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Supplementary Information for: The Fundamental Vibrational Frequencies and Spectroscopic Constants of the $C_2O_2H_2$ Isomers: Molecules Known in Simulated Interstellar Ice Analogues†

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CCSD(T)-F12b/cc-pCVTZ optimized geometries (in Å) and F12-TZ dipole moment projections (in a.u. at these geometries) for:

trans-glyoxal
C -0.6424352859 0.4019125850 0.0000000000
C 0.6424352859 -0.4019125850 0.0000000000
O -1.7180008163 -0.1409738275 0.0000000000
O 1.7180008163 0.1409738275 0.0000000000
H -0.5132913333 1.4954010318 0.0000000000
H 0.5132913333 -1.4954010318 0.0000000000

cis-glyoxal
C 0.0000000000 0.7663599838 0.5246719282
C 0.0000000000 -0.7663599838 0.5246719282
O 0.0000000000 1.4084991149 -0.4897529319
O 0.0000000000 -1.4084991149 -0.4897529319
H 0.0000000000 1.2407441956 1.5218351577
H 0.0000000000 -1.2407441956 1.5218351577
μ 0.0000000000 0.0000000000 1.39848436

cyc-H_2COCO
O 0.0000000000 -0.0934115742 -1.4630895097
C 0.0000000000 -0.0818693214 -0.2793384161
O 0.0000000000 0.8014549958 0.7122692605
C 0.0000000000 -0.6888785376 1.0314477161
H 0.9235868722 -1.0272523093 1.4778105299
H -0.9235868722 -1.0272523093 1.4778105299
μ 0.0000000000 -0.70816087 1.09361051

OCCHOH
H -1.6132126816 -0.0409298120 -0.7925423999
C -0.5541307570 0.0108017233 -0.5961099621
C -0.1327592374 0.0070381275 0.6565497044
O 0.2225260368 0.0002944791 1.7642376774
O 0.3655568072 -0.0624157886 -1.6330553958
H 0.4636036472 0.8144175491 -2.0099850730
μ -0.38090045 0.53246562 -0.42397192

HOCCOH
C -0.5978996172 -0.0089982104 -0.0209759699
C 0.5978996172 0.0089982104 -0.0209759699
O -1.9190018904 0.0479064026 -0.0209759699
O 1.9190018904 -0.0479064026 -0.0209759699
H -2.2567648023 -0.6182156620 0.5829169478
H 2.2567648023 0.6182156620 0.5829169478
μ 0.0000000000 0.0000000000 0.79797062

Table 1 Fermi resonances for *trans*-glyoxal

$\omega_5 + \omega_3 = \omega_6 + \omega_4 = \omega_7 + \omega_3 = \omega_1$
$\omega_5 + \omega_4 = \omega_6 + \omega_3 = \omega_2$
$2\omega_9 = \omega_{10} + \omega_7 = \omega_{11} + \omega_6 = \omega_3$
$\omega_{10} + \omega_6 = \omega_{11} + \omega_5 = \omega_4$
$\omega_{11} + \omega_7 = \omega_{12} + \omega_8 = \omega_6$
$2\omega_{10} = \omega_{12} + \omega_9 = \omega_7$
$\omega_{11} + \omega_9 = \omega_8$
$\omega_{12} + \omega_{10} = \omega_9$

Table 2 Coriolis resonances for *trans*-glyoxal

Modes	Axes
$\omega_8 = \omega_7$	A

Table 3 Fermi resonances for *cis*-glyoxal

$2\omega_5 = 2\omega_6 = \omega_1$
$\omega_6 + \omega_5 = \omega_2$
$\omega_9 + \omega_8 = \omega_{11} + \omega_6 = \omega_3$
$2\omega_8 = 2\omega_9 = \omega_4$
$2\omega_{10} = \omega_5$
$\omega_{12} + \omega_8 = \omega_7$
$\omega_{12} + \omega_{10} = \omega_9$
$2\omega_{12} = \omega_{11}$

Table 4 Coriolis resonances for *cis*-glyoxal

Modes	Axes
$\omega_9 = \omega_8$	C
$\omega_{12} = \omega_{11}$	B

Table 5 Fermi resonances for *cyc*-H_2COCO

$\omega_7 + \omega_3 = \omega_1$
$2\omega_4 = \omega_5 + \omega_3 = \omega_6 + \omega_3 = \omega_2$
$2\omega_8 = 2\omega_9 = \omega_9 + \omega_5 = \omega_9 + \omega_6 = \omega_{10} + \omega_5 = \omega_{10} + \omega_6 = \omega_3$
$2\omega_{10} = \omega_{10} + \omega_9 = \omega_{11} + \omega_9 = \omega_{12} + \omega_8 = \omega_4$
$2\omega_{12} = \omega_{11} + \omega_{10} = \omega_6$
$\omega_{12} + \omega_{10} = \omega_{12} + \omega_{11} = \omega_7$
$\omega_{12} + \omega_{10} = \omega_{12} + \omega_{11} = \omega_8$
$2\omega_{12} = \omega_9$

Table 6 Coriolis resonances for *cyc*-H_2COCO

Modes	Axes
$\omega_7 = \omega_5$	A
B	
$\omega_8 = \omega_6$	A
$\omega_8 = \omega_7$	C
$\omega_9 = \omega_8$	A
$\omega_{11} = \omega_{10}$	C
$\omega_{12} = \omega_{11}$	A

Table 7 Fermi resonances for OCCHOH

$\omega_6 + \omega_3 = \omega_2$
$2\omega_7 = \omega_7 + \omega_5 = \omega_7 + \omega_6 = \omega_9 + \omega_4 = \omega_3$
$2\omega_8 = \omega_{11} + \omega_5 = \omega_{11} + \omega_6 = \omega_{11} + \omega_7 = \omega_4$
$2\omega_9 = \omega_9 + \omega_8 = \omega_{11} + \omega_7 = \omega_{12} + \omega_6 = \omega_{12} + \omega_7 = \omega_5$
$2\omega_8 = 2\omega_9 = \omega_{10} + \omega_9 = \omega_{11} + \omega_7 = \omega_6$
$2\omega_{10} = \omega_{10} + \omega_9 = \omega_{11} + \omega_8 = \omega_{11} + \omega_9 = \omega_{12} + \omega_8 = \omega_7$
$2\omega_{11} = \omega_{11} + \omega_9 = \omega_{12} + \omega_9 = \omega_{12} + \omega_{11} = \omega_8$
$2\omega_{11} = \omega_{12} + \omega_{11} = \omega_9$
$2\omega_{11} = \omega_{10}$
$2\omega_{12} = \omega_{11}$

Table 8 Coriolis resonances for OCCHOH

Modes	Axes
$\omega_7 = \omega_6$	C
$\omega_9 = \omega_8$	A
B	
$\omega_{10} = \omega_8$	A

Table 9 Fermi resonances for HOCCOH

$2\omega_5 = 2\omega_6 = \omega_6 + \omega_4 = \omega_3$
$2\omega_8 = 2\omega_9 = \omega_7$
$2\omega_{12} = \omega_{11} + \omega_{10} = \omega_8$
$2\omega_{11} = \omega_{10}$

Table 10 Coriolis resonances for HOCCOH

Modes	Axes
$\omega_9 = \omega_8$	A
$\omega_{11} = \omega_9$	A
$\omega_{12} = \omega_8$	A
$\omega_{12} = \omega_{11}$	A

Table 11 Rotational Constants of *trans*-glyoxal

Const.	Units	TcCR	TcCR+DZ
A_1	MHz	55105.5	55089.9
B_1	MHz	4794.7	4794.3
C_1	MHz	4412.7	4412.2
A_2	MHz	55083.4	55067.8
B_2	MHz	4794.9	4794.5
C_2	MHz	4412.7	4412.2
A_3	MHz	55188.8	55176.1
B_3	MHz	4786.7	4786.2
C_3	MHz	4405.9	4405.4
A_4	MHz	55227.1	55215.7
B_4	MHz	4783.2	4782.7
C_4	MHz	4403.4	4402.9
A_5	MHz	55308.5	55296.2
B_5	MHz	4804.7	4804.3
C_5	MHz	4415.4	4415.0
A_6	MHz	55264.8	55252.3
B_6	MHz	4805.6	4805.2
C_6	MHz	4415.7	4415.2
A_7	MHz	55345.1	55333.2
B_7	MHz	4779.9	4779.3
C_7	MHz	4395.3	4394.7
A_8	MHz	55061.7	55049.8
B_8	MHz	4790.0	4789.7
C_8	MHz	4416.9	4416.6
A_9	MHz	55285.4	55273.1
B_9	MHz	4788.9	4788.5
C_9	MHz	4415.3	4414.8
A_{10}	MHz	55353.6	55342.2
B_{10}	MHz	4790.2	4789.6
C_{10}	MHz	4407.0	4406.5
A_{11}	MHz	57034.4	57023.6
B_{11}	MHz	4804.5	4804.1
C_{11}	MHz	4415.0	4414.5
A_{12}	MHz	53191.0	53181.4
B_{12}	MHz	4811.8	4811.2
C_{12}	MHz	4442.1	4441.5

Table 12 Rotational Constants for *cis*-glyxoal

Const.	Units	TcCR	TcCR+DZ
A_1	MHz	26761.8	26740.1
B_1	MHz	6164.5	6170.0
C_1	MHz	5018.7	5021.5
A_2	MHz	26780.2	26758.6
B_2	MHz	6162.8	6168.3
C_2	MHz	5017.8	5020.6
A_3	MHz	26632.6	26611.3
B_3	MHz	6181.3	6186.9
C_3	MHz	5024.7	5027.6
A_4	MHz	26620.1	26597.0
B_4	MHz	6174.9	6180.7
C_4	MHz	5018.9	5021.9
A_5	MHz	26736.9	26714.5
B_5	MHz	6194.8	6200.9
C_5	MHz	5031.9	5035.1
A_6	MHz	26707.5	26684.6
B_6	MHz	6202.7	6208.8
C_6	MHz	5028.4	5031.5
A_7	MHz	26688.8	26661.6
B_7	MHz	6175.8	6183.2
C_7	MHz	5032.5	5036.5
A_8	MHz	26809.1	26788.0
B_8	MHz	6143.2	6148.6
C_8	MHz	4999.4	5002.1
A_9	MHz	26783.3	26760.3
B_9	MHz	6186.4	6192.7
C_9	MHz	5024.5	5027.8
A_{10}	MHz	26716.7	26693.2
B_{10}	MHz	6165.9	6172.2
C_{10}	MHz	5028.1	5031.5
A_{11}	MHz	26960.4	26935.8
B_{11}	MHz	6169.2	6176.0
C_{11}	MHz	5017.6	5021.2
A_{12}	MHz	27069.4	27033.3
B_{12}	MHz	6111.1	6122.3
C_{12}	MHz	5030.9	5037.0

Table 13 Rotational Constants of *cyc*-H_2COCO

Const.	Units	TcCR
A_1	MHz	24931.6
B_1	MHz	8090.5
C_1	MHz	6368.7
A_2	MHz	24904.9
B_2	MHz	8091.3
C_2	MHz	6369.8
A_3	MHz	24878.9
B_3	MHz	8052.8
C_3	MHz	6340.8
A_4	MHz	24872.4
B_4	MHz	8103.2
C_4	MHz	6383.2
A_5	MHz	24933.0
B_5	MHz	8093.2
C_5	MHz	6357.2
A_6	MHz	24836.4
B_6	MHz	8093.2
C_6	MHz	6357.7
A_7	MHz	24710.9
B_7	MHz	8116.4
C_7	MHz	6371.5
A_8	MHz	24917.3
B_8	MHz	8093.5
C_8	MHz	6370.4
A_9	MHz	24918.7
B_9	MHz	8083.3
C_9	MHz	6360.8
A_{10}	MHz	24627.2
B_{10}	MHz	8127.3
C_{10}	MHz	6354.8
A_{11}	MHz	24965.1
B_{11}	MHz	8112.8
C_{11}	MHz	6369.8
A_{12}	MHz	24839.6
B_{12}	MHz	8113.2
C_{12}	MHz	6383.0

Table 14 Rotational Constants of OCCHOH

Const.	Units	TcCR	TcCR+DZ
A_1	MHz	48878.6	48706.7
B_1	MHz	4680.1	4685.4
C_1	MHz	4318.4	4321.8
A_2	MHz	49510.7	49339.2
B_2	MHz	4662.1	4667.4
C_2	MHz	4306.3	4309.6
A_3	MHz	48996.1	48824.9
B_3	MHz	4654.8	4659.9
C_3	MHz	4296.1	4299.2
A_4	MHz	48459.6	48277.5
B_4	MHz	4684.3	4689.8
C_4	MHz	4315.4	4318.8
A_5	MHz	49175.9	48999.7
B_5	MHz	4680.1	4685.7
C_5	MHz	4318.1	4321.5
A_6	MHz	48353.9	48159.5
B_6	MHz	4691.2	4697.1
C_6	MHz	4320.3	4324.0
A_7	MHz	49416.8	49243.0
B_7	MHz	4662.7	4668.1
C_7	MHz	4303.0	4306.3
A_8	MHz	49771.3	49595.3
B_8	MHz	4674.6	4680.3
C_8	MHz	4313.3	4316.9
A_9	MHz	49071.3	48885.2
B_9	MHz	4669.9	4675.9
C_9	MHz	4315.8	4319.6
A_{10}	MHz	48993.6	48765.8
B_{10}	MHz	4680.0	4687.2
C_{10}	MHz	4322.4	4326.9
A_{11}	MHz	49947.8	49700.0
B_{11}	MHz	4668.2	4675.8
C_{11}	MHz	4306.5	4311.2
A_{12}	MHz	49340.3	49079.6
B_{12}	MHz	4699.6	4707.9
C_{12}	MHz	4326.1	4331.3

Table 15 Rotational Constants of HOCCOH

Const.	Units	TcCR	TcCR+DZ
A_1	MHz	317178.4	317119.5
B_1	MHz	3674.7	3675.9
C_1	MHz	3664.9	3665.6
A_2	MHz	317211.3	317174.6
B_2	MHz	3674.7	3675.9
C_2	MHz	3664.8	3665.5
A_3	MHz	324037.6	324052.4
B_3	MHz	3656.3	3657.3
C_3	MHz	3646.6	3647.1
A_4	MHz	324836.3	324813.2
B_4	MHz	3665.5	3666.6
C_4	MHz	3656.0	3656.6
A_5	MHz	331974.6	332026.9
B_5	MHz	3675.2	3676.4
C_5	MHz	3664.8	3665.6
A_6	MHz	330702.4	330724.4
B_6	MHz	3668.7	3669.9
C_6	MHz	3658.4	3659.1
A_7	MHz	323685.1	323685.3
B_7	MHz	3668.9	3670.1
C_7	MHz	3659.1	3659.8
A_8	MHz	322066.2	321978.1
B_8	MHz	3684.6	3686.4
C_8	MHz	3674.3	3675.5
A_9	MHz	322144.9	322176.4
B_9	MHz	3684.6	3686.2
C_9	MHz	3674.9	3676.0
A_{10}	MHz	326103.9	326211.4
B_{10}	MHz	3675.0	3676.5
C_{10}	MHz	3663.2	3664.1
A_{11}	MHz	327098.3	327045.1
B_{11}	MHz	3684.7	3686.3
C_{11}	MHz	3676.6	3677.7
A_{12}	MHz	321002.2	321025.5
B_{12}	MHz	3686.1	3687.7
C_{12}	MHz	3675.4	3676.4