



Supplement of

First-principles modeling of the infrared spectrum of antigorite

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- * mode_4_53.1_cm-1.vesta
- * mode_500_486.1_cm-1.vesta
- * mode_501_486.3_cm-1.vesta

- * mode_502_487.8_cm-1.vesta
- * mode_503_488.3_cm-1.vesta
- * mode_504_489.9_cm-1.vesta
- * mode_505_491.9_cm-1.vesta
- * mode_506_492.6_cm-1.vesta
- * mode_507_492.9_cm-1.vesta
- * mode_508_493.3_cm-1.vesta
- * mode_509_495.5_cm-1.vesta
- * mode_50_163.7_cm-1.vesta
- * mode_510_497.8_cm-1.vesta
- * mode_511_498.6_cm-1.vesta
- * mode_512_500.0_cm-1.vesta
- * mode_513_500.1_cm-1.vesta
- * mode_514_501.6_cm-1.vesta
- * mode_515_502.5_cm-1.vesta
- * mode_516_503.4_cm-1.vesta
- * mode_517_504.1_cm-1.vesta
- * mode_518_504.5_cm-1.vesta
- * mode_519_505.1_cm-1.vesta
- * mode_51_164.6_cm-1.vesta
- * mode_520_506.0_cm-1.vesta
- * mode_521_507.1_cm-1.vesta
- * mode_522_507.9_cm-1.vesta
- * mode_523_509.4_cm-1.vesta
- * mode_524_509.6_cm-1.vesta
- * mode_525_510.1_cm-1.vesta
- * mode_526_512.1_cm-1.vesta
- * mode_527_513.0_cm-1.vesta
- * mode_528_515.6_cm-1.vesta
- * mode_529_516.8_cm-1.vesta
- * mode_52_165.7_cm-1.vesta
- * mode_530_518.0_cm-1.vesta
- * mode_531_519.0_cm-1.vesta
- * mode_532_519.5_cm-1.vesta
- * mode_533_519.8_cm-1.vesta
- * mode_534_520.1_cm-1.vesta
- * mode_535_521.3_cm-1.vesta
- * mode_536_521.6_cm-1.vesta
- * mode_537_526.3_cm-1.vesta
- * mode_538_528.4_cm-1.vesta
- * mode_539_529.4_cm-1.vesta
- * mode_53_167.7_cm-1.vesta
- * mode_540_532.4_cm-1.vesta
- * mode_541_534.3_cm-1.vesta
- * mode_542_536.5_cm-1.vesta
- * mode_543_538.1_cm-1.vesta
- * mode_544_541.0_cm-1.vesta

- * mode_545_543.8_cm-1.vesta
- * mode_546_544.3_cm-1.vesta
- * mode_547_545.7_cm-1.vesta
- * mode_548_547.7_cm-1.vesta
- * mode_549_548.9_cm-1.vesta
- * mode_54_168.9_cm-1.vesta
- * mode_550_555.4_cm-1.vesta
- * mode_551_557.9_cm-1.vesta
- * mode_552_589.9_cm-1.vesta
- * mode_553_591.7_cm-1.vesta
- * mode_554_596.8_cm-1.vesta
- * mode_555_599.1_cm-1.vesta
- * mode_556_600.2_cm-1.vesta
- * mode_557_601.4_cm-1.vesta
- * mode_558_607.8_cm-1.vesta
- * mode_559_609.6_cm-1.vesta
- * mode_55_169.4_cm-1.vesta
- * mode_560_610.1_cm-1.vesta
- * mode_561_611.4_cm-1.vesta
- * mode_562_611.7_cm-1.vesta
- * mode_563_612.5_cm-1.vesta
- * mode_564_613.8_cm-1.vesta
- * mode_565_616.0_cm-1.vesta
- * mode_566_616.5_cm-1.vesta
- * mode_567_616.7_cm-1.vesta
- * mode_568_617.8_cm-1.vesta
- * mode_569_619.0_cm-1.vesta
- * mode_56_170.4_cm-1.vesta
- * mode_570_619.8_cm-1.vesta
- * mode_571_620.6_cm-1.vesta
- * mode_572_620.8_cm-1.vesta
- * mode_573_622.5_cm-1.vesta
- * mode_574_622.5_cm-1.vesta
- * mode_575_622.7_cm-1.vesta
- * mode_576_623.8_cm-1.vesta
- * mode_577_624.4_cm-1.vesta
- * mode_578_624.8_cm-1.vesta
- * mode_579_625.4_cm-1.vesta
- * mode_57_171.8_cm-1.vesta
- * mode_580_626.8_cm-1.vesta
- * mode_581_627.0_cm-1.vesta
- * mode_582_628.4_cm-1.vesta
- * mode_583_629.9_cm-1.vesta
- * mode_584_630.8_cm-1.vesta
- * mode_585_631.7_cm-1.vesta
- * mode_586_633.2_cm-1.vesta
- * mode_587_643.2_cm-1.vesta

- * mode_588_644.3_cm-1.vesta
- * mode_589_645.0_cm-1.vesta
- * mode_58_172.6_cm-1.vesta
- * mode_590_646.9_cm-1.vesta
- * mode_591_650.3_cm-1.vesta
- * mode_592_650.9_cm-1.vesta
- * mode_593_651.2_cm-1.vesta
- * mode_594_653.2_cm-1.vesta
- * mode_595_653.8_cm-1.vesta
- * mode_596_655.2_cm-1.vesta
- * mode_597_657.8_cm-1.vesta
- * mode_598_657.9_cm-1.vesta
- * mode_599_658.1_cm-1.vesta
- * mode_59_173.0_cm-1.vesta
- * mode_5_64.7_cm-1.vesta
- * mode_600_659.0_cm-1.vesta
- * mode_601_659.8_cm-1.vesta
- * mode_602_659.8_cm-1.vesta
- * mode_603_660.7_cm-1.vesta
- * mode_604_661.3_cm-1.vesta
- * mode_605_661.7_cm-1.vesta
- * mode_606_662.2_cm-1.vesta
- * mode_607_663.3_cm-1.vesta
- * mode_608_663.4_cm-1.vesta
- * mode_609_666.2_cm-1.vesta
- * mode_60_173.6_cm-1.vesta
- * mode_610_666.7_cm-1.vesta
- * mode_611_667.7_cm-1.vesta
- * mode_612_668.0_cm-1.vesta
- * mode_613_669.7_cm-1.vesta
- * mode_614_670.4_cm-1.vesta
- * mode_615_670.8_cm-1.vesta
- * mode_616_672.3_cm-1.vesta
- * mode_617_672.8_cm-1.vesta
- * mode_618_673.6_cm-1.vesta
- * mode_619_674.2_cm-1.vesta
- * mode_61_176.6_cm-1.vesta
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- * mode_621_676.9_cm-1.vesta
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- * mode_623_680.0_cm-1.vesta
- * mode_624_681.2_cm-1.vesta
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- * mode_626_683.8_cm-1.vesta
- * mode_627_685.0_cm-1.vesta
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- * mode_629_686.9_cm-1.vesta

- * mode_62_178.1_cm-1.vesta
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- * mode_632_688.6_cm-1.vesta
- * mode_633_690.2_cm-1.vesta
- * mode_634_690.5_cm-1.vesta
- * mode_635_691.7_cm-1.vesta
- * mode_636_693.2_cm-1.vesta
- * mode_637_694.4_cm-1.vesta
- * mode_638_695.2_cm-1.vesta
- * mode_639_696.8_cm-1.vesta
- * mode_63_178.3_cm-1.vesta
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- * mode_641_699.0_cm-1.vesta
- * mode_642_699.2_cm-1.vesta
- * mode_643_701.2_cm-1.vesta
- * mode_644_703.3_cm-1.vesta
- * mode_645_704.7_cm-1.vesta
- * mode_646_706.7_cm-1.vesta
- * mode_647_707.6_cm-1.vesta
- * mode_648_708.7_cm-1.vesta
- * mode_649_709.4_cm-1.vesta
- * mode_64_179.6_cm-1.vesta
- * mode_650_713.3_cm-1.vesta
- * mode_651_714.2_cm-1.vesta
- * mode_652_715.3_cm-1.vesta
- * mode_653_715.6_cm-1.vesta
- * mode_654_717.1_cm-1.vesta
- * mode_655_717.9_cm-1.vesta
- * mode_656_718.0_cm-1.vesta
- * mode_657_719.9_cm-1.vesta
- * mode_658_721.4_cm-1.vesta
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- * mode_65_179.9_cm-1.vesta
- * mode_660_724.0_cm-1.vesta
- * mode_661_724.7_cm-1.vesta
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- * mode_664_730.8_cm-1.vesta
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- * mode_668_737.8_cm-1.vesta
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- * mode_672_740.9_cm-1.vesta
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- * mode_676_744.7_cm-1.vesta
- * mode_677_745.4_cm-1.vesta
- * mode_678_746.2_cm-1.vesta
- * mode_679_746.7_cm-1.vesta
- * mode_67_181.1_cm-1.vesta
- * mode_680_746.9_cm-1.vesta
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- * mode_682_756.4_cm-1.vesta
- * mode_683_758.9_cm-1.vesta
- * mode_684_760.5_cm-1.vesta
- * mode_685_766.5_cm-1.vesta
- * mode_686_767.5_cm-1.vesta
- * mode_687_772.4_cm-1.vesta
- * mode_688_772.9_cm-1.vesta
- * mode_689_776.5_cm-1.vesta
- * mode_68_182.0_cm-1.vesta
- * mode_690_777.4_cm-1.vesta
- * mode_691_777.6_cm-1.vesta
- * mode_692_781.4_cm-1.vesta
- * mode_693_782.2_cm-1.vesta
- * mode_694_785.8_cm-1.vesta
- * mode_695_786.7_cm-1.vesta
- * mode_696_786.9_cm-1.vesta
- * mode_697_787.5_cm-1.vesta
- * mode_698_790.9_cm-1.vesta
- * mode_699_791.8_cm-1.vesta
- * mode_69_183.7_cm-1.vesta
- * mode_6_65.0_cm-1.vesta
- * mode_700_792.9_cm-1.vesta
- * mode_701_795.9_cm-1.vesta
- * mode_702_800.9_cm-1.vesta
- * mode_703_802.5_cm-1.vesta
- * mode_704_803.1_cm-1.vesta
- * mode_705_803.7_cm-1.vesta
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- * mode_708_805.6_cm-1.vesta
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- * mode_713_810.5_cm-1.vesta

* mode_714_812.8_cm-1.vesta
* mode_715_813.1_cm-1.vesta
* mode_716_813.7_cm-1.vesta
* mode_717_815.1_cm-1.vesta
* mode_718_815.2_cm-1.vesta
* mode_719_815.9_cm-1.vesta
* mode_71_185.1_cm-1.vesta
* mode_720_817.8_cm-1.vesta
* mode_721_818.5_cm-1.vesta
* mode_722_819.1_cm-1.vesta
* mode_723_822.0_cm-1.vesta
* mode_724_824.6_cm-1.vesta
* mode_725_828.8_cm-1.vesta
* mode_726_830.6_cm-1.vesta
* mode_727_897.1_cm-1.vesta
* mode_728_898.5_cm-1.vesta
* mode_729_899.9_cm-1.vesta
* mode_72_186.2_cm-1.vesta
* mode_730_900.6_cm-1.vesta
* mode_731_900.8_cm-1.vesta
* mode_732_901.5_cm-1.vesta
* mode_733_902.5_cm-1.vesta
* mode_734_904.6_cm-1.vesta
* mode_735_908.8_cm-1.vesta
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* mode_739_923.7_cm-1.vesta
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* mode_74_187.4_cm-1.vesta
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* mode_756_963.9_cm-1.vesta

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- * mode_758_968.0_cm-1.vesta
- * mode_759_968.1_cm-1.vesta
- * mode_75_189.6_cm-1.vesta
- * mode_760_969.3_cm-1.vesta
- * mode_761_971.3_cm-1.vesta
- * mode_762_973.6_cm-1.vesta
- * mode_763_973.7_cm-1.vesta
- * mode_764_974.9_cm-1.vesta
- * mode_765_975.5_cm-1.vesta
- * mode_766_976.5_cm-1.vesta
- * mode_767_977.7_cm-1.vesta
- * mode_768_978.8_cm-1.vesta
- * mode_769_979.8_cm-1.vesta
- * mode_76_190.8_cm-1.vesta
- * mode_770_981.4_cm-1.vesta
- * mode_771_987.2_cm-1.vesta
- * mode_772_988.6_cm-1.vesta
- * mode_773_994.3_cm-1.vesta
- * mode_774_997.4_cm-1.vesta
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- * mode_777_1006.6_cm-1.vesta
- * mode_778_1009.6_cm-1.vesta
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- * mode_77_191.6_cm-1.vesta
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- * mode_784_1021.7_cm-1.vesta
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- * mode_790_1034.1_cm-1.vesta
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- * mode_792_1036.9_cm-1.vesta
- * mode_793_1037.5_cm-1.vesta
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- * mode_796_1043.9_cm-1.vesta
- * mode_797_1046.6_cm-1.vesta
- * mode_798_1048.2_cm-1.vesta
- * mode_799_1050.9_cm-1.vesta

- * mode_79_192.3_cm-1.vesta
- * mode_7_68.0_cm-1.vesta
- * mode_800_1051.9_cm-1.vesta
- * mode_801_1053.7_cm-1.vesta
- * mode_802_1055.0_cm-1.vesta
- * mode_803_1056.2_cm-1.vesta
- * mode_804_1064.0_cm-1.vesta
- * mode_805_1068.2_cm-1.vesta
- * mode_806_1076.5_cm-1.vesta
- * mode_807_1079.0_cm-1.vesta
- * mode_808_1086.0_cm-1.vesta
- * mode_809_1096.8_cm-1.vesta
- * mode_80_194.2_cm-1.vesta
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- * mode_811_1164.4_cm-1.vesta
- * mode_812_3649.2_cm-1.vesta
- * mode_813_3649.5_cm-1.vesta
- * mode_814_3665.1_cm-1.vesta
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- * mode_819_3681.7_cm-1.vesta
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- * mode_821_3681.9_cm-1.vesta
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- * mode_832_3696.0_cm-1.vesta
- * mode_833_3696.7_cm-1.vesta
- * mode_834_3697.8_cm-1.vesta
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- * mode_836_3705.1_cm-1.vesta
- * mode_837_3707.0_cm-1.vesta
- * mode_838_3712.6_cm-1.vesta
- * mode_839_3713.4_cm-1.vesta
- * mode_83_195.6_cm-1.vesta
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- * mode_841_3717.2_cm-1.vesta
- * mode_842_3717.9_cm-1.vesta
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- * mode_844_3724.4_cm-1.vesta
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- * mode_850_3728.8_cm-1.vesta
- * mode_851_3729.4_cm-1.vesta
- * mode_852_3729.9_cm-1.vesta
- * mode_853_3735.1_cm-1.vesta
- * mode_854_3740.2_cm-1.vesta
- * mode_855_3742.0_cm-1.vesta
- * mode_856_3747.6_cm-1.vesta
- * mode_857_3748.0_cm-1.vesta
- * mode_858_3756.0_cm-1.vesta
- * mode_859_3763.2_cm-1.vesta
- * mode_85_198.0_cm-1.vesta
- * mode_860_3763.5_cm-1.vesta
- * mode_861_3765.8_cm-1.vesta
- * mode_862_3766.7_cm-1.vesta
- * mode_863_3767.9_cm-1.vesta
- * mode_864_3770.2_cm-1.vesta
- * mode_865_3770.9_cm-1.vesta
- * mode_866_3772.5_cm-1.vesta
- * mode_867_3772.7_cm-1.vesta
- * mode_868_3773.1_cm-1.vesta
- * mode_869_3773.6_cm-1.vesta
- * mode_86_198.4_cm-1.vesta
- * mode_870_3775.2_cm-1.vesta
- * mode_871_3775.8_cm-1.vesta
- * mode_872_3777.7_cm-1.vesta
- * mode_873_3781.5_cm-1.vesta
- * mode_87_198.4_cm-1.vesta
- * mode_88_200.5_cm-1.vesta
- * mode_89_200.7_cm-1.vesta
- * mode_8_73.8_cm-1.vesta
- * mode_90_201.3_cm-1.vesta
- * mode_91_202.2_cm-1.vesta
- * mode_92_202.5_cm-1.vesta
- * mode_93_202.7_cm-1.vesta
- * mode_94_204.6_cm-1.vesta
- * mode_95_204.9_cm-1.vesta
- * mode_96_205.2_cm-1.vesta

- * mode_97_205.6_cm-1.vesta
- * mode_98_206.6_cm-1.vesta
- * mode_99_207.0_cm-1.vesta
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