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

Electronic Supplementary Information

Astrochemistry of Transition Metals? The Selected Cases of $[FeN]^+$, $[FeNH]^+$ and $[(CO)_2FeN]^+$]: Pathways toward CH_3NH_2 and HNCO

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```
#
# General Input Orca 2.9.1 for Optimization and Frequency calculations
#
%pal nprocs 2
    end

! UKS B2PLYP SlowConv TightSCF Grid4 NoFinalGrid
! Opt
%scf Maxiter=200
    end

%basis basis TZV
      newgto N "TZV(2d/sp)" end
      newgto C "TZV(2d/sp)" end
      newgto O "TZV(2d/sp)" end
      newgto H "TZV(p/s)" end
      end

* xyz 1 4
Fe       -0.90976        0.33981        0.00000 newgto "TZV(2f/sppd)" end
N         0.77979        0.72132        0.00000
H        -2.42220       -0.07507       -0.00115
*

$new_job
! UKS B2PLYP SlowConv TightSCF Grid4 NoFinalGrid MORead
! NumFreq
%base "FREQ_30_100_200_298_K"
%moinp "OPT.gbw"
%scf Maxiter=200
    end

%freq Temp 30, 100, 200, 298.15
     CentralDiff true
     Increment 0.003
     end

%basis basis TZV
      newgto Fe "TZV(2f/sppd)" end
      newgto N  "TZV(2d/sp)" end
      newgto C  "TZV(2d/sp)" end
      newgto O  "TZV(2d/sp)" end
      newgto H  "TZV(p/s)" end
      end

* xyzfile 1 4
```

```
#
# General Input Orca 2.9.1 for Minimum Energy Crossing Point search
#
%pal nprocs 2
    end

! UKS B2PLYP SlowConv TightSCF Grid4 NoFinalGrid
! Opt SurfCrossOpt
%geom MaxIter 150
     end
%mecp Mult 1
     end
%scf Maxiter=150
    end

%basis basis TZV
      newgto N "TZV(2d/sp)" end
      newgto C "TZV(2d/sp)" end
      newgto O "TZV(2d/sp)" end
      newgto H "TZV(p/s)" end
      end

* xyz 1 3
Fe     -1.390583     -0.081985     -0.022504 newgto "TZV(2f/sppd)" end
N       0.273220      0.182330      0.385391
C      -3.581820     -0.429323     -0.464172
H      -4.633764     -0.589122     -0.695506
H      -3.062602     -1.301273     -0.891282
H      -3.327189      0.520889     -0.959627
H      -3.532170     -0.381105      0.633649
*

$new_job

! UKS B2PLYP SlowConv TightSCF Grid4 NoFinalGrid MORead
! SurfCrossNumFreq
%base "FREQ_30_100_200_298_K"
%moinp "MECP_FREQ_PES2.gbw"
%scf Maxiter=200
    end
%mecp Mult 1
     end

%freq Temp 30, 100, 200, 298.15
      CentralDiff true
      Increment 0.0025
      end
```

```
%basis basis TZV
      newgto Fe "TZV(2f/sppd)" end
      newgto N  "TZV(2d/sp)" end
      newgto C  "TZV(2d/sp)" end
      newgto O  "TZV(2d/sp)" end
      newgto H  "TZV(p/s)" end
      end

* xyzfile 1 3
```

Energies = hartree

Calculated Energies: $[FeN]^+ + CH_4 + H \rightarrow Fe^+ + CH_3NH_2$ M=1

$[FeNH]^+ + CH_4 \rightarrow Fe^+ + CH_3NH_2$ M=2

	Reactants	Reactants	Reactants	Intermedia	Intermedia	Intermedia	Intermedia	TS_I	TS_II	TS_III	Products	Products	Products
M=1	$[FeN]^+$	CH_4	H	$[Fe\text{-}NH\text{-}CH_3]^+$	CH_4***$[FeN]^+$	$[HN\text{-}Fe\text{-}CH_3]^+$	$[H\text{-}Fe\text{-}NH\text{-}CH_3]^+$	C**Fe**N**H	N***CH_3	Fe**H**N	M=2 Fe^+	$CH_3\text{-}NH_2$	$[Fe^{***}NH_2\text{-}CH_3]^+$
E(el)	-1317.80355226	-40.48493205	-0.49861309	-1358.38204185	-1358.32728552	-1358.32702241	-1358.95396751	-1358.28286229	-1358.30287462	-1358.96036541	-1263.09477594	-95.80523172	-1359.02872693
E(ZPE)	0.00127564	0.04534893	0.00000000	0.05365559	0.04772007	0.04694083	0.05980267	0.04535452	0.04836099	0.06007328	-0.00000092	0.06461473	0.06798173
E(vib)	0.00000000	0.00000000	0.00000000	0.00000086	0.00004448	0.00000120	0.00000182	0.00000031	0.00000000	0.00000001	0.00000000	0.00000000	0.00000006
E(rot)	0.00009500	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00000000	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1317.80203911**	**-40.43929810**	**-0.49847058**	**-1358.32810038**	**-1358.27923595**	**-1358.27979536**	**-1358.89387800**	**-1358.23722244**	**-1358.25422861**	**-1358.90000710**	**-1263.09463435**	**-95.74033197**	**-1358.96046012**
H=U+k_B*T	**-1317.80194411**	**-40.43920310**	**-0.49837558**	**-1358.32800538**	**-1358.27914095**	**-1358.27970036**	**-1358.89378300**	**-1358.23712744**	**-1358.25413361**	**-1358.89991210**	**-1263.09453935**	**-95.74023697**	**-1358.96036512**
T*S(el)	0.00000000	0.00000000	0.00006585	0.00000000	0.00000000	0.00000000	0.00006585	0.00000000	0.00000000	0.00006585	0.00006585	0.00000000	0.00006585
T*S(vib)	0.00000000	0.00000000	0.00000000	0.00000099	0.00006208	0.00000140	0.00000213	0.00000035	0.00000000	0.00000001	0.00000000	0.00000000	0.00000006
T* S(rot)	0.00044621	0.00015936	0.00000000	0.00079680	0.00063744	0.00079680	0.00081274	0.00078087	0.00079680	0.00079680	0.00000000	0.00060557	0.00082867
T* S(trans)	0.00130230	0.00109264	0.00069829	0.00133176	0.00133176	0.00133176	0.00133342	0.00133176	0.00133176	0.00133342	0.00127041	0.00118678	0.00133342
T*S	**0.00174851**	**0.00125200**	**0.00076414**	**0.00212955**	**0.00203128**	**0.00212996**	**0.00221414**	**0.00211298**	**0.00212856**	**0.00219608**	**0.00133626**	**0.00179235**	**0.00222800**
H	-1317.80194411	-40.43920310	-0.49837558	-1358.32800538	-1358.27914095	-1358.27970036	-1358.89378300	-1358.23712744	-1358.25413361	-1358.89991210	-1263.09453935	-95.74023697	-1358.96036512
T*S	0.00174851	0.00125200	0.00076414	0.00212955	0.00203128	0.00212996	0.00221414	0.00211298	0.00212856	0.00219608	0.00133626	0.00179235	0.00222800
G=H-TS	**-1317.80369262**	**-40.44045510**	**-0.49913972**	**-1358.33013493**	**-1358.28117223**	**-1358.28183032**	**-1358.89599713**	**-1358.23924041**	**-1358.25626217**	**-1358.90210818**	**-1263.09587561**	**-95.74202932**	**-1358.96259312**

	Reactants	Intermedia	Intermedia	TS_II	TS_I
M=2	$[FeNH]^+$	CH_4***$[FeNH]^+$	$[H_2N\text{-}Fe\text{-}CH_3]^+$	H_2N***CH_3	CH_4***NH
E(el)	-1318.45493851	-1358.98315771	-1358.99377786	-1358.96462789	-1358.90976210
E(ZPE)	0.010114820	0.05795295	0.06135583	0.06094087	0.05379606
E(vib)	0.000000000	0.00003297	0.00000050	0.00002720	0.00000042
E(rot)	0.000142510	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.000142510	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1318.44453867**	**-1358.92488677**	**-1358.93213651**	**-1358.90337480**	**-1358.85568060**
H=U+k_B*T	**-1318.44444367**	**-1358.92479177**	**-1358.93204151**	**-1358.90327980**	**-1358.85558560**
T*S(el)	0.000065850	0.00006585	0.00006585	0.00006585	0.00006585
T*S(vib)	0.000000000	0.00004460	0.00000057	0.00003916	0.00000047
T* S(rot)	-0.000223105	0.00074899	0.00079680	0.00081274	0.00081274
T* S(trans)	0.001304340	0.00133342	0.00133342	0.00133342	0.00133342
T*S	**0.00114709**	**0.00219286**	**0.00219664**	**0.00225117**	**0.00221248**
H	-1318.44444367	-1358.92479177	-1358.93204151	-1358.90327980	-1358.85558560
T*S	0.00114709	0.00219286	0.00219664	0.00225117	0.00221248
G=H-TS	**-1318.44559075**	**-1358.92698463**	**-1358.93423815**	**-1358.90553096**	**-1358.85779807**

Calculated Energies: $[FeN]^+ + CH_4 + H \rightarrow Fe^+ + CH_3NH_2$ M=3

$[FeNH]^+ + CH_4 \rightarrow Fe^+ + CH_3NH_2$ M=4

	Reactants	Reactants	Reactants	Intermedia	Intermedia	Intermedia	Intermedia	TS_I	TS_II	TS_III	Products	Products	Products
M=3	$[FeN]^+$	CH_4	H	$[Fe\text{-}NH\text{-}CH_3]^+$	CH_4***$[FeN]^+$	$[HN\text{-}Fe\text{-}CH_3]^+$	$[H\text{-}Fe\text{-}NH\text{-}CH_3]^+$	C**Fe**N**H	N***CH_3	Fe**H**N	M=4 Fe^+	$CH_3\text{-}NH_2$	$[Fe^{***}NH_2\text{-}CH_3]^+$
E(el)	-1317.81984059	-40.48493205	-0.49861309	-1358.41389114	-1358.3385220	-1358.35444907	-1359.00425668	-1358.29310485	-1358.33592894	-1358.99027071	-1263.17954722	-95.80523172	-1359.0700064
E(ZPE)	0.00136354	0.04534893	0.00000000	0.05275756	0.04761258	0.04432060	0.05930821	0.04397538	0.04874853	0.05900237	-0.00000314	0.06461473	0.06802351
E(vib)	0.00000000	0.00000000	0.00000000	0.00000003	0.00002511	0.00000001	0.00000107	0.00000000	0.00000029	0.00000005	0.00000000	0.00000000	0.00000006
E(rot)	0.00009500	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00000000	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1317.81823954**	**-40.43929810**	**-0.49847058**	**-1358.36084853**	**-1358.29059929**	**-1358.30984344**	**-1358.94466238**	**-1358.24884445**	**-1358.28689510**	**-1358.93098327**	**-1263.17940785**	**-95.74033197**	**-1359.00169780**
H=U+k_B*T	**-1317.81814454**	**-40.43920310**	**-0.49837558**	**-1358.36075353**	**-1358.29050429**	**-1358.30974844**	**-1358.94456738**	**-1358.24874945**	**-1358.28680010**	**-1358.93088827**	**-1263.17931285**	**-95.74023697**	**-1359.00160280**
T*S(el)	0.00010437	0.00000000	0.00006585	0.00010437	0.00010437	0.00010437	0.00013170	0.00010437	0.00010437	0.00013170	0.00013170	0.00000000	0.00013170
T*S(vib)	0.00000000	0.00000000	0.00000000	0.00000004	0.00003359	0.00000001	0.00000123	0.00000000	0.00000033	0.00000006	0.00000000	0.00000000	0.00000006
T* S(rot)	0.00044621	0.00015936	0.00000000	0.00079680	0.00063744	0.00079680	0.00081274	0.00079680	0.00079680	0.00081274	0.00000000	0.00060557	0.00082867
T* S(trans)	0.00130230	0.00109264	0.00069829	0.00133176	0.00133176	0.00133176	0.00133342	0.00133176	0.00133176	0.00133342	0.00127041	0.00118678	0.00133342
T*S	**0.00185288**	**0.00125200**	**0.00076414**	**0.00223297**	**0.00210716**	**0.00223294**	**0.00227909**	**0.00223293**	**0.00223326**	**0.00227792**	**0.00140211**	**0.00179235**	**0.00229385**
H	-1317.81814454	-40.43920310	-0.49837558	-1358.36075353	-1358.29050429	-1358.30974844	-1358.94456738	-1358.24874945	-1358.28680010	-1358.93088827	-1263.17931285	-95.74023697	-1359.00160280
T*S	0.00185288	0.00125200	0.00076414	0.00223297	0.00210716	0.00223294	0.00227909	0.00223293	0.00223326	0.00227792	0.00140211	0.00179235	0.00229385
G=H-TS	**-1317.81999742**	**-40.44045510**	**-0.49913972**	**-1358.36298650**	**-1358.29261145**	**-1358.31198138**	**-1358.94684646**	**-1358.25098238**	**-1358.28903336**	**-1358.93316618**	**-1263.18071496**	**-95.74202932**	**-1359.00389665**

	Reactants	Intermedia	Intermedia	TS_II	TS_I
M=4	$[FeNH]^+$	CH_4***$[FeNH]^+$	$[H_2N\text{-}Fe\text{-}CH_3]^+$	H_2N***CH_3	CH_4***NH
E(el)	-1318.47383487	-1358.9949224	-1359.0253023	-1359.00568847	-1358.92701022
E(ZPE)	0.01106589	0.05777217	0.06038192	0.06188727	0.05780515
E(vib)	0.00000000	0.00000148	0.00001027	0.00000144	0.00000272
E(rot)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1318.46248396**	**-1358.93686373**	**-1358.96462508**	**-1358.94351474**	**-1358.86891733**
H=U+k_B*T	**-1318.46238896**	**-1358.93676873**	**-1358.96453008**	**-1358.94341974**	**-1358.86882233**
T*S(el)	0.0001317	0.00013170	0.00013170	0.00013170	0.00013170
T*S(vib)	0.00000000	0.00000171	0.00001304	0.00000168	0.00000324
T* S(rot)	-0.00014342	0.00078087	0.00081274	0.00081274	0.00079680
T* S(trans)	0.00130434	0.00133342	0.00133342	0.00133342	0.00133342
T*S	**0.00129262**	**0.00224770**	**0.00229090**	**0.00227954**	**0.00226516**
H	-1318.46238896	-1358.93676873	-1358.96453008	-1358.94341974	-1358.86882233
T*S	0.00129262	0.00224770	0.00229090	0.00227954	0.00226516
G=H-TS	**-1318.46368157**	**-1358.93901642**	**-1358.96682097**	**-1358.94569927**	**-1358.87108749**

Calculated Energies: $[FeN]^+ + CH_4 + H \rightarrow Fe^+ + CH_3NH_2$ M=5

$[FeNH]^+ + CH_4 \rightarrow Fe^+ + CH_3NH_2$ M=6

	Reactants	Reactants	Reactants	Intermedia	Intermedia	Intermedia	Intermedia	TS_I	TS_II	TS_III	Products	Products	Products
M=5	**$[FeN]^+$**	**CH_4**	**H**	**$[Fe\text{-}NH\text{-}CH_3]^+$**	**CH_4***$[FeN]^+$**	**$[HN\text{-}Fe\text{-}CH_3]^+$**	**$[H\text{-}Fe\text{-}NH\text{-}CH_3]^+$**	**C**Fe**N**H**	**N***CH_3**	**Fe**H**N**	**M=6 Fe^+**	**$CH_3\text{-}NH_2$**	**$[Fe^{***}NH_2\text{-}CH_3]^+$**
E(el)	-1317.77928248	-40.48493205	-0.49861309	-1358.43816893	-1358.32325297	-1358.36673959	-1358.99966158	-1358.29814080	-1358.35357513	-1358.95895279	-1263.18233615	-95.80523172	-1359.06364371
E(ZPE)	0.00145084	0.04534893	0.00000000	0.05306516	0.05046811	0.04918349	0.05827596	0.04512240	0.04955330	0.06348768	-0.00000581	0.06461473	0.06768366
E(vib)	0.00000000	0.00000000	0.00000000	0.00000156	0.00000842	0.00000790	0.00000052	0.00000011	0.00000304	0.00000001	0.00000000	0.00000000	0.00000030
E(rot)	0.00009500	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00000000	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1317.77759413**	**-40.43929810**	**-0.49847058**	**-1358.38481719**	**-1358.27249142**	**-1358.31726318**	**-1358.94110008**	**-1358.25273327**	**-1358.30373377**	**-1358.89518008**	**-1263.18219945**	**-95.74033197**	**-1358.99567473**
$H=U+k_B{*}T$	**-1317.77749913**	**-40.43920310**	**-0.49837558**	**-1358.38472219**	**-1358.27239642**	**-1358.31716818**	**-1358.94100508**	**-1358.25263827**	**-1358.30363877**	**-1358.89508508**	**-1263.18210445**	**-95.74023697**	**-1358.99557973**
T*S(el)	0.00015290	0.00000000	0.00006585	0.00015290	0.00015290	0.00015290	0.00017022	0.00015290	0.00015290	0.00017022	0.00017022	0.00000000	0.00017022
T*S(vib)	0.00000000	0.00000000	0.00000000	0.00000182	0.00001042	0.00000986	0.00000058	0.00000012	0.00000364	0.00000002	0.00000000	0.00000000	0.00000033
T* S(rot)	0.00039644	0.00015936	0.00000000	0.00079680	0.00079680	0.00079680	0.00082867	0.00079680	0.00079680	0.00082867	0.00000000	0.00060557	0.00084461
T* S(trans)	0.00130230	0.00109264	0.00069829	0.00133176	0.00133176	0.00133176	0.00133342	0.00133176	0.00133176	0.00133342	0.00127041	0.00118678	0.00133342
T*S	**0.00185164**	**0.00125200**	**0.00076414**	**0.00228328**	**0.00229188**	**0.00229132**	**0.00233289**	**0.00228158**	**0.00228510**	**0.00233233**	**0.00144063**	**0.00179235**	**0.00234858**
H	-1317.77749913	-40.43920310	-0.49837558	-1358.38472219	-1358.27239642	-1358.31716818	-1358.94100508	-1358.25263827	-1358.30363877	-1358.89508508	-1263.18210445	-95.74023697	-1358.99557973
T*S	0.00185164	0.00125200	0.00076414	0.00228328	0.00229188	0.00229132	0.00233289	0.00228158	0.00228510	0.00233233	0.00144063	0.00179235	0.00234858
G=H-TS	**-1317.77935077**	**-40.44045510**	**-0.49913972**	**-1358.38700547**	**-1358.27468830**	**-1358.31945950**	**-1358.94333797**	**-1358.25491985**	**-1358.30592387**	**-1358.89741741**	**-1263.18354508**	**-95.74202932**	**-1358.99792831**

	Reactants	Intermedia	Intermedia	TS_II	TS_I
M=6	**$[FeNH]^+$**	**CH_4***$[FeNH]^+$**	**$[H_2N\text{-}Fe\text{-}CH_3]^+$**	**H_2N***CH_3**	**CH_4***NH**
E(el)	-1318.49039309	-1359.01041252	-1359.02200693	-1358.97248212	-1358.94056780
E(ZPE)	0.01082110	0.05825507	0.05865434	0.06151328	0.05431437
E(vib)	0.00000000	0.00002062	0.00001115	0.00000000	0.00000038
E(rot)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-1318.47928697**	**-1358.95185181**	**-1358.96305642**	**-1358.91068382**	**-1358.88596803**
$H=U+k_B{*}T$	**-1318.47919197**	**-1358.95175681**	**-1358.96296142**	**-1358.91058882**	**-1358.88587303**
T*S(el)	0.00017022	0.00017022	0.00017022	0.00017022	0.00017022
T*S(vib)	0.00000000	0.00002691	0.00001437	0.00000000	0.00000043
T* S(rot)	-0.00007968	0.00078087	0.00079680	0.00084461	0.00082867
T* S(trans)	0.00130434	0.00133342	0.00133342	0.00133342	0.00133342
T*S	**0.00139488**	**0.00231142**	**0.00231481**	**0.00234825**	**0.00233274**
H	-1318.47919197	-1358.95175681	-1358.96296142	-1358.91058882	-1358.88587303
T*S	0.00139488	0.00231142	0.00231481	0.00234825	0.00233274
G=H-TS	**-1318.48058685**	**-1358.95406822**	**-1358.96527623**	**-1358.91293707**	**-1358.88820577**

Fig. 1	E_{el} (h)
MECP A	**-1358.323091**
MECP B	**-1358.322777**
MECP C	**-1359.000422**
MECP D	**-1358.998407**
MECP E	**-1359.062912**

Fig. 2	E_{el} (h)
MECP A	**-1359.018648**
MECP B	**-1359.062912**

Calculated Energies: $[(CO)_2FeN]^+ + H \rightarrow [FeCO]^+ + HNCO$ M=1

	Reactants	Reactants	Products	Products	Intermedia	Intermedia	TS_I	TS_II
M=1	**$[2(CO)-FeN]^+$**	**H**	**$[Fe-CO]^+$**	**HNCO**	**$[OC-Fe-NCO]^+$**	**$[OC-Fe(H)-NCO]^+$**	**N***CO**	**H***NCO**
E(el)	-403.67246890	-0.49861309	-235.64129481	-168.63688889	-403.69158443	-404.27838392	-403.62243425	-404.26216226
E(ZPE)	0.02119827	0.00000000	0.00669419	0.02132887	0.02083249	0.032076	0.02102507	0.02660227
E(vib)	0.00001499	0.00000000	0.00000000	0.00000000	0.00002668	0.00000763	0.00000514	0.00001073
E(rot)	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-403.65097062**	**-0.49847058**	**-235.63431560**	**-168.61527500**	**-403.67044024**	**-404.24601527**	**-403.60111902**	**-404.23526424**
$H=U+k_B*T$	**-403.65087562**	**-0.49837558**	**-235.63422060**	**-168.61518000**	**-403.67034524**	**-404.24592027**	**-403.60102402**	**-404.23516924**
T*S(el)	0.00000000	0.00006585	0.00006585	0.00000000	0.00000000	0.00006585	0.00000000	0.00006585
T*S(vib)	0.00001967	0.00000000	0.00000000	0.00000000	0.00003692	0.00000949	0.00000626	0.00001347
T* S(rot)	0.00092429	0.00000000	0.00006374	0.00055776	0.00101991	0.00094023	0.00098804	0.00100397
T* S(trans)	0.00138621	0.00069829	0.00132833	0.00123323	0.00138621	0.00138735	0.00138621	0.00138735
T*S	**0.00233017**	**0.00076414**	**0.00145792**	**0.00179099**	**0.00244304**	**0.00240292**	**0.00238051**	**0.00247064**
H	-403.65087562	-0.49837558	-235.63422060	-168.61518000	-403.67034524	-404.24592027	-403.60102402	-404.23516924
T*S	0.00233017	0.00076414	0.00145792	0.00179099	0.00244304	0.00240292	0.00238051	0.00247064
G=H-TS	**-403.65320579**	**-0.49913972**	**-235.63567852**	**-168.61697099**	**-403.67278827**	**-404.24832318**	**-403.60340452**	**-404.23763988**

Calculated Energies: $[(CO)_2FeN]^+ + H \rightarrow [FeCO]^+ + HNCO$ M=3

	Reactants	Reactants	Products	Products	Intermedia	Intermedia	TS_I	TS_II
M=3	**$[2(CO)-FeN]^+$**	**H**	**$[Fe-CO]^+$**	**HNCO**	**$[OC-Fe-NCO]^+$**	**$[OC-Fe(H)-NCO]^+$**	**N***CO**	**H***NCO**
E(el)	-403.63749587	-0.49861309	-235.6896194	-168.63688889	-403.71683605	-404.3026643	-403.62351336	-404.29996997
E(ZPE)	0.01635584	0.00000000	0.00665406	0.02132887	0.02069600	0.02698733	0.01838638	0.02567371
E(vib)	0.00002015	0.00000000	0.00000000	0.00000000	0.00002812	0.00002797	0.00000779	0.00001698
E(rot)	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-403.62083486**	**-0.49847058**	**-235.68268032**	**-168.61527500**	**-403.69582691**	**-404.27536398**	**-403.60483417**	**-404.27399426**
$H=U+k_B*T$	**-403.62073986**	**-0.49837558**	**-235.68258532**	**-168.61518000**	**-403.69573191**	**-404.27526898**	**-403.60473917**	**-404.27389926**
T*S(el)	0.00010437	0.00006585	0.00013170	0.00000000	0.00010437	0.0001317	0.00010437	0.00013170
T*S(vib)	0.00002651	0.00000000	0.00000000	0.00000000	0.00003899	0.0000399	0.00000966	0.00002257
T* S(rot)	0.00095616	0.00000000	0.00007968	0.00055776	0.00101991	0.000972099	0.00098804	0.00098804
T* S(trans)	0.00138621	0.00069829	0.00132833	0.00123323	0.00138621	0.00138735	0.00138621	0.00138735
T*S	**0.00247325**	**0.00076414**	**0.00153971**	**0.00179099**	**0.00254948**	**0.00253105**	**0.00248828**	**0.00252966**
H	-403.62073986	-0.49837558	-235.68258532	-168.61518000	-403.69573191	-404.27526898	-403.60473917	-404.27389926
T*S	0.00247325	0.00076414	0.00153971	0.00179099	0.00254948	0.00253105	0.00248828	0.00252966
G=H-TS	**-403.62321311**	**-0.49913972**	**-235.68412503**	**-168.61697099**	**-403.69828138**	**-404.27780002**	**-403.60722744**	**-404.27642891**

Calculated Energies: $[(CO)_2FeN]^+ + H \rightarrow [FeCO]^+ + HNCO$ M=5

	Reactants	Reactants	Products	Products	Intermedia	Intermedia	TS_I	TS_II
M=5	**$[2(CO)\text{-}FeN]^+$**	**H**	**$[Fe\text{-}CO]^+$**	**HNCO**	**$[OC\text{-}Fe\text{-}NCO]^+$**	**$[OC\text{-}Fe(H)\text{-}NCO]^+$**	**N***CO**	**H***NCO**
E(el)	-403.62772423	-0.49861309	-235.63986387	-168.63688889	-403.75982299	-404.28568284	-403.62418527	-404.25079613
E(ZPE)	0.01729825	0.00000000	0.00599105	0.02132887	0.02007295	0.02568167	0.01777675	0.02326971
E(vib)	0.00001333	0.00000000	0.00000018	0.00000000	0.00000210	0.00003779	0.00002475	0.00003278
E(rot)	0.00014251	0.00000000	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
E(trans)	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251	0.00014251
U	**-403.61012763**	**-0.49847058**	**-235.63358762**	**-168.61527500**	**-403.73946292**	**-404.25967836**	**-403.60609875**	**-404.22720862**
$H=U+k_B*T$	**-403.61003263**	**-0.49837558**	**-235.63349262**	**-168.61518000**	**-403.73936792**	**-404.25958336**	**-403.60600375**	**-404.22711362**
T*S(el)	0.00015290	0.00006585	0.00017022	0.00000000	0.00015290	0.00017022	0.00015290	0.00017022
T*S(vib)	0.00001695	0.00000000	0.00000020	0.00000000	0.00000243	0.00005534	0.00100397	0.00004500
T* S(rot)	0.00101991	0.00000000	0.00015936	0.00055776	0.00062151	0.00103584	0.00090060	0.00103584
T* S(trans)	0.00138621	0.00069829	0.00132833	0.00123323	0.00138621	0.00138735	0.00138621	0.00138735
T*S	**0.00257597**	**0.00076414**	**0.00165811**	**0.00179099**	**0.00216305**	**0.00264875**	**0.00344368**	**0.00263841**
H	-403.61003263	-0.49837558	-235.63349262	-168.61518000	-403.73936792	-404.25958336	-403.60600375	-404.22711362
T*S	0.00257597	0.00076414	0.00165811	0.00179099	0.00216305	0.00264875	0.00344368	0.00263841
G=H-TS	**-403.61260859**	**-0.49913972**	**-235.63515073**	**-168.61697099**	**-403.74153096**	**-404.26223211**	**-403.60944743**	**-404.22975203**

Fig. 3	E_{el} (h)
MECP A	**-403.6274483804**
MECP B	**-403.6276458568**
MECP C	**-404.2855097449**

Optimized cartesian coordinates of the products:

CH4

C	-0.428406	0.129750	-0.002498
H	0.658803	0.139147	0.004016
H	-0.795674	0.993106	-0.552036
H	-0.797196	0.167339	1.019711
H	-0.780628	-0.780742	-0.481275

H3C-NH2

C	-2.721952	1.216959	0.056667
N	-1.258357	1.221247	-0.011172
H	-3.213336	2.034667	-0.482834
H	-3.030599	1.268161	1.100108
H	-3.094686	0.275768	-0.345665
H	-0.896993	2.091490	0.359076
H	-0.956198	1.174969	-0.976341

HNCO

O	-4.254653	0.644160	-0.298537
C	-3.272578	1.264510	-0.172308
N	-2.181698	1.796004	-0.131814
H	-1.981001	2.651586	0.355210

Optimized cartesian coordinates: $[FeN]^+ + CH_4 + H \rightarrow Fe^+ + CH_3NH_2$

M=multiplicity

M=1 [FeN]+

Fe	-0.875043	0.347651	0.000000
N	0.745073	0.713479	0.000000

M=3 [FeN]+

Fe	-0.909758	0.339812	0.000000
N	0.779788	0.721318	0.000000

M=5 [FeN]+

Fe	-0.970544	0.326086	0.000000
N	0.840574	0.735044	0.000000

M=1 [FeN*CH4]+**

Fe	-1.448897	-0.094339	0.002914
N	0.139062	0.165358	0.319589
C	-3.547964	-0.424312	-0.456014
H	-4.594453	-0.579285	-0.708004
H	-3.015371	-1.297190	-0.875605
H	-3.273721	0.529733	-0.943330
H	-3.513565	-0.379552	0.646399

M=3 [FeN*CH4]+**

Fe	-1.390583	-0.081985	-0.022504
N	0.273220	0.182330	0.385391
C	-3.581820	-0.429323	-0.464172
H	-4.633764	-0.589122	-0.695506
H	-3.062602	-1.301273	-0.891282
H	-3.327189	0.520889	-0.959627
H	-3.532170	-0.381105	0.633649

M=5 [FeN*CH4]+**

Fe	-1.254923	-0.522776	-0.106549
N	-0.624759	0.787290	0.389286
C	-3.431588	-0.507520	-0.463445
H	-4.385571	0.020442	-0.473335
H	-3.580971	-1.545771	-0.750490
H	-2.849078	0.073092	-1.211130
H	-3.130320	-0.387157	0.601245

M=1 [H3C-Fe-NH]+

Fe	-2.598560	2.830401	0.454515
C	-2.837126	1.032371	0.021788
H	-3.612910	0.875522	0.791683
H	-2.044617	0.298025	0.074279
H	-3.243503	1.149295	-0.990950
N	-0.979362	3.011981	0.207874
H	-0.045923	2.787107	-0.151139

M=3 [H3C-Fe-NH]+

Fe	-2.513592	2.796916	0.776665
C	-2.811861	1.051623	0.023186
H	-3.746965	0.882389	0.581802
H	-2.041512	0.335190	0.285699
H	-2.977473	1.144209	-1.046838
N	-0.960174	3.141840	0.198137
H	-0.310423	2.632535	-0.410599

M=5 [H3C-Fe-NH]+

Fe	-2.465829	2.800670	0.870091
C	-2.771873	1.099971	0.037839
H	-3.750445	0.910429	0.505917
H	-2.036932	0.359944	0.339901
H	-2.857419	1.182941	-1.041449
N	-1.070395	3.028606	0.173803
H	-0.409107	2.602142	-0.478050

M=1 [H3C-HN-Fe]+

Fe	-0.910523	1.621307	0.884566
C	-3.309586	0.245323	-0.057188
N	-1.862988	0.412322	-0.016986
H	-1.390913	-0.280637	-0.593569
H	-3.583488	-0.743414	0.317369
H	-3.803050	0.999800	0.550724
H	-3.668862	0.330418	-1.084915

M=3 [H3C-HN-Fe]+

Fe	-0.817578	1.656154	0.927692
C	-3.319139	0.248769	-0.056666
N	-1.889330	0.423992	-0.013466
H	-1.444400	-0.276462	-0.610386
H	-3.567276	-0.754247	0.311498
H	-3.829581	0.997563	0.537658
H	-3.662108	0.289352	-1.096330

M=5 [H3C-HN-Fe]+

Fe	-0.875660	1.643672	0.864636
C	-3.320576	0.240807	-0.059145
N	-1.866756	0.413912	-0.006623
H	-1.389777	-0.286828	-0.568501
H	-3.587772	-0.754549	0.297997
H	-3.819529	0.981302	0.558995
H	-3.669342	0.346806	-1.087361

M=2 [H3C-HN-FeH]+

Fe	-2.815396	2.139211	-0.306778
N	-0.821618	2.452790	-0.508320
C	-0.036466	3.528476	0.027894
H	0.754102	3.114712	0.667964
H	-0.643190	4.231356	0.588144
H	0.485366	4.041286	-0.790320
H	-0.223014	1.816240	-1.038174
H	-4.303583	2.234048	0.065228

M=4 [H3C-HN-FeH]+

Fe	-2.846289	2.215631	-0.235533
N	-0.826163	2.476565	-0.466615
C	0.002240	3.538749	0.028839
H	0.821014	3.114779	0.624253
H	-0.562525	4.254725	0.615966
H	0.486258	4.041923	-0.819364
H	-0.264261	1.810978	-1.001177
H	-4.414073	2.104769	-0.040728

M=6 [H3C-HN-FeH]+

Fe	-2.775035	1.988869	-0.394603
N	-0.754573	2.358688	-0.573375
C	-0.116181	3.497911	0.026910
H	0.680456	3.157109	0.700197
H	-0.823339	4.116497	0.570508
H	0.382129	4.089944	-0.750866
H	-0.074788	1.790996	-1.080054
H	-4.122468	2.558106	0.206925

M=2 [H3C-H2N-Fe]+

Fe	-1.011549	0.322941	1.787661
C	-3.315630	0.242818	-0.070745
N	-1.828698	0.430857	-0.014942
H	-1.398698	-0.258375	-0.630720
H	-3.564706	-0.737040	0.325107
H	-3.793144	1.007591	0.534216
H	-3.674255	0.318570	-1.094549
H	-1.606462	1.329619	-0.441478

M=4 [H3C-H2N-Fe]+

Fe	-0.971412	0.327556	1.799562
C	-3.325358	0.242110	-0.075350
N	-1.837255	0.429402	-0.017097
H	-1.396992	-0.260956	-0.623252
H	-3.577829	-0.737057	0.318146
H	-3.805413	1.005863	0.527627
H	-3.674156	0.320062	-1.102355
H	-1.604725	1.330000	-0.432731

M=6 [H3C-H2N-Fe]+

Fe	-0.968532	0.312649	1.922596
C	-3.321387	0.243197	-0.079433
N	-1.832602	0.435084	-0.056268
H	-1.404146	-0.256042	-0.671751
H	-3.561591	-0.736910	0.323273
H	-3.789843	1.008857	0.532780
H	-3.702899	0.315107	-1.094328
H	-1.612140	1.335036	-0.482320

M=1 TS_I

Fe	-1.039355	0.000561	0.755380
N	0.360152	0.136052	0.141410
C	-0.859685	-1.535074	1.908355
H	-1.640975	-2.154225	1.453957
H	0.299845	-0.861676	0.950728
H	-1.174842	-1.039554	2.834103
H	0.012843	-2.152131	2.114859

M=3 TS_I

Fe	-1.023217	0.279768	0.862384
N	0.355781	0.020435	0.075701
C	-0.813692	-1.536699	1.882740
H	-1.512346	-2.196519	1.373545
H	0.112361	-1.002426	0.984120
H	-1.230471	-1.074859	2.781187
H	0.069566	-2.095747	2.199115

M=5 TS_I

Fe	-1.080802	0.126247	0.645106
N	0.408341	0.071430	0.226072
C	-0.834947	-1.529564	1.882270
H	-1.585237	-2.163242	1.412131
H	0.170745	-0.940022	1.088446
H	-1.171167	-1.042019	2.796498
H	0.051048	-2.128877	2.108268

M=1 TS_II

Fe	-2.163070	2.578231	1.456289
C	-2.611236	1.158040	0.026558
H	-3.680339	1.369862	0.024528
H	-2.318227	0.317985	0.656976
H	-2.244933	1.026180	-0.980337
N	-1.371169	2.800545	0.079571
H	-0.973026	2.733857	-0.855534

M=3 TS_II

Fe	-1.912463	2.383282	1.545348
C	-2.596485	1.203449	0.027266
H	-3.454191	0.967661	0.667684
H	-1.875713	0.392610	-0.035959
H	-2.954173	1.518750	-0.945085
N	-1.534208	2.963144	0.016135
H	-1.120726	2.672765	-0.872258

M=5 TS_II

Fe	-1.595350	2.205040	1.507154
C	-2.559033	1.152945	0.039309
H	-3.573055	1.237769	0.431825
H	-2.087560	0.204095	0.309538
H	-2.557899	1.256768	-1.034001
N	-1.431873	2.939168	0.064484
H	-1.643189	3.105876	-0.915178

M=2 TS_III

Fe	-2.614838	1.850034	0.548908
N	-1.094882	2.294184	-0.227486
C	-0.291053	3.500426	-0.008721
H	0.738541	3.181940	0.159881
H	-0.641876	4.040455	0.864866
H	-0.321162	4.150100	-0.883322
H	-0.802174	1.797121	-1.067365
H	-2.576354	2.743860	-0.681122

M=4 TS_III

Fe	-2.593052	1.899580	0.534396
N	-1.006219	2.231810	-0.174858
C	-0.266945	3.492026	-0.000058
H	0.779616	3.225673	0.159681
H	-0.613846	4.021752	0.883600
H	-0.346770	4.137956	-0.871483
H	-0.805679	1.804666	-1.076252
H	-2.750903	2.744658	-0.749388

M=6 TS_III

Fe	-2.696442	1.707961	0.671956
N	-1.068147	2.337888	-0.290074
C	-0.244927	3.509588	-0.028990
H	0.750639	3.164196	0.268135
H	-0.666835	4.102371	0.778233
H	-0.135587	4.122708	-0.922665
H	-0.792896	1.876854	-1.158787
H	-2.749603	2.736555	-0.612170

MECP_A

Fe	-1.422851	-0.182106	-0.365319
N	-0.441966	0.310941	0.756133
C	-3.435065	-0.451190	-0.504691
H	-4.495947	-0.364762	-0.280359
H	-3.268221	-1.386551	-1.059282
H	-3.198441	0.462945	-1.097940
H	-2.992418	-0.468865	0.537408

MECP_B

Fe	-1.293536	-0.531608	0.083418
N	-0.535739	0.795370	-0.033822
C	-3.440459	-0.513700	-0.396880
H	-4.377599	0.001061	-0.615283
H	-3.456455	-1.496222	-0.866018
H	-2.744708	0.220519	-0.888465
H	-3.408714	-0.557820	0.702633

MECP_C

Fe	-2.694721	1.961902	-0.442070
N	-0.784330	2.334388	-0.586424
C	-0.166669	3.485902	0.028915
H	0.617290	3.153775	0.718542
H	-0.894174	4.091433	0.561714
H	0.328014	4.089230	-0.740254
H	-0.087152	1.779603	-1.082464
H	-3.922057	2.661887	0.247684

MECP_D

Fe	-1.059720	0.348234	1.545542
C	-3.300827	0.241242	-0.044390
N	-1.826283	0.422228	0.058073
H	-1.400118	-0.270117	-0.570550
H	-3.575643	-0.739317	0.330217
H	-3.804145	1.002474	0.542524
H	-3.617575	0.326618	-1.085799
H	-1.608831	1.325619	-0.381067

MECP_E

Fe	-0.961534	0.295179	1.990909
C	-3.321405	0.250116	-0.085078
N	-1.831985	0.430830	-0.073997
H	-1.411830	-0.264302	-0.690978
H	-3.566102	-0.731949	0.311217
H	-3.778822	1.014405	0.538146
H	-3.714802	0.333533	-1.094350
H	-1.606659	1.329166	-0.501320

Optimized cartesian coordinates: $[FeNH]^+ + CH_4 \rightarrow Fe^+ + CH_3NH_2$
M = multiplicity

M=2 [FeNH]+

Fe	-1.605766	1.112297	-0.000050
N	0.146863	0.908135	0.000100
H	1.166823	0.789359	-0.000050

M=4 [FeNH]+

Fe	-1.570821	1.108201	-0.000116
N	0.134246	0.909655	0.000231
H	1.144496	0.791934	-0.000115

M=6 [FeNH]+

Fe	-1.558772	1.106775	-0.000238
N	0.129247	0.910282	0.000475
H	1.137446	0.792733	-0.000237

M=2 [FeNH*CH4]+**

Fe	-1.573392	0.017280	0.026235
N	0.040038	0.436930	0.495480
C	-3.542854	-0.434379	-0.471258
H	-4.569082	-0.674675	-0.732059
H	-2.932893	-1.280760	-0.848415
H	-3.319344	0.524585	-0.983400
H	-3.527494	-0.344379	0.634703
H	0.983201	0.702678	0.793245

M=4 [FeNH*CH4]+**

Fe	-1.587245	0.210025	0.336718
N	0.128364	0.390916	0.376945
C	-3.550877	-0.467032	-0.505117
H	-4.597246	-0.632681	-0.753067
H	-2.986312	-1.324173	-0.879084
H	-3.294605	0.476536	-1.010979
H	-3.575538	-0.408749	0.600222
H	1.021640	0.702436	0.748891

M=6 [FeNH*CH4]+**

Fe	-1.544226	0.090049	0.383438
N	0.107114	0.486687	0.511962
C	-3.564126	-0.463351	-0.544665
H	-4.642933	-0.579399	-0.639998
H	-3.096255	-1.359039	-0.955458
H	-3.312109	0.445188	-1.102542
H	-3.466740	-0.383439	0.563343
H	1.077456	0.710583	0.698449

M=2 [H2N-Fe-CH3]+

Fe	-1.417892	0.256552	0.885082
C	-2.768001	1.101807	-0.029443
H	-3.219648	0.236839	-0.538839
H	-2.574270	1.914624	-0.718171
H	-3.374724	1.433844	0.828111
N	-0.098702	1.110116	0.257100
H	0.826378	0.833195	0.584326
H	-0.061899	1.866251	-0.412615

M=4 [H2N-Fe-CH3]+

Fe	-1.432339	0.644093	1.165168
C	-2.858300	1.032990	-0.087961
H	-3.188434	0.033011	-0.379968
H	-2.581647	1.651749	-0.931645
H	-3.552510	1.533249	0.598000
N	0.095482	1.133671	0.452405
H	0.497372	0.606986	-0.318344
H	0.331617	2.117479	0.357895

M=6 [H2N-Fe-CH3]+

Fe	-1.248752	0.609592	-0.224974
C	-3.148321	0.990617	-0.098304
H	-3.712597	0.230700	0.438901
H	-3.409351	0.971847	-1.167231
H	-3.300914	1.988428	0.310344
N	0.374229	1.137509	0.404036
H	1.207266	1.328364	-0.146680
H	0.549681	1.496171	1.339459

M=2 [H3C-H2N-Fe]+

Fe	-1.011549	0.322941	1.787661
C	-3.315630	0.242818	-0.070745
N	-1.828698	0.430857	-0.014942
H	-1.398698	-0.258375	-0.630720
H	-3.564706	-0.737040	0.325107
H	-3.793144	1.007591	0.534216
H	-3.674255	0.318570	-1.094549
H	-1.606462	1.329619	-0.441478

M=4 [H3C-H2N-Fe]+

Fe	-0.971412	0.327556	1.799562
C	-3.325358	0.242110	-0.075350
N	-1.837255	0.429402	-0.017097
H	-1.396992	-0.260956	-0.623252
H	-3.577829	-0.737057	0.318146
H	-3.805413	1.005863	0.527627
H	-3.674156	0.320062	-1.102355
H	-1.604725	1.330000	-0.432731

M=6 [H3C-H2N-Fe]+

Fe	-0.968532	0.312649	1.922596
C	-3.321387	0.243197	-0.079433
N	-1.832602	0.435084	-0.056268
H	-1.404146	-0.256042	-0.671751
H	-3.561591	-0.736910	0.323273
H	-3.789843	1.008857	0.532780
H	-3.702899	0.315107	-1.094328
H	-1.612140	1.335036	-0.482320

M=2 TS_VII

Fe	-1.206349	-0.022991	0.443651
N	0.403758	-0.182453	-0.157087
C	-0.767440	-1.465211	1.872443
H	-1.682921	-2.014649	1.639311
H	0.108564	-1.014030	0.839841
H	-0.825395	-0.866202	2.778779
H	0.044432	-2.189237	1.966056
H	0.943389	0.647611	0.143106

M=4 TS_VII

Fe	-0.989006	0.217034	0.920673
N	0.401841	0.026587	0.085850
C	-0.851450	-1.470391	1.857274
H	-1.505325	-2.191055	1.365328
H	0.192215	-0.911617	0.977133
H	-1.279353	-1.164279	2.818777
H	0.054769	-2.016033	2.150240
H	0.994349	0.402593	-0.649174

M=6 TS_VII

Fe	-1.301263	0.141204	0.655407
N	0.317994	0.215202	0.011815
C	-0.806707	-1.520423	1.878790
H	-1.605885	-2.188837	1.552791
H	0.077092	-0.822176	0.954054
H	-1.020890	-1.087165	2.857079
H	0.095712	-2.127351	1.981184
H	1.261987	0.282385	-0.365021

M=2 TS_VI

Fe	-1.412363	0.368735	1.688703
C	-2.397203	1.059508	-0.131404
H	-2.809550	0.050651	-0.286221
H	-2.161097	1.507985	-1.097063
H	-3.059160	1.725967	0.440230
N	-0.477313	1.170222	0.373855
H	-0.047519	0.689859	-0.422774
H	-0.324554	2.180300	0.290225

M=4 TS_VI

Fe	-1.412363	0.368735	1.688703
C	-2.397203	1.059508	-0.131404
H	-2.809550	0.050651	-0.286221
H	-2.161097	1.507985	-1.097063
H	-3.059160	1.725967	0.440230
N	-0.477313	1.170222	0.373855
H	-0.047519	0.689859	-0.422774
H	-0.324554	2.180300	0.290225

M=6 TS_VI

Fe	-1.297789	0.428606	1.822385
C	-2.632602	1.072084	-0.244158
H	-2.870326	0.024429	-0.383192
H	-2.310152	1.604846	-1.121606
H	-3.225823	1.645202	0.460495
N	-0.403130	1.181992	0.347556
H	0.142549	0.644343	-0.326038
H	-0.091487	2.151725	0.300108

MECP_A

Fe	-1.302808	0.187239	0.498202
C	-2.994809	0.981855	-0.196708
H	-3.674738	0.143246	-0.014280
H	-2.825252	1.199293	-1.248005
H	-3.206528	1.860088	0.407039
N	0.153399	1.209659	0.537708
H	1.040583	0.974255	0.105097
H	0.121393	2.197592	0.766498

Optimized geometries: $[(CO)_2FeN]^+ + H \rightarrow [FeCO]^+ + HNCO$
M = multiplicity

M=1 [2COFeN]+

Fe	-1.073873	0.719145	0.368142
N	0.075473	0.406886	-0.266151
C	-1.276742	2.570101	0.118603
O	-1.300621	3.661276	-0.152053
C	-2.282522	-0.631672	-0.127265
O	-2.911244	-1.465056	-0.545146

M=3 [2COFeN]+

Fe	-1.013919	0.732428	-0.072644
N	0.600731	0.227215	0.002867
C	-1.346276	2.776965	0.012857
O	-1.408607	3.895424	0.065962
C	-2.454966	-0.747287	-0.255253
O	-3.146493	-1.624065	-0.357659

M=5 [2COFeN]+

Fe	-0.614919	0.806626	-0.026214
N	0.370180	-0.440274	-0.048651
C	-1.468509	2.785171	0.042079
O	-1.910489	3.814705	0.077052
C	-2.095580	-0.532008	-0.181668
O	-2.887103	-1.318921	-0.266608

M=1 [FeCO]+

Fe	-1.037864	0.842639	-0.068585
C	-1.284976	2.723413	0.012931
O	-1.432041	3.838766	0.061829

M=3 [FeCO]+

Fe	-1.037860	0.842522	-0.068555
C	-1.284819	2.722387	0.012816
O	-1.432203	3.839909	0.061914

M=5 [FeCO]+

Fe	-0.982560	0.472025	-0.084694
C	-1.311362	2.911479	0.021864
O	-1.460962	4.021312	0.069003

M=1 [OCN-FeCO]+

Fe	-1.153843	0.795447	-0.504712
N	0.528139	0.637081	-0.092592
C	1.423042	-0.133587	0.280663
O	2.311956	-0.781647	0.625026
C	-1.818283	-0.894750	-0.269156
O	-2.164002	-1.953993	-0.105699

M=3 [OCN-FeCO]+

Fe	-1.106676	0.567222	-0.441912
N	0.673461	0.418125	-0.010993
C	1.769092	-0.014225	0.330857
O	2.820006	-0.387435	0.649201
C	-2.202634	-0.989488	-0.333457
O	-2.826239	-1.925648	-0.260167

M=5 [OCN-FeCO]+

Fe	-0.682674	-0.534774	-0.106776
N	0.995519	-0.061115	0.161864
C	2.157235	0.253278	0.354448
O	3.260943	0.552742	0.536827
C	-2.769191	-1.121742	-0.425003
O	-3.834821	-1.419838	-0.587830

M=2 [OCN-FeH-CO]+

Fe	-1.733948	0.818965	-0.237901
N	-0.217558	0.744489	0.495449
C	0.714158	-0.097142	0.557065
O	1.630069	-0.775102	0.680559
C	-2.167086	-0.828169	-0.376330
O	-2.379943	-1.938272	-0.476042
H	-1.252861	0.421952	-1.492381

M=4 [OCN-FeH-CO]+

Fe	-1.460840	-0.051093	0.186651
N	0.104557	0.418003	0.741676
C	1.331089	0.398746	0.631556
O	2.482795	0.421500	0.586316
C	-3.151108	-0.825842	-0.777522
O	-4.002120	-1.276618	-1.347986
H	-0.711542	-0.737976	-0.870271

M=6 [OCN-FeH-CO]+

Fe	-0.537910	-1.342546	0.396945
N	0.752280	-0.150133	0.139396
C	1.834174	0.429641	0.154270
O	2.840920	0.994686	0.154972
C	-2.494828	-0.777467	-0.529898
O	-3.475582	-0.499195	-0.991562
H	-0.242104	-2.668556	1.226357

M=1 TS_I

Fe	-1.526105	0.705678	0.963256
N	-0.102386	0.953955	0.508762
C	-1.076373	2.192951	-0.072775
O	-1.108575	3.124875	-0.712572
C	-2.293697	-0.504310	-0.250586
O	-2.662393	-1.212468	-1.039954

M=3 TS_I

Fe	-1.548199	0.723654	0.961306
N	-0.127342	0.967528	0.445604
C	-1.093999	2.226505	-0.049422
O	-1.031203	3.175129	-0.674340
C	-2.290207	-0.549707	-0.265560
O	-2.678580	-1.282428	-1.021458

M=5 TS_I

Fe	-0.626467	0.870273	-0.022967
N	0.027218	-0.557111	-0.073368
C	-1.440637	2.877310	0.048801
O	-1.907631	3.895831	0.081709
C	-1.928401	-0.595880	-0.175900
O	-2.730500	-1.375123	-0.262286

M=2 TS_II

Fe	-1.720754	0.093751	0.400574
N	-0.001199	0.372639	0.686730
C	1.213442	0.283092	0.476056
O	2.358505	0.249528	0.349679
C	-2.931368	-0.800055	-0.766576
O	-3.591934	-1.350928	-1.491676
H	-0.733861	-0.501306	-0.504366

M=4 TS_II

Fe	-1.647877	0.059419	0.364221
N	0.035965	0.394020	0.717030
C	1.250546	0.314811	0.513838
O	2.397433	0.295992	0.401691
C	-3.053877	-0.830665	-0.799056
O	-3.759566	-1.355465	-1.494372
H	-0.629793	-0.531391	-0.552931

M=6 TS_II

Fe	-0.833678	-1.601555	0.174481
N	0.741585	-0.568956	0.162349
C	1.660650	0.237423	0.321988
O	2.563425	0.939901	0.485326
C	-2.643032	-0.807161	-0.578368
O	-3.587425	-0.372848	-0.995002
H	0.775426	-1.840376	0.979705

MECP_A

Fe	-0.604528	0.817511	-0.029537
N	0.385580	-0.413900	-0.058775
C	-1.475809	2.766094	0.041649
O	-1.926543	3.792100	0.076062
C	-2.096180	-0.530364	-0.175938
O	-2.888938	-1.316141	-0.257471

MECP_B

Fe	-0.645454	0.776316	-0.012224
N	0.475463	-0.338207	-0.005759
C	-1.483341	2.756067	0.041554
O	-1.886990	3.801440	0.069635
C	-2.135432	-0.548849	-0.197017
O	-2.930663	-1.331467	-0.300199

MECP_C

Fe	-0.584179	-1.150959	0.272815
N	0.778559	-0.031241	0.079753
C	1.926864	0.383877	0.208771
O	2.997654	0.803160	0.312220
C	-2.611838	-0.861878	-0.519643
O	-3.647324	-0.721033	-0.920062
H	-0.182786	-2.435496	1.116625