**Table III.**  B3LYP/cc-pVTZ calculated harmonic frequencies and infrared intensities of RDX decomposition species on the adiabatic singlet ground state potential energy surface.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **RDX** | | **i1** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 29.76 | 8.734 | 56.18 | 6.1487 |
| ν2 | 47.83 | 2.0036 | 60.72 | 0.3159 |
| ν3 | 63.46 | 2.3436 | 104.25 | 2.005 |
| ν4 | 78.46 | 0.2617 | 116.57 | 0.1376 |
| ν5 | 87.22 | 1.5664 | 156.46 | 4.2034 |
| ν6 | 118.29 | 0.9456 | 177.16 | 3.082 |
| ν7 | 205.22 | 3.1277 | 226.26 | 8.6251 |
| ν8 | 230.78 | 5.5047 | 312.8 | 1.7093 |
| ν9 | 249.7 | 1.7434 | 342.73 | 2.267 |
| ν10 | 338.05 | 1.437 | 396.29 | 0.8466 |
| ν11 | 360.36 | 3.9289 | 491.89 | 16.8395 |
| ν12 | 392.71 | 2.5485 | 557.9 | 3.7067 |
| ν13 | 415.02 | 1.4919 | 614.5 | 8.0332 |
| ν14 | 428.22 | 5.8062 | 624.98 | 4.521 |
| ν15 | 453.67 | 12.831 | 717.26 | 4.6658 |
| ν16 | 593.94 | 18.8045 | 767.16 | 7.9923 |
| ν17 | 607.48 | 21.0429 | 782.1 | 13.9221 |
| ν18 | 613.42 | 1.7884 | 832.65 | 20.1645 |
| ν19 | 645.42 | 4.5259 | 878.56 | 33.6642 |
| ν20 | 684.05 | 0.0335 | 933.89 | 124.1048 |
| ν21 | 763.35 | 1.1631 | 948.26 | 0.8453 |
| ν22 | 774.69 | 4.234 | 1001.18 | 0.5968 |
| ν23 | 779.65 | 44.8987 | 1004.73 | 244.3582 |
| ν24 | 795.32 | 9.8922 | 1033.21 | 152.8938 |
| ν25 | 847.78 | 2.4809 | 1061.84 | 103.0595 |
| ν26 | 868.66 | 26.348 | 1192.22 | 13.3066 |
| ν27 | 893.28 | 9.3538 | 1228.53 | 5.2746 |
| ν28 | 921.77 | 364.2882 | 1250.85 | 14.6375 |
| ν29 | 941.55 | 4.2217 | 1276.15 | 544.7074 |
| ν30 | 979.31 | 33.6716 | 1301.12 | 248.4076 |
| ν31 | 1017.07 | 181.4937 | 1310.66 | 99.6955 |
| ν32 | 1136.66 | 59.2749 | 1341.53 | 85.6041 |
| ν33 | 1151.39 | 91.2138 | 1385.92 | 7.5609 |
| ν34 | 1185.57 | 23.7189 | 1394.7 | 22.0378 |
| ν35 | 1228.5 | 25.8059 | 1433.01 | 28.8986 |
| ν36 | 1240.36 | 29.2388 | 1499.21 | 4.406 |
| ν37 | 1283.05 | 212.7402 | 1525.78 | 3.9805 |
| ν38 | 1295.97 | 258.9685 | 1615.09 | 217.6986 |
| ν39 | 1301.26 | 361.4362 | 1645.79 | 422.776 |
| ν40 | 1315.46 | 47.5426 | 1729.62 | 126.702 |
| ν41 | 1338.24 | 55.2666 | 2997.23 | 20.7383 |
| ν42 | 1354.61 | 22.5569 | 3009.21 | 20.5948 |
| ν43 | 1379.23 | 1.1924 | 3118.32 | 0.4289 |
| ν44 | 1408.32 | 29.1051 | 3184.69 | 6.2826 |
| ν45 | 1417.68 | 43.9747 | 3205.97 | 2.5881 |
| ν46 | 1493.21 | 51.5968 |  |  |
| ν47 | 1499.85 | 33.3449 |  |  |
| ν48 | 1513.06 | 13.352 |  |  |
| ν49 | 1622.19 | 197.2842 |  |  |
| ν50 | 1645.57 | 210.3287 |  |  |
| ν51 | 1646.02 | 479.0827 |  |  |
| ν52 | 3051.36 | 8.5695 |  |  |
| ν53 | 3076.99 | 10.3326 |  |  |
| ν54 | 3117.05 | 0.2252 |  |  |
| ν55 | 3164.46 | 7.5657 |  |  |
| ν56 | 3186.16 | 10.2461 |  |  |
| ν57 | 3189.37 | 3.2475 |  |  |
|  | **i2** | | **i3** | |
| ν1 | 44.1 | 3.0671 | 352.85 | 0 |
| ν2 | 111.73 | 2.5568 | 352.85 | 0 |
| ν3 | 161.71 | 0.0828 | 693.37 | 16.9269 |
| ν4 | 260.37 | 5.8798 | 693.37 | 16.9274 |
| ν5 | 341.79 | 0.4499 | 760.92 | 32.5027 |
| ν6 | 392.58 | 0.2646 | 956.07 | 0.0108 |
| ν7 | 549.35 | 1.024 | 1011.13 | 0 |
| ν8 | 592.95 | 30.8193 | 1049.27 | 0 |
| ν9 | 610.9 | 24.3073 | 1049.27 | 0 |
| ν10 | 702.51 | 0.163 | 1160.65 | 0 |
| ν11 | 769.12 | 9.8339 | 1166.57 | 0 |
| ν12 | 844.88 | 28.4888 | 1197.15 | 0.8359 |
| ν13 | 904.23 | 92.3904 | 1197.15 | 0.8365 |
| ν14 | 956.35 | 1.6974 | 1403.59 | 0 |
| ν15 | 989.79 | 143.6497 | 1443.41 | 71.921 |
| ν16 | 1012.49 | 1.2616 | 1443.41 | 71.9164 |
| ν17 | 1048.16 | 187.0982 | 1594.06 | 135.9882 |
| ν18 | 1082.6 | 8.5487 | 1594.06 | 135.9873 |
| ν19 | 1128.22 | 14.3755 | 3160.57 | 24.4705 |
| ν20 | 1259.29 | 245.0796 | 3160.57 | 24.4712 |
| ν21 | 1274.78 | 0 | 3165.81 | 0 |
| ν22 | 1303.9 | 366.7484 |  |  |
| ν23 | 1378.02 | 35.232 |  |  |
| ν24 | 1402.99 | 8.7991 |  |  |
| ν25 | 1432.31 | 11.179 |  |  |
| ν26 | 1518.58 | 1.0946 |  |  |
| ν27 | 1617.37 | 83.3818 |  |  |
| ν28 | 1646.85 | 339.9683 |  |  |
| ν29 | 1710.16 | 157.1705 |  |  |
| ν30 | 3040.83 | 17.7057 |  |  |
| ν31 | 3068.07 | 8.766 |  |  |
| ν32 | 3159.63 | 23.4002 |  |  |
| ν33 | 3199.9 | 3.379 |  |  |
|  | **i4** | | **i5** | |
| ν1 | 29.94 | 0.0406 | 49.48 | 2.2593 |
| ν2 | 39.88 | 6.7333 | 57.42 | 2.8551 |
| ν3 | 56.7 | 0.0083 | 90.62 | 1.3052 |
| ν4 | 65.81 | 0.0711 | 105.42 | 0.1142 |
| ν5 | 97.33 | 0.0157 | 137.04 | 7.2155 |
| ν6 | 119.96 | 0.7905 | 204.24 | 3.427 |
| ν7 | 165.47 | 1.171 | 231.48 | 5.5692 |
| ν8 | 174.08 | 8.2145 | 315.14 | 9.3763 |
| ν9 | 209.89 | 1.2374 | 348.61 | 4.8958 |
| ν10 | 222.88 | 6.0771 | 365.24 | 1.6539 |
| ν11 | 266.22 | 7.8056 | 426.04 | 26.4634 |
| ν12 | 292.85 | 18.3808 | 456.22 | 16.3828 |
| ν13 | 339.35 | 15.5039 | 483.99 | 0.6058 |
| ν14 | 351.96 | 11.2969 | 506.44 | 5.8426 |
| ν15 | 363.58 | 0.2304 | 604.69 | 15.5402 |
| ν16 | 439.34 | 4.9814 | 636.53 | 9.019 |
| ν17 | 446.18 | 15.1467 | 695.77 | 5.4013 |
| ν18 | 537.93 | 113.4037 | 744.99 | 11.8032 |
| ν19 | 611.99 | 65.8335 | 777.45 | 11.1673 |
| ν20 | 650.82 | 2.873 | 798.03 | 40.4526 |
| ν21 | 702.04 | 2.0741 | 807.09 | 11.7821 |
| ν22 | 750.07 | 224.044 | 871.31 | 107.8031 |
| ν23 | 775.63 | 1.9527 | 896.48 | 52.1462 |
| ν24 | 778.71 | 27.8302 | 918.81 | 10.0295 |
| ν25 | 822.44 | 63.819 | 990.76 | 215.0885 |
| ν26 | 887.84 | 13.0179 | 998.03 | 200.4734 |
| ν27 | 904.43 | 19.5391 | 1049.42 | 0.335 |
| ν28 | 956.75 | 18.9515 | 1160.79 | 18.3415 |
| ν29 | 999.09 | 320.8779 | 1222.63 | 21.3015 |
| ν30 | 1000.83 | 116.5283 | 1256.13 | 1.9651 |
| ν31 | 1038.38 | 4.7572 | 1282.77 | 455.0211 |
| ν32 | 1059.29 | 5.4607 | 1302.98 | 160.473 |
| ν33 | 1067.99 | 90.4169 | 1316.06 | 261.7621 |
| ν34 | 1160.98 | 7.7243 | 1322.62 | 9.6906 |
| ν35 | 1222.78 | 20.7291 | 1336.69 | 45.7379 |
| ν36 | 1234.34 | 10.1006 | 1362.23 | 10.4203 |
| ν37 | 1267.15 | 244.6208 | 1375.5 | 16.4506 |
| ν38 | 1281.53 | 366.0812 | 1420.46 | 46.0327 |
| ν39 | 1294.44 | 51.2907 | 1492.18 | 18.6056 |
| ν40 | 1303.45 | 79.0461 | 1506.96 | 16.3407 |
| ν41 | 1335.5 | 61.6404 | 1624.07 | 309.7545 |
| ν42 | 1338.97 | 190.6071 | 1640.08 | 24.4067 |
| ν43 | 1365.9 | 3.1085 | 1666.43 | 361.0923 |
| ν44 | 1419.5 | 2.2633 | 3026.73 | 18.5359 |
| ν45 | 1432.05 | 35.5929 | 3051.35 | 7.8014 |
| ν46 | 1512.21 | 2.8904 | 3166.52 | 2.5574 |
| ν47 | 1512.36 | 9.6065 | 3195.82 | 16.1458 |
| ν48 | 1526.18 | 4.1196 | 3267.14 | 14.9767 |
| ν49 | 1618.84 | 167.1853 |  |  |
| ν50 | 1631.08 | 459.9117 |  |  |
| ν51 | 1846.72 | 442.2349 |  |  |
| ν52 | 2930.97 | 7.6831 |  |  |
| ν53 | 2935.67 | 70.7631 |  |  |
| ν54 | 2957.86 | 48.2242 |  |  |
| ν55 | 3172.07 | 3.7473 |  |  |
| ν56 | 3174.16 | 0.3143 |  |  |
| ν57 | 3201.7 | 10.6209 |  |  |
|  | **i6** | | **i7** | |
| ν1 | 50.71 | 1.8649 | 41.49 | 1.8922 |
| ν2 | 60.21 | 3.9513 | 61.64 | 2.2592 |
| ν3 | 82.82 | 0.854 | 75.01 | 0.5523 |
| ν4 | 85.53 | 0.939 | 82.29 | 0.1898 |
| ν5 | 154.5 | 3.009 | 128.44 | 0.6409 |
| ν6 | 244.22 | 2.9658 | 171.58 | 0.8197 |
| ν7 | 281.78 | 6.0845 | 247.04 | 1.0186 |
| ν8 | 356.48 | 4.9305 | 315.87 | 5.593 |
| ν9 | 388.87 | 0.826 | 381.53 | 2.481 |
| ν10 | 424.56 | 16.8611 | 412.75 | 2.7315 |
| ν11 | 435.02 | 8.5225 | 444.86 | 52.3392 |
| ν12 | 491.7 | 11.2015 | 466.65 | 0.2239 |
| ν13 | 553.28 | 2.4306 | 498.57 | 30.0935 |
| ν14 | 593.33 | 19.5222 | 544.09 | 11.6077 |
| ν15 | 629 | 14.1801 | 595.38 | 6.6042 |
| ν16 | 682.09 | 0.8189 | 616.9 | 12.0122 |
| ν17 | 710.72 | 7.4033 | 649.54 | 2.6804 |
| ν18 | 768.35 | 7.032 | 737.71 | 39.3741 |
| ν19 | 777.6 | 16.2927 | 761 | 9.2371 |
| ν20 | 804.85 | 12.3423 | 776.44 | 0.1877 |
| ν21 | 839.43 | 53.5102 | 801.23 | 56.9279 |
| ν22 | 868.23 | 8.1621 | 833.51 | 46.311 |
| ν23 | 906.48 | 75.0515 | 884.89 | 86.5751 |
| ν24 | 940.57 | 115.7516 | 941.5 | 96.1471 |
| ν25 | 957.02 | 76.9408 | 990.65 | 56.7735 |
| ν26 | 995.5 | 271.043 | 1032.05 | 132.9844 |
| ν27 | 1044.21 | 27.2773 | 1051.81 | 146.9209 |
| ν28 | 1153.42 | 6.985 | 1167 | 24.9902 |
| ν29 | 1188.02 | 5.5156 | 1177.6 | 57.5568 |
| ν30 | 1210.29 | 14.3222 | 1226.54 | 191.71 |
| ν31 | 1254.3 | 20.4668 | 1262.48 | 342.744 |
| ν32 | 1293.57 | 239.0825 | 1297.27 | 29.1732 |
| ν33 | 1297.26 | 4.9548 | 1306.66 | 115.1093 |
| ν34 | 1301.36 | 270.2444 | 1329.68 | 184.1388 |
| ν35 | 1331.01 | 225.5396 | 1353.06 | 19.8056 |
| ν36 | 1346.57 | 11.2814 | 1403.23 | 19.1517 |
| ν37 | 1380.12 | 17.6269 | 1423.21 | 7.9897 |
| ν38 | 1413.12 | 7.465 | 1477.34 | 1.0303 |
| ν39 | 1439.6 | 16.9731 | 1502.96 | 59.6537 |
| ν40 | 1475.84 | 39.3003 | 1517.67 | 35.0567 |
| ν41 | 1492.55 | 26.0485 | 1653.24 | 172.3142 |
| ν42 | 1641.51 | 225.4255 | 1664.04 | 347.0832 |
| ν43 | 1653.9 | 406.424 | 1821.52 | 518.4556 |
| ν44 | 3068.37 | 7.8014 | 3024.28 | 31.1311 |
| ν45 | 3089.96 | 7.7504 | 3070.02 | 15.8846 |
| ν46 | 3166.59 | 6.4952 | 3154.75 | 1.6905 |
| ν47 | 3200.61 | 0.3561 | 3199.32 | 4.2659 |
| ν48 | 3213.01 | 9.2889 | 3612.94 | 60.8994 |
|  | **i8** | | **i9** | |
| ν1 | 65.09 | 0.1382 | 131.06 | 7.005 |
| ν2 | 85.13 | 0.3111 | 363.9 | 0.3341 |
| ν3 | 117.22 | 3.7928 | 493.07 | 2.7718 |
| ν4 | 171.5 | 2.4201 | 504.7 | 31.6941 |
| ν5 | 253.4 | 0.224 | 572.51 | 0.9293 |
| ν6 | 354.11 | 4.656 | 681.33 | 1.7674 |
| ν7 | 458.82 | 47.5679 | 737.38 | 41.1156 |
| ν8 | 469.19 | 19.18 | 818.7 | 36.1643 |
| ν9 | 516.88 | 4.7212 | 840.98 | 5.271 |
| ν10 | 566.53 | 35.7178 | 981.87 | 1.1628 |
| ν11 | 596.13 | 7.1624 | 984.51 | 16.5513 |
| ν12 | 652.42 | 10.8867 | 1041.46 | 0.1018 |
| ν13 | 744.89 | 28.2201 | 1058.59 | 18.6898 |
| ν14 | 774.92 | 14.8589 | 1134.29 | 36.7437 |
| ν15 | 829.56 | 15.0311 | 1221.41 | 39.6133 |
| ν16 | 903.81 | 107.2805 | 1395.15 | 63.301 |
| ν17 | 951.78 | 8.1835 | 1421.09 | 39.2649 |
| ν18 | 981.2 | 19.0292 | 1464.88 | 10.4754 |
| ν19 | 1033.2 | 58.1697 | 1551.82 | 258.4857 |
| ν20 | 1101.22 | 133.2625 | 1661.24 | 176.3489 |
| ν21 | 1111.28 | 6.7371 | 1812.63 | 629.7093 |
| ν22 | 1179.07 | 33.0417 | 3149.76 | 23.7822 |
| ν23 | 1211.48 | 444.2186 | 3156.76 | 5.1875 |
| ν24 | 1279.43 | 18.5981 | 3582.08 | 57.3427 |
| ν25 | 1310.12 | 222.9127 |  |  |
| ν26 | 1408.68 | 2.1397 |  |  |
| ν27 | 1439.62 | 19.6988 |  |  |
| ν28 | 1468.66 | 66.5208 |  |  |
| ν29 | 1515.1 | 15.6603 |  |  |
| ν30 | 1647.44 | 179.7335 |  |  |
| ν31 | 1754.32 | 228.048 |  |  |
| ν32 | 1831.31 | 493.315 |  |  |
| ν33 | 3022.55 | 20.9346 |  |  |
| ν34 | 3121.37 | 4.1272 |  |  |
| ν35 | 3150.39 | 14.6012 |  |  |
| ν36 | 3622.85 | 78.9362 |  |  |
|  | **i10** | | **i11** | |
| ν1 | 187.83 | 0.1679 | 51.32 | 0.4587 |
| ν2 | 375.57 | 1.0607 | 56.89 | 2.1952 |
| ν3 | 459.02 | 14.9335 | 77.63 | 0.8038 |
| ν4 | 558.77 | 52.1013 | 112.37 | 0.2138 |
| ν5 | 596.44 | 1.0945 | 199.37 | 3.7591 |
| ν6 | 598.34 | 48.7657 | 210.16 | 6.7759 |
| ν7 | 713.13 | 14.1468 | 238.32 | 3.6175 |
| ν8 | 850.69 | 36.7426 | 267.39 | 10.8594 |
| ν9 | 910.96 | 31.7822 | 332.77 | 6.0739 |
| ν10 | 995.84 | 2.0166 | 371.26 | 3.9523 |
| ν11 | 1007.8 | 15.9402 | 379.94 | 7.1975 |
| ν12 | 1049.6 | 0.0113 | 440.23 | 49.3913 |
| ν13 | 1152.64 | 61.1737 | 523.1 | 51.2144 |
| ν14 | 1182.71 | 1.067 | 543.93 | 7.0742 |
| ν15 | 1245.46 | 58.5985 | 599.21 | 12.2199 |
| ν16 | 1362.79 | 104.8003 | 620.38 | 17.1694 |
| ν17 | 1391.97 | 0.6263 | 650.67 | 1.657 |
| ν18 | 1424.62 | 42.4833 | 743.03 | 11.5442 |
| ν19 | 1489.51 | 321.0502 | 772.83 | 23.3391 |
| ν20 | 1600.68 | 333.3035 | 780.48 | 3.0185 |
| ν21 | 1622.1 | 223.6954 | 821.43 | 44.0232 |
| ν22 | 3162.48 | 23.1985 | 842.23 | 13.7239 |
| ν23 | 3166.03 | 9.2984 | 860.95 | 121.7952 |
| ν24 | 3760.99 | 98.3031 | 916.45 | 100.6876 |
| ν25 |  |  | 1004.46 | 272.8773 |
| ν26 |  |  | 1032.39 | 137.7314 |
| ν27 |  |  | 1048.39 | 20.5361 |
| ν28 |  |  | 1148.15 | 61.4822 |
| ν29 |  |  | 1191.07 | 46.1063 |
| ν30 |  |  | 1241.83 | 3.625 |
| ν31 |  |  | 1261.99 | 35.7662 |
| ν32 |  |  | 1277.14 | 267.5635 |
| ν33 |  |  | 1296.96 | 311.9107 |
| ν34 |  |  | 1306.26 | 91.5636 |
| ν35 |  |  | 1336.51 | 192.0303 |
| ν36 |  |  | 1374.06 | 29.586 |
| ν37 |  |  | 1420.78 | 1.2426 |
| ν38 |  |  | 1433.73 | 51.6585 |
| ν39 |  |  | 1501.8 | 15.5093 |
| ν40 |  |  | 1513.42 | 16.5152 |
| ν41 |  |  | 1612.8 | 248.513 |
| ν42 |  |  | 1676.46 | 365.019 |
| ν43 |  |  | 1758.15 | 373.9896 |
| ν44 |  |  | 3015.29 | 21.3264 |
| ν45 |  |  | 3033.59 | 20.1521 |
| ν46 |  |  | 3101.44 | 1.9334 |
| ν47 |  |  | 3200.08 | 12.3034 |
| ν48 |  |  | 3768.38 | 109.1528 |
|  | **i12** | | **tsi1** | |
| ν1 | 47.43 | 1.1501 | -1490.59 | 92.559 |
| ν2 | 77.08 | 0.8673 | 33.68 | 1.0477 |
| ν3 | 180.7 | 1.3869 | 49.42 | 0.2613 |
| ν4 | 275.71 | 0.0403 | 62.79 | 0.6236 |
| ν5 | 293.51 | 9.4844 | 82.41 | 0.0521 |
| ν6 | 344.44 | 9.3595 | 112.9 | 0.2285 |
| ν7 | 470.18 | 52.8788 | 127.35 | 2.1655 |
| ν8 | 489.03 | 74.0808 | 157.16 | 10.3627 |
| ν9 | 605.47 | 110.5799 | 206.96 | 3.0754 |
| ν10 | 628.56 | 55.0591 | 256.65 | 4.2427 |
| ν11 | 681.19 | 9.645 | 301.13 | 7.3435 |
| ν12 | 717.61 | 706.8151 | 348.21 | 0.0858 |
| ν13 | 768.66 | 55.4305 | 381.76 | 1.0456 |
| ν14 | 918.04 | 27.5629 | 407.37 | 6.5182 |
| ν15 | 967.37 | 3.1941 | 449.33 | 13.4141 |
| ν16 | 997.02 | 15.9245 | 472.4 | 27.0069 |
| ν17 | 1027.68 | 3.2614 | 512.6 | 3.1479 |
| ν18 | 1041.6 | 43.1783 | 554.17 | 4.8841 |
| ν19 | 1083.65 | 47.7162 | 598.28 | 7.8031 |
| ν20 | 1121.19 | 31.8735 | 604.83 | 8.3061 |
| ν21 | 1228.4 | 45.6003 | 640.78 | 8.8327 |
| ν22 | 1318.9 | 14.3933 | 686.44 | 13.156 |
| ν23 | 1384.69 | 72.8084 | 766.12 | 8.092 |
| ν24 | 1405.45 | 71.1872 | 770.86 | 6.7871 |
| ν25 | 1412.65 | 3.1888 | 810.22 | 77.8611 |
| ν26 | 1532.37 | 80.7342 | 821.42 | 17.8725 |
| ν27 | 1586.31 | 212.8841 | 867.67 | 0.9928 |
| ν28 | 1685.21 | 260.1496 | 911.41 | 58.2815 |
| ν29 | 1776.03 | 260.6913 | 928.94 | 36.7072 |
| ν30 | 3066.87 | 17.1199 | 933.88 | 162.5865 |
| ν31 | 3143.05 | 31.8768 | 963.74 | 62.2134 |
| ν32 | 3147.13 | 8.7511 | 1006.22 | 119.2534 |
| ν33 | 3610.71 | 38.3418 | 1031.87 | 68.4422 |
| ν34 |  |  | 1177.58 | 13.7533 |
| ν35 |  |  | 1199.96 | 15.2591 |
| ν36 |  |  | 1263.17 | 28.3395 |
| ν37 |  |  | 1277.94 | 133.9738 |
| ν38 |  |  | 1286.06 | 48.0223 |
| ν39 |  |  | 1291.71 | 282.6637 |
| ν40 |  |  | 1311.62 | 73.8371 |
| ν41 |  |  | 1319.28 | 138.2022 |
| ν42 |  |  | 1345.7 | 15.2053 |
| ν43 |  |  | 1365.03 | 183.4387 |
| ν44 |  |  | 1374.76 | 32.2139 |
| ν45 |  |  | 1408.08 | 19.5892 |
| ν46 |  |  | 1435.75 | 43.4688 |
| ν47 |  |  | 1480.84 | 29.2097 |
| ν48 |  |  | 1489.45 | 35.5134 |
| ν49 |  |  | 1559.63 | 208.3698 |
| ν50 |  |  | 1622.28 | 273.2635 |
| ν51 |  |  | 1646.99 | 325.9829 |
| ν52 |  |  | 1760.99 | 151.2273 |
| ν53 |  |  | 3026.57 | 4.8929 |
| ν54 |  |  | 3057.41 | 19.0375 |
| ν55 |  |  | 3066.45 | 2.9389 |
| ν56 |  |  | 3160.75 | 5.3367 |
| ν57 |  |  | 3192.78 | 11.9064 |
|  | **tsi1i2** | | **tsi2i3** | |
| ν1 | -1487.25 | 155.4532 | -972.19 | 125.1593 |
| ν2 | 35.88 | 3.235 | 79.62 | 0.8799 |
| ν3 | 74.56 | 0.048 | 120.65 | 1.2987 |
| ν4 | 121.35 | 0.3182 | 193.46 | 1.5435 |
| ν5 | 124.74 | 0.9632 | 225.79 | 6.5533 |
| ν6 | 142.18 | 4.9812 | 312.32 | 3.8331 |
| ν7 | 193.32 | 1.7348 | 409.85 | 2.0859 |
| ν8 | 244.27 | 13.9398 | 447.09 | 10.5266 |
| ν9 | 277.33 | 9.2969 | 534.49 | 0.6053 |
| ν10 | 381.56 | 2.2771 | 656.12 | 25.5666 |
| ν11 | 397.45 | 6.4266 | 677.14 | 18.6737 |
| ν12 | 458.96 | 10.5876 | 778.69 | 20.1415 |
| ν13 | 512.93 | 6.1132 | 809.2 | 166.1886 |
| ν14 | 559.09 | 0.1279 | 932.1 | 3.273 |
| ν15 | 623.24 | 13.2035 | 965.41 | 1.8403 |
| ν16 | 663.07 | 6.5108 | 1024.09 | 18.0266 |
| ν17 | 695.46 | 6.8934 | 1027.74 | 1.52 |
| ν18 | 776.52 | 14.8881 | 1082.03 | 10.9376 |
| ν19 | 818.65 | 98.643 | 1102.05 | 8.3957 |
| ν20 | 835.82 | 25.0251 | 1113.28 | 19.8007 |
| ν21 | 918.81 | 32.8773 | 1239.33 | 39.9389 |
| ν22 | 965.32 | 12.1487 | 1284.4 | 54.4648 |
| ν23 | 990.73 | 19.1338 | 1336.98 | 64.7843 |
| ν24 | 1018.32 | 20.0956 | 1353.73 | 146.3781 |
| ν25 | 1042.9 | 99.2184 | 1410.57 | 11.6917 |
| ν26 | 1053.67 | 57.715 | 1414.84 | 51.7489 |
| ν27 | 1154.18 | 39.7664 | 1468.75 | 15.7218 |
| ν28 | 1229.14 | 5.9797 | 1589.39 | 125.2144 |
| ν29 | 1262.84 | 128.8191 | 1670.25 | 320.8568 |
| ν30 | 1272.83 | 23.2501 | 1724.27 | 258.776 |
| ν31 | 1305.74 | 307.6414 | 3039.5 | 4.059 |
| ν32 | 1309.35 | 177.5123 | 3159.45 | 16.0768 |
| ν33 | 1351.03 | 125.1575 | 3163.26 | 13.696 |
| ν34 | 1378.05 | 81.3299 |  |  |
| ν35 | 1404.15 | 24.3707 |  |  |
| ν36 | 1473.61 | 70.7985 |  |  |
| ν37 | 1502.42 | 0.7867 |  |  |
| ν38 | 1554.95 | 245.947 |  |  |
| ν39 | 1606.62 | 306.155 |  |  |
| ν40 | 1648.66 | 96.7102 |  |  |
| ν41 | 1736.98 | 229.296 |  |  |
| ν42 | 2994.49 | 26.2044 |  |  |
| ν43 | 3060.72 | 3.1594 |  |  |
| ν44 | 3117.31 | 0.5097 |  |  |
| ν45 | 3173.63 | 6.7281 |  |  |
|  | **tsi2i12** | | **tsi4** | |
| ν1 | -1453.88 | 863.3398 | -478.71 | 4.0179 |
| ν2 | 68.31 | 0.6205 | 40.57 | 1.0235 |
| ν3 | 82.77 | 1.6824 | 43.95 | 0.7128 |
| ν4 | 100.02 | 2.0467 | 53.74 | 1.9522 |
| ν5 | 137.93 | 11.3738 | 73.5 | 0.2593 |
| ν6 | 224.37 | 8.0989 | 86.03 | 0.5725 |
| ν7 | 281.46 | 0.8309 | 97.4 | 0.3436 |
| ν8 | 311.29 | 0.5892 | 121.49 | 1.3505 |
| ν9 | 366.91 | 20.3667 | 139.31 | 4.2115 |
| ν10 | 627.53 | 18.8036 | 171.33 | 1.3786 |
| ν11 | 666.88 | 8.3412 | 202.16 | 4.2537 |
| ν12 | 678.8 | 13.4449 | 255.81 | 1.3286 |
| ν13 | 761.59 | 136.6369 | 258.94 | 19.5863 |
| ν14 | 796.04 | 98.0022 | 341.23 | 4.0297 |
| ν15 | 898.32 | 15.4456 | 378.98 | 12.5423 |
| ν16 | 960.78 | 9.5707 | 406.4 | 4.0928 |
| ν17 | 1024.84 | 1.4195 | 439 | 4.2268 |
| ν18 | 1046.39 | 24.5436 | 537.21 | 7.3874 |
| ν19 | 1083.43 | 25.2533 | 585.21 | 33.1506 |
| ν20 | 1104.41 | 54.2412 | 631.08 | 20.5917 |
| ν21 | 1124.89 | 25.2277 | 664.04 | 7.0054 |
| ν22 | 1247.35 | 275.8882 | 690.73 | 405.7552 |
| ν23 | 1341.58 | 207.0744 | 767.82 | 11.4652 |
| ν24 | 1363.09 | 22.3268 | 781.44 | 6.2584 |
| ν25 | 1391.42 | 62.246 | 809.21 | 28.8192 |
| ν26 | 1418.09 | 41.6912 | 852.54 | 22.7359 |
| ν27 | 1467.08 | 53.6692 | 866.93 | 15.7479 |
| ν28 | 1558.01 | 334.4965 | 895.55 | 42.0541 |
| ν29 | 1625.84 | 204.1946 | 911.31 | 28.147 |
| ν30 | 2007.21 | 7.8552 | 928.57 | 122.7544 |
| ν31 | 3174.43 | 9.2259 | 975.16 | 31.0407 |
| ν32 | 3187.72 | 1.7656 | 1012.67 | 284.3234 |
| ν33 | 3231.87 | 7.9738 | 1150.53 | 3.7438 |
| ν34 |  |  | 1165.25 | 122.2703 |
| ν35 |  |  | 1196.01 | 115.4664 |
| ν36 |  |  | 1201.82 | 65.0226 |
| ν37 |  |  | 1246.79 | 180.1523 |
| ν38 |  |  | 1254.02 | 82.9793 |
| ν39 |  |  | 1294.35 | 212.9011 |
| ν40 |  |  | 1310.53 | 228.4702 |
| ν41 |  |  | 1320.96 | 153.8637 |
| ν42 |  |  | 1342.59 | 140.4536 |
| ν43 |  |  | 1360 | 36.0108 |
| ν44 |  |  | 1378.09 | 78.4213 |
| ν45 |  |  | 1410.54 | 75.7959 |
| ν46 |  |  | 1429.4 | 19.1433 |
| ν47 |  |  | 1435.08 | 22.5995 |
| ν48 |  |  | 1495.95 | 23.365 |
| ν49 |  |  | 1614.67 | 273.3091 |
| ν50 |  |  | 1646.23 | 270.6936 |
| ν51 |  |  | 1721.54 | 326.5458 |
| ν52 |  |  | 2843.61 | 8.1421 |
| ν53 |  |  | 2907.92 | 9.5975 |
| ν54 |  |  | 3021.18 | 24.8873 |
| ν55 |  |  | 3065.61 | 11.8054 |
| ν56 |  |  | 3156.32 | 5.4936 |
| ν57 |  |  | 3201.16 | 7.787 |
|  | **tsi4i5** | | **tsi5i6** | |
| ν1 | -261.08 | 196.0403 | -534.56 | 50.7151 |
| ν2 | 18.81 | 0.2487 | 47.58 | 3.1182 |
| ν3 | 48.45 | 1.4761 | 65.99 | 3.0323 |
| ν4 | 55.32 | 5.0827 | 78.74 | 2.4689 |
| ν5 | 61.59 | 0.6003 | 84.37 | 2.9375 |
| ν6 | 91.35 | 1.2243 | 156.59 | 6.0302 |
| ν7 | 120.94 | 0.9528 | 233.18 | 8.4841 |
| ν8 | 133.58 | 2.8739 | 288.01 | 13.413 |
| ν9 | 164.01 | 4.8922 | 346.09 | 4.0242 |
| ν10 | 172.07 | 6.8515 | 375.67 | 11.2239 |
| ν11 | 178.44 | 8.2208 | 411.53 | 7.4658 |
| ν12 | 234.98 | 4.3335 | 429.61 | 1.7244 |
| ν13 | 298.35 | 21.572 | 470.71 | 18.0438 |
| ν14 | 354.69 | 4.8139 | 511.03 | 29.979 |
| ν15 | 373 | 0.3116 | 566.6 | 17.1767 |
| ν16 | 391.03 | 7.2634 | 631.02 | 12.8095 |
| ν17 | 454 | 8.2159 | 644.09 | 9.2296 |
| ν18 | 476.93 | 0.6645 | 756.69 | 7.7896 |
| ν19 | 565.84 | 10.4879 | 770.83 | 9.7061 |
| ν20 | 610.6 | 7.9267 | 806.54 | 79.6062 |
| ν21 | 654.21 | 19.4606 | 848.98 | 10.2948 |
| ν22 | 692.42 | 32.2345 | 872.33 | 39.4068 |
| ν23 | 763 | 11.5679 | 893.39 | 25.6692 |
| ν24 | 777.68 | 0.8512 | 911.91 | 224.4211 |
| ν25 | 783.78 | 42.6967 | 941.96 | 143.2884 |
| ν26 | 803.88 | 208.7999 | 955.64 | 35.1878 |
| ν27 | 877.98 | 28.6881 | 989.5 | 30.9586 |
| ν28 | 908.83 | 28.9431 | 1032.97 | 117.6187 |
| ν29 | 921.02 | 10.8297 | 1156.78 | 25.3079 |
| ν30 | 976.61 | 107.6962 | 1219.1 | 2.5637 |
| ν31 | 1016.21 | 418.0301 | 1278.29 | 178.5694 |
| ν32 | 1052.47 | 6.1913 | 1287.28 | 335.7176 |
| ν33 | 1114.24 | 4.4013 | 1311.01 | 229.304 |
| ν34 | 1178.01 | 9.1925 | 1327.5 | 68.4619 |
| ν35 | 1199.7 | 8.1209 | 1328.41 | 19.3378 |
| ν36 | 1219.56 | 14.4943 | 1345.18 | 83.4865 |
| ν37 | 1242.63 | 19.0994 | 1368.92 | 6.978 |
| ν38 | 1287.86 | 471.1696 | 1429.76 | 26.842 |
| ν39 | 1298.01 | 6.9339 | 1477.23 | 8.7337 |
| ν40 | 1316.42 | 64.9767 | 1504.25 | 24.0447 |
| ν41 | 1333.08 | 254.7892 | 1552.88 | 93.65 |
| ν42 | 1340.75 | 109.981 | 1658.52 | 271.9106 |
| ν43 | 1367.43 | 22.4962 | 1684.93 | 369.3933 |
| ν44 | 1373.33 | 18.7037 | 3064.99 | 13.4593 |
| ν45 | 1417.3 | 89.0337 | 3092.12 | 4.2282 |
| ν46 | 1455.23 | 136.5295 | 3171.51 | 1.1949 |
| ν47 | 1496.09 | 39.5021 | 3201.2 | 8.9662 |
| ν48 | 1513.28 | 1.3779 | 3253.79 | 12.7633 |
| ν49 | 1622.65 | 140.461 |  |  |
| ν50 | 1636.97 | 438.0541 |  |  |
| ν51 | 1709.84 | 97.8988 |  |  |
| ν52 | 1872.96 | 820.5213 |  |  |
| ν53 | 3003.83 | 3.1705 |  |  |
| ν54 | 3025.46 | 16.3173 |  |  |
| ν55 | 3043.12 | 11.0191 |  |  |
| ν56 | 3088.12 | 2.1465 |  |  |
| ν57 | 3195.7 | 15.1973 |  |  |
|  | **tsi6i7** | | **tsi7i8** | |
| ν1 | -665.24 | 17.7484 | -1437.07 | 140.3954 |
| ν2 | 45.47 | 0.3198 | 44.32 | 0.9587 |
| ν3 | 51.18 | 5.9149 | 58.42 | 1.1403 |
| ν4 | 93.5 | 0.647 | 79.95 | 0.1567 |
| ν5 | 112.18 | 1.767 | 110.03 | 1.6425 |
| ν6 | 146.49 | 9.063 | 147.56 | 2.0558 |
| ν7 | 210.22 | 1.0709 | 213.06 | 4.6584 |
| ν8 | 244.03 | 13.7519 | 225.62 | 15.7759 |
| ν9 | 294.27 | 0.929 | 253 | 0.1248 |
| ν10 | 338.44 | 3.5544 | 298.29 | 2.4432 |
| ν11 | 374.66 | 2.2502 | 355.86 | 3.9829 |
| ν12 | 400.98 | 9.0024 | 434.14 | 20.8715 |
| ν13 | 478.3 | 1.0743 | 463.13 | 39.6332 |
| ν14 | 533.25 | 3.443 | 484.63 | 41.451 |
| ν15 | 581.28 | 3.1988 | 501.51 | 3.9141 |
| ν16 | 611.07 | 3.0791 | 553.24 | 9.2437 |
| ν17 | 659.74 | 13.7749 | 580.99 | 5.5579 |
| ν18 | 752.46 | 16.6179 | 617.17 | 2.0812 |
| ν19 | 764.96 | 8.2301 | 649.6 | 6.8552 |
| ν20 | 776.97 | 41.2505 | 741.04 | 28.0983 |
| ν21 | 808.31 | 5.2218 | 771.31 | 6.5172 |
| ν22 | 837.75 | 25.6955 | 812.9 | 44.5425 |
| ν23 | 880.41 | 4.0272 | 832.19 | 19.2023 |
| ν24 | 920.08 | 148.2291 | 875.6 | 120.861 |
| ν25 | 947.03 | 384.0487 | 951.87 | 18.0911 |
| ν26 | 965.5 | 173.347 | 986.04 | 31.2243 |
| ν27 | 990.93 | 64.8819 | 1016.03 | 82.2994 |
| ν28 | 1047.06 | 14.0796 | 1058.22 | 98.4054 |
| ν29 | 1111.71 | 17.6634 | 1109.51 | 58.0313 |
| ν30 | 1164.08 | 20.206 | 1173.4 | 35.5471 |
| ν31 | 1189 | 16.8693 | 1230.53 | 348.4949 |
| ν32 | 1218.44 | 55.8338 | 1262.05 | 94.7004 |
| ν33 | 1242.82 | 84.5148 | 1275.87 | 48.0153 |
| ν34 | 1260.4 | 31.66 | 1307.53 | 219.7339 |
| ν35 | 1269.07 | 100.4352 | 1320.12 | 84.3328 |
| ν36 | 1290.89 | 127.8138 | 1355.63 | 115.5884 |
| ν37 | 1314.14 | 189.2901 | 1416.32 | 2.6512 |
| ν38 | 1335.17 | 143.5859 | 1437.07 | 24.5482 |
| ν39 | 1362.81 | 108.0117 | 1487.21 | 10.3089 |
| ν40 | 1398.17 | 31.1686 | 1513.18 | 38.0537 |
| ν41 | 1492.16 | 30.0026 | 1580.67 | 249.721 |
| ν42 | 1620.74 | 152.4163 | 1654.24 | 228.6216 |
| ν43 | 1646.99 | 383.0598 | 1751.69 | 197.1948 |
| ν44 | 2526.18 | 50.7493 | 1824.42 | 536.2607 |
| ν45 | 2885.18 | 23.9881 | 2986.69 | 8.6085 |
| ν46 | 2984.16 | 144.0044 | 3073.92 | 5.0237 |
| ν47 | 3049.56 | 9.3561 | 3150.75 | 0.3487 |
| ν48 | 3186.67 | 23.1841 | 3624.38 | 78.6579 |
|  | **tsi7i11** | | **tsi8i9** | |
| ν1 | -1920.27 | 590.7636 | -219.49 | 101.9682 |
| ν2 | 23.49 | 0.5233 | 87.73 | 5.6603 |
| ν3 | 53.12 | 4.2393 | 130.48 | 7.9464 |
| ν4 | 62.83 | 1.5932 | 216.13 | 12.2439 |
| ν5 | 102.92 | 0.4503 | 235.59 | 2.4356 |
| ν6 | 145.28 | 4.1626 | 343.3 | 9.0206 |
| ν7 | 179.55 | 7.8418 | 435.3 | 25.0608 |
| ν8 | 189.09 | 1.4992 | 453.23 | 17.4354 |
| ν9 | 275.32 | 4.3241 | 492.18 | 7.5481 |
| ν10 | 289.48 | 10.0136 | 533.5 | 12.262 |
| ν11 | 343.97 | 3.6239 | 574.99 | 4.2237 |
| ν12 | 361.77 | 0.9264 | 605.23 | 9.3838 |
| ν13 | 463.02 | 0.6499 | 627.64 | 67.5971 |
| ν14 | 551.94 | 1.9179 | 691.23 | 17.8842 |
| ν15 | 616.93 | 6.1819 | 733.3 | 37.3815 |
| ν16 | 654.44 | 0.4127 | 757 | 17.8909 |
| ν17 | 688.22 | 23.316 | 800.88 | 18.3724 |
| ν18 | 707.47 | 4.6611 | 872.82 | 33.2839 |
| ν19 | 762.98 | 8.3675 | 905.07 | 56.1651 |
| ν20 | 778.7 | 10.7886 | 961.22 | 38.2949 |
| ν21 | 834.62 | 43.3924 | 1058.93 | 28.4061 |
| ν22 | 856.87 | 6.085 | 1136.89 | 39.7469 |
| ν23 | 876.29 | 121.5294 | 1162.77 | 135.6362 |
| ν24 | 975.08 | 60.3029 | 1231.81 | 27.0331 |
| ν25 | 998.41 | 329.8161 | 1238.08 | 18.0528 |
| ν26 | 1048.95 | 46.896 | 1355.53 | 44.7043 |
| ν27 | 1067.72 | 24.1848 | 1399.58 | 136.3457 |
| ν28 | 1137.71 | 160.9728 | 1430.98 | 46.4397 |
| ν29 | 1172.85 | 44.2497 | 1463.02 | 72.7004 |
| ν30 | 1210.39 | 12.6979 | 1621.61 | 41.0064 |
| ν31 | 1248.29 | 30.4898 | 1661.44 | 369.9702 |
| ν32 | 1287.17 | 186.7763 | 1832.34 | 544.3744 |
| ν33 | 1292.78 | 289.3127 | 2808.09 | 113.3556 |
| ν34 | 1299.6 | 183.981 | 3158 | 3.5848 |
| ν35 | 1335.16 | 198.8817 | 3204.74 | 1.0226 |
| ν36 | 1371.94 | 25.226 | 3598.72 | 78.0757 |
| ν37 | 1428.65 | 8.8377 |  |  |
| ν38 | 1511.37 | 2.709 |  |  |
| ν39 | 1530.76 | 1.6909 |  |  |
| ν40 | 1564.13 | 112.1673 |  |  |
| ν41 | 1609.13 | 61.9877 |  |  |
| ν42 | 1633.09 | 524.1041 |  |  |
| ν43 | 1702.31 | 615.7894 |  |  |
| ν44 | 2137.72 | 34.5431 |  |  |
| ν45 | 2994.37 | 39.686 |  |  |
| ν46 | 3015.1 | 23.3362 |  |  |
| ν47 | 3111 | 2.1975 |  |  |
| ν48 | 3200 | 13.7901 |  |  |
|  | **tsi9i10** | | **tsi9i12** | |
| ν1 | -1864.75 | 619.984 | -775.54 | 957.8979 |
| ν2 | 161.81 | 0.8572 | 64.07 | 0.0285 |
| ν3 | 364.41 | 0.5424 | 92.06 | 1.7063 |
| ν4 | 520.13 | 11.8388 | 233.43 | 4.0038 |
| ν5 | 556.3 | 0.1017 | 291.24 | 57.3778 |
| ν6 | 619.58 | 1.9942 | 388.08 | 6.4071 |
| ν7 | 736.05 | 4.9795 | 466.96 | 15.3827 |
| ν8 | 810.15 | 14.1642 | 471.19 | 56.3987 |
| ν9 | 928.51 | 3.5262 | 496.94 | 18.371 |
| ν10 | 992.69 | 1.9302 | 554.2 | 246.3746 |
| ν11 | 1017.69 | 35.1128 | 613.15 | 27.8532 |
| ν12 | 1048.87 | 0.003 | 648.76 | 64.1936 |
| ν13 | 1112.89 | 67.5759 | 671.21 | 1.8602 |
| ν14 | 1148.22 | 7.598 | 735.4 | 26.1613 |
| ν15 | 1191.47 | 3.5197 | 961.17 | 7.7209 |
| ν16 | 1324.55 | 45.7016 | 968.33 | 8.9184 |
| ν17 | 1391.31 | 61.8012 | 1012.22 | 12.41 |
| ν18 | 1444.01 | 21.1904 | 1023.8 | 33.7726 |
| ν19 | 1520.55 | 347.7123 | 1051.15 | 28.957 |
| ν20 | 1581.87 | 6.2619 | 1095.81 | 57.4482 |
| ν21 | 1670.28 | 786.3833 | 1201.82 | 64.9249 |
| ν22 | 2106.43 | 42.1268 | 1271.98 | 14.7451 |
| ν23 | 3165.67 | 15.1959 | 1348.3 | 166.3775 |
| ν24 | 3177.92 | 6.9172 | 1401.69 | 101.6921 |
| ν25 |  |  | 1407.49 | 8.8457 |
| ν26 |  |  | 1483.43 | 87.9721 |
| ν27 |  |  | 1551 | 344.5111 |
| ν28 |  |  | 1617.59 | 108.708 |
| ν29 |  |  | 1658.18 | 196.1186 |
| ν30 |  |  | 1877.58 | 736.7581 |
| ν31 |  |  | 3142.28 | 26.6672 |
| ν32 |  |  | 3146.35 | 13.5973 |
| ν33 |  |  | 3601.92 | 44.7895 |
|  | **HNO** | | **HONO** | |
| ν1 | 1567.34 | 9.5052 | 587.76 | 96.6323 |
| ν2 | 1664.88 | 82.0273 | 616.14 | 127.6488 |
| ν3 | 2841.68 | 157.0875 | 825.57 | 131.8099 |
| v4 |  |  | 1300.92 | 182.8341 |
| v5 |  |  | 1783.17 | 165.6128 |
| v6 |  |  | 3760.86 | 71.636 |