

# Secondary Channels in the Thermal Decomposition of Monomethylhydrazine (CH<sub>3</sub>NHNH<sub>2</sub>)

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CH<sub>3</sub>NHNH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
C	-1.1799	-0.2405	-0.0023	263	355	421
N	0.0278	0.5683	-0.1206	781	904	980
N	1.2458	-0.1494	0.0542	1134	1136	1223
H	-2.0540	0.4155	-0.0378	1313	1447	1481
H	-1.2252	-0.8314	0.9295	1493	1521	1688
H	-1.2420	-0.9326	-0.8469	2928	3047	3090
H	0.0246	1.3178	0.5609	3401	3530	3548
H	1.1376	-0.9224	0.7139			
H	1.5235	-0.5358	-0.8416			
Rotational Constants (GHZ)				37.4502	9.5927	8.4925

TS1

Coordinates				Frequencies (cm-1)		
C	-1.2144	-0.2434	0.0362	-1515	232	271
N	0.0029	0.5435	-0.0809	369	640	790
N	1.2965	-0.4198	-0.0030	1035	1065	1165
H	-2.0915	0.3916	-0.1151	1307	1350	1446
H	-1.2513	-0.7282	1.0167	1478	1483	1502
H	-1.1941	-1.0193	-0.7282	2618	3023	3092
H	0.0611	1.3403	0.5415	3131	3396	3550
H	0.7394	0.4568	-0.9146			
H	1.9269	0.1536	0.5697			
Rotational Constants (GHZ)				35.7079	9.0049	7.8974

CH<sub>3</sub>NH<sub>2</sub>NH

Coordinates				Frequencies (cm-1)		
C	1.1877	-0.2587	-0.0259	263	355	417
N	-0.1102	0.4929	0.0474	787	857	908
N	-1.3216	-0.2740	-0.1339	1101	1135	1342
H	2.0386	0.4312	0.0177	1385	1427	1471
H	1.1789	-0.8212	-0.9569	1487	1498	1634
H	1.2202	-0.9510	0.8140	3014	3124	3161
H	-0.0811	1.0678	0.9065	3196	3381	3475
H	-0.1227	1.1661	-0.7185			
H	-1.3376	-0.8736	0.6982			
Rotational Constants (GHZ)				36.0732	9.3641	8.3310

## TS2

Coordinates				Frequencies (cm-1)		
C	-1.2082	0.2373	-0.0130	-1431	213	292
N	-0.1166	-0.7107	-0.0510	361	528	826
N	1.2552	0.2119	0.0319	918	993	1115
H	-1.2825	0.8618	-0.9228	1185	1418	1438
H	-2.1141	-0.3771	0.0349	1448	1505	1539
H	-1.2385	0.9123	0.8642	2632	2880	2904
H	0.8908	-0.4162	0.8656	3058	3511	3644
H	1.9265	-0.1257	-0.6443			
H	1.0964	1.2123	0.0140			
Rotational Constants (GHZ)				34.8336	9.0147	7.7849

CH<sub>3</sub>NNH<sub>3</sub>

Coordinates				Frequencies (cm-1)		
C	-1.1783	-0.1936	0.0000	278	332	412
N	-0.0492	0.6953	0.0002	752	1036	1065
N	1.0996	-0.1725	0.0000	1072	1132	1229
H	-2.0841	0.4164	-0.0034	1432	1449	1479
H	-1.2402	-0.8627	0.8929	1513	1585	1655
H	-1.2357	-0.8666	-0.8902	2757	2783	3015
H	1.1802	-0.7988	0.8311	3087	3089	3505
H	1.9261	0.4235	-0.0083			
H	1.1708	-0.8091	-0.8240			
Rotational Constants (GHZ)				37.0257	9.9881	8.6713

## TS3

Coordinates				Frequencies (cm-1)		
C	-1.1186	0.1751	-0.0672	-1276	519	583
N	0.0175	-0.5626	-0.0428	736	830	891
N	1.2014	0.0694	-0.0299	1005	1061	1125
H	-2.0376	-0.3321	0.2135	1209	1282	1366
H	-1.2053	0.9155	-0.8547	1397	1459	1510
H	-0.3504	1.2701	0.9188	1576	2042	3116
H	0.0095	-1.3566	0.5870	3212	3437	3551
H	0.5696	1.1666	0.8500			
H	1.1934	0.7384	-0.8023			
Rotational Constants (GHZ)				34.8028	10.9539	9.3941

CH<sub>2</sub>NH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
C	1.1800	-0.1719	-0.0001	479.9262	548.4486	652.6354
N	-0.0343	0.3317	0.0000	726.4482	969.2819	1066.274
N	-1.1681	-0.3264	0.0000	1232.3481	1375.927	1450.8423
H	2.0121	0.5120	0.0004	1494.408	1692.0453	3186.9038
H	1.2934	-1.2445	0.0001	3314.349	3404.518	3486.02
H	-0.0599	1.3544	0.0000			
H	-1.9087	0.3728	0.0000			
Rotational Constants (GHZ)				70.8610	11.1608	9.6421

H<sub>2</sub>

Coordinates				Frequencies (cm-1)		
H	0.0000	0.0000	0.3721	4418.7221		
H	0.0000	0.0000	-0.3721			
Rotational Constants (GHZ)				1811.2925		

## TS4

Coordinates				Frequencies (cm-1)		
C	-1.5745	-0.1877	0.0266	-1303	56	233
N	0.4266	0.6977	0.0327	378	493	626
N	1.3124	-0.2647	-0.0049	731	767	1079
H	-0.4427	0.5020	-0.6398	1161	1279	1383
H	1.5329	-0.7787	-0.8538	1417	1467	1690
H	1.6490	-0.6667	0.8632	2473	3038	3159
H	-1.5267	-0.3883	1.0897	3212	3438	3546
H	-2.3612	0.5204	-0.2315			
H	-1.5776	-1.0939	-0.5819			
Rotational Constants (GHZ)				34.6859	6.6868	6.0793

NNH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
N	0.7557	0.0000	0.0000	1024.236	1334.6141	1611.193
N	-0.4584	0.0000	0.0000	1746.3741	3003.8791	3036.9255
H	-1.0409	0.8677	0.0001			
H	-1.0409	-0.8677	0.0001			
Rotational Constants (GHZ)				333.0402	38.9311	34.8565

CH<sub>4</sub>

Coordinates				Frequencies (cm-1)		
C	0.0000	0.0000	0.0000	1339.948	1339.9483	1339.9487
H	0.6297	0.6297	0.6297	1558.3937	1558.3941	3025.4184
H	-0.6297	-0.6297	0.6297	3131.141	3131.1411	3131.1418
H	-0.6297	0.6297	-0.6297			
H	0.6297	-0.6297	-0.6297			
Rotational Constants (GHZ)				158.0586	158.0586	158.0586

## TS5

Coordinates				Frequencies (cm-1)		
N	0.1166	0.6330	-0.1841	-1072	217	476
H	0.0490	1.3355	0.5514	498	771	801
N	-1.1100	-0.2482	0.0229	921	1031	1050
H	-1.6031	-0.0788	0.9088	1152	1229	1402
H	-1.7758	-0.2076	-0.7587	1487	1525	1560
C	1.1846	-0.3373	0.0399	2132	3045	3129
H	1.8259	-0.4189	-0.8357	3297	3424	3458
H	1.7521	-0.1697	0.9586			
H	-0.4015	-1.1306	0.0650			
Rotational Constants (GHZ)				33.6735	10.0281	8.7201

CH<sub>2</sub>NH

Coordinates				Frequencies (cm-1)		
C	0.0561	0.5843	0.0000	1073	1105	1161
H	-0.8429	1.2121	0.0000	1370	1493	1708
H	1.0119	1.1113	0.0000	3011	3112	3432
N	0.0561	-0.6827	0.0000			
H	-0.8986	-1.0505	0.0000			
Rotational Constants (GHZ)				198.1566	34.9001	29.6738

NH<sub>3</sub>

Coordinates				Frequencies (cm-1)		
N	-0.0001	0.0000	-0.1090	1004	1668	1669
H	-0.9470	-0.0088	0.2544	3483	3609	3610
H	0.4662	0.8244	0.2541			
H	0.4815	-0.8156	0.2541			
Rotational Constants (GHZ)				300.2100	300.0133	186.3512

## TS6

Coordinates				Frequencies (cm-1)		
C	1.1923	0.2368	-0.0310	-1372	196	249
N	-0.0508	-0.5157	0.0516	458	615	856
N	-1.1994	0.0008	-0.2474	969	1110	1132
H	2.0428	-0.4290	0.1268	1239	1368	1403
H	1.2009	1.0234	0.7393	1454	1475	1493
H	1.2711	0.7052	-1.0127	1542	2331	2972
H	-0.0409	-1.3325	0.6592	3080	3126	3446
H	-1.2485	1.1475	0.0786			
H	-1.6283	1.0694	0.9651			
Rotational Constants (GHZ)				36.1148	9.6053	8.5491

CH<sub>3</sub>NHN

Coordinates				Frequencies (cm-1)		
C	-1.1356	-0.1541	0.0000	140	544	780
N	0.2742	0.3561	0.0000	837	1114	1142
N	1.2823	-0.3099	0.0000	1390	1470	1476
H	-1.6464	0.2176	-0.8917	1542	1667	2938
H	-1.6461	0.2165	0.8924	3031	3111	3163
H	-1.0856	-1.2407	-0.0006			
H	0.2959	1.4073	0.0000			
Rotational Constants (GHZ)				58.6373	10.62908	9.54307

CH<sub>3</sub>NHNH<sub>2</sub> (Roaming)

Coordinates				Frequencies (cm-1)		
C	-0.0066	-0.7119	-0.9376	-146	72	80
N	0.0802	0.6599	-1.3270	133	234	302
H	0.9731	-1.1789	-0.9640	355	945	1030
H	-0.3674	-0.7493	0.1052	1090	1343	1411
H	-0.7133	-1.2988	-1.5261	1482	1517	1549
H	-0.8671	0.9746	-1.5336	2881	3083	3168
N	-0.0828	0.0869	2.1094	3436	3483	3543
H	0.4615	0.7544	1.5592			
H	0.6282	-0.3969	2.6599			
Rotational Constants (GHZ)				3.8683	4.3494	24.2794

NHNH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
N	-0.7406	-0.1509	0.0230	513	695	1136
N	0.5952	0.0243	-0.0674	1236	1479	1669
H	-1.1508	0.7857	-0.0296	3418	3485	3635
H	1.0323	0.9017	0.1948			
H	1.1362	-0.8013	0.1455			
Rotational Constants (GHZ)				205.6241	30.6333	26.9976

CH<sub>3</sub>

Coordinates				Frequencies (cm-1)		
C	0.0000	0.0000	0.0000			
H	0.0000	1.0806	0.0000			
H	0.9358	-0.5403	0.0000			
H	-0.9358	-0.5403	0.0000			
Rotational Constants (GHZ)						

CH<sub>3</sub>NH

Coordinates				Frequencies (cm-1)		
C	0.6284	-0.0122	0.0000	253	951	1004
N	-0.8032	0.1531	0.0000	1044	1329	1392
H	1.1269	0.9588	-0.0005	1476	1483	2945
H	0.9683	-0.5833	0.8792	2978	3090	3384
H	0.9684	-0.5843	-0.8786			
H	-1.2119	-0.7896	0.0000			
Rotational Constants (GHZ)				125	25	24

NH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
N	0.0000	0.1424	0.0000	1507	3348	3440
H	0.8064	-0.4983	0.0000			
H	-0.8064	-0.4983	0.0000			
Rotational Constants (GHZ)				698.7633	385.5847	248.4742

TS1H

Coordinates				Frequencies (cm-1)		
N	0.1694	0.3183	-0.1756	-1064	223	497
H	0.2100	1.2969	-0.5026	572	634	744
H	1.1807	-0.4003	0.1343	966	1050	1147
C	-1.1668	-0.2529	0.0128	1160	1380	1410
H	-1.2737	-0.6329	1.0269	1459	1460	1511
H	-1.9014	0.5292	-0.1666	1593	3047	3130
H	-1.2707	-1.0778	-0.6966	3165	3277	3406
H	-0.2327	1.8963	0.7610			
H	2.0185	0.0794	-0.2100			
Rotational Constants (GHZ)				34.5671	10.0370	8.5880

trans-CH<sub>3</sub>NNH

Coordinates				Frequencies (cm-1)		
N	0.1924	-0.5006	0.0000	193	556	864
N	1.1207	0.3181	0.0000	928	1144	1171
C	-1.1305	0.1261	0.0000	1407	1469	1469
H	-1.6689	-0.2360	0.8802	1490	1658	3016
H	-1.0699	1.2183	0.0000	3096	3107	3279
H	-1.6689	-0.2360	-0.8802			
H	1.9989	-0.2254	0.0000			
Rotational Constants (GHZ)				60.8484	11.0603	9.9337

TS1M

Coordinates				Frequencies (cm-1)		
N	0.5512	0.5040	0.1264	-846	54	192
H	0.2603	1.1526	-0.5966	357	457	560
N	1.4820	-0.3347	-0.1875	643	844	935
H	1.6669	-0.9043	0.6424	1139	1348	1417
C	-1.7020	-0.1704	-0.0407	1429	1509	1670
H	-1.9743	-0.7159	0.8627	3038	3166	3193
H	-2.3553	0.6739	-0.2550	3282	3425	3582
H	-1.4998	-0.8139	-0.8920			
H	-0.1187	0.4451	0.9105			
Rotational Constants (GHZ)				37.6607	5.7496	5.3917



## trans-NHNH

Coordinates				Frequencies (cm-1)		
N	0.0000	-0.6194	0.0000	1346	1351	1591
H	-0.9897	-0.9218	0.0000	1653	3236	3267
N	0.0000	0.6194	0.0000			
H	0.9897	0.9218	0.0000			
Rotational Constants (GHZ)				304.2344	39.5731	35.0181

CH<sub>3</sub>NH<sub>2</sub>

Coordinates				Frequencies (cm-1)		
C	-0.7093	0.0000	0.0177	302	819	972
N	0.7503	0.0000	-0.1185	1054	1162	1341
H	-1.1166	0.8793	-0.4872	1459	1497	1517
H	-1.1166	-0.8790	-0.4876	1667	2963	3057
H	-1.0826	-0.0003	1.0527	3093	3507	3585
H	1.1595	0.8162	0.3229			
H	1.1595	-0.8162	0.3228			
Rotational Constants (GHZ)				103.8600	22.6806	21.7664

<sup>3</sup>NH

Coordinates				Frequencies (cm-1)		
N	0.0000	0.0000	0.1304			
H	0.0000	0.0000	-0.9131			
Rotational Constants (GHZ)						

## ISC1-CASSCF

Coordinates				Frequencies (cm-1)		
C	0.0000	-0.4376	-1.2284			
N	0.0000	0.6427	-0.2511			
H	0.8745	-1.0529	-1.0654			
H	-0.8745	-1.0529	-1.0654			
H	0.0000	-0.0780	-2.2552			
H	0.8121	1.2197	-0.3362			
H	-0.8121	1.2197	-0.3362			
N	0.0000	-0.3254	1.5220			
H	0.0000	0.5508	2.0350			
Rotational Constants (GHZ)						

## ISC1-MRCI

Coordinates

C	0.0022	-0.4637	-1.2145
N	-0.0021	0.6687	-0.2857
H	0.8364	-1.1214	-0.9411
H	-0.9181	-1.0368	-1.0475
H	0.0714	-0.1757	-2.2760
H	0.8509	1.2197	-0.3284
H	-0.8124	1.2725	-0.3925
N	-0.0034	-0.3208	1.5325
H	0.0208	0.5323	2.1313

Rotational Constants (GHZ)

Frequencies (cm-1)

## TS2H-a

Coordinates

C	1.1102	0.1283	0.0533	-1683	477	673
N	0.0416	-0.6953	-0.0435	768	856	1038
N	-1.0429	0.1371	0.0282	1081	1109	1131
H	2.0621	-0.3216	-0.2267	1227	1317	1369
H	1.2176	0.8236	0.9042	1444	1506	1530
H	0.6332	1.1361	-0.8015	1656	1667	2914
H	-0.4703	1.1597	-0.7472	3126	3295	3516
H	-1.9064	-0.3325	-0.2355			
H	-1.1882	0.6722	0.8944			

Rotational Constants (GHZ)

35.9836 11.3447 9.6121

CH<sub>2</sub>NNH<sub>2</sub>

Coordinates

C	-1.1554	0.1689	0.0083	429	515	639
N	-0.0818	-0.5158	0.0064	783	943	1065
N	1.1124	0.1430	-0.0903	1179	1309	1477
H	-2.0980	-0.3646	0.0317	1657	1691	3025
H	-1.1710	1.2640	-0.0204	3198	3446	3633
H	1.8655	-0.4108	0.2903			
H	1.1221	1.1080	0.2362			

Rotational Constants (GHZ)

65.7555 11.4119 9.8137

TS2H-b

Coordinates				Frequencies (cm-1)		
N	-0.0306	-0.6180	-0.1747	-924	179	288
N	1.0307	-0.0140	0.1898	503	654	721
H	1.9227	-0.4525	-0.0269	981	996	1091
H	1.7030	1.4034	-0.8765	1123	1306	1411
H	1.1017	0.9863	0.4505	1452	1475	1493
C	-1.2018	0.2017	0.0286	1662	2924	3000
H	-1.1683	1.0319	-0.7013	3137	3233	3546
H	-2.0920	-0.3961	-0.1569			
H	-1.2571	0.6415	1.0341			
Rotational Constants (GHZ)				36.4400	9.9204	8.7082

<sup>3</sup>NCH<sub>3</sub>

Coordinates				Frequencies (cm-1)		
C	0.0000	-0.5446	0.0000	961	961	1055
N	0.0000	0.8681	0.0000	1381	1418	1418
H	1.0298	-0.9365	0.0000	2931	2989	2989
H	-0.5149	-0.9365	0.8918			
H	-0.5149	-0.9365	-0.8918			
Rotational Constants (GHZ)				157.6111	27.9246	27.9245

ISC1-CASSCF

Coordinates				Frequencies (cm-1)		
C	0.0000	-0.4022	1.2521			
N	0.0000	0.7241	0.3761			
H	0.8901	-1.0326	1.1994			
H	0.0000	0.0729	2.2363			
H	-0.8901	-1.0326	1.1994			
N	0.0000	-0.1782	-1.4100			
H	0.0000	0.6402	-1.9830			
H	-0.8192	-0.7201	-1.6023			
H	0.8192	-0.7201	-1.6023			
Rotational Constants (GHZ)						

## ISC1-MRCI

Coordinates	Frequencies (cm-1)		
C	-0.3866	0.0001	-1.3078
N	0.7002	0.0088	-0.3714
H	-1.0072	0.9173	-1.3550
H	0.1908	-0.0250	-2.2496
H	-1.0361	-0.8987	-1.3148
N	-0.1768	0.0108	1.4594
H	0.6394	-0.1025	2.0618
H	-0.6559	-0.8902	1.4657
H	-0.7976	0.7268	1.8562
Rotational Constants (GHZ)			

CH<sub>3</sub>NNH<sub>2</sub>

Coordinates	Frequencies (cm-1)					
C	-1.1609	0.1567	0.0053	159	443	476
N	0.0615	-0.6133	-0.0374	636	957	1057
N	1.1345	0.1979	0.0822	1100	1279	1314
H	-2.0004	-0.5055	-0.2071	1426	1476	1480
H	-1.1652	0.9756	-0.7351	1652	2930	2982
H	-1.3156	0.6053	0.9983	3112	3409	3615
H	2.0072	-0.2625	-0.1361			
H	1.0680	1.1548	-0.2657			
Rotational Constants (GHZ)				46.7536	10.4536	9.0888

CH<sub>3</sub>NHNH

Coordinates	Frequencies (cm-1)					
C	-1.1748	-0.1676	0.0191	173	393	511
N	0.1387	0.4387	-0.0903	631	978	1125
N	1.1967	-0.3853	0.0130	1138	1292	1386
H	-1.9323	0.5541	-0.2930	1450	1477	1507
H	-1.3926	-0.5020	1.0415	1542	2997	3081
H	-1.2117	-1.0331	-0.6436	3123	3421	3494
H	0.2165	1.3961	0.2393			
H	2.0217	0.2165	0.0821			
Rotational Constants (GHZ)				48.2738	10.1162	8.8815



Coordinates				Frequencies (cm-1)		
C	-1.2306	-0.2539	0.0648	283	380	461
N	-0.0606	0.4668	-0.1250	623	730	874
N	1.1360	-0.2836	-0.0100	995	1174	1250
H	-2.1390	0.3300	0.1351	1333	1448	1507
H	-1.2485	-1.2513	-0.3517	1670	3145	3266
H	-0.0477	1.3680	0.3442	3422	3477	3576
H	1.8680	0.1801	-0.5348			
H	1.4225	-0.3859	0.9635			
Rotational Constants (GHZ)				48.3971	10.1566	8.9005