Table 2. Experimentally determined wavenumbers and linewidths of the $\nu_{975} = \nu_1(SiO_4)$, $\nu_{439} = \nu_2(SiO_4)$, $\nu_{356} = \nu_4(SiO_4)$, $\nu_{224}$, $\nu_{214}$, and $\nu_{202}$ Raman bands of fully crystalline synthetic zircon ($Zr_{0.987}Hf_{0.013}[SiO_4]$) as functions of temperature and pressure.

| $T$ (°C) | $P$ (MPa) | $\nu_{975}$ ($cm^{-1}$) | $\Gamma\nu_{975}$ ($cm^{-1}$) | $\nu_{439}$ ($cm^{-1}$) | $\Gamma\nu_{439}$ ($cm^{-1}$) | $\nu_{356}$ ($cm^{-1}$) | $\Gamma\nu_{356}$ ($cm^{-1}$) | $\nu_{224}$ ($cm^{-1}$) | $\Gamma\nu_{224}$ ($cm^{-1}$) | $\nu_{214}$ ($cm^{-1}$) | $\Gamma\nu_{214}$ ($cm^{-1}$) | $\nu_{202}$ ($cm^{-1}$) | $\Gamma\nu_{202}$ ($cm^{-1}$) | Experimental details |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 22 | 0.1 | 974.5 | 2.4 | 438.9 | 5.4 | 356.3 | 4.1 | 224.4 | 3.1 | 213.9 | 2.8 | 201.5 | 1.4 | TS1000 |
| 50 | 0.1 | 974.2 | 2.6 | 438.5 | 5.7 | 355.9 | 4.4 | 224.4 | 3.2 | 213.7 | 3.0 | 201.6 | 1.4 | TS1000 |
| 100 | 0.1 | 973.3 | 2.9 | 437.8 | 6.6 | 355.2 | 5.1 | 224.3 | 3.5 | 213.3 | 3.3 | 201.5 | 1.5 | TS1000 |
| 150 | 0.1 | 972.4 | 3.2 | 437.0 | 7.5 | 354.4 | 5.8 | 224.0 | 4.2 | 212.8 | 3.9 | 201.4 | 1.8 | TS1000 |
| 200 | 0.1 | 971.3 | 3.7 | 436.1 | 8.5 | 353.4 | 6.7 | 223.6 | 4.9 | 212.2 | 4.4 | 201.1 | 1.9 | TS1000 |
| 250 | 0.1 | 970.3 | 4.0 | 435.2 | 9.4 | 352.5 | 7.3 | 223.5 | 5.2 | 211.8 | 4.8 | 201.1 | 2.0 | TS1000 |
| 300 | 0.1 | 969.2 | 4.6 | 434.3 | 10.4 | 351.6 | 8.0 | 223.1 | 5.7 | 211.3 | 5.2 | 200.9 | 2.2 | TS1000 |
| 350 | 0.1 | 968.2 | 5.1 | 433.5 | 11.3 | 350.8 | 8.8 | 222.7 | 5.8 | 210.8 | 5.7 | 200.8 | 2.4 | TS1000 |
| 400 | 0.1 | 966.9 | 5.7 | 432.7 | 12.4 | 349.9 | 9.9 | 222.5 | 6.7 | 210.2 | 6.1 | 200.6 | 2.6 | TS1000 |
| 450 | 0.1 | 965.8 | 6.1 | 431.8 | 13.6 | 348.9 | 10.7 | 222.2 | 7.0 | 209.7 | 6.7 | 200.4 | 2.7 | TS1000 |
| 500 | 0.1 | 964.6 | 6.7 | 431.0 | 14.5 | 347.9 | 11.3 | 221.9 | 7.1 | 209.1 | 7.1 | 200.2 | 2.7 | TS1000 |
| 550 | 0.1 | 963.5 | 7.5 | 430.2 | 15.6 | 346.8 | 12.2 | 221.6 | 7.7 | 208.6 | 7.6 | 200.0 | 2.9 | TS1000 |
| 600 | 0.1 | 962.4 | 8.1 | 429.5 | 16.8 | 345.9 | 13.3 | 221.4 | 8.5 | 208.2 | 8.1 | 199.9 | 3.2 | TS1000 |
| 650 | 0.1 | 961.2 | 9.1 | 428.2 | 18.2 | 344.9 | 13.6 | 221.1 | 8.5 | 207.7 | 9.4 | 199.7 | 3.2 | TS1000 |
| 700 | 0.1 | 959.7 | 9.4 | 427.3 | 18.5 | 344.1 | 14.5 | 220.6 | 9.7 | 207.0 | 10.1 | 199.5 | 3.6 | TS1000 |
| 750 | 0.1 | 958.7 | 10.0 | 426.9 | 20.0 | 343.1 | 15.7 | 220.5 | 10.0 | 206.5 | 10.5 | 199.2 | 4.0 | TS1000 |
| 800 | 0.1 | 958.0 | 11.6 | 426.1 | 21.4 | 341.9 | 16.3 | 220.2 | 10.9 | 206.0 | 11.0 | 199.1 | 4.2 | TS1000 |
| 850 | 0.1 | 956.5 | 12.1 | 425.2 | 23.2 | 341.0 | 17.4 | 220.1 | 10.7 | 205.3 | 12.6 | 198.8 | 3.9 | TS1000 |
| 900 | 0.1 | 955.4 | 13.1 | 424.6 | 23.9 | 340.1 | 18.0 | 219.6 | 12.0 | 204.6 | 13.7 | 198.6 | 4.1 | TS1000 |
| 950 | 0.1 | 953.6 | n.r. | 423.9 | n.r. | 339.3 | n.r. | n.r. | n.r. | n.r. | n.r. | n.r. | n.r. | TS1000 |
| 25.5 | 0.1 | 974.7 | 2.9 | 439.0 | 5.6 | 356.4 | 4.4 | 224.5 | n.r. | 214.0 | 3.3 | 201.7 | n.r. | HDAC |
| 25.3 | 0.1 | 974.5 | 2.7 | 439.0 | 5.6 | 356.3 | 4.4 | 224.6 | n.r. | 213.9 | 3.2 | 201.7 | n.r. | HDAC |
| 98.8 | 0.1 | 973.4 | 3.2 | 437.9 | 6.8 | 355.2 | 5.5 | 224.3 | n.r. | 213.4 | 4.2 | 201.6 | n.r. | HDAC |
| 98.8 | 0.1 | 973.3 | 3.3 | 437.8 | 6.8 | 355.1 | 5.6 | 224.1 | n.r. | 213.4 | 4.0 | 201.6 | n.r. | HDAC |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 197.6 | 0.1 | 971.3 | 4.1 | 436.2 | 8.6 | 353.4 | 6.9 | 223.6 | n.r. | 212.3 | 5.1 | 201.3 | n.r. | HDAC |
| 197.6 | 0.1 | 971.5 | 3.8 | 436.3 | 8.5 | 353.5 | 6.7 | 223.9 | n.r. | 212.5 | 4.9 | 201.4 | n.r. | HDAC |
| 296.4 | 0.1 | 969.4 | 4.6 | 434.6 | 10.4 | 351.8 | 7.9 | 223.2 | n.r. | 211.5 | 5.7 | 201.1 | n.r. | HDAC |
| 395.2 | 0.1 | 967.4 | 5.6 | 433.0 | 12.3 | 350.1 | 9.6 | 222.7 | n.r. | 210.7 | 6.3 | 201.0 | n.r. | HDAC |
| 494 | 0.1 | 964.8 | 6.8 | 431.0 | 14.5 | 348.0 | 11.5 | 222.1 | n.r. | 209.5 | 7.5 | 200.6 | n.r. | HDAC |
| 592.9 | 0.1 | 962.7 | 8.1 | 429.6 | 16.4 | 346.4 | 12.8 | 221.6 | n.r. | 208.7 | 8.3 | 200.3 | n.r. | HDAC |
| 691.6 | 0.1 | 960.4 | 9.2 | 427.9 | 18.4 | 344.5 | 14.3 | 221.1 | n.r. | 207.8 | 9.5 | 199.9 | n.r. | HDAC |
| 741 | 0.1 | 959.2 | 10.0 | 427.0 | 19.7 | 343.4 | 15.1 | 220.4 | n.r. | 207.1 | 9.8 | 199.6 | n.r. | HDAC |
| 26.8 | 0.1 | 974.4 | 2.7 | 438.8 | 5.6 | 356.2 | 4.4 | n.r. | n.r. | 213.7 | n.r. | n.r. | n.r. | HDAC,W |
| 26.5 | 46 | 974.8 | 2.7 | 439.0 | 5.5 | 356.6 | 4.2 | n.r. | n.r. | 213.9 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.5 | 88 | 974.9 | 2.7 | 439.0 | 5.6 | 356.7 | 4.3 | n.r. | n.r. | 213.9 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.2 | 173 | 975.5 | 2.7 | 439.2 | 5.6 | 357.2 | 4.3 | n.r. | n.r. | 214.1 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.3 | 265 | 976.0 | 2.8 | 439.3 | 5.7 | 357.7 | 4.3 | n.r. | n.r. | 214.3 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.6 | 440 | 976.8 | 2.8 | 439.6 | 5.6 | 358.5 | 4.3 | n.r. | n.r. | 214.6 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.5 | 606 | 977.7 | 2.8 | 439.8 | 5.6 | 359.2 | 4.3 | n.r. | n.r. | 214.8 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.6 | 874 | 979.0 | 2.7 | 440.1 | 5.5 | 360.5 | 4.2 | n.r. | n.r. | 215.2 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.6 | 1100 | 980.4 | 3.1 | 440.6 | 5.7 | 361.7 | 4.4 | n.r. | n.r. | 215.8 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.7 | 1264 | 981.1 | 2.7 | 440.6 | 5.5 | 362.3 | 4.1 | n.r. | n.r. | 215.8 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.7 | 1439 | 982.2 | 2.9 | 441.1 | 5.6 | 363.4 | 4.2 | n.r. | n.r. | 216.3 | n.r. | n.r. | n.r. | HDAC,W,C |
| 27.0 | 1303 | 981.5 | 2.8 | 440.9 | 5.4 | 362.8 | 4.2 | n.r. | n.r. | 215.9 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.9 | 1682 | 983.4 | 2.9 | 441.4 | 5.5 | 364.5 | 4.3 | n.r. | n.r. | 216.6 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.8 | 1682 | 983.4 | 2.8 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | HDAC,W,C |
| 27.0 | 1948 | 984.7 | 2.9 | 441.7 | 5.5 | 365.8 | 4.4 | n.r. | n.r. | 217.0 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.9 | 1948 | 984.7 | 2.9 | 441.6 | 5.4 | 365.6 | 4.1 | n.r. | n.r. | 216.9 | n.r. | n.r. | n.r. | HDAC,W,C |
| 26.7 | 1978 | 984.7 | 2.9 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | HDAC,W,C |
| 24.2 | 0.1 | 974.2 | 2.4 | 438.7 | 5.4 | 356.0 | 4.0 | 224.1 | 3.0 | 213.5 | 2.9 | 201.2 | 1.4 | DAC,MEW |
| 23.1 | 41 | 974.4 | 2.4 | 438.8 | 5.5 | 356.2 | 4.0 | 224.2 | 3.1 | 213.6 | 2.9 | 201.3 | 1.4 | DAC,MEW, |
| 22.8 | 241 | 975.6 | 2.4 | 439.1 | 5.4 | 357.3 | 4.0 | 224.2 | 3.1 | 214.1 | 2.9 | 201.2 | 1.4 | DAC,MEW, |
| 22.9 | 1217 | 980.5 | 2.4 | 440.3 | 5.3 | 361.9 | 3.9 | 224.3 | 3.2 | 215.4 | 2.8 | 200.8 | 1.5 | DAC,MEW, |
| 23.0 | 1503 | 982.1 | 2.4 | 440.8 | 5.4 | 363.3 | 3.8 | 224.5 | 3.2 | 216.0 | 3.0 | 200.8 | 1.5 | DAC,MEW, |
| 23.1 | 2516 | 987.5 | 2.2 | 442.2 | 5.5 | 368.1 | 3.8 | 224.6 | 3.1 | 217.4 | 2.9 | 200.3 | 1.4 | DAC,MEW, |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.2 | 3258 | 991.1 | 2.1 | 443.2 | 5.4 | 371.4 | 3.7 | 224.7 | 3.2 | 218.5 | 2.9 | 199.9 | 1.5 | DAC,MEW, |
| 23.2 | 3953 | 994.6 | 2.1 | 444.2 | 5.5 | 374.2 | 3.6 | 224.8 | 3.2 | 219.6 | 3.1 | 199.6 | 1.6 | DAC,MEW, |
| 23.2 | 4403 | 996.9 | 2.1 | 444.8 | 5.7 | 376.4 | 3.6 | 225.0 | 3.2 | 220.3 | 3.2 | 199.5 | 1.6 | DAC,MEW, |
| 23.2 | 4903 | 999.7 | 2.0 | 445.6 | 5.6 | 378.6 | 3.5 | 225.2 | 3.1 | 220.6 | 2.8 | 199.2 | 1.6 | DAC,MEW, |
| 23.2 | 5579 | 1,003.2 | 2.0 | 446.8 | 6.0 | 381.7 | 3.6 | 225.4 | 3.2 | 221.9 | 3.5 | 198.8 | 1.7 | DAC,MEW, |
| 23.3 | 6126 | 1,005.9 | 1.8 | 447.7 | 5.9 | 384.1 | 3.5 | 225.6 | 3.1 | 222.5 | 3.2 | 198.7 | 1.7 | DAC,MEW, |
| 23.4 | 6645 | 1,008.3 | 2.1 | 448.5 | 5.9 | 386.1 | 3.6 | 225.7 | 3.1 | 223.2 | 3.6 | 198.3 | 1.7 | DAC,MEW, |
| 23.4 | 44 | 974.5 | 2.4 | 438.9 | 5.4 | 356.2 | 4.0 | 224.4 | 2.9 | 213.8 | 3.0 | 201.5 | 1.3 | DAC,MEW, |
| 21.8 | 0.1 | 974.6 | 2.4 | 438.9 | 5.2 | 356.3 | 3.8 | 224.4 | 3.0 | 213.9 | 2.7 | 201.6 | 1.3 | HDAC,W |
| 200 | 120 | 972.0 | 3.5 | 436.2 | 8.5 | 354.0 | 6.5 | 223.4 | 5.1 | 212.5 | 4.2 | 201.1 | 1.7 | HDAC,W,Ec |
| 200 | 360 | 972.9 | 3.6 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | HDAC,E,Q |
| 300 | 9 | 969.4 | 4.3 | 434.4 | 10.2 | 351.8 | 8.3 | 223.1 | 5.9 | 211.4 | 5.3 | 201.0 | 2.1 | HDAC,W,Ec |
| 300 | 149 | 970.0 | 4.4 | 434.5 | 10.3 | 352.5 | 7.9 | 223.1 | 5.9 | 211.6 | 5.2 | 200.9 | 2.1 | HDAC,W,Ec |
| 300 | 310 | 970.8 | 4.3 | 434.7 | 10.2 | 353.2 | 8.1 | 222.9 | 6.0 | 211.7 | 5.1 | 200.8 | 2.0 | HDAC,W,Ec |
| 300 | 304 | 970.7 | 4.8 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | HDAC,E,Q |
| 400 | 108 | 967.5 | 5.5 | 432.6 | 12.3 | 350.3 | 9.7 | 222.4 | 6.7 | 210.4 | 6.1 | 200.5 | 2.3 | HDAC,W,Ec |
| 400 | 309 | 968.8 | 5.4 | 432.9 | 12.2 | 351.4 | 9.6 | 222.5 | 6.3 | 210.8 | 6.1 | 200.5 | 2.3 | HDAC,W,Ec |
| 400 | 502 | 969.6 | 5.3 | 433.2 | 12.2 | 352.3 | 9.3 | 222.4 | 5.9 | 210.9 | 5.9 | 200.4 | 2.2 | HDAC,W,Ec |
| 500 | 213 | 965.9 | 6.6 | 431.1 | 14.2 | 349.0 | 11.3 | 221.9 | 7.7 | 209.5 | 6.9 | 200.2 | 2.5 | HDAC,W,Ec |
| 500 | 466 | 967.2 | 6.3 | 431.6 | 13.8 | 350.5 | 11.0 | 222.0 | 7.9 | 209.9 | 7.1 | 200.2 | 2.8 | HDAC,W,Ec |
| 500 | 854 | 969.3 | 6.2 | 431.8 | 14.0 | 352.2 | 11.2 | 222.1 | 8.0 | 210.6 | 6.7 | 200.1 | 2.7 | HDAC,W,Ec |
| 500 | 652 | 968.4 | 5.9 | 431.7 | 14.1 | 351.4 | 11.2 | 221.9 | 7.0 | 210.3 | 6.9 | 200.1 | 2.5 | HDAC,W,Ec |
| 600 | 316 | 964.0 | 7.7 | 429.4 | 16.4 | 347.6 | 13.2 | 221.3 | 8.8 | 208.6 | 8.1 | 199.7 | 2.9 | HDAC,W,Ec |
| 600 | 618 | 965.5 | 7.1 | 430.0 | 15.9 | 349.1 | 13.3 | 221.6 | 9.0 | 209.1 | 7.5 | 199.8 | 3.0 | HDAC,W,Ec |
| 600 | 1052 | 967.8 | 7.4 | 430.2 | 16.2 | 351.3 | 12.6 | 221.5 | 9.0 | 210.0 | 7.4 | 199.7 | 3.0 | HDAC,W,Ec |
| 600 | 829 | 966.9 | 7.7 | 430.2 | 16.0 | 350.3 | 13.3 | 221.5 | 8.3 | 209.5 | 8.1 | 199.8 | 2.8 | HDAC,W,Ec |
| 700 | 437 | 962.0 | 8.9 | 428.0 | 18.8 | 346.3 | 14.9 | 220.8 | 10.5 | 207.8 | 8.9 | 199.4 | 3.3 | HDAC,W,Ec |
| 700 | 765 | 964.0 | 9.5 | 428.4 | 18.5 | 347.9 | 14.9 | 221.1 | 9.9 | 208.2 | 9.1 | 199.3 | 3.5 | HDAC,W,Ec |
| 700 | 1242 | 966.4 | 9.5 | 428.6 | 18.1 | 350.4 | 14.9 | 221.0 | 10.9 | 208.9 | 8.0 | 199.2 | 3.4 | HDAC,W,Ec |

*Notes:* $T$ = temperature; $P$ = pressure; $\nu_i$ = determined wavenumber of the $\nu_i$ Raman band of zircon; $\Gamma\nu_i$ = full width at half maximum of the $\nu_i$ Raman band o zircon (not corrected for spectral resolution). TS1000 = Linkam TS1000 heating stage, HDAC, = hydrothermal diamond-anvil cell, DAC = piston-cylinde diamond-anvil cell. Pressure medium: W = water; MEW = 16:3:1 mixture of methanol, ethanol, and distilled water; E = ethanol. Pressure determinatio technique: Q = wavenumber shift of the 464 $cm^{-1}$ Raman line of quartz using equation (2) of Schmidt and Ziemann (2000); EoS = liquid-vapo homogenization temperature after isochoric cooling and equation of state of $H_2O$ (Wagner and Pruß 2002). n.d. = not determined; n.r. = not reported becaus fitting results were inaccurate due to lower spectral quality or unresolvable overlap with plasma line.