

Supplementary information

A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl Radical (CH_3CC ; X^2A_1) with Ethylene (H_2CCH_2 ; X^1A_{1g}) and the Formation of 1-Penten-3-yne ($\text{CH}_2\text{CHCCCH}_3$; $\text{X}^1\text{A}'$)

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Optimized Cartesian coordinates (in Å) and calculated vibrational frequencies (in cm⁻¹) of the reactants, products, intermediates, and transition states in the 1-propynyl plus ethylene reaction; point groups and electronic ground states are also given.

Reactants

C₂H₄, D_{2h}, ¹A_{1g}

6	0	-0.663585	0.000000	0.000000
6	0	0.663426	0.000000	0.000000
1	0	-1.2360973	0.9225588	0.000000
1	0	-1.2360973	-0.9225588	0.000000
1	0	1.2360973	-0.9225588	0.000000
1	0	1.2360973	0.9225588	0.000000

Frequencies

840.4073	955.5511	966.0451
1066.4178	1248.6545	1385.0246
1481.1861	1700.2203	3122.6829
3138.2058	3193.6533	3222.3305

C₃H₃, C_{3v}, ²A₁

H	0.000000	1.021621	-1.512622
C	0.000000	0.000000	-1.133496
C	0.000000	0.000000	0.336404
H	0.884750	-0.510811	-1.512622
H	-0.884750	-0.510811	-1.512622
C	0.000000	0.000000	1.553404

Frequencies

125.	125.	934.
1009.	1009.	1410.
1479.	1479.	2190.
3054.	3133.	3133.

Products

p1, C₁, ¹A

6	0	2.412835	0.467137	0.000090
6	0	1.466252	-0.478208	-0.000286
6	0	0.065922	-0.231158	0.000896
6	0	-1.129112	-0.061591	0.000074
6	0	-2.568466	0.159753	-0.000500
1	0	2.166425	1.523264	0.000275
1	0	3.464364	0.202797	-0.001432
1	0	1.766397	-1.525073	-0.000632
1	0	-2.906494	0.572510	0.955207
1	0	-2.861032	0.863949	-0.785333
1	0	-3.114252	-0.773045	-0.169728

Frequencies

14.5923	140.7524	185.3916
327.5848	378.8949	539.7050
698.8686	723.3435	930.3995
1006.6882	1054.6076	1058.8481

1064.4256	1198.6176	1329.4444
1429.7840	1457.4707	1495.1518
1495.4054	1676.6979	2334.9605
3024.4957	3077.1205	3082.6455
3126.6112	3145.2144	3232.0848

p2, C_s, ¹A'

6	0	2.303006	0.468267	-0.000056
6	0	1.208813	-0.562208	-0.000058
6	0	-0.081242	-0.297947	0.000273
6	0	-1.319936	-0.040173	0.000131
6	0	-2.608442	0.223353	-0.000177
1	0	2.946875	0.351156	0.878968
1	0	1.901450	1.482108	-0.000365
1	0	2.947227	0.350689	-0.878726
1	0	1.523935	-1.606052	-0.000405
1	0	-3.351380	-0.569480	-0.000164
1	0	-2.981299	1.243831	0.000016

Frequencies

140.2495	143.9206	227.7823
314.3685	487.5495	530.8085
572.8298	802.1213	843.1650
857.6205	1038.5717	1044.2669
1057.0052	1114.3047	1331.0923
1417.6150	1458.9503	1497.6416
1505.9957	1702.6157	2199.5772
3018.0836	3059.3352	3105.7725
3116.9552	3125.3681	3189.3916

p3, C_s, ¹A'

6	0	-2.497817	-0.194376	-0.000081
6	0	-1.246966	0.164856	0.000064
6	0	0.015734	0.524038	0.000093
6	0	1.140868	-0.407567	0.000078
6	0	2.423626	-0.032686	-0.000083
1	0	-3.046891	-0.350952	-0.925810
1	0	-3.047166	-0.351077	0.925438
1	0	0.252330	1.588276	0.000162
1	0	0.888272	-1.465254	0.000199
1	0	3.226780	-0.760655	-0.000093
1	0	2.714005	1.014070	-0.000322

Frequencies

128.6648	166.1215	347.7932
401.9535	507.6400	568.5394
731.4523	869.4481	903.7782
919.8823	923.4832	1021.4790
1030.5881	1117.3237	1192.8015
1318.2218	1344.3802	1452.9101
1494.0295	1686.6520	2035.7348
3105.7778	3114.7545	3134.3633

3152.3162 3173.2942 3221.3942

p4, C_s, ¹A'

6	0	0.534359	-1.062117	0.000042
6	0	1.498651	0.121478	-0.000168
6	0	0.518068	1.045864	0.000006
6	0	-0.552437	0.036009	0.000255
6	0	-1.882004	0.030344	-0.000133
1	0	0.554012	-1.697982	-0.891018
1	0	0.554407	-1.697349	0.891570
1	0	2.581033	0.179846	-0.000569
1	0	0.509659	2.130706	0.000514
1	0	-2.444653	-0.897645	-0.000102
1	0	-2.454277	0.952953	-0.000407

Frequencies

219.6216	346.3393	491.5043
706.1112	717.6776	773.9944
874.5550	878.7935	912.3367
938.8758	975.7586	1020.7172
1106.2067	1111.7806	1191.4664
1220.0940	1320.5431	1451.4861
1486.5685	1592.3423	1740.4855
3034.0189	3075.0580	3131.6679
3179.7111	3210.9853	3211.6255

p5, C_{2v}, ¹A₁

6	0	1.181322	-0.272975	0.000338
6	0	0.727847	0.994273	0.000106
6	0	-0.741114	0.984520	-0.000059
6	0	-1.177507	-0.288684	-0.000080
6	0	0.008109	-1.215833	-0.000016
1	0	2.215632	-0.592729	-0.000265
1	0	1.335894	1.891560	-0.000683
1	0	-1.361078	1.873585	0.000143
1	0	-2.207441	-0.622301	0.000448
1	0	0.013086	-1.878139	-0.876888
1	0	0.011961	-1.879778	0.875509

Frequencies

349.4174	521.4491	678.9551
704.1414	817.9793	819.7035
921.6188	925.3197	940.9081
942.0991	972.7377	1013.6376
1115.3978	1133.2492	1137.7369
1274.8306	1321.0652	1404.7178
1431.5497	1556.6425	1643.8042
3015.1893	3035.2267	3184.8479
3195.3132	3213.9413	3220.7796

p6, C_s, ¹A'

6	0	2.184841	-0.459797	0.000417
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6	0	1.083919	0.234051	-0.000811
6	0	-0.026527	0.932333	-0.000249
6	0	-1.397106	0.394185	0.000350
6	0	-1.748395	-0.893883	-0.000152
1	0	2.669530	-0.764426	-0.924595
1	0	2.667868	-0.762898	0.926838
1	0	0.064645	2.017764	-0.000305
1	0	-2.179881	1.149258	0.001379
1	0	-1.011343	-1.691084	-0.001189
1	0	-2.791209	-1.189946	0.000539

Frequencies

62.5193	151.6007	320.0225
394.9380	502.1432	656.1715
713.7252	866.7064	909.2917
913.7683	924.4344	1021.8746
1023.2850	1055.9846	1161.0927
1344.1389	1385.6667	1454.1760
1486.1395	1685.7322	2032.3349
3103.8464	3120.9419	3137.0130
3150.5625	3170.9233	3223.4803

p7, C_{2v}, ¹A₁

6	0	1.494067	0.762275	-0.000095
6	0	1.494269	-0.762150	-0.000117
6	0	0.226447	-0.000123	0.000277
6	0	-1.058833	-0.000198	0.000261
6	0	-2.365990	0.000074	-0.000131
1	0	1.783047	1.274967	0.913043
1	0	1.782453	1.275106	-0.913345
1	0	1.782938	-1.274842	-0.913372
1	0	1.783452	-1.274585	0.913132
1	0	-2.936137	-0.000025	0.925069
1	0	-2.935515	0.000113	-0.925702

Frequencies

185.3946	187.3977	368.9275
561.7255	566.0530	651.4645
779.5575	842.2678	933.2625
936.2030	1009.3500	1031.9106
1049.4251	1070.1438	1088.5983
1179.7254	1373.6994	1465.0666
1480.0041	1544.8297	2107.1665
3101.7821	3102.5578	3113.8233
3174.7486	3183.0247	3189.0583

Intermediates

i1, C₁, ¹A

6	0	2.288265	0.657820	-0.000005
6	0	1.477863	-0.606339	0.000052
1	0	2.466020	1.187964	0.927897
1	0	2.467571	1.187022	-0.928144

1	0	1.727257	-1.215898	-0.876907
1	0	1.727219	-1.215792	0.877108
6	0	0.032266	-0.335009	0.000039
6	0	-1.144547	-0.080584	0.000033
6	0	-2.571468	0.221372	-0.000008
1	0	-3.038893	-0.061698	0.947922
1	0	-2.751029	1.290318	-0.150005
1	0	-3.092413	-0.315482	-0.798534

Frequencies

25.0971	91.3661	127.4193
197.3995	291.3774	381.2467
463.6284	571.6792	745.5827
780.4665	1042.3699	1061.4431
1062.9018	1096.3492	1153.6019
1294.2792	1321.3529	1431.8406
1467.0569	1485.5884	1498.4652
1498.5593	2350.7478	3010.9068
3024.7163	3039.6632	3078.6137
3079.1912	3140.8889	3246.9948

i2, C₁, ¹A

6	0	-2.399951	0.487194	0.000477
6	0	-1.340100	-0.572603	0.001864
6	0	0.007077	-0.310185	-0.001525
6	0	1.207181	-0.069870	-0.006771
6	0	2.634542	0.209635	0.002048
1	0	-3.051664	0.399126	-0.878279
1	0	-1.967259	1.488708	0.000426
1	0	-1.663089	-1.611031	0.005061
1	0	3.193740	-0.549627	-0.554192
1	0	2.854399	1.181856	-0.450203
1	0	3.034712	0.226237	1.022642
1	0	-3.053329	0.399707	0.877990

Frequencies

17.8957	78.7730	134.7538
171.8081	305.4275	390.8366
534.6272	581.3148	733.2365
981.6293	1014.1412	1041.7795
1059.3579	1109.5417	1238.9884
1416.1093	1419.0351	1433.4677
1490.1188	1493.1595	1494.5976
1514.5101	2149.8115	2998.1976
3009.8082	3030.1157	3056.7073
3073.8572	3109.8021	3140.0830

i3, C_s, ²A'

6	0	-0.602569	0.954419	0.000075
6	0	-1.666602	-0.201492	0.000070
6	0	-0.427579	-1.071374	-0.000199
6	0	0.501033	-0.118058	-0.000037

6	0	1.982208	-0.014071	0.000000
1	0	-0.631618	1.581505	-0.897255
1	0	-0.631554	1.581312	0.897545
1	0	-2.294039	-0.256971	0.892273
1	0	-2.294139	-0.256753	-0.892076
1	0	2.344573	0.530187	-0.879319
1	0	2.344665	0.528398	0.880391
1	0	2.443168	-1.004218	-0.001014

Frequencies

152.9762	212.9875	314.5903
406.3108	650.2554	807.3783
847.1772	879.8139	990.4285
997.7135	1030.1953	1057.5808
1104.1248	1130.5530	1170.0126
1206.7255	1245.2527	1423.9253
1475.8793	1494.3407	1498.7281
1503.9955	1700.5028	3014.6650
3019.3643	3059.5515	3059.6757
3072.4881	3103.4360	3106.9243

i4, C_s, ²A'

6	0	-2.100748	0.710885	-0.000006
6	0	-1.486984	-0.475615	0.000012
6	0	-0.035019	-0.712230	-0.000017
6	0	0.927852	0.187177	0.000017
6	0	2.391543	0.266486	0.000003
1	0	-3.182525	0.783808	0.000022
1	0	-1.544396	1.643091	-0.000056
1	0	-2.098069	-1.375844	0.000051
1	0	2.767495	0.797848	-0.880928
1	0	2.767517	0.797776	0.880967
1	0	2.844073	-0.737815	-0.000046
1	0	0.266043	-1.769082	-0.000062

Frequencies

17.3942	161.7137	170.2754
210.8171	336.6416	594.0050
616.4883	812.3662	871.1628
919.1050	1005.7045	1023.5762
1039.3748	1052.8037	1130.7563
1313.3407	1345.6393	1413.4904
1453.6684	1469.8396	1490.3503
1676.6492	1737.8713	2962.5330
2999.1632	3044.0132	3065.0680
3134.5019	3143.6795	3221.9623

i5, C_s, ²A''

6	0	-2.077996	-0.622064	0.000134
6	0	-1.361571	0.539174	0.000120
6	0	0.047250	0.689254	-0.000296
6	0	1.007415	-0.354182	-0.000257

6	0	2.351281	-0.158505	0.000274
1	0	-3.161299	-0.606420	0.000322
1	0	-1.609830	-1.600288	-0.000048
1	0	-1.929867	1.467593	0.000352
1	0	0.432857	1.706217	-0.000554
1	0	3.047181	-0.989170	0.000292
1	0	0.643859	-1.379704	-0.000933
1	0	2.778822	0.839711	0.000717

Frequencies

140.3470	219.6396	236.0154
396.6513	576.2881	612.7927
621.3443	810.2525	834.9941
865.0951	923.4160	993.9130
1006.7881	1044.8268	1102.1672
1198.4038	1274.7032	1319.1819
1387.2661	1453.8754	1490.2144
1555.8896	1599.7731	3128.6356
3135.1311	3140.7146	3149.7473
3153.8103	3226.8577	3231.7040

i6, C_s, 2A''

6	0	-0.636770	-1.050700	0.000132
6	0	-1.602785	0.137835	-0.000553
6	0	-0.539427	1.043429	0.000155
6	0	0.441100	0.046786	0.001128
6	0	1.923057	0.002390	-0.000288
1	0	-0.664375	-1.689900	0.890310
1	0	-0.662812	-1.689037	-0.890783
1	0	-2.681103	0.221817	-0.000503
1	0	2.315773	-0.533119	0.874367
1	0	2.314276	-0.523762	-0.881385
1	0	2.353353	1.007389	0.004545
1	0	-0.486158	2.128174	0.000005

Frequencies

115.9174	204.4059	313.5536
407.3383	491.5221	648.9638
866.1406	879.9623	932.2882
938.1144	983.6047	1032.8148
1054.7651	1097.6392	1168.6245
1207.1977	1265.9238	1368.3132
1419.9289	1463.9160	1485.7267
1493.2072	1535.6806	2990.7120
3019.1845	3019.8327	3054.8683
3087.1638	3172.2644	3222.8819

i7, C_s, 2A''

6	0	1.644522	-0.857151	0.114435
6	0	1.283954	0.436240	-0.105834
6	0	-0.000056	1.038010	-0.000033
6	0	-1.284055	0.436306	0.105674

1	0	2.677052	-1.167107	0.000458
1	0	0.948696	-1.610394	0.460699
1	0	2.087089	1.126844	-0.360431
1	0	-0.000045	2.125146	0.000684
1	0	-2.087270	1.126853	0.360187
6	0	-1.644396	-0.857284	-0.114346
1	0	-0.948494	-1.610487	-0.460574
1	0	-2.676841	-1.167577	-0.000394

Frequencies

131.4346	243.2599	276.3547
378.2287	570.6494	589.8829
699.8784	799.1252	858.9677
864.0971	901.8146	983.0130
999.3600	1015.0480	1129.5670
1183.6625	1271.9681	1319.9803
1424.7333	1458.9882	1481.6036
1566.7283	1608.2827	3117.9844
3123.0181	3149.9586	3151.7990
3159.6657	3234.7608	3245.9855

i8, C_{2v}, ²B₁

6	0	-0.971144	0.779378	0.000105
6	0	0.491373	1.145554	-0.000027
6	0	1.274042	0.000256	-0.000014
6	0	0.491897	-1.145400	0.000050
6	0	-0.970877	-0.779724	-0.000115
1	0	-1.492560	1.187841	0.874846
1	0	-1.492822	1.188260	-0.874303
1	0	0.859133	2.164185	-0.000355
1	0	2.359045	0.000526	0.000104
1	0	0.859927	-2.163923	0.000182
1	0	-1.492370	-1.188733	0.874342
1	0	-1.492104	-1.188541	-0.874810

Frequencies

123.3985	449.5643	589.1850
628.7035	728.6058	809.7195
811.6027	908.2287	912.7549
938.2719	999.8375	1029.8342
1074.8056	1107.6384	1155.1607
1234.1435	1283.7912	1308.2313
1323.3094	1407.0676	1484.9853
1486.2507	1508.3013	3000.6401
3010.5385	3014.3774	3033.4642
3178.7623	3200.8294	3212.8516

i9, C₁, ¹A

6	0	1.899691	0.682555	-0.153016
6	0	1.344921	-0.533038	0.099453
6	0	-0.033914	-0.803289	-0.097932
6	0	-1.012165	0.108340	0.404529

6	0	-2.210690	0.179966	-0.217939
1	0	1.283009	1.556175	-0.338770
1	0	2.966452	0.796952	-0.320018
1	0	2.011840	-1.388623	0.214381
1	0	-0.801005	0.797790	1.230613
1	0	-2.443813	-0.515718	-1.016732
1	0	-2.943536	0.946216	0.019960

Frequencies

76.8546	181.5283	271.5523
351.7344	459.8707	681.8327
714.1864	876.7780	908.8932
960.6529	991.6463	1010.9743
1049.6789	1112.9804	1279.0171
1310.5675	1328.7039	1430.4383
1446.0937	1567.8124	1613.1988
3033.9176	3105.3683	3130.1829
3134.7083	3217.0264	3233.9782

i10, C_s, ¹A'

6	0	2.497705	-0.194507	0.000145
6	0	1.246926	0.164982	0.000165
6	0	-0.015732	0.524341	0.000128
6	0	-1.140747	-0.407481	-0.000114
6	0	-2.423591	-0.032903	-0.000264
1	0	3.046858	-0.351260	-0.925495
1	0	3.046813	-0.351526	0.925771
1	0	-0.252358	1.588544	0.000239
1	0	-0.887885	-1.465097	-0.000204
1	0	-3.226590	-0.761044	-0.000484
1	0	-2.714210	1.013787	-0.000187

Frequencies

128.6602	166.1351	347.8241
401.9350	507.6192	568.5615
731.4593	869.4492	903.7062
919.8570	923.4752	1021.4832
1030.5796	1117.2865	1192.7059
1318.1900	1344.3368	1452.9084
1493.9940	1686.6494	2035.6997
3105.7645	3115.0159	3134.3630
3152.3867	3173.2835	3221.3814

i11, C_s, ¹A'

6	0	2.184841	-0.459797	0.000417
6	0	1.083919	0.234051	-0.000811
6	0	-0.026527	0.932333	-0.000249
6	0	-1.397106	0.394185	0.000350
6	0	-1.748395	-0.893883	-0.000152
1	0	2.669530	-0.764426	-0.924595
1	0	2.667868	-0.762898	0.926838
1	0	0.064645	2.017764	-0.000305

1	0	-2.179881	1.149258	0.001379
1	0	-1.011343	-1.691084	-0.001189
1	0	-2.791209	-1.189946	0.000539

Frequencies

62.5193	151.6007	320.0225
394.9380	502.1432	656.1715
713.7252	866.7064	909.2917
913.7683	924.4344	1021.8746
1023.2850	1055.9846	1161.0927
1344.1389	1385.6667	1454.1760
1486.1395	1685.7322	2032.3349
3103.8464	3120.9419	3137.0130
3150.5625	3170.9233	3223.4803

i12, C₁, ¹A

6	0	-2.241216	-0.131670	0.068287
6	0	-0.927239	-0.368599	-0.083675
6	0	0.054867	0.679499	-0.034642
6	0	1.425029	0.491624	-0.057571
6	0	1.933474	-0.817453	0.031592
1	0	-2.975927	-0.923849	-0.022831
1	0	-2.622222	0.859421	0.298950
1	0	-0.327591	1.695737	0.067308
1	0	2.043378	1.396936	-0.058444
1	0	-0.547633	-1.368570	-0.268206
1	0	2.960507	-0.780085	0.439276

Frequencies

140.0756	246.6940	273.8385
397.6968	473.3084	621.2836
670.8267	881.6230	942.4640
959.5706	998.9138	1050.9007
1070.6903	1109.6898	1205.9229
1255.8101	1306.2696	1415.2648
1486.1333	1552.8097	1663.0042
2963.9707	3033.5865	3128.4711
3134.9705	3182.1207	3224.9065

i13, C₁, ¹A

6	0	-1.678806	-0.666687	0.318155
6	0	-1.164620	0.361031	-0.416185
6	0	0.000010	1.037066	0.000015
1	0	-1.108939	-1.111499	1.125840
1	0	-2.713535	-0.979907	0.213084
1	0	-1.782898	0.814067	-1.190965
6	0	1.164603	0.361024	0.416189
6	0	1.678822	-0.666626	-0.318201
1	0	1.782794	0.813888	1.191122
1	0	1.109007	-1.111432	-1.125929
1	0	2.713513	-0.979958	-0.212985

Frequencies

131.1141	220.1593	270.7440
423.0526	535.2423	612.7921
767.2402	876.7220	908.8984
937.5597	943.1908	993.5179
1043.3998	1114.8836	1303.2866
1308.1686	1342.5473	1423.9227
1463.2672	1551.9825	1568.0228
3116.9522	3117.8269	3135.2657
3136.3894	3230.0223	3230.3721

i14, C₁, ¹A

6	0	-0.764664	0.897763	-0.210528
6	0	-1.104006	-0.548923	0.077213
6	0	-0.000303	-1.342816	0.000008
6	0	1.103737	-0.549364	-0.077307
6	0	0.765072	0.897412	0.210542
1	0	-1.398687	1.583284	0.362407
1	0	-0.847450	1.193232	-1.263912
1	0	-2.066654	-0.837777	0.493247
1	0	2.066395	-0.838655	-0.492948
1	0	0.848009	1.192720	1.263952
1	0	1.399371	1.582769	-0.362316

Frequencies

220.7227	404.7667	602.0977
609.9614	795.8698	844.2964
877.6538	880.8425	933.3874
955.9878	1031.7894	1126.9170
1175.6573	1207.1872	1225.0967
1280.5302	1314.7263	1436.9621
1478.4719	1499.6507	1549.9015
3017.1894	3017.5492	3056.9077
3065.2012	3149.1803	3151.5028

i15, C₁, ¹A

6	0	1.105415	-0.640780	0.209717
6	0	0.888618	0.819404	0.003070
6	0	-0.449484	1.079498	-0.182542
6	0	-1.358689	-0.127016	0.271440
6	0	-0.292346	-0.817458	-0.379230
1	0	1.201787	-0.977847	1.248952
1	0	1.895827	-1.103938	-0.386105
1	0	1.660879	1.578232	-0.119481
1	0	-2.334178	-0.139639	-0.203107
1	0	-1.417050	-0.178974	1.358094
1	0	-0.368340	-1.059729	-1.433082

Frequencies

242.3878	412.2271	491.2915
544.0247	649.6578	809.2293
896.2513	931.5056	948.7042

999.6102	1049.7270	1091.7964
1139.4439	1183.2783	1236.9517
1261.0040	1279.3522	1411.1007
1492.1640	1513.9867	1519.4654
3012.9975	3079.4359	3095.2405
3114.4895	3176.0759	3195.0938

i16, C₁, ¹A

6	0	0.130521	0.844982	0.081501
6	0	1.482037	0.194651	-0.092227
6	0	1.989521	-0.995388	-0.133954
6	0	-2.073569	-0.298900	-0.277419
6	0	-0.958141	-0.136608	0.424517
1	0	-0.124270	1.394419	-0.830659
1	0	0.219312	1.594635	0.878017
1	0	2.378444	0.832366	-0.222763
1	0	-2.833598	-1.012506	0.022080
1	0	-2.272699	0.272360	-1.180131
1	0	-0.789399	-0.733698	1.318946

Frequencies

81.8377	131.3614	155.1149
335.2826	427.4946	545.8995
646.9833	849.7441	901.5935
941.0771	948.1791	1012.5654
1027.5279	1147.4323	1259.5032
1324.5574	1343.9402	1460.4560
1486.7127	1718.9561	1792.3281
2979.6778	3017.0001	3058.5129
3129.1699	3140.8993	3214.4181

i17, C_s, ¹A'

6	0	-1.329406	0.123647	-0.000196
6	0	-1.487932	-1.163183	0.000237
6	0	1.431915	-0.865804	-0.000079
6	0	1.185875	0.437006	-0.000015
6	0	-0.170191	1.085148	0.000114
1	0	-2.353916	0.533561	-0.000829
1	0	2.442887	-1.258967	-0.000070
1	0	2.018521	1.138654	0.000011
1	0	-0.260486	1.748088	-0.870438
1	0	-0.260527	1.747452	0.871161
1	0	0.631956	-1.609679	-0.000200

Frequencies

139.5972	179.4997	219.6322
340.6595	526.8435	586.2635
588.8070	843.5027	926.6353
929.8582	965.8756	994.4932
1014.4862	1081.0927	1240.7783
1321.8466	1369.7867	1460.6026
1478.9122	1720.6259	1779.6371

3011.7626	3020.0298	3026.8523
3061.8964	3135.5537	3198.0356

Transition states

TS i2_p1, C₁, ²A

6	0	2.327038	0.350558	-0.268096
6	0	1.381948	-0.543276	0.058352
6	0	-0.014577	-0.275306	0.026709
6	0	-1.200395	-0.068495	0.010978
6	0	-2.633104	0.193988	-0.010595
1	0	3.376105	0.078297	-0.260309
1	0	2.069970	1.337615	-0.635941
1	0	1.676350	-1.537180	0.386881
1	0	-3.159848	-0.447564	0.700092
1	0	-2.842110	1.234308	0.250904
1	0	-3.049023	0.007736	-1.004367
1	0	2.763095	1.381974	1.658651

Frequencies

455.1315i	71.7138	134.7601
153.1992	232.6918	272.3847
335.9403	412.1280	549.8892
723.8608	732.8306	953.6737
1002.4521	1057.6642	1062.1866
1071.3775	1205.4851	1322.8455
1433.4576	1453.7029	1501.5912
1504.0002	1661.7534	2368.2148
3053.0493	3120.9401	3129.1166
3166.8936	3179.1468	3264.6642

TS i1_i2, C₁, ²A

6	0	2.415954	0.539516	0.047078
6	0	1.382264	-0.539498	0.001529
6	0	-0.004067	-0.283741	0.019143
6	0	-1.195671	-0.065774	0.008455
6	0	-2.629308	0.191616	0.002061
1	0	3.432287	0.279941	0.306305
1	0	2.106587	1.573711	0.007451
1	0	1.989628	-0.155339	-1.037486
1	0	1.725964	-1.540235	0.244275
1	0	-3.144364	-0.410162	0.757946
1	0	-2.843714	1.242485	0.219622
1	0	-3.081412	-0.043113	-0.967710

Frequencies

1915.4340i	21.7053	133.0822
176.5031	308.2868	330.3486
475.3504	521.1165	627.3663
714.4908	780.3501	1006.5881
1054.2968	1060.6249	1105.7329
1228.9923	1261.1813	1401.3951
1429.6764	1434.4112	1493.4854

1497.9780	2168.3522	2286.6377
3015.1603	3062.3185	3074.7064
3152.4319	3160.8849	3285.2249

TS i1_i3, C_s, ²A'

6	0	1.056734	1.055424	-0.000074
6	0	1.625004	-0.365051	0.000151
6	0	0.287301	-1.033532	-0.000191
6	0	-0.710406	-0.261543	-0.000069
6	0	-2.114378	0.145433	0.000079
1	0	1.080711	1.623551	0.924327
1	0	1.080626	1.623183	-0.924706
1	0	2.226756	-0.607467	-0.880762
1	0	2.226232	-0.607375	0.881443
1	0	-2.365242	0.734718	0.886365
1	0	-2.365058	0.736017	-0.885394
1	0	-2.749552	-0.747011	-0.000646

Frequencies

714.3000 <i>i</i>	116.6511	177.0583
232.9853	292.0664	476.1543
623.6566	747.9255	808.2940
827.4436	980.8935	1015.9509
1055.7597	1086.2884	1114.3642
1220.6349	1274.0820	1415.3082
1436.8829	1479.8441	1497.5145
1500.1080	1911.0748	3024.7697
3042.1642	3074.0152	3083.6210
3088.7443	3113.8612	3225.0400

TS i1_i4, C₁, ²A

6	0	-2.416056	0.520105	-0.004630
6	0	-1.460217	-0.466218	-0.066122
6	0	-0.034419	-0.262459	-0.008769
6	0	1.162166	-0.014967	-0.145661
6	0	2.595418	0.176851	0.025746
1	0	-3.466833	0.261059	-0.030592
1	0	-2.150407	1.559821	0.140566
1	0	-0.670933	-0.753876	1.173259
1	0	-1.765335	-1.486196	-0.288142
1	0	3.165082	-0.455031	-0.662722
1	0	2.879528	1.213379	-0.180984
1	0	2.927545	-0.059025	1.045232

Frequencies

1626.0971 <i>i</i>	73.1473	122.4105
137.3819	313.6731	406.0116
529.7625	603.2648	641.3662
707.4805	747.5373	829.8161
1032.8195	1048.4076	1061.2707
1065.9894	1188.9712	1308.5219
1424.6441	1433.6864	1490.2850

1493.4650	1553.4272	2172.7982
2996.5580	3054.4442	3076.8165
3139.7761	3153.1091	3247.9421

TS i4_p1, C_s, ²A'

6	0	2.302754	-0.621595	0.000081
6	0	1.504679	0.451522	-0.000134
6	0	0.073636	0.379796	-0.000007
6	0	-1.078548	-0.019821	-0.000053
6	0	-2.507523	-0.279340	-0.000012
1	0	3.381283	-0.510112	-0.000048
1	0	1.906625	-1.631015	0.000393
1	0	1.942763	1.444887	-0.000424
1	0	-0.309541	2.269601	0.000826
1	0	-2.810967	-0.848754	-0.883773
1	0	-2.810783	-0.849490	0.883336
1	0	-3.069364	0.661503	0.000436

Frequencies

643.7849i	16.0886	87.1182
147.2772	196.4159	337.4294
399.1672	527.1600	610.1888
696.0325	717.4437	934.5572
1012.8077	1044.6430	1051.7024
1060.8923	1202.5503	1332.8996
1425.4803	1451.4596	1487.3443
1491.0445	1668.5651	2235.0876
3017.6825	3071.7931	3080.3592
3144.9053	3165.5691	3234.2738

TS i2_p2, C₁, ²A

6	0	-2.372256	0.486770	-0.007869
6	0	-1.300664	-0.558634	0.080779
6	0	-0.012124	-0.318919	-0.020431
6	0	1.224394	-0.077308	-0.119449
6	0	2.515080	0.171587	-0.202619
1	0	-3.065874	0.259162	-0.823671
1	0	-1.950061	1.477922	-0.176005
1	0	-2.961643	0.511665	0.914556
1	0	-1.623161	-1.586597	0.240105
1	0	3.246738	-0.629056	-0.162556
1	0	2.883947	1.175082	-0.389785
1	0	3.143481	0.570852	2.014888

Frequencies

374.1942i	131.7611	139.6858
166.3844	184.9955	266.6547
317.1979	534.0058	540.5406
589.3891	809.4870	859.8930
892.3789	1042.1819	1048.2618
1065.0497	1128.8366	1323.4431
1425.5381	1461.0728	1505.8864

1509.9632	1713.5909	2189.9144
3044.8789	3103.2615	3144.5314
3152.3123	3161.4471	3236.6830

TS i4_i5, C₁, ²A

6	0	2.014039	-0.718591	0.035204
6	0	1.416127	0.486977	0.067607
6	0	0.006949	0.761121	-0.112300
6	0	-0.977111	-0.158891	-0.294564
6	0	-2.316255	-0.232902	0.127903
1	0	3.080005	-0.821740	0.202493
1	0	1.458029	-1.624192	-0.184841
1	0	2.037163	1.360463	0.258022
1	0	-0.282464	1.814922	-0.171742
1	0	-3.002641	-0.908577	-0.375595
1	0	-1.391666	-1.116507	0.487408
1	0	-2.760917	0.469343	0.841155

1787.4289i	150.0953	182.8898
200.9152	328.9447	504.9027
625.3356	666.8807	816.5259
885.7285	907.7672	948.8430
1012.3083	1043.4596	1061.9804
1159.0661	1182.4492	1324.3978
1350.8206	1451.1165	1493.5609
1526.8393	1648.5546	2142.2827
3020.7993	3055.3319	3134.0513
3141.9589	3161.5684	3225.3452

TS i3_i6, C₁, ²A

6	0	-0.597113	1.049418	0.008274
6	0	-1.553680	-0.135957	-0.032049
6	0	-0.527470	-1.153176	-0.113139
6	0	0.451365	-0.060880	-0.013831
6	0	1.929626	-0.043587	0.009625
1	0	-0.643810	1.697987	-0.876029
1	0	-0.621783	1.687849	0.898166
1	0	-1.306005	-1.009233	0.915772
1	0	-2.632218	-0.212121	-0.147174
1	0	2.348351	0.534383	-0.825516
1	0	2.315268	0.426629	0.925883
1	0	2.323828	-1.060400	-0.044385

Frequencies

1233.8396i	95.0019	163.5845
322.8532	389.1484	640.0288
747.7264	866.7429	876.4911
930.0729	946.8588	1002.4386
1027.7889	1111.6486	1165.2500
1224.5085	1241.2756	1313.8368
1353.4502	1414.9333	1464.5329
1480.4125	1492.8847	2094.7123

2982.9866	3012.0886	3014.5513
3060.6989	3104.7709	3157.3533

TS i4_i6, C₁, ²A

6	0	-1.295338	-0.986853	-0.077283
6	0	-1.524893	0.395079	0.075281
6	0	-0.252408	1.008700	-0.114856
1	0	-1.857705	-1.733017	0.486524
1	0	-0.872324	-1.360349	-1.001118
1	0	-2.402929	0.840831	0.534172
1	0	-0.024387	2.036115	-0.397624
6	0	0.620158	0.000850	0.130424
6	0	2.076395	-0.232827	0.042198
1	0	2.495123	-0.567242	0.997693
1	0	2.310740	-1.007921	-0.695767
1	0	2.608003	0.681890	-0.258462

Frequencies

690.8638i	130.0488	234.2471
252.7724	457.5432	627.8148
666.8348	756.2711	873.2861
914.8565	929.0850	1007.2579
1040.3270	1045.8165	1070.2426
1192.0573	1299.7673	1405.0010
1410.9692	1472.7581	1488.2515
1525.4872	1588.4826	2979.6294
3046.1886	3060.2748	3092.2481
3119.9371	3161.8103	3194.9711

TS i5_i7, C₁, ²A

6	0	-1.728819	-0.878998	0.053662
6	0	-1.342088	0.430642	-0.149693
6	0	-0.054676	0.936944	0.000790
1	0	-2.758756	-1.186041	-0.082329
1	0	-1.016088	-1.641418	0.346239
1	0	-2.109548	1.139165	-0.457004
1	0	0.105637	1.997229	-0.182345
6	0	1.109174	0.149434	0.460296
6	0	1.984152	-0.462453	-0.334884
1	0	1.255157	0.086061	1.541459
1	0	2.827860	-1.013172	0.069264
1	0	1.889276	-0.435232	-1.416313

Frequencies

168.4178i	209.1495	242.2837
438.6149	502.5384	521.7312
674.4822	722.1376	797.3508
915.8922	948.2212	987.0610
1010.7785	1035.9200	1086.2238
1170.9448	1235.8155	1323.2581
1414.0887	1448.1237	1469.8148
1530.9041	1694.8746	3080.0420

3125.9348	3130.1336	3143.4631
3151.0550	3212.4426	3240.2754

TS i5_p3, C₁, ²A

6	0	2.446479	-0.279163	-0.091644
6	0	1.219205	0.157663	-0.027847
6	0	-0.055972	0.477145	-0.201560
6	0	-1.171586	-0.395894	0.123113
6	0	-2.456817	-0.048970	-0.021310
1	0	3.146983	-0.181596	0.730592
1	0	2.810872	-0.759475	-0.997537
1	0	1.370633	1.186580	1.812406
1	0	-0.291958	1.478917	-0.559763
1	0	-0.918192	-1.384769	0.496966
1	0	-3.259577	-0.735855	0.220518
1	0	-2.746616	0.931509	-0.387698

Frequencies

535.7194i	109.0942	132.0522
180.5769	394.5771	410.0850
434.1939	527.7824	577.3346
726.1459	883.8120	896.8376
920.9558	926.4479	1017.8247
1028.2215	1108.5018	1194.5195
1318.6706	1343.8199	1452.2266
1488.3948	1668.1700	1979.9752
3113.7229	3121.3108	3137.3352
3157.2277	3195.4103	3225.1671

TS i7_i8, C₁, ²A

6	0	1.186883	-0.832485	0.232129
6	0	1.166216	0.484051	-0.170582
6	0	-0.068699	1.202424	0.084055
6	0	-1.181006	0.435036	0.087253
6	0	-1.057282	-1.010569	-0.198724
1	0	1.900741	-1.536623	-0.188726
1	0	0.788421	-1.116545	1.198286
1	0	1.885332	0.869437	-0.889306
1	0	-0.110351	2.283927	0.176637
1	0	-2.162616	0.876021	0.259335
1	0	-1.070517	-1.318896	-1.243441
1	0	-1.507684	-1.728064	0.482432

Frequencies

664.0256i	211.1516	405.5334
451.2543	509.8537	641.0945
713.4212	731.6345	773.3953
867.8536	933.1978	958.1684
987.0691	1011.5938	1047.5376
1072.7464	1167.4681	1248.4852
1379.0849	1429.7879	1456.3026
1542.9448	1598.2682	3089.3519

3115.8509	3124.3808	3145.9614
3170.7307	3173.5753	3204.3919

TS i6_p4, C₁, ²A

6	0	-0.589442	-1.061573	-0.013451
6	0	-1.555454	0.112791	0.073065
6	0	-0.590326	1.044826	-0.011070
6	0	0.474677	0.040660	-0.106390
6	0	1.807931	0.037630	-0.183888
1	0	-0.522185	-1.688985	0.878713
1	0	-0.680722	-1.691963	-0.901105
1	0	-2.633108	0.161530	0.169987
1	0	-0.587312	2.127980	-0.007001
1	0	2.358961	-0.891025	-0.278271
1	0	2.369846	0.961488	-0.263059
1	0	2.410209	-0.025030	1.851137

Frequencies

467.4144i	165.9846	205.5651
290.8743	344.4019	496.5250
719.9974	758.5257	796.8401
886.0091	922.3448	929.7243
963.8891	989.5787	1020.7205
1114.2315	1116.3767	1206.2035
1223.0591	1334.6128	1451.7850
1487.4349	1619.7200	1727.0274
3075.0837	3127.9909	3155.5985
3208.9634	3239.3431	3246.3072

TS i8_p5, C₁, ²A

6	0	-1.158357	0.017926	-0.143116
6	0	-0.405645	1.140787	-0.107615
6	0	0.999308	0.774147	0.040445
6	0	1.108635	-0.565103	0.061524
6	0	-0.250860	-1.179115	-0.089608
1	0	-1.774566	0.029768	1.933299
1	0	-2.222021	-0.037670	-0.331185
1	0	-0.778051	2.156100	-0.166479
1	0	1.814091	1.483392	0.120620
1	0	2.022171	-1.136062	0.165976
1	0	-0.497198	-1.866559	0.726505
1	0	-0.322914	-1.760812	-1.018506

Frequencies

508.4633i	232.6940	298.9192
377.1882	526.0279	694.5577
770.5335	819.5560	822.2006
920.1854	939.1052	961.3748
968.1171	984.9154	1031.7064
1114.3274	1136.5456	1148.1800
1287.1151	1333.7608	1415.8275
1439.7872	1549.8819	1653.1867

3051.3095	3099.9399	3220.0401
3231.1576	3248.8938	3255.9883

TS i7_p6, C₁, ²A

6	0	-2.136084	-0.492168	-0.156938
6	0	-1.057128	0.220938	0.007391
6	0	0.060503	0.925816	-0.073949
6	0	1.422671	0.387720	-0.090554
6	0	1.771710	-0.895289	0.052509
1	0	-2.729608	-0.858013	0.674232
1	0	-2.482100	-0.741115	-1.158391
1	0	-1.174056	0.451799	2.143516
1	0	-0.034604	2.010491	-0.088674
1	0	2.203897	1.130877	-0.231493
1	0	1.035236	-1.675988	0.214383
1	0	2.811202	-1.200155	0.015667

Frequencies

498.6004i	73.7314	129.1269
161.7628	375.9380	398.0426
410.5682	522.5301	655.1662
711.9156	880.4026	899.6266
920.1778	926.3654	1017.1987
1018.7858	1051.4993	1154.4379
1340.4570	1385.0246	1453.4387
1477.4355	1670.8337	1982.1035
3111.4180	3126.1568	3139.7751
3152.8866	3191.8228	3227.3212

TS i1_p1, C₁, ²A

6	0	-2.356525	-0.554186	0.036307
6	0	-1.431621	0.416562	-0.168981
6	0	-0.022744	0.204186	-0.079792
6	0	1.171100	0.041617	-0.034166
6	0	2.612004	-0.158390	0.034661
1	0	-2.078361	-1.530703	0.414786
1	0	-3.410073	-0.358436	-0.124666
1	0	-1.745447	1.346789	-0.636690
1	0	-1.611386	1.481524	1.454478
1	0	2.963354	-0.144431	1.071001
1	0	2.901214	-1.120014	-0.399746
1	0	3.147416	0.626536	-0.507341

Frequencies

746.7916i	32.5389	139.7541
172.5366	322.9905	349.0111
412.0885	437.1067	537.6796
671.6971	721.1210	889.5501
1024.0141	1050.7239	1059.5875
1064.0525	1190.8712	1302.0614
1430.0129	1447.1485	1495.2409
1495.5360	1596.2585	2341.0204

3026.1037	3079.9850	3084.1646
3139.6569	3150.1644	3243.8613

TS i1_p7, C_s, ²A'

6	0	-1.510576	0.810040	-0.000057
6	0	-1.629255	-0.705403	0.000037
6	0	-0.306890	-0.047596	-0.000022
6	0	0.970552	-0.141543	0.000008
6	0	2.286098	-0.177346	0.000032
1	0	-1.751462	1.341440	-0.915256
1	0	-1.751433	1.341555	0.915082
1	0	-1.951743	-1.192515	0.914874
1	0	-1.951776	-1.192623	-0.914732
1	0	2.841393	-0.275770	-0.927175
1	0	2.841361	-0.275660	0.927271
1	0	2.864087	1.824665	-0.000049

Frequencies

513.4156i	156.2699	177.1858
233.0303	313.1771	370.5872
569.2306	658.9576	676.2946
789.8832	901.8050	933.4300
950.7775	1016.7176	1042.1825
1058.9950	1079.0459	1093.6082
1190.7174	1367.8828	1468.9383
1485.3687	1544.6976	2109.7687
3135.5624	3138.3192	3153.0426
3218.1077	3231.8241	3237.2924

TS p1_i9, C₁, ¹A

6	0	2.342442	0.510879	0.059514
6	0	1.416351	-0.474596	-0.027832
6	0	0.045391	-0.298440	-0.188436
6	0	-1.189188	-0.139471	0.038223
6	0	-2.553911	0.239138	-0.093800
1	0	2.063458	1.558344	0.068922
1	0	3.399747	0.276170	0.067846
1	0	1.763737	-1.507435	-0.065598
1	0	-1.458716	-0.209866	1.149507
1	0	-2.814261	1.283344	-0.230330
1	0	-3.320475	-0.425618	0.283635

Frequencies

833.3676i	101.3902	150.9472
257.6607	326.4471	488.0054
544.5989	580.7431	666.4332
764.0316	794.1218	848.9501
976.3891	1043.6237	1067.7131
1249.6470	1308.6267	1453.3605
1465.2434	1604.5149	2002.2963
2665.8739	3113.9526	3137.9945
3148.6052	3238.0132	3239.1298

TS i9_i10, C₁, ¹A

6	0	2.489194	0.119350	-0.189351
6	0	1.209421	-0.106983	0.075772
6	0	-0.061740	-0.516302	0.130212
6	0	-1.199050	0.401058	0.096487
6	0	-2.424304	-0.073585	-0.153705
1	0	2.854436	0.001463	-1.202487
1	0	3.190403	0.424651	0.574888
1	0	0.789474	-0.291434	1.224212
1	0	-1.047894	1.478485	0.194151
1	0	-2.592970	-1.140638	-0.252335
1	0	-3.274570	0.586246	-0.294922

Frequencies

808.8255i	63.5329	168.4580
355.9364	431.8686	536.7202
548.8807	705.6063	724.4337
862.1774	885.8593	990.0917
1007.2399	1081.8705	1113.4335
1216.9459	1329.6033	1436.6303
1464.3800	1666.4778	1867.0169
2262.0889	3081.6591	3140.9354
3158.3894	3231.5467	3245.2986

TS i10_i11, C₁, ¹A

6	0	2.343730	-0.406353	0.130687
6	0	1.179732	0.131537	-0.100192
6	0	0.013703	0.670787	-0.332543
6	0	-1.242942	0.294979	0.379806
6	0	-2.153230	-0.546621	-0.098957
1	0	3.019524	-0.000623	0.879011
1	0	2.683848	-1.282898	-0.414312
1	0	-0.053566	1.462037	-1.080939
1	0	-1.410384	0.771344	1.345286
1	0	-2.026024	-1.043401	-1.056091
1	0	-3.059355	-0.772433	0.454239

Frequencies

154.0185i	179.4887	301.0425
358.0214	498.3091	613.2659
694.6721	860.7164	874.9515
921.9422	950.2100	1013.2348
1029.0418	1088.0065	1153.0222
1325.3124	1340.3552	1449.6822
1484.6809	1700.2818	2054.3647
3097.1365	3114.9003	3118.4977
3133.6964	3184.7445	3214.4743

TS i11_i12, C₁, ¹A

6	0	-2.121331	0.265950	0.107747
6	0	-0.822776	-0.088655	-0.145641

6	0	0.125617	0.931305	-0.096078
6	0	1.429559	0.408768	0.079386
6	0	1.544972	-0.947940	-0.066944
1	0	-2.654221	-1.139099	-0.255514
1	0	-2.683977	0.417310	0.739314
1	0	-0.097505	1.985084	-0.232162
1	0	2.275129	1.055655	0.312953
1	0	-0.052854	-1.046488	-0.369591
1	0	2.277181	-1.497627	0.534171

Frequencies

1097.2722 <i>i</i>	244.2033	342.8084
424.1996	475.7972	664.7558
736.0946	787.0722	876.7381
893.8683	943.7594	958.0513
1005.2966	1077.0155	1130.3121
1169.4036	1195.0092	1380.8759
1466.5881	1490.4650	1721.6570
1831.5311	3079.2929	3116.8428
3128.9041	3180.4368	3196.8222

TS i12_p5, C₁, ¹A

6	0	1.931255	-0.458119	-0.313166
6	0	1.051594	0.193139	0.440098
6	0	-0.159497	0.888666	-0.041508
6	0	-1.408600	0.344782	-0.125286
6	0	-1.607043	-1.020818	0.211548
1	0	2.819510	-0.904172	0.120581
1	0	1.792325	-0.582859	-1.382385
1	0	1.232915	0.296071	1.511177
1	0	-0.017595	1.913762	-0.389092
1	0	-2.203198	0.989870	-0.518904
1	0	-2.470216	-1.398572	-0.371490

Frequencies

240.5498 <i>i</i>	205.9290	234.6041
365.8134	438.7771	507.1942
700.1238	838.2837	918.0924
938.6363	973.2317	993.6023
1074.8706	1091.2854	1144.0307
1233.7416	1314.9200	1431.7920
1465.6432	1576.3170	1708.0891
2944.1485	3033.0861	3107.9122
3111.8890	3138.6287	3222.0028

TS i9_i13, C₁, ¹A

6	0	1.510096	0.870480	0.169964
6	0	1.360649	-0.449617	-0.074869
6	0	0.069556	-1.073160	-0.213620
1	0	0.665623	1.484311	0.467259
1	0	2.463010	1.375194	0.032284
1	0	2.237728	-1.038687	-0.339622

6	0	-1.121181	-0.471077	0.253838
6	0	-1.748645	0.652503	-0.174369
1	0	-1.692924	-1.136435	0.909207
1	0	-1.319805	1.289069	-0.940908
1	0	-2.776486	0.851777	0.106114

Frequencies

220.4711 <i>i</i>	184.6999	249.8227
393.8817	466.6459	610.6447
733.5730	818.1952	876.1199
942.5098	1005.0634	1032.1618
1036.2737	1094.4293	1270.1636
1293.0517	1343.0995	1433.0043
1462.5714	1577.3289	1601.6378
3068.6857	3118.5855	3129.4908
3136.8892	3218.0341	3223.7436

TS i13_i14, C₁, ¹A

6	0	1.094211	-0.831374	-0.322985
6	0	1.098966	0.483709	0.209290
6	0	0.000032	1.298569	-0.000011
6	0	-1.098941	0.483748	-0.209281
6	0	-1.094254	-0.831321	0.323004
1	0	1.850953	-1.548485	0.000309
1	0	0.702339	-1.031111	-1.310771
1	0	1.924309	0.769547	0.862982
1	0	-1.924231	0.769583	-0.863024
1	0	-0.702470	-1.031071	1.310821
1	0	-1.850983	-1.548442	-0.000417

Frequencies

471.4690 <i>i</i>	339.9278	448.4303
560.1148	673.6019	686.9734
724.5266	892.0580	931.5127
959.2705	988.8936	1003.1529
1015.1351	1138.2509	1163.8984
1197.6461	1306.1393	1389.4086
1462.5218	1519.0999	1526.7075
3095.4106	3096.1164	3117.6310
3117.8368	3227.7024	3227.7643

TS i14_i15, C₁, ¹A

6	0	-0.619057	1.021263	0.011193
6	0	-1.166135	-0.406670	0.051996
6	0	-0.217371	-1.380414	-0.051659
6	0	1.059861	-0.584082	-0.039991
6	0	0.841064	0.837452	-0.047321
1	0	-0.977175	1.811060	0.683591
1	0	-0.884642	1.356541	-1.009508
1	0	-2.240313	-0.558711	-0.002275
1	0	2.054062	-1.002167	-0.186420
1	0	1.069144	-0.154073	1.070254

1	0	1.588756	1.622056	-0.100947
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Frequencies

977.2674i	358.8121	485.1896
614.9816	703.6479	784.7415
805.8309	857.8909	877.9707
886.6630	927.9955	987.3493
1035.2632	1039.2717	1223.4587
1242.2881	1269.6261	1314.3677
1351.0251	1398.3561	1444.2162
2427.0069	2964.4718	3034.9801
3148.6154	3161.5424	3190.4527

TS i15_i16, C₁, ¹A

6	0	1.197809	0.478617	0.045514
6	0	0.217079	1.363628	-0.216526
6	0	-0.640285	-0.676061	-0.386069
6	0	0.752856	-0.942697	0.174379
6	0	-1.482178	0.141387	0.287063
1	0	2.229880	0.828752	0.078829
1	0	-0.820459	-0.905484	-1.431582
1	0	1.324928	-1.643483	-0.439897
1	0	0.743406	-1.328884	1.200972
1	0	-2.370260	0.541884	-0.185723
1	0	-1.379182	0.317972	1.351230

Frequencies

266.9294i	275.4210	335.0871
444.0050	650.9071	734.3985
790.3895	925.4443	937.7015
967.1524	979.9531	999.9746
1097.8234	1136.7979	1205.2719
1298.8802	1313.7900	1451.4715
1500.9978	1592.9886	1634.8810
3015.8501	3071.7685	3120.9374
3155.7607	3179.9009	3244.5840

TS i16_i17, C₁, ¹A

6	0	-1.375117	0.079931	0.084658
6	0	-1.661902	-1.131006	-0.273349
6	0	-0.185940	1.001795	0.151715
1	0	-2.366317	0.446308	0.421311
1	0	-0.408550	1.893982	-0.440852
1	0	-0.074470	1.353913	1.184208
6	0	1.683046	-0.693134	0.220057
6	0	1.108037	0.369904	-0.330091
1	0	2.611859	-1.096498	-0.168599
1	0	1.246034	-1.212548	1.068654
1	0	1.582698	0.849906	-1.182662

Frequencies

143.2436i	114.7243	152.4744
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301.6002	463.4210	553.3920
650.7021 <i>i</i>	843.0894	911.6097
936.8535	954.5132	1011.7154
1015.3797	1121.2083	1253.6237
1342.2549	1361.8615	1457.4701
1496.7691	1714.5651	1797.0185
2968.6888	3025.2990	3063.7828
3131.3961	3148.1267	3215.5641

TS i17_p5, C_s, ¹A'

6	0	1.248113	0.013245	0.000006
6	0	0.888618	-1.255838	-0.000005
6	0	-1.157909	-0.772342	-0.000008
6	0	-1.085495	0.544633	-0.000025
6	0	0.273845	1.163890	-0.000004
1	0	2.315347	0.225690	0.000038
1	0	-2.036912	-1.410516	0.000112
1	0	-1.975045	1.172211	0.000029
1	0	0.420379	1.812339	0.875124
1	0	0.420461	1.812434	-0.875045
1	0	-0.147259	-1.773688	-0.000046

Frequencies

1123.8655 <i>i</i>	321.9649	419.2117
474.1546	522.5805	654.3117
704.6967	778.0634	813.8329
880.4673	916.8535	964.7284
972.8015	1053.6996	1179.3394
1193.7741	1267.4413	1335.2285
1462.2691	1631.4910	1675.0588
2652.4760	3007.6517	3025.8793
3134.9430	3149.3892	3180.5767