

SupMat without 636 transitions.txt

07/04/2023

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All frequencies and uncertainties are given in kHz.  
Meas. freq.: Frequencies measured in this work. They are reported with their 1-sigma uncertainty UncMeas.  
Calc. freq.: Frequencies calculated from the effective Hamiltonian constants fitted in this work for the 20013  
and 20012 states (given below) and from the effective Hamiltonian constants given in Table 2 of  
Wu2020 for the ground state. Frequencies marked with \* are calculated with the experimental value  
of the upper energy level.  
Cal-Meas. : Calc. freq.-Meas. freq.  
Rec. freq. : Frequencies that are recommended to be used.  
Unc. : 1-sigma uncertainty of the recommended frequencies.

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Effective Hamiltonian constants in MHz

State 20012

	Value	Unc.
G	1.492317285961E+08	4.87117E-04
B	1.158798150755E+04	6.38182E-06
D	4.080361306835E-03	2.23925E-08
H	2.187291242079E-08	3.24045E-11
L	1.448393706292E-13	2.31815E-14
M	1.384541996722E-16	8.66453E-18
N	-2.122605726631E-20	1.61851E-21
O	3.097547539876E-24	1.19073E-25
Nfit/Nmeas	54/63	
J"max	74	
RMS of the fit (Hz)	1100	

State 20013

	Value	Unc.
G	1.455079611574E+08	3.44628E-04
B	1.163787718148E+04	3.79995E-06
D	5.451340885814E-03	1.01443E-08
H	1.817775758405E-08	1.06746E-11
L	-3.178611468350E-14	5.1997E-15
M	-2.460270770993E-17	1.17745E-18
N	9.771626705837E-22	1.00257E-22
Nfit/Nmeas	40/44	
J"max	70	
RMS of the fit (Hz)	808	

Wu2020: Wu H, Hu C-L, Wang J, Sun YR, Tan Y, Liu A-W, Hu S-M. A well-isolated vibrational state of CO<sub>2</sub> verified by near-infrared saturated spectroscopy with kHz accuracy. Phys Chem Chem Phys 2020;22:2841-2848. Doi: 10.1039/C9CP05121J

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20013-00001 band

Assig.	Meas. freq.	UncMeas	Calc. freq	Cal-Meas	Rec. freq.	Unc.
P(70)			143551036296.4*		143551036296.4	14.6
P(68)			143617406813.3*		143617406813.3	6.5
P(66)			143683041703.1*		143683041703.1	7.7
P(64)			143747954381.8		143747954381.8	3.2
P(62)			143812158059.4		143812158059.4	3.2
P(60)			143875665697.1		143875665697.1	3.2
P(58)			143938490004.9		143938490004.9	3.2
P(56)			144000643426.9		144000643426.9	3.2
P(54)			144062138129.1		144062138129.1	3.1
P(52)			144122985985.2		144122985985.2	3.3
P(50)			144183198562.5		144183198562.5	3.2
P(48)			144242787108.0		144242787108.0	3.2
P(46)			144301762533.8		144301762533.8	3.2
P(44)			144360135402.7		144360135402.7	3.2
P(42)			144417915913.1		144417915913.1	3.2
P(40)			144475113885.4		144475113885.4	3.2
P(38)			144531738746.9		144531738746.9	3.2
P(36)			144587799518.3		144587799518.3	3.2
P(34)			144643304799.6		144643304799.6	3.2
P(32)			144698262757.2		144698262757.2	3.2
P(30)			144752681110.6		144752681110.6	3.2
P(28)			144806567120.6		144806567120.6	3.2
P(26)			144859927577.1		144859927577.1	3.2
P(24)			144912768788.5		144912768788.5	3.2
P(22)			144965096570.8		144965096570.8	3.2
P(20)			145016916238.1		145016916238.1	3.2
P(18)			145068232593.8		145068232593.8	3.2
P(16)	145119049920.6	3.0	145119049921.9	1.3	145119049921.9	3.2
P(14)	145169371981.4	3.4	145169371980.1	-1.3	145169371980.1	3.2
P(12)	145219201993.0	3.5	145219201992.5	-0.5	145219201992.5	3.2
P(10)	145268542644.7	3.4	145268542644.3	-0.4	145268542644.3	3.2
P(8)	145317396075.5	3.6	145317396076.3	0.8	145317396076.3	3.2
P(6)	145365763879.6	3.2	145365763880.8	1.2	145365763880.8	3.2
P(4)	145413647096.5	3.1	145413647098.1	1.6	145413647098.1	3.2
P(2)	145461046214.5	3.4	145461046213.9	-0.6	145461046213.9	3.2
R(0)	145531236890.1	3.4	145531236890.0	-0.1	145531236890.0	3.2

R(2)	145577424223.3	3.1	145577424222.6	-0.7	145577424222.6	3.2
R(4)	145623124768.3	2.9	145623124766.6	-1.7	145623124766.6	3.2
R(6)	145668336501.3	3.0	145668336501.0	-0.3	145668336501.0	3.2
R(8)	145713056851.0	2.9	145713056850.1	-0.9	145713056850.1	3.2
R(10)	145757282685.6	3.4	145757282686.2	0.6	145757282686.2	3.2
R(12)	145801010333.2	3.0	145801010333.3	0.1	145801010333.3	3.2
R(14)	145844235571.7	2.9	145844235571.2	-0.5	145844235571.2	3.2
R(16)	145886953640.9	2.9	145886953640.7	-0.2	145886953640.7	3.2
R(18)	145929159249.7	3.0	145929159249.5	-0.2	145929159249.5	3.2
R(20)	145970846578.6	2.9	145970846578.6	0.0	145970846578.6	3.2
R(22)	146012009289.8	2.9	146012009290.4	0.6	146012009290.4	3.2
R(24)	146052640536.8	2.9	146052640536.5	-0.3	146052640536.5	3.2
R(26)	146092732967.0	3.1	146092732966.7	-0.3	146092732966.7	3.2
R(28)	146132278738.5	3.0	146132278739.0	0.5	146132278739.0	3.2
R(30)	146171269531.1	3.3	146171269529.7	-1.4	146171269529.7	3.2
R(32)	146209696545.2	3.1	146209696545.1	-0.1	146209696545.1	3.2
R(34)	146247550532.3	3.0	146247550532.4	0.1	146247550532.4	3.2
R(36)	146284821792.1	2.9	146284821792.6	0.5	146284821792.6	3.2
R(38)	146321500193.2	3.0	146321500193.5	0.3	146321500193.5	3.2
R(40)	146357575182.8	2.9	146357575182.3	-0.5	146357575182.3	3.2
R(42)	146393035800.0	3.0	146393035800.1	0.1	146393035800.1	3.2
R(44)	146427870697.5	3.0	146427870695.4	-2.1	146427870695.4	3.2
R(46)	146462068137.7	2.9	146462068138.8	1.1	146462068138.8	3.2
R(48)	146495616036.8	3.0	146495616037.3	0.5	146495616037.3	3.2
R(50)	146528501949.4	3.2	146528501948.7	-0.7	146528501948.7	3.2
R(52)	146560713096.8	3.3	146560713096.7	-0.1	146560713096.7	3.2
R(54)	146592236384.6	3.5	146592236384.7	0.1	146592236384.7	3.2
R(56)	146623058410.3	3.2	146623058410.6	0.3	146623058410.6	3.2
R(58)	146653165481.7	3.8	146653165480.5	-1.2	146653165480.5	3.2
R(60)	146682543621.6	3.4	146682543622.5	0.9	146682543622.5	3.2
R(62)	146711178600.3	3.4	146711178599.9	-0.4	146711178599.9	3.2
R(64)	146739055925.1	7.7			146739055925.1	7.7
R(66)	146766160861.4	6.5			146766160861.4	6.5
R(68)	146792478469.7	14.6			146792478469.7	14.6

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20012-00001 band

Assig.	Meas. freq.	UncMeas	Calc. freq	Cal-Meas	Rec. freq.	Unc.
P(74)	146911623361.5	8.7			146911623361.5	8.7
P(72)	146989515840.3	4.0			146989515840.3	4.0
P(70)	147066640733.3	3.5			147066640733.3	3.5
P(68)	147142980565.8	3.5			147142980565.8	3.5
P(66)	147218521294.3	3.4			147218521294.3	3.4

P(64)	147293251422.9	3.7	147293251423.0	0.1	147293251423.0	3.2
P(62)	147367161400.9	3.3	147367161402.0	1.1	147367161402.0	3.2
P(60)	147440243211.6	3.3	147440243210.7	-0.9	147440243210.7	3.2
P(58)	147512490048.1	3.3	147512490047.3	-0.8	147512490047.3	3.2
P(56)	147583896096.4	3.3	147583896095.9	-0.5	147583896095.9	3.2
P(54)	147654456358.4	3.3	147654456358.3	-0.1	147654456358.3	3.2
P(52)	147724166519.3	3.0	147724166519.9	0.6	147724166519.9	3.2
P(50)	147793022842.6	3.1	147793022843.2	0.6	147793022843.2	3.2
P(48)	147861022080.7	3.0	147861022082.0	1.3	147861022082.0	3.2
P(46)	147928161407.1	3.1	147928161410.7	3.6	147928161407.1	3.1
P(44)	147994438380.1	3.3	147994438365.6	-14.5	147994438380.1	3.3
P(42)	148059850796.9	3.0	148059850795.5	-1.4	148059850795.5	3.2
P(40)	148124396819.3	2.9	148124396819.2	-0.1	148124396819.2	3.2
P(38)	148188074787.2	2.9	148188074788.6	1.4	148188074788.6	3.2
P(36)	148250883255.1	2.8	148250883256.5	1.4	148250883256.5	3.2
P(34)	148312820947.2	2.9	148312820948.2	1.0	148312820948.2	3.2
P(32)	148373886735.5	2.9	148373886735.6	0.1	148373886735.6	3.2
P(30)	148434079613.5	2.9	148434079614.7	1.2	148434079614.7	3.2
P(28)	148493398682.7	3.9	148493398684.8	2.1	148493398684.8	3.2
P(26)	148551843131.1	2.9	148551843130.4	-0.7	148551843130.4	3.2
P(24)	148609412204.0	3.0	148609412203.9	-0.1	148609412203.9	3.2
P(22)	148666105210.8	3.1	148666105211.2	0.4	148666105211.2	3.2
P(20)	148721921498.3	3.0	148721921497.9	-0.4	148721921497.9	3.2
P(18)	148776860436.3	3.0	148776860437.2	0.9	148776860437.2	3.2
P(16)	148830921417.8	3.0	148830921419.1	1.3	148830921419.1	3.2
P(14)	148884103839.8	3.2	148884103841.0	1.2	148884103841.0	3.2
P(12)	148936407097.7	3.1	148936407098.8	1.1	148936407098.8	3.2
P(10)	148987830579.6	3.6	148987830580.0	0.4	148987830580.0	3.2
P(8)	149038373657.5	2.9	149038373657.3	-0.2	149038373657.3	3.2
P(6)	149088035683.0	2.9	149088035683.3	0.3	149088035683.3	3.2
P(4)	149136815987.3	2.9	149136815986.2	-1.1	149136815986.2	3.2
P(2)	149184713867.3	3.0	149184713866.8	-0.5	149184713866.8	3.2
R(0)	149254904543.6	3.1	149254904542.8	-0.8	149254904542.8	3.2
R(2)	149300593110.5	2.9	149300593110.6	0.1	149300593110.6	3.2
R(4)	149345396570.0	2.9	149345396569.1	-0.9	149345396569.1	3.2
R(6)	149389314083.5	2.9	149389314082.0	-1.5	149389314082.0	3.2
R(8)	149432344784.5	3.1	149432344785.8	1.3	149432344785.8	3.2
R(10)	149474487792.4	3.1	149474487792.4	0.0	149474487792.4	3.2
R(12)	149515742194.7	3.0	149515742194.1	-0.6	149515742194.1	3.2
R(14)	149556107069.8	3.2	149556107068.4	-1.4	149556107068.4	3.2
R(16)	149595581482.8	3.1	149595581484.1	1.3	149595581484.1	3.2
R(18)	149634164511.2	3.0	149634164509.2	-2.0	149634164509.2	3.2
R(20)	149671855220.4	3.1	149671855219.0	-1.4	149671855219.0	3.2
R(22)	149708652707.4	2.9	149708652705.8	-1.6	149708652705.8	3.2
R(24)	149744556091.7	3.1	149744556089.7	-2.0	149744556089.7	3.2

R(26)	149779564532.6	3.2	149779564531.0	-1.6	149779564531.0	3.2
R(28)	149813677243.6	3.1	149813677243.1	-0.5	149813677243.1	3.2
R(30)	149846893508.5	3.1	149846893508.2	-0.3	149846893508.2	3.2
R(32)	149879212692.8	3.0	149879212693.7	0.9	149879212693.7	3.2
R(34)	149910634270.4	3.0	149910634270.6	0.2	149910634270.6	3.2
R(36)	149941157834.1	3.3	149941157834.3	0.2	149941157834.3	3.2
R(38)	149970783128.6	3.1	149970783127.3	-1.3	149970783127.3	3.2
R(40)	149999510067.7	3.2	149999510064.7	-3.0	149999510064.7	3.2
R(42)	150027338777.9	3.2	150027338763.0	-14.9	150027338777.9	3.2
R(44)	150054269570.1	3.2	150054269572.3	2.2	150054269570.1	3.2
R(46)	150080303113.5	3.3	150080303112.8	-0.7	150080303112.8	3.2
R(48)	150105440317.6	3.1	150105440318.0	0.4	150105440318.0	3.2
R(50)	150129682483.6	3.2	150129682483.4	-0.2	150129682483.4	3.2
R(52)			150153031325.9		150153031325.9	3.2
R(54)			150175489053.7		150175489053.7	3.2
R(56)			150197058453.0		150197058453.0	3.2
R(58)			150217742994.1		150217742994.1	3.2
R(60)			150237546965.1		150237546965.1	3.2
R(62)			150256475641.1		150256475641.1	3.2
R(64)			150274535516.2*		150274535516.2	3.4
R(66)			150291734614.4*		150291734614.4	3.5
R(68)			150308082906.4*		150308082906.4	3.5
R(70)			150323592911.2*		150323592911.2	4.0
R(72)			150338280579.2*		150338280579.2	8.7

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20012-00001 band of 12C18O16O

Assig.	Meas. freq.	UncMeas	Calc. freq	Cal-Meas	Rec. freq.	Unc.
R(11)	147293250931.5	3.7			147293250931.5	3.7
P(12)	146765882700.7	3.7			146765882700.7	3.7

