

Electronic Supplementary Information

**The Cooperative Role of Innocent Ligand in *N*-heterocyclic  
Carbene Manganese Catalyzed Carbon Dioxide  
Hydrogenation**

Yaru Jing,<sup>a</sup> Jiahao Liu,<sup>b</sup> Zongren Ye,<sup>b</sup> Jiaqi Su,<sup>a</sup> Yan Liu<sup>\*a</sup> and Zhuofeng Ke<sup>\*b</sup>

<sup>a</sup>School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, P. R. China

<sup>b</sup>School of Materials Science and Engineering, PCFM Lab, Sun Yat-sen University, Guangzhou 510275, P. R. China.

Corresponding authors:

E-mail: kezhf3@mail.sysu.edu.cn

E-mail: yanliu@gdut.edu.cn

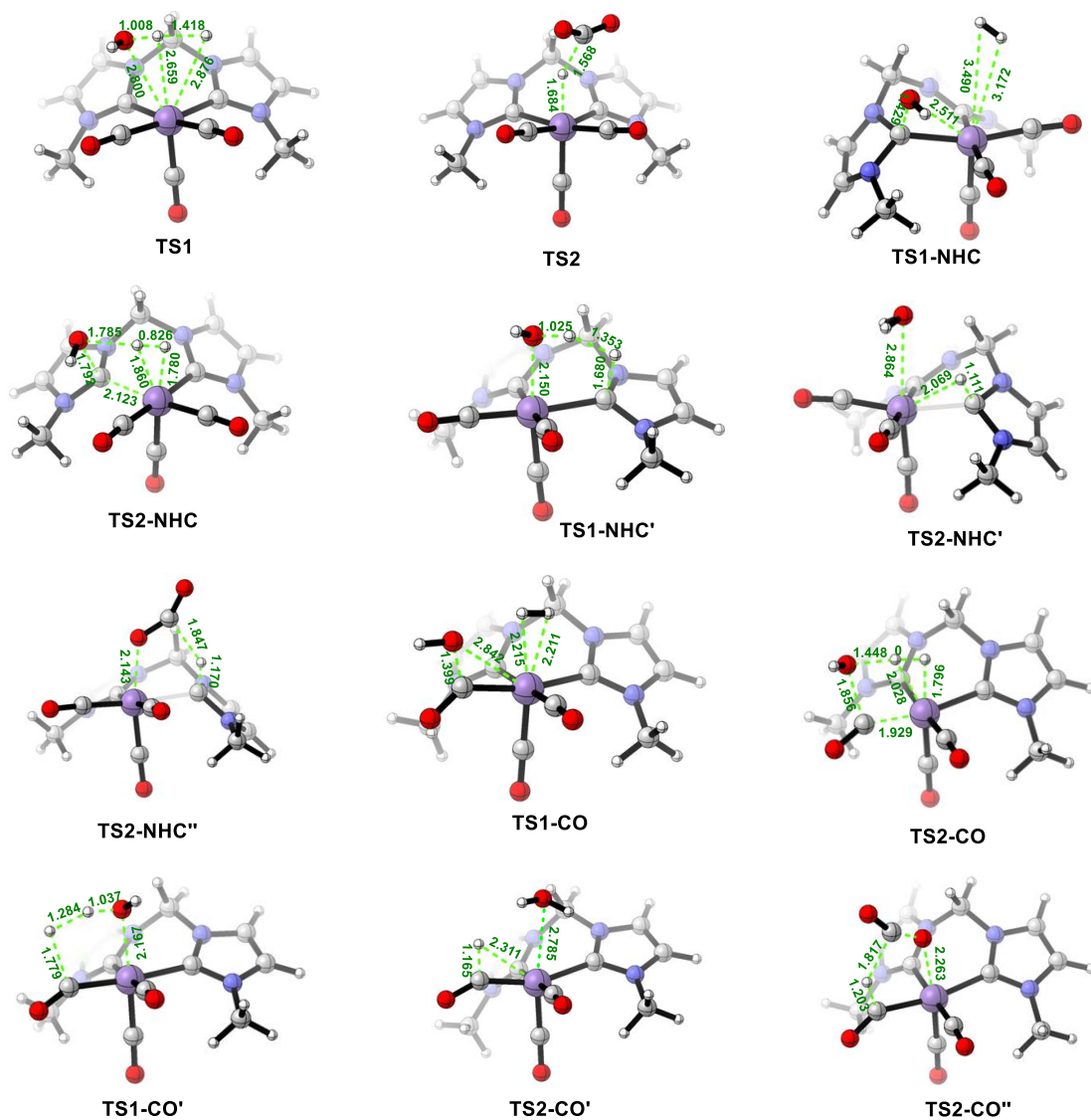


Fig. S1 3D structures of all transition states in the manuscript.

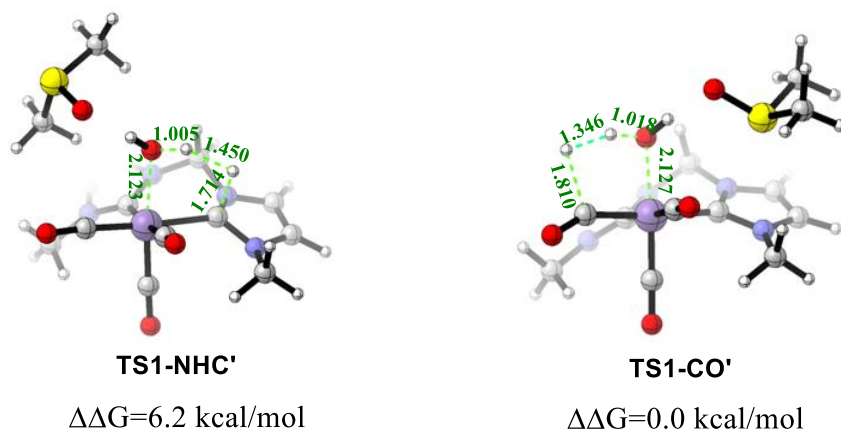


Fig. S2 3D structures of TS1-NHC' and TS1-CO' using the explicit solvent model.

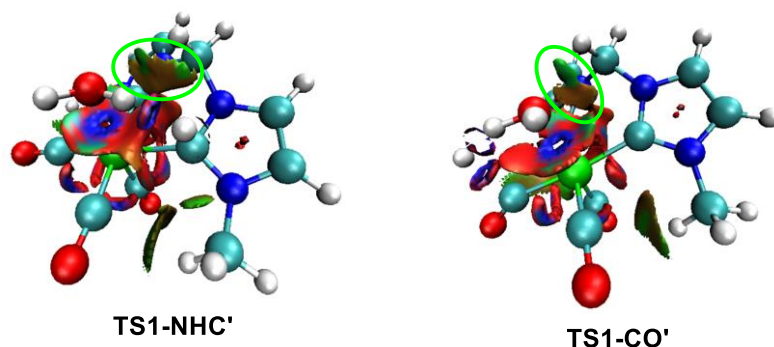


Fig. S3 Noncovalent interaction analyses of TS1-NHC' and TS1-CO'.

### Cartesian coordinates of all intermediates and transition states

<b>Cat</b>				C	-0.001130	-0.673435	-2.088037
N	1.186117	1.924474	0.464431	O	-0.002584	-0.613402	-3.259405
N	2.605367	0.905085	-0.760960	Mn	0.000051	-0.764616	-0.343440
C	-0.000630	2.209354	1.240919	Br	0.001755	-1.012682	2.294724
C	2.267115	2.776970	0.340632	<b>I</b>			
C	3.168153	2.126133	-0.434282	N	-1.200617	1.863768	-0.403493
C	1.374451	0.751538	-0.201371	N	-2.602315	0.623627	0.622975
C	-1.375843	0.750207	-0.200021	C	-0.017904	2.288568	-1.124586
C	-2.268797	2.775780	0.341079	C	-2.283714	2.670842	-0.109980
C	-3.170070	2.124150	-0.432879	C	-3.174968	1.881570	0.537634
N	-2.607032	0.903115	-0.759187	C	-1.376518	0.587047	0.033170
N	-1.187617	1.923562	0.465133	C	1.373229	0.606539	0.017613
H	-0.000134	1.573610	2.131054	C	2.237878	2.710392	-0.099998
H	-0.000950	3.263129	1.513855	C	3.145870	1.930774	0.536464
C	-3.296359	-0.088123	-1.562724	N	2.599120	0.660608	0.606845
H	-4.069374	0.410838	-2.146885	N	1.171657	1.885169	-0.402722
H	-2.598665	-0.575428	-2.243877	H	-0.015210	1.767398	-2.085736
H	-3.765970	-0.843347	-0.928208	H	-0.027610	3.374067	-1.213791
H	4.144331	2.416705	-0.789900	C	3.295055	-0.467376	1.194977
H	2.287568	3.750235	0.805536	H	3.938521	-0.111390	2.000492
H	-2.289327	3.749322	0.805401	H	2.574821	-1.176229	1.602228
H	-4.146583	2.414141	-0.788057	H	3.911376	-0.975055	0.448188
C	-1.260395	-2.044696	-0.283507	H	-4.149353	2.093529	0.949580
O	-2.023148	-2.924618	-0.233678	H	-2.313498	3.713897	-0.383435
C	1.262468	-2.042687	-0.285473	H	2.246468	3.757283	-0.359784
O	2.027160	-2.920998	-0.236639	H	4.115729	2.158204	0.950773
C	3.294311	-0.085517	-1.565626	O	-0.088245	-0.287129	-2.236661
H	3.762895	-0.842197	-0.932095	C	1.279679	-2.079315	-0.686945
H	2.596559	-0.571066	-2.248014	O	2.081428	-2.867667	-1.007933
H	4.068053	0.413754	-2.148548	C	-1.264775	-2.076163	-0.718985

O	-2.067270	-2.843558	-1.077678	H	-3.090624	0.168705	-2.242547
C	-3.273753	-0.502535	1.240928	H	0.584106	-0.573273	-2.647975
H	-2.546728	-1.280588	1.467470				
H	-3.751838	-0.179673	2.167127	<b>TS1</b>			
H	-4.036148	-0.910855	0.572175	N	1.245305	1.875751	0.380226
C	0.013800	-1.364774	1.453262	N	2.699360	0.593886	-0.516361
O	0.020058	-1.686051	2.583997	C	0.042696	2.293572	1.061343
Mn	0.007437	-0.906095	-0.249990	C	2.354996	2.664069	0.146603
H	0.801602	-0.448604	-2.565904	C	3.275828	1.848949	-0.423436
				C	1.441583	0.585131	-0.003756
<b>I-1</b>				C	-1.297870	0.635290	-0.165903
N	-1.170968	1.878127	-0.293702	C	-2.175601	2.730169	-0.029288
N	-2.550010	0.617080	0.737703	C	-3.047103	1.962917	-0.728338
C	-0.013043	2.322389	-1.044204	N	-2.492126	0.697859	-0.809710
C	-2.271231	2.664659	-0.008756	N	-1.116869	1.903598	0.292486
C	-3.148022	1.861586	0.642729	H	0.009469	1.807673	2.043725
C	-1.326116	0.599847	0.145107	H	0.049775	3.375568	1.178738
C	1.415987	0.606151	0.005295	C	-3.161481	-0.409524	-1.465368
C	2.286946	2.706921	-0.119875	H	-3.725325	-0.030167	-2.318117
C	3.218488	1.913124	0.461980	H	-2.427836	-1.130358	-1.823813
N	2.667729	0.645125	0.538241	H	-3.849923	-0.906215	-0.777305
N	1.202583	1.891933	-0.386217	H	4.274892	2.042596	-0.781175
H	-0.050932	1.847491	-2.027015	H	2.377879	3.712935	0.396217
H	-0.021020	3.410764	-1.092965	H	-2.199926	3.770004	0.255484
C	3.381635	-0.494140	1.080931	H	-3.995422	2.197634	-1.185870
H	4.063865	-0.151507	1.859806	O	-1.224296	-0.260270	2.645910
H	2.674816	-1.201550	1.513122	C	-1.315948	-2.046670	0.503083
H	3.959721	-0.997658	0.301698	O	-2.154646	-2.838257	0.669905
H	-4.124220	2.058242	1.057828	C	1.248950	-2.100109	0.735602
H	-2.318061	3.707219	-0.281858	O	2.002211	-2.938226	1.029412
H	2.289765	3.757493	-0.364585	C	3.414945	-0.562378	-1.021108
H	4.208180	2.128764	0.833419	H	2.716657	-1.273825	-1.459032
O	-0.185205	-0.233958	-2.180570	H	4.117866	-0.239598	-1.789433
C	1.274434	-2.070471	-0.727703	H	3.969231	-1.052177	-0.216533
O	2.056504	-2.862130	-1.088134	C	0.145050	-1.356801	-1.448084
C	-1.262427	-2.060719	-0.645338	O	0.222398	-1.669845	-2.574133
O	-2.067212	-2.835642	-0.980899	Mn	0.022219	-0.878682	0.215826
C	-3.212111	-0.532641	1.319796	H	-0.226796	-0.270471	2.792253
H	-2.468430	-1.252010	1.660849	H	1.190400	-0.223249	2.761110
H	-3.815335	-0.212355	2.170284	H	-1.507726	-1.125849	2.964754
H	-3.863280	-1.014153	0.584196				
C	0.112927	-1.387074	1.474218	<b>I-2</b>			
O	0.163659	-1.734488	2.595927	N	-1.237885	1.891957	-0.470315
Mn	0.031611	-0.896051	-0.217299	N	-2.796717	0.658539	0.307703
H	-2.350927	0.051211	-2.339612	C	0.043212	2.289106	-1.002891

C	-2.327899	2.723995	-0.289630	N	1.182123	1.861027	-0.487491
C	-3.317307	1.937855	0.198005	H	0.000233	1.785901	-2.190822
C	-1.502821	0.603788	-0.111477	H	0.000075	3.352297	-1.318483
C	1.207359	0.544553	0.266942	C	3.269416	-0.517665	1.121026
C	2.160480	2.617347	0.310393	H	3.752266	-0.202407	2.047396
C	2.960431	1.783485	1.017408	H	2.544510	-1.299255	1.342333
N	2.361785	0.533887	0.989053	H	4.028822	-0.917905	0.444014
N	1.102349	1.844214	-0.129608	H	-4.116263	2.094218	0.890398
H	0.181004	1.823536	-1.985884	H	-2.273079	3.724595	-0.417423
H	0.077661	3.373610	-1.093588	H	2.273497	3.724425	-0.417786
C	2.956773	-0.630242	1.614553	H	4.116768	2.093882	0.889753
H	3.396259	-0.342738	2.570814	C	1.277357	-2.039336	-0.889675
H	2.192473	-1.386601	1.785849	O	2.100123	-2.779196	-1.272412
H	3.740688	-1.051465	0.978377	C	-1.277595	-2.038878	-0.889952
H	-4.332398	2.165537	0.483311	O	-2.100716	-2.778274	-1.272818
H	-2.292973	3.777332	-0.519091	C	-3.269338	-0.517488	1.121111
H	2.234825	3.670347	0.088534	H	-2.544627	-1.299536	1.341439
H	3.883335	1.960715	1.547459	H	-3.751049	-0.202464	2.048155
O	2.746261	0.176732	-2.398167	H	-4.029592	-0.916976	0.444621
C	1.149868	-2.086955	-0.590839	C	-0.000133	-1.445979	1.337664
O	1.963934	-2.880699	-0.869583	O	-0.000137	-1.827685	2.447429
C	-1.360910	-2.015848	-0.905059	Mn	-0.000003	-0.917342	-0.362898
O	-2.136877	-2.754313	-1.376320	H	0.000364	-0.358234	-1.890053
C	-3.580755	-0.471731	0.763977				
H	-2.923559	-1.221609	1.202666	<b>II-1</b>			
H	-4.292160	-0.133637	1.518409	N	-1.513833	1.678095	-0.848116
H	-4.131554	-0.922712	-0.065390	N	-3.070585	0.382724	-0.172407
C	-0.368479	-1.432391	1.462415	C	-0.195477	2.152540	-1.192467
O	-0.515399	-1.798973	2.566403	C	-2.696066	2.369281	-1.041906
Mn	-0.139051	-0.912363	-0.225878	C	-3.682654	1.543530	-0.617805
H	1.839445	-0.066777	-2.153662	C	-1.717233	0.440298	-0.312653
H	0.063063	-0.340852	-1.738295	C	0.831597	0.820179	0.592771
H	3.250381	-0.115542	-1.631856	C	1.541715	2.983039	0.422724
<b>II</b>				C	2.239813	2.399140	1.426679
N	-1.182092	1.860995	-0.487784	N	1.788570	1.092948	1.521261
N	-2.590459	0.612557	0.519661	N	0.693573	2.006338	-0.065772
C	0.000082	2.269188	-1.207784	H	0.192255	1.551233	-2.023601
C	-2.253938	2.675213	-0.169147	H	-0.251863	3.202072	-1.477242
C	-3.147912	1.880076	0.465629	C	2.338792	0.135060	2.456959
C	-1.366347	0.573866	-0.076421	H	2.622134	0.649539	3.376236
C	1.366315	0.573909	-0.076062	H	1.590520	-0.622909	2.685462
C	2.254266	2.675069	-0.169411	H	3.223128	-0.352780	2.036637
C	3.148283	1.879859	0.465231	H	-4.752882	1.673459	-0.579798
N	2.590608	0.612458	0.519623	H	-2.719589	3.367472	-1.450282

H	1.558184	3.984815	0.022876	H	3.681317	-0.628631	-1.572310
H	2.995550	2.789418	2.090219	H	2.138347	-0.676361	-2.454091
C	1.269432	-1.846575	0.220075	H	3.377050	0.516667	-2.895447
O	2.239591	-2.503800	0.241190	C	-0.401912	-0.966050	-1.995367
C	-1.107181	-2.209480	-0.632358	O	-0.600712	-1.085661	-3.143903
O	-1.660854	-3.098505	-1.156534	Mn	-0.096366	-0.816624	-0.254883
C	-3.813196	-0.747000	0.347441	H	0.181130	-0.591641	1.390352
H	-4.234663	-1.342155	-0.467110	C	1.001038	-0.981999	2.668356
H	-3.148662	-1.373825	0.940045	O	0.361209	-1.851378	3.184813
H	-4.626484	-0.388402	0.980470	O	1.949768	-0.249015	2.656232
C	-0.754615	-1.223296	1.779623				
O	-1.099967	-1.511502	2.864192	<b>III</b>			
Mn	-0.212631	-0.868854	0.119912	N	1.176643	1.818831	-0.236044
H	0.274907	-0.488253	-1.376588	N	2.383626	0.392686	-1.272007
C	2.981470	-0.505169	-2.130868	C	0.119710	2.426739	0.547278
O	2.720119	-1.311654	-2.935984	C	2.253870	2.521419	-0.744923
O	3.287460	0.310666	-1.351512	C	3.019956	1.614202	-1.397079
				C	1.241377	0.492557	-0.542357
<b>TS2</b>				C	-1.469847	0.634078	-0.105287
N	1.093404	1.899300	0.299214	C	-2.274261	2.762966	-0.067175
N	2.340601	0.932062	-1.138343	C	-3.291967	1.947245	-0.432395
C	0.029734	2.132278	1.248153	N	-2.781905	0.661781	-0.459995
C	2.136608	2.770680	0.051255	N	-1.176636	1.943556	0.122393
C	2.928078	2.153964	-0.859379	H	0.266876	2.202126	1.605911
C	1.201957	0.745570	-0.417321	H	0.152971	3.504036	0.389386
C	-1.499035	0.637784	0.032074	C	-3.596732	-0.493809	-0.784761
C	-2.364191	2.642349	0.690700	H	-4.350663	-0.202337	-1.516488
C	-3.351867	1.951444	0.071840	H	-2.976957	-1.281215	-1.211292
N	-2.807125	0.741984	-0.326382	H	-4.097799	-0.874976	0.108444
N	-1.250169	1.824219	0.654655	H	3.943831	1.722233	-1.943428
H	0.187377	1.495929	2.123971	H	2.364146	3.584871	-0.602386
H	0.042413	3.178882	1.547324	H	-2.222481	3.831814	0.067798
C	-3.581319	-0.288327	-0.990601	H	-4.319078	2.158174	-0.685135
H	-4.353588	0.182221	-1.599724	C	-1.354671	-1.980122	0.825863
H	-2.934270	-0.883756	-1.633449	O	-2.116643	-2.708034	1.323267
H	-4.058015	-0.945119	-0.258243	C	1.121953	-2.167987	0.369052
H	3.838653	2.470725	-1.343589	O	1.866834	-3.046368	0.555515
H	2.209876	3.733143	0.532597	C	2.930520	-0.840611	-1.803560
H	-2.344806	3.621654	1.142539	H	3.530175	-1.353119	-1.046952
H	-4.380029	2.206113	-0.131726	H	2.125310	-1.497785	-2.131250
C	-1.245526	-2.101853	0.209456	H	3.564452	-0.607543	-2.658986
O	-1.962479	-2.962284	0.540414	C	-0.432513	-1.470656	-1.543341
C	1.257917	-1.978472	-0.230651	O	-0.632237	-1.844615	-2.634897
O	2.128677	-2.754251	-0.159783	Mn	-0.121294	-0.900735	0.092389
C	2.917690	-0.021780	-2.065569	H	2.188140	-0.451445	1.919722

C	1.372880	0.090770	2.473648	C	0.522574	-2.172265	-1.389395
O	0.189202	-0.073527	1.999301	C	2.868919	-1.992919	-0.500591
O	1.669055	0.778147	3.449904	C	3.535233	-1.069676	0.234228
<b>TS1-NHC</b>				C	1.494096	-0.197120	-0.249055
N	-1.637855	1.552950	-0.581164	C	-1.462326	-1.017495	-0.495483
N	-2.676842	0.038533	0.509483	C	-0.517182	-2.676376	0.783763
C	-0.545971	2.259374	-1.250503	C	-1.520224	-2.128410	1.502992
C	-2.865481	2.092274	-0.253821	N	-2.244738	-1.285034	0.678185
C	-3.525409	1.126954	0.432925	N	-0.616361	-2.185048	-0.526801
C	-1.488927	0.282296	-0.120856	H	0.232622	-1.713338	-2.337714
C	1.366751	0.874933	-0.501638	H	0.871722	-3.188020	-1.581847
C	1.003655	2.835438	0.620002	C	-3.203214	-0.336009	1.162733
C	2.113731	2.270221	1.133980	H	-2.732549	0.582007	1.547566
N	2.507467	1.206207	0.315198	H	-3.882899	-0.053056	0.354570
N	0.682526	2.135205	-0.547503	H	-3.789506	-0.790280	1.963871
H	-0.420501	1.846536	-2.254306	H	4.525370	-1.076882	0.663009
H	-0.826163	3.310299	-1.326006	H	3.148718	-2.977811	-0.841675
C	3.363838	0.172855	0.834054	H	0.193258	-3.447260	1.043936
H	2.829388	-0.521907	1.501332	H	-1.834172	-2.328911	2.517698
H	3.802996	-0.405083	0.016409	O	-2.261391	-0.956123	-1.654711
H	4.181431	0.638256	1.388618	C	-1.715261	1.845325	-0.581745
H	-4.509611	1.112087	0.875128	O	-2.705647	2.465509	-0.679174
H	-3.148985	3.092833	-0.541556	C	0.746224	2.512027	-0.525426
H	0.470933	3.730842	0.903452	O	1.242949	3.571998	-0.581669
H	2.716780	2.569789	1.978543	C	3.073733	1.221279	1.080012
O	1.599172	0.481776	-1.855386	H	3.881146	0.982973	1.772632
C	1.586813	-2.010926	-0.356113	H	3.426040	1.978722	0.375169
O	2.397221	-2.861669	-0.336299	H	2.233115	1.624355	1.643660
C	-0.830292	-2.325662	-0.660838	C	-0.245919	0.984716	1.354489
O	-1.424857	-3.318915	-0.844834	O	-0.235270	1.040633	2.525082
C	-3.057680	-1.195277	1.169155	Mn	-0.157624	0.983211	-0.413590
H	-3.702947	-0.961973	2.017058	H	-0.253486	0.303563	-2.007376
H	-3.600127	-1.850865	0.482676	H	0.142328	1.017564	-2.119969
H	-2.171587	-1.714745	1.529779	H	-2.245436	-0.041517	-1.959022
C	0.249818	-0.954206	1.445642	<b>TS2-NHC</b>			
O	0.259567	-1.019527	2.620608	N	-1.287751	1.858017	-0.556866
Mn	0.191844	-0.890449	-0.292517	N	-2.732333	0.607023	0.398253
H	-0.745104	-0.480973	-3.629239	C	-0.013295	2.301141	-1.118512
H	-0.820935	-1.141316	-3.287694	C	-2.377599	2.662273	-0.296725
H	2.147366	-0.315757	-1.838014	C	-3.295745	1.866282	0.305087
<b>I-NHC</b>				C	-1.481577	0.579532	-0.141571
N	1.638258	-1.435948	-0.795762	C	1.404937	0.535220	-0.179788
N	2.685594	0.010747	0.382932	C	2.030302	2.705956	0.294617
				C	2.904594	1.890411	0.913935







**TS2-NHC"**

N	0.729726	2.115574	0.176290
N	2.287131	1.153719	-1.021767
C	-0.301350	2.267393	1.134459
C	1.104979	3.018232	-0.807814
C	2.077405	2.421876	-1.535739
C	1.372938	0.869055	0.008068
C	-1.554957	0.350518	0.155103
C	-2.764584	2.213527	0.665031
C	-3.603382	1.334320	0.064995
N	-2.852953	0.217124	-0.246315
N	-1.529006	1.596231	0.707307
H	0.031775	1.842756	2.091937
H	-0.532789	3.323003	1.274368
C	-3.419419	-0.945786	-0.902290
H	-4.329979	-0.645817	-1.421388
H	-2.714326	-1.349696	-1.629222
H	-3.665391	-1.722246	-0.174593
H	2.666055	2.795258	-2.359978
H	0.678843	4.007859	-0.864050
H	-2.922839	3.206105	1.057091
H	-4.653408	1.398221	-0.174227
C	-0.968789	-2.417465	0.129206
O	-1.521767	-3.448378	0.174808
C	1.482600	-1.986014	-0.132377
O	2.385791	-2.726547	-0.192225
C	3.166855	0.175093	-1.592583
H	2.616746	-0.581910	-2.168622
H	3.873048	0.672959	-2.258294
H	3.733261	-0.338375	-0.809201
C	-0.096252	-0.810922	-1.758234
O	-0.180880	-0.687374	-2.922240
Mn	0.025715	-0.941979	-0.022808
H	1.858092	0.538754	1.020457
C	1.369013	-0.274714	2.605126
O	2.102401	-0.247277	3.543283
O	0.349882	-0.698750	2.081324

**TS1-CO**

N	-1.942956	1.311523	-0.603394
N	-2.804665	-0.321844	0.468777
C	-0.973235	2.144600	-1.284488
C	-3.267888	1.649692	-0.390910
C	-3.812119	0.610601	0.288184

C	-1.627204	0.082753	-0.086137
C	0.876398	1.153533	0.018343
C	0.838043	3.435526	-0.126766
C	1.889955	3.089167	0.654228
N	1.896601	1.707614	0.729491
N	0.234859	2.247178	-0.496804
H	-0.738745	1.718031	-2.264172
H	-1.395576	3.139473	-1.418802
C	2.817461	0.969962	1.573160
H	2.496256	1.020847	2.617417
H	2.850035	-0.068939	1.246609
H	3.813160	1.410276	1.491016
H	-4.809894	0.454572	0.668037
H	-3.686508	2.583681	-0.731641
H	0.472992	4.394860	-0.458689
H	2.629257	3.690547	1.160201
O	2.273814	-1.224885	-2.163554
C	2.069895	-1.338562	-0.783937
O	3.024650	-1.770098	-0.141667
C	-0.336221	-2.425888	-0.563535
O	-0.650628	-3.550582	-0.709355
C	-3.000506	-1.592606	1.135429
H	-2.084417	-1.876993	1.653407
H	-3.807544	-1.496122	1.862711
H	-3.259658	-2.375146	0.417120
C	0.443211	-1.224603	1.378864
O	0.609853	-1.569524	2.495362
Mn	0.211291	-0.769724	-0.262281
H	0.263404	-0.495856	-2.459796
H	-0.472460	-0.356012	-2.323505
H	3.192305	-1.515771	-2.310283

**I-CO**

N	-1.997351	1.269725	-0.593440
N	-2.793239	-0.436097	0.414881
C	-1.060844	2.136958	-1.274847
C	-3.324951	1.563642	-0.335360
C	-3.827599	0.477807	0.301063
C	-1.638308	0.028649	-0.140965
C	0.837894	1.182989	-0.018643
C	0.715832	3.465665	-0.102049
C	1.792491	3.137895	0.651696
N	1.848826	1.755039	0.691530
N	0.152386	2.265954	-0.498278
H	-0.825090	1.721898	-2.259721

H	-1.510089	3.121001	-1.399791	H	1.367534	4.189482	-0.278359
C	2.829464	1.038292	1.483147	H	3.381237	2.988140	1.226351
H	2.600462	1.137781	2.547839	O	2.254086	-0.771227	-2.102973
H	2.818090	-0.013948	1.205360	C	1.741958	-1.705996	-0.582997
H	3.822724	1.453099	1.298855	O	2.526940	-2.558350	-0.352426
H	-4.813188	0.275681	0.690977	C	-0.804659	-2.300863	-0.675553
H	-3.774671	2.501852	-0.621043	O	-1.337166	-3.313800	-0.934296
H	0.310452	4.419751	-0.401051	C	-3.329094	-1.109491	0.908219
H	2.519876	3.751870	1.159811	H	-2.537140	-1.595781	1.477531
O	2.528590	-1.021985	-2.014297	H	-4.170552	-0.905835	1.570864
C	2.120185	-1.340152	-0.715342	H	-3.660885	-1.780738	0.111875
O	2.941035	-1.955173	-0.038659	C	0.042802	-1.289950	1.439306
C	-0.248021	-2.435055	-0.587330	O	0.026168	-1.629250	2.566998
O	-0.495292	-3.576769	-0.727393	Mn	0.066629	-0.815764	-0.236092
C	-2.944316	-1.744633	1.018032	H	0.841696	-0.452112	-2.074917
H	-2.059840	-1.987345	1.608213	H	-0.011278	-0.274540	-1.946867
H	-3.818464	-1.736411	1.669513	H	2.465366	-1.483159	-2.724052
H	-3.078798	-2.512748	0.251883				
C	0.411742	-1.121890	1.385340	<b>I-CO'</b>			
O	0.547025	-1.388235	2.522631	N	-1.168797	1.895053	-0.461314
Mn	0.221418	-0.752588	-0.308156	N	-2.591798	0.723126	0.615469
H	0.505653	-0.294994	-2.010056	C	0.019591	2.272469	-1.199417
H	-0.286781	-0.417634	-1.972859	C	-2.235457	2.733340	-0.198604
H	3.427575	-1.391210	-2.093590	C	-3.140373	1.986667	0.480055
				C	-1.367499	0.639655	0.026839
<b>TS2-CO</b>				C	1.384618	0.616317	0.016717
N	-1.642131	1.648911	-0.553682	C	2.282768	2.697865	-0.203050
N	-2.847399	0.142620	0.359968	C	3.176022	1.937428	0.475104
C	-0.512947	2.305108	-1.171249	N	2.609228	0.681206	0.607264
C	-2.881948	2.226126	-0.345896	N	1.204411	1.874880	-0.468475
C	-3.645522	1.266450	0.229700	H	0.015533	1.733561	-2.149139
C	-1.592864	0.350816	-0.129477	H	0.027933	3.354456	-1.324497
C	1.070321	0.931414	0.120981	C	3.287706	-0.414479	1.271193
C	1.533637	3.162842	0.008276	H	3.763495	-0.049609	2.182850
C	2.511523	2.575020	0.739453	H	2.566918	-1.187625	1.531043
N	2.208113	1.226045	0.803747	H	4.052938	-0.844485	0.619518
N	0.668991	2.144929	-0.353754	H	-4.109553	2.233938	0.884516
H	-0.332751	1.865025	-2.157545	H	-2.245929	3.765668	-0.511097
H	-0.731289	3.366595	-1.279997	H	2.308271	3.730121	-0.515079
C	3.062451	0.251788	1.452287	H	4.148629	2.169256	0.880574
H	2.456710	-0.552527	1.868088	O	0.013870	-0.385187	-2.205338
H	3.771764	-0.173106	0.736978	C	1.257621	-2.095749	-0.571206
H	3.613192	0.739849	2.256779	O	2.056105	-2.898751	-0.851952
H	-4.670935	1.279253	0.564358	C	-1.282113	-2.098405	-0.509156
H	-3.095590	3.247446	-0.619460	O	-2.083053	-2.919619	-0.732742

C	-3.286913	-0.371792	1.263996	H	0.888520	-0.746669	-2.573028
H	-2.566812	-1.060558	1.704509	H	1.859254	-1.565424	-2.384486
H	-3.925517	0.027529	2.052789	H	-0.674764	-0.574567	-2.809695
H	-3.908277	-0.915096	0.547211				
C	0.010080	-1.234092	1.549460	<b>H-CO'</b>			
O	0.016435	-1.472022	2.699844	N	-1.488596	1.754563	-0.359295
Mn	-0.008042	-0.887424	-0.178530	N	-2.661985	0.300891	0.670678
H	0.009366	-2.255568	-3.197380	C	-0.395957	2.380698	-1.074923
H	-0.051572	-2.933512	-3.538317	C	-2.641050	2.407229	0.042763
H	-0.918843	-0.413039	-2.444927	C	-3.387007	1.479786	0.691220
				C	-1.471352	0.438657	0.016871
<b>TS1-CO'</b>				C	1.239161	0.823275	-0.054649
N	-1.324909	1.873440	-0.333372	C	1.776473	3.045866	-0.023090
N	-2.657082	0.490837	0.598124	C	2.767113	2.375300	0.613340
C	-0.167463	2.434884	-0.994413	N	2.424306	1.035071	0.584629
C	-2.445283	2.602168	0.024375	N	0.862837	2.086734	-0.421404
C	-3.290672	1.721193	0.611497	H	-0.370382	2.016820	-2.101840
C	-1.432389	0.555509	0.004845	H	-0.547526	3.459341	-1.069731
C	1.311546	0.726612	0.027284	C	3.201456	0.014611	1.262592
C	2.089171	2.869295	-0.011217	H	3.044641	0.076713	2.342991
C	3.038980	2.099041	0.572414	H	2.900594	-0.968792	0.904087
N	2.545123	0.807512	0.595326	H	4.262274	0.170262	1.054150
N	1.049640	2.015655	-0.329645	H	-4.352238	1.550809	1.168353
H	-0.141840	2.107280	-2.033767	H	-2.817002	3.451191	-0.165450
H	-0.231423	3.521043	-0.945924	H	1.641841	4.094309	-0.239996
C	3.299544	-0.315800	1.116978	H	3.676150	2.722334	1.079909
H	4.035039	0.054752	1.831281	O	-0.182784	-0.233443	-2.443270
H	2.632395	-1.011870	1.623579	C	1.598793	-1.870009	-1.018997
H	3.818049	-0.839725	0.310476	O	2.515235	-2.560820	-0.586369
H	-4.270647	1.852619	1.042504	C	-0.882300	-2.334885	-0.525691
H	-2.527616	3.660639	-0.166750	O	-1.444889	-3.366791	-0.617303
H	2.051139	3.926326	-0.223233	C	-3.136943	-0.942480	1.241653
H	4.005940	2.347302	0.981487	H	-2.312770	-1.459527	1.734984
O	0.061572	-0.166815	-2.335928	H	-3.915773	-0.724982	1.972971
C	1.435928	-2.040896	-0.723754	H	-3.549393	-1.594806	0.467361
O	2.112259	-2.970041	-0.456323	C	0.346209	-1.357528	1.317247
C	-1.132704	-2.160458	-0.658988	O	0.523717	-1.728647	2.426025
O	-1.834537	-3.073620	-0.875859	Mn	0.078651	-0.859524	-0.312553
C	-3.257849	-0.712742	1.138639	H	0.485867	-0.763578	-2.916630
H	-2.495218	-1.325948	1.618388	H	1.584024	-1.815768	-2.190385
H	-4.005177	-0.431569	1.880832	H	-1.030317	-0.612556	-2.711871
H	-3.742970	-1.294561	0.351144				
C	0.086862	-1.354255	1.359115	<b>TS2-CO'</b>			
O	0.152882	-1.720707	2.475814	N	-1.375617	1.816480	-0.299119
Mn	0.014339	-0.843583	-0.299125	N	-2.606375	0.442055	0.771003

C	-0.259391	2.351642	-1.048646	N	-1.964703	1.642750	-1.001522
C	-2.475880	2.539977	0.124358	N	-0.483235	2.195999	0.433051
C	-3.259058	1.662202	0.799101	H	0.363898	1.617444	2.254830
C	-1.426896	0.505358	0.088080	H	0.945770	3.156568	1.584019
C	1.298279	0.746892	-0.003736	C	-2.753913	0.924780	-1.984877
C	1.980674	2.924037	-0.063093	H	-2.485518	1.252697	-2.992765
C	2.955705	2.203121	0.544611	H	-2.570487	-0.142970	-1.889795
N	2.525239	0.889271	0.570022	H	-3.814672	1.125715	-1.820131
N	0.985623	2.020891	-0.384381	H	4.824268	0.966140	-0.251552
H	-0.260941	1.922587	-2.052229	H	3.342872	2.869774	1.139941
H	-0.353133	3.434803	-1.106243	H	-0.949148	4.298327	0.600944
C	3.267667	-0.175456	1.218655	H	-2.875390	3.578751	-1.279632
H	4.334767	-0.019089	1.051276	C	-1.872414	-1.615446	-0.002873
H	3.075179	-0.173517	2.294711	O	-2.724980	-2.137842	-0.692230
H	2.968647	-1.133652	0.795235	C	0.587123	-2.389073	0.015296
H	-4.206410	1.793567	1.298685	O	0.997535	-3.487628	0.077765
H	-2.594670	3.590852	-0.089413	C	3.284831	-1.180734	-1.094741
H	1.908213	3.973004	-0.305125	H	2.539907	-1.400430	-1.860893
H	3.906097	2.501321	0.959484	H	4.247279	-0.999685	-1.573649
O	-0.868852	-0.183280	-2.765783	H	3.376566	-2.043603	-0.430657
C	1.486309	-1.748587	-1.117367	C	-0.081684	-0.946010	-1.857545
O	2.466247	-2.474729	-1.041885	O	-0.076870	-1.085737	-3.028911
C	-0.989766	-2.293787	-0.444040	Mn	-0.123060	-0.765608	-0.145961
O	-1.629941	-3.278508	-0.528091	H	-2.121449	-1.661451	1.173090
C	-3.133093	-0.766296	1.372436	C	-1.314888	-1.081188	2.694805
H	-2.321895	-1.324109	1.842913	O	-0.398374	-0.597304	2.094212
H	-3.870986	-0.496479	2.128263	O	-1.976870	-1.396949	3.618897
H	-3.609228	-1.400601	0.620153				
C	0.386352	-1.474139	1.341511				
O	0.600524	-1.921964	2.415895				
Mn	0.070287	-0.881326	-0.238229				
H	-0.548416	-1.010950	-3.149072				
H	1.238821	-1.337819	-2.179119				
H	-1.654549	-0.449602	-2.268785				

**TS2-CO''**

N	1.759439	1.460210	0.711757
N	2.895112	0.002424	-0.354185
C	0.646083	2.138752	1.338537
C	3.059558	1.933264	0.685213
C	3.778404	1.003128	0.010364
C	1.627607	0.256977	0.077759
C	-0.953900	1.113967	-0.258707
C	-1.180333	3.352338	0.136306
C	-2.119345	2.998734	-0.773923