

Supplementary Information

Electrochemical Reduction of CO₂ and N₂ to synthesize urea on Metal-Nitrogen- Doped Carbon Catalysts: A Theoretical Study

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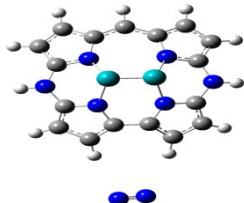
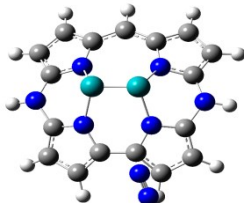
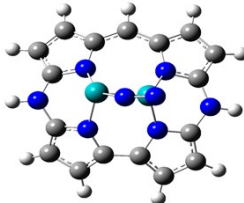
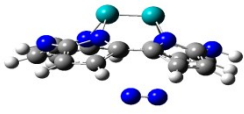
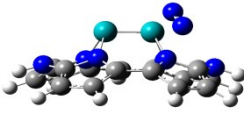
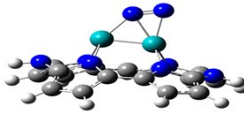
	IS1	TS1	FS1
Top view			
Side view			
Energy(eV)	-33569.79171	-33569.59515	-33571.29797

Table S1 Initial state, transition state, and final state ($* \rightarrow *N_2$). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

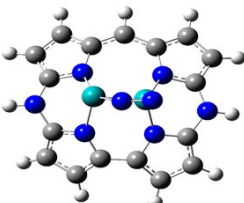
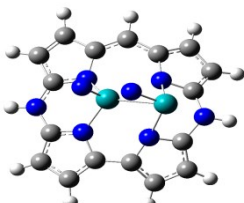
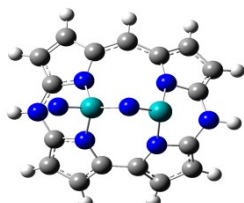
	IS2	TS2	FS2
Top view			
Side view			
Energy(eV)	-33571.29797	-33569.41866	-33570.70557

Table S2 Initial state, transition state, and final state ($*N_2 \rightarrow *NN$). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

	IS3	TS3	FS3
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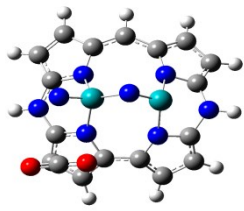
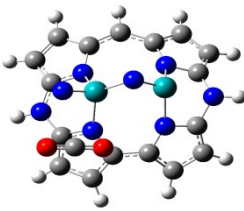
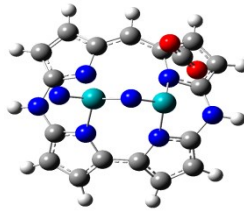
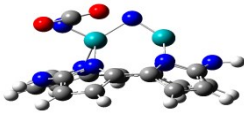
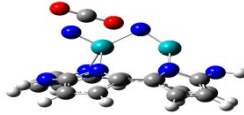
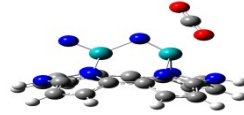
Top view			
Side view			
Energy(eV)	-38697.27763	-38697.18981	-38697.4631

Table S3 Initial state, transition state, and final state (*NN $\rightarrow$ *NCO₂N). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

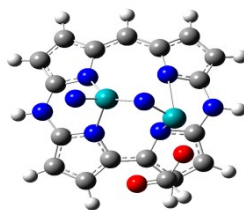
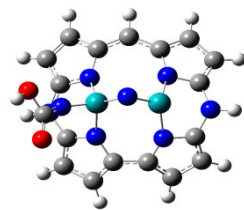
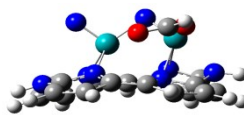
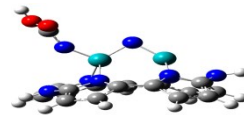
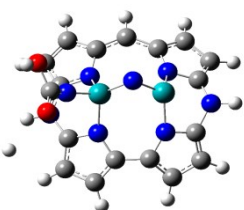
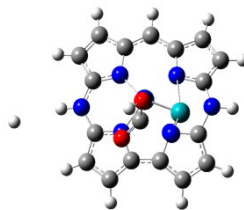
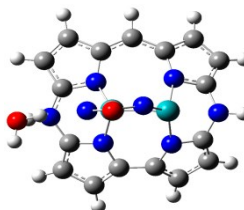
	IS4	TS4	FS4
Top view			
Side view			
Energy(eV)	-38712.59866	-38712.33775	-38713.40591

Table S4 Initial state, transition state, and final state (*NCO₂N $\rightarrow$ *NCOOHN). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

	IS5	TS5	FS5
Top view			

Side view			
Energy(eV)	-38727.212	-38726.5487	-38728.91704

Table S5 Initial state, transition state, and final state (*NCOOHN $\rightarrow$ *NCON). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

	IS6	TS6	FS6
Top view			
Side view			
Energy(eV)	-36667.57047	-36667.19989	-36668.87993

Table S6 Initial state, transition state, and final state (*NCON $\rightarrow$ *NCONH). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

	IS7	TS7	FS7
Top view			
Side view			
Energy(eV)	-36684.08306	-36683.44709	-36685.74765

Table S7 Initial state, transition state, and final state (*NCONH $\rightarrow$ *HNCONH). V atom, green; N

atoms, blue; C atoms, gray; O, red; And the H atom, white.

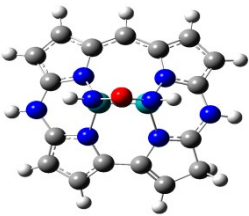
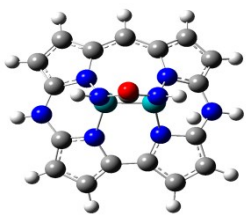
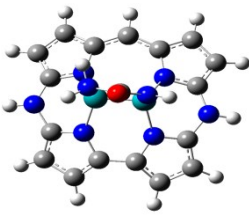
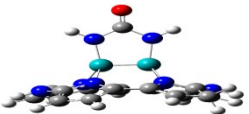
	IS8	TS8	FS8
Top view			
Side view			
Energy(eV)	-36701.45379	-36699.8814	-36701.20752

Table S8 Initial state, transition state, and final state (*HNCONH → *HNCONH₂). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

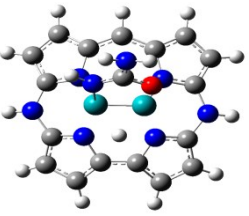
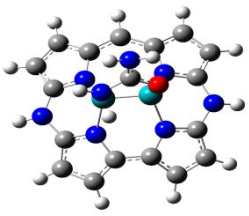
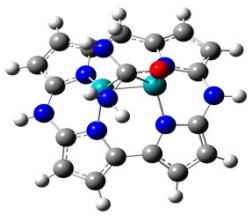
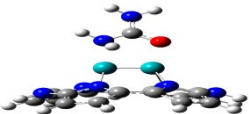
	IS9	TS9	FS9
Top view			
Side view			
Energy(eV)	-36717.39735	-36715.49001	-36716.44542

Table S9 Initial state, transition state, and final state (*HNCONH₂ → *H₂NCONH₂). V atom, green; N atoms, blue; C atoms, gray; O, red; And the H atom, white.

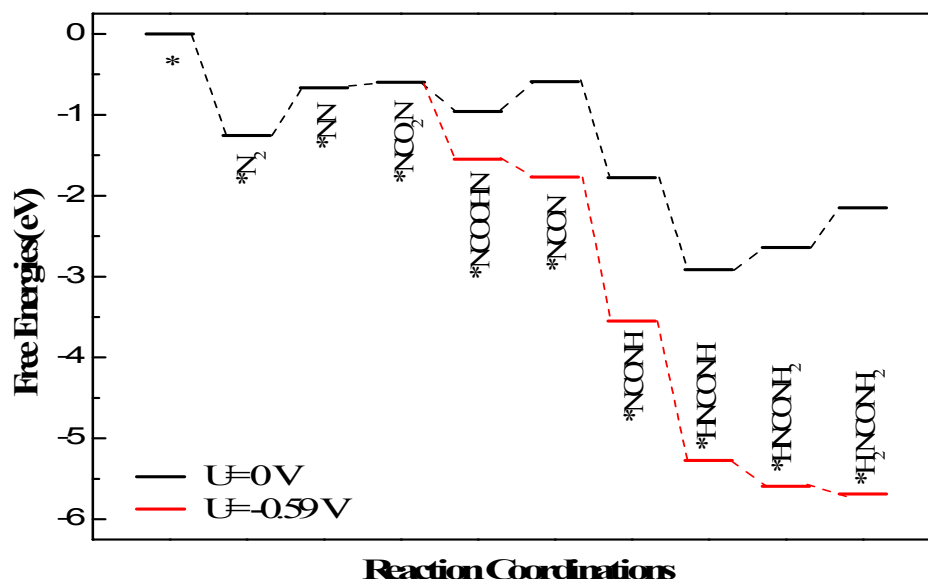


Figure S1 The free energy distribution of $\text{N}_2 + \text{CO}_2 \rightarrow \text{CO}(\text{NH}_2)_2$ on $\text{V}_2\text{N}_6\text{C}$ catalyst under the applied electric potential of -0.59V .

The coordinates of $\text{V}_2\text{N}_6\text{C}$ and each of the intermediates in Figure 5 were shown below.

The coordinates of $\text{V}_2\text{N}_6\text{C}^*$

$\text{N}, 0, 1.2943032176, 1.4775038481, -0.2037876146$
 $\text{N}, 0, 1.4201677657, -1.3107384594, -0.4262667579$
 $\text{N}, 0, -1.7252022015, -1.2375950641, -0.1218036713$
 $\text{N}, 0, -1.4298284953, 1.5416937877, 0.0625516919$
 $\text{C}, 0, 0.6384055323, 2.6398234064, -0.6271009288$
 $\text{C}, 0, 1.5368420583, 3.3706651802, -1.4089522893$
 $\text{C}, 0, 2.7338132079, 2.5907641172, -1.5660925552$
 $\text{C}, 0, 2.5261178061, 1.4194502576, -0.8500172661$
 $\text{C}, 0, 2.6784771288, -1.0660913575, -0.9187728061$
 $\text{C}, 0, 3.2048998093, -2.2399616139, -1.5316342202$
 $\text{C}, 0, 2.1926027592, -3.199442643, -1.458964709$
 $\text{C}, 0, 1.0542484186, -2.6095589252, -0.8244881735$
 $\text{C}, 0, -0.2482830624, -3.1433788844, -0.813762844$
 $\text{C}, 0, -1.5029647338, -2.5498506224, -0.5777960218$
 $\text{C}, 0, -2.7677506877, -3.0830273403, -0.9801798257$
 $\text{C}, 0, -3.729718155, -2.0772738978, -0.8604442976$
 $\text{C}, 0, -3.0418266932, -0.9326247196, -0.3637321481$
 $\text{C}, 0, -2.7635955398, 1.5420470547, -0.3364945526$
 $\text{C}, 0, -3.0504421105, 2.7227718978, -1.0079236637$
 $\text{C}, 0, -1.8109530345, 3.4464773594, -1.087542377$
 $\text{C}, 0, -0.8142964663, 2.6736878051, -0.4863826804$
 $\text{H}, 0, -4.0033170767, 3.0153785234, -1.4508383961$
 $\text{H}, 0, -1.6621996016, 4.3909280939, -1.6121954059$
 $\text{H}, 0, 1.3345525278, 4.3248490692, -1.8967884936$

H,0,3.5971374265,2.8426763116,-2.1833202066
H,0,-4.7802511352,-2.1255062888,-1.1490912631
H,0,-2.9219963087,-4.0831191534,-1.3889544422
H,0,2.2188233863,-4.2041795681,-1.8842839531
H,0,4.1771638099,-2.3357234636,-2.0161884849
H,0,-0.308424411,-4.172355032,-1.1897862321
H,0,4.1905701449,0.2592031454,-1.2258006373
H,0,-4.5218343469,0.4627571304,-0.3744856173
N,0,-3.5321728096,0.3546157502,-0.1557555273
N,0,3.2576428059,0.1964247641,-0.8200718677
V,0,-0.9313665983,0.0409550483,1.1256596215
V,0,0.9411026634,-0.0019815172,0.9441646169

The coordinates of *N₂

N,0,1.4310583964,1.52017261,0.3310421604
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N,0,-1.5440920342,-1.277337822,0.0876864573
N,0,-1.3384681205,1.4316979258,0.2238116668
C,0,0.7494494755,2.5853763002,-0.2595705597
C,0,1.6460754212,3.2546728147,-1.1063084503
C,0,2.8728963676,2.5224772495,-1.1156506772
C,0,2.6828993017,1.4549316713,-0.2422678007
C,0,2.9324858626,-0.9761669479,-0.3021763431
C,0,3.5225189298,-2.0911318326,-0.9461593198
C,0,2.5194403183,-3.0688683014,-1.0127000588
C,0,1.3281741728,-2.5313670555,-0.4367065907
C,0,0.0438337671,-3.1173075271,-0.5097526879
C,0,-1.2416915522,-2.5846087258,-0.3324430094
C,0,-2.4687604583,-3.1820798073,-0.7763506605
C,0,-3.4795942158,-2.226724003,-0.7151582698
C,0,-2.8628145141,-1.0348759522,-0.2288933537
C,0,-2.6634288002,1.4461000032,-0.2138789361
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C,0,-0.7050798438,2.579950655,-0.2424071985
H,0,-3.8616069162,2.9673593847,-1.3136988772
H,0,-1.5226336699,4.3507205158,-1.3117811987
H,0,1.4159386768,4.1270406651,-1.7189655703
H,0,3.7644488399,2.7422693347,-1.7039983431
H,0,-4.5123819782,-2.3290347812,-1.0494234406
H,0,-2.5573363144,-4.1936838246,-1.1757080505
H,0,2.5967369483,-4.0485180986,-1.4874745449
H,0,4.5373278131,-2.1512604685,-1.3401638582
H,0,0.0479383648,-4.1445721305,-0.8941643643
H,0,4.4614081863,0.377278665,-0.0742471006

H,0,-4.3760244017,0.3137983204,-0.4242985224
N,0,-3.3942097676,0.2397420933,-0.1608205432
N,0,3.4564524752,0.2819577804,0.071728854
N,0,-1.1529846341,0.258759603,3.3404929134
N,0,0.0494353967,0.3212678924,3.0674113658
V,0,-0.9206293927,0.0156719449,1.3948286717
V,0,1.1608221144,-0.0148249677,1.5155413339

The coordinates of *NN

N,0,-1.3435716253,-1.4906979247,0.1897342149
N,0,-1.624044965,1.1788869293,0.0986224832
N,0,1.6742695192,1.3504023046,0.0149993541
N,0,1.547498683,-1.4643098162,0.1478727053
C,0,-0.631905578,-2.5256650585,-0.3888722737
C,0,-1.540824946,-3.3165790813,-1.1456277966
C,0,-2.8019567071,-2.6922234315,-1.1109547428
C,0,-2.6200458885,-1.5311761698,-0.3300432481
C,0,-2.9144359001,0.9179835459,-0.2615536633
C,0,-3.5708583134,2.1110214131,-0.7163658437
C,0,-2.6011802396,3.0967540829,-0.707042892
C,0,-1.3545247214,2.5083486897,-0.2615121272
C,0,-0.1029990744,3.0932699233,-0.4640743626
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C,0,3.322062535,2.146660988,-1.3605630408
C,0,2.9164621005,1.086488487,-0.5419545567
C,0,2.7638742506,-1.3461326026,-0.5156387632
C,0,2.8769275366,-2.3358185646,-1.4838054295
C,0,1.6558499874,-3.0736191597,-1.4354111726
C,0,0.8121969999,-2.4790191089,-0.4800284835
H,0,3.7116747368,-2.4967689534,-2.166439182
H,0,1.3843241234,-3.8968873869,-2.0965157972
H,0,-1.2805988863,-4.209743574,-1.7144160444
H,0,-3.7003732195,-2.9845742407,-1.6546082095
H,0,4.2456731057,2.2135851003,-1.9352975915
H,0,2.2207860255,4.0296889346,-1.8631411262
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H,0,-4.5988091736,2.1889635995,-1.0716877735
H,0,-0.1603744915,4.1245816295,-0.8332889009
H,0,-4.3582011368,-0.4713857563,-0.6297918732
H,0,4.5159456971,-0.2165633902,-0.1866554677
N,0,3.4991364165,-0.1628809971,-0.1158695772
N,0,-3.3945540763,-0.3708436362,-0.3120850981
N,0,0.5519724256,0.0503100506,2.5829088588
N,0,-2.2978419235,-0.1757132291,2.4891012241

V,0,1.6930304273,-0.0096273503,1.3975888975
V,0,-1.0471682563,-0.0707307275,1.5474598095

The coordinates of *NCO₂N

N,0,-1.5854850987,-1.6259261763,-0.2459397837
N,0,-1.8987206096,1.0350049822,-0.3359752053
N,0,1.3070398382,1.2362247536,0.2428732311
N,0,1.2388808208,-1.4893956468,0.2917863168
C,0,-0.7396640455,-2.645510269,-0.6422009148
C,0,-1.4307680711,-3.4467610461,-1.6066272437
C,0,-2.6642317117,-2.8375151653,-1.8707402482
C,0,-2.6880686028,-1.6747918802,-1.0556700475
C,0,-3.0549812211,0.7601731061,-0.9965386973
C,0,-3.6266215723,1.949291179,-1.5587722194
C,0,-2.726011541,2.9628924959,-1.2752716149
C,0,-1.6087191743,2.3864365594,-0.5623354688
C,0,-0.3621872388,3.0115899458,-0.4279082835
C,0,0.9471242056,2.5127055853,-0.1991294104
C,0,2.1341450887,3.1551094109,-0.6762505679
C,0,3.1928170228,2.238466117,-0.5988343159
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N,0,3.2092408198,-0.1887724164,0.3277878725
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N,0,-0.3200900426,-0.2255368784,2.5748723751
N,0,-3.0624057357,-0.3895791937,1.8397909724
V,0,1.0952199334,-0.1124698237,1.71751265
V,0,-1.6324912371,-0.2465366117,1.2047740562
C,0,1.2864543383,1.6949040718,4.0988285114
O,0,0.6217322832,2.1021429173,4.9716047815
O,0,2.0268458915,1.3171941305,3.2416015542

The coordinates of *NCOOHN

N,0,-1.0942749382,-1.4392060566,0.1384832279
N,0,-1.3661769175,1.240717474,0.0598325632
N,0,1.8538935409,1.2874264789,-0.2238157558
N,0,1.7226774377,-1.5616541046,0.0289659758
C,0,-0.4773272229,-2.5783136958,-0.3589101096
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C,0,-2.6880363431,-2.6844054891,-0.9516486795
C,0,-2.4071271023,-1.4694592984,-0.3031451937
C,0,-2.6744617668,0.9848139595,-0.2690665099
C,0,-3.3306241254,2.1833917486,-0.7017530044
C,0,-2.3512154135,3.1605505874,-0.7278805311
C,0,-1.0953333294,2.5658208977,-0.3252047171
C,0,0.156629274,3.1175477898,-0.5988064654
C,0,1.4550946682,2.5390761695,-0.6995984602
C,0,2.5261276593,3.0428391677,-1.483359069
C,0,3.5433575289,2.0596903768,-1.5561065386
C,0,3.094410358,0.9899659718,-0.7762942222
C,0,2.912208221,-1.4705701103,-0.6827584754
C,0,2.9856547191,-2.4997521473,-1.6091707536
C,0,1.7631973142,-3.2378651595,-1.4741984265
C,0,0.9611040609,-2.5998800485,-0.515142616
H,0,3.7883215699,-2.69665349,-2.3204220178
H,0,1.46476532,-4.0845210484,-2.0931836825
H,0,-1.277207992,-4.332628285,-1.4861237924
H,0,-3.6315517877,-2.9822078389,-1.4092630348
H,0,4.475964206,2.1154355749,-2.1174416993
H,0,2.5215656242,4.0034486217,-2.0009468867
H,0,-2.4602978348,4.1796869465,-1.1018938068
H,0,-4.3685214983,2.2700786468,-1.0244863344
H,0,0.1135634414,4.1509489045,-0.9635653219
H,0,-4.1429802924,-0.3959559971,-0.5521464053
H,0,4.6546484317,-0.3224722101,-0.3020741176
N,0,3.6370891343,-0.2664197267,-0.3452811724
N,0,-3.1601791057,-0.2964322709,-0.2998275791
N,0,0.7162576353,0.1982720306,2.4251248335
N,0,-2.0488179336,-0.2265479162,2.5735862112
V,0,1.7956991335,-0.037769767,1.1431383761
V,0,-0.7834665894,-0.0056500754,1.4583131612
C,0,-2.5131765848,-0.6418395872,3.7954257795
O,0,-2.524142429,-1.8020379563,4.2064970408
O,0,-3.0190906439,0.4056905299,4.529702101
H,0,-3.3176020959,-0.0201144984,5.3654369003

The coordinates of *NCON

N,0,-1.3145684961,-1.4714011267,-0.0967431975
N,0,-1.5846961765,1.2222842424,-0.329136797
N,0,1.5585995799,1.3486587452,0.0061644185
N,0,1.43373237,-1.5718553477,0.2390160905
C,0,-0.64367804,-2.6096806401,-0.5287746886
C,0,-1.5783082462,-3.4293374898,-1.1919370068
C,0,-2.8232266622,-2.7453393267,-1.2344520015
C,0,-2.6078933108,-1.5189473046,-0.592261935
C,0,-2.8912172737,0.9451381219,-0.6431400309
C,0,-3.5465514627,2.1326607996,-1.1003786086
C,0,-2.5734774102,3.1219389023,-1.1285690237
C,0,-1.3246484253,2.5556261035,-0.6863648625
C,0,-0.0547077174,3.1258592058,-0.7844872741
C,0,1.2386061082,2.5546853542,-0.6230467237
C,0,2.4186355842,3.0189611878,-1.2735438916
C,0,3.4288860611,2.0483252664,-1.1203542732
C,0,2.8575472357,1.0387617703,-0.3310535211
C,0,2.7176009329,-1.4166161087,-0.2542929603
C,0,2.9755623922,-2.3743922802,-1.2265918758
C,0,1.7692181126,-3.1387199974,-1.3462570277
C,0,0.8069496055,-2.5840660748,-0.4868932548
H,0,3.8877521682,-2.5026847599,-1.8097663528
H,0,1.5985438542,-3.9477523186,-2.0573920262
H,0,-1.3679999208,-4.4020166153,-1.6373330823
H,0,-3.7345466166,-3.072684037,-1.7351929175
H,0,4.4349924803,2.0643825935,-1.5388121548
H,0,2.4840123714,3.9336175815,-1.8647543438
H,0,-2.6977801106,4.1437195068,-1.4899507437
H,0,-4.5833130503,2.2108483343,-1.4284021662
H,0,-0.0461780404,4.1473843414,-1.1822210898
H,0,-4.3463752421,-0.4552717893,-0.8930348854
H,0,4.2988461057,-0.2274933388,0.5149899971
N,0,3.3138337711,-0.1954504452,0.2464542848
N,0,-3.3706946451,-0.3432764042,-0.6196565771
N,0,0.2882441791,0.3170023784,2.8136307335
N,0,-1.9262190264,0.057996746,2.4600674121
V,0,1.2888655926,-0.0321915204,1.4113714775
V,0,-0.8952702819,0.0345495519,1.0216910676
O,0,-1.1054798958,0.0254241269,4.6907794463
C,0,-0.9809919043,0.1152974553,3.4771627164

The coordinates of *NCONH

N,0,1.22802483,1.5965366733,-0.2423442313
N,0,1.610857517,-1.2287148645,-0.5389890736
N,0,-1.5446036979,-1.3294309136,-0.3334352707

N,0,-1.5080020912,1.4129143267,-0.0708371609
C,0,0.4586273918,2.6587538874,-0.7384859773
C,0,1.2718990355,3.3860818025,-1.614514591
C,0,2.5281512138,2.699662707,-1.7458236636
C,0,2.4483238804,1.6019960522,-0.9062213341
C,0,2.8187038672,-0.8353952462,-1.0583508041
C,0,3.3546122658,-1.8294676267,-1.8942626871
C,0,2.405376771,-2.873156025,-1.8895335496
C,0,1.2932220829,-2.4717177659,-1.0949686751
C,0,0.0306362233,-3.1202186821,-1.055565592
C,0,-1.2447523006,-2.6368701476,-0.7522443085
C,0,-2.491274224,-3.29082614,-1.0558028765
C,0,-3.5184629342,-2.372487691,-0.8954929183
C,0,-2.8946902507,-1.1479839716,-0.4908235769
C,0,-2.8436466986,1.3368892012,-0.4355603568
C,0,-3.2329271357,2.532143709,-1.0471601096
C,0,-2.0506098238,3.3258258959,-1.1383854881
C,0,-0.9856164578,2.5960554875,-0.5822200334
H,0,-4.2136684991,2.7732276546,-1.4581007845
H,0,-1.9747313333,4.2972376482,-1.6279921319
H,0,0.9680750271,4.2648280675,-2.1844290822
H,0,3.3561109493,2.9775679381,-2.3986537023
H,0,-4.5792619443,-2.5161272558,-1.1038370497
H,0,-2.5837036768,-4.3126133293,-1.4266811211
H,0,2.4595239047,-3.799118403,-2.4644714281
H,0,4.2915798191,-1.7884996154,-2.449537364
H,0,0.0395283384,-4.1375112618,-1.4650447047
H,0,4.2600815209,0.5889186491,-0.5517559122
H,0,-4.4949554303,0.1076400815,-0.5398133997
N,0,-3.4927372909,0.0918379058,-0.3552837705
N,0,3.2506576769,0.4469687519,-0.5981436801
N,0,-0.0180574641,-0.3895209226,2.4769579548
N,0,2.1074651039,0.1769020629,2.7037022668
V,0,-0.7567910236,-0.0470596315,0.9270871584
V,0,1.3709809492,0.0706778755,0.9215339457
O,0,0.8601364798,-0.3098639251,4.6639025929
C,0,1.0032646877,-0.1730542474,3.4548835852
H,0,3.0010442215,0.3108659487,3.1862822059

The coordinates of *HNCONH

N,0,1.320540021,1.5398184366,-0.4088151596
N,0,1.648535737,-1.1597996241,-0.7047326641
N,0,-1.4580002564,-1.3583461409,-0.2496518443
N,0,-1.3983124678,1.3659445373,-0.0106989162
C,0,0.5393481594,2.6594425905,-0.6948815635

C,0,1.3121398714,3.543156646,-1.5046391265
C,0,2.5284139122,2.9022007498,-1.7981233757
C,0,2.4654593267,1.6404960716,-1.1482082595
C,0,2.8263836344,-0.8112434701,-1.2982163569
C,0,3.4246476947,-1.9373603954,-1.9434202405
C,0,2.5297882855,-2.9905552806,-1.7713733244
C,0,1.3924783609,-2.4932102715,-1.0487887536
C,0,0.1479120925,-3.1474635359,-0.9414393469
C,0,-1.1468720346,-2.6556043175,-0.6765719566
C,0,-2.3720120971,-3.3040051772,-1.0527559226
C,0,-3.4027155384,-2.373857697,-0.9427101259
C,0,-2.7902247814,-1.1702755319,-0.4752319601
C,0,-2.7100337906,1.3096802115,-0.3900641564
C,0,-3.112848749,2.5417030727,-0.9715000942
C,0,-1.9531863837,3.3344918485,-1.0261582929
C,0,-0.8773747393,2.5688668838,-0.4873797406
H,0,-4.0967054233,2.7861060561,-1.3732363588
H,0,-1.8712739848,4.3240172979,-1.4766664983
H,0,0.9822122438,4.5063330221,-1.8948524987
H,0,3.3179067326,3.2598568001,-2.4598504915
H,0,-4.4505302822,-2.5068912145,-1.2149696563
H,0,-2.4520788719,-4.321709538,-1.4376781162
H,0,2.6225860014,-3.9971248033,-2.1818653688
H,0,4.3589161133,-1.9436095774,-2.5063087228
H,0,0.1637663212,-4.1884798137,-1.2874927868
H,0,4.1221850762,0.663895291,-1.8694709163
H,0,-4.3685122142,0.1211623565,-0.6257029374
N,0,-3.3834361763,0.0864664278,-0.3671999142
N,0,3.2642869596,0.5113742604,-1.3411328733
N,0,-0.6231975993,-0.2635911429,3.0123231849
N,0,1.650711541,-0.118441549,2.6792886449
V,0,-0.7057187568,-0.1088125795,1.1103274249
V,0,1.1665224026,0.0108358623,0.8361199485
O,0,0.8186638885,-0.3358881563,4.8646553817
C,0,0.6348776243,-0.2502087071,3.6471200851
H,0,2.5775250456,-0.0943069058,3.117380305
H,0,-1.3817917886,-0.3487252727,3.6969893253

The coordinates of *HNCONH₂

N,0,-1.3565653391,-1.3320282367,-0.0092526851
N,0,-1.4983457341,1.2696509541,-0.9018556608
N,0,1.6730211149,1.1634474664,-0.9423173823
N,0,1.3892003879,-1.4184647364,-0.0450110487
C,0,-0.7550263883,-2.5856183062,-0.167643516
C,0,-1.7418550253,-3.4766538093,-0.5998934737

C,0,-2.9545234014,-2.7349012623,-0.8133927471
C,0,-2.6607019164,-1.4186156649,-0.4789211031
C,0,-2.807345484,0.964968727,-1.1702231302
C,0,-3.3926734802,1.9731974121,-1.9909266333
C,0,-2.3698175207,2.8825845233,-2.2709527424
C,0,-1.1709230787,2.4203155935,-1.6420153335
C,0,0.1292542074,2.8938088646,-1.9043963065
C,0,1.4005111925,2.3347975925,-1.673361378
C,0,2.6123845754,2.72351526,-2.3276989327
C,0,3.583386706,1.7532521911,-2.0724774165
C,0,2.9551900379,0.7790636032,-1.2419083916
C,0,2.6756448869,-1.5909196556,-0.5430873643
C,0,2.8774545887,-2.9252292222,-0.8740001554
C,0,1.6246291759,-3.5855397373,-0.6304733374
C,0,0.7050038728,-2.6312498123,-0.1841944233
H,0,3.7735607274,-3.3700680234,-1.3087443938
H,0,1.4084425119,-4.6326094809,-0.846558764
H,0,-1.5980426738,-4.5337500901,-0.8273313761
H,0,-3.8862402615,-3.1187111501,-1.2313134008
H,0,4.5953229613,1.7037800296,-2.476265628
H,0,2.7175527024,3.5910093227,-2.9816592598
H,0,-2.4361087106,3.7526321335,-2.9265962912
H,0,-4.4141684308,1.9843403481,-2.3731400619
H,0,0.1524614153,3.800541965,-2.5221620703
H,0,-4.3482014315,-0.3511362034,-0.9948222783
H,0,4.4161698283,-0.6306802191,-1.0994367283
N,0,3.4644883601,-0.4342836237,-0.7932794705
N,0,-3.3840234898,-0.210831261,-0.6963867457
V,0,1.0416665856,0.3064835005,0.7020032363
V,0,-0.8642444237,0.366624094,0.7219010211
C,0,0.272466839,1.0163219276,3.2765915671
O,0,1.3674670788,0.8387281405,2.5974222172
N,0,0.4113329324,1.3392336883,4.5970388005
H,0,-0.3793653493,1.2707881253,5.2315786641
H,0,1.3404578366,1.2313020575,4.9968726153
N,0,-0.9197427863,0.91028531,2.6659783137
H,0,-1.7383775997,1.0674366646,3.2624701955

The coordinates of *H₂NCONH₂

N,0,-1.379941037,-1.4591626255,-0.1553651272
N,0,-1.604794072,1.2164538648,-0.4079654693
N,0,1.5656951764,1.2729033362,-0.4756306071
N,0,1.3895590235,-1.4975778909,-0.1414133444
C,0,-0.745564448,-2.6274642449,-0.5692049366
C,0,-1.6958611836,-3.443375584,-1.2122358103

C,0,-2.9230253305,-2.7233730319,-1.2614213446
C,0,-2.6638256061,-1.4951086665,-0.6405339425
C,0,-2.8994763199,0.9524458249,-0.7391795737
C,0,-3.5454614973,2.1250494232,-1.2566755646
C,0,-2.5698681387,3.1096229127,-1.2963550069
C,0,-1.3384832362,2.5344837206,-0.8152644716
C,0,-0.0730123145,3.1047365548,-0.9969422662
C,0,1.2290484817,2.546484073,-0.9548170984
C,0,2.3904081161,3.0879335248,-1.5752326211
C,0,3.4041633277,2.1122298438,-1.5504134995
C,0,2.8525146576,0.99821519,-0.8808238953
C,0,2.6531435845,-1.4638644471,-0.7297500029
C,0,2.8473093507,-2.612656199,-1.4774441543
C,0,1.6224531899,-3.3639828979,-1.3832946639
C,0,0.7115512041,-2.6260666495,-0.6232808404
H,0,3.7261745522,-2.8735610034,-2.0687240535
H,0,1.4075214005,-4.2923851435,-1.9136851715
H,0,-1.5028203285,-4.4146826136,-1.6691385008
H,0,-3.8499862953,-3.0327735336,-1.7466393957
H,0,4.3964418524,2.1749474118,-1.9981017299
H,0,2.4411387087,4.0629703365,-2.0630324402
H,0,-2.6682753502,4.1123101891,-1.7159601288
H,0,-4.5748039904,2.188096808,-1.6127805783
H,0,-0.0977495403,4.1320813015,-1.3816444568
H,0,-4.4036529642,-0.4100135992,-0.9137214776
H,0,4.4037778774,-0.3399110888,-0.7362900779
N,0,3.4060729949,-0.2567477654,-0.5446950391
N,0,-3.4450461297,-0.311831254,-0.5845539806
V,0,1.1698027603,0.025347696,0.9677949745
C,0,0.1848480861,0.1504949642,2.7957442081
O,0,1.5226827928,0.1305122446,2.8642752566
N,0,-0.6613284754,-0.998191636,3.0415666641
H,0,-0.1411627387,-1.8800577485,3.0178402638
H,0,-1.2890634037,-0.9647015344,3.8566473218
N,0,-0.6370748759,1.3334952607,2.9522301803
H,0,-1.2206968557,1.3818168125,3.7999078927
H,0,-0.0882265274,2.1921852575,2.8554603607
V,0,-0.9272164784,0.0284036065,1.0691921489

The coordinates of *N₂-CO₂

N,0,-1.8019175498,-0.9765687377,0.0025654661
N,0,-1.1512888257,1.5152010468,-0.6082748367
N,0,1.8993702109,0.5027860394,-0.5481394657
N,0,0.8226921656,-1.8471864059,-0.0046446649
C,0,-1.5508115551,-2.3338412548,-0.1921079956

C,0,-2.7232990198,-2.9283200786,-0.7445655814
C,0,-3.6553215648,-1.9026206412,-0.9740550143
C,0,-3.018401804,-0.7056193166,-0.5558715603
C,0,-2.439625672,1.632974869,-1.032228326
C,0,-2.6311272422,2.8406420491,-1.7680511369
C,0,-1.3777076957,3.4432240137,-1.8272400846
C,0,-0.4408788333,2.5943571258,-1.146106292
C,0,0.9619531429,2.7106794301,-1.2607745859
C,0,2.0097461698,1.7840326047,-1.0947186068
C,0,3.28578061,1.8812966466,-1.7545290114
C,0,3.897380478,0.6354767037,-1.6820038576
C,0,2.9852905785,-0.1954222766,-0.9553827535
C,0,1.9645116428,-2.3794820321,-0.5210582377
C,0,1.7530590243,-3.7271813382,-0.9200851735
C,0,0.3882287017,-3.9793759008,-0.7103225365
C,0,-0.1923396716,-2.7879566574,-0.1859648286
H,0,2.4879760216,-4.3951157724,-1.3707139351
H,0,-0.1507356937,-4.8878520667,-0.9793617312
H,0,-2.837119159,-3.9773789628,-1.0180497907
H,0,-4.6312954778,-1.9897917325,-1.4522154658
H,0,4.8411217442,0.3255215132,-2.1321657308
H,0,3.6450299813,2.7549245741,-2.3004352457
H,0,-1.1162047887,4.3513973881,-2.3722953561
H,0,-3.5581317509,3.1761555628,-2.2340615317
H,0,1.2791826499,3.6469486662,-1.737033076
H,0,-4.3025286484,0.7836957456,-1.1759683981
H,0,3.9199384952,-2.0218434799,-1.0740553525
N,0,3.0843598753,-1.5637136414,-0.7163302576
N,0,-3.3708875634,0.6237338278,-0.7972659716
C,0,0.4853027534,1.6292246487,1.9823059344
O,0,1.6771376092,1.5293652981,2.3477383542
O,0,-0.6151489256,2.162199395,2.3022375864
N,0,-0.132244725,-0.8762242802,2.6075152199
N,0,-1.0708066576,-0.9691195076,3.293167877
V,0,-0.9437611637,0.4602113753,1.0729932237
V,0,0.9637211335,-0.1984544404,1.1164627309

The coordinates of *N₂-COOH

N,0,-0.8310169599,-1.8927275771,-0.3153103523
N,0,-1.8233781654,0.5838101311,-0.257569394
N,0,1.2236057648,1.5404327479,-0.3980748585
N,0,1.8671035295,-1.0315307344,-0.3646585382
C,0,0.1319147188,-2.7294969833,-0.8477107063
C,0,-0.5373632524,-3.7539262133,-1.5757908114
C,0,-1.9238622469,-3.4838394839,-1.5501318538

C,0,-2.0483124461,-2.2876997682,-0.8130293199
C,0,-2.9958606976,-0.0146988704,-0.6389552949
C,0,-3.9558286979,0.9590893762,-1.0518028774
C,0,-3.2944004875,2.1817590267,-0.9933095459
C,0,-1.9496263339,1.9480835562,-0.5512488113
C,0,-0.8957310663,2.8775178943,-0.6345467526
C,0,0.5039085325,2.725194281,-0.642775181
C,0,1.4277973869,3.6925190891,-1.153213708
C,0,2.6721350993,3.0771336289,-1.2894851262
C,0,2.5013491356,1.73569884,-0.83785957
C,0,3.0331489018,-0.6481882044,-0.9673534484
C,0,3.5343008423,-1.6857154103,-1.7608367131
C,0,2.5815660936,-2.7450999855,-1.6832666878
C,0,1.5175524425,-2.3077245078,-0.8805738
H,0,4.4371061876,-1.6656234797,-2.3730924621
H,0,2.6183322231,-3.6774196235,-2.2471121285
H,0,-0.0550862119,-4.5749882326,-2.1078848559
H,0,-2.7121223547,-4.0234291012,-2.0751082814
H,0,3.5825364259,3.5026886621,-1.7131232312
H,0,1.1622325945,4.7021790066,-1.4707211699
H,0,-3.6880194879,3.1496920916,-1.3076346077
H,0,-4.9665380948,0.761258337,-1.409882161
H,0,-1.2253229376,3.8938392153,-0.8841943787
H,0,-4.0084305788,-1.7292756602,-1.0778524604
H,0,4.3599296496,0.9413390969,-1.1650729746
N,0,3.4401490781,0.7041992124,-0.7991369824
N,0,-3.1160304552,-1.3945731235,-0.7164345715
C,0,-0.3721152611,1.2169256572,2.4201224402
O,0,0.8912650797,1.2899065434,2.6877094262
O,0,-1.1195192408,2.2701272934,2.7939759955
H,0,-0.5048689679,2.9286748517,3.2165181878
N,0,0.6037183407,-1.4106005931,2.2797834063
N,0,-0.4061632733,-1.9188947358,2.6046919401
V,0,-0.7691059324,-0.4522357183,1.0558939305
V,0,1.1234451235,0.1318524675,0.9994562893

The coordinates of *N₂-CO

N,0,1.4034428673,1.4193650667,-0.1861517705
N,0,1.4815714931,-1.2323525085,-0.4376669955
N,0,-1.7013735712,-1.1601569254,-0.2598193953
N,0,-1.3986200311,1.4728167626,-0.048140934
C,0,0.7196688405,2.5785450029,-0.547154594
C,0,1.6070292575,3.3897002256,-1.3178090826
C,0,2.7951658623,2.6655308077,-1.5093098785
C,0,2.5992749964,1.4286210136,-0.8421941545

C,0,2.7330093953,-1.0251691544,-0.940344125
C,0,3.2578109678,-2.2191441339,-1.5185915686
C,0,2.2438554455,-3.1664798668,-1.4061317839
C,0,1.1143862129,-2.5416900559,-0.7792412381
C,0,-0.1899848036,-3.0804158437,-0.7773079794
C,0,-1.4578188101,-2.4831938891,-0.6390190326
C,0,-2.6823563733,-3.0375921102,-1.1530165446
C,0,-3.6354114812,-2.026069897,-1.1599559235
C,0,-2.9724163665,-0.871138151,-0.6316725358
C,0,-2.6549126874,1.5581957834,-0.5545181348
C,0,-2.8681687001,2.8188224822,-1.1822161619
C,0,-1.635247733,3.4813059758,-1.1238896172
C,0,-0.7113711086,2.6111839652,-0.4649742593
H,0,-3.7807661699,3.1570426852,-1.67416428
H,0,-1.3943803959,4.4441159004,-1.5747405359
H,0,1.3650099053,4.3592358493,-1.7534938692
H,0,3.6557034602,2.9532903559,-2.1137947855
H,0,-4.6553853287,-2.0696267371,-1.5438973624
H,0,-2.7970463718,-4.0463836807,-1.5526268717
H,0,2.2538273954,-4.1826102485,-1.8032693548
H,0,4.2285081889,-2.3324706593,-2.0024449549
H,0,-0.2283938874,-4.1256645003,-1.1086225337
H,0,4.2379674688,0.2953540866,-1.3754363548
H,0,-4.4220191711,0.5536185868,-0.9029941423
N,0,-3.4744203991,0.4247890955,-0.5536412882
N,0,3.3239148309,0.2370693237,-0.9300577428
O,0,1.1095332931,1.3390680063,3.0279287013
C,0,0.0166521725,1.0734835572,2.5685146224
N,0,0.9521773153,-2.029865759,2.6096364908
N,0,-0.0315802498,-1.5232317238,2.2369292192
V,0,-0.9169745507,-0.0065223129,1.2434777105
V,0,1.0660628214,-0.0341003751,1.1117250416

The coordinates of *NCONH₂

N,0,1.3049440817,1.3751964188,-0.3033175193
N,0,1.5685477227,-1.3222464857,-0.7267217821
N,0,-1.5669400692,-1.4364757685,-0.3281433052
N,0,-1.4229698202,1.3481492419,0.178031818
C,0,0.5893421749,2.5388812179,-0.5611940855
C,0,1.4242921975,3.404503509,-1.2921590743
C,0,2.6488202953,2.7225311212,-1.5578160814
C,0,2.5148711745,1.4636482525,-0.9681634533
C,0,2.7980041277,-0.9869414529,-1.2343283335
C,0,3.369264631,-2.0924742195,-1.9344422293
C,0,2.4074483637,-3.0979737074,-1.9091724271

C,0,1.2555156677,-2.6068154933,-1.208331917
C,0,-0.0203627153,-3.1896655198,-1.2358830677
C,0,-1.2981161923,-2.6708834406,-0.935928467
C,0,-2.5437660654,-3.2088749674,-1.3784208948
C,0,-3.5494196824,-2.2691641718,-1.1136565729
C,0,-2.9064711583,-1.1760351219,-0.4807555471
C,0,-2.7553254565,1.2797270841,-0.2184021059
C,0,-3.0925517991,2.4328871054,-0.9090724291
C,0,-1.8928347618,3.2230968015,-0.9845826208
C,0,-0.858580587,2.5036266724,-0.3818661646
H,0,-4.0571638776,2.6736413457,-1.3577407583
H,0,-1.7899384743,4.1679462852,-1.5192881637
H,0,1.1486484629,4.3899626138,-1.6691456833
H,0,3.4814176328,3.0809882561,-2.1641193543
H,0,-4.6051337759,-2.3339128765,-1.3781459822
H,0,-2.6620466574,-4.1559842444,-1.9071903244
H,0,2.4635259762,-4.0643400146,-2.4126873985
H,0,4.331501365,-2.1028828877,-2.4473587881
H,0,-0.0437646475,-4.1839880421,-1.6983339344
H,0,4.2230831613,0.4403526091,-1.5126768455
H,0,-4.448301386,0.089170569,-0.0105829614
N,0,-3.4304887439,0.0348114307,0.0185254732
N,0,3.3082006948,0.2954092763,-1.0875086975
N,0,0.1627977254,-0.674504182,2.5663283626
N,0,1.7975765019,0.9227432389,2.5767244418
V,0,-0.8862900315,-0.2432034556,1.0663231827
V,0,1.1320218742,-0.1999331151,0.8340321938
O,0,1.3965968997,-0.3740587958,4.5541995729
C,0,1.0669171924,-0.1000623648,3.4090513565
H,0,1.3163257624,1.8330927171,2.5557077923
H,0,2.7598353061,1.0703818111,2.9074633054

The coordinates of *NNH

N,0,-1.328611826,-1.4636064832,0.0723743029
N,0,-1.5948618233,1.1917956949,-0.1087187408
N,0,1.6972382964,1.3280342648,0.025267741
N,0,1.5593498851,-1.5208840288,0.2464896805
C,0,-0.6120517278,-2.5516624643,-0.3957247536
C,0,-1.4901292429,-3.3695957848,-1.1602477433
C,0,-2.7350549026,-2.7195588548,-1.233044298
C,0,-2.5700705195,-1.5162769878,-0.509372225
C,0,-2.8600706462,0.9273818542,-0.5362267508
C,0,-3.4829743777,2.1126071258,-1.0614025578
C,0,-2.5122444459,3.0949513605,-1.0171641859
C,0,-1.2976908113,2.5087217254,-0.4816987453

C,0,-0.031478707,3.0794820153,-0.6116221199
C,0,1.2864553791,2.5269437852,-0.5639824568
C,0,2.3872922912,3.0087181635,-1.3229323446
C,0,3.4327830788,2.0541764436,-1.2823599637
C,0,2.9715070531,1.0339097101,-0.4495480096
C,0,2.8055053095,-1.4314622021,-0.3612226065
C,0,2.944709234,-2.4180639445,-1.3275350618
C,0,1.713030485,-3.1411441396,-1.3197137261
C,0,0.8331969999,-2.5299382542,-0.4063946524
H,0,3.800104468,-2.59147811,-1.9808826305
H,0,1.4552126503,-3.9602003402,-1.9916969959
H,0,-1.2185829195,-4.3016620998,-1.6568291862
H,0,-3.6112383542,-3.028189713,-1.8037887051
H,0,4.3874149432,2.0953091328,-1.8064986744
H,0,2.3804255971,3.9299882121,-1.9076971524
H,0,-2.588445512,4.1069318546,-1.4180491913
H,0,-4.4880723699,2.1851541734,-1.4784835238
H,0,-0.0492670151,4.1018433217,-1.0087218032
H,0,-4.287632333,-0.4681612823,-0.9469594564
H,0,4.4524912037,-0.258566541,0.3158544409
N,0,3.4628872423,-0.2176184541,0.0690464672
N,0,-3.3441392781,-0.357509423,-0.5777718737
N,0,0.4072465358,0.1615594429,2.6500192588
N,0,-2.3534336881,-0.1095368964,2.2960919079
V,0,1.6582803502,-0.0035992867,1.4007691606
V,0,-1.0539425311,-0.0007826353,1.4133735523
H,0,0.2936368183,0.2206243752,3.6696388029

The coordinates of *HNNH

N,0,1.2582444882,1.4480330872,-0.0384396294
N,0,1.63125642,-1.2024944192,-0.1461257241
N,0,-1.6742483089,-1.3683476303,0.046959938
N,0,-1.532702844,1.4791378034,0.2167010438
C,0,0.552140671,2.5804590488,-0.4304127048
C,0,1.413561287,3.4140382245,-1.1777187974
C,0,2.6542963,2.7497605737,-1.3158144978
C,0,2.4970630526,1.5227808383,-0.6505562755
C,0,2.8597306927,-0.9139529487,-0.6765435334
C,0,3.4622046645,-2.0944337685,-1.2234168711
C,0,2.5122147693,-3.0949941126,-1.0987685575
C,0,1.3257604567,-2.5320162779,-0.4929421729
C,0,0.0550088285,-3.1050532868,-0.5974654819
C,0,-1.2653964154,-2.5679765505,-0.5265477742
C,0,-2.3786022668,-3.0762787283,-1.2635070724
C,0,-3.4259039678,-2.131987001,-1.2103967384

C,0,-2.9420051154,-1.0976398274,-0.3925844115
C,0,-2.8092339283,1.3632745067,-0.3153854628
C,0,-3.0624701052,2.4198046904,-1.1751399059
C,0,-1.8523826047,3.1951520197,-1.1991252798
C,0,-0.8972400268,2.5595984051,-0.3894263014
H,0,-3.9754661814,2.6207901525,-1.7366652593
H,0,-1.6736080723,4.0638407901,-1.8340435687
H,0,1.1354958807,4.3595079435,-1.6449188323
H,0,3.511713687,3.0689943937,-1.9095346909
H,0,-4.3922482177,-2.1825804551,-1.7119635787
H,0,-2.3696446418,-3.998620156,-1.8469071861
H,0,2.578432495,-4.1066637566,-1.502634002
H,0,4.4309662105,-2.1539583441,-1.7205563161
H,0,0.0764669145,-4.1271271013,-0.9963954361
H,0,4.2235683365,0.520132832,-1.1614727505
H,0,-4.4473516227,0.1860734088,0.3191392195
N,0,-3.4421612422,0.1445090017,0.1438288144
N,0,3.2977527141,0.3805632727,-0.7606097153
N,0,-0.1540350991,-0.4315849956,2.5526338672
N,0,2.5396377542,0.3663653152,2.2538529093
V,0,-1.4872586651,0.0201541645,1.4281629583
V,0,1.1887773175,0.0048812507,1.3500864225
H,0,-0.0337802136,-0.9065217281,3.4588023839
H,0,2.9936156285,0.884430615,3.0208031416

The coordinates of *NNH₂

N,0,-1.2941050615,-1.4058916238,0.0462175612
N,0,-1.6353828711,1.2082131164,-0.0759079356
N,0,1.6829404753,1.3198237689,0.0466290959
N,0,1.5480567444,-1.5043547395,0.2113794384
C,0,-0.5972757136,-2.5144840752,-0.4201778762
C,0,-1.4838170058,-3.3445624634,-1.1735692776
C,0,-2.7158388012,-2.689374737,-1.2362117133
C,0,-2.5309692687,-1.4710566469,-0.5224036521
C,0,-2.8832496443,0.9452166671,-0.5325965287
C,0,-3.4936903974,2.1229171736,-1.0870848557
C,0,-2.522981649,3.1067528812,-1.0281830158
C,0,-1.3257872674,2.5210115192,-0.4568219194
C,0,-0.0478621109,3.0711686947,-0.6013387487
C,0,1.2650531328,2.5134396864,-0.5538491724
C,0,2.3600844646,2.9923459079,-1.3321308661
C,0,3.4009711123,2.0395946888,-1.2911131243
C,0,2.9373477234,1.0280717546,-0.4399588137
C,0,2.7965739696,-1.4260508838,-0.3490924085
C,0,2.9714855097,-2.4369794574,-1.3009429111

C,0,1.7417083609,-3.1496624178,-1.3268104595
C,0,0.8377809221,-2.5130731167,-0.4407460081
H,0,3.8484467084,-2.6220374904,-1.9219579566
H,0,1.5007709784,-3.979797766,-1.9912195574
H,0,-1.2138163231,-4.2779976508,-1.6679183641
H,0,-3.6065571221,-2.9932207767,-1.7874342872
H,0,4.3515613643,2.0718801832,-1.8234236067
H,0,2.3414905198,3.9024174267,-1.9338796813
H,0,-2.5858650963,4.1128004158,-1.4461436444
H,0,-4.4856825335,2.188982061,-1.53556499
H,0,-0.0581491597,4.0856549287,-1.0196992935
H,0,-4.2912372079,-0.4844166104,-0.9425607645
H,0,4.4627196469,-0.2493000873,0.2382061142
N,0,3.4503065546,-0.2103648423,0.1029573962
N,0,-3.354122682,-0.3477342721,-0.5688689999
N,0,0.4277671817,0.3478180714,2.947265517
N,0,-2.3673465353,-0.2826212847,2.3498522994
V,0,1.6467656364,-0.0369608044,1.4625990767
V,0,-1.08065522,0.0651588596,1.509346331
H,0,0.2142766461,-0.2913930814,3.7239471939
H,0,0.3755404093,1.3046103429,3.3346630888

The coordinates of *H₂NNH

N,0,-1.3410079062,-1.4792568691,-0.3420171854
N,0,-1.5576917594,1.1438369974,-0.0799205225
N,0,1.6556588226,1.3557794128,0.0857097731
N,0,1.2785152298,-1.5139364185,0.1895434138
C,0,-0.7013729464,-2.6342724789,-0.7258896689
C,0,-1.6425124067,-3.4479307177,-1.4015901312
C,0,-2.8707877169,-2.737449499,-1.43646841
C,0,-2.62181924,-1.5096347132,-0.7824022411
C,0,-2.8474111228,0.9202063925,-0.4754375783
C,0,-3.5005730184,2.1533921783,-0.828117324
C,0,-2.5302966239,3.1305895523,-0.7439257638
C,0,-1.2880904799,2.4984922556,-0.3462304588
C,0,-0.0365489202,3.0931840257,-0.5327938344
C,0,1.2754920293,2.527180545,-0.5566890664
C,0,2.4040395964,2.9542355002,-1.3095606016
C,0,3.4299047241,1.9761171144,-1.1973872813
C,0,2.9222837201,1.0160275215,-0.3155466504
C,0,2.6225846028,-1.4246047933,-0.2038120523
C,0,2.9650280982,-2.4755932943,-1.0380239144
C,0,1.7721788204,-3.2389952958,-1.2210834479
C,0,0.7341923367,-2.6059394373,-0.5297387615
H,0,3.9388760104,-2.6560251191,-1.4943801241

H,0,1.655770338,-4.0968602069,-1.8837292578
H,0,-1.4558831032,-4.4280416654,-1.8412366482
H,0,-3.7945428688,-3.0503170623,-1.9244715751
H,0,4.3947406267,1.9755563851,-1.7041725118
H,0,2.4428608236,3.8549235614,-1.9245942442
H,0,-2.629802295,4.1797646375,-1.0271532653
H,0,-4.5277333835,2.2579996123,-1.180523855
H,0,-0.0860697744,4.1306222965,-0.8859632849
H,0,-4.3377744695,-0.3725545966,-0.9794407104
H,0,4.2632216674,-0.3584816408,0.5772778586
N,0,3.2890868592,-0.2464643174,0.2909086434
N,0,-3.3703981107,-0.3352462752,-0.6643219699
N,0,0.3051954593,1.1219793231,2.5956634459
N,0,-1.6405023771,-0.7966104327,2.4173375622
V,0,1.3903252145,0.0637236941,1.4677296285
V,0,-0.725702281,-0.3040465319,1.0858232014
H,0,-0.1564830554,0.9094754446,3.4843138616
H,0,0.2009140013,2.1227248354,2.3828185567
H,0,-1.6454247214,-0.7978750905,3.4508864556

The coordinates of *H₂NNH₂

N,0,-1.2634582101,-1.4677765154,-0.0294285564
N,0,-1.5767959842,1.1727760359,0.0488287546
N,0,1.6929895912,1.2457812218,0.0380828991
N,0,1.5421022141,-1.6410352752,0.2449744128
C,0,-0.6043798826,-2.6176989895,-0.4512626285
C,0,-1.5251860522,-3.4242536602,-1.1530311546
C,0,-2.7582249192,-2.7258746455,-1.2215492539
C,0,-2.5346604794,-1.5060761675,-0.5656915981
C,0,-2.8307383989,0.9308700656,-0.4525585655
C,0,-3.4340534214,2.1420459585,-0.921581
C,0,-2.4589274272,3.1199169273,-0.8002076853
C,0,-1.2617876093,2.5092782841,-0.270197872
C,0,0.0159711298,3.0586785034,-0.4457474996
C,0,1.3187282913,2.4788714561,-0.4778876134
C,0,2.4339787771,2.9763928027,-1.2246371185
C,0,3.4534263946,2.0024535208,-1.2120872183
C,0,2.947730698,0.954565994,-0.4187204721
C,0,2.7760753956,-1.4998237094,-0.3482732677
C,0,2.9484519022,-2.4284798863,-1.3746191723
C,0,1.72909794,-3.1642522876,-1.4135290142
C,0,0.8496942779,-2.6137261885,-0.4545529036
H,0,3.8191766493,-2.5603644786,-2.0178436086
H,0,1.4777063995,-3.9469250438,-2.1306782769
H,0,-1.302521989,-4.3821082563,-1.6247638855

H,0,-3.6616829807,-3.0308020017,-1.7515210141
H,0,4.4173357513,2.04405654,-1.7193668721
H,0,2.4451427821,3.915534386,-1.7809005129
H,0,-2.5182366905,4.1459140624,-1.1676234479
H,0,-4.4207765673,2.2361077913,-1.3768779635
H,0,-0.0056614996,4.0940023249,-0.8092430896
H,0,-4.2520870603,-0.436117343,-0.964974464
H,0,4.4466700156,-0.3455068977,0.2696740194
N,0,3.4348357703,-0.2938394915,0.1324880232
N,0,-3.3235079232,-0.3464101496,-0.5572311123
N,0,0.2810351273,1.0038686365,2.5039659495
N,0,-2.3153741534,-0.6388381005,2.7172085462
V,0,1.6235570626,-0.0881220852,1.4919662478
V,0,-1.0545492291,-0.1511376311,1.4407418475
H,0,0.0806834157,0.9138850031,3.5071624579
H,0,0.2815168943,2.0051143732,2.2621746618
H,0,-3.1882811413,-0.1343899281,2.8999276886
H,0,-2.3364914311,-1.5603063354,3.171436613

The coordinates of *H₂NCO₂NH₂

N,0,-1.6191703746,-1.3622819197,-0.5450664247
N,0,-1.9733740385,1.1805625068,0.054272535
N,0,0.7768898906,1.5162962148,-0.8096711456
N,0,0.8447860592,-1.1519841244,-0.8655270141
C,0,-1.0694741584,-2.5571957494,-0.9664435425
C,0,-2.0837511146,-3.5298932256,-1.0001141495
C,0,-3.2971388354,-2.9000548006,-0.5794067835
C,0,-2.9564091187,-1.5673591158,-0.3103797556
C,0,-3.2816086539,0.8089926073,0.1965039911
C,0,-4.1288160938,1.9597361114,0.3646754401
C,0,-3.3037822165,3.0609150999,0.2581204767
C,0,-1.9639572642,2.5842537317,0.0207682995
C,0,-0.8687946066,3.339924222,-0.3795613938
C,0,0.3813400531,2.8638642932,-0.8584812779
C,0,1.3691735332,3.612247841,-1.5492026949
C,0,2.3898856979,2.7284804942,-1.9431436566
C,0,1.9862178373,1.4688958715,-1.4706222181
C,0,2.0387085555,-0.9859971552,-1.5585730862
C,0,2.3604318394,-2.121748269,-2.2887837555
C,0,1.2718061526,-3.0259199583,-2.0970550926
C,0,0.3440608665,-2.4098046556,-1.2550118223
H,0,3.2399272216,-2.2691524401,-2.9151685311
H,0,1.1433856314,-3.98613467,-2.5970267872
H,0,-1.975373246,-4.5742972092,-1.2942137117
H,0,-4.2879937447,-3.3528506385,-0.5331717662

H,0,3.298174253,2.9560770034,-2.5007571891
H,0,1.3040919936,4.6766174651,-1.7805344195
H,0,-3.6009793903,4.110419872,0.2733638917
H,0,-5.2120824458,1.94185959,0.4912480993
H,0,-1.012625027,4.4251802869,-0.4198009622
H,0,-4.7148868172,-0.6363174849,0.2383086398
H,0,3.6941693115,0.2814755683,-1.6415102759
N,0,2.7240631147,0.2518607939,-1.3206364924
N,0,-3.7175561836,-0.4820156224,0.1038014765
N,0,0.612775177,1.1673658898,1.7825045563
N,0,-0.7429878855,-1.1175113152,1.8346065466
V,0,1.9233489615,0.2332094212,0.6739833543
V,0,-0.4293161566,-0.0737555586,0.3406357924
H,0,0.4502037636,0.9557508612,2.7721785687
H,0,0.4044826384,2.1590808823,1.6050725847
H,0,-1.3172496289,-1.9659609027,1.7943361573
H,0,-0.0856764414,-1.1644930412,2.6305837323
C,0,2.2465737861,-0.9656175725,2.1962924456
O,0,3.3368810224,-0.8979012091,1.4775592382
O,0,1.9080820819,-1.4967499902,3.2477701225

The coordinates of *H₂NCOOHNH₂

N,0,1.5493569915,1.3650224238,-0.542142052
N,0,1.5606603035,-1.2708183537,-0.5273776945
N,0,-1.4993900456,-1.4235052055,0.2139026192
N,0,-0.8247403117,1.3759446018,0.2875729087
C,0,1.0021701339,2.6153257613,-0.6687778721
C,0,1.9491459276,3.4491435227,-1.3021999406
C,0,3.0992660406,2.6518128212,-1.5809258805
C,0,2.7878569349,1.3622773991,-1.1054345444
C,0,2.8193756316,-1.0924713873,-1.0461006341
C,0,3.3733389006,-2.336444203,-1.5069480088
C,0,2.3764974116,-3.2763196415,-1.3501459132
C,0,1.2202447652,-2.6179959549,-0.7871210504
C,0,-0.0616083684,-3.1799419257,-0.787607152
C,0,-1.3277654614,-2.5722640118,-0.5375507705
C,0,-2.5753335332,-2.8507823704,-1.1801181519
C,0,-3.4706334666,-1.7993987362,-0.8838823404
C,0,-2.7478559245,-0.9535138599,-0.0222103995
C,0,-2.2220613748,1.4267311546,0.230147778
C,0,-2.6616720074,2.6672189976,-0.2055289669
C,0,-1.4886150912,3.4244330876,-0.494249862
C,0,-0.3799412142,2.620730991,-0.2250352961
H,0,-3.6985732864,2.9750677388,-0.3421656376
H,0,-1.4584514846,4.4141137943,-0.9508990864

H,0,1.830179793,4.5050537492,-1.5479033676
H,0,3.9937084683,2.9610563946,-2.1228186456
H,0,-4.4866994454,-1.6679838523,-1.2549969517
H,0,-2.7562984198,-3.6753047496,-1.8717343307
H,0,2.4010916124,-4.3199912012,-1.668119474
H,0,4.3538411351,-2.4670406424,-1.9673250808
H,0,-0.1047784102,-4.1957323385,-1.1997185524
H,0,4.3406837741,0.1109684225,-1.6549873072
H,0,-3.8463990669,0.4666241072,1.1115989349
N,0,-2.9203213145,0.2704473945,0.7239359678
N,0,3.4225598802,0.1270043959,-1.2157691155
N,0,0.3609473897,-1.4857192243,2.0635353205
N,0,1.9778799456,0.8004209067,2.0252926086
V,0,-1.1117957688,-0.2267607028,1.842698446
V,0,0.7956500203,0.1156443313,0.7744096832
H,0,0.9780783485,-1.5727124918,2.8751375571
H,0,0.3078427335,-2.3948710749,1.5881795227
H,0,2.7053221624,1.4606712497,1.7317106039
H,0,1.8714799282,0.8119707967,3.0436920657
C,0,-0.8611181878,0.4271172873,3.6646430642
O,0,-1.731652156,1.2442605435,3.2793396487
O,0,-0.3297906486,0.5266603414,4.8988334465
H,0,0.2799300357,-0.2343001762,5.0045808337