

Supplementary Information

Reaction Mechanism of the Selective Reduction of CO₂ to CO by a Tetraaza [Co^{II}N₄H]²⁺ Complex in the Presence of Protons.

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1 Geometries

1.1 [CoIN4H]²⁺

1	N	0.04648500	-0.07670200	0.02420900	9	H	3.33735400	-0.30983300	1.90500100
2	C	-0.01514100	-0.08658900	1.41794500	10	H	1.20888200	-0.13077500	3.17006800
3	C	1.05204900	0.02699200	-2.05003900	11	H	1.96327000	-0.85765200	-3.79434400
4	C	1.26375600	-0.02984800	-0.65566800	12	C	-1.57059600	0.11181400	-0.88394000
5	C	2.44851900	-0.03288000	0.07734800	13	C	-1.34733500	0.16561100	1.86761700
6	C	1.17174200	-0.08990000	2.14764200	14	N	-0.39909200	0.13149900	-2.39805900
7	C	2.40360500	-0.06781200	1.47833500	15	C	1.98518400	-0.02878700	-3.14881500
8	H	3.40673700	-0.00220700	-0.43159900	16	N	-3.28550000	0.46807400	-1.86631200
9	H	3.32726400	-0.06703400	2.04796300	17	N	-2.26007900	0.26032600	0.89678900
10	H	1.14662400	-0.10339700	3.23274700	18	C	-1.67451500	0.22419300	3.33215200
11	H	2.09518200	0.99549400	-3.69119400	19	C	-0.75493900	0.29041800	-3.80949300
12	Co	-1.46977600	-0.06078600	-0.91033600	20	H	1.88599200	-0.90424100	-3.80264000
13	C	-1.35684700	-0.07921900	1.85593000	21	H	2.97131500	-0.07502300	-2.68569700
14	N	-0.26775600	0.01430500	-2.38125600	22	C	-4.33566200	1.13573000	-1.07617600
15	C	2.16564700	0.10337300	-3.05458300	23	C	-3.13556400	1.03847600	-3.21718200
16	N	-3.17370300	-0.20901900	-1.96406500	24	H	-3.55593200	-0.52393000	-1.97291700
17	N	-2.24556600	-0.07271100	0.82524100	25	C	-3.64510700	0.49556000	1.31039000
18	C	-1.75561600	-0.06870700	3.30372500	26	H	-2.20182300	1.14940100	3.59492500
19	C	-0.59311000	0.16957500	-3.79241400	27	H	-2.31995600	-0.60991500	3.63431200
20	H	2.18543700	-0.76524000	-3.72801300	28	H	-0.77005600	0.17645500	3.93930600
21	H	3.13339400	0.14088400	-2.55175100	29	C	-2.24886800	0.13856000	-4.07852100
22	C	-4.40153200	0.25011100	-1.26976900	30	H	-0.21725500	-0.43946500	-4.42771700
23	C	-3.11736800	0.29890000	-3.35677400	31	H	-0.43049800	1.28697300	-4.14992000
24	H	-3.24746000	-1.22779000	-2.03371300	32	H	-5.24393700	1.23882300	-1.68867700
25	C	-3.65349000	0.03779600	1.17420100	33	H	-4.00231800	2.14935000	-0.81788700
26	H	-2.37962500	0.79792600	3.55996100	34	C	-4.65370600	0.32267200	0.17897200
27	H	-2.32503300	-0.96439800	3.59011700	35	H	-4.12699200	1.13641400	-3.68435300
28	H	-0.87264500	-0.03174400	3.94384800	36	H	-2.71469300	2.04942400	-3.13776100
29	C	-1.98528200	-0.34633700	-4.14854400	37	H	-3.72921100	1.51865900	1.71057700
30	H	0.12757600	-0.35867300	-4.42935600	38	H	-3.92454100	-0.18110300	2.12786800
31	H	-0.53446100	1.23268600	-4.08456200	39	H	-2.42346500	0.36996400	-5.13534500
32	H	-5.27138100	0.06483700	-1.91734300	40	H	-2.54780000	-0.90411200	-3.92310500
33	H	-4.32304700	1.33374600	-1.13028400	41	H	-4.72323800	-0.73591100	-0.09488100
34	C	-4.58890300	-0.45275700	0.07016500	42	H	-5.63684800	0.62225700	0.55926300
35	H	-4.08110800	0.10322700	-3.85023800	43	C	-1.89380100	-1.89882100	-0.98883500
36	H	-2.98857000	1.38585500	-3.31367600	44	O	-0.99566700	-2.53950300	-0.47377100
37	H	-3.91265800	1.08730600	1.40078800	45	O	-2.96680300	-2.15696000	-1.56659800
38	H	-3.88826600	-0.53282100	2.08204500					
39	H	-2.16223700	-0.15847400	-5.21415800					
40	H	-2.02389100	-1.43657500	-4.01504300					
41	H	-4.46723300	-1.53634800	-0.06784500					
42	H	-5.62376300	-0.29672200	0.39697000					

1.4 [CoIN4H]-CO₂ (Back)

1	N	0.02112800	-0.06833700	0.01333400	2	C	0.02632300	-0.09108800	1.38091300
2	C	0.87326600	0.00091300	-2.13209900	3	C	1.17139900	-0.09018700	-0.72633000
4	C	1.17139900	-0.09018700	-0.72633000	4	C	2.40127100	-0.19178200	-0.07496500
5	C	2.40127100	-0.19178200	-0.07496500	6	C	1.24083800	-0.19370400	2.06042800
6	C	1.24083800	-0.19370400	2.06042800	7	C	2.42937200	-0.25015400	1.32315600
7	C	2.42937200	-0.25015400	1.32315600	8	H	3.32719400	-0.21907100	-0.63839200
8	H	3.32719400	-0.21907100	-0.63839200	9	H	3.38039600	-0.32711500	1.83979800
9	H	3.38039600	-0.32711500	1.83979800	10	H	1.27047800	-0.22098200	3.14398200
10	H	1.27047800	-0.22098200	3.14398200	11	H	1.89628700	0.10250400	-3.74215600
11	H	1.89628700	0.10250400	-3.74215600	12	C	-1.56528600	0.13789200	-0.85695200
12	C	-1.56528600	0.13789200	-0.85695200	13	C	-1.31786700	0.01138300	1.89030200
13	C	-1.31786700	0.01138300	1.89030200	14	N	-0.43365500	0.04721300	-2.39711900
14	N	-0.43365500	0.04721300	-2.39711900	15	C	1.95197400	0.07513000	-3.17645900
15	C	1.95197400	0.07513000	-3.17645900	16	N	-3.30363400	-0.30503300	-1.81803900
16	N	-3.30363400	-0.30503300	-1.81803900	17	N	-2.23461700	0.09641400	0.92473100
17	N	-2.23461700	0.09641400	0.92473100	18	C	-1.62175800	0.04253400	3.36262400
18	C	-1.62175800	0.04253400	3.36262400	19	C	-0.85854100	0.27035100	-3.77516200
19	C	-0.85854100	0.27035100	-3.77516200	20	H	1.88507600	-0.74734400	-3.89944700
20	H	1.88507600	-0.74734400	-3.89944700	21	H	2.94098500	0.02817500	-2.71963200
21	H	2.94098500	0.02817500	-2.71963200	22	C	-4.56220100	0.03001600	-1.10341900
22	C	-4.56220100	0.03001600	-1.10341900	23	C	-3.36706200	0.19930300	-3.21275500
23	C	-3.36706200	0.19930300	-3.21275500	24	H	-3.27095100	-1.32536900	-1.88025100
24	H	-3.27095100	-1.32536900	-1.88025100	25	C	-3.63575300	0.30012600	1.27322700
25	C	-3.63575300	0.30012600	1.27322700	26	H	-2.12823500	0.97038500	3.65243700
26	H	-2.12823500	0.97038500	3.65243700	27	H	-2.26790400	-0.79028000	3.66660100
27	H	-2.26790400	-0.79028000	3.66660100	28	H	-0.70461800	-0.02629800	3.94873300
28	H	-0.70461800	-0.02629800	3.94873300	29	C	-2.22849300	-0.33651700	-4.07572100
29	C	-2.22849300	-0.33651700	-4.07572100	30	H	-0.13560200	-0.14150900	-4.48785300
30	H	-0.13560200	-0.14150900	-4.48785300	31	H	-0.90062200	1.35504700	-3.95637400
31	H	-0.90062200	1.35504700	-3.95637400	32	H	-5.41217300	-0.40060300	-1.65375700
32	H	-5.41217300	-0.40060300	-1.65375700	33	H	-4.64826300	1.11749800	-1.12549300
33	H	-4.64826300	1.11749800	-1.12549300	34	C	-4.57797500	-0.46428000	0.33948400
34	C	-4.57797500	-0.46428000	0.33948400	35	H	-4.33023600	-0.08849300	-3.66002900
35	H	-4.33023600	-0.08849300	-3.66002900	36	H	-3.33539400	1.29005200	-3.14933700
36	H	-3.33539400	1.29005200	-3.14933700	37	H	-3.85290500	1.37368800	1.19299500
37	H	-3.85290500	1.37368800	1.19299500	38	H	-3.84017600	-0.00507000	2.30438800
38	H	-3.84017600	-0.00507000	2.30438800	39	H	-2.46896800	-0.12459000	-5.12424200
39	H	-2.46896800	-0.12459000	-5.12424200	40	H	-2.17531800	-1.43113600	-3.98661300
40	H	-2.17531800	-1.43113600	-3.98661300	41	H	-4.34988700	-1.53874000	0.38224400
41	H	-4.34988700	-1.53874000	0.38224400	42	H	-5.60051900	-0.34849700	0.71876500
42	H	-5.60051900	-0.34849700	0.71876500	43	C	-1.62290300	2.15398500	-0.94080100
43	C	-1.62290300	2.15398500	-0.94080100	44	O	-2.80693600	2.48228600	-1.07770600
44	O	-2.80693600	2.48228600	-1.07770600	45	O	-0.53399100	2.69444000	-0.85699200
45	O	-0.53399100	2.69444000	-0.85699200					

1.5 TS-[CoIN4H]-COO-H⁺ (Front)

1	N	0.00432700	0.01719800	-0.00744000	1	N	0.00432700	0.01719800	-0.00744000
2	C	0.00615900	0.02522800	1.33834700	2	C	0.00615900	0.02522800	1.33834700
3	C	0.83784800	0.01233000	-2.16876900	3	C	0.83784800	0.01233000	-2.16876900
4	C	1.13938300	-0.03753900	-0.72745200	4	C	1.13938300	-0.03753900	-0.72745200
5	C	2.37709300	-0.10971200	-0.08409500	5	C	2.37709300	-0.10971200	-0.08409500
6	C	1.21133900	-0.04238100	2.03933600	6	C	1.21133900	-0.04238100	2.03933600
7	C	2.40148700	-0.11685800	1.31187300	7	C	2.40148700	-0.11685800	1.31187300
8	H	3.29996600	-0.16528700	-0.64796200	8	H	3.29996600	-0.16528700	-0.64796200
9	H	3.34977100	-0.17868900	1.83435600	9	H	3.34977100	-0.17868900	1.83435600
10	H	1.23084400	-0.04536800	3.12207500	10	H	1.23084400	-0.04536800	3.12207500
11	H	2.91387200	-0.08836000	-2.74534000	11	H	2.91387200	-0.08836000	-2.74534000
12	Co	-1.61117200	0.01274700	-0.89118200	12	Co	-1.61117200	0.01274700	-0.89118200
13	C	-1.36956000	0.12150600	1.85633000	13	C	-1.36956000	0.12150600	1.85633000
14	N	-0.44105000	0.05747500	-2.43989500	14	N	-0.44105000	0.05747500	-2.43989500
15	C	1.92539400	0.04157200	-3.19995600	15	C	1.92539400	0.04157200	-3.19995600

16	N	-3.34484300	0.22346300	-1.84867000
17	N	-2.28554100	0.14293700	0.92390500
18	C	-1.65230300	0.20486600	3.32609000
19	C	-0.83557200	0.19890600	-3.85176500
20	H	1.81687300	0.90652000	-3.86262000
21	H	1.88686900	-0.85549800	-3.82896600
22	C	-4.44457000	0.82207200	-1.05210100
23	C	-3.24119200	0.82207400	-3.20404800
24	H	-3.58134700	-0.76511700	-1.98604900
25	C	-3.68845200	0.30115800	1.34202300
26	H	-2.29546100	1.05956000	3.55771300
27	H	-2.17224100	-0.69756900	3.66915100
28	H	-0.73778700	0.30402500	3.90913000
29	C	-2.32570600	-0.01539900	-4.09602900
30	H	-0.26672600	-0.50208800	-4.47185200
31	H	-0.55589300	1.21177800	-4.17559200
32	H	-5.35858200	0.83580500	-1.65890100
33	H	-4.19122800	1.86455500	-0.82556600
34	C	-4.68603600	0.01753800	0.22421500
35	H	-4.24255300	0.87047600	-3.64979300
36	H	-2.87846700	1.85254300	-3.10936800
37	H	-3.82146500	1.33392300	1.69477200
38	H	-3.90320900	-0.35642600	2.19101900
39	H	-2.52274200	0.24028800	-5.14194600
40	H	-2.57633600	-1.07550500	-3.98062700
41	H	-4.69111500	-1.05261200	-0.01438000
42	H	-5.68343100	0.25328700	0.60840600
43	C	-1.71548900	-2.11870700	-0.87378900
44	O	-0.87443400	-2.58025100	-0.13912500
45	O	-2.62764600	-2.41748500	-1.62430200
46	H	-1.20148200	-4.75966700	-0.26727100

1.6 [CoIN4H]-COOH (Front)

1	N	0.03632000	-0.14126600	0.00795400
2	C	0.02344000	-0.08148100	1.39403200
3	C	0.93685200	-0.03021000	-2.11341900
4	C	1.20486300	0.03293000	-0.71932000
5	C	2.40132400	0.26150000	-0.04168800
6	C	1.21690400	0.14724200	2.07718000
7	C	2.40691600	0.31751500	1.35804700
8	H	3.32456500	0.40428700	-0.59320000
9	H	3.33579400	0.50174900	1.88716000
10	H	1.22612700	0.20149100	3.16062500
11	H	1.77960700	0.96055400	-3.84561800
12	Co	-1.48693000	-0.57595600	-0.86689400
13	C	-1.29905500	-0.24791000	1.88686600
14	N	-0.36690400	-0.22930100	-2.38788700
15	C	1.99779500	0.12797600	-3.16523800
16	N	-3.25226300	-0.58780400	-1.85458800
17	N	-2.20764100	-0.40846700	0.90528300
18	C	-1.64263900	-0.22791200	3.34907300
19	C	-0.73998300	-0.23110400	-3.80349200
20	H	2.10102000	-0.77179300	-3.78543100
21	H	2.97000100	0.32377700	-2.71072000
22	C	-4.41506400	-0.12533000	-1.07296400
23	C	-3.22071900	-0.00310300	-3.20905800
24	H	-3.35028600	-1.60805100	-1.96821500
25	C	-3.60609400	-0.51513700	1.32482000
26	H	-2.37295500	0.55512400	3.58835100
27	H	-2.07456200	-1.17963700	3.68465700
28	H	-0.75455200	-0.04195600	3.95477300
29	C	-2.16640900	-0.70312300	-4.06418500
30	H	-0.05838300	-0.86372900	-4.38709100
31	H	-0.62784400	0.79112700	-4.19793100
32	H	-5.32549100	-0.23162200	-1.68166100
33	H	-4.29208200	0.94160300	-0.85024500
34	C	-4.55222900	-0.94503000	0.20890100
35	H	-4.21128900	-0.11598500	-3.67480100
36	H	-3.01754700	1.07165700	-3.12781800
37	H	-3.93385300	0.46353600	1.70948700
38	H	-3.71221700	-1.22466200	2.15590700
39	H	-2.38920700	-0.52794300	-5.12280300
40	H	-2.23873000	-1.78415200	-3.89917600
41	H	-4.39383500	-2.00308900	-0.02936100
42	H	-5.57755700	-0.85402600	0.58494800
43	C	-1.50433200	-2.48256000	-0.97993100
44	O	-0.45490900	-3.15717300	-0.42377600
45	O	-2.37791200	-3.15996800	-1.50953800
46	H	0.13673900	-2.48508300	-0.05290300

1.7 TS-[CoIN4H]-COOH-H⁺ (Front)

1	N	-0.01141400	0.00586900	-0.00112700
2	C	-0.00842200	0.00820100	1.34326500
3	C	0.81851700	-0.00670900	-2.18815800
4	C	1.10159100	-0.18150000	-0.73751400
5	C	2.31557500	-0.45544000	-0.10427500
6	C	1.17506900	-0.26265100	2.03449300
7	C	2.33647200	-0.50757500	1.29443300
8	H	3.22496500	-0.61654300	-0.67030800
9	H	3.26663800	-0.72374600	1.80978300
10	H	1.20530600	-0.27525700	3.11713700
11	H	1.99841500	0.79858000	-3.78561800
12	Co	-1.59445100	0.46269600	-0.88666000
13	C	-1.33851500	0.39678400	1.88445300
14	N	-0.42532600	0.28774000	-2.45640200
15	C	1.89595500	-0.13296000	-3.21699300
16	N	-3.16799700	1.25573000	-1.80075200
17	N	-2.21880600	0.69382400	0.96865900
18	C	-1.58742300	0.48409700	3.35563100
19	C	-0.79279500	0.54589900	-3.86580900
20	H	1.65002500	-0.92041100	-3.93927100
21	H	2.86366000	-0.36895800	-2.77806300
22	C	-3.93828300	2.19929700	-0.93114800
23	C	-2.88532500	1.83438600	-3.14794600
24	H	-3.78712500	0.45548700	-1.95465500
25	C	-3.53264400	1.21165700	1.40928900

26	H	-1.81323000	1.51647500	3.64922700
27	H	-2.45510200	-0.12364100	3.63586600
28	H	-0.73545300	0.14415700	3.94175400
29	C	-2.28440600	0.78018100	-4.07459400
30	H	-0.46001200	-0.29423800	-4.48512100
31	H	-0.23193300	1.43002100	-4.19694500
32	H	-4.74978400	2.62884800	-1.52799300
33	H	-3.27998600	3.02554000	-0.63798200
34	C	-4.52275700	1.47012700	0.27614800
35	H	-3.82625200	2.20664400	-3.56659800
36	H	-2.22080600	2.69754300	-3.02752000
37	H	-3.34239400	2.14855400	1.94957400
38	H	-3.97492600	0.51319600	2.12768900
39	H	-2.41711700	1.10386600	-5.11124000
40	H	-2.84155000	-0.16026300	-3.98205700
41	H	-4.98553700	0.53281200	-0.04892000
42	H	-5.32999000	2.07973800	0.69278300
43	C	-2.31434800	-1.31527900	-0.98546100
44	O	-1.51509300	-2.37800900	-0.96115200
45	O	-3.50860700	-1.42239300	-1.06005900
46	H	-0.58034300	-2.13961000	-0.89923500
47	H	-4.11502100	-3.76041600	-1.14309900

1.8 [CoIN4H]-HCOOH (Front)

1	N	0.00752400	-0.14953500	0.00105900
2	C	0.00122500	-0.07900000	1.35123300
3	C	0.88410200	-0.00618200	-2.16368700
4	C	1.15409400	-0.12425700	-0.71475400
5	C	2.38797800	-0.12887800	-0.05912400
6	C	1.20680100	-0.08315400	2.05743800
7	C	2.40436400	-0.12596500	1.33831700
8	H	3.31762600	-0.11647700	-0.61454100
9	H	3.35164800	-0.12855800	1.86703900
10	H	1.22251800	-0.03557800	3.13933000
11	H	1.96626900	1.00644500	-3.71568900
12	Co	-1.62697300	-0.11656100	-0.91200200
13	C	-1.37083300	0.08320900	1.87768600
14	N	-0.38504600	0.08610400	-2.45740800
15	C	1.99247700	0.05658100	-3.16957500
16	N	-3.31993900	0.34204000	-1.86775000
17	N	-2.28539000	0.16182600	0.94897300
18	C	-1.64301800	0.20195000	3.34602200
19	C	-0.75801600	0.30376800	-3.86671900
20	H	1.89099000	-0.74247500	-3.91270600
21	H	2.97478100	-0.03915200	-2.71031500
22	C	-4.31986900	1.07487400	-1.03113400
23	C	-3.12073900	1.02394100	-3.18396100
24	H	-3.75648100	-0.55581600	-2.08972300
25	C	-3.67601600	0.42303300	1.36244800
26	H	-2.09555800	1.17281800	3.57846100
27	H	-2.35000200	-0.56775100	3.67532100
28	H	-0.73909700	0.10159900	3.94417800
29	C	-2.25674300	0.18567200	-4.12246200
30	H	-0.22047500	-0.40095500	-4.51011100
31	H	-0.41905300	1.31082500	-4.14559000
32	H	-5.21741600	1.24212000	-1.63644500
33	H	-3.90669600	2.05863400	-0.78389200
34	C	-4.68157700	0.28595400	0.22496600
35	H	-4.10455000	1.19232800	-3.63542200
36	H	-2.67619900	2.00755300	-2.99850600
37	H	-3.71422000	1.44556400	1.76203500
38	H	-3.95694100	-0.24755000	2.18163400
39	H	-2.43705800	0.51352900	-5.15061800
40	H	-2.57378700	-0.86380100	-4.08348400
41	H	-4.83374500	-0.77004500	-0.03055300
42	H	-5.64544300	0.64450000	0.59805800
43	C	-1.93490100	-2.09585300	-1.03319400
44	O	-1.18957300	-3.08063000	-0.58695300
45	O	-3.00503300	-2.57090100	-1.61782100
46	H	-0.38994300	-2.75013800	-0.14887800
47	H	-3.04308600	-3.55287900	-1.60994700

1.9 TS-[CoIN4H]-COO-H₂ Formation (Front)

1	N	0.00988400	-0.06710900	-0.00088200
2	C	-0.00635600	-0.07828800	1.34175500
3	C	0.86178700	-0.00576300	-2.17354300
4	C	1.14236200	-0.12357600	-0.72012500
5	C	2.37307700	-0.24186100	-0.07078700
6	C	1.19125400	-0.19456000	2.05059700
7	C	2.38403200	-0.28688900	1.32672700
8	H	3.30165600	-0.29624400	-0.62550800
9	H	3.32718300	-0.38305100	1.85429000
10	H	1.20753900	-0.21185400	3.13338300
11	H	1.90433600	0.95109200	-3.78527700
12	Co	-1.62377500	0.02022300	-0.91313600
13	C	-1.38725400	0.08191900	1.86340300
14	N	-0.40687200	0.08835500	-2.46689400
15	C	1.96545400	0.03839700	-3.18226900
16	N	-3.33082900	0.37444700	-1.87227000
17	N	-2.30264000	0.16307700	0.93626500
18	C	-1.66294600	0.17988100	3.33037600
19	C	-0.78657000	0.29983200	-3.87817700
20	H	1.88981500	-0.80878200	-3.874

34	C	-4.70271000	0.27889400	0.20889900	17	N	-2.26882500	-0.31533100	0.92617400
35	H	-4.14219500	1.17648800	-3.65127000	18	C	-1.63778900	-0.11261000	3.31278100
36	H	-2.72094600	2.02650500	-3.04609000	19	C	-0.78928200	-0.04287800	-3.89150400
37	H	-3.74257800	1.43592500	1.75458200	20	H	2.93673900	0.30436900	-2.72981400
38	H	-3.97304400	-0.26308900	2.16146300	21	H	1.74378300	0.95795000	-3.85816000
39	H	-2.46542700	0.49508200	-5.16250300	22	C	-4.42510600	0.22561100	-1.06757400
40	H	-2.60435800	-0.86794900	-4.07781400	23	C	-3.24111800	0.28006500	-3.22378600
41	H	-4.84558300	-0.77641500	-0.05428600	24	H	-3.56665600	-1.34384400	-2.03196800
42	H	-5.66917400	0.62442800	0.58794200	25	C	-3.68627000	-0.24244200	1.34069800
43	C	-1.85418600	-2.06992100	-0.99459900	26	H	-2.31723500	0.72295000	3.51223700
44	O	-0.99033700	-2.77271500	-0.46284400	27	H	-2.13032000	-1.02169900	3.67924900
45	O	-2.84602600	-2.52832300	-1.57031900	28	H	-0.73372800	0.03976200	3.89934600
46	H	-1.63005700	-3.98076300	-0.80817800	29	C	-2.24558400	-0.41591400	-4.14491100
47	H	-2.46478500	-3.89455200	-1.30537800	30	H	-0.13913100	-0.65252300	-4.52647700
					31	H	-0.62667500	1.00527700	-4.17656400
					32	H	-5.32896900	0.21420100	-1.68575300
					33	H	-4.18575500	1.27645600	-0.86852300
					34	C	-4.67376200	-0.55085900	0.22087000
					35	H	-4.24246600	0.24365600	-3.66556700
					36	H	-2.98936900	1.33776300	-3.08587800
					37	H	-3.86413800	0.77468600	1.71530600
					38	H	-3.85796100	-0.92623800	2.17814200
					39	H	-2.47568100	-0.13744900	-5.17791500
					40	H	-2.38232400	-1.50356300	-4.09276500
					41	H	-4.69514100	-1.62435400	0.01116300
					42	H	-5.67003600	-0.29137700	0.59151100
					43	C	-1.50180700	-2.35806300	-0.71486400
					44	O	-0.55440100	-2.90577300	-0.21987700
					45	O	-2.70917500	-2.93552900	-0.91661700
					46	H	-2.64960000	-3.87833800	-0.66180700
					47	H	-1.00050300	-2.56122700	-2.58624800

1.10 Formate + Catalyst (Front)

1	N	-0.05061400	-0.21301700	-0.04215500
2	C	-0.04102300	-0.25160200	1.34217200
3	C	0.83030100	-0.07684500	-2.16112700
4	C	1.12329400	-0.18042900	-0.77399300
5	C	2.35185300	-0.24318900	-0.10928300
6	C	1.18262100	-0.31798800	2.01944000
7	C	2.37410800	-0.31782000	1.28842800
8	H	3.28088900	-0.22950400	-0.66901000
9	H	3.32516900	-0.36807900	1.80944000
10	H	1.20830700	-0.36218900	3.10294700
11	H	1.79354300	0.89054900	-3.84882000
12	Co	-1.61803900	-0.11228100	-0.90305400
13	C	-1.36866200	-0.20280000	1.84161100
14	N	-0.50329400	-0.04711300	-2.41750600
15	C	1.89482400	-0.00218400	-3.21850000
16	N	-3.36834800	-0.27162500	-1.85767700
17	N	-2.30443500	-0.14681900	0.85311300
18	C	-1.69096600	-0.19185600	3.30896200
19	C	-0.89867600	0.11617100	-3.81202000
20	H	1.88257200	-0.87066500	-3.89202100
21	H	2.88517600	0.03541800	-2.76195200
22	C	-4.55167500	0.23532900	-1.12034900
23	C	-3.39589000	0.20037200	-3.26250400
24	H	-3.46664900	-1.29119100	-1.88981900
25	C	-3.68868800	0.02946500	1.28144600
26	H	-2.26402200	0.69698400	3.60386400
27	H	-2.27902800	-1.06683700	3.61868200
28	H	-0.77446900	-0.19616000	3.90103400
29	C	-2.29281200	-0.43332300	-4.10606400
30	H	-0.19498100	-0.38514800	-4.48722600
31	H	-0.88009300	1.18455800	-4.08676100
32	H	-5.45537100	0.06035100	-1.72359400
33	H	-4.44168800	1.31972100	-1.00761500
34	C	-4.70208300	-0.43544300	0.23967100
35	H	-4.37885500	-0.02855700	-3.70155500
36	H	-3.29220100	1.29136600	-3.25474700
37	H	-3.87889600	1.09334400	1.50322900
38	H	-3.89235800	-0.51557800	2.21142300
39	H	-2.52166900	-0.25870300	-5.15881800
40	H	-2.30168400	-1.52170500	-3.95362900
41	H	-4.63793900	-1.52358600	0.11268400
42	H	-5.70874300	-0.22329800	0.61898200
43	C	-2.16273200	-3.62493000	-0.25934600
44	O	-1.89086700	-4.69632400	0.21697000
45	O	-3.13125400	-3.45494100	-1.20598300
46	H	-3.49957700	-4.33919900	-1.38092300
47	H	-1.70602000	-2.65195800	-0.02865100

1.11 TS-[CoIN4H]-Formate Formation (Front)

1	N	0.05643300	-0.21808500	-0.00881300
2	C	0.04093400	-0.21150800	1.33108000
3	C	0.88539300	-0.07671400	-2.18386300
4	C	1.18214700	-0.13494600	-0.73059600
5	C	2.41915300	-0.08251900	-0.08387400
6	C	1.24225900	-0.15895300	2.04000100
7	C	2.43671100	-0.10861200	1.31389800
8	H	3.34640500	-0.02553000	-0.64077900
9	H	3.38487400	-0.07802500	1.84038000
10	H	1.26121100	-0.15982200	3.12289600
11	H	2.06556400	-0.77571300	-3.82523200
12	Co	-1.57669500	-0.42336900	-0.91486400
13	C	-1.35015300	-0.22897900	1.85015400
14	N	-0.38248100	-0.18410000	-2.47691400
15	C	1.97028900	0.11725700	-3.19443000
16	N	-3.30717300	-0.36652500	-1.87423900

1.12 TS-[CoIN4H]-Bicarbonate Formation (Front)

1	N	0.05720500	-0.11018200	-0.01432000
2	C	0.04762200	-0.03806800	1.32798700
3	C	0.88799000	-0.00924900	-2.19586600
4	C	1.18573700	-0.02451600	-0.74137500
5	C	2.42090600	0.08586700	-0.09900400
6	C	1.25061000	0.07139600	2.02855000
7	C	2.44227400	0.11886500	1.29876900
8	H	3.34515600	0.14877900	-0.66021700
9	H	3.39012300	0.19820200	1.82070900
10	H	1.27052800	0.12174800	3.11024300
11	H	2.94465200	0.33042000	-2.75637800
12	Co	-1.57005200	-0.34197300	-0.90582100
13	C	-1.33985200	-0.04365200	1.85807300
14	N	-0.38015600	-0.13094600	-2.47987800
15	C	1.96821600	-0.18214200	-3.21398100
16	N	-3.30713800	-0.39432600	-1.86250900
17	N	-2.26024800	-0.15933200	0.94190100
18	C	-1.61811400	0.09999900	3.32088400
19	C	-0.80065900	-0.02173100	-3.89100000
20	H	1.75490800	1.05114500	-3.84594900
21	H	2.03540500	-0.68881400	-3.87671800
22	C	-4.45631600	0.15765000	-1.07589400
23	C	-3.26929100	0.20969100	-3.23265000
24	H	-3.51805600	-1.38892000	-2.00125800
25	C	-3.67774700	-0.11508400	1.35136800
26	H	-2.33996000	0.90171400	3.50591900
27	H	-2.05283100	-0.82617100	3.71754400
28	H	-0.71786600	0.31839300	3.89270000
29	C	-2.23845800	-0.47242400	-4.12787100
30	H	-0.12580000	-0.60233300	-4.52790300
31	H	-0.69224800	1.03103300	-4.18617600
32	H	-5.36336200	0.05251700	-1.68033700
33	H	-4.28910700	1.23040800	-0.92851500
34	C	-4.63456600	-0.56919800	0.25408900
35	H	-4.26551100	0.10900500	-3.67625000
36	H	-3.06786700	1.28183500	-3.13153400
37	H	-3.90850100	0.92084500	1.63539000
38	H	-3.82454900	-0.73333600	2.24231100
39	H	-2.48018000	-0.24269600	-5.17014400
40	H	-2.32590000	-1.56186400	-4.03508100
41	H	-4.56237100	-1.65279100	0.10170500
42	H	-5.65079500	-0.38538800	0.61575500
43	C	-1.55348500	-2.57465500	-0.57563400
44	O	-1.41964100	-3.08156500	0.46497600
45	O	-2.64275400	-3.24605700	-1.75420600
46	H	-2.70812900	-4.22086000	-1.70108500