

MECHANISM AND KINETICS FOR THE REACTION OF FULMINIC ACID, HCNO, WITH AN AMINO RADICAL, NH₂

Electronic Supplementary Information (ESI)

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Table 1S: Theoretical predictions of detailed energies for reactants, intermediates, main transition states, and products of the NH₂ + HCNO reaction at two different levels of theory, based on B3LYP/6-311++G(3df,2p) geometries. ZPE energies are reported unscaled.

Species	Single point energy (a.u.)		ZPE (a.u)
	B3LYP/6-311++G(3df,2p)	CCSD(T)/6-311++G(3df,2p)	B3LYP/6-311++G(3df,2p)
RA (HCNO + NH ₂)	-224.5459851	-224.1151106	0.03835
IS1a	-224.6306090	-224.1978849	0.0496250
IS1b	-224.6260708	-224.1926265	0.0492070
IS2	-224.5968285	-224.1660697	0.0484830
IS3	-224.6031760	-224.1809438	0.0495460
IS4	-224.5660223	-224.1439595	0.0494080
IS5	-224.5661142	-224.1428490	0.0483540
IS6	-224.6838731	-224.2559547	0.0487540
IS7	-224.5225560	-224.0946478	0.0467900
IS8	-224.5918294	-224.1619080	0.0482770
IS9	-224.6222702	-224.1940854	0.0492080
IS10	-224.5948163	-224.1684902	0.0487400
IS11	-224.6319800	-224.2009768	0.0496690
IS12	-224.5088412	-224.0834568	0.0493800
IS13	-224.5879391	-224.1555916	0.0490730
IS14	-224.5241348	-224.0946369	0.0475640
IS15	-224.6563635	-224.2251084	0.0483300
COM	-224.5602149	-224.1335264	0.0459860
T0/1	-224.5475708	-224.1151834	0.0419350
T1P2	-224.5584972	-224.1255360	0.0454990
TS1a1b	-224.6088076	-224.1733465	0.0479610
T1/3	-224.5919506	-224.1628796	0.0485000
T3/5	-224.5220159	-224.0997802	0.0440170
T5/11	-224.5507627	-224.0967573	0.0470210
T1/14	-224.4798838	-224.0466219	0.0461240
T0/14	-224.5070322	-224.0718792	0.0440810
T1/13	-224.5218810	-224.0859811	0.0434380
T3/4	-224.4969937	-224.0736093	0.0431880
T4/5	-224.4928708	-224.0691289	0.0437120
T3/6	-224.5021811	-224.0977841	0.0436590
T13/2	-224.5081842	-224.0730413	0.0420420
T1/2	-224.5558530	-224.1245719	0.0445540

T2/9	-224.5004920	-224.0859632	0.0428260
T1/9	-224.6094549	-224.1794579	0.0455530
T9/11	-224.5423503	-224.1124289	0.0429010
T9/8	-224.5162422	-224.0861485	0.0434370
T8/11	-224.5193931	-224.0858586	0.0425630
T8/10	-224.5224857	-224.0951830	0.0432550
T9/10	-224.5425578	-224.1157574	0.0436050
T1/11	-224.5674679	-224.1334808	0.0437590
T10/11	-224.5635132	-224.1333378	0.0434460
T13/11	-224.5076308	-224.0751034	0.0426980
T11/12	-224.4999074	-224.0702315	0.0473260
T0P1	-224.5389932	-224.1001565	0.0399330
T1P2	-224.5208769	-224.0903786	0.0431770
T6P5	-224.6010086	-224.1713166	0.0431180
T2P6	-224.5844499	-224.1508256	0.0451740
T2P7	-224.5249715	-224.0923699	0.0390180
T2P1	-224.5320986	-224.1023910	0.0451390
T9P9	-224.5189107	-224.0851976	0.0408390
T9P10	-224.5300367	-224.1012076	0.0439900
T9P7	-224.5239401	-224.0942970	0.0390350
T9P3	-224.5403994	-224.1021710	0.0390050
T10P13	-224.5711614	-224.1429171	0.0458620
T10P12	-224.5239808	-224.1011971	0.0401310
T11P11	-224.5161818	-224.0818715	0.0370300
T11P2	-224.5332479	-224.0964529	0.0416260
T12P8	-224.4590712	-224.0344895	0.0402500
T15P5	-224.5773819	-224.1454873	0.0432790
T7P4	-224.5191811	-224.0893723	0.0448480
T0/7	-224.5094322	-224.0735797	0.0440310
T4/13	-224.5344529	-224.1032303	0.0472540
T4/6	-224.5574008	-224.1198093	0.0477550
T14/15	-224.4761955	---	0.0456990
PR1 (NH ₃ + CNO)	-224.5528932	-224.1231702	0.0421760
PR2 (NO + H ₂ NCH)	-224.5541362	-224.1307392	0.0441220
PR3 (H ₂ + HNCNO)	-224.5610737	-224.1215139	0.0339110
PR4 (HCN + NH ₂ O)	-224.6070958	-224.1794864	0.0426640
PR5 (NCO + NH ₃)	-224.6534521	-224.2240906	0.0442720
PR6 (NH ₂ CN + OH)	-224.6106582	-224.1868732	0.0424550
PR7 (H + HNCNOH)	-224.5282142	-224.1009447	0.0376090
PR8 (H + HCN(H)NO _{-cy})	-224.4639870	-224.0463126	0.0388900
PR9 (HNCN + H ₂ O)	-224.6494389	-224.2206469	0.0409680
PR10 (H ₂ O + NC(H)N)	-224.5791887	-224.1577961	0.0408470
PR11 (NO + H ₂ + HCN)	-224.5803626	-224.1626196	0.0308860
PR12 (H + HON(H)CN)	-224.5303816	-224.1106783	0.0387160
PR13 (HNOH + HCN)	-224.5921157	-224.1683452	0.0433310
PR14 (CH ₂ NH + NO)	-224.6092523	-224.1874963	0.0442970

Table 2S: Gibbs free energies (ΔG^0) and entropies (ΔS^0) for the $\text{NH}_2 + \text{HCNO}$ reaction products at the CCSD(T)/CBS//B3LYP/6-311++G(3df,2p) level of theory.

Species	$\Delta G^0(298.15\text{K})$ (kcal mol ⁻¹)	$\Delta S^0(298.15\text{K})$ (cal mol ⁻¹ K ⁻¹)
PR1 ($\text{NH}_3 + \text{CNO}$)	-2.1	-2.8
PR2 ($\text{NO} + \text{singlet H}_2\text{NCH}$)	-9.6	10.8
PR3 ($\text{H}_2 + \text{HNCNO}$)	-7.5	-5.9
PR4 ($\text{HCN} + \text{NH}_2\text{O}$)	-42.3	-38.6
PR5 ($\text{NCO} + \text{NH}_3$)	-67.5	-65.3
PR6 ($\text{NH}_2\text{CN} + \text{OH}$)	-46.6	-43.8
PR7 ($\text{H} + \text{HNCNOH}$)	7.5	7.8
PR8 ($\text{H} + \text{HCN(H)NO}_{\text{cy}}$)	44.0	43.0
PR9 ($\text{HNCN} + \text{H}_2\text{O}$)	-69.7	-66.3
PR10 ($\text{H}_2\text{O} + \text{NC(H)N}$)	-29.9	-26.4
PR11 ($\text{NO} + \text{H}_2 + \text{HCN}$)	-42.4	-31.7
PR12 ($\text{H} + \text{HON(H)CN}$)	2.3	2.6
PR13 ($\text{HNOH} + \text{HCN}$)	-34.8	-31.4
PR14 ($\text{CH}_2\text{NH} + \text{NO}$)	-45.2	-42.0

Table 3S: Vibrational wavenumbers (unscaled) for the reactants, intermediates, transition states and products of the $\text{NH}_2 + \text{HCNO}$ reaction, as obtained using B3LYP/6-311++G(3df,2p).

HCNO	257.1878 1291.1961	560.4896 2321.6017	566.2711 3490.0419
NH_2	1530.7356	3364.1399	3452.5462
IS1a	245.8404 562.9239 1055.2741 1446.9104 3222.5661	323.1408 690.1620 1184.0126 1634.8006 3561.4419	383.2262 827.0218 1248.1288 1730.6023 3666.8806
IS1b	256.5027 567.0565 1041.6339 1427.7923 3133.1882	311.5198 671.6791 1233.1337 1641.1208 3541.8016	350.7944 779.1578 1263.4254 1739.7680 3640.7233
IS2	218.6318 360.0477 921.1254 1414.8584 3518.8738	270.5163 516.1151 1128.1833 1622.5008 3692.9317	314.4058 584.4783 1205.7640 1690.6406 3822.3443
IS3	334.5107 676.4591 1052.0326 1316.0073 3141.2025	435.4690 708.6757 1138.0097 1472.5951 3542.5818	497.7824 906.6136 1239.8157 1647.7736 3638.6650
IS4	181.3128 683.4229 997.6250 1338.0738 3335.3387	437.5937 772.3188 1152.4682 1440.9762 3519.2495	497.9628 872.8648 1221.9628 1632.2669 3603.9700
IS5	341.1119 711.2236 1097.3591 1291.0894 3119.7603	472.4579 749.2034 1134.0257 1344.5581 3353.4039	539.4318 1025.8498 1201.9547 1390.6768 3452.7238
IS6	322.0281 506.3173 917.9155 1387.8237 3466.0630	351.1602 553.6893 1052.5776 1583.7904 3593.0931	424.7678 713.7538 1148.6892 1656.2497 3722.7573
IS7	114.1030 611.9473 869.9442 1285.0677 3184.9507	261.5355 698.3956 1026.3598 1629.5985 3449.4791	297.0109 709.8351 1157.7808 1702.9908 3539.3353
IS8	154.7316 483.3645 950.5071 1387.2109 3479.8784	314.1179 584.4091 1080.5210 1434.7203 3554.2390	329.2344 662.6868 1198.1149 1781.9264 3795.4677
IS9	213.8027 608.8795 1059.9976 1374.3553 3105.4156	372.5496 821.5755 1102.2771 1416.3098 3426.1861	512.4252 1028.7439 1226.3423 1530.1924 3800.6203
IS10	149.0551 543.6560 1026.5359 1389.7098 3043.9252	359.5598 760.7333 1141.7371 1453.4743 3511.8695	382.0907 902.1205 1248.2820 1678.6014 3802.8671
IS11	195.2875 601.0260 1070.8313 1386.9322 3152.8786	368.6866 816.5047 1234.7151 1486.4829 3396.7230	583.5173 1052.4979 1367.3767 1649.8271 3438.6751
IS12	262.0667 865.6584 1031.4586 1294.5477 3143.1655	699.7663 918.9672 1106.0076 1315.4975 3356.1997	790.2111 1004.8580 1149.0820 1324.2718 3413.6473

IS13	187.7481 594.1286 1015.0685 1384.2358 3214.2067	384.4452 641.1937 1232.3273 1506.5915 3369.3660	564.0413 759.0954 1366.4281 1663.6911 3657.9352
IS14	135.3303 542.5050 969.4992 1297.1264 3245.7236	340.5053 587.6920 1066.4874 1571.0638 3449.3438	439.3579 777.6975 1235.6374 1689.2635 3531.1488
IS15	102.4116 480.3209 1055.1233 1423.5878 2816.0721	195.5274 660.7955 1229.4639 1639.3708 3459.6370	386.5387 990.3029 1385.2635 1708.1527 3681.6999
COM	57.6132 249.2748 1045.8992 1470.0732 2961.6584	120.8434 320.5524 1139.6368 1672.9383 3411.1662	174.6230 831.1307 1355.5399 1879.9560 3494.3969
T0/1	186.4355i 365.4774 504.8963 1278.8871 3376.4358	95.2275 411.4846 559.3941 1536.2314 3446.4624	99.2063 443.5710 569.2644 2256.3647 3464.5240
T1P2	288.3880i 223.2256 994.9510 1453.1836 2987.5872	98.1758 464.3330 1089.0588 1655.7778 3403.6101	215.6925 795.0471 1330.7355 1734.9886 3525.4442
TS1a1b	458.8183i 441.9413 974.5001 1430.8959 3055.0665	259.3467 658.7221 1182.8434 1634.2966 3528.9361	291.3070 770.9224 1202.9444 1988.1442 3632.5249
T1/3	363.5824i 520.2442 1006.2697 1332.2289 3168.4198	455.4132 617.3771 1141.0084 1512.7634 3569.5690	473.0291 898.1093 1252.4480 1649.4174 3692.6463
T3/5	2118.1925i 744.8104 1052.5288 1231.2467 1947.9590	512.3434 796.4632 1059.2654 1349.7417 3191.9621	621.9151 862.3050 1136.9900 1368.5867 3444.9342
T5/11	773.4376i 648.3169 1054.1703 1350.3486 3179.9526	303.9420 780.7472 1099.5192 1360.0672 3334.5924	482.3907 1027.4622 1176.7341 1392.1859 3449.2263
T1/14	735.7101i 542.3265 905.6740 1130.9237 3008.5766	393.4739 612.7387 1027.4298 1472.3691 3494.8193	476.9609 848.7349 1111.2408 1589.1078 3631.7639
T0/14	598.9041i 389.9455 836.1289 1224.5556 3281.1016	93.0853 522.0797 882.7410 1514.4974 3407.8823	343.5824 579.3452 910.5089 1842.9069 3520.8931
T1/13	1386.9802i 387.9600 932.5296 1346.4103 1948.5576	329.4265 533.7511 1091.2117 1508.7417 3516.8953	344.6182 623.0972 1174.7903 1629.4349 3699.8124
T3/4	2141.5467i 463.3254 909.7292 1245.8037 2087.1510	283.3306 559.7666 1010.4515 1475.1609 3486.6777	374.8739 602.3345 1209.8286 1620.1323 3628.8923
T4/5	1999.0975i 516.6015 984.0017 1208.1698	373.5464 671.2304 1144.3161 1319.1985	462.0710 912.6751 1160.1859 1459.9398

	2188.2232	3347.6509	3439.7183
T3/6	2884.6734i	127.0110	419.5647
	483.3125	609.2167	751.5311
	899.4139	1049.9595	1123.4628
	1281.6259	1348.3061	1625.3350
	2282.5479	3529.7776	3633.1262
T13/2	1962.7946i	184.7884	294.3532
	338.4444	393.1484	495.1383
	570.1562	909.3001	1137.0647
	1168.0323	1589.5192	1637.3519
	2544.2782	3510.0048	3682.6149
T1/2	1725.4126i	186.6956	429.2407
	533.0635	664.9204	760.9861
	1014.4870	1153.7630	1154.8700
	1334.6353	1487.5602	1646.2022
	1991.2116	3517.2692	3681.9954
T2/9	2014.0324i	236.2691	309.1788
	362.3728	406.7271	591.7416
	938.9661	1088.4276	1111.5339
	1134.0913	1416.2705	1730.6982
	2215.7914	3428.6133	3827.9135
T1/9	1516.5392i	400.7607	621.7769
	748.3963	871.5128	939.2031
	1014.4314	1119.7782	1156.7646
	1263.6382	1365.8824	1563.7495
	2065.5782	3210.9426	3652.8412
T9/11	2112.9038i	166.9104	312.0022
	367.3171	613.3276	772.9756
	986.0624	1045.1703	1143.3430
	1248.3412	1378.6073	1593.9397
	2663.0513	3038.1321	3501.9674
T9/8	1941.5635i	230.0880	373.4500
	430.9179	575.0553	783.4716
	907.6328	1006.7219	1079.6024
	1166.8200	1424.5710	1690.1363
	2074.3143	3521.7691	3802.2289
T8/11	1937.6246i	249.9347	437.8382
	547.6506	663.7726	796.6567
	873.4786	922.3566	982.6204
	1155.6697	1282.3467	1865.2376
	1975.5915	3455.5270	3474.3626
T8/10	1879.2278i	233.6144	298.2888
	351.1123	485.1823	554.0129
	673.5953	1041.6803	1130.5178
	1391.3158	1434.7951	1694.6967
	2447.1842	3450.7076	3800.2143
T9/10	2033.9623i	238.2189	379.2686
	461.5303	748.8477	915.8613
	954.2851	1021.2063	1207.8656
	1213.6834	1388.3500	1625.6715
	2003.0186	3184.4781	3797.9612
T1/11	1812.4177i	228.4665	450.4869
	478.9131	769.1015	930.7125
	1018.7067	1097.4755	1098.0004
	1324.7715	1475.5083	1496.0929
	2010.4987	3204.3132	3625.1189
T10/11	2494.4114i	354.3496	417.8520
	480.3323	788.2033	848.2077
	888.5107	1132.6205	1143.2881
	1293.9038	1402.1416	1611.5899
	2097.4796	3099.6952	3512.5917
T13/11	1883.7309i	211.4920	357.3405
	498.5377	623.5344	656.6653
	943.6785	1083.3354	1268.6101
	1368.3268	1423.8781	1499.9110
	2399.8553	3171.2019	3235.8740
T11/12	1107.2852i	307.7505	630.8746
	737.2873	900.9223	945.5932
	990.7589	1094.9497	1149.8520
	1221.0683	1347.3150	1397.4902
	3169.9851	3434.8142	3445.1675
TOP1	1455.1289i	100.1967	140.5168
	377.7310	505.0786	512.8879
	579.2993	721.0040	1214.4205

	1244.8442 2179.9612	1422.4398 3428.4410	1575.9201 3525.6813
T6P5	1688.8938i 578.4806 766.2053 1188.3860 2122.4236	286.2919 614.3671 797.6350 1499.5885 3485.1052	394.4647 697.3753 973.4388 1896.2788 3626.5378
T2P6	569.8012i 247.7526 550.3957 1169.8167 3524.3320	123.7350 335.5129 1040.5995 1630.7030 3638.3538	226.2408 447.1154 1131.1245 1958.7030 3804.9006
T2P7	697.9235i 319.5706 673.8932 1043.9168 2115.9853	197.6669 356.2835 746.7507 1233.6737 3531.5581	233.3628 507.7329 876.8134 1463.6253 3826.2358
T2P1	1329.6563i 642.4897 995.9941 1519.9407 1962.1884	229.2430 787.8532 1050.3554 1538.7185 3469.8262	470.2528 910.6440 1074.2285 1609.8374 3552.1398
T9P9	1605.2265i 491.6416 691.0091 1181.3134 1666.0468	317.2856 561.0494 938.4731 1210.8807 3540.9874	357.8573 603.1643 1053.3973 1595.8018 3717.3293
T9P10	819.3625i 562.4227 915.6856 1262.2132 2220.7894	427.5344 749.0665 998.5155 1403.4201 3063.4593	485.4842 843.5973 1135.2557 1478.2508 3760.3436
T9P7	736.0735i 345.0485 683.8235 1028.2883 2050.4989	119.0907 441.5258 755.7127 1216.9886 3527.9290	270.4241 511.0707 895.4966 1463.9785 3824.7124
T9P3	968.0714i 508.5566 801.0134 1111.0290 1792.5818	166.9397 646.5211 853.4999 1233.1300 2621.2926	433.1672 762.0578 1086.8651 1484.8982 3619.7742
T10P13	541.2619i 366.1791 902.2928 1285.5763 3263.9312	114.0481 458.3770 980.8578 1545.9465 3422.5617	277.8424 785.1659 1027.4199 1914.1778 3786.8639
T10P12	753.7957i 328.2439 606.2060 1094.8499 2218.8160	129.5889 499.3345 722.3888 1389.0132 3523.3207	305.9446 520.1066 1017.9925 1464.8700 3794.8179
T11P11	1269.9342i 506.1500 796.0288 1114.7830 1918.8173	132.9042 623.2637 864.7134 1215.1552 2234.4311	195.6389 647.2233 963.9223 1735.8422 3305.3320
T11P2	871.0501i 242.3748 982.7169 1291.5156 2344.4507	165.8123 585.3896 983.8554 1384.7389 3086.0090	191.0705 645.6023 1108.4168 1775.9516 3484.0154
T12P8	867.6895i 616.3031 874.0773 1099.6512 1528.9175	337.3245 725.7629 987.0440 1243.5385 3259.6725	383.1914 771.3662 1041.1924 1336.1135 3463.5526
T15P5	1042.0619i 514.7071 948.2228 1207.9911 1848.9981	299.9914 646.5770 1014.9568 1465.3419 3451.2896	419.3989 822.1579 1193.6797 1616.7924 3547.1871
T7P4	661.6499i 321.9221	139.1890 570.8896	282.8723 679.6422

	765.2171 1300.2645 3285.0718	833.5416 1639.6536 3459.9246	1103.1205 1745.1977 3559.6140
T0/7	675.5341i 396.0474 867.7958 1120.2160 3221.5255	98.8317 554.2318 915.2275 1539.8839 3420.7974	231.1410 622.5117 958.0028 1866.2151 3514.9223
T4/13	791.4771i 512.3009 941.8811 1287.0341 3436.4834	248.6141 545.0117 1068.8382 1558.3885 3493.2567	421.1095 786.7926 1147.7490 1629.4693 3665.0750
T4/6	1860.5324i 490.4290 976.8655 1267.3597 3457.1945	195.9462 648.5659 1052.3506 1459.4571 3543.0779	444.0316 925.9593 1234.4620 1630.2366 3636.1701
T14/15	593.7432i 470.5673 866.0343 1336.7208 3016.8145	115.1657 728.2331 999.3814 1370.6986 3476.2806	459.5992 822.0730 1192.0940 1627.1412 3578.6129
T1P14	1840.9446i 584.7236 1006.0509 1280.4856 2342.1448	211.7512 607.5516 1135.3122 1363.9646 3103.7775	354.6674 970.2872 1144.5636 1454.2959 3392.9918
CNO	325.9029	1210.1211	1947.6060
NH ₃	1026.6259 3478.4097	1665.6128 3596.7302	1665.6129 3596.7304
NO	1978.9435		
H ₂ NCH	809.4749 1381.8003 2924.6559	1072.7798 1437.9751 3378.8839	1153.2050 1688.1216 3541.3736
H ₂	4420.4114		
HNCNO	182.7010 452.3805 1517.9645	217.5911 961.3307 2259.8090	322.7425 1058.4437 3492.1062
HCN	760.9965 3436.6842	760.9968	2199.3121
NH ₂ O	284.8289 1662.2109	1269.8909 3419.3444	1383.9772 3549.1412
OCN	512.9636 1994.4574	597.0145	1298.9170
OH	3722.2830		
H ₂ NCN	410.6416 1095.6855 2351.0391	486.3178 1188.7559 3551.7717	556.9405 1629.8717 3642.4583
HNCNOH	243.1700 684.7921 992.2473 2175.0552	295.0929 719.8384 1245.0642 3519.7913	450.8909 881.1172 1470.4406 3830.8526
HCN(H)ON _{cy}	570.9691 876.4713 1102.6970 1616.2019	757.6183 984.7012 1252.2887 3248.9267	789.8296 1057.2801 1338.3334 3475.5904
HNCN	468.2427 1204.2242	497.6008 1906.9165	1057.3822 3472.1078
H ₂ O	1627.0107	3822.8922	3926.4178
NC(H)N	723.2614 1203.8996	850.5294 1636.8386	930.9604 3208.0630
HON(H)CN	241.8334 602.6260 1095.2926 2329.1129	318.5039 729.6368 1385.5129 3531.5960	493.4235 1008.0393 1464.8959 3793.9117
HNOH	739.2592 1574.6842	1111.1148 3381.2419	1271.6253 3784.1966

CH ₂ NH	1072.3988	1101.3451	1162.5240
	1366.0461	1492.0285	1710.0267
	3013.2202	3107.9333	3439.4716

Table 4S: Cartesian coordinates (Å) for reactants, intermediates, transition states and products of the $\text{NH}_2 + \text{HCNO}$ reaction, optimized using B3LYP/6-311++G(3df,2p).

HCNO	C	-1.175443000	-0.000294000	0.000019000
	H	-2.235396000	0.001115000	0.000036000
	N	-0.020541000	0.000042000	-0.000047000
	O	1.178980000	0.000045000	0.000022000
NH_2	N	0.000000000	0.000000000	0.141616000
	H	0.000000000	0.805662000	-0.495657000
	H	0.000000000	-0.805662000	-0.495657000
IS1a	C	-0.523235000	0.618410000	-0.004333000
	N	0.748835000	0.519767000	0.020774000
	O	1.468716000	-0.498136000	-0.002273000
	N	-1.377763000	-0.468409000	-0.080388000
	H	-0.966475000	-1.360146000	0.152218000
	H	-2.292118000	-0.333877000	0.320505000
	H	-0.949233000	1.609146000	-0.011243000
IS1b	C	0.435656000	0.413161000	-0.007315000
	H	0.372675000	1.496195000	-0.044277000
	N	1.702244000	-0.152442000	-0.091632000
	H	1.723989000	-1.149759000	0.067664000
	H	2.409280000	0.329289000	0.443770000
	N	-0.624587000	-0.290683000	0.040376000
	O	-1.832934000	-0.006602000	-0.008060000
IS2	C	0.497631000	-0.351683000	-0.082018000
	N	-0.506361000	0.398330000	-0.148851000
	O	-1.749031000	-0.204689000	0.128987000
	H	-2.374896000	0.461075000	-0.174219000
	N	1.770965000	0.018438000	0.076129000
	H	2.019767000	0.943695000	0.399234000
	H	2.509363000	-0.574537000	-0.255751000
IS3	C	-0.152330000	0.010010000	0.458590000
	O	0.971513000	-0.646907000	-0.206154000
	N	0.931823000	0.734117000	-0.078889000
	N	-1.400510000	0.082557000	-0.147254000
	H	-1.365789000	0.237237000	-1.145137000
	H	-2.034175000	-0.664103000	0.098730000
	H	-0.177349000	-0.174650000	1.527101000
IS4	C	-0.139295000	0.000781000	-0.428960000
	O	0.813099000	0.806416000	0.080503000
	H	0.867354000	-1.012193000	0.947895000
	N	1.017800000	-0.712933000	-0.024264000
	N	-1.400395000	-0.079449000	0.174098000
	H	-1.844292000	0.829416000	0.237254000
	H	-2.013921000	-0.726565000	-0.304258000
IS5	C	-0.260849000	-0.132963000	0.435581000
	O	0.840064000	-0.694242000	-0.259748000
	H	0.681607000	1.204492000	-0.752969000
	N	0.900195000	0.706041000	0.119313000
	N	-1.373215000	0.075118000	-0.336631000
	H	-2.203400000	0.103070000	0.258600000
	H	-0.322483000	-0.423964000	1.480097000
IS6	C	0.048975000	0.075169000	0.015540000
	O	0.480682000	1.221327000	-0.026207000
	N	0.923717000	-1.000715000	-0.079021000
	H	1.758863000	-0.770178000	0.463000000
	N	-1.266792000	-0.248588000	0.051735000
	H	-1.945737000	0.489270000	-0.026049000
	H	-1.550908000	-1.195600000	-0.129533000
IS7	C	1.391263000	-0.586574000	-0.000008000
	H	2.457952000	-0.768934000	-0.000016000
	O	-0.526976000	0.695283000	-0.000001000
	N	0.844089000	0.513415000	0.000010000
	N	-1.255611000	-0.558956000	-0.000009000
	H	-1.854481000	-0.477591000	0.818142000
	H	-1.854586000	-0.477504000	-0.818078000
IS8	C	0.650624000	-0.314374000	0.059012000
	N	-0.470869000	0.430574000	0.141698000
	N	1.826847000	0.065662000	-0.051127000
	H	-0.469982000	1.334166000	-0.322189000
	H	2.580159000	-0.609083000	-0.013813000
	O	-1.671108000	-0.251248000	-0.166030000

	H	-2.136906000	-0.302504000	0.676179000
IS9	C	-0.587459000	0.374908000	0.000016000
	H	-0.351549000	1.438411000	-0.000036000
	N	0.447170000	-0.507021000	-0.000186000
	O	1.626161000	0.187851000	0.000120000
	H	2.305581000	-0.497040000	-0.000094000
	N	-1.816604000	-0.015201000	-0.000067000
	H	-1.852526000	-1.038072000	0.000844000
IS10	C	-0.726313000	-0.338588000	0.110083000
	H	-0.548464000	-1.398326000	0.313285000
	N	-1.875225000	0.086026000	-0.149143000
	N	0.414928000	0.463388000	0.249171000
	H	0.329517000	1.345798000	-0.244783000
	O	1.578179000	-0.194594000	-0.242967000
	H	2.173467000	-0.205094000	0.514538000
IS11	C	0.594034000	-0.415903000	0.000014000
	O	-1.731771000	-0.137641000	-0.000031000
	N	-0.563588000	0.357717000	0.000039000
	N	1.785543000	0.021875000	-0.000020000
	H	-0.471839000	1.376133000	0.000023000
	H	1.835663000	1.042414000	-0.000045000
	H	0.372456000	-1.479149000	0.000054000
IS12	C	0.105682000	0.997242000	-0.120268000
	H	0.292695000	1.919088000	0.417082000
	O	-0.111707000	-1.010575000	0.019856000
	N	1.009481000	-0.096435000	-0.146373000
	H	1.606696000	-0.195714000	0.678583000
	N	-1.002766000	0.140894000	0.155668000
	H	-1.686833000	0.066559000	-0.597963000
IS13	C	0.496860000	-0.592421000	0.000034000
	N	1.634479000	0.084496000	-0.000031000
	H	1.721056000	1.102614000	0.000281000
	H	2.501375000	-0.424924000	-0.000059000
	O	-1.779576000	-0.112603000	0.000020000
	N	-0.567381000	0.270160000	-0.000042000
	H	-0.436668000	1.295071000	-0.000075000
IS14	H	0.459018000	2.117463000	-0.000002000
	C	0.829670000	1.106400000	0.000000000
	N	0.184928000	0.005413000	0.000000000
	O	0.654524000	-1.161178000	0.000001000
	N	-1.260923000	0.171597000	-0.000002000
	H	-1.570630000	-0.352747000	0.816070000
	H	-1.570630000	-0.352768000	-0.816060000
IS15	C	-0.640025000	0.297892000	0.000040000
	O	-1.782220000	-0.102048000	0.000847000
	N	0.453575000	-0.539362000	0.001320000
	H	-0.406860000	1.387936000	0.000051000
	N	1.603308000	0.105992000	-0.011888000
	H	1.663997000	1.119187000	0.028198000
	H	2.442594000	-0.444502000	0.038709000
COM	C	1.147886000	0.758507000	-0.000044000
	H	1.950765000	1.513070000	0.000399000
	N	1.671802000	-0.425141000	-0.000091000
	H	1.046980000	-1.227991000	-0.000361000
	H	2.664937000	-0.645426000	0.000172000
	N	-1.083873000	-0.389586000	0.000281000
	O	-2.083187000	0.189049000	-0.000159000
T0/1	C	0.073501000	0.898843000	-0.000007000
	H	0.612709000	1.814241000	-0.000032000
	N	-0.869309000	0.215525000	-0.000003000
	O	-1.765489000	-0.582280000	0.000009000
	N	2.180439000	-0.319282000	-0.000034000
	H	1.946057000	-0.911568000	-0.804436000
	H	1.946227000	-0.911188000	0.804696000
T1P2	C	0.849933000	0.677246000	0.000001000
	H	1.387551000	1.636733000	-0.000011000
	N	1.652099000	-0.334408000	0.000003000
	H	1.223743000	-1.260732000	0.000013000
	H	2.665067000	-0.301704000	-0.000005000
	N	-0.911233000	-0.415300000	-0.000010000
	O	-1.945253000	0.138772000	0.000006000
T1a1b	C	0.522097000	0.514837000	-0.010398000
	H	0.752554000	1.580555000	-0.039066000
	N	1.641499000	-0.335377000	-0.092182000
	H	1.445297000	-1.302037000	0.126875000

	H	2.443817000	0.005366000	0.419262000
	N	-0.663268000	0.128352000	0.034333000
	O	-1.827733000	-0.240466000	-0.004967000
T1/3	H	-0.217697000	-1.046161000	1.056847000
	C	-0.303329000	-0.185832000	0.404961000
	N	0.747524000	0.678255000	0.231865000
	O	1.359933000	-0.367315000	-0.351969000
	N	-1.470454000	0.026535000	-0.189650000
	H	-1.575502000	0.826284000	-0.794297000
	H	-2.205771000	-0.660133000	-0.172068000
T3/5	H	-0.154962000	-0.943775000	1.366964000
	C	-0.145393000	-0.371691000	0.449593000
	N	0.646268000	0.809042000	0.235888000
	O	0.976231000	-0.448737000	-0.391997000
	H	-0.393425000	1.052040000	-0.517610000
	N	-1.263043000	-0.019716000	-0.331671000
	H	-2.071677000	0.186493000	0.259549000
T5/11	H	0.328598000	-0.431105000	1.475766000
	C	0.389231000	-0.235279000	0.413457000
	N	-0.791008000	-0.581584000	-0.382231000
	O	-0.971938000	0.745887000	0.057634000
	H	-1.399883000	-1.160420000	0.208519000
	N	1.521924000	0.114275000	-0.119299000
	H	1.394985000	0.307267000	-1.115393000
T1/14	C	-0.651749000	1.104895000	0.222824000
	H	-1.355884000	1.335504000	-0.586724000
	O	1.420997000	-0.105095000	0.051451000
	N	0.237172000	0.150709000	-0.237193000
	N	-0.861341000	-0.788370000	0.048432000
	H	-1.055615000	-1.377959000	-0.751483000
	H	-0.676796000	-1.282524000	0.910983000
T0/14	H	0.760649000	1.922477000	-0.000001000
	C	-0.143909000	1.343917000	0.000005000
	N	-0.359533000	0.123612000	-0.000001000
	O	-1.232484000	-0.704668000	-0.000002000
	N	1.285401000	-0.670568000	-0.000008000
	H	1.740775000	-0.260013000	0.817547000
	H	1.740823000	-0.259928000	-0.817494000
T1/13	C	-0.507763000	-0.524888000	-0.133686000
	N	0.618665000	0.210224000	0.148173000
	O	1.804476000	0.039699000	-0.121104000
	H	0.145636000	-0.594354000	1.064854000
	N	-1.662834000	0.163518000	-0.060326000
	H	-1.705148000	1.163420000	0.088058000
	H	-2.520542000	-0.353525000	0.003113000
T3/4	C	0.131337000	-0.022805000	0.321765000
	O	-0.916399000	0.781577000	-0.093935000
	N	-0.944522000	-0.753379000	-0.180180000
	H	-0.629144000	-0.790452000	1.075109000
	N	1.450828000	-0.064856000	-0.037777000
	H	1.621058000	-0.312526000	-1.007048000
	H	2.007113000	0.714838000	0.278524000
T4/5	C	0.184155000	0.009535000	0.294028000
	O	-0.828564000	0.821224000	-0.073901000
	H	-0.970645000	-1.019532000	-0.926296000
	N	-0.994687000	-0.713402000	0.054705000
	N	1.476660000	-0.166167000	-0.201284000
	H	1.908098000	0.758137000	-0.283459000
	H	1.212322000	-0.208621000	1.062851000
T3/6	C	0.019488000	0.005438000	0.180850000
	O	0.841064000	-0.966313000	-0.107530000
	N	0.874434000	1.057635000	-0.096163000
	H	0.198091000	0.295209000	1.307550000
	N	-1.354522000	-0.036159000	-0.147714000
	H	-1.902476000	-0.617389000	0.471104000
	H	-1.780440000	0.869725000	-0.296370000
T13/2	C	0.531679000	-0.430403000	-0.065571000
	N	-0.535787000	0.228618000	-0.201069000
	O	-1.853530000	-0.136518000	0.143258000
	N	1.753104000	0.074772000	0.075329000
	H	1.922701000	1.031088000	0.358842000
	H	2.554392000	-0.507593000	-0.089319000
	H	-1.360148000	1.027335000	-0.141981000
T1/2	C	0.380301000	-0.349542000	-0.000336000
	N	-0.575947000	0.610945000	-0.000268000

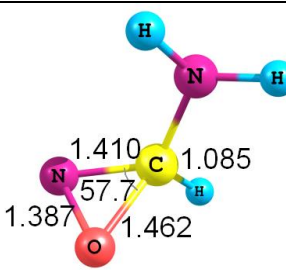
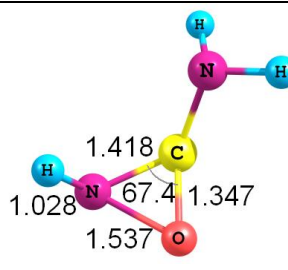
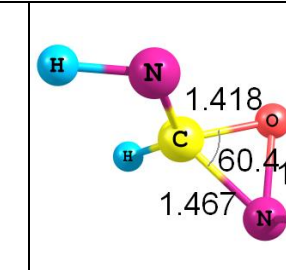
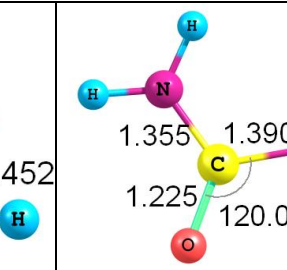
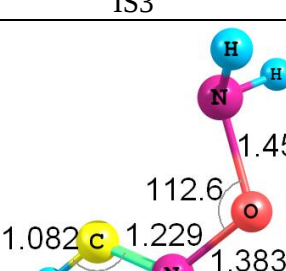
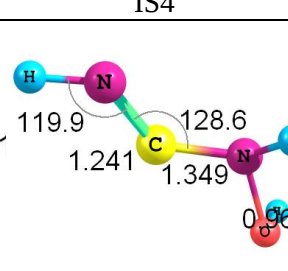
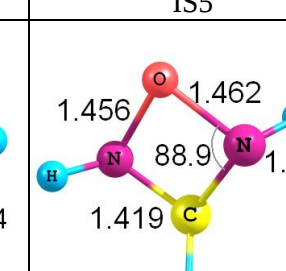
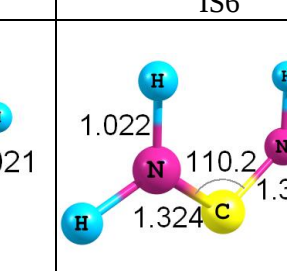
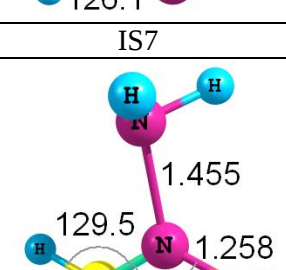
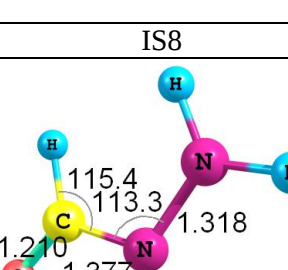
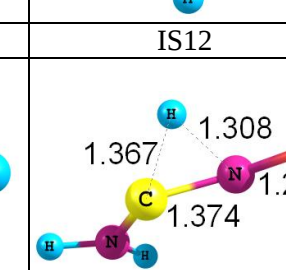
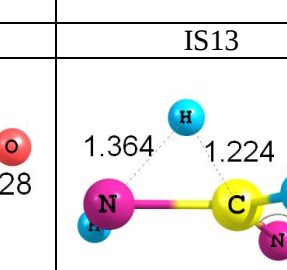
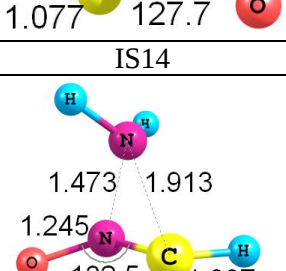
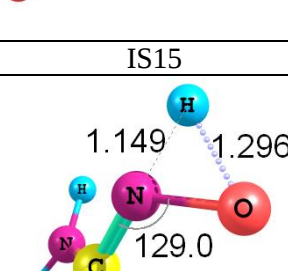
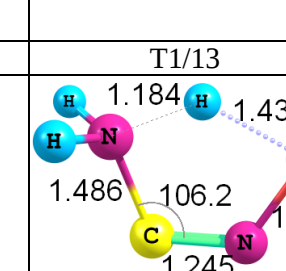
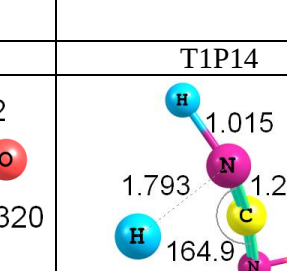
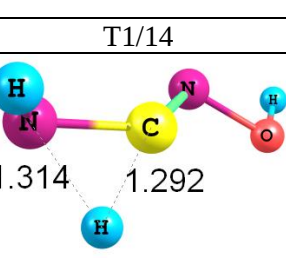
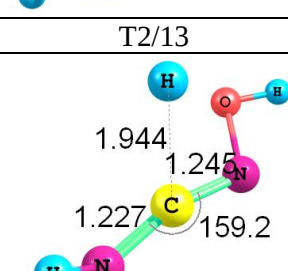
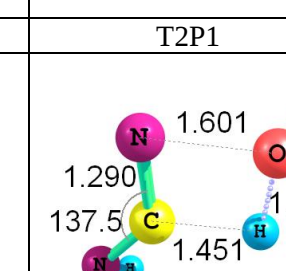
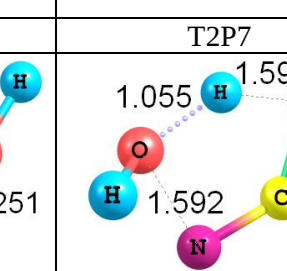
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	N	0.523930000	-0.446787000	-0.093942000
	O	1.714429000	0.233176000	0.029157000
	H	1.504564000	-0.959014000	0.275116000
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	H	0.093458000	0.375717000	1.156908000
	N	-1.801435000	-0.026962000	-0.234438000
	H	-2.531104000	-0.397117000	0.367510000
T8/11	C	0.497294000	-0.149533000	-0.015199000
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	H	-0.410718000	-1.122599000	0.030095000
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	H	2.139500000	-0.373349000	0.601623000
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	N	-1.569198000	-0.355673000	-0.258406000
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	N	1.551133000	-0.265896000	-0.000206000
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	N	0.606884000	0.628618000	-0.072802000
	O	1.186824000	-0.561407000	0.019456000
	H	0.231351000	-1.112145000	-0.081463000
	H	1.187122000	1.385310000	0.278773000
	N	-1.246001000	-0.670585000	0.018645000
T13/11	C	-0.540127000	-0.496939000	-0.118908000
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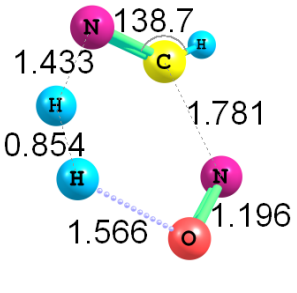
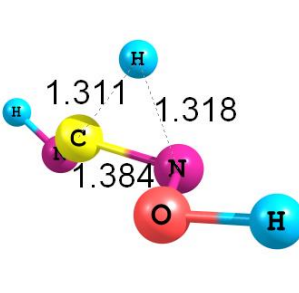
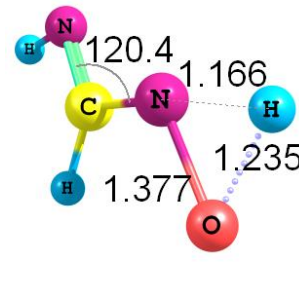
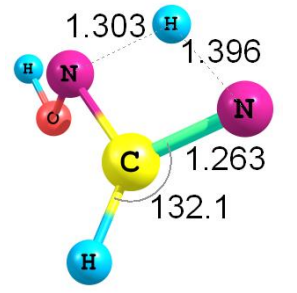
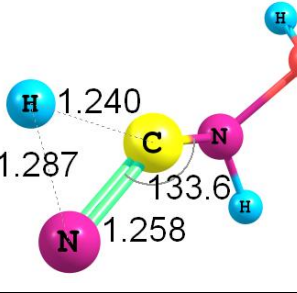
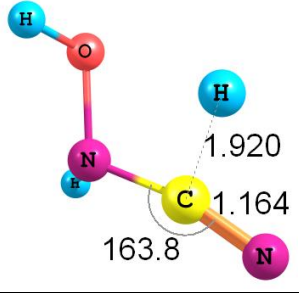
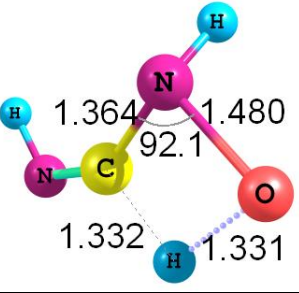
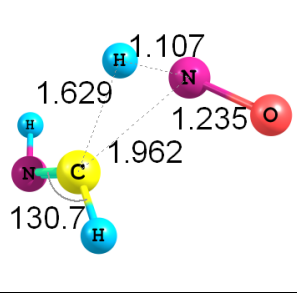
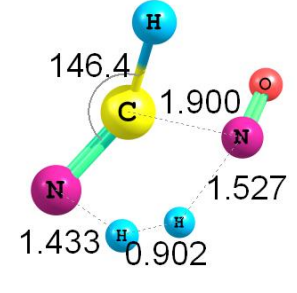
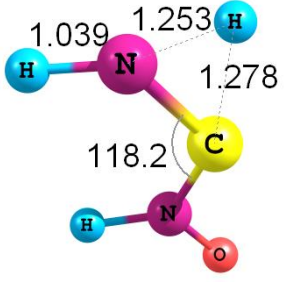
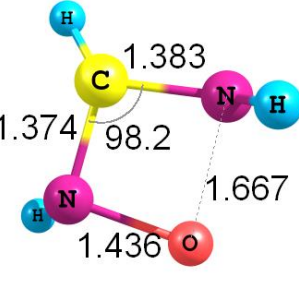
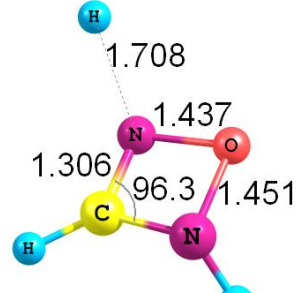
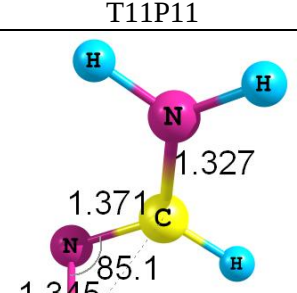
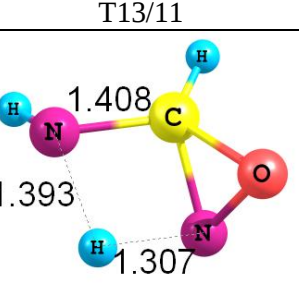
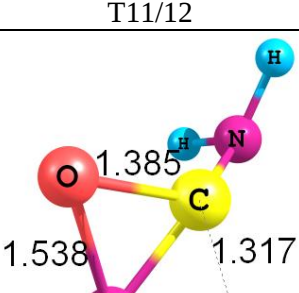
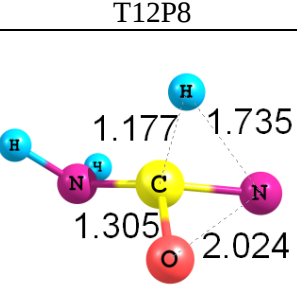
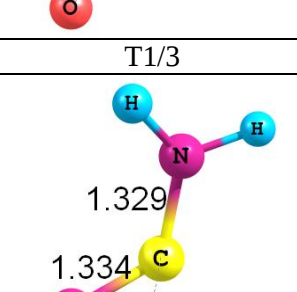
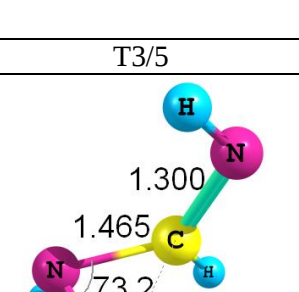
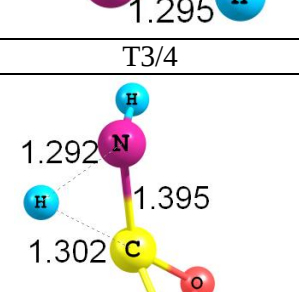
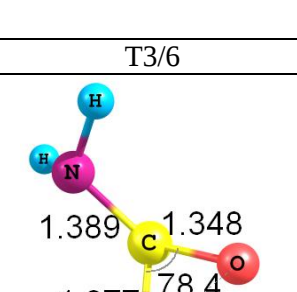
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	H	1.370568000	-1.106310000	0.853733000
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	N	0.062503000	-0.522090000	0.000000000
H ₂	H	0.000000000	0.000000000	0.371401000
	H	0.000000000	0.000000000	-0.371401000
HNCNO	C	0.585854000	0.075592000	0.000214000
	N	1.823071000	-0.135501000	-0.001884000
	H	2.394333000	0.706962000	0.001617000
	N	-0.596518000	-0.072094000	0.004473000
	O	-1.811916000	0.036581000	-0.002628000
HCN	C	0.000000000	0.000000000	-0.496840000
	N	0.000000000	0.000000000	0.649153000
	H	0.000000000	0.000000000	-1.563030000
NH ₂ O	N	0.014698000	0.540261000	0.000000000
	H	-0.110237000	1.039251000	0.875231000
	H	-0.110237000	1.039251000	-0.875231000
	O	0.014698000	-0.732541000	0.000000000
OCN	O	0.000000000	0.000000000	1.134133000
	N	0.000000000	0.000000000	-1.261731000
	C	0.000000000	0.000000000	-0.040157000
OH	O	0.000000000	0.000000000	0.108214000
	H	0.000000000	0.000000000	-0.865716000
H ₂ NCN	C	0.000000000	0.221082000	0.000000000
	N	-0.011430000	1.375529000	0.000000000
	N	0.078737000	-1.116000000	0.000000000
	H	-0.235573000	-1.571597000	0.844107000
	H	-0.235573000	-1.571597000	-0.844107000
HNCNOH	C	-0.616874000	0.110069000	0.014152000
	N	0.527312000	0.558333000	0.016630000
	O	1.571245000	-0.397717000	-0.001449000
	H	2.354680000	0.161380000	0.013917000
	N	-1.795611000	-0.172995000	-0.130246000
	H	-2.345306000	-0.337420000	0.708078000
HCN(H)ON _{cy}	O	0.746864000	-0.664802000	-0.000677000
	N	0.581785000	0.771440000	-0.125901000
	H	1.063021000	1.236581000	0.642649000
	C	-0.780031000	0.502364000	0.011374000
	H	-1.636441000	1.155801000	-0.007648000
	N	-0.684829000	-0.784032000	0.026212000
HNCN	C	0.000000000	0.109104000	0.000000000
	N	-0.074548000	1.294792000	0.000000000
	N	-0.049580000	-1.159091000	0.000000000
	H	0.868900000	-1.604531000	0.000000000
H ₂ O	O	0.000000000	0.000000000	0.116715000
	H	0.000000000	0.763273000	-0.466858000
	H	0.000000000	-0.763273000	-0.466858000
NC(H)N	C	-0.000147000	0.637852000	-0.000008000
	H	-0.000501000	1.719588000	0.000042000
	N	-0.783097000	-0.396373000	0.000018000
	N	0.783294000	-0.396013000	-0.000017000
HON(H)CN	C	-0.772418000	0.098437000	0.009981000
	N	-1.861913000	-0.281995000	-0.015917000
	N	0.482998000	0.571638000	0.132545000
	H	0.675458000	1.362709000	-0.471152000
	O	1.465428000	-0.427008000	-0.140144000
	H	1.888033000	-0.564764000	0.716023000
HNOH	N	-0.704381000	-0.177179000	-0.000033000
	H	-1.137135000	0.753148000	0.000242000

	O	0.623370000	0.148551000	-0.000034000
	H	1.080844000	-0.701303000	0.000261000
CH ₂ NH	C	-0.585082000	0.029119000	-0.000005000
	H	-1.071299000	1.008816000	0.000004000
	H	-1.245605000	-0.837013000	-0.000022000
	N	0.665120000	-0.154113000	0.000004000
	H	1.171556000	0.732276000	0.000020000

 IS3	 IS4	 IS5	 IS6
 IS7	 IS8	 IS12	 IS13
 IS14	 IS15	 T1/13	 T1P14
 T1/14	 T2/13	 T2P1	 T2P7
 T2/9	 T9P7	 T9P9	 T9P10

 T9P11	 T9/8	 T9/11	 T9/10
 T8/10	 T10P12	 T8/11	 T11P2
 T11P11	 T13/11	 T8/11	 T11P2
 T11P11	 T13/11	 T11/12	 T12P8
 T1/3	 T3/5	 T3/4	 T3/6
 T13/4	 T11/5	 T4/5	 T4/6

T5/6	T6P5	T0/7	T7P4
T0/14	T14/15	T15P5	PR4
PR5	PR7	PR8	PR9
PR10	PR11	PR12	PR14

Figure 1S: Optimized geometries of additional transition states and intermediates on the HCNO + NH₂ PES, calculated using B3LYP/6-311++G(3df,2p). (Bond lengths in Å and angles in degree).

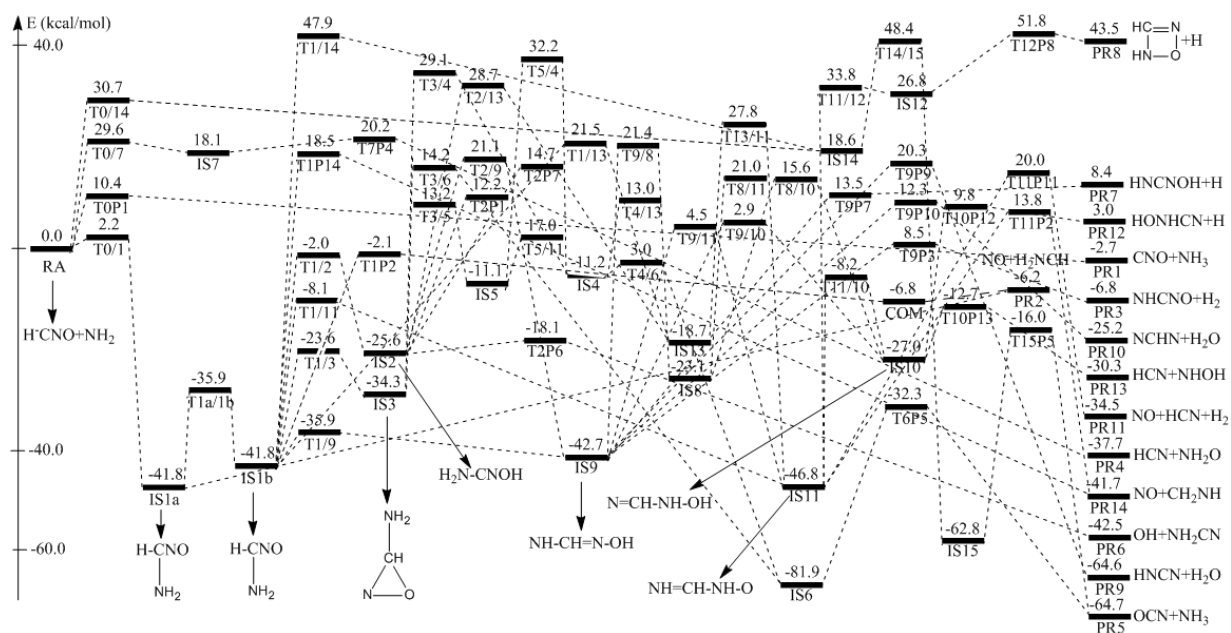


Figure 2S. Detailed potential energy surface of the $\text{HCNO} + \text{NH}_2$ reaction calculated using the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) + ZPVE methodology

Table 5S: Theoretical predication of relative energies ΔE (kcal/mol) for reactants, intermediates, main transition states, and products of the $\text{NH}_2 + \text{HCNO}$ reaction at two different levels of theory

Species	ΔE (kcal/mol)	ΔE (kcal/mol)
	B3LYP/6-311++G(3df,2p)	CCSD(T)/6-311++G(3df,2p)
RA(HCNO + NH_2)	0.0	0.0
IS1a	-46.0	-44.9
IS1b	-43.4	-41.8
IS2	-25.5	-25.6
IS3	-28.9	-34.3
IS4	-5.6	-11.2
IS5	-6.4	-11.1
IS6	-80.0	-81.9
IS7	20.0	18.1
IS8	-22.5	-23.1
IS9	-41.1	-42.7
IS10	-24.1	-27.0
IS11	-46.9	-46.8
IS12	30.2	26.8
IS13	-19.6	-18.7
IS14	19.5	18.6
IS15	-63.0	-62.8
COM	-4.1	-6.8
T0/1	1.3	2.2
T1P2	-3.4	-2.1
T1a1b	-33.4	-30.5
T1/3	-22.5	-23.6
T3/5	18.6	13.2
T5/11	2.4	17.0
T1/14	46.4	47.9
T0/14	28.0	30.7
T1/13	18.3	21.5
T3/4	33.8	29.1
T4/5	36.7	32.2
T3/6	30.8	14.2
T13/2	26.0	28.7
T1/2	-2.3	-2.0
T2/9	31.4	21.1
T1/9	-35.3	-35.9
T9/11	5.1	4.5
T9/8	21.9	21.4
T8/11	19.3	21.0
T8/10	17.8	15.6
T9/10	5.4	2.9
T1/11	-10.1	-8.1
T10/11	-7.8	-8.2
T13/11	26.8	27.8

T11/12	34.5	33.8
T0P1	5.4	10.4
T1P12	18.8	18.5
T6P5	-31.5	-32.3
T2P6	-19.9	-18.1
T2P7	13.6	14.7
T2P1	13.0	12.2
T9P9	18.6	20.3
T9P10	13.5	12.3
T9P7	14.3	13.5
T9P3	3.9	8.5
T10P13	-11.1	-12.7
T10P12	14.9	9.8
T11P11	17.9	20.0
T11P2	10.0	13.8
T12P8	55.7	51.8
T15P5	-16.6	-16.0
T7P4	20.9	20.2
T0/7	26.5	29.6
T4/13	12.8	13.0
T4/6	-1.3	3.0
T14/15	48.4	---
PR1 (NH ₃ + CNO)	-1.9	-2.7
PR2 (NO + H ₂ NCH)	-1.5	-6.2
PR3 (H ₂ + HNCNO)	-12.3	-6.8
PR4 (HCN + NH ₂ O)	-35.6	-37.7
PR5 (NCO + NH ₃)	-63.7	-64.7
PR6 (NH ₂ CN + OH)	-38.0	-42.5
PR7 (H + HNCNOH)	10.7	8.4
PR8 (H + HCN(H)NO _{cy})	51.8	43.5
PR9 (HNCN + H ₂ O)	-63.3	-64.6
PR10 (H ₂ O + NC(H)N)	-19.3	-25.2
PR11 (NO + H ₂ + HCN)	-26.3	-34.5
PR12 (H + HON(H)CN)	10.0	3.0
PR13 (HNOH + HCN)	-25.8	-30.3
PR14 (CH ₂ NH + NO)	-36.0	-41.7

Figure 3S: Energy profile (kcal/mol) for the dissociation of **IS1a** ($Z\text{-H}_2\text{NCHNO}$) to H_2NCH + NO , as a function of the C–N distance ($\text{\AA}$). Blue curve: B3LYP/6-311++G(3df,2p) energies, red curve: CCSD(T)/aug-cc-pVTZ//B3LYP energies. Both are ZPE-corrected using B3LYP vibrational information.

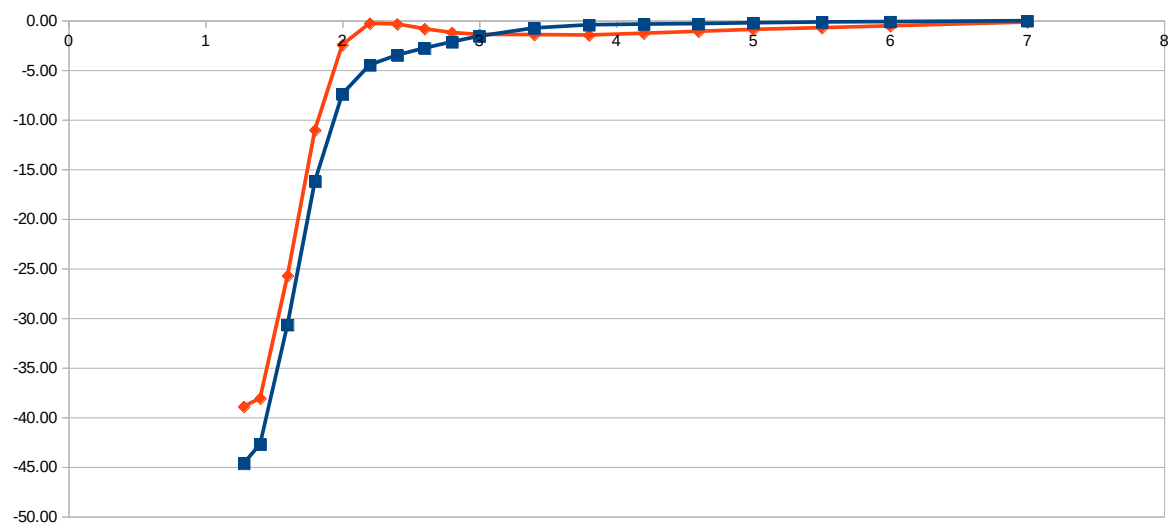


Table 6S: Product distribution (fraction) with errors (absolute fraction) as a function of temperature and pressure.

Temperature K	Pressure Bar	IS1a	IS1b	IS9	IS10	IS11	H2NCH+NO PR2	OH+H2NCN PR6	HCN+NHOH PR13	CNO+NH3 PR1
3000	9.866E-5	4.26E-08 ± 1.64E-08	1.2E-08 ± 3.48E-09	1.41E-08 ± 4.14E-09	1.04E-11 ± 1.35E-11	2.43E-09 ± 3.79E-09	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.36E-02	4.81E-02 ± 8.82E-03	2.88E-01 ± 5.3E-02
3000	3.120E-4	1.41E-07 ± 5.4E-08	3.9E-08 ± 1.12E-08	4.59E-08 ± 1.34E-08	3.33E-11 ± 4.31E-11	1.54E-09 ± 1.16E-08	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.36E-02	4.81E-02 ± 8.82E-03	2.88E-01 ± 5.3E-02
3000	9.866E-4	4.64E-07 ± 1.79E-07	1.27E-07 ± 3.64E-08	1.5E-07 ± 4.38E-08	1.07E-10 ± 1.37E-10	3.22E-08 ± 3.47E-08	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.36E-02	4.81E-02 ± 8.82E-03	2.88E-01 ± 5.3E-02
3000	3.120E-3	1.54E-06 ± 5.97E-07	4.15E-07 ± 1.19E-07	4.94E-07 ± 1.45E-07	3.51E-10 ± 4.42E-10	1.03E-07 ± 1.03E-07	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.82E-03	2.88E-01 ± 5.3E-02
3000	9.866E-3	5.21E-06 ± 2.03E-06	1.38E-06 ± 3.97E-07	1.66E-06 ± 4.98E-07	1.18E-09 ± 1.45E-09	3.48E-07 ± 3.2E-07	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.83E-03	2.88E-01 ± 5.3E-02
3000	3.120E-2	1.8E-05 ± 6.96E-06	4.7E-06 ± 1.36E-06	5.69E-06 ± 1.73E-06	4.19E-09 ± 4.92E-09	1.28E-06 ± 1.07E-06	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.83E-03	2.88E-01 ± 5.3E-02
3000	9.866E-2	6.26E-05 ± 2.38E-05	1.63E-05 ± 4.67E-06	1.99E-05 ± 5.94E-06	1.59E-08 ± 1.76E-08	4.96E-06 ± 3.86E-06	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.83E-03	2.88E-01 ± 5.3E-02
3000	3.120E-1	2.15E-04 ± 7.86E-05	5.67E-05 ± 1.54E-05	7.03E-05 ± 1.96E-05	6.36E-08 ± 6.64E-08	1.96E-05 ± 1.44E-05	6.12E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.83E-03	2.88E-01 ± 5.3E-02
3000	9.866E-1	7.95E-04 ± 2.44E-04	1.94E-04 ± 4.7E-05	2.42E-04 ± 6E-05	2.63E-07 ± 2.58E-07	7.6E-05 ± 5.33E-05	6.11E-01 ± 5.23E-02	5.19E-02 ± 1.35E-02	4.81E-02 ± 8.81E-03	2.88E-01 ± 5.3E-02
3000	3.120E+0	2.14E-03 ± 7.04E-04	6.34E-04 ± 1.32E-04	7.9E-04 ± 1.67E-04	1.08E-06 ± 9.89E-07	2.74E-04 ± 1.85E-04	6.09E-01 ± 5.22E-02	5.19E-02 ± 1.35E-02	4.78E-02 ± 8.73E-03	2.88E-01 ± 5.3E-02
3000	9.866E+0	5.91E-03 ± 1.87E-03	1.93E-03 ± 3.44E-04	2.37E-03 ± 4.28E-04	4.24E-06 ± 3.6E-06	8.91E-04 ± 5.69E-04	6.03E-01 ± 5.19E-02	5.18E-02 ± 1.33E-02	4.7E-02 ± 8.52E-03	2.87E-01 ± 5.28E-02
3000	3.120E+1	1.45E-02 ± 4.56E-03	5.36E-03 ± 8.25E-04	6.41E-03 ± 9.93E-04	1.55E-05 ± 1.19E-05	2.52E-03 ± 1.49E-03	5.91E-01 ± 5.1E-02	5.17E-02 ± 1.3E-02	4.51E-02 ± 8.06E-03	2.84E-01 ± 5.23E-02
3000	9.866E+1	3.19E-02 ± 1.03E-02	1.35E-02 ± 1.81E-03	1.53E-02 ± 2.06E-03	4.97E-05 ± 3.35E-05	5.99E-03 ± 3.13E-03	5.65E-01 ± 4.88E-02	5.1E-02 ± 1.23E-02	4.12E-02 ± 7.33E-03	2.76E-01 ± 5.13E-02
1714	9.866E-5	4.59E-08 ± 7.7E-08	1.35E-08 ± 1.93E-08	1.93E-08 ± 2.81E-08	1.38E-13 ± 5.4E-13	7.7E-09 ± 1.65E-08	8.02E-01 ± 4.4E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.24E-02	6.39E-02 ± 2.82E-02
1714	3.120E-4	1.79E-07 ± 2.9E-07	7.2E-08 ± 7.21E-08	7.52E-08 ± 1.05E-07	6.65E-13 ± 2.42E-12	3.59E-08 ± 6.44E-08	8.02E-01 ± 4.4E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.24E-02	6.39E-02 ± 2.82E-02
1714	9.866E-4	7E-07 ± 1.1E-06	2.06E-07 ± 2.73E-07	2.94E-07 ± 3.99E-07	2.92E-12 ± 1.03E-11	1.46E-07 ± 2.36E-07	8.02E-01 ± 4.4E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.24E-02	6.39E-02 ± 2.82E-02
1714	3.120E-3	2.87E-06 ± 4.35E-06	8.44E-07 ± 1.09E-06	1.21E-06 ± 1.59E-06	1.32E-11 ± 4.59E-11	5.9E-07 ± 9.5E-07	8.02E-01 ± 4.4E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.24E-02	6.39E-02 ± 2.82E-02
1714	9.866E-3	3.11E-05 ± 1.89E-05	3.86E-06 ± 4.75E-06	5.53E-06 ± 6.94E-06	7.25E-11 ± 2.49E-10	2.8E-06 ± 4.39E-06	8.02E-01 ± 4.4E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.25E-02	6.39E-02 ± 2.82E-02
1714	3.120E-2	6.74E-05 ± 9.01E-05	2E-05 ± 2.33E-05	2.86E-05 ± 3.38E-05	5.14E-10 ± 1.73E-09	1.61E-05 ± 2.36E-05	8.02E-01 ± 4.41E-02	5.35E-02 ± 2.13E-02	8.03E-02 ± 2.25E-02	6.39E-02 ± 2.82E-02
1714	9.866E-2	3.68E-04 ± 4.37E-04	1.11E-04 ± 1.14E-04	1.59E-04 ± 1.65E-04	4.49E-09 ± 1.45E-08	1.03E-04 ± 1.31E-04	8.02E-01 ± 4.43E-02	5.34E-02 ± 2.13E-02	8.03E-02 ± 2.25E-02	6.39E-02 ± 2.82E-02
1714	3.120E-1	1.88E-03 ± 1.9E-03	5.84E-04 ± 4.86E-04	8.34E-04 ± 7.15E-04	4.07E-08 ± 1.18E-07	6.09E-04 ± 6.44E-04	7.99E-01 ± 4.5E-02	5.32E-02 ± 2.12E-02	7.98E-02 ± 2.23E-02	6.37E-02 ± 2.81E-02
1714	9.866E-1	7.95E-03 ± 6.64E-03	2.59E-03 ± 1.71E-03	3.68E-03 ± 2.52E-03	3.1E-07 ± 7.57E-07	2.8E-03 ± 2.35E-03	7.89E-01 ± 4.69E-02	5.25E-02 ± 2.08E-02	7.78E-02 ± 2.16E-02	6.34E-02 ± 2.8E-02
1714	3.120E+0	2.65E-02 ± 1.81E-02	9.2E-03 ± 4.64E-03	1.28E-02 ± 6.82E-03	1.74E-06 ± 3.46E-06	9.25E-03 ± 5.89E-03	7.57E-01 ± 5.36E-02	5.07E-02 ± 1.98E-02	7.15E-02 ± 1.97E-02	6.26E-02 ± 2.77E-02
1714	9.866E+0	6.94E-02 ± 3.78E-02	2.6E-02 ± 9.64E-03	3.47E-02 ± 1.4E-02	5.53E-10 ± 1.12E-05	2.15E-02 ± 1E-02	6.84E-01 ± 6.59E-02	4.65E-02 ± 2.31E-02	5.8E-02 ± 1.69E-02	6.04E-02 ± 2.69E-02
1714	3.120E+1	1.43E-01 ± 6.02E-02	5.85E-02 ± 1.52E-02	7.32E-02 ± 1.2E-02	1.98E-05 ± 2.57E-05	3.51E-02 ± 1.14E-02	5.57E-01 ± 8.85E-02	3.9E-02 ± 1.46E-02	3.85E-02 ± 1.46E-02	5.61E-02 ± 2.54E-02
1714	9.866E+1	2.36E-01 ± 7.22E-02	1.06E-01 ± 1.74E-02	1.22E-01 ± 2.37E-02	4.06E-05 ± 4.28E-05	4E-02 ± 1.05E-02	3.97E-01 ± 9.41E-02	2.89E-02 ± 1.12E-02	1.99E-02 ± 1.01E-02	4.92E-02 ± 2.31E-02
1200	9.866E-5	1.29E-08 ± 4.38E-08	3.23E-09 ± 1.06E-08	4.61E-09 ± 1.55E-08	1.72E-14 ± 1.56E-13	2.85E-09 ± 9.94E-09	8.44E-01 ± 4.58E-02	4.49E-02 ± 2.31E-02	9.37E-02 ± 3.32E-02	1.7E-02 ± 1.22E-02
1200	3.120E-4	6.63E-08 ± 2.06E-07	1.66E-08 ± 4.99E-08	2.37E-08 ± 7.32E-08	9.92E-14 ± 7.77E-13	1.66E-08 ± 5.06E-08	8.44E-01 ± 4.58E-02	4.49E-02 ± 2.31E-02	9.37E-02 ± 3.32E-02	1.7E-02 ± 1.22E-02
1200	9.866E-4	3.5E-07 ± 1.02E-06	8.77E-08 ± 2.48E-07	1.25E-07 ± 3.63E-07	5.53E-13 ± 4E-12	8.97E-08 ± 2.61E-07	8.44E-01 ± 4.58E-02	4.49E-02 ± 2.31E-02	9.37E-02 ± 3.32E-02	1.7E-02 ± 1.22E-02
1200	3.120E-3	2.15E-06 ± 5.97E-06	5.39E-07 ± 1.45E-06	7.7E-07 ± 2.12E-06	3.78E-12 ± 2.6E-11	5.69E-07 ± 1.64E-06	8.44E-01 ± 4.58E-02	4.49E-02 ± 2.31E-02	9.37E-02 ± 3.32E-02	1.7E-02 ± 1.22E-02
1200	9.866E-3	1.71E-05 ± 4.32E-05	4.28E-06 ± 1.06E-05	6.12E-06 ± 1.54E-05	4.03E-11 ± 2.56E-10	5.21E-06 ± 1.38E-05	8.44E-01 ± 4.59E-02	4.49E-02 ± 2.31E-02	9.37E-02 ± 3.32E-02	1.69E-02 ± 1.22E-02
1200	3.120E-2	1.63E-04 ± 3.43E-04	4.12E-05 ± 8.46E-05	5.88E-05 ± 1.23E-04	6.36E-10 ± 3.6E-09	6.04E-05 ± 1.28E-04	8.44E-01 ± 4.61E-02	4.48E-02 ± 2.31E-02	9.37E-02 ± 3.33E-02	1.69E-02 ± 1.22E-02
1200	9.866E-2	1.45E-03 ± 2.28E-03	3.72E-04 ± 5.7E-04	5.31E-04 ± 8.28E-04	1.08E-08 ± 5.34E-08	6.14E-04 ± 9.24E-04	8.42E-01 ± 4.75E-02	4.46E-02 ± 2.29E-02	9.33E-02 ± 3.31E-02	1.69E-02 ± 1.22E-02
1200	3.120E-1	9.5E-03 ± 1.03E-02	2.49E-03 ± 2.64E-03	3.54E-03 ± 3.85E-03	1.39E-07 ± 5.63E-07	4.03E-03 ± 4.2E-03	8.3E-01 ± 5.42E-02	4.37E-02 ± 2.24E-02	9.05E-02 ± 3.18E-02	1.68E-02 ± 1.21E-02
1200	9.866E-1	4.12E-02 ± 3.17E-02	1.42E-02 ± 8.37E-03	1.59E-02 ± 1.23E-02	1.09E-06 ± 3.34E-06	1.54E-02 ± 1.07E-02	7.79E-01 ± 7.57E-02	4.1E-02 ± 2.08E-02	7.96E-02 ± 2.78E-02	1.64E-02 ± 1.19E-02
1200	3.120E+0	1.19E-01 ± 6.25E-02	3.45E-02 ± 1.76E-02	4.77E-02 ± 2.57E-02	4.8E-06 ± 1.1E-05	3.43E-02 ± 1.65E-02	6.56E-01 ± 1.06E-01	3.5E-02 ± 1.73E-02	5.69E-02 ± 2.29E-02	1.57E-02 ± 1.15E-02
1200	9.866E+0	2.41E-01 ± 7.9E-02	7.54E-02 ± 2.46E-02	9.99E-02 ± 3.5E-02	1.24E-05 ± 2.18E-05	4.64E-02 ± 1.58E-02	4.68E-01 ± 1.26E-01	2.56E-02 ± 1.3E-02	2.99E-02 ± 1.67E-02	1.44E-02 ± 1.08E-02
1200	3.120E+1	3.63E-01 ± 6.58E-02	1.26E-01 ± 2.46E-02	1.56E-01 ± 3.29E-02	2.03E-05 ± 2.79E-05	4.05E-02 ± 1.51E-02	2.75E-01 ± 1.05E-01	1.56E-02 ± 8.54E-03	1.1E-02 ± 8.43E-03	1.28E-02 ± 9.8E-03
1200	9.866E+1	4.44E-01 ± 3.74E-02	1.75E-01 ± 1.99E-02	1.97E-01 ± 2.32E-02	2.33E-05 ± 2.53E-05	2.46E-02 ± 1.21E-02	1.37E-01 ± 6.51E-02	7.87E-03 ± 4.77E-03	2.84E-03 ± 2.84E-03	1.14E-02 ± 8.88E-03
923	9.866E-5	7.47E-09 ± 4.15E-08	1.87E-09 ± 1.04E-08	2.63E-09 ± 1.49E-08	8.01E-15 ± 1.39E-13	1.93E-09 ± 1.07E-08	8.56E-01 ± 5.12E-02	3.79E-02 ± 2.29E-02	1E-01 ± 4.08E-02	5.53E-03 ± 5.7E-03
923	3.120E-4	4.82E-08 ± 2.35E-07	1.2E-08 ± 5.89E-08	1.7E-08 ± 8.42E-08	5.27E-14 ± 7.3E-13	1.36E-08 ± 6.6E-08	8.56E-01 ± 5.12E-02	3.79E-02 ± 2.29E-02	1E-01 ± 4.08E-02	5.53E-03 ± 5.7E-03
923	9.866E-4	3.35E-07 ± 1.48E-06	8.38E-08 ± 3.71E-07	1.18E-07 ± 5.29E-07	3.81E-13 ± 4.52E-12	9.85E-08 ± 4.41E-07	8.56E-01 ± 5.12E-02	3.79E-02 ± 2.29E-02	1E-01 ± 4.08E-02	5.53E-03 ± 5.7E-03
923	3.120E-3	3.06E-06 ± 1.19E-05	7.64E-07 ± 2.99E-06	1.08E-06 ± 4.26E-06	4.15E-12 ± 4.18E-11	1E-06 ± 4.05E-06	8.56E-01 ± 5.12E-02	3.79E-02 ± 2.29E-02	1E-01 ± 4.08E-02	5.53E-03 ± 5.7E-03
923	9.866E-3	3.85E-05 ± 1.23E-04	9.63E-06 ± 3.08E-05	1.36E-05 ± 4.38E-05	7.76E-11 ± 6.3E-10	1.55E-05 ± 4.92E-05	8.56E-01 ± 5.14E-02	3.79E-02 ± 2.29E-02	1E-01 ± 4.09E-02	5.52E-03 ± 5.7E-03
923	3.120E-2	5.2E-04 ± 1.2E-03	1.31E-04 ± 3.04E-04	1.85E-04 ± 4.31E-04	1.84E-09 ± 1.22E-08	2.47E-04 ± 5.34E-04	8.56E-01 ± 5.23E-02	3.77E-02 ± 2.28E-02	1E-01 ± 4.1E-02	5.52E-03 ± 5.69E-03
923	9.866E-2	5.18E-03 ± 7.92E-03	1.32E-03 ± 2.03E-03	1.86E-03 ± 2.88E-03	3.57E-08 ± 2E-07	2.53E-03 ± 3.42E-03	8.48E-01 ± 5.83E-02	3.7E-02 ± 2.24E-02	9.84E-02 ± 4.01E-02	5.49E-03 ± 6.67E-03
923	3.120E-1	3.11E-02 ± 2.96E-02	8.12E-03 ± 7.79E-03	1.14E-02 ± 1.11E-02	4.13E-07 ± 1.8E-06	1.33E-02 ± 1.13E-02	8.07E-01 ± 8.32E-02	3.5E-02 ± 2.09E-02	8.89E-02 ± 3.57E-02	5.42E-03 ± 5.62E-03
923	9.866E-1	1.1E-01 ± 6.77E-02	2.99E-02 ± 1.88E-02	4.16E-02 ± 2.67E-02	2.42E-06 ± 7.63E-06	3.51E-02 ± 1.82E-02	6.84E-01 ± 1.22E-01	2.98E-02 ± 1.75E-02	6.43E-02 ± 2.82E-02	5.26E-03 ± 5.49E-03
923	3.120E+0	2.45E-01 ± 8.97E-02	7.06E-02 ± 2.73E-02	9.64E-02 ± 3.8E-02	7.11E-06 ± 1.64E-05	5.02E-02 ± 1.94E-02	4.79E-01 ± 1.44E-01	2.13E-02 ± 1.27E-02	3.28E-02 ± 2.01E-02	4.97E-03 ± 2.56E-03
923	9.866E+0	3.83E-01 ± 7.29E-02	1.2E-01 ± 2.67E-02	1.57E-01 ± 3.44E-02	1.18E-05 ± 2.07E-05	4.29E-02 ± 1.85E-02	2.69E-01 ± 1.16E-01	1.24E-02 ± 7.85E-03	1.12E-02 ± 9.43E-03	4.62E-03 ± 4.96E-03
923	3.120E+1	4.72E-01 ± 3.9E-02	1.65E-01 ± 2.11E-02	2.01E-01 ± 2.19E-02	1.3E-05 ± 1.78E-05	2.47E-02 ± 1.38E-02	1.25E-01 ± 6.68E-02	5.85E-03 ± 4.05E-03	2.6E-03 ± 2.84E-03	4.32E-03 ± 4.69E-03
923	9.866E+1	5.07E-01 ± 1.41E-02	2.02E-01 ± 1.65E-02	2.23E-01 ± 1.1E-02	1.03E-05 ± 1.1E-05	1.06E-02 ± 7.24E-03	5.04E-02 ± 3.05E-02	2.32E-03 ± 1.76E-03	4.27E-04 ± 5.97E-04	4.14E-03 ± 4.51E-03
750	9.866E-5	8.32E-09 ± 6.2E-08	2.09E-09 ± 1.57E-08	2.91E-09 ± 2.2E-08	8.04E-15 ± 2E-13	2.36E-09 ± 1.76E-08	8.61E-01 ± 5.6E-02			

632	3.120E+0	4.3E-01 ± 7.53E-02	1.26E-01 ± 2.64E-02	1.68E-01 ± 3.32E-02	6.58E-06 ± 1.47E-05	4.15E-02 ± 2.24E-02	2.19E-01 ± 1.17E-01	7.26E-03 ± 5.77E-03	7.81E-03 ± 8.02E-03	7.33E-04 ± 1.31E-03
632	9.866E+0	5.12E-01 ± 3.46E-02	1.64E-01 ± 1.85E-02	2.09E-01 ± 1.82E-02	6.3E-06 ± 1.08E-05	2.04E-02 ± 1.4E-02	8.96E-02 ± 5.75E-02	3.01E-03 ± 2.56E-03	1.42E-03 ± 1.83E-03	7.18E-04 ± 1.29E-03
632	3.120E+1	5.37E-01 ± 1.08E-02	1.93E-01 ± 1.44E-02	2.28E-01 ± 7.8E-03	4.42E-06 ± 5.88E-06	7.77E-03 ± 6.14E-03	3.27E-02 ± 2.27E-02	1.07E-03 ± 9.58E-04	1.87E-04 ± 2.84E-04	7.1E-04 ± 1.28E-03
632	9.866E+1	5.32E-01 ± 7.47E-03	2.17E-01 ± 1.29E-02	2.35E-01 ± 2.81E-03	2.22E-06 ± 2.37E-06	2.54E-03 ± 2.19E-03	1.16E-02 ± 8.13E-03	3.39E-04 ± 3.18E-04	1.85E-05 ± 3.31E-05	7.07E-04 ± 1.27E-03
545	9.866E-5	1.78E-08 ± 1.69E-07	4.49E-09 ± 4.31E-08	6.18E-09 ± 5.91E-08	1.5E-14 ± 4.95E-13	5.55E-09 ± 5.33E-08	8.65E-01 ± 6.37E-02	2.6E-02 ± 2.07E-02	1.09E-01 ± 5.51E-02	3.2E-04 ± 6.99E-04
545	3.120E-4	1.57E-07 ± 1.2E-06	3.96E-08 ± 3.06E-07	5.44E-08 ± 4.21E-07	1.26E-13 ± 3.04E-12	5.22E-08 ± 4.06E-07	8.65E-01 ± 6.37E-02	2.6E-02 ± 2.07E-02	1.09E-01 ± 5.51E-02	3.2E-04 ± 6.99E-04
545	9.866E-4	1.7E-06 ± 1.04E-05	4.28E-07 ± 2.65E-06	5.89E-07 ± 3.64E-06	1.49E-12 ± 2.66E-11	6.24E-07 ± 3.91E-06	8.65E-01 ± 6.38E-02	2.6E-02 ± 2.07E-02	1.09E-01 ± 5.52E-02	3.2E-04 ± 6.99E-04
545	3.120E-3	2.69E-05 ± 1.25E-04	6.77E-06 ± 3.17E-05	9.3E-06 ± 4.35E-05	3.17E-11 ± 3.92E-10	1.2E-05 ± 5.41E-05	8.65E-01 ± 6.4E-02	2.59E-02 ± 2.06E-02	1.09E-01 ± 5.54E-02	3.2E-04 ± 6.98E-04
545	9.866E-3	5.08E-04 ± 1.61E-03	1.28E-04 ± 4.09E-04	1.76E-04 ± 5.62E-04	9.49E-10 ± 8.34E-09	2.7E-04 ± 7.66E-04	8.64E-01 ± 6.55E-02	2.57E-02 ± 2.05E-02	1.09E-01 ± 5.56E-02	3.2E-04 ± 6.98E-04
545	3.120E-2	7.02E-03 ± 1.34E-02	1.78E-03 ± 3.43E-03	2.45E-03 ± 4.71E-03	2.34E-08 ± 1.68E-07	3.81E-03 ± 6.06E-03	8.54E-01 ± 7.79E-02	2.49E-02 ± 1.98E-02	1.06E-01 ± 5.39E-02	3.19E-04 ± 6.97E-04
545	9.866E-2	4.95E-02 ± 5.25E-02	1.28E-02 ± 1.37E-02	1.75E-02 ± 1.88E-02	3.06E-07 ± 1.82E-06	2.22E-02 ± 1.91E-02	7.86E-01 ± 1.27E-01	2.24E-02 ± 1.77E-02	8.95E-02 ± 4.52E-02	3.17E-04 ± 6.94E-04
545	3.120E-1	1.73E-01 ± 1.02E-01	4.58E-02 ± 2.78E-02	6.28E-02 ± 3.79E-02	1.75E-06 ± 7.62E-06	5.13E-02 ± 2.55E-02	5.98E-01 ± 1.74E-01	1.69E-02 ± 1.32E-02	5.22E-02 ± 3.27E-02	3.13E-04 ± 6.87E-04
545	9.866E-1	3.46E-01 ± 1.04E-01	9.55E-02 ± 3.12E-02	1.3E-01 ± 4.15E-02	4.32E-06 ± 1.31E-05	5.47E-02 ± 2.65E-02	3.46E-01 ± 1.6E-01	9.89E-03 ± 8.14E-03	1.84E-02 ± 1.65E-02	3.08E-04 ± 6.78E-04
545	3.120E+0	4.76E-01 ± 6.17E-02	1.4E-01 ± 2.3E-02	1.86E-01 ± 2.77E-02	5.45E-06 ± 1.21E-05	3.33E-02 ± 2.11E-02	1.55E-01 ± 9.47E-02	4.52E-03 ± 3.97E-03	4.02E-03 ± 4.78E-03	3.03E-04 ± 6.69E-04
545	9.866E+0	5.34E-01 ± 2.36E-02	1.72E-01 ± 1.56E-02	2.18E-01 ± 1.34E-02	4.51E-06 ± 7.7E-06	1.42E-02 ± 1.09E-02	5.86E-02 ± 4.1E-02	1.71E-03 ± 1.59E-03	6.01E-04 ± 8.63E-04	3E-04 ± 6.63E-04
545	3.120E+1	5.45E-01 ± 7.48E-03	1.97E-01 ± 1.31E-02	2.32E-01 ± 5.33E-03	2.82E-06 ± 3.71E-06	5E-03 ± 4.23E-03	2.06E-02 ± 1.5E-02	5.71E-04 ± 5.52E-04	6.86E-05 ± 1.12E-04	2.99E-04 ± 6.61E-04
545	9.866E+1	5.34E-01 ± 8.46E-03	2.2E-01 ± 1.22E-02	2.37E-01 ± 1.74E-03	1.2E-06 ± 1.32E-06	1.55E-03 ± 1.41E-03	7.28E-03 ± 5.23E-03	1.73E-04 ± 1.74E-04	5.94E-06 ± 1.14E-05	2.98E-04 ± 6.6E-04
480	9.866E-5	2.79E-08 ± 2.74E-07	7.01E-09 ± 6.98E-08	9.62E-09 ± 9.55E-08	2.22E-14 ± 7.63E-13	8.9E-09 ± 8.89E-08	8.66E-01 ± 6.67E-02	2.37E-02 ± 2E-02	1.1E-01 ± 5.84E-02	1.32E-04 ± 3.51E-04
480	3.120E-4	2.57E-07 ± 2.01E-06	6.47E-08 ± 5.13E-07	8.89E-08 ± 7.02E-07	1.96E-13 ± 4.9E-12	8.77E-08 ± 6.99E-07	8.66E-01 ± 6.67E-02	2.37E-02 ± 2E-02	1.1E-01 ± 5.84E-02	1.32E-04 ± 3.51E-04
480	9.866E-4	3E-06 ± 1.84E-05	7.55E-07 ± 4.69E-06	1.04E-06 ± 6.43E-06	2.56E-12 ± 4.6E-11	1.14E-06 ± 7.16E-06	8.66E-01 ± 6.68E-02	2.37E-02 ± 2E-02	1.1E-01 ± 5.85E-02	1.32E-04 ± 3.51E-04
480	3.120E-3	5.11E-05 ± 2.32E-04	1.29E-05 ± 5.89E-05	1.77E-05 ± 8.07E-05	5.98E-11 ± 7.27E-10	2.38E-05 ± 1.04E-04	8.66E-01 ± 6.71E-02	2.36E-02 ± 1.99E-02	1.1E-01 ± 5.87E-02	1.32E-04 ± 3.51E-04
480	9.866E-3	9.77E-04 ± 2.93E-03	2.47E-04 ± 7.46E-04	3.39E-04 ± 1.02E-03	1.83E-09 ± 1.58E-08	5.32E-04 ± 1.41E-03	8.65E-01 ± 6.99E-02	2.33E-02 ± 1.97E-02	1.1E-01 ± 5.89E-02	1.32E-04 ± 3.51E-04
480	3.120E-2	1.24E-02 ± 2.17E-02	3.45E-03 ± 5.55E-03	4.33E-03 ± 7.61E-03	4.13E-08 ± 2.98E-07	6.65E-03 ± 9.47E-03	8.46E-01 ± 9.09E-02	2.28E-02 ± 1.87E-02	1.05E-01 ± 5.57E-02	1.31E-04 ± 3.5E-04
480	9.866E-2	7.58E-02 ± 7.08E-02	1.96E-02 ± 1.85E-02	2.68E-02 ± 2.53E-02	4.55E-07 ± 2.7E-06	3.17E-02 ± 2.35E-02	7.46E-01 ± 1.53E-01	1.9E-02 ± 1.59E-02	8.14E-02 ± 4.36E-02	1.31E-04 ± 3.49E-04
480	3.120E-1	2.2E-01 ± 1.14E-01	6.03E-02 ± 3.16E-02	8.24E-02 ± 4.28E-02	2.1E-06 ± 8.96E-06	5.81E-02 ± 2.82E-02	5.19E-01 ± 1.84E-01	1.31E-02 ± 1.11E-02	4E-02 ± 2.94E-02	1.29E-04 ± 3.46E-04
480	9.866E-1	4E-01 ± 9.66E-02	1.11E-01 ± 2.96E-02	1.51E-01 ± 3.89E-02	4.17E-06 ± 1.24E-05	5E-02 ± 2.74E-02	2.7E-01 ± 1.46E-01	6.91E-03 ± 6.2E-03	1.14E-02 ± 1.2E-02	1.28E-04 ± 3.43E-04
480	3.120E+0	5.08E-01 ± 4.85E-02	1.51E-01 ± 1.96E-02	1.99E-01 ± 2.25E-02	4.45E-06 ± 9.78E-06	2.59E-02 ± 1.85E-02	1.11E-01 ± 7.49E-02	2.87E-03 ± 2.74E-03	2.06E-03 ± 2.75E-03	1.27E-04 ± 3.4E-04
480	9.866E+0	5.47E-01 ± 1.59E-02	1.77E-01 ± 1.37E-02	2.24E-01 ± 9.96E-03	3.31E-06 ± 5.56E-06	1.01E-02 ± 8.27E-03	3.98E-02 ± 2.96E-02	1.02E-03 ± 1.01E-03	2.68E-04 ± 4.15E-04	1.26E-04 ± 3.39E-04
480	3.120E+1	5.48E-01 ± 7.1E-03	2E-01 ± 1.24E-02	2.34E-01 ± 3.82E-03	1.87E-06 ± 2.43E-06	3.35E-03 ± 2.97E-03	1.37E-02 ± 1.04E-02	3.27E-04 ± 3.36E-04	2.75E-05 ± 4.78E-05	1.26E-04 ± 3.38E-04
480	9.866E+1	5.35E-01 ± 8.54E-03	2.22E-01 ± 1.16E-02	2.37E-01 ± 1.38E-03	6.78E-07 ± 7.84E-07	1E-03 ± 9.47E-04	4.89E-03 ± 3.61E-03	9.58E-05 ± 1.03E-04	2.11E-06 ± 4.35E-06	1.26E-04 ± 3.38E-04
429	9.866E-5	4.22E-08 ± 4.2E-07	1.06E-08 ± 1.07E-07	1.46E-08 ± 1.46E-07	3.21E-14 ± 1.12E-12	1.38E-08 ± 1.39E-07	8.67E-01 ± 6.92E-02	2.19E-02 ± 1.94E-02	1.11E-01 ± 6.11E-02	5.49E-05 ± 1.76E-04
429	3.120E-4	4.04E-07 ± 3.17E-06	1.02E-07 ± 8.08E-07	1.39E-07 ± 1.1E-06	2.97E-13 ± 7.49E-12	1.4E-07 ± 1.13E-06	8.67E-01 ± 6.92E-02	2.19E-02 ± 1.94E-02	1.11E-01 ± 6.11E-02	5.49E-05 ± 1.76E-04
429	9.866E-4	5E-06 ± 3.04E-05	1.26E-06 ± 7.74E-06	1.72E-06 ± 1.06E-05	4.2E-12 ± 7.47E-11	1.97E-06 ± 1.21E-05	8.67E-01 ± 6.93E-02	2.19E-02 ± 1.94E-02	1.11E-01 ± 6.12E-02	5.49E-05 ± 1.76E-04
429	3.120E-3	8.96E-05 ± 3.95E-04	2.26E-05 ± 1E-04	3.09E-05 ± 1.37E-04	1.05E-10 ± 1.24E-09	4.32E-05 ± 1.8E-04	8.67E-01 ± 6.98E-02	2.17E-02 ± 1.93E-02	1.11E-01 ± 6.15E-02	5.49E-05 ± 1.76E-04
429	9.866E-3	1.7E-03 ± 4.82E-03	4.29E-04 ± 1.23E-03	5.88E-04 ± 1.68E-03	3.19E-09 ± 2.72E-08	9.38E-04 ± 2.31E-03	8.64E-01 ± 7.43E-02	2.13E-02 ± 1.9E-02	1.11E-01 ± 6.15E-02	5.49E-05 ± 1.76E-04
429	3.120E-2	1.97E-02 ± 3.15E-02	5E-03 ± 8.09E-03	6.86E-03 ± 1.11E-02	6.53E-08 ± 4.74E-07	1.03E-02 ± 1.32E-02	8.35E-01 ± 1.06E-01	2E-02 ± 1.77E-02	1.03E-01 ± 5.64E-02	5.48E-05 ± 1.75E-04
429	9.866E-2	1.05E-01 ± 8.72E-02	2.72E-02 ± 2.28E-02	3.72E-02 ± 3.12E-02	6.18E-07 ± 3.61E-06	4.07E-02 ± 2.69E-02	7.01E-01 ± 1.75E-01	1.63E-02 ± 1.43E-02	7.25E-02 ± 4.14E-02	5.45E-05 ± 1.75E-04
429	3.120E-1	2.76E-01 ± 1.2E-01	7.35E-02 ± 3.35E-02	1E-01 ± 4.52E-02	2.32E-06 ± 9.75E-06	6.09E-02 ± 3.01E-02	4.48E-01 ± 1.88E-01	1.03E-02 ± 9.32E-03	3.02E-02 ± 2.56E-02	5.41E-05 ± 1.74E-04
429	9.866E-1	4.41E-01 ± 8.7E-02	1.23E-01 ± 2.72E-02	1.66E-01 ± 3.53E-02	3.86E-06 ± 1.13E-05	4.42E-02 ± 2.73E-02	2.14E-01 ± 1.3E-01	4.95E-03 ± 4.78E-03	7.22E-03 ± 8.52E-03	5.37E-05 ± 1.73E-04
429	3.120E+0	5.29E-01 ± 3.81E-02	1.57E-01 ± 1.7E-02	2.08E-01 ± 1.84E-02	3.65E-06 ± 7.93E-06	2.04E-02 ± 1.58E-02	8.25E-02 ± 6E-02	1.92E-03 ± 1.96E-03	1.12E-03 ± 1.63E-03	5.35E-05 ± 1.72E-04
429	9.866E+0	5.54E-01 ± 1.2E-02	1.81E-01 ± 1.25E-02	2.28E-01 ± 7.75E-03	2.51E-06 ± 4.16E-06	7.41E-03 ± 6.43E-03	2.87E-02 ± 2.23E-02	6.51E-04 ± 6.87E-04	1.32E-04 ± 2.18E-04	5.33E-05 ± 1.72E-04
429	3.120E+1	5.5E-01 ± 8.12E-03	2.02E-01 ± 1.2E-02	2.35E-01 ± 2.91E-03	1.31E-06 ± 1.68E-06	2.39E-03 ± 2.2E-03	9.83E-03 ± 7.68E-03	2.04E-04 ± 2.21E-04	1.26E-05 ± 2.3E-05	5.33E-05 ± 1.71E-04
429	9.866E+1	5.35E-01 ± 8.07E-03	2.23E-01 ± 1.09E-02	2.37E-01 ± 2.08E-03	4.06E-07 ± 4.99E-07	7E-04 ± 6.81E-04	3.54E-03 ± 2.68E-03	5.83E-05 ± 6.58E-05	8.66E-07 ± 1.91E-06	5.33E-05 ± 1.71E-04
387	9.866E-5	6.15E-08 ± 6.13E-07	1.55E-08 ± 1.56E-07	2.12E-08 ± 2.13E-07	4.51E-14 ± 1.58E-12	2.03E-08 ± 2.07E-07	8.68E-01 ± 7.13E-02	2.05E-02 ± 1.89E-02	1.12E-01 ± 6.34E-02	2.3E-05 ± 8.77E-05
387	3.120E-4	6.06E-07 ± 4.73E-06	1.52E-07 ± 1.21E-06	2.09E-07 ± 1.65E-06	4.35E-13 ± 1.09E-11	2.14E-07 ± 1.71E-06	8.68E-01 ± 7.13E-02	2.04E-02 ± 1.89E-02	1.12E-01 ± 6.34E-02	2.3E-05 ± 8.77E-05
387	9.866E-4	7.87E-06 ± 4.71E-05	1.98E-06 ± 1.2E-05	2.71E-06 ± 1.64E-05	6.56E-12 ± 1.15E-10	3.18E-06 ± 1.92E-05	8.68E-01 ± 7.14E-02	2.04E-02 ± 1.88E-02	1.12E-01 ± 6.36E-02	2.3E-05 ± 8.77E-05
387	3.120E-3	1.46E-04 ± 6.26E-04	3.69E-05 ± 1.59E-04	5.05E-05 ± 2.17E-04	1.72E-10 ± 1.98E-09	7.23E-05 ± 2.89E-04	8.67E-01 ± 7.22E-02	2.03E-02 ± 1.87E-02	1.12E-01 ± 6.39E-02	2.3E-05 ± 8.77E-05
387	9.866E-3	2.71E-03 ± 7.29E-03	6.85E-04 ± 1.86E-03	9.38E-04 ± 2.54E-03	5.14E-09 ± 4.33E-08	1.51E-03 ± 3.48E-03	8.63E-01 ± 7.91E-02	1.98E-02 ± 1.83E-02	1.11E-01 ± 6.36E-02	2.3E-05 ± 8.76E-05
387	3.120E-2	2.87E-02 ± 4.24E-02	7.3E-03 ± 1.09E-02	9.99E-03 ± 1.49E-02	9.56E-08 ± 6.9E-07	1.47E-02 ± 1.71E-02	8.21E-01 ± 1.22E-01	1.81E-02 ± 1.67E-02	1.01E-01 ± 5.63E-02	2.3E-05 ± 8.75E-05
387	9.866E-2	1.35E-01 ± 1.02E-01	3.51E-02 ± 2.69E-02	4.8E-02 ± 3.66E-02	7.66E-07 ± 4.47E-06	4.86E-02 ± 2.93E-02	6.55E-01 ± 1.93E-01	1.4E-02 ± 1.28E-02	6.37E-02 ± 4.06E-02	2.29E-05 ± 8.73E-05
387	3.120E-1	3.19E-01 ± 1.22E-01	8.51E-02 ± 3.4E-02	1.16E-01 ± 4.58E-02	2.44E-06 ± 1.01E-05	6.1E-02 ± 3.16E-02	3.88E-01 ± 1.87E-01	8.2E-03 ± 7.88E-03	2.27E-02 ± 2.18E-02	2.28E-05 ± 8.69E-05
387	9.866E-1	4.71E-01 ± 7.7E-02	1.32E-01 ± 2.47E-02	1.78E-01 ± 3.16E-02	3.53E-06 ± 1.02E-05	3.85E-02 ± 2.61E-02	1.72E-01 ± 1.15E-01	3.65E-03 ± 3.75E-03	4.69E-03 ± 6.07E-03	2.27E-05 ± 8.66E-05
387	3.120E+0	5.42E-01 ± 3.03E-02	1.62E-01 ± 1.5E-02	2.14E-01 ± 1.53E-02	3.04E-06 ± 6.52E-06	1.63E-02 ± 1.35E-02	6.37E-02 ± 4.89E-02	1.34E-03 ± 1.45E-03	6.54E-04 ± 1.01E-03	2.26E-05 ± 8.63E-05
387	9.866E+0	5.58E-01 ± 9.57E-03	1.84E-01 ± 1.17E-02	2.3E-01 ± 6.26E-03	1.98E-06 ± 3.23E-06	5.7E-03 ± 5.14E-03	2.1			

324	9.866E+1	5.35E-01 ± 6.85E-03	2.26E-01 ± 8.55E-03	2.36E-01 ± 5.93E-03	1.18E-07 ± 1.72E-07	3.17E-04 ± 3.33E-04	1.79E-03 ± 1.44E-03	1.95E-05 ± 2.48E-05	1.13E-07 ± 2.88E-07	4.06E-06 ± 2.14E-05
300	9.866E-5	1.54E-07 ± 1.5E-06	3.86E-08 ± 3.81E-07	5.29E-08 ± 5.2E-07	1.04E-13 ± 3.57E-12	5.24E-08 ± 5.2E-07	8.69E-01 ± 7.58E-02	1.76E-02 ± 1.77E-02	1.14E-01 ± 6.85E-02	1.74E-06 ± 1.07E-05
300	3.120E-4	1.62E-06 ± 1.22E-05	4.06E-07 ± 3.1E-06	5.56E-07 ± 4.22E-06	1.11E-12 ± 2.68E-11	5.94E-07 ± 4.56E-06	8.69E-01 ± 7.59E-02	1.75E-02 ± 1.76E-02	1.14E-01 ± 6.86E-02	1.74E-06 ± 1.07E-05
300	9.866E-4	2.34E-05 ± 1.32E-04	5.88E-06 ± 3.35E-05	8.05E-06 ± 4.57E-05	1.94E-11 ± 3.17E-10	1E-05 ± 5.58E-05	8.69E-01 ± 7.62E-02	1.75E-02 ± 1.76E-02	1.14E-01 ± 6.88E-02	1.74E-06 ± 1.07E-05
300	3.120E-3	4.6E-04 ± 1.79E-03	1.16E-04 ± 4.55E-04	1.59E-04 ± 6.21E-04	5.52E-10 ± 5.91E-09	2.39E-04 ± 8.43E-04	8.68E-01 ± 7.81E-02	1.72E-02 ± 1.74E-02	1.14E-01 ± 6.93E-02	1.73E-06 ± 1.07E-05
300	9.866E-3	7.7E-03 ± 1.78E-02	1.94E-03 ± 4.53E-03	2.66E-03 ± 6.19E-03	1.5E-08 ± 1.23E-07	4.29E-03 ± 8.22E-03	8.56E-01 ± 9.6E-02	1.64E-02 ± 1.66E-02	1.11E-01 ± 6.71E-02	1.73E-06 ± 1.07E-05
300	3.120E-2	6.3E-02 ± 7.5E-02	1.6E-02 ± 1.93E-02	2.2E-02 ± 2.63E-02	2.1E-07 ± 1.51E-06	2.94E-02 ± 2.68E-02	7.67E-01 ± 1.69E-01	1.4E-02 ± 1.41E-02	8.88E-02 ± 5.34E-02	1.73E-06 ± 1.07E-05
300	9.866E-2	2.21E-01 ± 1.29E-01	5.75E-02 ± 3.45E-02	7.86E-02 ± 4.68E-02	1.13E-06 ± 6.42E-06	6.3E-02 ± 3.38E-02	5.29E-01 ± 2.18E-01	9.26E-03 ± 9.55E-03	4.18E-02 ± 3.51E-02	1.73E-06 ± 1.06E-05
300	3.120E-1	4.1E-01 ± 1.11E-01	1.1E-01 ± 3.13E-02	1.5E-01 ± 4.21E-02	2.45E-06 ± 9.65E-06	5.34E-02 ± 3.32E-02	2.62E-01 ± 1.65E-01	4.52E-03 ± 5E-03	1.03E-02 ± 1.28E-02	1.72E-06 ± 1.06E-05
300	9.866E-1	5.23E-01 ± 5.29E-02	1.47E-01 ± 1.86E-02	1.99E-01 ± 2.28E-02	2.66E-06 ± 7.39E-06	2.59E-02 ± 2.1E-02	1.02E-01 ± 7.94E-02	1.75E-03 ± 2.04E-03	1.58E-03 ± 2.42E-03	1.72E-06 ± 1.06E-05
300	3.120E+0	5.61E-01 ± 1.72E-02	1.7E-01 ± 1.18E-02	2.23E-01 ± 9.94E-03	1.96E-06 ± 4.05E-06	9.54E-03 ± 8.76E-03	3.52E-02 ± 2.97E-02	5.94E-04 ± 7.14E-04	1.84E-04 ± 3.14E-04	1.72E-06 ± 1.06E-05
300	9.866E+0	5.63E-01 ± 7.21E-03	1.88E-01 ± 1.08E-02	2.33E-01 ± 3.95E-03	1.13E-06 ± 1.77E-06	3.13E-03 ± 3.03E-03	1.18E-02 ± 1.01E-02	1.88E-04 ± 2.31E-04	1.82E-05 ± 3.33E-05	1.72E-06 ± 1.06E-05
300	3.120E+1	5.49E-01 ± 1.02E-02	2.08E-01 ± 1.17E-02	2.37E-01 ± 1.43E-03	4.38E-07 ± 5.75E-07	9.53E-04 ± 9.58E-04	4.1E-03 ± 3.43E-03	5.61E-05 ± 7.03E-05	1.39E-06 ± 2.93E-06	1.72E-06 ± 1.06E-05
300	9.866E+1	5.36E-01 ± 7.58E-03	2.27E-01 ± 7.73E-03	2.35E-01 ± 7.45E-03	8.5E-08 ± 1.29E-07	2.6E-04 ± 2.79E-04	1.52E-03 ± 1.24E-03	1.48E-05 ± 1.94E-05	6.68E-08 ± 1.77E-07	1.72E-06 ± 1.06E-05
MAXIMUM YIELD		0.563	0.227	0.237	< 0.001	0.063	0.869	0.053	0.114	0.288

Table 7S: Rate coefficient of the $\text{HCNO} + \text{NH}_2$ reaction ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), with uncertainty interval, as a function of temperature and pressure.

Temperature K	Pressure Bar	k(T,P) $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Uncertainty interval	
			Lower band	Upper band
3000	9.866E-5	1.058E-10	6.6E-11	1.1E-10
3000	3.120E-4	1.058E-10	6.6E-11	1.1E-10
3000	9.866E-4	1.058E-10	6.6E-11	1.1E-10
3000	3.120E-3	1.058E-10	6.6E-11	1.1E-10
3000	9.866E-3	1.058E-10	6.6E-11	1.1E-10
3000	3.120E-2	1.058E-10	6.6E-11	1.1E-10
3000	9.866E-2	1.059E-10	6.6E-11	1.1E-10
3000	3.120E-1	1.059E-10	6.6E-11	1.1E-10
3000	9.866E-1	1.059E-10	6.6E-11	1.1E-10
3000	3.120E+0	1.060E-10	6.6E-11	1.1E-10
3000	9.866E+0	1.063E-10	6.6E-11	1.1E-10
3000	3.120E+1	1.072E-10	6.6E-11	1.2E-10
3000	9.866E+1	1.096E-10	6.7E-11	1.2E-10
1714	9.866E-5	4.342E-11	2.1E-11	5.0E-11
1714	3.120E-4	4.342E-11	2.1E-11	5.0E-11
1714	9.866E-4	4.342E-11	2.1E-11	5.0E-11
1714	3.120E-3	4.342E-11	2.1E-11	5.0E-11
1714	9.866E-3	4.342E-11	2.1E-11	5.0E-11
1714	3.120E-2	4.343E-11	2.1E-11	5.0E-11
1714	9.866E-2	4.346E-11	2.1E-11	5.0E-11
1714	3.120E-1	4.353E-11	2.1E-11	5.0E-11
1714	9.866E-1	4.374E-11	2.1E-11	5.1E-11
1714	3.120E+0	4.430E-11	2.1E-11	5.2E-11
1714	9.866E+0	4.576E-11	2.1E-11	5.4E-11
1714	3.120E+1	4.914E-11	2.1E-11	5.9E-11
1714	9.866E+1	5.559E-11	2.2E-11	6.8E-11
1200	9.866E-5	2.998E-11	1.1E-11	4.1E-11
1200	3.120E-4	2.998E-11	1.1E-11	4.1E-11
1200	9.866E-4	2.998E-11	1.1E-11	4.1E-11
1200	3.120E-3	2.998E-11	1.1E-11	4.1E-11
1200	9.866E-3	2.999E-11	1.1E-11	4.1E-11
1200	3.120E-2	3.001E-11	1.1E-11	4.1E-11
1200	9.866E-2	3.008E-11	1.1E-11	4.1E-11
1200	3.120E-1	3.029E-11	1.1E-11	4.1E-11
1200	9.866E-1	3.089E-11	1.1E-11	4.2E-11
1200	3.120E+0	3.236E-11	1.1E-11	4.5E-11
1200	9.866E+0	3.524E-11	1.1E-11	5.0E-11
1200	3.120E+1	3.955E-11	1.1E-11	5.8E-11
1200	9.866E+1	4.437E-11	1.1E-11	6.6E-11
923	9.866E-5	2.247E-11	7.1E-12	3.6E-11
923	3.120E-4	2.247E-11	7.1E-12	3.6E-11
923	9.866E-4	2.247E-11	7.1E-12	3.6E-11
923	3.120E-3	2.248E-11	7.1E-12	3.6E-11
923	9.866E-3	2.249E-11	7.1E-12	3.6E-11
923	3.120E-2	2.252E-11	7.1E-12	3.6E-11
923	9.866E-2	2.262E-11	7.1E-12	3.6E-11
923	3.120E-1	2.291E-11	7.1E-12	3.7E-11
923	9.866E-1	2.362E-11	7.1E-12	3.8E-11
923	3.120E+0	2.498E-11	7.1E-12	4.1E-11
923	9.866E+0	2.685E-11	7.1E-12	4.5E-11
923	3.120E+1	2.869E-11	7.1E-12	4.9E-11
923	9.866E+1	2.999E-11	7.1E-12	5.1E-11
750	9.866E-5	1.751E-11	4.9E-12	3.2E-11
750	3.120E-4	1.751E-11	4.9E-12	3.2E-11
750	9.866E-4	1.751E-11	4.9E-12	3.2E-11
750	3.120E-3	1.751E-11	4.9E-12	3.2E-11
750	9.866E-3	1.752E-11	4.9E-12	3.2E-11
750	3.120E-2	1.756E-11	4.9E-12	3.3E-11
750	9.866E-2	1.766E-11	4.9E-12	3.3E-11
750	3.120E-1	1.794E-11	4.9E-12	3.4E-11
750	9.866E-1	1.850E-11	4.8E-12	3.5E-11
750	3.120E+0	1.932E-11	4.8E-12	3.7E-11
750	9.866E+0	2.014E-11	4.8E-12	3.9E-11

750	3.120E+1	2.071E-11	4.8E-12	4.0E-11
750	9.866E+1	2.101E-11	4.8E-12	4.1E-11
632	9.866E-5	1.415E-11	3.6E-12	3.0E-11
632	3.120E-4	1.416E-11	3.6E-12	3.0E-11
632	9.866E-4	1.416E-11	3.6E-12	3.0E-11
632	3.120E-3	1.416E-11	3.6E-12	3.0E-11
632	9.866E-3	1.417E-11	3.6E-12	3.0E-11
632	3.120E-2	1.420E-11	3.6E-12	3.0E-11
632	9.866E-2	1.430E-11	3.5E-12	3.1E-11
632	3.120E-1	1.451E-11	3.5E-12	3.1E-11
632	9.866E-1	1.488E-11	3.5E-12	3.2E-11
632	3.120E+0	1.529E-11	3.5E-12	3.4E-11
632	9.866E+0	1.561E-11	3.5E-12	3.4E-11
632	3.120E+1	1.578E-11	3.5E-12	3.5E-11
632	9.866E+1	1.585E-11	3.5E-12	3.5E-11
545	9.866E-5	1.186E-11	2.7E-12	2.9E-11
545	3.120E-4	1.186E-11	2.7E-12	2.9E-11
545	9.866E-4	1.186E-11	2.7E-12	2.9E-11
545	3.120E-3	1.187E-11	2.7E-12	2.9E-11
545	9.866E-3	1.188E-11	2.7E-12	2.9E-11
545	3.120E-2	1.190E-11	2.7E-12	2.9E-11
545	9.866E-2	1.198E-11	2.7E-12	3.0E-11
545	3.120E-1	1.213E-11	2.7E-12	3.0E-11
545	9.866E-1	1.234E-11	2.7E-12	3.1E-11
545	3.120E+0	1.254E-11	2.7E-12	3.1E-11
545	9.866E+0	1.266E-11	2.7E-12	3.2E-11
545	3.120E+1	1.272E-11	2.7E-12	3.2E-11
545	9.866E+1	1.274E-11	2.7E-12	3.2E-11
480	9.866E-5	1.027E-11	2.2E-12	2.9E-11
480	3.120E-4	1.027E-11	2.2E-12	2.9E-11
480	9.866E-4	1.027E-11	2.2E-12	2.9E-11
480	3.120E-3	1.028E-11	2.2E-12	2.9E-11
480	9.866E-3	1.028E-11	2.2E-12	2.9E-11
480	3.120E-2	1.031E-11	2.2E-12	2.9E-11
480	9.866E-2	1.036E-11	2.2E-12	2.9E-11
480	3.120E-1	1.047E-11	2.2E-12	3.0E-11
480	9.866E-1	1.059E-11	2.2E-12	3.0E-11
480	3.120E+0	1.068E-11	2.2E-12	3.0E-11
480	9.866E+0	1.073E-11	2.2E-12	3.1E-11
480	3.120E+1	1.075E-11	2.2E-12	3.1E-11
480	9.866E+1	1.076E-11	2.2E-12	3.1E-11
429	9.866E-5	9.159E-12	1.8E-12	2.9E-11
429	3.120E-4	9.160E-12	1.8E-12	2.9E-11
429	9.866E-4	9.160E-12	1.8E-12	2.9E-11
429	3.120E-3	9.162E-12	1.8E-12	2.9E-11
429	9.866E-3	9.169E-12	1.8E-12	2.9E-11
429	3.120E-2	9.188E-12	1.8E-12	2.9E-11
429	9.866E-2	9.231E-12	1.8E-12	3.0E-11
429	3.120E-1	9.299E-12	1.8E-12	3.0E-11
429	9.866E-1	9.369E-12	1.8E-12	3.0E-11
429	3.120E+0	9.415E-12	1.8E-12	3.0E-11
429	9.866E+0	9.437E-12	1.8E-12	3.1E-11
429	3.120E+1	9.445E-12	1.8E-12	3.1E-11
429	9.866E+1	9.448E-12	1.8E-12	3.1E-11
387	9.866E-5	8.375E-12	1.5E-12	3.0E-11
387	3.120E-4	8.375E-12	1.5E-12	3.0E-11
387	9.866E-4	8.376E-12	1.5E-12	3.0E-11
387	3.120E-3	8.378E-12	1.5E-12	3.0E-11
387	9.866E-3	8.384E-12	1.5E-12	3.0E-11
387	3.120E-2	8.399E-12	1.5E-12	3.1E-11
387	9.866E-2	8.431E-12	1.5E-12	3.1E-11
387	3.120E-1	8.477E-12	1.5E-12	3.1E-11
387	9.866E-1	8.517E-12	1.5E-12	3.1E-11
387	3.120E+0	8.541E-12	1.5E-12	3.1E-11
387	9.866E+0	8.551E-12	1.5E-12	3.1E-11
387	3.120E+1	8.554E-12	1.5E-12	3.1E-11
387	9.866E+1	8.556E-12	1.5E-12	3.1E-11
353	9.866E-5	7.827E-12	1.5E-12	3.2E-11
353	3.120E-4	7.828E-12	1.5E-12	3.2E-11

353	9.866E-4	7.828E-12	1.5E-12	3.2E-11
353	3.120E-3	7.830E-12	1.5E-12	3.2E-11
353	9.866E-3	7.835E-12	1.5E-12	3.2E-11
353	3.120E-2	7.847E-12	1.5E-12	3.2E-11
353	9.866E-2	7.871E-12	1.5E-12	3.3E-11
353	3.120E-1	7.902E-12	1.5E-12	3.3E-11
353	9.866E-1	7.926E-12	1.5E-12	3.3E-11
353	3.120E+0	7.939E-12	1.5E-12	3.3E-11
353	9.866E+0	7.944E-12	1.5E-12	3.3E-11
353	3.120E+1	7.945E-12	1.5E-12	3.3E-11
353	9.866E+1	7.946E-12	1.5E-12	3.3E-11
324	9.866E-5	7.455E-12	1.3E-12	3.5E-11
324	3.120E-4	7.455E-12	1.3E-12	3.5E-11
324	9.866E-4	7.456E-12	1.3E-12	3.5E-11
324	3.120E-3	7.457E-12	1.3E-12	3.5E-11
324	9.866E-3	7.461E-12	1.3E-12	3.5E-11
324	3.120E-2	7.471E-12	1.3E-12	3.5E-11
324	9.866E-2	7.490E-12	1.3E-12	3.5E-11
324	3.120E-1	7.511E-12	1.3E-12	3.5E-11
324	9.866E-1	7.526E-12	1.3E-12	3.5E-11
324	3.120E+0	7.533E-12	1.3E-12	3.6E-11
324	9.866E+0	7.535E-12	1.3E-12	3.6E-11
324	3.120E+1	7.536E-12	1.3E-12	3.6E-11
324	9.866E+1	7.537E-12	1.3E-12	3.6E-11
300	9.866E-5	7.218E-12	1.2E-12	3.8E-11
300	3.120E-4	7.218E-12	1.2E-12	3.8E-11
300	9.866E-4	7.218E-12	1.2E-12	3.8E-11
300	3.120E-3	7.219E-12	1.2E-12	3.8E-11
300	9.866E-3	7.223E-12	1.2E-12	3.8E-11
300	3.120E-2	7.232E-12	1.2E-12	3.9E-11
300	9.866E-2	7.246E-12	1.2E-12	3.9E-11
300	3.120E-1	7.260E-12	1.2E-12	3.9E-11
300	9.866E-1	7.270E-12	1.2E-12	3.9E-11
300	3.120E+0	7.274E-12	1.2E-12	3.9E-11
300	9.866E+0	7.275E-12	1.2E-12	3.9E-11
300	3.120E+1	7.276E-12	1.2E-12	3.9E-11
300	9.866E+1	7.276E-12	1.2E-12	3.9E-11

Analytical expressions for the product yields $Y(T,P)$

This section gives equations fitted to the product yields, as tabulated in Table 6S and depicted in Figure 5 in the main text, for specific temperature and pressure ranges. Product yields are given as fractions, where pressure is expressed in Bar, and temperature in Kelvin.

The title reaction can be included in a kinetic model as a set of independent reactions, each giving a different product, combining the total rate coefficient as given in the main text, with the yield expressions Y_{product} described below. Each product channel is then included as follows:



$$k_{\text{tot}}(T) = 1.36 \times 10^{-15} T^{1.40} \exp(170 \text{ K} / T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

Analytical expressions for the product yields are given for the low-pressure regime, where collisional stabilisation of the adducts is negligible and only dissociation products are formed. We also give Kooij-style equations for the product yields at 1 bar and 100 bar, for the temperature range 700 to 2000K. Finally, we describe a set of equations that allows for interpolation of the product yields between the 1 bar and 100 bar values.

a) Low pressure regime ($P < 0.1 \text{ Bar}$; $T = 300 - 3000 \text{ K}$)

$$Y_{\text{H}_2\text{NCH}+\text{NO}}(T,P<0.1 \text{ Bar}) = 0.856 \times (1 - \exp(-4080\text{K}/T))$$

$$Y_{\text{OH}+\text{H}_2\text{NCN}}(T,P<0.1 \text{ Bar}) = 0.053 - 12.8\text{K}/T$$

$$Y_{\text{HCN}+\text{NHOH}}(T,P<0.1 \text{ Bar}) = 0.111 \times (1 - \exp(-1500\text{K}/T))$$

$$Y_{\text{CNO}+\text{NH}_3}(T,P<0.1 \text{ Bar}) = 2.1 \times \exp(-6000\text{K}/T)$$

Yields of ISa, ISb, IS9, IS10, and IS11 are below 1% and are considered negligible.

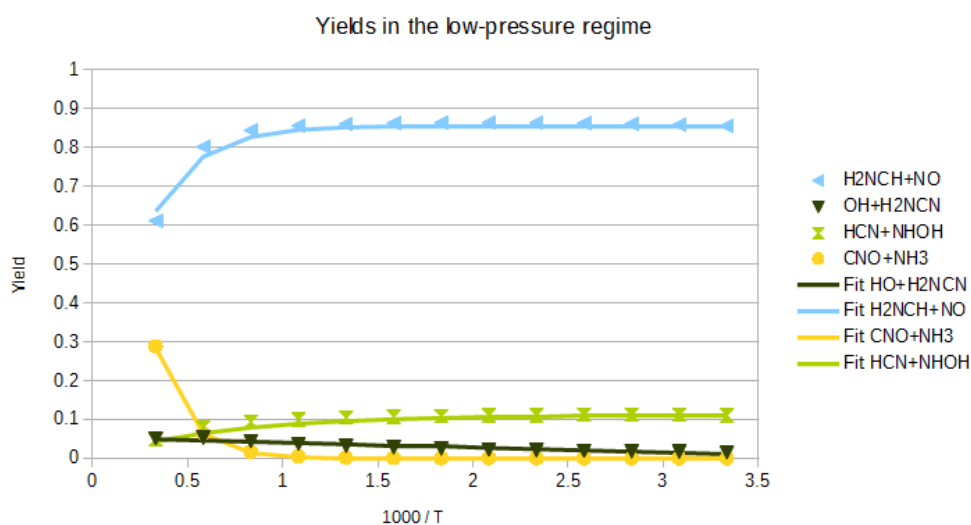


Figure 4S: Quality of fit for the product yields of the dominant products of the $\text{HCNO}+\text{NH}_2$ reaction in the low-pressure regime.

b) Combustion reaction conditions (P = 1 - 100 Bar ; T = 700 - 2000 K)

The pressure dependence is implemented by an interpolation between Kooij-style expressions for the product yield at the limiting pressures 1 Bar and 100 Bar. A logarithmic interpolation across the pressure-dependent rate coefficients at a given temperature is performed by the following equation:

$$P_{dep}^{\log} = \frac{\log(P) - \log(P_1)}{\log(P_2) - \log(P_1)}$$

where pressure $P_1 = 1$ Bar and $P_2 = 100$ Bar. For many product yields, the pressure interpolation is fitter better by mixing a linear and a logarithmic dependence on pressure. For the pressure range of 1 Bar to 100 Bar, and a pressure P expressed in Bar, we find the following interpolation expression, easiest to implement using Briggsian logarithms (base 10):

$$P_{dep}^{mixed} = \left(\frac{1000}{T} - 0.5 \right) \left(\frac{\log(P) - \log(1)}{\log(100) - \log(1)} \right) + \left(1.5 - \frac{1000}{T} \right) \left(\frac{P - 1}{100 - 1} \right)$$

The temperature- and pressure-dependent product yield $Y(T,P)$ across the reaction condition domain defined above is then obtained by interpolation between Kooij expressions for the 1 Bar and 100 Bar product yields, using one of the above pressure dependencies, as follows:

$$Y(T, P) = Y(T, P = 1barr) + [Y(T, P = 100barr) - Y(T, P = 1barr)] \times P_{dep}$$

The fitting by these formulas is relatively poor, with errors up to 9% absolute on the predicted yield, though this is not necessarily outside the uncertainty interval predicted by our error analysis. Figure 5S shows the fitting quality, using both a linear and a logarithmic scale. The sum of the yields is not guaranteed to be exactly 1, but should remain within the uncertainty interval. For a more accurate fit it is recommended that the tabulated data (Table 6S) is used either as a lookup table, a lookup table with (linear) interpolation, or by fitting more free-form polynomials (e.g. Chebychev functions) to the table data across the desired range of reaction conditions, depending on the capabilities of the modeling software. The interpolation equations given in this section are unlikely to be reliable outside the indicated reaction conditions.

Below, we provide the limiting Arrhenius expressions for each product at 1 and 100 bar, indicate which pressure interpolation formula to use, and give an estimate of the maximum fitting error (absolute error on the product yield).

IS1a:

$$Y_{IS1a}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 6.45 \times 10^3 \times T^{-2.42} \times \exp(2230K/T)$$

$$Y_{IS1a}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 1.47 \times 10^{23} \times T^{-7.10} \times \exp(-5320K/T)$$

Pressure interpolation: P_{dep}^{mixed}

Maximum absolute fitting error: 5 %

IS1b:

$$Y_{IS1b}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 0.154 \times T^{-1.23} \times \exp(3340K/T)$$

$$Y_{IS1b}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 1.62 \times 10^{18} \times T^{-5.80} \times \exp(-4090K/T)$$

Pressure interpolation: P_{dep}^{mixed}

Maximum absolute fitting error: 2 %

IS9:

$$Y_{IS9}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 0.415 \times T^{-1.31} \times \exp(3210K/T)$$

$$Y_{IS9}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 2.74 \times 10^{18} \times T^{-5.83} \times \exp(-4170K/T)$$

Pressure interpolation: P_{dep}^{mixed}

Maximum absolute fitting error: 3 %

IS10, IS11:

Negligible yields < 5%

H₂NCH+NO:

$$Y_{H2NCH+NO}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 21.5 \times T^{-0.41} \times \exp(-390K/T)$$

$$Y_{H2NCH+NO}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 9.40 \times 10^4 \times T^{-1.32} \times \exp(-3470K/T)$$

Pressure interpolation: P_{dep}^{mixed}

Maximum absolute fitting error: 9 %

OH+H₂NCN:

$$Y_{OH+H2NCN}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 6.25 \times 10^{-2} \times T^{-0.03} \times \exp(-690K/T)$$

$$Y_{OH+H2NCN}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 436 \times T^{-0.93} \times \exp(-3780K/T)$$

Pressure interpolation: P_{dep}^{log}

Maximum absolute fitting error: 1 %

HCN+NHOH:

$$Y_{HCN+NHOH}(P = 1 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 208 \times T^{-0.99} \times \exp(-820K/T)$$

$$Y_{HCN+NHOH}(P = 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 9.70 \times 10^8 \times T^{-2.65} \times \exp(-6530K/T)$$

Pressure interpolation: P_{dep}^{log}

Maximum absolute fitting error: 2 %

CNO+NH₃:

The yield of this product is not very pressure-dependent, and can be expressed as a simple Kooij expression:

$$Y_{CNO+NH_3} (P = 1 - 100 \text{ Bar} ; T = 700 - 2000 \text{ K}) = 1.81 \times 10^{-9} \times T^{2.48} \times \exp(-1930K/T)$$

Maximum absolute fitting error: 4 %

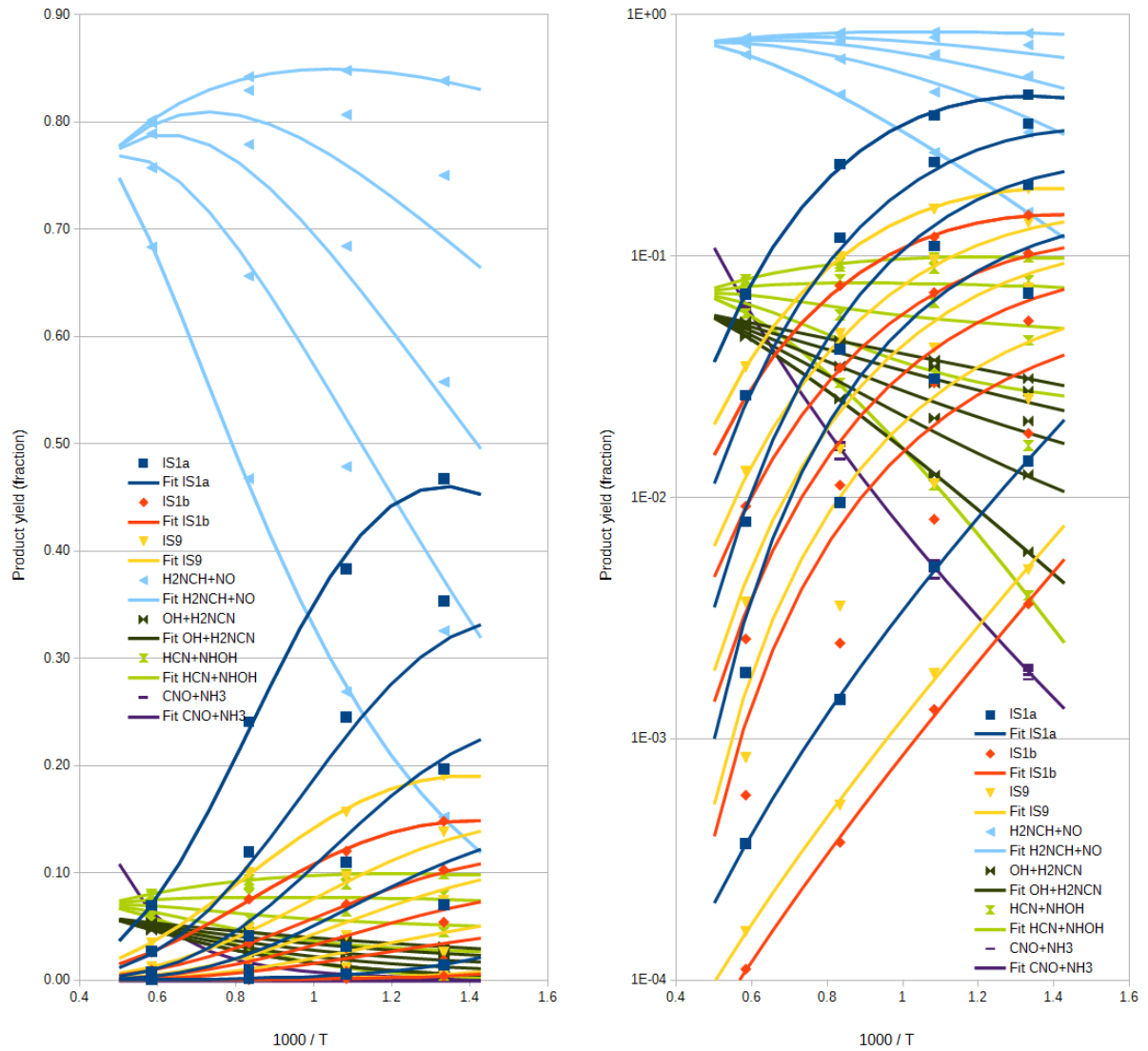


Figure 5S: Quality of fit for the product yields of the dominant products of the HCNO+NH₂ reaction at reaction conditions relevant for combustion systems, shown for clarity using a linear (left panel) and logarithmic (right panel) scale. For each product, temperature- and pressure-dependent reference yields (symbols) are shown as a function of temperature and pressure ($P = 1, 3.3, 10, 33.3, 100$ Bar). The fits obtained using the expressions described above are shown as lines.

Extensive quantum chemical data for the key intermediates, products and transition states, obtained at the B3LYP/6-311++G(3df,2p) level of theory, as well as CCSD(T) calculations with aug-cc-pVxZ (x=D,T,Q) basis sets.

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*****
B3LYP/6-311++G(3df,2p) geometries
*****

COM
---
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.96810608
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.94136668
T1 diagnostic: 0.021372
E(MP2/Aug-CC-pVDZ) (Hartree): -223.91000903
E(MP3/Aug-CC-pVDZ) (Hartree): -223.92624402
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.91352525
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.92832955
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.26763264
E(UHF/Aug-CC-pVDZ) (Hartree): -223.26248398
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.15312244
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.11539453
T1 diagnostic: 0.020556
E(MP2/Aug-CC-pVTZ) (Hartree): -224.09428493
E(MP3/Aug-CC-pVTZ) (Hartree): -224.10429243
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.09805390
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.10648906
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.31807569
E(UHF/Aug-CC-pVTZ) (Hartree): -223.31255115
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.20871604
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.16846458
T1 diagnostic: 0.020359
E(MP2/Aug-CC-pVQZ) (Hartree): -224.15555455
E(MP3/Aug-CC-pVQZ) (Hartree): -224.15905943
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.15938323
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.16127903
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.33225999
E(UHF/Aug-CC-pVQZ) (Hartree): -223.32666739
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.56021684
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      1.148191      0.758426      0.000149
  H      1.950912      1.513186      0.000289
  N      1.672628     -0.425018     -0.000020
  H      1.048337     -1.228250     -0.000163
  H      2.665888     -0.644839     -0.000026
  N     -1.084755     -0.389962     -0.000088
  O     -2.083675      0.189276     -0.000029
Rotational constants (GHz):  30.8544500   3.3141400   2.9926900
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
   55.8692      118.0515      168.6170
  242.7890      313.8689      814.4076
 1024.8470      1116.7824      1328.5983
 1440.4875      1639.3996      1842.9546
 2901.6560      3342.9472      3424.5003
Zero-point correction (Hartree): 0.045972

HCNO
----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -168.19100343
E(CCSD/Aug-CC-pVDZ) (Hartree): -168.16625316
T1 diagnostic: 0.020972
E(MP2/Aug-CC-pVDZ) (Hartree): -168.16915940
E(MP3/Aug-CC-pVDZ) (Hartree): -168.15613865
E(RHF/Aug-CC-pVDZ) (Hartree): -167.65688740
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -168.33454446
E(CCSD/Aug-CC-pVTZ) (Hartree): -168.30070149
T1 diagnostic: 0.020254
E(MP2/Aug-CC-pVTZ) (Hartree): -168.31166478
E(MP3/Aug-CC-pVTZ) (Hartree): -168.29321238

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E(RHF/Aug-CC-pVTZ) (Hartree): -167.69816390
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -168.37725127
 E(CCSD/Aug-CC-pVQZ) (Hartree): -168.34137401
 T1 diagnostic: 0.019967
 E(MP2/Aug-CC-pVQZ) (Hartree): -168.35833497
 E(MP3/Aug-CC-pVQZ) (Hartree): -168.33510871
 E(RHF/Aug-CC-pVQZ) (Hartree): -167.70883087
 E(RB3LYP/6-311++G(3df,2p)) (Hartree): -168.64134754
 Point group : C*v
 Electronic state : 1-SG
 Cartesian coordinates (Angs):

C	-0.000000	-0.000000	1.175443
H	-0.000000	-0.000000	2.235396
N	-0.000000	-0.000000	0.020541
O	0.000000	0.000000	-1.178980

 Rotational constants (GHz): 0.0000000 11.5538771 11.5538771
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

251.6484 (PI)	251.6484 (PI)	554.9426 (PI)
554.9426 (PI)	1265.2481 (SG)	2275.2682 (SG)
3420.4352 (SG)		

 Zero-point correction (Hartree): 0.019932

NH2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -55.75180452
 E(CCSD/Aug-CC-pVDZ) (Hartree): -55.74788363
 T1 diagnostic: 0.011190
 E(MP2/Aug-CC-pVDZ) (Hartree): -55.72843611
 E(MP3/Aug-CC-pVDZ) (Hartree): -55.74472831
 E(PMP2/Aug-CC-pVDZ) (Hartree): -55.73033840
 E(PMP3/Aug-CC-pVDZ) (Hartree): -55.74585939
 E(PUHF/Aug-CC-pVDZ) (Hartree): -55.57803673
 E(UHF/Aug-CC-pVDZ) (Hartree): -55.57498439
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -55.79984500
 E(CCSD/Aug-CC-pVTZ) (Hartree): -55.79361938
 T1 diagnostic: 0.010262
 E(MP2/Aug-CC-pVTZ) (Hartree): -55.77659658
 E(MP3/Aug-CC-pVTZ) (Hartree): -55.79161411
 E(PMP2/Aug-CC-pVTZ) (Hartree): -55.77867898
 E(PMP3/Aug-CC-pVTZ) (Hartree): -55.79280535
 E(PUHF/Aug-CC-pVTZ) (Hartree): -55.59127155
 E(UHF/Aug-CC-pVTZ) (Hartree): -55.58789955
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -55.81307639
 E(CCSD/Aug-CC-pVQZ) (Hartree): -55.80633132
 T1 diagnostic: 0.010192
 E(MP2/Aug-CC-pVQZ) (Hartree): -55.79156513
 E(MP3/Aug-CC-pVQZ) (Hartree): -55.80469160
 E(PMP2/Aug-CC-pVQZ) (Hartree): -55.79366374
 E(PMP3/Aug-CC-pVQZ) (Hartree): -55.80587888
 E(PUHF/Aug-CC-pVQZ) (Hartree): -55.59462639
 E(UHF/Aug-CC-pVQZ) (Hartree): -55.59122870
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -55.90463983
 Point group : C2V
 Electronic state : 2-B1
 Cartesian coordinates (Angs):

N	-0.000000	0.000000	0.141616
H	0.000000	0.805662	-0.495657
H	-0.000000	-0.805662	-0.495657

 Rotational constants (GHz): 706.2452800 386.2747300 249.7022500
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

1500.2151	3297.9782	3384.6644
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 Zero-point correction (Hartree): 0.019022

NO

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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -129.62419543
 E(CCSD/Aug-CC-pVDZ) (Hartree): -129.61104179
 T1 diagnostic: 0.024689
 E(MP2/Aug-CC-pVDZ) (Hartree): -129.60211232
 E(MP3/Aug-CC-pVDZ) (Hartree): -129.60083143
 E(PMP2/Aug-CC-pVDZ) (Hartree): -129.60661127
 E(PMP3/Aug-CC-pVDZ) (Hartree): -129.60375124
 E(PUHF/Aug-CC-pVDZ) (Hartree): -129.27647974
 E(UHF/Aug-CC-pVDZ) (Hartree): -129.27061302
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -129.72594612

E(CCSD/Aug-CC-pVTZ) (Hartree): -129.70671664
 T1 diagnostic: 0.024514
 E(MP2/Aug-CC-pVTZ) (Hartree): -129.70213064
 E(MP3/Aug-CC-pVTZ) (Hartree): -129.69797992
 E(PMP2/Aug-CC-pVTZ) (Hartree): -129.70700465
 E(PMP3/Aug-CC-pVTZ) (Hartree): -129.70112760
 E(PUHF/Aug-CC-pVTZ) (Hartree): -129.30557279
 E(UHF/Aug-CC-pVTZ) (Hartree): -129.29924182
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -129.75804240
 E(CCSD/Aug-CC-pVQZ) (Hartree): -129.73742149
 T1 diagnostic: 0.024617
 E(MP2/Aug-CC-pVQZ) (Hartree): -129.73649846
 E(MP3/Aug-CC-pVQZ) (Hartree): -129.72959791
 E(PMP2/Aug-CC-pVQZ) (Hartree): -129.74147018
 E(PMP3/Aug-CC-pVQZ) (Hartree): -129.73279943
 E(PUHF/Aug-CC-pVQZ) (Hartree): -129.31426099
 E(UHF/Aug-CC-pVQZ) (Hartree): -129.30782651
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -129.93990141
 Point group : C*V
 Cartesian coordinates (Angs):
 N 0.000000 0.000000 -0.610415
 O 0.000000 0.000000 0.534113
 Rotational constants (GHz): 0.0000000 51.6715452 51.6715452
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
 1940.8083 (SG)
 Zero-point correction (Hartree): 0.004512

 NH2CH.singlet

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -94.34054425
 E(CCSD/Aug-CC-pVDZ) (Hartree): -94.32897586
 T1 diagnostic: 0.017461
 E(MP2/Aug-CC-pVDZ) (Hartree): -94.30267071
 E(MP3/Aug-CC-pVDZ) (Hartree): -94.32330109
 E(RHF/Aug-CC-pVDZ) (Hartree): -93.99826947
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -94.42371023
 E(CCSD/Aug-CC-pVTZ) (Hartree): -94.40734832
 T1 diagnostic: 0.016438
 E(MP2/Aug-CC-pVTZ) (Hartree): -94.38658476
 E(MP3/Aug-CC-pVTZ) (Hartree): -94.40400359
 E(RHF/Aug-CC-pVTZ) (Hartree): -94.02018004
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -94.44738053
 E(CCSD/Aug-CC-pVQZ) (Hartree): -94.42993450
 T1 diagnostic: 0.016192
 E(MP2/Aug-CC-pVQZ) (Hartree): -94.41352257
 E(MP3/Aug-CC-pVQZ) (Hartree): -94.42728671
 E(RHF/Aug-CC-pVQZ) (Hartree): -94.02590863
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -94.61423659
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 C 0.062503 0.783788 0.000000
 H -0.995455 1.102305 0.000000
 H -0.758805 -1.127032 0.000000
 H 0.941715 -1.023375 0.000000
 N 0.062503 -0.522090 0.000000
 Rotational constants (GHz): 206.2049200 34.1173600 29.2738900
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
 793.3731 (A'') 1051.7306 (A') 1130.6401 (A'')
 1354.6036 (A') 1409.2565 (A') 1654.4215 (A')
 2865.1234 (A') 3311.7002 (A') 3471.0558 (A')
 Zero-point correction (Hartree): 0.039617

 NH2CH.triplet

 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -94.56181642
 Electronic state : 3-A
 Cartesian coordinates (Angs):
 C -0.768214 -0.000522 0.170659
 H -1.560733 0.001788 -0.576433
 H 1.090850 -0.836060 0.135304
 H 1.090337 0.836148 0.137317
 N 0.569833 0.000180 -0.102877
 Rotational constants (GHz): 231.0796200 29.1536000 28.1294500
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

506.7454	570.3829	1043.7791
1068.9111	1246.7102	1591.7194
3006.3922	3405.2104	3470.5686

Zero-point correction (Hartree): 0.036986

IS1a

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.02672359
 E(CCSD/Aug-CC-pVDZ) (Hartree): -223.99941835
 T1 diagnostic: 0.037769
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.96125635
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.98072841
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.97276548
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.98963727
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.32837238
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.31519427
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.21699886
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.17823836
 T1 diagnostic: 0.037245
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.14992951
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.16377577
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.16177752
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.17291169
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.38007093
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.36650341
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.27399265
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.23257584
 T1 diagnostic: 0.037273
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.21209602
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.21968360
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.22406611
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.22889218
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.39439482
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.38069335
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.63060649
 Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.523235	0.618410	-0.004333
N	0.748835	0.519767	0.020774
O	1.468716	-0.498136	-0.002273
N	-1.377763	-0.468409	-0.080388
H	-0.966475	-1.360146	0.152218
H	-2.292118	-0.333876	0.320505
H	-0.949232	1.609146	-0.011243

Rotational constants (GHz): 25.0126400 6.3736700 5.1003100

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

240.5630	313.6684	375.4734
550.0185	676.1196	810.0031
1033.9952	1160.3116	1223.2231
1417.9706	1602.2849	1696.0297
3157.0938	3490.0815	3593.3175

Zero-point correction (Hartree): 0.049609

IS1b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.02137772
 E(CCSD/Aug-CC-pVDZ) (Hartree): -223.99419115
 T1 diagnostic: 0.038291
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.95497357
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.97492292
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.96777092
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.98498256
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.32505412
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.31052353
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.21164788
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.17303683
 T1 diagnostic: 0.037875
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.14359821
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.15795879
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.15674607
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.16825301
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.37692818
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.36199900
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.26856189
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.22729425

T1 diagnostic: 0.037939
E(MP2/Aug-CC-pVQZ) (Hartree): -224.20566229
E(MP3/Aug-CC-pVQZ) (Hartree): -224.21376253
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.21893718
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.22413216
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.39124715
E(UHF/Aug-CC-pVQZ) (Hartree): -223.37617890
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.62607172
Electronic state : 2-A
Cartesian coordinates (Angs):
C 0.435656 0.413161 -0.007315
H 0.372675 1.496195 -0.044277
N 1.702244 -0.152442 -0.091632
H 1.723989 -1.149759 0.067664
H 2.409280 0.329289 0.443770
N -0.624587 -0.290683 0.040376
O -1.832934 -0.006602 -0.008060
Rotational constants (GHz): 66.7154900 4.5509700 4.2842200
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
250.5503 305.4815 343.6526
555.7870 658.2326 763.0765
1020.9877 1208.4070 1238.2624
1399.1152 1608.5117 1704.9955
3069.5988 3471.1637 3568.1587
Zero-point correction (Hartree): 0.049204

IS2

E(CCS2D(T)/Aug-CC-pVDZ) (Hartree): -223.99581437
E(CCS2D/Aug-CC-pVDZ) (Hartree): -223.96856259
T1 diagnostic: 0.025830
E(MP2/Aug-CC-pVDZ) (Hartree): -223.94258468
E(MP3/Aug-CC-pVDZ) (Hartree): -223.95686674
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.94570174
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.95909847
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.28402087
E(UHF/Aug-CC-pVDZ) (Hartree): -223.27999403
E(CCS2D(T)/Aug-CC-pVTZ) (Hartree): -224.18601778
E(CCS2D/Aug-CC-pVTZ) (Hartree): -224.14722364
T1 diagnostic: 0.024843
E(MP2/Aug-CC-pVTZ) (Hartree): -224.13158470
E(MP3/Aug-CC-pVTZ) (Hartree): -224.13962338
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.13487573
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.14196531
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.33541972
E(UHF/Aug-CC-pVTZ) (Hartree): -223.33119307
E(CCS2D(T)/Aug-CC-pVQZ) (Hartree): -224.24329876
E(CCS2D/Aug-CC-pVQZ) (Hartree): -224.20186135
T1 diagnostic: 0.024502
E(MP2/Aug-CC-pVQZ) (Hartree): -224.19431197
E(MP3/Aug-CC-pVQZ) (Hartree): -224.19601100
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.19764446
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.19837330
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.34953144
E(UHF/Aug-CC-pVQZ) (Hartree): -223.34526086
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.59683259
Electronic state : 2-A
Cartesian coordinates (Angs):
C 0.497642 -0.351753 -0.082048
N -0.506338 0.398285 -0.148895
O -1.749030 -0.204589 0.129196
H -2.374935 0.460599 -0.175151
N 1.770908 0.018620 0.075744
H 2.019832 0.943230 0.400558
H 2.509501 -0.574933 -0.254630
Rotational constants (GHz): 74.2882400 4.3404700 4.1653700
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
213.5874 264.8499 308.1013
352.7324 505.6164 572.8847
902.7643 1105.5957 1181.7390
1386.7832 1590.1642 1656.8520
3449.1396 3619.2493 3745.1450
Zero-point correction (Hartree): 0.048481

IS9

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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.02613116
E(CCSD/Aug-CC-pVDZ) (Hartree): -224.00034446
  T1 diagnostic: 0.034176
E(MP2/Aug-CC-pVDZ) (Hartree): -223.95553764
E(MP3/Aug-CC-pVDZ) (Hartree): -223.98028587
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.97278359
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.99290820
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.34715738
E(UHF/Aug-CC-pVDZ) (Hartree): -223.32686438
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.21408960
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.17716337
  T1 diagnostic: 0.033540
E(MP2/Aug-CC-pVTZ) (Hartree): -224.14196995
E(MP3/Aug-CC-pVTZ) (Hartree): -224.16141169
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.15965821
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.17437063
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.39695436
E(UHF/Aug-CC-pVTZ) (Hartree): -223.37616962
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.27058515
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.23105314
  T1 diagnostic: 0.033403
E(MP2/Aug-CC-pVQZ) (Hartree): -224.20371195
E(MP3/Aug-CC-pVQZ) (Hartree): -224.21700999
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.22147671
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.23000595
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.41094412
E(UHF/Aug-CC-pVQZ) (Hartree): -223.39007576
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.62227014
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      -0.587459      0.374908      0.000016
  H      -0.351549      1.438411     -0.000036
  N       0.447170     -0.507021     -0.000186
  O       1.626161      0.187851      0.000120
  H       2.305581     -0.497040     -0.000094
  N      -1.816604     -0.015201     -0.000067
  H      -1.852526     -1.038072      0.000844
Rotational constants (GHz): 54.4976200 4.8412500 4.4462700
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
  209.4287      364.8439      499.2689
  596.6097      804.9503     1007.9171
  1038.7221     1080.3000     1201.3015
  1346.7967     1387.9385     1499.6263
  3042.4333     3358.9581     3723.1597
Zero-point correction (Hartree): 0.049195

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IS10

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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.00081617
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.97611630
  T1 diagnostic: 0.027852
E(MP2/Aug-CC-pVDZ) (Hartree): -223.93655961
E(MP3/Aug-CC-pVDZ) (Hartree): -223.96147750
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.94603281
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.96873589
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.31481284
E(UHF/Aug-CC-pVDZ) (Hartree): -223.30394058
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.18873235
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.15307193
  T1 diagnostic: 0.027371
E(MP2/Aug-CC-pVTZ) (Hartree): -224.12336277
E(MP3/Aug-CC-pVTZ) (Hartree): -224.14268868
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.13293216
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.14998062
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.36463379
E(UHF/Aug-CC-pVTZ) (Hartree): -223.35363763
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.24472920
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.20651972
  T1 diagnostic: 0.027432
E(MP2/Aug-CC-pVQZ) (Hartree): -224.18469813
E(MP3/Aug-CC-pVQZ) (Hartree): -224.19776043
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.19433543
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.20508284
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.37843996

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E(UHF/Aug-CC-pVQZ) (Hartree): -223.36736846
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.59481394
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.726313	-0.338588	0.110083
H	-0.548464	-1.398326	0.313285
N	-1.875225	0.086026	-0.149143
N	0.414928	0.463388	0.249171
H	0.329517	1.345798	-0.244783
O	1.578179	-0.194594	-0.242967
H	2.173467	-0.205094	0.514538

 Rotational constants (GHz): 43.5432100 4.7898900 4.5130000
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

145.7678	352.5107	375.7967
532.9312	746.0449	884.3264
1006.0215	1118.9333	1223.2420
1361.5320	1424.8152	1645.2120
2981.9103	3442.5209	3726.0909

 Zero-point correction (Hartree): 0.048743

IS11

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.03108427
 E(CCSD/Aug-CC-pVDZ) (Hartree): -224.00499553
 T1 diagnostic: 0.028081
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.97000361
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.99015449
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.97981366
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.99698752
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.33765445
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.32577134
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.22041945
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.18313208
 T1 diagnostic: 0.027740
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.15767950
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.17229237
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.16778355
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.17932095
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.38844305
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.37621115
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.27722572
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.23732504
 T1 diagnostic: 0.027767
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.21973597
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.22806407
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.22991549
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.23512913
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.40256498
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.39024734
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.63197882
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.594034	-0.415903	0.000014
O	-1.731771	-0.137641	-0.000031
N	-0.563588	0.357717	0.000039
N	1.785543	0.021875	-0.000020
H	-0.471839	1.376133	0.000023
H	1.835663	1.042414	-0.000045
H	0.372456	-1.479149	0.000054

 Rotational constants (GHz): 53.9609300 4.8125800 4.4185100
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

191.6795	360.4126	570.3149
589.1626	800.0409	1030.7875
1049.2864	1209.5421	1340.1295
1359.5228	1456.8864	1616.8568
3088.9967	3330.3880	3371.0209

 Zero-point correction (Hartree): 0.049666

T0_1

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.94402587
 E(CCSD/Aug-CC-pVDZ) (Hartree): -223.91390760
 T1 diagnostic: 0.038755
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.87963884
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.89012427

E(PMP2/Aug-CC-pVDZ) (Hartree): -223.89657195
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.90295706
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.24559431
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.22643039
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.13503866
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.09338235
 T1 diagnostic: 0.038609
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.06907211
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.07351678
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.08669172
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.08686194
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.29987655
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.27995170
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.19087507
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.14658634
 T1 diagnostic: 0.038718
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.13013394
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.12820585
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.14794394
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.14167121
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.31404594
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.29391475
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.54757413
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.073501	0.898843	-0.000007
H	0.612709	1.814241	-0.000032
N	-0.869309	0.215525	-0.000003
O	-1.765489	-0.582280	0.000009
N	2.180439	-0.319282	-0.000034
H	1.946057	-0.911568	-0.804436
H	1.946227	-0.911188	0.804696

 Rotational constants (GHz): 21.5598800 3.7130300 3.2201900
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i182.6419	90.9086	97.3570
358.5200	403.3918	434.9019
495.1833	548.5801	558.1144
1253.1954	1505.4653	2211.3293
3309.9943	3377.7803	3396.3624

 Zero-point correction (Hartree): 0.041939

T0P1

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.93088268
 E(CCSD/Aug-CC-pVDZ) (Hartree): -223.89754133
 T1 diagnostic: 0.042835
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.86703391
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.87372398
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.88242648
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.88523829
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.21496386
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.19747721
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.12050357
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.07534009
 T1 diagnostic: 0.042178
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.05506838
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.05565182
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.07130907
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.06781782
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.26808776
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.24966456
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.17617863
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.12833407
 T1 diagnostic: 0.042043
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.11612882
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.11021855
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.13254943
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.12250229
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.28219235
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.26357451
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.53899037
 Electronic state : 2-A
 Cartesian coordinates (Angs):

H	-1.301574	0.597977	-0.000001
C	-0.052231	0.759809	0.000000

N	0.943322	0.126876	0.000000
O	2.024889	-0.400543	0.000000
N	-2.358882	-0.179948	0.000000
H	-2.337615	-0.790492	-0.818830
H	-2.337615	-0.790491	0.818831

Rotational constants (GHz): 38.6645500 2.9810500 2.8092500
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i1425.3982	97.9071	130.1306
369.9695	494.5445	501.9235
567.7622	705.7567	1189.8273
1219.8525	1393.7432	1544.2489
2136.4152	3360.3811	3455.7285

Zero-point correction (Hartree): 0.039910

TS10P13

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.97664213
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.94839150
T1 diagnostic: 0.038955
E(MP2/Aug-CC-pVDZ) (Hartree): -223.90154517
E(MP3/Aug-CC-pVDZ) (Hartree): -223.92330039
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.92373871
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.93973850
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.28769868
E(UHF/Aug-CC-pVDZ) (Hartree): -223.26184333
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.16414090
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.12445181
T1 diagnostic: 0.038581
E(MP2/Aug-CC-pVTZ) (Hartree): -224.08754201
E(MP3/Aug-CC-pVTZ) (Hartree): -224.10359025
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.11017548
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.12032087
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.33843557
E(UHF/Aug-CC-pVTZ) (Hartree): -223.31209110
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.21980492
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.17745026
T1 diagnostic: 0.038576
E(MP2/Aug-CC-pVQZ) (Hartree): -224.14845357
E(MP3/Aug-CC-pVQZ) (Hartree): -224.15822259
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.17120591
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.17500583
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.35222949
E(UHF/Aug-CC-pVQZ) (Hartree): -223.32575669
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.57116285
Electronic state : 2-A

Cartesian coordinates (Angs):

C	-1.023931	0.478297	0.128833
H	0.400590	-1.238361	0.387950
H	-0.893097	1.507058	0.414060
N	0.635208	-0.259708	0.574837
O	1.573456	0.013811	-0.404562
H	1.936177	0.876088	-0.167700
N	-1.762026	-0.329585	-0.313525

Rotational constants (GHz): 26.6496100 4.3876600 4.3635600
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i530.3456	112.1349	272.3466
358.3999	447.1251	769.6480
884.1816	961.1180	1006.9342
1259.5433	1515.0308	1875.8992
3197.6435	3355.4323	3709.6719

Zero-point correction (Hartree): 0.045854

TS11_10

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.96485211
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.93417385
T1 diagnostic: 0.040870
E(MP2/Aug-CC-pVDZ) (Hartree): -223.89968547
E(MP3/Aug-CC-pVDZ) (Hartree): -223.91419441
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.91282013
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.92353617
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.25352829
E(UHF/Aug-CC-pVDZ) (Hartree): -223.23794294
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.15451821
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.11206493

T1 diagnostic: 0.039944
E(MP2/Aug-CC-pVTZ) (Hartree): -224.08783298
E(MP3/Aug-CC-pVTZ) (Hartree): -224.09646741
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.10146548
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.10616697
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.30396591
E(UHF/Aug-CC-pVTZ) (Hartree): -223.28782142
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.21106633
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.16587039
T1 diagnostic: 0.039658
E(MP2/Aug-CC-pVQZ) (Hartree): -224.14978070
E(MP3/Aug-CC-pVQZ) (Hartree): -224.15207181
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.16348985
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.16180492
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.31777257
E(UHF/Aug-CC-pVQZ) (Hartree): -223.30154271
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.56351105
Electronic state : 2-A
Cartesian coordinates (Angs):
H -1.364999 1.464519 0.005430
C -0.845708 0.507891 0.003451
N 0.606884 0.628618 -0.072802
O 1.186824 -0.561408 0.019456
H 0.231351 -1.112145 -0.081463
H 1.187123 1.385309 0.278773
N -1.246001 -0.670585 0.018645
Rotational constants (GHz): 19.8836500 8.2132000 5.8336500
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
i2444.6479 347.1473 409.7589
470.7256 772.4323 831.2459
870.7292 1109.5572 1120.2239
1267.6301 1374.0674 1579.2184
2054.2032 3036.5263 3443.2454
Zero-point correction (Hartree): 0.043440

TS1_11

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.96361904
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.93252698
T1 diagnostic: 0.029600
E(MP2/Aug-CC-pVDZ) (Hartree): -223.90788582
E(MP3/Aug-CC-pVDZ) (Hartree): -223.91833102
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.91578447
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.92367648
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.24206202
E(UHF/Aug-CC-pVDZ) (Hartree): -223.23213791
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.15336522
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.11044969
T1 diagnostic: 0.028776
E(MP2/Aug-CC-pVTZ) (Hartree): -224.09633391
E(MP3/Aug-CC-pVTZ) (Hartree): -224.10059628
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.10444286
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.10607398
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.29228647
E(UHF/Aug-CC-pVTZ) (Hartree): -223.28209311
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.21043669
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.16478355
T1 diagnostic: 0.028594
E(MP2/Aug-CC-pVQZ) (Hartree): -224.15883620
E(MP3/Aug-CC-pVQZ) (Hartree): -224.15668145
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.16699545
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.16217707
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.30621364
E(UHF/Aug-CC-pVQZ) (Hartree): -223.29596106
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.56747003
Electronic state : 2-A
Cartesian coordinates (Angs):
C 0.535062 0.553169 -0.000015
H 0.504169 1.634280 0.000118
H 0.563333 -1.170735 0.000075
N -0.532287 -0.295490 0.000214
O -1.740860 0.015401 -0.000099
N 1.551133 -0.265896 -0.000206
H 2.517084 0.023938 0.000638
Rotational constants (GHz): 50.7540900 5.2469900 4.7553800

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i1776.2254	223.1909	440.3759
469.3603	753.7101	911.7404
997.9637	1075.5217	1077.1676
1298.2072	1445.9115	1466.2179
1970.5533	3139.4123	3552.2358

Zero-point correction (Hartree): 0.043754

TS1_2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.95731737
 E(CCSD(Aug-CC-pVDZ) (Hartree): -223.92660424
 T1 diagnostic: 0.023228

E(MP2/Aug-CC-pVDZ) (Hartree): -223.90513899
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.91536511
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.90934432
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.91761239
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.23199910
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.22569725
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.14563210
 E(CCSD(Aug-CC-pVTZ) (Hartree): -224.10317727
 T1 diagnostic: 0.022365

E(MP2/Aug-CC-pVTZ) (Hartree): -224.09255842
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.09626041
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.09700627
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.09857300
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.28106756
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.27440017
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.20223063
 E(CCSD(Aug-CC-pVQZ) (Hartree): -224.15706012
 T1 diagnostic: 0.022157

E(MP2/Aug-CC-pVQZ) (Hartree): -224.15473333
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.15195473
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.15922040
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.15426261
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.29472904
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.28800864
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.55585415

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.380301	-0.349542	-0.000336
N	-0.575947	0.610945	-0.000268
O	-1.664804	-0.163927	0.000271
H	-0.827014	-1.103987	0.000076
N	1.654164	-0.003256	0.000001
H	2.370869	-0.708016	0.000417
H	1.945247	0.966843	0.001216

Rotational constants (GHz): 51.7070900 5.1045000 4.6458700

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i1690.3097	182.6266	420.6759
521.4603	650.8427	745.7938
993.9339	1131.5515	1131.6231
1307.8940	1457.8579	1613.0593
1951.5840	3446.9330	3608.6393

Zero-point correction (Hartree): 0.044551

TS1_9

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.01126982
 E(CCSD(Aug-CC-pVDZ) (Hartree): -223.98107750
 T1 diagnostic: 0.030917

E(MP2/Aug-CC-pVDZ) (Hartree): -223.95610401
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.96681671
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.96316006
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.97137413
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.28869151
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.27985051
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.20072919
 E(CCSD(Aug-CC-pVTZ) (Hartree): -224.15862327
 T1 diagnostic: 0.030057

E(MP2/Aug-CC-pVTZ) (Hartree): -224.14440037
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.14863605
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.15166830
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.15331260
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.33804862

E(UHF/Aug-CC-pVTZ) (Hartree): -223.32893696
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.25770837
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.21285371
 T1 diagnostic: 0.029785
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.20686334
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.20468714
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.21418873
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.20938628
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.35184190
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.34266277
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.60945225
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.625961	0.639829	0.000001
H	1.168414	1.574314	0.000001
N	1.114652	-0.555072	-0.000003
H	-0.022814	-1.097291	0.000003
H	2.102552	-0.745060	0.000010
N	-0.761683	0.676858	-0.000001
O	-1.184337	-0.552930	0.000001

 Rotational constants (GHz): 20.3785600 8.6658600 6.0802600
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i1485.8087	392.6921	609.2013
733.3270	853.9095	920.7250
993.9905	1097.4416	1133.7542
1238.1808	1338.4672	1532.2847
2022.8144	3145.9483	3579.7324

 Zero-point correction (Hartree): 0.045546

TS1a_1b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.00004572
 E(CCSD/Aug-CC-pVDZ) (Hartree): -223.97222772
 T1 diagnostic: 0.032020
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.94031002
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.95548980
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.95422434
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.96612705
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.29973381
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.28367667
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.19232588
 E(CCSD/Aug-CC-pVTZ) (Hartree): -224.15289084
 T1 diagnostic: 0.031557
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.13113608
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.14026799
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.14529894
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.15103975
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.35241490
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.33606439
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.24924029
 E(CCSD/Aug-CC-pVQZ) (Hartree): -224.20713479
 T1 diagnostic: 0.031620
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.19324000
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.19604445
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.20753881
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.20689108
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.36665020
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.35014832
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.60880922
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.522097	0.514837	-0.010398
H	0.752554	1.580555	-0.039066
N	1.641499	-0.335377	-0.092182
H	1.445297	-1.302037	0.126875
H	2.443817	0.005366	0.419262
N	-0.663268	0.128352	0.034333
O	-1.827733	-0.240466	-0.004967

 Rotational constants (GHz): 48.3783000 4.6254800 4.2437400
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i449.7978	255.0033	287.2057
433.4296	646.6596	755.3622
955.0863	1159.1679	1179.0005
1402.4525	1601.5402	1948.3444
2993.0327	3458.4763	3560.0209

Zero-point correction (Hartree): 0.047969

TS1P2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.95991910
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.93032792
T1 diagnostic: 0.025068
E(MP2/Aug-CC-pVDZ) (Hartree): -223.90141799
E(MP3/Aug-CC-pVDZ) (Hartree): -223.91514718
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.90471888
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.91690075
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.24949554
E(UHF/Aug-CC-pVDZ) (Hartree): -223.24422768
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.14578442
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.10499674
T1 diagnostic: 0.023913
E(MP2/Aug-CC-pVTZ) (Hartree): -224.08658448
E(MP3/Aug-CC-pVTZ) (Hartree): -224.09408594
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.09010552
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.09588880
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.29958694
E(UHF/Aug-CC-pVTZ) (Hartree): -223.29394419
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.20167895
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.15830161
T1 diagnostic: 0.023622
E(MP2/Aug-CC-pVQZ) (Hartree): -224.14815587
E(MP3/Aug-CC-pVQZ) (Hartree): -224.14915005
E(PMP2/Aug-CC-pVQZ) (Hartree): -224.15171586
E(PMP3/Aug-CC-pVQZ) (Hartree): -224.15095019
E(PUHF/Aug-CC-pVQZ) (Hartree): -223.31361283
E(UHF/Aug-CC-pVQZ) (Hartree): -223.30791161
E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.55849381
Electronic state : 2-A
Cartesian coordinates (Angs):
C -0.849933 0.677246 -0.000001
H -1.387551 1.636733 0.000011
N -1.652099 -0.334408 -0.000003
H -1.223743 -1.260732 -0.000013
H -2.665067 -0.301704 0.000005
N 0.911233 -0.415300 0.000010
O 1.945253 0.138772 -0.000006
Rotational constants (GHz): 35.6241400 3.9120000 3.5249100
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)
i282.6838 97.3189 209.7872
216.9891 455.0478 778.5484
974.3741 1067.5243 1303.8999
1424.1090 1622.0815 1700.2264
2926.8231 3336.0518 3455.4374
Zero-point correction (Hartree): 0.045489

TS2P6

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -223.98212528
E(CCSD/Aug-CC-pVDZ) (Hartree): -223.95403692
T1 diagnostic: 0.037008
E(MP2/Aug-CC-pVDZ) (Hartree): -223.91082386
E(MP3/Aug-CC-pVDZ) (Hartree): -223.93021279
E(PMP2/Aug-CC-pVDZ) (Hartree): -223.93054885
E(PMP3/Aug-CC-pVDZ) (Hartree): -223.94468197
E(PUHF/Aug-CC-pVDZ) (Hartree): -223.29113591
E(UHF/Aug-CC-pVDZ) (Hartree): -223.26818388
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -224.17234374
E(CCSD/Aug-CC-pVTZ) (Hartree): -224.13274911
T1 diagnostic: 0.036347
E(MP2/Aug-CC-pVTZ) (Hartree): -224.09937465
E(MP3/Aug-CC-pVTZ) (Hartree): -224.11337492
E(PMP2/Aug-CC-pVTZ) (Hartree): -224.11958206
E(PMP3/Aug-CC-pVTZ) (Hartree): -224.12819946
E(PUHF/Aug-CC-pVTZ) (Hartree): -223.34342009
E(UHF/Aug-CC-pVTZ) (Hartree): -223.31993212
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -224.22875032
E(CCSD/Aug-CC-pVQZ) (Hartree): -224.18648295
T1 diagnostic: 0.036294
E(MP2/Aug-CC-pVQZ) (Hartree): -224.16096377
E(MP3/Aug-CC-pVQZ) (Hartree): -224.16875306

E(PMP2/Aug-CC-pVQZ) (Hartree): -224.18127396
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.18362816
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.35721848
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.33361834
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.58444758
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.531387	-0.053255	-0.028426
N	-0.496131	0.560770	-0.034650
O	-1.864346	-0.354286	0.034640
H	-2.495831	0.374838	-0.008440
N	1.858261	-0.112918	-0.033423
H	2.386618	0.659106	0.349994
H	2.300751	-1.015092	0.028396

 Rotational constants (GHz): 60.2023200 3.9402200 3.7075300
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i558.6036	116.9991	221.4543
239.6032	328.4980	437.9638
539.3169	1019.5321	1108.2588
1145.9822	1598.0295	1919.4029
3454.1559	3565.5630	3727.1638

 Zero-point correction (Hartree): 0.045149

TS9P3

E(CCS(DT)/Aug-CC-pVDZ) (Hartree): -223.93374177
 E(CCS(DT)/Aug-CC-pVDZ) (Hartree): -223.89738481
 T1 diagnostic: 0.033189
 E(MP2/Aug-CC-pVDZ) (Hartree): -223.87766377
 E(MP3/Aug-CC-pVDZ) (Hartree): -223.87959183
 E(PMP2/Aug-CC-pVDZ) (Hartree): -223.89202683
 E(PMP3/Aug-CC-pVDZ) (Hartree): -223.89016328
 E(PUHF/Aug-CC-pVDZ) (Hartree): -223.19884838
 E(UHF/Aug-CC-pVDZ) (Hartree): -223.18185607
 E(CCS(DT)/Aug-CC-pVTZ) (Hartree): -224.12219893
 E(CCS(DT)/Aug-CC-pVTZ) (Hartree): -224.07365129
 T1 diagnostic: 0.032966
 E(MP2/Aug-CC-pVTZ) (Hartree): -224.06512280
 E(MP3/Aug-CC-pVTZ) (Hartree): -224.05990105
 E(PMP2/Aug-CC-pVTZ) (Hartree): -224.08000970
 E(PMP3/Aug-CC-pVTZ) (Hartree): -224.07083208
 E(PUHF/Aug-CC-pVTZ) (Hartree): -223.24956962
 E(UHF/Aug-CC-pVTZ) (Hartree): -223.23199040
 E(CCS(DT)/Aug-CC-pVQZ) (Hartree): -224.17885843
 E(CCS(DT)/Aug-CC-pVQZ) (Hartree): -224.12747138
 T1 diagnostic: 0.032998
 E(MP2/Aug-CC-pVQZ) (Hartree): -224.12707717
 E(MP3/Aug-CC-pVQZ) (Hartree): -224.11534754
 E(PMP2/Aug-CC-pVQZ) (Hartree): -224.14213255
 E(PMP3/Aug-CC-pVQZ) (Hartree): -224.12637915
 E(PUHF/Aug-CC-pVQZ) (Hartree): -223.26375408
 E(UHF/Aug-CC-pVQZ) (Hartree): -223.24599207
 E(UB3LYP/6-311++G(3df,2p)) (Hartree): -224.54039969
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.574960	0.100884	0.000001
H	0.964807	1.427527	0.000001
H	0.102780	1.535340	0.000005
N	0.578418	-0.557628	0.000002
O	1.657016	0.075887	-0.000002
N	-1.782063	-0.128822	-0.000002
H	-2.448441	0.629880	-0.000001

 Rotational constants (GHz): 53.6806100 4.8594700 4.4560800
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9800)

i947.7016	163.4030	424.7172
497.9231	633.2569	746.9881
786.0649	836.5147	1064.1906
1088.9556	1208.5788	1455.3809
1756.6417	2569.1515	3548.2463

 Zero-point correction (Hartree): 0.039008