98463600	0.00000000	-1.14629200
O	-1.98463600	0.00000000	-1.14629200
O	0.00000000	-1.98463600	-1.14629200
O	0.00000000	1.98463600	-1.14629200
C	0.00000000	2.50910700	-0.00524800
C	0.00000000	-2.50910700	-0.00524800
C	-2.50910700	0.00000000	-0.00524800
C	2.50910700	0.00000000	-0.00524800
H	0.00000000	-3.61415100	-0.00362400
H	-3.61415100	0.00000000	-0.00362400
H	0.00000000	3.61415100	-0.00362400
H	3.61415100	0.00000000	-0.00362400

$[Fe\text{-}Ni(CO_2H)_4]^-$ Doublet E= -3528.07 a. u.

Ni	0.00000000	0.00000000	-1.13154200
Fe	-0.00000100	-0.00000100	1.24136300
O	0.00000100	2.04586300	-1.09566200
O	0.00000100	-2.04586200	-1.09566000
O	2.04586300	0.00000100	-1.09566200
O	-2.04586200	0.00000100	-1.09566000
O	-2.10356100	-0.00000200	1.15168300
O	2.10355800	-0.00000200	1.15168200
O	-0.00000200	-2.10356100	1.15168300
O	-0.00000200	2.10355800	1.15168200
C	0.00001300	2.62395300	0.01252300

C	0.00001300	-2.62395500	0.01252400
C	2.62395300	0.00001300	0.01252300
C	-2.62395500	0.00001300	0.01252400
H	-0.00000800	-3.73161100	-0.01622300
H	3.73160900	-0.00000800	-0.01622200
H	-0.00000800	3.73160900	-0.01622200
H	-3.73161100	-0.00000800	-0.01622300

NO/Fe-Co(CO_2H)$_4$	Triplet	E= -3532.15 a. u.
Co	-0.00095000	-0.00476500	1.05893500
Fe	-0.02123300	-0.00937500	-1.37014700
O	-1.35423600	1.34624200	1.05084700
O	1.34933400	-1.36177400	1.02318900
O	-1.35625300	-1.35716800	1.04532500
O	1.35677500	1.34145800	1.02868400
O	1.35323800	1.37401700	-1.21704100
O	-1.40537100	-1.36324200	-1.19816700
O	1.36038600	-1.36851800	-1.22080700
O	-1.38807000	1.37886200	-1.19462800
C	-1.77171600	1.75336800	-0.05894900
C	1.74864900	-1.76558700	-0.09284300
C	-1.77591800	-1.75919100	-0.06387600
C	1.75709400	1.74715400	-0.08792900
H	2.52007600	-2.54516900	-0.08814500
H	-2.55002000	-2.53593300	-0.04627900
H	-2.55357100	2.52249800	-0.03607000
H	2.54189800	2.51355400	-0.07811900
N	-0.03719500	0.19542700	-3.52168600
O	-0.04409000	-0.37287900	-4.51021100

NO/Fe-Ni(CO_2H)	Quartet	E= -3657.87 a. u.
Ni	-0.00195800	0.06945400	1.90347600
Fe	0.00740500	2.79437700	1.90085600

O	-0.00099400	0.07820100	0.01952900
O	-0.00285800	0.08187100	3.78741800
O	1.88959000	0.06271000	1.90442500
O	-1.89355600	0.07580200	1.90253900
O	-1.99317000	2.31927600	1.89994500
O	2.00473100	2.30545800	1.90267700
O	0.00446900	2.32421900	3.91312700
O	0.00719900	2.32030400	-0.11052400
C	0.00333000	1.17152000	-0.60043800
C	0.00039500	1.17638800	4.40526700
C	2.50228600	1.15798500	1.90390100
C	-2.49866200	1.17527500	1.90094500
H	-0.00049200	1.09863000	5.50061600
H	3.59808600	1.08860200	1.90460600
H	0.00369000	1.09163600	-1.69563400
H	-3.59491600	1.11348000	1.90037800
N	0.01347300	4.57495100	1.89914100
O	0.01718400	5.72304800	1.89807000

NO/Fe-Cu(CO_2H)$_4$	Triplet	E= -3789.86 a. u.
Cu	-1.58147800	0.01571600	0.19968600
Fe	1.07789000	-0.01520100	-0.19952300
O	-1.42180200	-1.94043400	0.22454900
O	-1.38494200	1.96750600	0.12884300
O	-1.25455000	0.06020300	2.12123600
O	-1.84556100	-0.02992700	-1.72548300
O	0.37651700	-0.12681800	-2.04391000
O	0.96093600	0.10991300	1.75304100
O	0.83008900	1.92723200	-0.28409600
O	0.81563200	-1.95121100	-0.04440100
C	-0.30295100	-2.49392100	0.11620100
C	-0.27255100	2.49550200	-0.10342900
C	-0.05764100	0.11041100	2.48427400

C	-0.81287700	-0.10443000	-2.43283700
H	-0.25716600	3.59236000	-0.15642900
H	0.12634300	0.16219300	3.56518800
H	-0.29670500	-3.59093600	0.16773000
H	-0.96912000	-0.15666700	-3.51834400
N	2.85256300	-0.03059400	-0.36955300
O	3.91649900	-0.00379800	0.06274200

NO/[Fe-Co$(CO_2H)_4$]$^-$	Quartet	E= -3532.27 a. u.
Co	0.00727000	-0.01430600	1.07166200
Fe	0.02033700	0.04513300	-1.91514300
O	-1.27822500	1.40945800	1.12590200
O	1.29249900	-1.43936100	1.08121500
O	-1.41747000	-1.29986300	1.07114400
O	1.43173700	1.27003800	1.13571600
O	1.33649700	1.55616300	-1.09137800
O	-1.30305700	-1.49741500	-1.16468600
O	1.54378000	-1.29027000	-1.14712000
O	-1.51046100	1.34909500	-1.10868800
C	-1.77929000	1.77130300	0.02366300
C	1.80298700	-1.75727000	-0.03021200
C	-1.75258200	-1.78356200	-0.04719300
C	1.77636700	1.79772300	0.04040400
H	2.57164600	-2.54873200	0.02884600
H	-2.54302300	-2.55372500	0.00567300
H	-2.54863700	2.55984900	0.10759900
H	2.56614000	2.56510200	0.13057300
N	0.02879400	0.08132600	-3.71444800
O	0.03451400	0.10589300	-4.90757000

NO/[Fe-Ni$(CO_2H)_4$]$^-$	Triplet	E= -3657.81 a. u.
Ni	-0.02527500	0.05539900	1.92601000
Fe	0.01930900	2.53222100	1.83306400
O	-0.16191500	0.01833300	-0.11048600

O	0.11712300	0.10891400	3.95523100
O	2.01233600	0.05851000	1.78218700
O	-2.05599300	0.07895600	2.06282300
O	-1.96109600	2.29648600	1.69186600
O	1.98460500	2.30022900	1.96414100
O	-0.11085500	2.34348500	3.82086600
O	0.16262500	2.24389300	-0.12553900
C	0.00796400	1.11782500	-0.66484000
C	-0.00639800	1.25040100	4.43299500
C	2.54538700	1.17708600	1.88034800
C	-2.55382200	1.20193200	1.86983700
H	-0.03012900	1.33461000	5.53478200
H	3.64970600	1.20981700	1.89868900
H	0.03155300	1.12740100	-1.76951800
H	-3.65691700	1.26581500	1.84502000
N	-0.14230900	4.35192400	1.92428100
O	-0.64550800	5.33869000	2.32002500

Fe-Ni$(BTC)_4$ Triplet E= -5953.80 a. u.

Ni	0.00000000	0.00000000	1.15159000
Fe	0.00000000	0.00000000	-1.30769000
O	6.21866900	-0.23501500	3.60982500
O	-1.91319700	0.09437500	1.08484900
O	0.01813700	1.93497500	-1.17435200
O	1.91319700	-0.09437500	1.08484900
O	-0.01813700	-1.93497500	-1.17435200
O	1.93653300	-0.01013200	-1.15622700
O	-0.09163800	-1.89840500	1.06688100
O	-1.93653300	0.01013200	-1.15622700
O	0.09163800	1.89840500	1.06688100
O	0.21290600	8.00234400	2.62265600
O	8.08525500	-0.08989700	-2.54008300
O	-0.21290600	-8.00234400	2.62265600
O	8.02814900	-0.23599500	2.59959600

O	-0.05643400	-8.09415000	-2.51597700
O	-8.02814900	0.23599500	2.59959600
O	0.05643400	8.09415000	-2.51597700
O	0.00000000	-6.31431800	-3.57616600
O	-6.21866900	0.23501500	3.60982500
O	0.00000000	6.31431800	-3.57616600
O	0.22354400	6.18588200	3.62038700
O	6.29846800	-0.02299400	-3.58771900
O	-0.22354400	-6.18588200	3.62038700
C	0.19466900	6.75593100	2.50603700
C	6.83596400	-0.06784900	-2.45787200
C	-0.19466900	-6.75593100	2.50603700
C	6.78107600	-0.21128300	2.49139400
C	-0.04247600	-6.84423000	-2.44271000
C	-6.78107600	0.21128300	2.49139400
C	0.04247600	6.84423000	-2.44271000
C	-2.50235600	0.06166000	-0.03079200
C	0.06171700	2.49485900	-0.04671800
C	2.50235600	-0.06166000	-0.03079200
C	-0.06171700	-2.49485900	-0.04671800
C	-4.70082700	0.06585600	-1.20811300
C	0.12772200	4.65720700	1.19705200
C	4.70082700	-0.06585600	-1.20811300
C	-0.12772200	-4.65720700	1.19705200
C	4.67373900	-0.13465200	1.19675600
C	-0.05396700	-4.70048600	-1.20774300
C	-4.67373900	0.13465200	1.19675600
C	0.05396700	4.70048600	-1.20774300
H	-4.16653400	0.02920600	-2.15039600
H	0.14951800	4.09598000	2.12404000
H	4.16653400	-0.02920600	-2.15039600
H	-0.14951800	-4.09598000	2.12404000
H	4.11838200	-0.15110000	2.12739100

H	-0.01800700	-4.17259700	-2.15367400
H	-4.11838200	0.15110000	2.12739100
H	0.01800700	4.17259700	-2.15367400
C	-3.99087300	0.08744000	-0.01323300
C	0.08165600	3.98261000	-0.01764600
C	3.99087300	-0.08744000	-0.01323300
C	-0.08165600	-3.98261000	-0.01764600
C	-6.77961900	0.13917700	0.01661600
C	0.11802600	6.77102500	0.03129800
C	6.77961900	-0.13917700	0.01661600
C	-0.11802600	-6.77102500	0.03129800
C	-6.09013700	0.09150900	-1.18808100
C	0.14550000	6.04665700	1.21597500
C	6.09013700	-0.09150900	-1.18808100
C	-0.14550000	-6.04665700	1.21597500
C	6.06320300	-0.16070700	1.20625100
C	-0.07222600	-6.08965700	-1.17810400
C	-6.06320300	0.16070700	1.20625100
C	0.07222600	6.08965700	-1.17810400
C	-6.83596400	0.06784900	-2.45787200
H	-7.86465300	0.15931100	0.02833500
H	0.13222500	7.85605400	0.05043900
H	-0.13222500	-7.85605400	0.05043900
H	7.86465300	-0.15931100	0.02833500
O	-8.08525500	0.08989700	-2.54008300
O	-6.29846800	0.02299400	-3.58771900

$Fe\text{-}Ni(BDC)_4$ Triplet E= -5202.65 a. u.

Ni	0.00000000	0.00000000	1.08112300
Fe	0.00000000	0.00000000	-1.31606500
O	-1.87543200	0.00000200	1.02296200
O	0.00000800	1.94158900	-1.22225500
O	1.87543200	-0.00000200	1.02296200

O	-0.00000800	-1.94158900	-1.22225500
O	1.94152200	-0.00000800	-1.22227000
O	-0.00000300	-1.87541200	1.02297000
O	-1.94152200	0.00000800	-1.22227000
O	0.00000300	1.87541200	1.02297000
C	-2.48769600	0.00000500	-0.08569100
C	0.00000600	2.48771700	-0.08566200
C	2.48769600	-0.00000500	-0.08569100
C	-0.00000600	-2.48771700	-0.08566200
C	-4.70526600	0.00000700	-1.21861700
C	0.00000400	4.62884600	1.19939600
C	4.70526600	-0.00000700	-1.21861700
C	-0.00000400	-4.62884600	1.19939600
C	4.62889100	0.00000200	1.19923700
C	-0.00000100	-4.70535800	-1.21844900
C	-4.62889100	-0.00000200	1.19923700
C	0.00000100	4.70535800	-1.21844900
H	-4.17588600	0.00001100	-2.16256200
H	0.00000600	4.04261500	2.10910300
H	4.17588600	-0.00001100	-2.16256200
H	-0.00000600	-4.04261500	2.10910300
H	4.04271000	0.00000500	2.10897700
H	0.00000000	-4.17603000	-2.16242400
H	-4.04271000	-0.00000500	2.10897700
H	0.00000000	4.17603000	-2.16242400
C	-3.97516400	0.00000400	-0.03161900
C	0.00000400	3.97519400	-0.03149600
C	3.97516400	-0.00000400	-0.03161900
C	-0.00000400	-3.97519400	-0.03149600
C	-6.73611300	-0.00000200	0.05554800
C	-0.00000400	6.73613100	0.05582900
C	6.73611300	0.00000200	0.05554800
C	0.00000400	-6.73613100	0.05582900

C	-6.08714100	0.00000400	-1.17579700
C	0.00000000	6.01059900	1.24380600
C	6.08714100	-0.00000400	-1.17579700
C	0.00000000	-6.01059900	1.24380600
C	6.01064200	0.00000500	1.24356900
C	0.00000300	-6.08723400	-1.17554800
C	-6.01064200	-0.00000500	1.24356900
C	-0.00000300	6.08723400	-1.17554800
H	6.67002200	-0.00000600	-2.08973100
H	6.53480900	0.00001000	2.19239400
H	-6.53480900	-0.00001000	2.19239400
H	-6.67002200	0.00000600	-2.08973100
H	-0.00000700	6.67017100	-2.08944900
H	0.00000000	6.53471400	2.19266000
H	0.00000000	-6.53471400	2.19266000
H	0.00000700	-6.67017100	-2.08944900
C	0.00000900	-8.20588400	0.10244600
C	-8.20585300	-0.00000500	0.10208800
C	-0.00000900	8.20588400	0.10244600
C	8.20585300	0.00000500	0.10208800
O	-0.00002100	8.88100300	1.15892500
O	-0.00000400	8.94652800	-0.90924800
O	-8.88102900	-0.00001400	1.15854000
O	-8.94646100	0.00000200	-0.90963300
O	8.94646100	-0.00000200	-0.90963300
O	8.88102900	0.00001400	1.15854000
O	0.00000400	-8.94652800	-0.90924800
O	0.00002100	-8.88100300	1.15892500