

Supporting Information

for

**A Combined Experimental and Computational
Investigation of the Elementary Reaction of Ground
State Atomic Carbon (C; 3P_j) with Pyridine
(C₅H₅N; X¹A₁) via Ring Expansion and Ring
Degradation Pathways**

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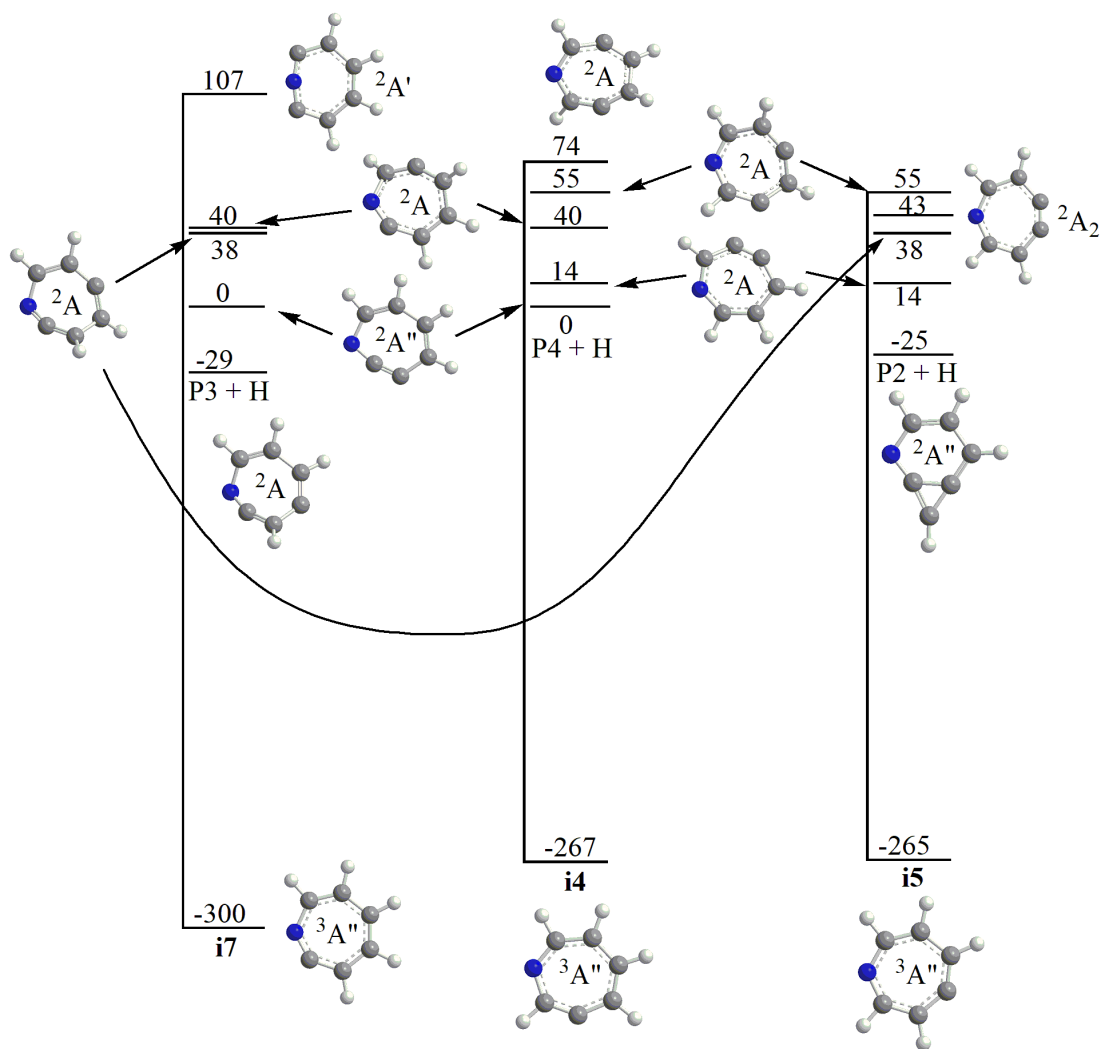


Figure S1. Optimized structures, electronic states, and relative energies (kJ mol^{-1}) of various H loss products originating from seven-member ring $\text{C}_6\text{H}_5\text{N}$ isomers (directly or via a bicyclic intermediate). All relative energies are calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G** + ZPE(B3LYP/6-311G**) level of theory.

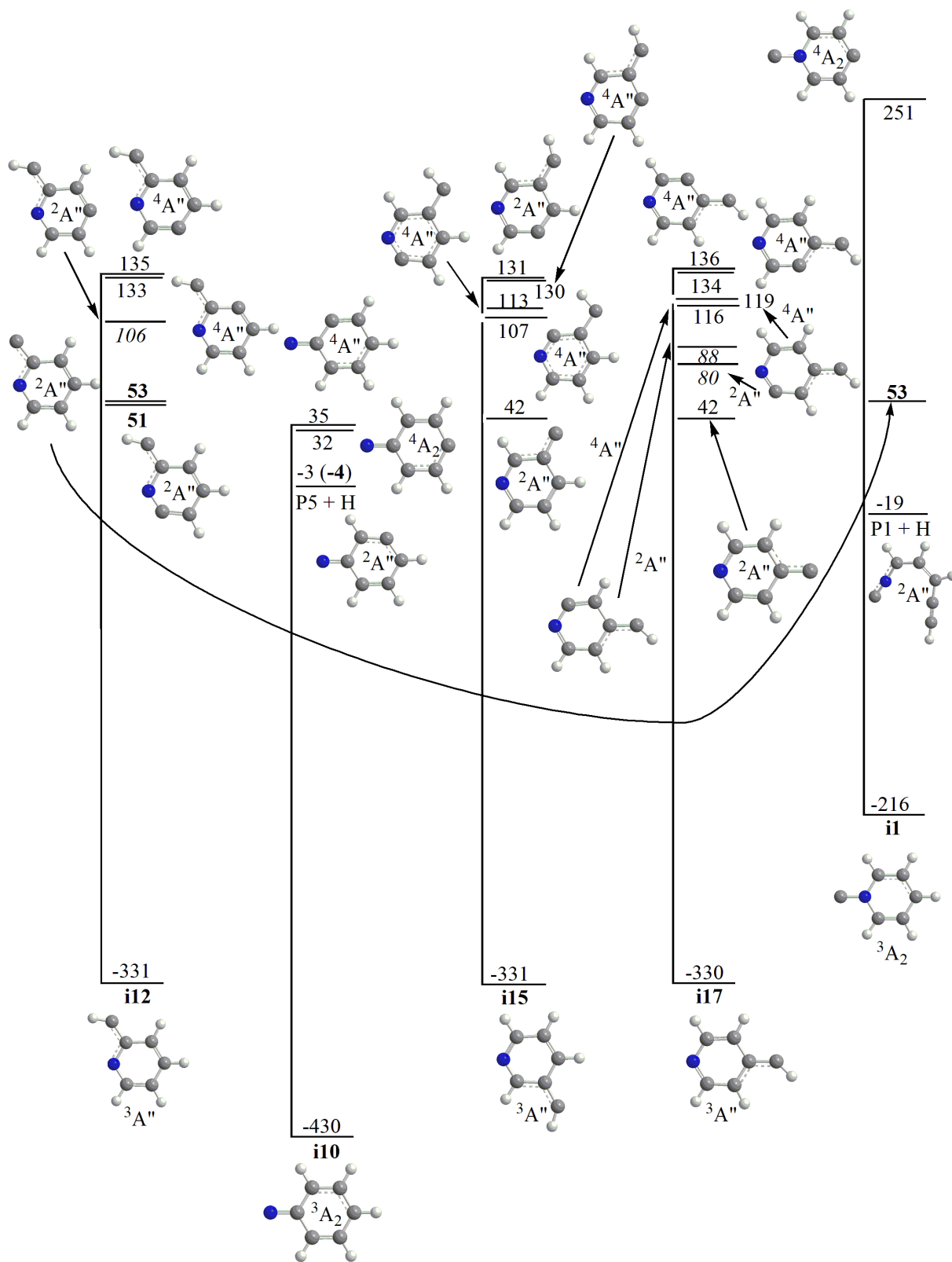
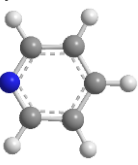
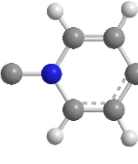
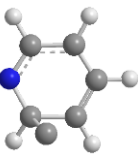


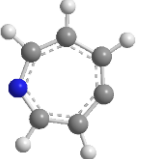
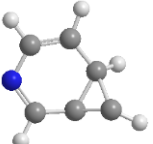
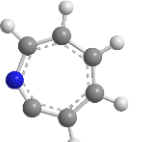


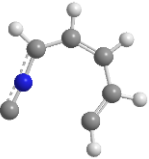
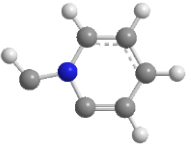
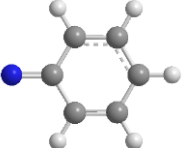

Figure S2. Optimized structures, electronic states, and relative energies (kJ mol⁻¹) of various H loss products originating from six-member ring C₆H₅N isomers. All geometries have been

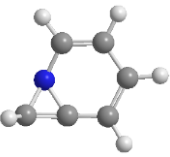
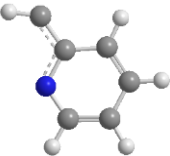
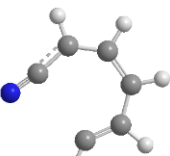
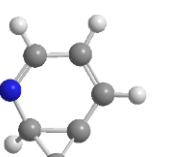
optimized at the B3LYP/6-311G** level of theory and ZPE(B3LYP/6-311G**) are included in relative energies. Plain numbers show relative energies (in kJ mol^{-1}) refined at the CCSD(T)-F12/cc-pVTZ-f12// level for structures with low T1 diagnostics (≤ 0.03). Bold numbers show relative energies refined at the CASPT2(10,10)/cc-pVTZ level for structures with high T1 diagnostics (> 0.03). For some high-energy isomers with high T1 diagnostics relative energies were not recalculated at CASPT2 and only B3LYP relative energies are shown in italics. Both doublet and quartet states were calculated for all structures but only ground states are shown for most of the isomers.

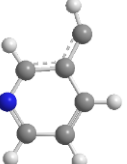
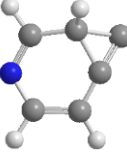
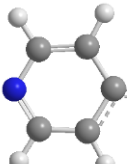
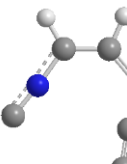
Table S1. Optimized Cartesian coordinates (in Å) and vibrational frequencies (in cm⁻¹) for all stationary structures.

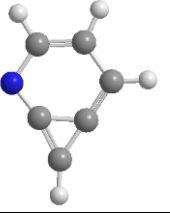
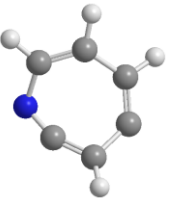
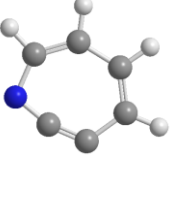
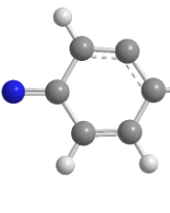
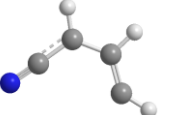
Structure	Coordinates					Frequencies		
 pyridine	N	0	-0.834319	1.367320	0.000000	384.7154	419.8249	616.3411
	C	0	0.499780	1.368574	0.000000	670.3636	720.2160	764.5095
	C	0	-1.445574	0.181745	0.000000	899.8933	958.8629	1004.8281
	C	0	-0.768304	-1.032182	0.000000	1010.3357	1016.4418	1046.9834
	C	0	0.619802	-1.015869	0.000000	1076.1929	1093.5069	1170.0157
	C	0	1.269366	0.211108	0.000000	1241.4553	1282.0483	1383.8055
	H	0	0.975927	2.342786	0.000000	1471.6464	1511.6606	1619.0546
	H	0	-2.529715	0.203878	0.000000	1624.9221	3143.2573	3145.9151
	H	0	-1.318936	-1.962668	0.000000	3168.1610	3183.7993	3192.1408
	H	0	1.183278	-1.939547	0.000000			
H	0	2.348696	0.274856	0.000000				
 i1	C	0	2.435371	-0.000258	0.000000	164.9983	413.3711	424.8794
	N	0	1.088871	0.000318	0.000000	438.6485	531.0614	636.4993
	C	0	0.354595	1.204687	0.000000	651.6354	724.8691	798.5405
	C	0	-1.012272	1.205242	0.000000	818.2660	840.4223	964.6513
	C	0	-1.736483	-0.000339	0.000000	970.8708	971.6223	1024.7141
	C	0	-1.011883	-1.205868	0.000000	1069.3011	1145.7573	1171.0647
	C	0	0.355143	-1.203810	0.000000	1256.0717	1269.8885	1344.8449
	H	0	0.969905	2.092200	0.000000	1417.0260	1453.5879	1530.6643
	H	0	-1.526426	2.158889	0.000000	1609.7256	3184.6435	3188.4575
	H	0	-2.817914	-0.000293	0.000000	3211.8663	3231.5200	3233.8657
H	0	-1.525307	-2.159794	0.000000				
H	0	0.970812	-2.091157	0.000000				
 i2	C	0	1.524847	-0.055222	1.092217	176.6015	249.7012	308.4993
	C	0	1.024782	-0.618591	-0.312365	404.6350	477.4094	598.0213
	N	0	-0.122888	-1.425888	-0.244290	620.5536	667.9294	737.4824
	C	0	-1.255250	-0.845793	0.055256	858.9905	925.7852	950.4390
	C	0	-1.426431	0.559460	0.195402	965.7545	990.3617	998.2505
	C	0	-0.364931	1.396116	-0.124939	1019.3625	1074.8210	1161.8943
	C	0	0.884109	0.843196	-0.423702	1165.7585	1273.0777	1353.1343
	H	0	1.857028	-1.083014	-0.841182	1410.7107	1458.5228	1512.2804
	H	0	-2.122541	-1.496098	0.147768	1573.7096	3089.2670	3134.6593
	H	0	-2.395334	0.962400	0.462060	3174.5681	3198.0645	3202.9997
H	0	-0.506790	2.470164	-0.172858				
H	0	1.705099	1.452772	-0.776970				
 i3	C	0	1.554055	0.014087	1.067239	201.4119	243.4475	284.3405
	C	0	1.077586	-0.568087	-0.328173	365.7807	465.4965	579.5379
	C	0	-0.139478	-1.362893	-0.197713	629.9740	645.9427	751.3494
	N	0	-1.322511	-0.885377	0.088241	883.1580	900.5020	928.9002
	C	0	-1.450824	0.470249	0.167878	961.3727	971.6900	992.0283
	C	0	-0.425437	1.364674	-0.122107	1039.7031	1057.2536	1150.3847
	C	0	0.857703	0.888159	-0.412527	1218.5384	1307.1531	1358.9115
	H	0	1.899647	-1.000043	-0.898790	1397.9866	1476.6274	1503.6886

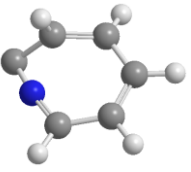
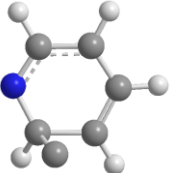
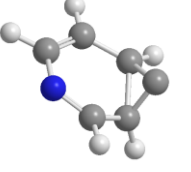
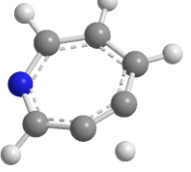
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	H	0	-2.438324	0.833481	0.430244	3171.3856	3188.0788	3211.0057
	H	0	-0.630857	2.428824	-0.141832			
	H	0	1.643085	1.542461	-0.763921			
i4 	N	0	-1.651690	0.238512	0.000081	161.9719	242.5488	389.2884
	C	0	-1.223871	-1.076754	-0.000087	462.1876	511.3477	542.8661
	C	0	0.040429	-1.537864	-0.000056	675.6403	728.3557	813.0199
	C	0	1.350571	-0.990521	0.000012	822.3820	881.5428	892.2583
	C	0	1.577239	0.355047	0.000047	897.8780	966.9321	978.3956
	C	0	0.586621	1.389566	-0.000076	1002.9530	1043.2551	1203.8243
	C	0	-0.803141	1.272684	-0.000197	1240.0898	1355.9473	1426.2294
	H	0	-2.044065	-1.791373	0.000414	1449.5248	1500.5706	1577.1702
	H	0	2.195603	-1.671156	0.000165	1613.2741	3103.4687	3129.0909
	H	0	2.612614	0.685160	0.000200	3141.6486	3164.4391	3175.3749
	H	0	0.960665	2.407347	0.000046			
	H	0	-1.330075	2.227490	0.000746			
i5 	N	0	-0.753784	1.395954	-0.000209	177.5102	235.7181	393.9006
	C	0	1.540131	0.361662	-0.000057	458.5576	528.7043	549.5271
	C	0	1.290351	-1.067817	0.000158	666.9648	712.2231	762.1826
	C	0	0.050301	-1.574718	0.000238	853.0966	863.6776	864.4522
	C	0	-1.255225	-1.055867	0.000161	899.1023	973.7017	989.4208
	C	0	0.611531	1.373257	-0.000205	1002.0591	1009.8945	1178.2798
	C	0	-1.534964	0.311609	-0.000047	1284.1446	1314.0179	1447.0781
	H	0	2.581119	0.669629	-0.000103	1454.3521	1468.7677	1564.4752
	H	0	2.150907	-1.730879	0.000255	1626.6425	3094.3874	3118.7884
	H	0	-2.098442	-1.738121	0.000263	3141.0381	3162.0624	3165.8025
	H	0	1.027946	2.379403	-0.000353			
	H	0	-2.597787	0.559534	-0.000087			
i6 	N	0	-1.531737	-0.749957	-0.026697	181.5517	312.4800	383.6410
	C	0	-0.335947	-1.383350	-0.062336	479.8638	525.6838	581.4093
	C	0	0.856135	-0.722505	-0.223222	629.6739	651.5058	775.7653
	C	0	1.952419	-0.168236	0.433761	812.4069	828.0808	891.0241
	C	0	0.935232	0.786930	-0.260237	917.3826	977.8189	1003.7535
	C	0	-0.348148	1.387514	0.085051	1013.5971	1057.8208	1106.8407
	C	0	-1.479887	0.598681	0.120408	1188.6940	1224.6520	1304.0142
	H	0	-0.354452	-2.459271	0.093928	1374.5223	1431.9077	1490.9136
	H	0	3.014207	-0.143506	0.212924	1621.0437	3013.3701	3135.4335
	H	0	1.477007	1.316183	-1.051295	3144.6071	3152.7979	3170.3427
	H	0	-0.447140	2.467497	0.105965			
	H	0	-2.446288	1.074583	0.264813			
i7 	C	0	0.225886	-1.551407	-0.000199	127.2684	292.5469	379.9664
	N	0	-1.003154	-1.295530	-0.000171	457.7407	495.9075	566.1637
	C	0	-1.606163	-0.035409	0.000159	664.5184	766.1148	779.3475
	C	0	-0.985245	1.174616	0.000046	813.4693	843.1710	896.3135
	C	0	0.421984	1.475175	-0.000165	925.8095	979.1864	990.8563
	C	0	1.479526	0.581883	0.000037	998.6575	1083.5229	1189.0818
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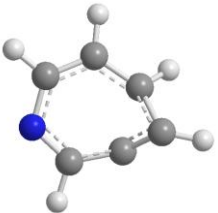
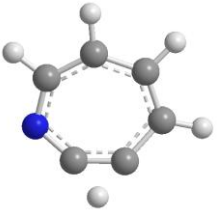
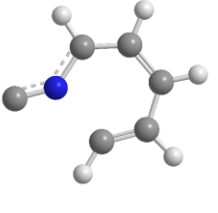
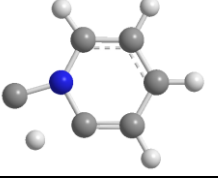
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i8		C 0 2.071260 1.304330 -0.164548 N 0 1.582947 0.240040 -0.034561 C 0 1.139914 -1.044453 0.102805 C 0 -0.159761 -1.482167 0.049087 C 0 -1.400741 -0.827783 -0.098417 C 0 -1.752486 0.550961 -0.072178 C 0 -0.994942 1.619262 0.207354 H 0 1.935790 -1.768298 0.232151 H 0 -0.234080 -2.564105 0.111343 H 0 -2.241154 -1.500730 -0.234188 H 0 -1.149277 2.685756 0.265698 H 0 -2.811368 0.746193 -0.277703	38.2706 222.1687 515.9354 704.1927 879.4303 958.4903 1265.3163 1446.1004 2137.7934 3165.3391	129.9165 315.0407 552.6061 756.8603 890.3856 1023.9120 1295.0390 1524.9291 3021.7427 3183.6094	197.2476 343.5650 596.5429 790.0232 906.4561 1202.8434 1385.8913 1563.5564 3145.1717 3247.7369
i9		C 0 -2.310965 -0.274429 -0.000247 N 0 -0.986537 -0.003632 -0.000095 C 0 -0.313645 1.202741 0.000089 C 0 1.059677 1.181466 0.000218 C 0 1.738900 -0.047629 0.000159 C 0 1.013570 -1.245924 -0.000029 C 0 -0.373303 -1.231334 -0.000153 H 0 -0.921161 2.098559 0.000125 H 0 1.604875 2.116988 0.000366 H 0 2.823318 -0.060572 0.000261 H 0 1.535131 -2.196328 -0.000078 H 0 -3.021811 0.557433 -0.000230	190.3144 455.8465 591.3889 791.3443 939.5529 1050.7421 1240.6606 1408.5268 1579.1558 3178.6946	355.0032 498.1136 685.4638 853.1481 982.5786 1116.0480 1248.9648 1450.4347 3056.2751 3191.3721	394.9966 591.0752 764.4275 855.6124 1004.4195 1168.3808 1329.2637 1529.1105 3165.2176 3207.0405
i10		C 0 -1.071960 0.000000 -0.000003 N 0 -2.394540 0.000000 -0.000002 C 0 1.044358 1.214520 -0.000001 C 0 1.743996 0.000000 -0.000003 C 0 1.044358 -1.214520 0.000000 C 0 -0.335953 -1.230858 0.000003 C 0 -0.335954 1.230858 0.000005 H 0 1.591376 2.150642 -0.000005 H 0 2.827528 0.000000 0.000009 H 0 1.591378 -2.150641 -0.000006 H 0 -0.890785 -2.160798 0.000002 H 0 -0.890785 2.160798 0.000001	205.7375 484.0709 675.2440 831.3166 980.0321 1091.7647 1268.9411 1443.2048 1587.9807 3190.0463	377.0318 525.2811 764.6728 909.4474 994.8198 1168.6668 1308.7356 1461.0915 3168.0017 3197.7688	399.1832 615.9360 821.5701 974.3187 1026.9423 1174.1875 1339.2612 1557.8661 3174.4404 3200.4452
i11		C 0 -2.012352 -0.147407 0.164856 N 0 -0.924717 0.603339 -0.382173 C 0 0.149556 1.415467 0.037477 C 0 1.376248 0.800271 0.104392 C 0 1.542893 -0.605084 -0.016023 C 0 0.382357 -1.437757 0.010460	222.6913 491.7940 641.6772 720.6564 932.7786 997.6839	330.7409 578.8252 702.8344 839.6531 942.5652 1058.4472	406.9296 591.2966 704.7623 896.3959 984.4712 1113.6692

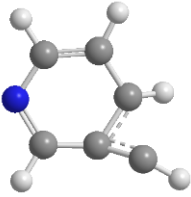
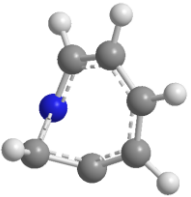
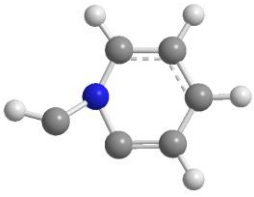
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i12 	C 0 -1.003520 0.071591 -0.000146 N 0 -0.439102 -1.174684 -0.000004 C 0 0.884373 -1.250311 -0.000034 C 0 1.737961 -0.139978 0.000028 C 0 1.166202 1.134194 0.000004 C 0 -0.211452 1.251178 -0.000020 C 0 -2.400618 0.124843 0.000098 H 0 1.300964 -2.254980 0.000128 H 0 2.812375 -0.277084 0.000134 H 0 1.791988 2.019786 0.000064 H 0 -0.698324 2.218859 0.000044 H 0 -3.170971 -0.632890 0.000080	192.1092 344.0962 406.1016 461.1990 556.5702 558.0947 634.2497 734.8839 783.3155 830.5515 884.0070 902.3249 974.6122 979.0370 1000.2071 1050.6931 1113.5904 1166.4015 1246.6489 1285.3986 1346.6523 1437.5211 1456.7562 1569.1407 1587.0023 3136.7373 3169.5873 3189.5214 3196.4473 3236.2349
i13 	C 0 1.598630 -0.004933 -0.000004 C 0 0.890085 -1.224936 0.000016 C 0 -0.468980 -1.457516 0.000004 C 0 -1.586687 -0.602207 -0.000020 N 0 2.308964 0.914337 -0.000022 H 0 1.540210 -2.094034 0.000035 H 0 -0.725104 -2.513153 0.000010 H 0 -2.545372 -1.110119 -0.000045 C 0 -1.659385 0.819344 -0.000011 C 0 -0.645588 1.691171 0.000040 H 0 -2.675879 1.228379 -0.000045 H 0 -0.525057 2.763033 0.000054	23.8615 154.1813 175.6683 217.5300 372.8295 406.7143 551.3248 558.8858 604.0784 714.2888 741.2190 801.2919 864.9553 900.3797 904.0300 984.7908 1001.1958 1191.1021 1258.5358 1284.8859 1376.5381 1451.5467 1526.0205 1561.6213 2246.6595 3026.9962 3143.4699 3161.9680 3172.3920 3256.6829
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i15	C 0 -1.030600 0.099928 -0.000058 C 0 -0.343858 -1.160737 0.000011 N 0 0.971691 -1.290906 0.000013 C 0 1.719651 -0.175759 -0.000025 C 0 1.170020 1.110160 0.000006	196.1210 344.0621 396.8514 458.9272 522.6031 554.0416 630.8822 702.9371 802.6046 827.9110 870.5344 906.3899 933.3927 990.3316 998.8909

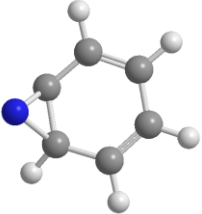
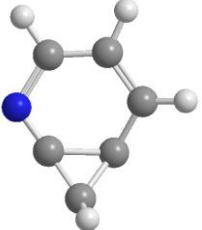
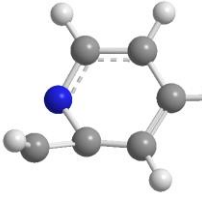
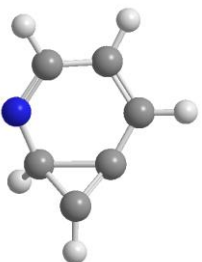
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i16 	N 0 -1.479580 0.735972 -0.134454 C 0 0.947323 0.731184 0.284088 C 0 1.975128 -0.185897 -0.381648 C 0 0.827835 -0.764681 0.162954 C 0 -0.352500 -1.412448 0.048170 C 0 -0.327564 1.378302 -0.118247 C 0 -1.532974 -0.593959 0.061824 H 0 1.399220 1.206314 1.164227 H 0 3.034491 -0.234728 -0.159373 H 0 -0.416002 -2.456502 -0.243029 H 0 -0.363456 2.458338 -0.238427 H 0 -2.520676 -1.040233 0.074932	206.6249 337.7551 377.0890 499.3784 520.3171 564.3692 602.5288 631.0182 732.1643 785.6400 806.5028 839.3166 913.2996 935.8052 953.9730 1006.3438 1046.3159 1104.3853 1176.9331 1212.2285 1303.4350 1352.9326 1368.5662 1461.7380 1695.7840 2984.2513 3132.8224 3149.8680 3170.3584 3177.6746
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P1 	C 0 1.438918 1.899610 0.000046 N 0 1.411357 0.721142 0.000037 C 0 1.473625 -0.640052 -0.000070 C 0 0.384900 -1.488030 -0.000006 C 0 -0.983631 -1.197892 0.000083 C 0 -1.585564 0.060842 -0.000085 C 0 -2.175372 1.118917 -0.000058 H 0 2.477646 -1.046412 -0.000136 H 0 0.642644 -2.541796 -0.000004 H 0 -1.660915 -2.046658 0.000256 H 0 -2.656129 2.066503 0.000170	96.5873 111.4311 178.7838 296.4102 316.7045 402.4288 494.9863 510.3228 608.1408 667.9296 691.5234 774.8451 796.9663 933.4353 958.5165 992.8409 1182.6728 1246.2188 1392.4827 1462.8062 1504.3705 2112.9131 2134.7655 3149.5550 3170.6162 3191.4529 3471.1199
P2	N 0 -0.193135 -1.504908 -0.000034 C 0 -1.464329 0.618344 -0.000133 C 0 -0.321421 1.469487 -0.000083 C 0 0.854254 0.741848 0.000408 C 0 2.038947 -0.012785 -0.000287	255.3288 349.0871 472.9556 529.8263 541.8931 586.6338 723.3771 745.6772 755.8433 871.4892 957.4680 962.6263 987.7379 1024.2055 1034.4497

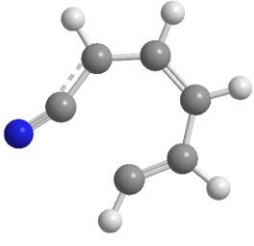
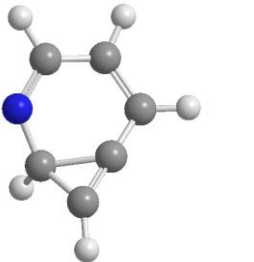
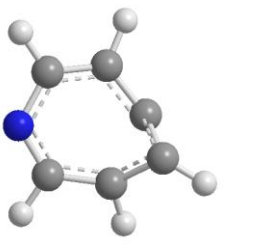
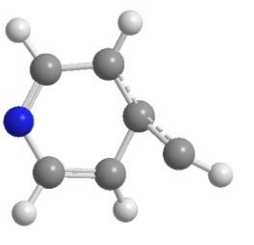
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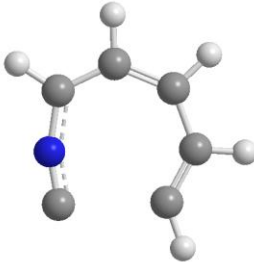
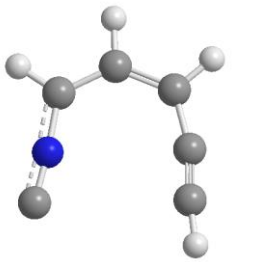
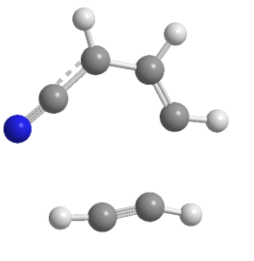
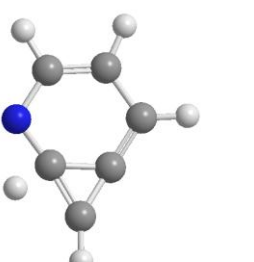
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	N 0 0.955066 0.746590 -0.123091	363.7259	397.8557	453.8227
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	C 0 -1.414424 0.703579 0.018548	726.7776	738.7219	833.8472
	C 0 -1.453903 -0.673155 -0.085463	897.5012	934.5384	1003.0617
	C 0 -0.258754 -1.442784 -0.062518	1045.6359	1064.3711	1141.8749
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	H 0 -0.178517 -2.376163 -0.609499			
	H 0 1.018806 -0.680802 1.563054			
ts i2-i4 	C 0 1.584484 -0.098861 0.978594	672.1020 <i>i</i>	234.0062	290.6095
	C 0 1.046148 -0.632531 -0.287436	396.1827	509.2666	584.8472
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	H 0 -0.578550 2.474168 -0.228470			
	H 0 1.681458 1.530817 -0.711469			
ts i3-i5 	C 0 -1.407045 0.120656 -0.817521	529.9191 <i>i</i>	302.7667	332.4626
	C 0 -1.230494 -0.253606 0.543482	500.6566	551.5072	566.8808
	C 0 -0.275026 -1.296147 0.062766	654.0004	741.6234	826.8922
	N 0 1.025113 -1.155668 -0.112435	854.0745	885.1623	927.7222
	C 0 1.550947 0.101126 0.022124	953.9469	958.2015	989.1635
	C 0 0.799316 1.240980 0.044306	1028.3159	1100.0352	1156.7865
	C 0 -0.650716 1.133667 -0.021344	1207.7716	1245.3122	1311.1062
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	H 0 1.263502 2.213249 0.155892			
	H 0 -1.233842 2.007512 0.262844			
ts i4-i5 	N 0 1.313984 0.910023 0.048672	1791.9280 <i>i</i>	145.5264	274.9316
	C 0 1.598624 -0.350937 0.128018	372.8071	408.2128	472.5121
	C 0 0.641005 -1.413395 -0.195249	544.5668	573.9062	687.9237
	C 0 -0.678610 -1.419193 -0.169432	732.9080	792.6245	824.0033
	C 0 -1.629058 -0.384492 0.141386	841.7261	880.0086	924.0648
	C 0 -1.217706 0.935363 0.024754	956.8652	986.1340	1070.3791
	C 0 0.077488 1.475317 -0.125221	1163.5950	1288.9223	1387.5680
	H 0 2.618427 -0.618043 0.389803	1423.4272	1488.8814	1532.9053
	H 0 -2.668908 -0.621667 0.322779	1733.0122	2184.0973	3123.6204

	H 0 -2.002807 1.689043 0.055073 H 0 0.128586 2.549510 -0.268262 H 0 -0.023645 -2.424989 0.334365	3146.9223 3162.2873 3197.2267
ts i4-i6 	N 0 -1.534403 -0.666465 0.092721 C 0 -0.448963 -1.373425 -0.148403 C 0 0.866561 -0.887797 -0.296122 C 0 1.784526 -0.238311 0.539099 C 0 1.034788 0.804040 -0.225628 C 0 -0.256928 1.397699 -0.050399 C 0 -1.407624 0.688234 0.176114 H 0 -0.589716 -2.446388 -0.275937 H 0 2.865933 -0.275839 0.437576 H 0 1.701013 1.358375 -0.888272 H 0 -0.333368 2.464287 -0.237275 H 0 -2.337196 1.222184 0.346900	343.9356i 155.7638 284.4748 473.9085 490.9987 604.2787 626.6603 757.2921 812.7887 852.5822 863.5439 900.8485 950.1975 960.9834 975.0089 1063.4727 1088.9197 1151.0702 1239.4030 1307.6268 1382.1020 1406.5357 1440.8957 1497.1248 1560.7205 3076.3337 3110.7948 3122.3017 3151.3430 3169.5392
ts i4-i7 	C 0 0.635808 -1.350103 -0.178492 N 0 1.634708 -0.497164 0.167283 C 0 1.324951 0.794763 0.037152 C 0 0.090162 1.455911 -0.125598 C 0 -1.238348 0.956482 0.013794 C 0 -1.647862 -0.351341 0.128044 C 0 -0.688861 -1.377519 -0.176589 H 0 2.188558 1.455576 0.117854 H 0 0.172989 2.534175 -0.208790 H 0 -2.012674 1.719295 0.068026 H 0 -2.680732 -0.593449 0.342367 H 0 0.033810 -2.404605 0.319686	1848.4815i 171.3091 296.7401 374.8754 437.4550 506.8797 563.7186 579.8656 711.3754 769.0887 816.8749 877.7284 902.9369 930.0277 956.3165 977.9874 1030.5337 1117.2152 1189.8434 1233.9035 1402.1918 1416.9098 1495.9635 1548.6749 1718.0046 2102.9342 3107.7221 3128.2515 3169.0819 3194.8217
ts i1-i8 	C 0 -2.474064 0.405607 -0.000029 N 0 -1.317443 0.022174 -0.000003 C 0 -0.625271 -1.188957 0.000016 C 0 0.736916 -1.336357 0.000006 C 0 1.705386 -0.318840 -0.000016 C 0 1.369882 1.059983 -0.000008 C 0 0.097959 1.483355 0.000032 H 0 -1.274169 -2.054621 0.000032 H 0 1.085908 -2.363359 0.000016 H 0 2.750915 -0.601475 -0.000037 H 0 2.183068 1.788962 -0.000029 H 0 -0.388469 2.446531 0.000042	538.2470i 90.1196 279.5780 332.0898 368.9139 394.8859 548.6819 566.2754 613.5068 713.0558 800.2650 837.3113 903.3878 907.4884 951.7079 958.0513 1037.4968 1154.9078 1227.3062 1267.1264 1362.3337 1430.9697 1522.1842 1571.2124 1727.2413 3072.1081 3167.6415 3190.2272 3204.2125 3247.3712
ts i1-i9 	C 0 2.367494 0.027624 0.000093 N 0 0.995823 0.197813 -0.000130 C 0 0.176441 1.297499 -0.000011 C 0 -1.186171 1.076936 0.000025 C 0 -1.700658 -0.226168 0.000012 C 0 -0.821316 -1.331718 0.000002 C 0 0.534022 -1.101727 -0.000051 H 0 0.652681 2.267843 0.000037	1660.1688i 169.2181 408.6088 447.6237 479.2083 583.0585 655.0759 670.4045 753.2607 840.0908 867.9250 928.8108 930.7929 973.2357 1025.6029 1042.1738 1099.1460 1142.9413 1181.5431 1245.1993 1324.2493 1414.5161 1436.6154 1526.3068

	H 0 -1.853350 1.929850 0.000100 H 0 -2.772800 -0.381718 0.000056 H 0 -1.203097 -2.344929 0.000070 H 0 1.986939 -1.310409 0.000237	1575.8196 3194.1289	1978.8713 3200.8130	3180.0600 3223.3727
ts i6-i15 	N 0 -1.455610 -0.873384 -0.032374 C 0 -0.196168 -1.376357 -0.073146 C 0 0.906298 -0.569133 -0.244963 C 0 2.040852 -0.147966 0.432559 C 0 0.795756 0.886736 -0.276166 C 0 -0.497456 1.375056 0.096533 C 0 -1.547773 0.461619 0.127634 H 0 -0.085811 -2.441540 0.109118 H 0 3.085462 0.001970 0.181467 H 0 1.435210 1.503526 -0.904765 H 0 -0.695914 2.436336 0.188914 H 0 -2.558730 0.833663 0.277174	527.1031 <i>i</i> 392.3832 639.7582 786.6008 912.5456 1036.8585 1186.7889 1395.3369 1609.9922 3149.4361	240.5870 550.3932 665.6018 820.6308 943.8523 1088.7286 1232.6775 1446.0503 3097.1505 3160.6656	361.1178 589.6732 758.5564 880.2033 979.2915 1119.9695 1332.2943 1474.4868 3138.8121 3180.8894
ts i4-i11 	C 0 -1.663585 -0.175739 0.527248 N 0 -1.081142 0.740256 -0.322454 C 0 0.071317 1.427888 -0.199636 C 0 1.266487 0.848237 0.184668 C 0 1.438856 -0.545857 0.177704 C 0 0.430424 -1.430111 -0.199646 C 0 -0.905980 -1.064427 -0.329658 H 0 -1.559559 -0.091409 1.611801 H 0 0.041929 2.456970 -0.548699 H 0 2.128340 1.489317 0.329601 H 0 2.435348 -0.941829 0.344327 H 0 0.696825 -2.454788 -0.443927	179.1433 291.9058 649.9608 683.7027 812.5860 957.4068 1002.8831 1047.1945 1254.9157 1431.4549 1694.9738 1717.7148 3104.3945 3128.2777	233.8262 363.6961 649.9608 775.0243 887.8073 957.4068 1002.8831 1238.3034 1254.9157 1431.4549 1694.9738 3100.8922 3110.0730 3128.2777	263.8547 363.6961 673.1933 812.5860 941.3255 980.9307 1012.1621 1240.7181 1387.8830 1469.4725 1699.9728 3104.3945 3120.9842 3135.1456
ts i9-i11 	C 0 2.138199 -0.211370 -0.293334 N 0 0.943690 0.284642 0.145707 C 0 0.095187 1.341847 0.066072 C 0 -1.243669 1.033254 -0.006162 C 0 -1.637102 -0.328769 -0.120116 C 0 -0.723412 -1.367455 -0.026766 C 0 0.620104 -1.051660 0.300043 H 0 3.099295 0.302472 -0.176060 H 0 0.516095 2.337906 0.015108 H 0 -1.981490 1.823606 -0.032788 H 0 -2.690620 -0.552028 -0.253640 H 0 -1.044945 -2.399532 -0.090987	701.8836 <i>i</i> 404.2358 627.3833 839.9285 911.9175 1022.8164 1169.8231 1427.4645 1566.8771 3191.6356	223.2087 464.0439 682.0667 854.3658 974.7094 1081.5555 1219.8288 1439.4351 3011.0821 3195.0923	372.0130 526.1293 734.6249 906.8363 1008.1962 1159.6546 1360.6188 1536.1450 3162.2244 3213.2015
ts i7-i10	C 0 0.944759 -0.691217 -0.388906 C 0 -0.246325 -1.407008 -0.113103 C 0 -1.447587 -0.748784 0.029251 C 0 -1.455206 0.678349 0.126718 C 0 -0.314917 1.419388 0.009008	355.5215 <i>i</i> 422.6649 620.5984 815.0383 939.3290	312.8529 514.1802 721.3816 870.5071 973.1030	333.5195 562.0529 752.2424 932.2290 995.0845

	C 0 0.964913 0.780217 -0.269576 N 0 1.849467 -0.211943 0.567757 H 0 -0.182863 -2.484018 0.012941 H 0 -2.376120 -1.298000 0.130561 H 0 -2.399972 1.182541 0.301025 H 0 -0.361796 2.502754 0.007077 H 0 1.700660 1.394653 -0.786258	1022.8469 1073.1665 1169.7024 1196.5772 1272.8292 1365.4864 1381.1102 1421.3397 1490.1073 1600.1735 3094.5476 3149.8764 3161.4284 3177.5481 3188.1819
ts i7-i12 	C 0 0.812181 -0.800517 -0.013425 N 0 -0.241385 -1.502304 0.000275 C 0 -1.429872 -0.708577 -0.025571 C 0 -1.436296 0.673433 0.102710 C 0 -0.254156 1.446353 0.103995 C 0 0.909120 -0.729848 -0.455186 C 0 1.950775 -0.094701 0.223361 H 0 -2.346550 -1.281838 -0.039033 H 0 -2.394857 1.149525 0.287943 H 0 -0.229027 2.454181 0.502769 H 0 0.908598 0.671200 -1.548155 H 0 2.441019 0.048016 1.179244	354.6532/ 239.9102 359.5492 415.0684 465.2577 516.2361 562.6960 632.4491 665.2291 734.3201 798.7660 843.4869 910.1263 957.3059 984.0334 1019.8485 1065.7680 1104.0795 1186.9909 1232.4630 1291.2717 1350.9322 1394.2180 1454.7063 1753.1555 3025.9888 3150.1998 3170.3500 3174.4334 3212.6287
ts i11-i12 	C 0 2.133768 0.096031 0.210228 N 0 0.791450 -0.826817 -0.369652 C 0 -0.395121 -1.400429 0.022898 C 0 -1.521666 -0.568428 0.151428 C 0 -1.445810 0.811048 0.014605 C 0 -0.149780 1.423754 -0.072638 C 0 0.882370 0.539947 -0.197463 H 0 2.669647 -0.014771 1.141231 H 0 -0.428858 -2.475211 0.133531 H 0 -2.479026 -1.034722 0.358124 H 0 -2.336864 1.420622 0.086726 H 0 0.012381 2.480265 0.093606	825.6078/ 243.0780 326.3901 416.3466 484.6854 572.7081 584.6358 624.8812 683.7665 751.1323 761.6121 826.8940 875.3525 942.6138 950.2415 1008.4503 1033.2305 1123.0753 1150.9084 1171.5481 1344.6825 1374.9958 1458.6103 1494.2860 1638.9997 3169.4452 3194.1934 3206.2145 3210.8562 3234.2227
ts i5-i14 	N 0 0.139708 1.422908 0.048153 C 0 1.563664 -0.528106 -0.054177 C 0 0.472322 -1.414188 -0.100011 C 0 -0.797776 -0.907170 -0.066352 C 0 -1.866565 -0.219339 0.418234 C 0 1.312310 0.842275 0.171024 C 0 -1.006276 0.743722 -0.317650 H 0 2.580424 -0.896436 -0.065678 H 0 0.627019 -2.486402 -0.011251 H 0 -2.929331 -0.331596 0.231452 H 0 2.139100 1.501233 0.426340 H 0 -1.461231 1.149691 -1.224342	402.9764/ 202.2085 335.1868 459.5116 479.5662 498.3002 568.2774 582.0096 702.5994 816.4692 831.2160 896.1834 919.6015 959.8583 965.9779 1049.2624 1071.6498 1111.1066 1173.6166 1299.1035 1356.4955 1392.1926 1441.5333 1516.6953 1671.7630 3053.9502 3131.4996 3137.0895 3146.9815 3208.6382
ts i10-i13	C 0 -1.439405 0.139119 0.000006 N 0 -2.429784 -0.492728 0.000011	306.7486/ 84.8859 244.7325 258.2516 371.5129 416.2203

	C 0 0.166459 -1.568333 -0.000018 C 0 1.412166 -1.077859 0.000005 C 0 1.718933 0.309660 0.000008 C 0 0.779085 1.351651 -0.000004 C 0 -0.597104 1.280956 -0.000007 H 0 -0.285441 -2.547553 -0.000024 H 0 2.256235 -1.773411 0.000024 H 0 2.766205 0.589270 0.000019 H 0 1.186005 2.357893 -0.000009 H 0 -1.155333 2.211731 -0.000017	541.6310 561.0378 618.2123 719.1991 771.3740 810.6060 868.2014 903.6178 927.0415 979.5211 1012.0356 1168.6510 1231.7323 1265.1813 1361.9312 1439.7687 1524.4212 1561.8924 2088.6155 3052.3433 3153.4251 3167.7469 3183.2638 3258.0043
ts i14-i15 	N 0 -0.136295 -1.394579 0.125073 C 0 -1.559349 0.542643 -0.093426 C 0 -0.450630 1.421844 -0.099084 C 0 0.758644 0.805566 0.104378 C 0 1.928392 0.209453 0.301207 C 0 -1.330919 -0.827769 0.160584 C 0 0.989889 -0.735295 -0.357899 H 0 -2.573088 0.913313 -0.165399 H 0 -0.568116 2.497032 -0.019531 H 0 2.989118 0.372636 0.192786 H 0 -2.163338 -1.483973 0.398670 H 0 1.253328 -1.035613 -1.376591	188.0281 <i>i</i> 255.7917 306.4724 381.1382 464.8407 509.1819 519.9612 566.5842 688.3214 783.2092 794.8495 893.2744 902.0888 936.9275 970.9055 1026.6490 1047.8687 1077.2366 1149.2213 1278.2137 1331.4462 1379.1341 1444.0738 1488.2564 1734.0171 3032.9676 3150.6438 3159.9695 3207.4017 3226.5202
ts i5-i16 	N 0 1.411675 0.802399 0.178803 C 0 -1.032718 0.792372 -0.179198 C 0 -1.720809 -0.293112 0.571200 C 0 -0.887353 -0.908676 -0.388982 C 0 0.432797 -1.372788 -0.199087 C 0 0.270950 1.382303 -0.084607 C 0 1.482253 -0.553252 0.151796 H 0 -1.735927 1.399441 -0.748188 H 0 -2.806236 -0.312619 0.577011 H 0 0.605488 -2.439742 -0.305575 H 0 0.325837 2.435266 -0.357910 H 0 2.458396 -0.980225 0.356301	322.5047 <i>i</i> 189.6307 293.0547 474.2229 498.2093 608.1737 676.6210 771.9334 802.7213 830.9620 890.2365 917.0249 946.4355 957.7593 990.2631 1073.6724 1100.7769 1135.0379 1245.3341 1295.9728 1387.4953 1415.0336 1445.1311 1486.4608 1550.5485 3095.0378 3119.7401 3138.8030 3150.9138 3171.4218
ts i16-i17 	N 0 -1.567612 -0.584230 0.155379 C 0 0.800220 -0.854653 -0.292103 C 0 2.058295 0.175412 0.413554 C 0 0.892270 0.594867 -0.221851 C 0 -0.202184 1.401396 -0.080059 C 0 -0.492773 -1.368562 0.094648 C 0 -1.460350 0.736623 -0.034570 H 0 1.433895 -1.455848 -0.942129 H 0 3.113554 0.111469 0.171189 H 0 -0.112992 2.453746 0.167284 H 0 -0.645919 -2.429030 0.271834 H 0 -2.388124 1.298770 -0.033549	633.3525 <i>i</i> 237.8638 359.7017 415.1057 537.2000 590.2092 611.0126 659.4384 744.4801 758.9662 795.5705 829.6909 874.6949 913.6110 944.1941 1011.0947 1073.3326 1112.1000 1198.8798 1216.4119 1358.1049 1365.7565 1392.3347 1471.1935 1645.1162 3089.1027 3148.1359 3159.2049 3163.0324 3172.7468
ts i7-i8	6 0 1.008887 1.798796 -0.115256	244.9447 <i>i</i> 48.2017 229.8160

	7	0	1.422292	0.692593	-0.037989	272.0448	311.9049	363.6532
	6	0	1.492259	-0.667055	0.065961	525.4216	576.6208	607.8666
	6	0	0.388172	-1.484462	0.033329	701.3502	786.6618	800.1099
	6	0	-0.988777	-1.195272	-0.059127	891.1360	904.2778	927.9114
	6	0	-1.715689	0.032290	-0.040643	956.0047	1033.9808	1192.3684
	6	0	-1.319115	1.302047	0.151162	1245.4371	1282.4050	1374.0413
	1	0	2.488378	-1.082142	0.146585	1437.4612	1521.3188	1553.2475
	1	0	0.630645	-2.542962	0.066398	2077.4746	3023.1575	3145.0635
	1	0	-1.617287	-2.074920	-0.152054	3165.7192	3198.7639	3238.2287
	1	0	-2.794394	-0.103768	-0.179719			
	1	0	-1.857811	2.237573	0.172150			
ts i8-P1 	C	0	-1.710924	1.703923	0.086153	706.9138/	22.0614	99.4907
	N	0	-1.523315	0.541629	0.035639	122.3484	191.6218	303.2868
	C	0	-1.403010	-0.814582	-0.022848	335.2621	425.2952	494.8802
	C	0	-0.218867	-1.521711	-0.039334	507.7753	547.8577	599.2050
	C	0	1.114402	-1.093438	-0.013420	651.2559	695.7713	785.1794
	C	0	1.574247	0.233001	0.004103	798.3653	931.1348	960.6147
	C	0	1.698262	1.441975	-0.144498	989.4405	1183.6580	1255.4660
	H	0	-2.346053	-1.346884	-0.051389	1392.9118	1462.4282	1503.8784
	H	0	-0.354019	-2.597776	-0.075112	2010.7712	2136.0296	3162.6753
	H	0	1.871735	-1.868203	-0.005870	3178.6501	3190.3090	3457.2526
	H	0	1.914704	2.482139	-0.190518			
	H	0	3.252176	-0.155696	0.852479			
ts i13-P6 	C	0	1.329658	-0.878309	-0.000049	360.3594/	13.4659	44.9057
	C	0	1.673389	0.483449	-0.000113	139.1333	172.7038	263.2601
	C	0	0.782326	1.562499	-0.000076	289.4689	443.9194	497.9712
	C	0	-0.581713	1.578761	0.000021	598.9500	632.1653	650.3960
	N	0	1.098117	-2.015569	0.000002	695.2811	730.1635	783.9778
	C	0	-2.288410	0.013226	0.000101	801.8106	921.4838	932.1819
	C	0	-1.931626	-1.149469	0.000123	1016.0490	1169.8478	1247.8700
	H	0	2.736988	0.692399	-0.000197	1427.5463	1453.2669	1936.7701
	H	0	1.269953	2.541548	-0.000134	2253.4976	3055.7590	3179.0366
	H	0	-1.195579	2.471800	0.000050	3185.4369	3390.6409	3473.0601
	H	0	-2.971881	0.830140	0.000096			
	H	0	-1.428045	-2.087855	0.000134			
ts i14-P2 	N	0	0.178658	-1.487835	-0.114714	858.5000/	234.0808	282.5946
	C	0	1.512285	0.588954	0.029874	337.2956	478.5391	512.3688
	C	0	0.392926	1.477097	0.038228	537.3878	559.1527	596.3348
	C	0	-0.801155	0.793353	0.026893	708.4556	752.9934	770.5158
	C	0	-2.007474	0.109250	-0.158275	869.8271	941.9884	961.6571
	C	0	1.363826	-0.795800	-0.064134	980.8477	1009.9215	1024.2001
	C	0	-0.830941	-0.620396	0.041683	1065.3403	1129.3893	1239.2750
	H	0	2.518208	0.991415	0.049454	1312.8846	1445.6820	1458.1051
	H	0	0.504761	2.553442	0.006509	1487.1856	1717.0305	3164.9572
	H	0	-3.072796	0.149105	-0.321012	3180.9585	3194.9412	3240.2080
	H	0	2.251500	-1.417178	-0.123980			
	H	0	-1.229077	-1.176685	1.706416			