

Electronic Supplementary Information (ESI) for Physical Chemistry Chemical Physics.

Table S1. ω B97XD, and CCSD(T) calculated total energies at 0K, zero-point energy corrections (ZPE), ω B97XD/6-311+G** optimized Cartesian coordinates, unscaled vibrational frequencies (ν_i), moments of inertia (I_i), and rotational constants (B_i) of all species involved in the studied $N(^2D) + C_6H_6$ dissociation mechanisms.

Species, point group, electronic state	Energies, a.u.	i	I_i , a.u.	B_i , GHz	Cartesian coordinates, angstroms				ν_i , cm ⁻¹
					Atom	X	Y	Z	
N ² D	ZPE(ω B97XD/6-311+G**) = 0.000000 E(ω B97XD/6-311+G**) = - 54.474822 E(CCSD(T)/cc-pVDZ) = -54.372388 E(CCSD(T)/cc-pVTZ) = -54.413737	A B C							
H ² S	ZPE(ω B97XD/6-311+G**) = 0.000000 E(ω B97XD/6-311+G**) = - 0.5026683 E(CCSD(T)/cc-pVDZ) = -0.499278 E(CCSD(T)/cc-pVTZ) = -0.499810	A B C							
CH $C_{\infty v}$ ² Σ	ZPE(ω B97XD/6-311+G**) = 0.006484 E(ω B97XD/6-311+G**) = -	A B C	0.00000 4.20419 4.20419	429.3	C H	0.000000 0.000000	0.000000 0.000000	0.160755 -0.964527	2846

	38.473621 E(CCSD(T)/cc-pVDZ) = -38.379858 E(CCSD(T)/cc-pVTZ) = -38.410379								
NH ₂ C _{2v} ² B ₁	ZPE(ω B97XD/6-311+G**) = 0.019176 E(ω B97XD/6-311+G**) = - 55.8761271 E(CCSD(T)/cc-pVDZ) = -55.732670 E(CCSD(T)/cc-pVTZ) = -55.793602	A B C	2.55949 4.66395 7.22344	705.1 387.0 249.8	H N H	0.000000 0.000000 0.000000	0.804953 0.000000 -0.804953	-0.496053 0.141729 -0.496053	1506, 3408, 3504
HCN C _{∞v} ¹ Σ^+	ZPE(ω B97XD/6-311+G**) = 0.016458 E(ω B97XD/6-311+G**) = - 93.414274 E(CCSD(T)/cc-pVDZ) = -93.187539 E(CCSD(T)/cc-pVTZ) = -93.274805	A B C	0.00000 40.15915 40.15915	44.9	C H N	0.000000 0.000000 0.000000	0.000000 0.000000 0.000000	-0.496912 -1.564400 0.649410	765, 765, 2228, 3467
HNC C _{∞v} ¹ Σ^+	ZPE(ω B97XD/6-311+G**) = 0.015973 E(ω B97XD/6-311+G**) = - 93.393024 E(CCSD(T)/cc-pVDZ) = -93.163065 E(CCSD(T)/cc-pVTZ) =	A B C	0.00000 39.63020 39.63020	45.5	C N H	0.000000 0.000000 0.000000	0.000000 0.000000 0.000000	-0.738340 0.428946 1.427419	522, 522, 2123, 3843

	-93.251281								
C_2H_2 $D_{\infty h}$ $^1\Sigma_g^+$	ZPE(ω B97XD/6-311+G**) = 0.027186 E(ω B97XD/6-311+G**) = - 77.320062 E(CCSD(T)/cc-pVDZ) = -77.108631 E(CCSD(T)/cc-pVTZ) = -77.187356	A B C	0.00000 50.62058 50.62058	35.7	C H C H	0.000000 0.000000 0.000000 0.000000	0.000000 0.000000 0.000000 0.000000	-0.598659 -1.662905 0.598659 1.662905	682, 682, 768, 768, 2082, 3422, 3530
HCNH C_s $^2A'$	ZPE(ω B97XD/6-311+G**) = 0.026050 E(ω B97XD/6-311+G**) = -93.959317 E(CCSD(T)/cc-pVDZ) = -93.716405 E(CCSD(T)/cc-pVTZ) = -93.809107	A B C	4.34839 46.32768 50.67607	415.0 39.0 35.6	C H N H	0.000051 0.894400 0.000051 -0.895068	0.645788 1.280245 -0.583315 -1.071768	0.000000 0.000000 0.000000 0.000000	898, 980, 1185, 1824, 3052, 3495
C_4H_4N C_s $^2A''$	ZPE(ω B97XD/6-311+G**) = 0.068463 E(ω B97XD/6-311+G**) = - 209.488386 E(CCSD(T)/cc-pVDZ) = -208.931505 E(CCSD(T)/cc-pVTZ) = - 209.131673	A B C	179.67211 203.53533 383.20744	10.0 8.9 4.7	C C C C N H H H H	0.000000 -1.162051 -0.659200 0.787218 1.153386 -0.007415 -2.196029 -1.194419 1.528361	1.141671 0.265972 -0.993501 -0.827019 0.460541 2.225080 0.577269 -1.931341 -1.617527	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	496, 544, 689, 713, 830, 851, 885, 925, 949, 1052, 1097, 1101, 1219, 1299, 1370, 1467, 1587, 3225, 3230, 3251, 3273
C_5H_4 C_1	ZPE(ω B97XD/6-311+G**) = 0.067566	A B	169.50529 215.46843	10.6 8.4	C C	0.737716 -0.739269	0.868225 0.867178	-0.000000 0.000000	513, 589, 600, 687, 724, 824, 894, 912, 947, 1003, 1061,

³ A	E(ω B97XD/6-311+G**) = -192.751136 E(CCSD(T)/cc-pVDZ) = -192.227143 E(CCSD(T)/cc-pVTZ) = -192.406394	C	384.97373	4.7	C C C H H H H	-1.185644 0.001193 1.186264 1.351677 -1.354484 -2.204630 2.205878	-0.425132 -1.213978 -0.423740 1.759480 1.757550 -0.777789 -0.774567	0.000006 0.000003 -0.000008 0.000018 -0.000011 -0.000018 0.000011	1134, 1146, 1268, 1377, 1479, 1509, 3220, 3232, 3268, 3272
C ₅ H ₅ C _s ² A''	ZPE(ω B97XD/6-311+G**) = 0.078340 E(ω B97XD/6-311+G**) = -193.440410 E(CCSD(T)/cc-pVDZ) = -192.906161 E(CCSD(T)/cc-pVTZ) = -193.092876	A B C	193.16101 211.12572 404.28673	9.3 8.5 4.5	C C C C C H H H H H	-0.740625 -1.163746 0.000000 1.168590 0.735975 -1.366050 -2.184774 0.009404 2.192043 1.348205	0.938721 -0.364619 -1.183870 -0.339548 0.949905 1.821402 -0.715410 -2.266641 -0.684048 1.841164	-0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000	58, 500, 521, 688, 735, 829, 849, 910, 922, 929, 959, 1062, 1082, 1152, 1224, 1298, 1400, 1505, 1560, 3220, 3226, 3238, 3255, 3263
C ₆ H ₄ C _{2v} ¹ A ₁	ZPE(ω B97XD/6-311+G**) = 0.075681 E(ω B97XD/6-311+G**) = -230.876088 E(CCSD(T)/cc-pVDZ) = -230.258243 E(CCSD(T)/cc-pVTZ) = -230.476868	A B C	254.43804 314.28831 568.72635	7.1 5.7 3.2	C C C C C C H H H H	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	0.701891 1.456966 0.619842 -0.619842 -1.456966 -0.701891 1.224913 2.539093 -2.539093 -1.224913	1.051932 -0.132810 -1.230313 -1.230313 -0.132810 1.051932 2.002719 -0.135574 -0.135574 2.002719	392, 404, 454, 608, 627, 751, 847, 875, 938, 987, 1008, 1081, 1121, 1175, 1271, 1314, 1443, 1497, 1500, 2055, 3195, 3210, 3231, 3235
C ₅ H ₅ N	ZPE(ω B97XD/6-311+G**) =	A	296.51464	6.1	C	0.000000	1.137393	0.719365	386, 419, 620, 673, 718, 766,

C _{2v} 1A ₁	0.089341	B	308.00489	5.9	C	0.000000	-1.137393	0.719365	902, 971, 1022, 1023, 1024, 1057, 1090, 1107, 1174, 1254, 1294, 1386, 1485, 1527, 1655, 1661, 3173, 3176, 3202, 3221, 3228
	E(ω B97XD/6-311+G**) = -	C	604.51953	3.0	C	0.000000	-1.193179	-0.669825	
	248.255864				C	0.000000	0.000000	-1.379287	
	E(CCSD(T)/cc-pVDZ) =				C	0.000000	1.193179	-0.669825	
	-247.592802				H	0.000000	2.052906	1.304442	
	E(CCSD(T)/cc-pVTZ) = -				H	0.000000	-2.052906	1.304442	
	247.831796				H	0.000000	-2.150493	-1.177133	
					H	0.000000	0.000000	-2.463703	
					H	0.000000	2.150493	-1.177133	
					N	0.000000	0.000000	1.412904	
C ₅ H ₅ CN C _s 1A'	ZPE(ω B97XD/6-311+G**) =	A	265.7339	6.8	C	0.377863	-1.655652	0.734410	124, 169, 386, 488, 530, 601, 704, 734, 814, 836, 902, 979, 982, 1002, 1040, 1047, 1110, 1134, 1217, 1282, 1304, 1399, 1600, 1675, 2394, 3045, 3221, 3232, 3258, 3262
	0.092190	B	852.7411	2.1	C	0.377863	-1.655652	-0.734410	
	E(ω B97XD/6-311+G**) =	C	1016.2205	1.8	C	0.377863	-0.395164	-1.184103	
	-286.306814				C	-0.658614	1.534488	0.000000	
	E(CCSD(T)/cc-pVDZ) =				C	0.417030	0.544255	0.000000	
	-285.553774				C	0.377863	-0.395164	1.184103	
	E(CCSD(T)/cc-pVTZ) = -				H	0.377641	-2.546639	1.348116	
	285.824384				H	0.377641	-2.546639	-1.348116	
					H	0.368598	-0.054349	-2.209222	
					H	1.370357	1.091896	0.000000	
					H	0.368598	-0.054349	2.209222	
					N	-1.497435	2.321059	0.000000	
C ₄ H ₄ NCCH C _{2v} 1A ₁	ZPE(ω B97XD/6-311+G**) =	A	198.14813	9.1	C	0.000000	1.128218	-0.501044	135, 172, 467, 558, 574, 613, 619, 621, 709, 729, 745, 872, 887, 915, 976, 1070, 1097, 1121, 1289, 1335, 1355, 1450, 1538,1603, 2285, 3256, 3269, 3297, 3301, 3490
	0.091914	B	874.71503	2.1	C	0.000000	0.714231	-1.799656	
	E(ω B97XD/6-311+G**) = -	C	1072.8632	1.7	C	0.000000	-0.714231	-1.799656	
	286.266271				C	0.000000	-1.128218	-0.501044	
	E(CCSD(T)/cc-pVDZ) =				C	0.000000	0.000000	1.651734	
	-285.499866				C	0.000000	0.000000	2.849742	

	E(CCSD(T)/cc-pVTZ) = - 285.778012				H H H H H N	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	2.109094 1.360138 -1.360138 -2.109094 0.000000 0.000000	-0.055176 -2.663594 -2.663594 -0.055176 3.912474 0.303516	
C ₆ H ₅ N C _s ³ A''	ZPE(ω B97XD/6-311+G**) = 0.091635 E(ω B97XD/6-311+G**) = - 286.270401 E(CCSD(T)/cc-pVDZ) = -285.505359 E(CCSD(T)/cc-pVTZ) = -285.776201	A B C	322.04769 617.85387 939.90156	5.6 2.9 1.9	C C C C C C H H H H H N	-0.000048 -1.212144 -1.228495 -0.000000 1.228483 1.212080 -0.000074 -2.147948 -2.159712 2.159713 2.147860 0.000130	-1.738386 -1.041536 0.336818 1.064851 0.336753 -1.041599 -2.822024 -1.588738 0.890344 0.890256 -1.588841 2.388228	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	208, 380, 400, 484, 528, 620, 670, 760, 829, 843, 916, 980, 995, 1005, 1039, 1104, 1174, 1179, 1285, 1312, 1343, 1456, 1473, 1585, 1612, 3192, 3200, 3212, 3219, 3223
C ₆ H ₆ D _{6h} ¹ A _{1g}	ZPE(ω B97XD/6-311+G**) = 0.101186 E(ω B97XD/6-311+G**) = - 232.220915 E(CCSD(T)/cc-pVDZ) = -231.579882 E(CCSD(T)/cc-pVTZ) = - 231.805638	A B C	314.80040 314.80040 629.60081	5.7 5.7 2.9	C C C C C C H H H H	0.000000 1.204418 1.204418 0.000000 -1.204418 -1.204418 0.000000 2.143557 2.143557 0.000000	1.390742 0.695371 -0.695371 -1.390742 -0.695371 0.695371 2.475166 1.237583 -1.237583 -2.475166	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	412, 412, 625, 625, 691, 726, 874, 874, 1004, 1004, 1024, 1026, 1031, 1072, 1072, 1182, 1210, 1210, 1341, 1387, 1525, 1525, 1668, 1668, 3186, 3196, 3196, 3213, 3213, 3224

					H	-2.143557	-1.237583	0.000000	
					H	-2.143557	1.237583	0.000000	
i1	ZPE(ω B97XD/6-311+G**) =	A	384.99028	4.7	C	-1.006712	1.223719	-0.032659	108, 211, 312, 416, 545, 584,
C ₁	0.100758	B	587.65636	3.1	C	-1.693966	-0.000004	-0.205544	591, 682, 757, 824, 866, 959,
² A	E(ω B97XD/6-311+G**) = -	C	867.49151	2.1	C	-1.006703	-1.223723	-0.032657	983, 988, 996, 998, 1051,
	286.797519				C	0.317176	-1.258464	0.281704	1105, 1181, 1205, 1230, 1276,
	E(CCSD(T)/cc-pVDZ) =				C	0.317172	1.258468	0.281702	1344, 1398, 1454, 1549, 1606,
	-286.028658				H	-1.550744	2.156313	-0.138285	2968, 3191, 3195, 3213, 3217,
	E(CCSD(T)/cc-pVTZ) = -				H	-2.746931	-0.000008	-0.458099	3225
	286.299122				H	-1.550730	-2.156320	-0.138283	
					H	0.837121	-2.200855	0.407311	
					H	0.837111	2.200862	0.407312	
					C	1.145103	0.000003	0.383070	
					H	1.763492	0.000005	1.295851	
					N	1.996894	0.000001	-0.775644	
i2	ZPE(ω B97XD/6-311+G**) =	A	389.00510	4.6	C	0.235585	0.253636	1.425856	254, 254, 444, 514, 617, 626,
C _s	0.103673	B	493.16866	3.7	C	0.034971	-1.042752	0.761682	702, 761, 798, 848, 937, 951,
² A'	E(ω B97XD/6-311+G**) = -	C	778.51021	2.3	C	0.034971	-1.042752	-0.761682	989, 999, 1010, 1021, 1029,
	286.844564				C	0.235585	0.253636	-1.425856	1094, 1198, 1208, 1220, 1333,
	E(CCSD(T)/cc-pVDZ) =				C	0.235585	1.400400	-0.725897	1366, 1407, 1461, 1638, 1715,
	-286.074352				C	0.235585	1.400400	0.725897	3139, 3147, 3192, 3201, 3215,
	E(CCSD(T)/cc-pVTZ) = -				H	0.401267	0.251822	2.497037	3222
	286.349640				H	0.358492	-1.933125	1.295913	
					H	0.358492	-1.933125	-1.295913	
					H	0.401267	0.251822	-2.497037	
					H	0.355028	2.347220	-1.240439	
					H	0.355028	2.347220	1.240439	
					N	-1.186179	-1.238178	0.000000	

i3	ZPE(ω B97XD/6-311+G**) =	A	378.35400	4.8	C	-1.340097	0.846859	0.186010	196, 310, 448, 535, 591, 607,
C ₁	0.104214	B	509.43419	3.5	C	-1.515627	-0.594858	0.094263	682, 789, 808, 843, 916, 936,
2A	E(ω B97XD/6-311+G**) = -	C	795.82714	2.3	C	-0.488037	-1.419491	-0.190993	945, 999, 1009, 1019, 1045,
	286.825024				C	0.829333	-0.835581	-0.350907	1127, 1138, 1201, 1212, 1325,
	E(CCSD(T)/cc-pVDZ) =				C	1.020873	0.635494	-0.396360	1418, 1419, 1480, 1603, 1693,
	-286.051836				C	-0.166065	1.445322	-0.086758	3141, 3178, 3186, 3202, 3209,
	E(CCSD(T)/cc-pVTZ) =				H	-2.212936	1.450500	0.410448	3534
	-286.329669				H	-2.512732	-1.000164	0.232790	
					H	-0.633930	-2.487286	-0.310149	
					H	2.585625	-0.337737	0.552916	
					H	1.746400	1.052848	-1.089739	
					H	-0.099136	2.526634	-0.150202	
					N	1.583490	-0.238752	0.688916	
i4	ZPE(ω B97XD/6-311+G**) =	A	323.74504	5.6	C	0.021119	-1.800634	0.000000	196, 389, 425, 487, 538, 620,
C _s	0.104286	B	650.74160	2.8	C	1.228307	-1.092815	0.000000	664, 687, 771, 834, 839, 917,
2A''	E(ω B97XD/6-311+G**) = -	C	974.48663	1.9	C	1.226875	0.284278	0.000000	990, 994, 1004, 1037, 1100,
	286.922642				C	0.000000	1.016441	0.000000	1172, 1178, 1189, 1327, 1340,
	E(CCSD(T)/cc-pVDZ) =				C	-1.217377	0.265053	0.000000	1369, 1481, 1500, 1593, 1611,
	-286.148113				C	-1.197276	-1.112272	0.000000	3188, 3199, 3207, 3218, 3226,
	E(CCSD(T)/cc-pVTZ) = -				H	0.028757	-2.884573	0.000000	3486
	286.424791				H	2.168473	-1.632664	0.000000	
					H	2.148662	0.854046	0.000000	
					H	-0.880486	2.735211	0.000000	
					H	-2.161337	0.801672	0.000000	
					H	-2.129112	-1.666601	0.000000	
					N	0.065023	2.347514	0.000000	
i5	ZPE(ω B97XD/6-311+G**) =	A	317.43597	5.7	C	-1.703545	0.022312	-0.520268	154, 254, 447, 461, 569, 625,
C ₁	0.101840	B	698.96716	2.6	C	-1.066038	-1.135966	-0.102110	686, 711, 747, 801, 835, 918,

² A	E(ω B97XD/6-311+G**) = - 286.844014 E(CCSD(T)/cc-pVDZ) = -286.069679 E(CCSD(T)/cc-pVTZ) = - 286.347052	C	813.39824	2.2	C C C C H H H H H N H	0.142988 1.181819 0.158133 -1.044232 -2.586781 -1.360897 0.441636 0.475995 -1.326517 2.246878 2.613663	-0.800104 -0.028026 0.773039 1.157382 0.040051 -2.149287 -1.396577 1.339260 2.182382 -0.109598 0.819537	0.687597 -0.015655 0.708358 -0.066507 -1.146002 -0.335562 1.544198 1.578560 -0.262573 -0.663925 -0.879634	931, 936, 981, 1011, 1028, 1069, 1072, 1115, 1228, 1258, 1286, 1323, 1401, 1474, 1866, 3162, 3168, 3216, 3241, 3251, 3477
i6 C ₁ ² A	ZPE(ω B97XD/6-311+G**) = 0.101376 E(ω B97XD/6-311+G**) = - 286.842254 E(CCSD(T)/cc-pVDZ) = -286.074093 E(CCSD(T)/cc-pVTZ) = -286.350064	A B C	249.15872 914.80256 1092.1974	7.2 2.0 1.7	C C C C C C H H H H H N H	1.793033 1.793049 0.578515 -1.544450 -0.321620 0.578489 2.648907 2.648935 0.253545 -0.640791 0.253499 -2.757437 -3.124135	-0.733561 0.733537 1.178549 0.000023 0.000012 -1.178546 -1.348455 1.348413 2.205995 0.000014 -2.205986 -0.000003 -0.000047	-0.181424 -0.181424 0.168544 -0.428972 0.442469 0.168545 -0.427720 -0.427722 0.253282 1.499154 0.253285 -0.254519 0.704922	56, 128, 322, 389, 493, 555, 715, 719, 750, 819, 839, 895, 942, 977, 977, 1007, 1025, 1036, 1111, 1131, 1218, 1231, 1310, 1404, 1592, 1673, 1895, 2977, 3217, 3229, 3253, 3258, 3353
i7 C _s ² A''	ZPE(ω B97XD/6-311+G**) = 0.103644 E(ω B97XD/6-311+G**) = - 286.830507	A B C	342.26708 481.11868 710.89611	5.3 3.8 2.5	C C C C	0.005166 0.699202 0.005166 0.005166	-0.537034 -1.248082 -0.537034 0.937149	1.099101 0.000000 -1.099101 -1.179650	313, 366, 541, 565, 596, 663, 693, 705, 810, 814, 883, 948, 969, 1003, 1032, 1042, 1118, 1122, 1155, 1168, 1250, 1266,

	E(CCSD(T)/cc-pVDZ) = -286.058067 E(CCSD(T)/cc-pVTZ) = - 286.335071				C C H H H H H H N	-0.006426 0.005166 -0.091980 1.302785 -0.091980 -0.012445 -0.029081 -0.012445 -0.763643	1.657145 0.937149 -1.072958 -2.145376 -1.072958 1.412710 2.740651 1.412710 -1.218649	0.000000 1.179650 2.037727 0.000000 -2.037727 -2.151968 0.000000 2.151968 0.000000	1343, 1385, 1472, 1489, 1537, 3183, 3184, 3205, 3211, 3227, 3236
i8 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.103041 E(ω B97XD/6-311+G**) = - 286.811832 E(CCSD(T)/cc-pVDZ) = -286.040039 E(CCSD(T)/cc-pVTZ) = - 286.316918	A B C	376.81811 493.98962 781.72558	4.8 3.7 2.3	C C C C C C H H H H H H N	-0.313324 1.588833 0.972468 -0.306379 -1.416544 -1.430948 -0.303189 2.606938 1.573043 -0.320934 -2.346789 -2.375256 0.943078	-1.406266 -0.050911 0.745620 1.432097 0.734222 -0.721808 -2.474093 -0.204575 1.144743 2.515796 1.249713 -1.248046 -0.768751	-0.159243 0.692363 -0.371712 -0.084797 0.188452 0.102480 -0.343290 1.029519 -1.187405 -0.133044 0.398230 0.173642 -0.306130	198, 262, 423, 504, 599, 621, 653, 727, 779, 817, 875, 955, 965, 982, 1001, 1033, 1061, 1089, 1123, 1201, 1218, 1330, 1388, 1429, 1466, 1651, 1721, 3128, 3191, 3198, 3203, 3214, 3227
i9 C_s $^2A''$	ZPE(ω B97XD/6-311+G**) = 0.102921 E(ω B97XD/6-311+G**) = - 286.830972 E(CCSD(T)/cc-pVDZ) = -286.057554	A B C	314.41508 619.60099 934.01607	5.7 2.9 1.9	C N C C C C	1.200756 0.000000 -1.188281 -1.180403 0.028184 1.221900	0.309498 1.032798 0.281869 -1.082495 -1.793431 -1.053195	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	155, 401, 446, 469, 543, 643, 646, 697, 729, 805, 838, 856, 969, 978, 997, 1040, 1085, 1147, 1197, 1234, 1319, 1332, 1377, 1462, 1487, 1550, 1631, 2966, 3216, 3223, 3239, 3244,

	E(CCSD(T)/cc-pVTZ) = - 286.333881				H H H H H C H 0.982638	2.076682 -2.092949 -2.130811 0.040179 2.183405 0.068868 - 0.982638	0.941287 0.873550 -1.602369 -2.875037 -1.551481 2.380593 2.727423	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	3258
i10 C ₁ ²A	ZPE(ω B97XD/6-311+G**) = 0.104932 E(ω B97XD/6-311+G**) = - 286.888755 E(CCSD(T)/cc-pVDZ) = - 286.109459 E(CCSD(T)/cc-pVTZ) = -286.388922	A B C	297.54927 697.83813 993.86070	6.1 2.6 1.8	C C C C C H H H H H N H	1.864457 1.199468 -0.167235 -0.967709 -0.274596 1.115338 2.947686 1.750958 -2.758556 -0.838552 1.619253 -2.357227 -2.838536	0.009946 -1.221434 -1.197092 -0.069255 1.150762 1.181153 0.044703 -2.155593 -1.000028 2.079425 2.141141 -0.129553 0.672735	0.007992 0.003554 -0.005462 -0.010186 -0.006292 0.003911 0.014738 0.007921 0.237172 -0.016278 0.007484 -0.073356 0.301347	214, 290, 375, 412, 514, 529, 587, 633, 693, 742, 837, 845, 936, 984, 986, 1053, 1072, 1156, 1185, 1282, 1332, 1343, 1482, 1506, 1605, 1659, 1686, 3175, 3192, 3206, 3221, 3612, 3716
i11 C ₁ ²A	ZPE(ω B97XD/6-311+G**) = 0.102121 E(ω B97XD/6-311+G**) = - 286.884648 E(CCSD(T)/cc-pVDZ) = -286.114242 E(CCSD(T)/cc-pVTZ) =	A B C	242.42339 882.32490 1124.7483	7.4 2.0 1.6	C C C C C C H	-1.967335 -1.686499 -0.346470 1.676848 0.268441 -0.777083 -2.956048	-0.509683 0.936431 1.110816 -0.527339 -0.216025 -1.185468 -0.948670	0.000078 -0.000004 -0.000084 -0.000113 -0.000067 0.000028 0.000175	106, 214, 239, 485, 522, 544, 571, 717, 722, 735, 828, 901, 918, 936, 1000, 1034, 1103, 1117, 1143, 1260, 1296, 1310, 1417, 1451, 1467, 1589, 1596, 3118, 3236, 3243, 3257, 3265, 3486

	-286.390223				H	-2.439098	1.712417	-0.000022	
					H	0.180180	2.054350	-0.000192	
					H	1.930713	-1.589583	-0.000372	
					H	-0.634526	-2.256409	0.000074	
					N	2.656775	0.301586	0.000134	
					H	2.313943	1.264407	0.000372	
i12	ZPE(ω B97XD/6-311+G**) =	A	451.30839	4.0	C	0.000000	0.677580	-1.463316	157, 230, 410, 476, 535, 544,
C_{2v}	0.103113	B	482.65129	3.7	C	0.000000	-0.677580	-1.463316	663, 695, 793, 858, 876, 898,
2B_1	E(ω B97XD/6-311+G**) = -	C	933.95968	1.9	C	0.000000	-1.538754	-0.313555	922, 992, 1003, 1004, 1031,
	286.888327				C	0.000000	-1.186895	1.016327	1040, 1240, 1267, 1318, 1431,
	E(CCSD(T)/cc-pVDZ) =				C	0.000000	1.186895	1.016327	1489, 1492, 1549, 1609, 1673,
	-286.114231				C	0.000000	1.538754	-0.313555	3144, 3147, 3177, 3190, 3198,
	E(CCSD(T)/cc-pVTZ) = -				H	0.000000	1.174643	-2.428660	3209
	286.390514				H	0.000000	-1.174643	-2.428660	
					H	0.000000	-2.605379	-0.512997	
					H	0.000000	-2.024512	1.713172	
					H	0.000000	2.024512	1.713172	
					H	0.000000	2.605379	-0.512997	
					N	0.000000	0.000000	1.654785	
i13	ZPE(ω B97XD/6-311+G**) =	A	311.71811	5.8	C	0.324161	-0.789125	0.510690	243, 265, 472, 357, 627, 659,
C_1	0.103017	B	534.86529	3.4	C	-0.998743	-1.139540	-0.084204	725, 753, 804, 850, 908, 923,
2A	E(ω B97XD/6-311+G**) =	C	734.20616	2.5	C	-1.694790	0.033125	-0.327009	936, 945, 1025, 1055, 1077,
	-286.838254				C	-0.930128	1.132095	0.036989	1113, 1120, 1199, 1232, 1294,
	E(CCSD(T)/cc-pVDZ) =				C	1.458253	0.698859	-0.278338	1297, 1346, 1400, 1484, 1641,
	-286.064316				C	1.560201	-0.626956	-0.373151	3050, 3224, 3230, 3253, 3264,
	E(CCSD(T)/cc-pVTZ) = -				H	0.520922	-1.256877	1.482353	3268
	286.341699				H	-1.354733	-2.147367	-0.239088	
					H	-2.693803	0.095199	-0.739177	

					H	-1.157576	2.182791	-0.065263	
					H	1.984923	1.571896	-0.641128	
					H	2.270710	-1.318487	-0.799449	
					N	0.302262	0.717442	0.584557	
i14	ZPE(ω B97XD/6-311+G**) =	A	221.75223	8.1	C	0.300711	1.071109	0.000002	81, 217, 235, 514, 588, 623,
C ₁	0.102010	B	830.84718	2.2	C	1.658351	0.912913	-0.000005	641, 641, 702, 745, 813, 861,
² A	E(ω B97XD/6-311+G**) = -	C	1052.5994	1.7	C	1.926834	-0.487586	-0.000007	862, 891, 908, 1003, 1083,
	286.844788				C	0.721417	-1.130476	-0.000002	1101, 1121, 1258, 1308, 1342,
	E(CCSD(T)/cc-pVDZ) =				C	-1.646086	-0.465848	0.000008	1418, 1459, 1543, 1596, 1710,
	-286.072465				C	-2.620492	0.411632	-0.000001	3121, 3258, 3266, 3278, 3288,
	E(CCSD(T)/cc-pVTZ) = -				H	-0.314627	1.956591	0.000006	3304
	286.350009				H	2.385271	1.710189	-0.000007	
					H	2.895426	-0.962418	-0.000012	
					H	0.478675	-2.181493	-0.000002	
					H	-1.862956	-1.535050	0.000020	
					H	-3.697270	0.392747	0.000001	
					N	-0.275562	-0.178718	0.000004	
i15	ZPE(ω B97XD/6-311+G**) =	A	328.15801	5.50	C	-0.344677	0.799672	0.584632	241, 272, 463, 521, 662, 689,
C ₁	0.103177	B	542.96037	3.32	C	0.985676	1.151443	-0.001080	722, 790, 859, 886, 920, 931,
² A	E(ω B97XD/6-311+G**) = -	C	726.64487	2.48	C	1.672504	-0.009038	-0.334026	966, 990, 1008, 1052, 1072,
	286.854415				C	0.949711	-1.148531	-0.011781	1097, 1192, 1204, 1248, 1280,
	E(CCSD(T)/cc-pVDZ) = -				C	-1.465367	0.577333	-0.413634	1316, 1332, 1407, 1480, 1677,
	286.085152				H	-0.610283	1.324913	1.505264	3086, 3099, 3147, 3206, 3231,
	E(CCSD(T)/cc-pVTZ) = -				H	1.335642	2.161551	-0.166157	3242
	286.359689				H	2.647583	-0.020620	-0.806728	
					H	1.256448	-2.168471	-0.198359	
					H	-2.087680	1.253634	-0.999051	
					N	-1.491397	-0.700311	-0.447623	

					C	-0.369862	-0.762558	0.564422	
					H	-0.669838	-1.298750	1.467190	
i16	ZPE(ω B97XD/6-311+G**) =	A	257.21054	7.0	C	-0.362286	-1.710001	0.733900	95, 128, 314, 388, 517, 567,
C_s	0.101745	B	872.75954	2.1	C	-0.362286	-0.444330	1.178047	736, 740, 817, 840, 860, 933,
$^2A'$	E(ω B97XD/6-311+G**) = -	C	1041.9634	1.7	C	-0.356404	0.493843	0.000000	979, 982, 1010, 1040, 1044,
	286.862509				C	0.900666	1.357274	0.000000	1110, 1128, 1180, 1252, 1266,
	E(CCSD(T)/cc-pVDZ) =				C	-0.362286	-0.444330	-1.178047	1310, 1402, 1583, 1665, 1737,
	-286.098098				C	-0.362286	-1.710001	-0.733900	3019, 3082, 3214, 3225, 3247,
	E(CCSD(T)/cc-pVTZ) = -				H	-0.367403	-2.601090	1.348289	3252
	286.371129				H	-0.358217	-0.108197	2.205684	
					H	-1.231402	1.152674	0.000000	
					H	1.856680	0.812808	0.000000	
					H	-0.358217	-0.108197	-2.205684	
					H	-0.367403	-2.601090	-1.348289	
					N	0.893607	2.599767	0.000000	
i17	ZPE(ω B97XD/6-311+G**) =	A	315.88932	5.71321	C	-1.672432	0.013139	-0.509597	145, 271, 410, 470, 561, 636,
C_1	0.100447	B	660.73671	2.73141	C	-1.028488	-1.139536	-0.087645	698, 721, 754, 799, 825, 869,
2A	E(ω B97XD/6-311+G**) = -	C	772.89813	2.33503	C	0.173434	-0.770792	0.690788	928, 958, 978, 1010, 1057,
	286.771718				C	0.174725	0.762818	0.705417	1092, 1095, 1160, 1177, 1282,
	E(CCSD(T)/cc-pVDZ) = -				C	-1.016661	1.156577	-0.060469	1318, 1332, 1414, 1475, 1597,
	285.996870				H	-2.551895	0.024174	-1.140705	2956, 3188, 3199, 3220, 3244,
	E(CCSD(T)/cc-pVTZ) = -				H	-1.311258	-2.156256	-0.318632	3254
	286.273167				H	0.546117	-1.371500	1.512685	
					H	0.576811	1.346310	1.524842	
					H	-1.300590	2.179448	-0.262249	
					H	2.595636	0.886815	-0.968218	
					N	1.172389	-0.031229	-0.049684	
					C	2.242497	-0.137270	-0.738483	

i18	ZPE(ω B97XD/6-311+G**) =	A	282.69762	6.38400	C	1.784132	-0.522465	-0.353318	74, 178, 257, 419, 538, 571,
C ₁	0.101497	B	790.35057	2.28347	C	1.550152	0.923620	-0.189349	665, 707, 739, 810, 853, 905,
² A	E(ω B97XD/6-311+G**) = -	C	966.58858	1.86712	C	0.326872	1.123633	0.313947	975, 977, 990, 1030, 1062,
	286.832894				C	-0.316470	-0.215845	0.580761	1105, 1112, 1149, 1245, 1294,
	E(CCSD(T)/cc-pVDZ) = -				C	0.702734	-1.196599	0.053098	1319, 1402, 1607, 1679, 1863,
	286.066457				H	2.695697	-0.954850	-0.745002	3018, 3062, 3215, 3226, 3250,
	E(CCSD(T)/cc-pVTZ) = -				H	2.267612	1.692110	-0.447144	3255
	286.341537				H	-0.151255	2.066593	0.538203	
					H	-0.381184	-0.358849	1.670363	
					H	0.546813	-2.266003	0.053277	
					H	-3.384466	0.140478	-0.886701	
					N	-1.653834	-0.451622	0.056128	
					C'	-2.383484	0.361302	-0.501121	
TS1	ZPE(ω B97XD/6-311+G**) =	A	393.38265	4.6	C	0.838702	1.297746	-0.014477	282 <i>i</i> , 179, 274, 401, 554, 575,
C ₁	0.100429	B	558.91899	3.2	C	1.649165	0.188241	0.202254	591, 686, 755, 831, 880, 953,
² A	E(ω B97XD/6-311+G**) = -	C	828.40774	2.2	C	1.113162	-1.129014	0.052611	966, 981, 993, 997, 1046,
	286.796505				C	-0.185188	-1.335059	-0.261601	1128, 1168, 1191, 1231, 1285,
	E(CCSD(T)/cc-pVDZ) =				C	-0.491925	1.153662	-0.366498	1344, 1396, 1452, 1524, 1627,
	-286.026964				H	1.257598	2.294476	0.069541	3018, 3192, 3196, 3213, 3225,
	E(CCSD(T)/cc-pVTZ) = -				H	2.691540	0.316715	0.466457	3231
	286.297771				H	1.774734	-1.980186	0.173445	
					H	-0.580777	-2.337263	-0.379564	
					H	-1.116752	2.017903	-0.552618	
					C	-1.156867	-0.190775	-0.388126	
					H	-1.869297	-0.333299	-1.211406	
					N	-1.822764	0.016122	0.869881	
TS2	ZPE(ω B97XD/6-311+G**) =	A	382.06117	4.7	C	-1.254973	0.918869	0.177101	1912 <i>i</i> , 240, 316, 444, 548, 591,
C ₁	0.099587	B	498.90167	3.6	C	-1.543505	-0.501064	0.089307	631, 701, 767, 802, 836, 934,

² A	E(ω B97XD/6-311+G**) = - 286.766736 E(CCSD(T)/cc-pVDZ) = -285.996246 E(CCSD(T)/cc-pVTZ) = - 286.273472	C	780.14691	2.3	C C C C H H H H H H N	-0.578341 0.774713 1.108974 -0.045169 -2.075714 -2.572479 -0.784512 1.951258 1.871544 0.086474 1.536176	-1.395481 -0.875107 0.572177 1.435150 1.590264 -0.826614 -2.442575 -1.174187 0.937609 2.509334 -0.217299	-0.197404 -0.291616 -0.405348 -0.123827 0.404754 0.199651 -0.378220 0.118284 -1.087125 -0.196868 0.778607	942, 982, 994, 1005, 1014, 1095, 1155, 1187, 1221, 1332, 1385, 1422, 1466, 1609, 1692, 2425, 3152, 3189, 3198, 3213, 3226
TS3 C ₁ ² A	ZPE(ω B97XD/6-311+G**) = 0.101601 E(ω B97XD/6-311+G**) = - 286.816189 E(CCSD(T)/cc-pVDZ) = - 286.040337 E(CCSD(T)/cc-pVTZ) = - 286.319052	A B C	354.25540 556.91681 853.72639	5.1 3.2 2.1	C C C C C C H H H H H H N	1.543496 1.469854 0.218729 -0.855860 -0.797751 0.445035 2.514335 2.378235 0.094567 -2.769197 -1.438496 0.537348 -1.922545	-0.600439 0.808704 1.430968 0.590666 -0.825723 -1.421979 -1.038591 1.397004 2.489550 -0.008482 -1.372464 -2.492323 0.161732	0.149876 -0.033804 -0.097177 -0.278268 -0.365101 0.079061 0.358152 0.020371 0.102234 -0.025644 -1.050630 0.221754 0.520893	567 <i>i</i> , 209, 366, 441, 537, 574, 637, 702, 765, 783, 862, 906, 925, 994, 1006, 1025, 1077, 1088, 1154, 1163, 1208, 1298, 1357, 1427, 1451, 1553, 1654, 3160, 3188, 3197, 3209, 3217, 3465
TS4 C ₁ ² A	ZPE(ω B97XD/6-311+G**) = 0.100711 E(ω B97XD/6-311+G**) = - 286.828121	A B C	307.92586 697.78865 895.23026	5.9 2.6 2.0	C C C C	-1.781250 -1.127456 0.202333 1.132238	0.008937 -1.135641 -0.970659 -0.058303	-0.401260 -0.049157 0.527700 -0.076682	667 <i>i</i> , 172, 306, 420, 493, 557, 610, 711, 743, 775, 827, 881, 890, 934, 978, 991, 1058, 1089, 1115, 1135, 1232, 1283,

	E(CCSD(T)/cc-pVDZ) = -286.052908 E(CCSD(T)/cc-pVTZ) = - 286.331424				C C H H H H H N H	0.248305 -1.074263 -2.752915 -1.537678 0.554607 0.708376 -1.534528 2.321535 2.711948	0.990688 1.170970 0.030942 -2.131275 -1.610115 1.723085 2.152163 -0.141474 0.789564	0.457497 -0.014904 -0.874873 -0.171704 1.332880 1.115991 0.010777 -0.490190 -0.640908	1344, 1378, 1423, 1545, 1804, 3171, 3178, 3207, 3212, 3248, 3494
TS5 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.099974 E(ω B97XD/6-311+G**) = - 286.815403 E(CCSD(T)/cc-pVDZ) = -286.040323 E(CCSD(T)/cc-pVTZ) = -286.318000	A B C	294.22430 767.23403 896.89497	6.1 2.4 2.0	C C C C C C H H H H H N H	-1.736230 -1.401199 -0.199270 1.259544 0.261044 -0.793813 -2.595504 -1.948090 0.271820 0.587272 -0.758328 2.434720 3.059328	0.401166 -0.969369 -1.023776 -0.035680 0.402497 1.218706 0.735400 -1.824040 -1.896720 0.697758 2.297355 -0.083200 -0.611376	-0.441733 -0.208927 0.475331 -0.192678 0.771644 0.094121 -1.008981 -0.580624 0.903768 1.775016 0.038199 -0.567842 -0.139028	643 <i>i</i> , 149, 259, 341, 409, 560, 720, 727, 753, 791, 825, 857, 900, 961, 969, 1005, 1032, 1061, 1104, 1108, 1153, 1252, 1306, 1402, 1428, 1573, 1862, 3048, 3223, 3244, 3253, 3263, 3346
TS6 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.093097 E(ω B97XD/6-311+G**) = - 286.795285 E(CCSD(T)/cc-pVDZ) = -286.036390	A B C	261.96646 916.87338 1084.0436	6.9 2.0 1.7	C C C C C	-1.773352 -1.773369 -0.590071 1.570227 0.279431 -0.590041	0.734162 -0.734135 -1.184051 -0.000053 0.000002 1.184063	-0.246614 -0.246596 0.188223 -0.135089 0.546935 0.188187	1150 <i>i</i> , 47, 116, 200, 286, 482, 499, 605, 612, 708, 745, 817, 837, 902, 982, 983, 1005, 1033, 1045, 1112, 1135, 1216, 1274, 1307, 1403, 1600, 1677, 2243, 3008, 3224, 3235, 3262,

	E(CCSD(T)/cc-pVTZ) = - 286.309846				H H H H H N H	-2.609793 -2.609823 -0.268085 0.474942 -0.268038 2.675183 3.817563	1.348198 -1.348157 -2.209308 0.000016 2.209314 -0.000057 0.000407	-0.553184 -0.553160 0.299668 1.631688 0.299621 -0.499004 0.598117	3266
TS7 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.102208 E(ω B97XD/6-311+G**) = - 286.816067 E(CCSD(T)/cc-pVDZ) = -286.044322 E(CCSD(T)/cc-pVTZ) = - 286.259615	A B C	359.61156 484.12519 730.14552	5.0 3.7 2.5	C C C C C C H H H H H H N	-0.398841 -1.244981 -0.593696 0.877051 1.643994 0.987590 -0.891208 -2.114601 -1.167327 1.306053 2.725342 1.532583 -1.288221	-1.234885 -0.133311 1.082881 1.220196 0.104529 -1.151766 -2.191549 -0.210877 2.003476 2.211616 0.161662 -2.050889 0.107243	-0.134021 -0.582639 -0.035452 -0.079155 -0.011893 0.050138 0.001951 -1.225531 -0.098149 -0.160119 0.026408 0.310114 0.843351	658 <i>i</i> , 317, 349, 519, 570, 633, 693, 754, 804, 827, 920, 955, 972, 989, 1013, 1040, 1052, 1094, 1159, 1173, 1225, 1312, 1346, 1406, 1476, 1478, 1606, 3163, 3179, 3196, 3202, 3215, 3225
TS8 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.101610 E(ω B97XD/6-311+G**) = - 286.792214 E(CCSD(T)/cc-pVDZ) = -286.019146 E(CCSD(T)/cc-pVTZ) = - 286.296434	A B C	360.66560 484.05450 737.06036	5.0 3.7 2.4	C C C C C C H H	0.298336 1.386214 0.637608 -0.830948 -1.633798 -1.027561 0.756880 2.356810	1.267240 -0.107104 -1.053951 -1.258018 -0.188010 1.116786 2.249306 -0.118360	0.179024 -0.728307 0.090759 0.037937 -0.074767 -0.121626 0.206831 -1.207573	678 <i>i</i> , 302, 350, 524, 563, 628, 650, 715, 750, 792, 890, 931, 949, 975, 996, 1005, 1052, 1062, 1111, 1177, 1236, 1280, 1373, 1427, 1457, 1508, 1669, 3159, 3199, 3207, 3212, 3221, 3228

					H	1.213813	-1.896254	0.464440	
					H	-1.214924	-2.265680	0.139432	
					H	-2.711512	-0.289647	-0.123823	
					H	-1.603290	1.991832	-0.394243	
					N	1.174731	0.238163	0.659545	
TS9	ZPE(ω B97XD/6-311+G**) =	A	355.13020	5.1	C	-0.030927	1.385432	-0.193536	819 <i>i</i> , 219, 357, 414, 525, 584,
C ₁	0.100697	B	539.93571	3.3	C	-2.003476	-0.108778	0.491351	627, 674, 713, 783, 825, 891,
² A	E(ω B97XD/6-311+G**) = -	C	833.45565	2.2	C	-0.614469	-1.000418	-0.397049	921, 964, 971, 991, 1012,
	286.764776				C	0.687981	-1.367225	0.049164	1092, 1170, 1181, 1280, 1341,
	E(CCSD(T)/cc-pVDZ) = -				C	1.595747	-0.357136	0.248669	1394, 1453, 1525, 1551, 1626,
	285.993888				C	1.263787	1.013646	-0.004348	3023, 3198, 3207, 3221, 3223,
	E(CCSD(T)/cc-pVTZ) = -				H	-0.402206	2.398475	-0.275612	3242
	286.270920				H	-2.897200	0.495078	0.695440	
					H	-1.115908	-1.493975	-1.217671	
					H	0.978001	-2.408073	0.129233	
					H	2.617452	-0.598878	0.517328	
					H	2.041783	1.765987	-0.012629	
					N	-0.944826	0.349751	-0.143086	
TS10	ZPE(ω B97XD/6-311+G**) =	A	328.08539	5.5	C	1.778653	-0.154276	0.000026	1811 <i>i</i> , 137, 241, 430, 488, 534,
C ₁	0.098600	B	633.41037	2.8	C	0.993092	-1.310017	0.000032	588, 640, 652, 773, 851, 872,
² A	E(ω B97XD/6-311+G**) = -	C	961.49575	1.9	C	-0.394138	-1.209578	-0.000067	967, 989, 1003, 1025, 1077,
	286.816358				C	-0.930373	0.128468	-0.000036	1119, 1155, 1184, 1292, 1308,
	E(CCSD(T)/cc-pVDZ) =				C	-0.154315	1.315342	-0.000025	1413, 1439, 1493, 1590, 1600,
	-286.041121				C	1.208080	1.141225	-0.000004	2067, 3178, 3192, 3201, 3215,
	E(CCSD(T)/cc-pVTZ) =				H	2.861142	-0.238716	0.000027	3567
	-286.317585				H	1.483460	-2.278811	0.000060	
					H	-1.940697	-1.289229	0.000005	
					H	-0.604493	2.301746	-0.000003	

					H	1.864346	2.004511	0.000007	
					N	-2.245289	-0.086953	0.000009	
					H	-2.952719	0.642183	0.000289	
TS11	ZPE(ω B97XD/6-311+G**) =	A	393.94897	4.6	C	1.339836	-0.732980	-0.609936	503 <i>i</i> , 87, 126, 189, 284, 457,
C ₁	0.098063	B	776.84249	2.3	C	1.340110	0.731181	-0.611719	559, 567, 584, 741, 741, 781,
² A	E(ω B97XD/6-311+G**) = -	C	804.95370	2.2	C	0.590926	1.170380	0.431012	838, 894, 934, 936, 974, 999,
	286.818866				C	-1.862213	0.000962	0.335919	1054, 1101, 1145, 1284, 1309,
	E(CCSD(T)/cc-pVDZ) =				C	0.045375	0.001432	1.111235	1405, 1529, 1593, 2007, 3228,
	-286.051967				C	0.590485	-1.169368	0.433850	3232, 3241, 3257, 3264, 3705
	E(CCSD(T)/cc-pVTZ) = -				H	1.871887	-1.353106	-1.319295	
	286.328282				H	1.872467	1.349384	-1.322525	
					H	0.392690	2.195142	0.708899	
					H	-0.250464	0.002744	2.150787	
					H	0.391763	-2.193381	0.714142	
					N	-2.118360	-0.001132	-0.818961	
					H	-1.716933	-0.002503	-1.741442	
TS12	ZPE(ω B97XD/6-311+G**) =	A	233.26215	7.7	C	1.943699	0.563727	0.126810	1783 <i>i</i> , 147, 169, 329, 462, 549,
C ₁	0.097078	B	936.61418	1.9	C	1.742987	-0.878035	0.036420	599, 625, 712, 741, 768, 825,
² A	E(ω B97XD/6-311+G**) = -	C	1148.0462	1.6	C	0.423799	-1.150099	-0.099335	900, 938, 957, 985, 1000,
	286.782675				C	-1.675699	0.375485	-0.086529	1031, 1102, 1115, 1207, 1280,
	E(CCSD(T)/cc-pVDZ) =				C	-0.277427	0.139180	-0.115876	1330, 1425, 1522, 1624, 1827,
	-286.007027				C	0.748558	1.186465	0.025822	2041, 3229, 3240, 3259, 3264,
	E(CCSD(T)/cc-pVTZ) = -				H	2.903070	1.047109	0.247141	3409
	286.286169				H	2.537586	-1.611979	0.064869	
					H	-0.054605	-2.112225	-0.204241	
					H	-0.928469	0.604256	-1.189382	
					H	0.539248	2.246010	0.051924	
					N	-2.798519	-0.109909	0.121540	

					H	-2.842696	-0.824144	0.855041	
TS13	ZPE(ω B97XD/6-311+G**) =	A	400.37851	4.5	C	1.412351	-0.702152	0.162277	507 <i>i</i> , 264, 297, 468, 476, 642,
C ₁	0.102041	B	486.43794	3.7	C	1.412350	0.702152	0.162277	665, 726, 790, 870, 881, 945,
² A	E(ω B97XD/6-311+G**) = -	C	797.68088	2.3	C	0.301685	1.424225	-0.214211	956, 977, 997, 1001, 1072,
	286.836234				C	-1.009412	0.907958	-0.215579	1123, 1214, 1231, 1233, 1340,
	E(CCSD(T)/cc-pVDZ) =				C	-1.009412	-0.907960	-0.215577	1395, 1443, 1487, 1571, 1647,
	-286.064138				C	0.301685	-1.424224	-0.214212	3136, 3139, 3187, 3196, 3205,
	E(CCSD(T)/cc-pVTZ) =				H	2.362293	-1.216310	0.258554	3215
	-286.340138				H	2.362292	1.216311	0.258557	
					H	0.420743	2.436291	-0.585572	
					H	-1.799939	1.476046	-0.704098	
					H	-1.799939	-1.476049	-0.704093	
					H	0.420744	-2.436290	-0.585574	
					N	-1.488811	0.000000	0.753196	
TS14	ZPE(ω B97XD/6-311+G**) =	A	362.33634	5.0	C	-0.338503	1.134635	0.389060	627 <i>i</i> , 240, 302, 447, 532, 631,
C ₁	0.101135	B	501.72545	3.6	C	1.006039	1.136705	-0.047932	732, 739, 775, 795, 842, 908,
² A	E(ω B97XD/6-311+G**) = -	C	750.45376	2.4	C	1.600995	-0.097337	-0.377486	937, 942, 1015, 1026, 1072,
	286.801509				C	0.870633	-1.178022	0.050452	1110, 1126, 1179, 1209, 1315,
	E(CCSD(T)/cc-pVDZ) = -				C	-1.402810	-0.740099	-0.212490	1363, 1396, 1470, 1518, 1682,
	286.031811				C	-1.488310	0.569335	-0.392216	3094, 3166, 3181, 3196, 3221,
	E(CCSD(T)/cc-pVTZ) = -				H	-0.599708	1.931081	1.090883	3230
	286.308228				H	1.615385	2.027040	0.072698	
					H	2.584471	-0.192147	-0.820523	
					H	1.180049	-2.215132	-0.052758	
					H	-1.921728	-1.585571	-0.650246	
					H	-2.191043	1.157852	-0.968279	
					N	-0.307957	-0.867775	0.695986	
TS15	ZPE(ω B97XD/6-311+G**) =	A	295.81936	6.1	C	0.046672	-0.883981	0.479277	701 <i>i</i> , 206, 317, 438, 587, 685,

C_1	0.101154	B	611.22438	3.0	C	-1.233289	-1.055050	-0.053829	728, 747, 771, 792, 823, 864,
2A	$E(\omega B97XD/6-311+G^{**}) = -$ 286.801448 $E(CCSD(T)/cc-pVDZ) =$ -286.029066 $E(CCSD(T)/cc-pVTZ) =$ -286.306874	C	794.94063	2.3	C	-1.740841	0.233019	-0.366094	902, 915, 922, 980, 1067,
					C	-0.799580	1.161275	-0.011166	1085, 1107, 1200, 1223, 1263,
					C	1.582512	0.600553	-0.026805	1334, 1389, 1451, 1540, 1641,
					C	1.796811	-0.595954	-0.543588	3186, 3225, 3229, 3248, 3264,
					H	0.520937	-1.540447	1.196417	3275
					H	-1.754540	-1.994905	-0.153658	
					H	-2.710144	0.453073	-0.789251	
					H	-0.783960	2.228658	-0.171477	
					H	2.168797	1.512345	0.013967	
					H	2.649465	-1.087219	-0.997143	
					N	0.285105	0.524189	0.576340	
TS16	$ZPE(\omega B97XD/6-311+G^{**}) =$ 0.096839	A	297.76074	6.1	C	-0.356231	0.928537	-0.546764	643 <i>i</i> , 86, 92, 166, 298, 534,
C_1		B	856.91967	2.1	C	-1.564912	0.944969	0.078840	572, 619, 691, 702, 755, 776,
2A	$E(\omega B97XD/6-311+G^{**}) = -$ 286.777278 $E(CCSD(T)/cc-pVDZ) =$ -286.005905 $E(CCSD(T)/cc-pVTZ) =$ -286.284794	C	1007.5140	1.8	C	-1.820087	-0.406392	0.476324	790, 844, 877, 898, 903, 984,
					C	-0.730496	-1.166668	0.057733	1020, 1088, 1140, 1195, 1296,
					C	2.094377	-0.445779	-0.098834	1385, 1435, 1547, 1907, 3236,
					C	2.336683	0.512475	0.620098	3255, 3261, 3281, 3394, 3482
					H	0.224056	1.734165	-0.969782	
					H	-2.207167	1.798255	0.235568	
					H	-2.727471	-0.788347	0.923658	
					H	-0.578842	-2.232586	0.147376	
					H	2.318178	-1.340984	-0.635382	
					H	2.379694	1.386215	1.227376	
					N	0.119364	-0.394224	-0.636171	
TS17	$ZPE(\omega B97XD/6-311+G^{**}) =$ 0.093208	A	216.19303	8.3	C	-0.463619	-1.121676	0.067520	851 <i>i</i> , 85, 145, 231, 482, 506,
C_1		B	882.75259	2.0	C	-1.784646	-0.796208	0.015662	558, 561, 619, 623, 633, 711,
2A	$E(\omega B97XD/6-311+G^{**}) = -$	C	1090.7071	1.7	C	-1.876917	0.626623	-0.062939	720, 747, 872, 887, 914, 981,

	286.755315 E(CCSD(T)/cc-pVDZ) = -285.988858 E(CCSD(T)/cc-pVTZ) = -286.269198				C C C H H H H H H N	-0.609657 1.622071 2.783382 0.045292 -2.603989 -2.780914 -0.231999 1.844821 3.836462 0.266663	1.125742 0.103557 -0.210415 -2.068875 -1.497420 1.212323 2.133343 1.812271 -0.352704 0.056475	-0.055364 0.014711 -0.121782 0.131853 0.034363 -0.116889 -0.102459 0.880455 -0.157332 0.026165	1072, 1094, 1117, 1283, 1325, 1359, 1455, 1533, 1610, 2184, 3261, 3273, 3293, 3299, 3478
TS18 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.101149 E(ω B97XD/6-311+G**) = - 286.811064 E(CCSD(T)/cc-pVDZ) = - 286.042606 E(CCSD(T)/cc-pVTZ) = - 286.317676	A B C	369.54304 513.79660 759.42760	4.88 3.51 2.38	C C C C C H H H H H N C H	-0.374715 0.976204 1.602643 0.944641 -1.437549 -0.704362 1.576533 2.058732 -0.069484 -2.177459 -2.141514 -1.429253 -0.375792 -0.668122	1.134317 1.170520 -0.047188 -1.176987 0.503342 1.967661 2.058732 -0.069484 -2.177459 1.068047 -0.767044 -0.937526 -1.357061	0.428133 0.020686 -0.365529 0.013771 -0.407471 1.051239 0.191345 -0.822006 -0.115549 -1.022596 -0.368711 0.600016 1.560909	797 <i>i</i> , 226, 309, 444, 514, 590, 687, 726, 753, 834, 882, 917, 965, 978, 997, 1011, 1055, 1082, 1140, 1181, 1294, 1321, 1382, 1414, 1453, 1563, 1717, 3108, 3121, 3151, 3180, 3188, 3214
TS19 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.101324 E(ω B97XD/6-311+G**) = - 286.829450 E(CCSD(T)/cc-pVDZ) = -	A B C	335.92792 583.76356 751.50709	5.37241 3.09156 2.40150	C C C C C	-0.359250 0.842059 1.656883 1.117346 -1.537437	0.617409 1.198640 0.191806 -1.083364 0.533848	0.682748 0.001438 -0.406983 -0.036597 -0.252598	758 <i>i</i> , 241, 270, 402, 550, 689, 736, 788, 793, 834, 874, 893, 908, 984, 996, 1020, 1054, 1102, 1120, 1220, 1223, 1260, 1319, 1383, 1427, 1566, 1696,

	286.063041 E(CCSD(T)/cc-pVTZ) = - 286.337233				H H H H H N C H	-0.566832 0.988779 2.587215 1.578170 -2.173799 -1.638217 -0.112173 -0.590583	1.023051 2.256215 0.327597 -2.039098 1.352940 -0.667717 -0.896412 -1.618240	1.677256 -0.169282 -0.944716 -0.243223 -0.600107 -0.626848 0.584621 1.232230	3084, 3095, 3220, 3233, 3245, 3253
TS20 C_1 2A	ZPE(ω B97XD/6-311+G**) = 0.098545 E(ω B97XD/6-311+G**) = - 286.835031 E(CCSD(T)/cc-pVDZ) = -286.070931 E(CCSD(T)/cc-pVTZ) = - 286.346196	A B C	304.42864 876.05453 995.22613	5.9 2.1 1.8	C C C C C H H H H H H N	-1.626903 -0.566338 0.182662 1.620638 -0.566789 -1.627186 -2.367355 -0.283087 0.815630 0.989733 -0.284056 -2.367914 2.714363	-0.733261 -1.172827 0.000231 0.000224 1.172892 0.732810 -1.350523 -2.196464 0.000408 0.000523 2.196672 1.349710 -0.000106	-0.352588 0.367195 0.814995 -0.598674 0.367020 -0.352692 -0.843568 0.562783 1.692115 -1.475774 0.562613 -0.843714 -0.160855	716i, 79, 141, 244, 293, 541, 562, 745, 752, 754, 783, 838, 868, 943, 950, 955, 968, 1002, 1049, 1100, 1144, 1289, 1311, 1402, 1533, 1597, 1923, 3229, 3232, 3243, 3257, 3261, 3268
TS21 C_s $^2A'$	ZPE(ω B97XD/6-311+G**) = 0.093683 E(ω B97XD/6-311+G**) = - 286.7989883 E(CCSD(T)/cc-pVDZ) = - 286.041936 E(CCSD(T)/cc-pVTZ) = -	A B C	265.56714 889.81567 1052.9502	6.8 2.0 1.7	C C C C C C H	-0.384433 -0.384433 -0.423702 0.659440 -0.384433 -0.384433 -0.382223	-1.696505 -0.435074 0.502263 1.503268 -0.435074 -1.696505 -2.587642	0.734150 1.183170 0.000000 0.000000 -1.183170 -0.734150 1.347773	939i, 108, 145, 218, 441, 497, 497, 558, 608, 711, 738, 815, 838, 908, 979, 983, 1001, 1039, 1044, 1110, 1133, 1228, 1268, 1306, 1400, 1598, 1674, 2254, 3051, 3220, 3231, 3257, 3261

	286.315005				H	-0.375252	-0.094151	2.208370	
					H	-1.368646	1.063352	0.000000	
					H	2.034412	0.265451	0.000000	
					H	-0.375252	-0.094151	-2.208370	
					H	-0.382223	-2.587642	-1.347773	
					N	1.237306	2.511507	0.000000	
TS22	ZPE(ω B97XD/6-311+G**) =	A	322.85986	5.6	C	-1.679275	0.005330	-0.459042	837 <i>i</i> , 160, 313, 450, 483, 533,
C_s	0.099381	B	635.41783	2.8	C	-1.073235	-1.137356	-0.049892	596, 696, 730, 743, 846, 858,
$^2A'$	E(ω B97XD/6-311+G**) = -	C	813.09996	2.2	C	0.209464	-0.932484	0.618156	885, 941, 975, 994, 1048,
	286.745025				C	0.277427	0.987490	0.499042	1102, 1128, 1154, 1208, 1302,
	E(CCSD(T)/cc-pVDZ) = -				C	-0.997295	1.185946	-0.015828	1366, 1408, 1433, 1583, 1608,
	285.970808				H	-2.613823	0.032603	-1.002806	2968, 3208, 3210, 3219, 3230,
	E(CCSD(T)/cc-pVTZ) = -				H	-1.471776	-2.134203	-0.193642	3243
	286.247917				H	0.578970	-1.503786	1.461600	
					H	0.803827	1.685653	1.137509	
					H	-1.490561	2.146311	0.074318	
					H	2.581221	0.849712	-0.844148	
					N	1.104207	-0.087891	-0.046178	
					C	2.243364	-0.185769	-0.644034	
TS23	ZPE(ω B97XD/6-311+G**) =	A	314.26845	5.7	C	1.662572	-0.238179	-0.515992	703 <i>i</i> , 132, 238, 386, 443, 589,
C_1	0.098420	B	686.15289	2.6	C	1.192527	1.059506	-0.193814	667, 686, 720, 796, 818, 831,
2A	E(ω B97XD/6-311+G**) = -	C	799.63459	2.3	C	0.045741	0.929811	0.612970	883, 940, 972, 980, 999, 1066,
	286.761357				C	-0.226749	-0.555211	0.783065	1097, 1111, 1185, 1276, 1308,
	E(CCSD(T)/cc-pVDZ) = -				C	0.874481	-1.209983	0.040728	1349, 1429, 1523, 1737, 2923,
	285.986140				H	2.519897	-0.433956	-1.148132	3141, 3217, 3246, 3253, 3263
	E(CCSD(T)/cc-pVTZ) = -				H	1.601024	1.993159	-0.549696	
	286.263234				H	-0.429245	1.691430	1.212915	
					H	-0.614192	-0.984893	1.704463	

					H	0.991117	-2.279630	-0.050436	
					H	-2.895578	-0.803992	-0.779885	
					N	-1.239227	0.021794	-0.076783	
					C	-2.298310	0.124942	-0.702248	
TS24	ZPE(ω B97XD/6-311+G**) =	A	367.25370	4.9	C	1.426148	-0.735248	-0.514856	830 <i>i</i> , 104, 133, 238, 345, 530,
C ₁	0.098434	B	738.07429	2.4	C	1.426158	0.735191	-0.514917	559, 595, 717, 739, 756, 808,
² A	E(ω B97XD/6-311+G**) = -	C	795.22392	2.3	C	0.539497	1.173203	0.400850	842, 946, 953, 962, 1022,
	286.809222				C	-0.141605	0.000045	0.978336	1038, 1069, 1111, 1142, 1292,
	E(CCSD(T)/cc-pVDZ) = -				C	0.539478	-1.173171	0.400944	1332, 1401, 1552, 1634, 1869,
	286.043362				H	2.052102	-1.351636	-1.146607	3204, 3218, 3229, 3249, 3256,
	E(CCSD(T)/cc-pVTZ) = -				H	2.052119	1.351516	-1.146723	3359
	286.319386				H	0.291513	2.197627	0.638065	
					H	-0.438377	0.000089	2.020101	
					H	0.291486	-2.197571	0.638256	
					H	-2.641823	-0.000121	-1.748662	
					N	-1.798060	0.000049	0.252267	
					C	-1.959777	-0.000061	-0.920405	
TS25	ZPE(ω B97XD/6-311+G**) =	A	326.84688	5.52167	C	-0.014211	0.960439	0.557002	746 <i>i</i> , 230, 256, 403, 550, 662,
C ₁	0.100533	B	612.67307	2.94568	C	1.213939	1.065202	-0.054213	719, 727, 767, 814, 842, 864,
² A	E(ω B97XD/6-311+G**) = -	C	777.75514	2.32045	C	1.674216	-0.259557	-0.422347	901, 977, 988, 1020, 1046,
	286.807395				C	0.789318	-1.196789	-0.024493	1093, 1102, 1119, 1258, 1272,
	E(CCSD(T)/cc-pVDZ) = -				C	-1.710674	0.528350	-0.593537	1320, 1391, 1438, 1601, 1713,
	286.039672				H	-0.470234	1.722814	1.175526	3067, 3072, 3211, 3217, 3237,
	E(CCSD(T)/cc-pVTZ) = -				H	1.747885	1.983945	-0.255672	3250
	286.314417				H	2.599136	-0.456929	-0.950139	
					H	0.846521	-2.262720	-0.193448	
					H	-2.467812	0.915173	-1.283862	
					N	-1.605262	-0.630450	-0.136419	

					C	-0.368098	-0.529679	0.666893	
					H	-0.525603	-0.896924	1.686698	

Table S2. Rate constants (s^{-1}) for various unimolecular reaction steps for isomerization and dissociation of $\text{C}_6\text{H}_6\text{N}$ intermediates involved in the $\text{N}(^2\text{D}) + \text{C}_6\text{H}_6$ reaction, calculated using RRKM theory under single collision condition at $E_c = 0 \sim 10 \text{ kcal mol}^{-1}$.

Rate constants	Collision energy (kcal mol^{-1})						
	σ^a	0	2	4	6	8	10
$\text{i1} \rightarrow \text{TS1} \rightarrow \text{i2}, k_1$	1	3.28×10^{12}	3.30×10^{12}	3.32×10^{12}	3.35×10^{12}	3.37×10^{12}	3.39×10^{12}
$\text{i2} \rightarrow \text{TS1} \rightarrow \text{i1}, k_{-1}$	1	3.78×10^9	4.56×10^9	5.45×10^9	6.47×10^9	7.62×10^9	8.92×10^9
$\text{i2} \rightarrow \text{TS2} \rightarrow \text{i3}, k_2$	1	2.77×10^7	3.76×10^7	5.02×10^7	6.62×10^7	8.61×10^7	1.11×10^8
$\text{i3} \rightarrow \text{TS2} \rightarrow \text{i2}, k_{-2}$	1	4.88×10^8	6.30×10^8	8.01×10^8	1.01×10^9	1.25×10^9	1.54×10^9
$\text{i3} \rightarrow \text{TS3} \rightarrow \text{i4}, k_3$	1	4.96×10^{12}	5.12×10^{12}	5.27×10^{12}	5.43×10^{12}	5.58×10^{12}	5.73×10^{12}
$\text{i4} \rightarrow \text{TS3} \rightarrow \text{i3}, k_{-3}$	1	1.75×10^7	2.16×10^7	2.64×10^7	3.22×10^7	3.90×10^7	4.69×10^7
$\text{i4} \rightarrow \text{VTS1} \rightarrow \text{C}_6\text{H}_5\text{N} + \text{H}, k_{v1}$	1	3.03×10^3	4.85×10^3	7.62×10^3	1.17×10^4	1.78×10^4	2.64×10^4
$\text{i4} \rightarrow \text{TS4} \rightarrow \text{i5}, k_4$	1	3.57×10^7	4.41×10^7	5.42×10^7	6.62×10^7	8.03×10^7	9.69×10^7
$\text{i5} \rightarrow \text{TS4} \rightarrow \text{i4}, k_{-4}$	1	1.54×10^{11}	1.67×10^{11}	1.81×10^{11}	1.95×10^{11}	2.10×10^{11}	2.25×10^{11}
$\text{i5} \rightarrow \text{TS5} \rightarrow \text{i6}, k_5$	1	2.56×10^{11}	2.78×10^{11}	3.01×10^{11}	3.25×10^{11}	3.50×10^{11}	3.76×10^{11}
$\text{i6} \rightarrow \text{TS5} \rightarrow \text{i5}, k_{-5}$	1	2.26×10^{10}	2.47×10^{10}	2.69×10^{10}	2.91×10^{10}	3.16×10^{10}	3.41×10^{10}
$\text{i6} \rightarrow \text{TS6} \rightarrow \text{C}_5\text{H}_5\text{CN} + \text{H}, k_6$	1	5.49×10^{11}	6.19×10^{11}	6.94×10^{11}	7.75×10^{11}	8.61×10^{11}	9.54×10^{11}
$\text{i2} \rightarrow \text{TS7} \rightarrow \text{i7}, k_7$	1	1.33×10^{11}	1.44×10^{11}	1.55×10^{11}	1.66×10^{11}	1.78×10^{11}	1.90×10^{11}
$\text{i7} \rightarrow \text{TS7} \rightarrow \text{i2}, k_{-7}$	1	1.88×10^{12}	1.96×10^{12}	2.04×10^{12}	2.13×10^{12}	2.21×10^{12}	2.29×10^{12}
$\text{i7} \rightarrow \text{TS8} \rightarrow \text{i8}, k_8$	1	2.77×10^{10}	3.19×10^{10}	3.65×10^{10}	4.14×10^{10}	4.69×10^{10}	5.27×10^{10}

$i8 \rightarrow TS8 \rightarrow i, k_8$	1	1.93×10^{11}	2.10×10^{11}	2.27×10^{11}	2.45×10^{11}	2.63×10^{11}	2.82×10^{11}
$i8 \rightarrow TS9 \rightarrow i9, k_9$	1	1.31×10^9	1.66×10^9	2.09×10^9	2.59×10^9	3.17×10^9	3.85×10^9
$i9 \rightarrow TS9 \rightarrow i8, k_9$	1	7.49×10^7	1.00×10^8	1.33×10^8	1.72×10^8	2.22×10^8	2.81×10^8
$i9 \rightarrow VTS2 \rightarrow C_5H_5N + CH, k_{v2}$	1	2.54×10^7	4.23×10^7	6.81×10^7	1.06×10^8	1.62×10^8	2.40×10^8
$i4 \rightarrow TS10 \rightarrow i10, k_{10}$	1	5.82×10^7	7.22×10^7	8.90×10^7	1.09×10^8	1.33×10^8	1.60×10^8
$i10 \rightarrow TS10 \rightarrow i4, k_{-10}$	1	1.42×10^9	1.68×10^9	1.97×10^9	2.30×10^9	2.67×10^9	3.09×10^9
$i10 \rightarrow VTS3 \rightarrow C_6H_4 + NH_2, k_{v3}$	1	1.68×10^6	2.58×10^6	3.88×10^6	5.72×10^6	8.28×10^6	1.18×10^7
$i6 \rightarrow TS11 \rightarrow C_5H_5 + HNC, k_{11}$	1	3.63×10^{12}	3.86×10^{12}	4.09×10^{12}	4.32×10^{12}	4.56×10^{12}	4.80×10^{12}
$i6 \rightarrow TS12 \rightarrow i11, k_{12}$	1	2.06×10^8	2.56×10^8	3.15×10^8	3.84×10^8	4.65×10^8	5.59×10^8
$i11 \rightarrow TS12 \rightarrow i6, k_{-12}$	1	2.58×10^6	3.47×10^6	4.61×10^6	6.05×10^6	7.86×10^6	1.01×10^7
$i11 \rightarrow VTS4 \rightarrow C_5H_4 + HCNH, k_{v4}$	1	8.65×10^1	2.07×10^2	4.64×10^2	9.86×10^2	1.99×10^3	3.85×10^3
$i2 \rightarrow TS13 \rightarrow i12, k_{13}$	1	4.49×10^{12}	4.59×10^{12}	4.69×10^{12}	4.79×10^{12}	4.89×10^{12}	4.99×10^{12}
$i12 \rightarrow TS13 \rightarrow i2, k_{-13}$	1	1.42×10^9	1.57×10^9	1.73×10^9	1.91×10^9	2.09×10^9	2.29×10^9
$i12 \rightarrow TS14 \rightarrow i13, k_{14}$	1	8.99×10^6	1.10×10^7	1.34×10^7	1.62×10^7	1.95×10^7	2.32×10^7
$i13 \rightarrow TS14 \rightarrow i12, k_{-14}$	1	4.59×10^{10}	5.11×10^{10}	5.67×10^{10}	6.26×10^{10}	6.89×10^{10}	7.55×10^{10}
$i13 \rightarrow TS15 \rightarrow i14, k_{15}$	1	5.11×10^{10}	5.71×10^{10}	6.35×10^{10}	7.04×10^{10}	7.76×10^{10}	8.53×10^{10}
$i14 \rightarrow TS15 \rightarrow i13, k_{-15}$	1	1.58×10^9	1.80×10^9	2.04×10^9	2.30×10^9	2.58×10^9	2.89×10^9
$i14 \rightarrow TS16 \rightarrow C_4H_4N + C_2H_2, k_{16}$	1	4.50×10^9	5.71×10^9	7.15×10^9	8.88×10^9	1.09×10^{10}	1.33×10^{10}
$i14 \rightarrow TS17 \rightarrow C_4H_4NCCH + H, k_{17}$	1	2.00×10^8	2.75×10^8	3.73×10^8	4.98×10^8	6.56×10^8	8.55×10^8

i12 $\rightarrow$ TS18 $\rightarrow$ i15, k_{18}	1	4.76×10^7	5.64×10^7	6.65×10^7	7.80×10^7	9.09×10^7	1.05×10^8
i15 $\rightarrow$ TS18 $\rightarrow$ i12, k_{18}	1	4.08×10^{10}	4.57×10^{10}	5.11×10^{10}	5.67×10^{10}	6.28×10^{10}	6.94×10^{10}
i15 $\rightarrow$ TS19 $\rightarrow$ i16, k_{19}	1	9.36×10^{11}	9.88×10^{11}	1.04×10^{12}	1.10×10^{12}	1.15×10^{12}	1.21×10^{12}
i16 $\rightarrow$ TS19 $\rightarrow$ i15, k_{19}	1	1.33×10^{10}	1.44×10^{10}	1.55×10^{10}	1.66×10^{10}	1.78×10^{10}	1.91×10^{10}
i16 $\rightarrow$ TS20 $\rightarrow$ C ₅ H ₅ + HCN, k_{20}	1	3.28×10^{12}	3.45×10^{12}	3.63×10^{12}	3.81×10^{12}	4.00×10^{12}	4.19×10^{12}
i16 $\rightarrow$ TS21 $\rightarrow$ C ₅ H ₅ CN + H, k_{21}	1	4.88×10^{10}	5.64×10^{10}	6.46×10^{10}	7.39×10^{10}	8.39×10^{10}	9.50×10^{10}
i9 $\rightarrow$ TS22 $\rightarrow$ i17, k_{22}	1	2.36×10^5	4.04×10^5	6.68×10^5	1.07×10^6	1.66×10^6	2.51×10^6
i17 $\rightarrow$ TS22 $\rightarrow$ i9, k_{22}	1	1.20×10^{10}	1.56×10^{10}	1.99×10^{10}	2.48×10^{10}	3.05×10^{10}	3.69×10^{10}
i17 $\rightarrow$ TS23 $\rightarrow$ i18, k_{23}	1	2.93×10^{12}	3.17×10^{12}	3.40×10^{12}	3.64×10^{12}	3.88×10^{12}	4.11×10^{12}
i18 $\rightarrow$ TS23 $\rightarrow$ i17, k_{23}	1	1.84×10^6	2.67×10^6	3.80×10^6	5.30×10^6	7.27×10^6	9.81×10^6
i18 $\rightarrow$ TS24 $\rightarrow$ C ₅ H ₅ + HCN, k_{24}	1	1.86×10^{12}	1.98×10^{12}	2.11×10^{12}	2.24×10^{12}	2.38×10^{12}	2.52×10^{12}
i15 $\rightarrow$ TS25 $\rightarrow$ i18, k_{25}	1	3.25×10^{10}	3.69×10^{10}	4.17×10^{10}	4.69×10^{10}	5.24×10^{10}	5.85×10^{10}
i18 $\rightarrow$ TS25 $\rightarrow$ i15, k_{25}	1	2.17×10^{10}	2.36×10^{10}	2.56×10^{10}	2.76×10^{10}	2.98×10^{10}	3.20×10^{10}
