Justification of the Estimated ZPVE Correction Added to the PCM Single-Point Energy:

The ZPVE corrections to the gas-phase energies are nearly the same with different numbers of solvent molecules, zero, one, or two. For example, the relative energy of the transition structure (TS) for the first step without solvent is 62.9 (without) and 60.4 kcal/mol (with ZPVE correction). The relative energy of the TS with one water molecule is 40.5 (without) and 38.0 kcal/mol (with ZPVE). With two water molecules, the TS relative energy is 39.9 (without) and 37.6 kcal/mol (with ZPVE correction). Consequently, the average ZPVE correction (~2.5 kcal/mol) was added to the PCM single-point energy.

Coordinates and energies of all compounds computed at B3LYP/6-311+G**

HCN
SCF= -93.45449 ZPVE= 10.2 Kcal/mol
Sum of electronic and thermal Free Energies= -93.45749
3

H	0.0000000	0.0000000	1.5651243
C	0.0000000	0.0000000	0.4983373
N	0.0000000	0.0000000	-0.6507355

$C_2H_2N_2$
SCF= -186.92409 ZPVE= 24.7 Kcal/mol
Sum of electronic and thermal Free Energies= -186.91045
6

C	-0.7010345	-0.2725596	-0.0036864
C	0.7457894	-0.3144583	-0.0184271
N	1.5080202	0.7007488	0.0115429
H	1.1852588	-1.3106961	-0.0562984
H	0.9751612	1.5732958	0.0470383
N	-1.8550130	-0.2351049	0.0087344

$C_3H_3N_3$
SCF= -280.40402 ZPVE= 38.7 Kcal/mol
Sum of electronic and thermal Free Energies= -280.37192
9

C	0.8562459	-0.9323890	0.1261996
C	-0.1755945	0.0552559	0.5327859
N	0.3508068	1.3242121	1.0230851
H	0.9223483	1.7838204	0.3217362
N	1.7051847	-1.6653887	-0.1393156
H	0.9118995	1.1801976	1.8556947
C	-1.1107518	0.2898706	-0.5827061
N	-1.8414341	0.4787850	-1.4519050
H	-0.7555468	-0.4037017	1.3418411

$C_4H_4N_4$ (DAMN)

SCF= -373.89828 ZPVE= 52.5 Kcal/mol
Sum of electronic and thermal Free Energies= -373.847439
12

C	0.2616578	1.6323310	0.0495592
C	-0.5846320	0.5040696	-0.1294077
N	-1.9428523	0.7408644	-0.3756887
H	-2.1742906	1.7054559	-0.5661355
N	0.8976318	2.5885012	0.1872197
C	-0.1241489	-0.7728156	0.0041379
N	-0.9989609	-1.8562977	-0.1444361
H	-2.3512943	0.1129480	-1.0600092
H	-1.8974374	-1.7231904	0.3076793

C	1.2520363	-1.0584653	0.2180756
N	2.3570634	-1.3545045	0.3881907
H	-0.5966311	-2.7558742	0.0772776

$C_4H_4N_4$ (AICN higher energy isomer)

SCF=-373.92556 ZPVE= 54.2 Kcal/mol
Sum of electronic and zero-point Energies= -373.839187
12

N	1.724237	0.238272	0.005614
C	1.641210	-1.142088	0.005032
C	0.443886	0.726688	-0.001440
H	2.563291	0.792163	-0.075364
N	0.407117	-1.551741	-0.004173
C	-0.365418	-0.398089	-0.002653
N	0.160405	2.079521	-0.083867
H	2.519741	-1.768155	0.023876
C	-1.779618	-0.384403	0.004981
N	-2.934294	-0.304194	0.015067
H	-0.832189	2.272002	-0.129822
H	0.606539	2.658337	0.617301

$C_4H_4N_4$ (AICN isomer)
SCF= -373.93163 ZPVE= 52.2 Kcal/mol
Sum of electronic and thermal Free Energies= -373.876240
12

N	-0.6781766	1.0854557	-0.8007630
C	-0.4865136	-0.0654503	-0.0270124
C	0.8901503	-0.1180906	0.1849263
N	1.6185782	-1.0783325	0.8383477
N	1.5020771	0.9415256	-0.4217186
C	0.5389991	1.6340536	-0.9992949
H	2.5507931	-0.7983021	1.1032485
H	1.1368585	-1.6520899	1.5132997
C	-1.5166132	-0.9120400	0.4016007
H	0.6811147	2.5400638	-1.5684078
N	-2.3511340	-1.6268862	0.7740017
H	-1.5643145	1.4271535	-1.1385338

$C_5H_5N_5$ (adenine)
SCF= -467.45139 ZPVE= 69.7 Kcal/mol
Sum of electronic and thermal Free Energies= -467.37303
15

N	-0.0600112	1.8172610	-1.8542740
C	-0.0209635	1.2070087	-0.6477496
C	-0.0165709	-0.1955525	-0.5119839
C	0.0257518	-0.6838289	0.7956995
N	0.0620482	0.0409382	1.9172120
C	0.0535540	1.3488228	1.6547490
N	0.0149520	1.9611166	0.4619945
N	-0.0463733	-1.2286168	-1.4328749
C	-0.0226933	-2.3125196	-0.7011880
N	0.0211491	-2.0535728	0.6534849
H	-0.0613159	2.8226452	-1.8946311
H	-0.0873719	1.2731578	-2.6996847
H	0.0814369	2.0087435	2.5162921
H	-0.0350546	-3.3226220	-1.0831358
H	0.0454747	-2.7253907	1.4052004

Uncatalyzed pathway: first step N-C bond formation

Reactant

15

N	-0.4493914	-1.7862208	0.4032184
C	-1.4019533	-1.8837493	-0.5055676
C	-0.3272923	-0.4570006	0.6729776
N	-1.9094203	-0.6787649	-0.8430704
C	-1.2274648	0.2790655	-0.0889903
N	0.6480861	0.0059444	1.5463203
H	-1.7522595	-2.8057325	-0.9434498
C	-1.4816117	1.6578820	-0.1374003
C	3.3967314	0.2002681	-0.3026206
N	-1.6724384	2.8011366	-0.1495033
N	4.3528566	0.2497230	-0.9396782
H	2.5043764	0.1544944	0.2986871
H	0.4500175	0.9062197	1.9652479
H	0.8977537	-0.6865256	2.2423896
H	-2.6381924	-0.4899779	-1.5142755

Product

15

N	-1.002360	-1.769248	-0.002491
C	-2.224580	-1.269068	0.008381
C	-0.160474	-0.692050	-0.009063
N	-2.225153	0.080142	0.009353
C	-0.889454	0.499891	-0.000577
N	1.198609	-0.928428	-0.024598
H	-3.135027	-1.852582	0.016635
C	-0.527274	1.858864	0.000747
C	2.233483	-0.001124	-0.021458
N	-0.232415	2.988195	0.003489
N	3.484154	-0.241097	0.026910
H	1.897168	1.034592	-0.068187
H	3.677520	-1.249038	0.075125
H	1.437369	-1.913599	0.008638
H	-3.027076	0.694604	0.010981

Pathway catalyzed by one explicit water: first step

Reactant

18

N	-1.1426300	-1.7428920	0.9238350
C	-2.1733660	-1.8344800	0.1058290
C	-0.5618930	-0.5347000	0.6666060
N	-2.3039310	-0.7445850	-0.6798220
C	-1.2637470	0.1269020	-0.3417500
N	0.5917270	-0.1443250	1.3115350
H	-2.8501680	-2.6733940	0.0501060
C	-1.0630750	1.3902070	-0.9086750
C	3.1294120	-1.2107470	-0.4746790
N	-0.8447700	2.4478950	-1.3331390
N	4.0215950	-1.5835410	-1.0969180
H	1.9451740	3.2602690	1.0085700
H	2.2899140	-0.8672260	0.1109710
O	1.1087840	2.7850630	1.0304670
H	0.7712030	0.8599930	1.3515210
H	0.7108250	-0.6088750	2.2027980
H	0.6104570	3.0803320	0.2553800
H	-3.0056010	-0.5825490	-1.3855110

Product

18

N	0.310063	-1.683648	-0.018735
C	-0.847055	-2.322239	-0.019093
C	0.010119	-0.340538	-0.007828
N	-1.890581	-1.473475	-0.005150
C	-1.377594	-0.168562	0.002188
N	1.045346	0.561684	-0.008922
H	-0.964026	-3.396994	-0.029420
C	-2.218342	0.958671	0.017267
C	0.947655	1.947673	0.001347
N	-2.932706	1.881479	0.031208
N	1.910077	2.783382	-0.026577
H	2.818609	2.306569	-0.069449
H	-0.073200	2.327139	0.041667
O	3.146514	-1.392366	-0.051240
H	3.466339	-1.571745	0.846401
H	1.975618	0.123161	-0.037928
H	2.292962	-1.875206	-0.102558
H	-2.872504	-1.709978	-0.004852

Pathway catalyzed by two explicit NH_3: Geometry for the stationary points

Reactant 1
SCF energy -580.58826 ZPVE=112.1 kcal/mol
23

N	0.7775208	-2.3346511	-0.3626348
C	2.0126452	-1.9516455	-0.0562079
C	0.0531576	-1.1824480	-0.4524746
N	2.1401451	-0.6187926	0.0579651
C	0.8766311	-0.0791852	-0.1955139
N	-1.3074960	-1.2007819	-0.7058730
H	2.8446359	-2.6277006	0.0901917
C	0.6281035	1.3021561	-0.1911079
C	-3.4157834	-0.4168815	1.4647668
N	0.4242729	2.4540935	-0.1966095
N	-4.2799061	0.0720007	2.0617859
H	-3.2598344	1.5560932	-0.8392808
H	-2.6137430	-0.8446117	0.8650003
N	-2.4980519	1.4046861	-1.5004759
H	-1.6947882	-0.3488307	-1.1481828
H	-1.5883582	-2.0584154	-1.1705363
H	-1.7783961	2.0907635	-1.2701847
H	2.9653133	-0.0334680	0.2888589
N	3.9813076	1.5101290	0.6510234
H	3.2974694	2.2564988	0.5187694
H	4.3312451	1.6033431	1.6036185
H	-2.8588887	1.6500669	-2.4213549
H	4.7622736	1.7174988	0.0300577

Product 1
SCF energy -580.59733 ZPVE= 114.8 kcal/mol
23

N	0.5380686	-1.6804782	-0.0410001
C	-0.7251067	-2.0896491	-0.0318143
C	0.4834928	-0.3102324	-0.0132453
N	-1.6020868	-1.0762910	0.0002091
C	-0.8545185	0.1058812	0.0132251
N	1.6601053	0.4033133	-0.0151099
H	-1.0333108	-3.1264912	-0.0481079
C	-1.4980677	1.3557061	0.0468616
C	1.7932651	1.7802515	0.0096564
N	-2.0951499	2.3601501	0.0749637
N	2.8830075	2.4480375	0.0078792
H	3.6942375	1.8183341	-0.0151924
H	0.8504380	2.3280410	0.0329253
N	3.6424627	-1.7310823	-0.0822394
H	4.1857014	-2.0341820	0.7243269
H	2.5145098	-0.1814511	-0.0381542

H 2.7679333 -2.2619077 -0.0808659
H -2.6420489 -1.0780593 0.0143512
N -4.3901460 -0.4187670 0.0535579
H -4.2205910 0.5882391 0.0727997
H -4.9766355 -0.5995702 -0.7600360
H 4.1647444 -2.0040541 -0.9130023
H -4.9531978 -0.6348192 0.8750304

Product 2
SCF energy -580.59938 ZPVE= 114.6 kcal/mol
23

N 0.5470162 -1.6943651 -0.0404760
C -0.7162506 -2.1011067 -0.0310701
C 0.4963951 -0.3235140 -0.0131450
N -1.5933896 -1.0877580 0.0008392
C -0.8439658 0.0937095 0.0133333
N 1.6671682 0.3933278 -0.0153067
H -1.0254343 -3.1377755 -0.0469963
C -1.4844931 1.3440942 0.0463891
C 1.7809672 1.7651506 0.0097643
N -2.0733300 2.3542194 0.0740813
N 2.9301031 2.3280243 0.0049642
H 0.8219689 2.2923110 0.0331473
N 3.6311865 -1.7274761 -0.0833220
H 4.1937086 -1.9888832 0.7239016
H 2.5389532 -0.1725440 -0.0382343
H 2.7901664 -2.3069300 -0.0830496
H -2.6323039 -1.0893952 0.0152361
N -4.3846968 -0.4227755 0.0522323
H -4.2100984 0.5833359 0.0693389
H -4.9716697 -0.6025610 -0.7611973
H 4.1713117 -1.9571540 -0.9151196
H -4.9491524 -0.6342614 0.8739328
H 2.8082300 3.3414793 0.0263250

Product 3
SCF energy -580.59836 ZPVE=115.1 kcal/mol
23

N -1.0817155 -1.4578182 -0.0000462
C 0.0541714 -2.1400721 -0.0000797
C -0.7195080 -0.1316085 0.0000036
N 1.1334007 -1.3449388 -0.0000021
C 0.6762144 -0.0208997 -0.0000097
N -1.7389206 0.8003702 0.0000086
H 0.1236729 -3.2196977 -0.0001250
C 1.6640474 0.9930286 -0.0000004
N 2.6514957 1.6166151 0.0000114
N -0.4657267 2.7434386 -0.0000370
C -1.6040669 2.1620536 -0.0000196
H -2.5795586 2.6635491 -0.0000161
H 2.1453217 -1.5903889 0.0000145
H -0.5737341 3.7569434 -0.0000450
H -2.6873908 0.3931962 0.0000270
N -4.1023932 -0.9022778 0.0000566
H -3.3271185 -1.5711766 0.0002540
H -4.6758380 -1.0984025 0.8188047
N 3.9982311 -1.4012399 0.0000522
H 4.0163345 -0.3786824 0.0000600
H 4.5241267 -1.7053736 -0.8179998
H -4.6756646 -1.0986331 -0.8187594
H 4.5240990 -1.7053904 0.8181158

Product 4
SCF energy -580.59952 ZPVE= 117.0 kcal/mol
23

N	-1.2315914	-1.5956975	0.0000142
C	-0.0202466	-2.2091646	0.0000774
C	-0.8641358	-0.2996013	0.0000155
N	1.0649727	-1.4137775	0.0000118
C	0.5279618	-0.1590068	0.0000143
N	-1.7296316	0.7922223	0.0000027
H	0.0635440	-3.2898551	0.0001202
C	1.1565036	1.1484047	-0.0000070
N	2.3464128	1.5960941	-0.0000353
N	0.1192417	2.1738073	-0.0000174
C	-1.2040224	1.9990641	-0.0000126
H	-1.8512494	2.8676290	-0.0000266
H	3.1605320	-1.4002459	-0.0000190
H	0.5011316	3.1135034	-0.0000340
H	-2.7608702	0.5795373	-0.0000000
N	-4.0974276	-0.6243806	-0.0000034
H	-3.3977278	-1.3790830	-0.0001385
H	-4.6888885	-0.7553622	0.8192222
N	4.0811468	-0.9451714	-0.0000317
H	3.0412143	0.8310009	-0.0000429
H	4.5865622	-1.2859122	-0.8166198
H	-4.6890405	-0.7551943	-0.8191458
H	4.5865642	-1.2858713	0.8165722

Product 5
SCF energy -580.62037 ZPVE= 116.9 kcal/mol
23

C	1.1862486	1.2119970	0.1833399
N	2.2556706	0.2557368	0.2283003
C	2.1439459	-1.0940289	0.1387414
N	1.0249117	-1.7483918	-0.0052626
C	-0.0543404	-0.8984977	-0.0574632
C	-0.0687720	0.4889857	0.0223635
N	-1.3627014	0.9544738	-0.0726485
C	-2.1005299	-0.1319352	-0.2059371
N	-1.3616775	-1.2823031	-0.2034099
N	1.5067004	2.4403155	0.2856031
H	-1.6425740	-2.2751120	-0.2880723
H	-3.1772635	-0.1412933	-0.3082292
H	3.0789460	-1.6465765	0.1947074
H	-1.6266591	4.4757320	0.9279795
H	0.6838654	3.0587846	0.2441787
N	-1.1749429	4.0436622	0.1234510
H	-1.5569111	3.0982578	0.0313330
N	-1.1021130	-4.1036839	-0.3439265
H	-1.1583915	-4.6468376	-1.2040282
H	-0.1271354	-3.8108457	-0.2348597
H	-1.4718875	4.5716971	-0.6956853
H	-1.3117748	-4.7417695	0.4221328
H	3.1695371	0.6801721	0.3395278

Product5 isomer
SCF energy -580.62934 ZPVE= 117.4 kcal/mol
23

C	0.2921620	0.9146654	-1.1484508
N	1.5214850	0.4801912	-0.5961963
C	1.6474487	-0.3601815	0.4609225
N	0.6668844	-0.9016712	1.1368992
C	-0.5535971	-0.5159231	0.6459012
C	-0.8131332	0.3333973	-0.4231455
N	-2.1685501	0.4797159	-0.6138347
C	-2.7079131	-0.2704478	0.3265667
N	-1.7802909	-0.8979308	1.1202009
N	0.3173764	1.7175539	-2.1577462
H	-1.8904505	-1.5379901	1.9244264
H	-3.7706586	-0.3992838	0.4832491
H	2.6714626	-0.5852447	0.7489385
H	2.3721110	2.1139449	-2.6459738

H -0.6432490 1.9311708 -2.4310663
N 3.3206007 1.8686665 -2.3329139
H 3.8081533 1.4562345 -3.1269359
N -0.9931238 -2.5959657 3.2587659
H -1.0002896 -3.6141864 3.2247432
H -0.0947591 -2.2876398 2.8756984
H 3.8031200 2.7374607 -2.1078525
H -1.0052584 -2.3342845 4.2433252
H 2.3693429 0.8568369 -1.0655409

Product 6
SCF energy -580.6444 ZPVE= 117.0 kcal/mol

23

C 0.3904778 0.7279752 -1.0844384
N 1.6058574 0.3517178 -0.6138063
C 1.6613613 -0.4095615 0.4906999
N 0.6615501 -0.8802330 1.2391079
C -0.5345427 -0.4933679 0.7518225
C -0.7577246 0.2944396 -0.3806815
N -2.1115508 0.4952247 -0.5871632
C -2.6771943 -0.1605029 0.4031991
N -1.7830060 -0.7783406 1.2457500
N 0.3186156 1.4907755 -2.1902184
H -1.9231921 -1.3538198 2.0923003
H -3.7449940 -0.2270206 0.5677217
H 2.6650543 -0.6774744 0.8170652
H 1.1816469 1.7807303 -2.6666207
H -0.5906122 1.7641297 -2.5301298
N 3.1342529 1.8399634 -2.8760150
H 3.6432687 1.3092883 -3.5811712
N -1.0185612 -2.3470088 3.4808134
H -1.0504242 -3.3646944 3.5193876
H -0.1243799 -2.0899628 3.0501428
H 3.7016442 2.6568108 -2.6551463
H -0.9919187 -2.0178805 4.4447375
H 3.0895370 1.2613067 -2.0311763

Pathway catalyzed by two explicit H_2O: Geometry for the stationary points

Reactant1

SCF energy -620.33657 ZPVE= 95.9kcal/mol
21

N 0.7987381 -2.4315784 -0.4717619
C 2.0277950 -2.0495572 -0.1449131
C 0.0590670 -1.2870652 -0.5117988
N 2.1338919 -0.7208441 0.0338200
C 0.8645732 -0.1858353 -0.1986522
N -1.2990186 -1.3071556 -0.7707148
H 2.8694065 -2.7192004 -0.0295217
C 0.5976061 1.1885423 -0.1382070
C -3.2336664 -0.1519412 1.3908435
N 0.3752568 2.3368830 -0.0999092
N -3.9441632 0.6491930 1.8332887
H -3.0556561 1.5223018 -0.5798627
H -2.5608235 -0.8534715 0.9100390
O -2.4063640 1.3807758 -1.2883512
H -1.6847182 -0.4359114 -1.1530288
H -1.5777568 -2.1349985 -1.2868003
H -1.6899694 2.0064214 -1.0835266
H 2.9380126 -0.1371356 0.2810408
O 3.6336104 1.6093142 0.6665475
H 3.0045204 2.2236455 0.2509864
H 3.5938287 1.8372825 1.6084085

Product 1
SCF energy -620.34791 ZPVE= 98.8 kcal/mol
21

N	0.6281384	-1.6610750	0.0011135
C	-0.6101962	-2.1306489	-0.0152692
C	0.5214249	-0.2946530	0.0076830
N	-1.5224884	-1.1501397	-0.0186070
C	-0.8279745	0.0634801	-0.0039940
N	1.6675636	0.4640419	0.0223764
H	-0.8734754	-3.1768508	-0.0254836
C	-1.5238144	1.2810654	0.0014817
C	1.7453469	1.8488051	0.0246454
N	-2.1712976	2.2438059	0.0073326
N	2.8028635	2.5553783	0.0207334
H	3.6487234	1.9802515	0.0093765
H	0.7813592	2.3542318	0.0326232
O	3.4528851	-1.8383826	-0.0572337
H	3.9754419	-2.3487638	0.5676630
H	2.5332452	-0.0788560	0.0218635
H	2.5403107	-2.1831283	-0.0142744
H	-2.5411460	-1.2077622	-0.0333174
O	-4.2608495	-0.3210695	-0.0048368
H	-4.1401920	0.6376796	0.0240903
H	-5.1227294	-0.4735562	-0.4039013

Product 2

SCF energy -620.35019 ZPVE= 98.8 kcal/mol

21

N	-0.9448683	-0.2384849	1.4981009
C	-2.0665053	-0.1853640	0.7967007
C	0.0790047	-0.0822846	0.6007378
N	-1.8390412	-0.0070184	-0.5112215
C	-0.4530679	0.0665233	-0.6837143
N	1.3747452	-0.0923062	1.0494521
H	-3.0583001	-0.2731024	1.2123249
C	0.0985921	0.2622250	-1.9571073
C	2.5111026	0.0153392	0.2746702
N	0.4850211	0.4263873	-3.0393952
N	3.6663429	-0.0211050	0.8084492
H	2.3186204	0.1282540	-0.7941229
O	0.6046765	-0.3374472	3.8658406
H	1.4968425	-0.1907035	2.0605862
H	-0.2150092	-0.3967833	3.3413848
H	-2.5014366	0.0714401	-1.2826909
O	-2.8265414	0.3605388	-3.1745586
H	-1.9911108	0.4740486	-3.6472679
H	-3.4713394	0.0726168	-3.8276364
H	4.3885665	0.0727167	0.0985914
H	0.5979296	-1.0741615	4.4831543

Product 3
SCF energy -620.35103 ZPVE= 99.5kcal/mol

21

N	0.9796877	-1.5424473	-0.0163168
C	-0.2010565	-2.1363945	0.0113008
C	0.7327466	-0.1916570	-0.0201441
N	-1.2056854	-1.2503679	0.0249754
C	-0.6437140	0.0320258	0.0048240
N	1.8236560	0.6527901	-0.0478033
H	-0.3572978	-3.2037622	0.0233538
C	-1.5426050	1.1206625	-0.0061872
N	-2.4788051	1.8044238	-0.0194294
N	0.7074618	2.6765984	0.0715222

C	1.7977313	2.0227482	0.0072087
H	2.8029232	2.4533889	-0.0115672
H	-2.2143087	-1.4167908	0.0496627
H	0.8664504	3.6791820	0.1042963
H	2.7249503	0.1779911	-0.0757560
O	3.7967086	-1.4843321	-0.0161172
H	2.9031529	-1.8827999	-0.0294288
H	4.3212767	-1.9544047	-0.6701507
O	-4.0386524	-0.8237379	0.0153962
H	-3.9439663	0.1414873	-0.0183253
H	-4.8104492	-1.0010206	0.5610322

Product 4
SCF energy -620.32589 ZPVE= 99.3 kcal/mol

21

N	-1.1219009	-1.3931561	0.0165569
C	-0.0197794	-2.1466904	0.0233250
C	-0.8035301	-0.0217261	0.0043222
N	1.0297622	-1.3473085	0.0186770
C	0.6105501	-0.0025959	0.0074432
N	-1.8144925	0.8396881	-0.0101289
H	0.0083555	-3.2227162	0.0295468
C	1.6355869	0.9638532	-0.0085583
N	2.6825377	1.4682934	-0.0205524
N	-0.3470157	2.6630117	-0.0064275
C	-1.5358592	2.1771737	-0.0224302
H	-2.4384398	2.7966583	-0.0471805
H	2.0225800	-1.6145810	0.0259583
H	-2.1036877	-1.6965207	0.0228573
O	3.8327770	-1.2806582	-0.0407805
H	3.8485319	-0.3076630	-0.0631783
H	-0.3467138	3.6797746	-0.0220261
H	4.5917845	-1.5565350	0.4812438
O	-3.8289793	-1.0193410	-0.0746655
H	-3.3652823	-0.1414582	-0.0485309
H	-4.5715549	-0.9707517	0.5333904

Product 5
SCF energy -620.37754 ZPVE= 101.5 kcal/mol

21

N	-1.3101087	-1.3591847	0.1211849
C	-2.1318239	-0.2685160	0.0555463
C	-0.0258804	-0.8863510	0.0626771
N	-1.4593916	0.8593370	-0.0417881
C	-0.1333162	0.4901795	-0.0375414
N	1.1159393	-1.6442991	0.0998092
H	-3.2068421	-0.3534750	0.0842945
C	1.0693315	1.3020181	-0.1118800
N	1.2848812	2.5511151	-0.1990443
N	2.2094514	0.4362689	-0.0719633
C	2.1930115	-0.9146313	0.0288893
H	3.1637095	-1.3983614	0.0500158
H	-1.8258505	2.7435824	-0.1580224
H	-1.5435449	-2.3475138	0.1998776
O	-1.6575313	3.7060645	-0.1932349
H	0.4170128	3.0906972	-0.2144847
H	3.0960998	0.9226629	-0.1157726
H	-2.1386454	4.0335030	-0.9580799
O	-0.4390525	-4.0222049	0.3807808
H	0.3891744	-3.5150301	0.2822119
H	-0.2917781	-4.8857990	-0.0139444

Product 5 isomer
SCF energy -620.38559 ZPVE=101.8 kcal/mol

21

C	0.3517585	0.8826537	-1.0991348
N	1.5455358	0.3818300	-0.5283882
C	1.6129156	-0.4752058	0.5195344
N	0.5876852	-0.9719995	1.1554753
C	-0.6012861	-0.5275102	0.6468596
C	-0.7944479	0.3456081	-0.4126459
N	-2.1345866	0.5586290	-0.6291251
C	-2.7358638	-0.1715794	0.2827919
N	-1.8547630	-0.8540741	1.0860882
N	0.4384143	1.6987258	-2.0898505
H	-2.0335483	-1.4849758	1.8648123
H	-3.8042261	-0.2495953	0.4142553
H	2.6141489	-0.7509557	0.8312152
H	2.2273901	2.0519858	-2.4807359
H	-0.4861660	1.9853742	-2.4001743
O	3.1784815	1.8967684	-2.2645358
H	3.6417062	1.7751291	-3.0977110
O	-0.8061776	-2.4668182	3.1512581
H	-0.6067113	-3.3453084	3.4854276
H	-0.0149983	-2.1555474	2.6717918
H	2.4095169	0.7187152	-0.9664885

Product 6
SCF energy -620.40083 ZPVE= 101.4 kcal/mol

21

C	0.5024850	0.8573444	-0.9415640
N	1.6319625	0.3440734	-0.4001523
C	1.5344245	-0.5654677	0.5796856
N	0.4300314	-1.0681148	1.1271335
C	-0.6826310	-0.5495730	0.5784302
C	-0.7349175	0.4000668	-0.4411904
N	-2.0430307	0.7108959	-0.7586932
C	-2.7546763	-0.0349140	0.0515274
N	-1.9906306	-0.8204814	0.8845522
N	0.5980050	1.7690243	-1.9245842
H	-2.2758564	-1.4835453	1.6019097
H	-3.8336246	-0.0554665	0.0883185
H	2.4767908	-0.9335860	0.9728889
H	3.1494038	1.2052443	-1.2470294
H	1.5139030	2.0817135	-2.2320587
H	-0.2420767	2.1710221	-2.3060398
O	3.5122014	1.8692228	-1.8701422
H	4.2375653	1.4447864	-2.3363783
O	-1.1682481	-2.5989901	2.9069147
H	-1.0142530	-3.4991476	3.2054409
H	-0.3359495	-2.2854039	2.4996433

Full citation for text ref. 21

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