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## Using computed infrared intensities for the reduction of vibrational configuration interaction bases<sup>†</sup>

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The Adaptive Vibrational Configuration Interaction (A-VCI) algorithm is an iterative process that computes the anharmonic spectrum of a molecule using nested bases to discretize the Hamiltonian operator. For large molecular systems, the size of the discretization space and the computation time quickly become prohibitive. It is therefore necessary to develop new methods to further limit the number of basis functions. Most of the time, the interpretation of an experimental infrared spectrum does not require the calculation of all eigenvalues but only those corresponding to vibrational states with significant intensity. In this paper, a technique that uses infrared intensities is introduced to select a subset of eigenvalues to be precisely calculated. Thus, we build smaller nested bases and reduce both the memory footprint and the computational time. We validate the advantages of this new approach on a well-studied 7-atom molecular system ( $C_2H_4O$ ), and we apply it on a larger 10-atom molecule ( $C_4H_4N_2$ ).

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<sup>†</sup> Electronic Supplementary Information (ESI) available: [The supplementary material contains the PES, Coriolis and dipole moment coefficients used in this work for  $C_2H_4O$  and  $C_4H_4N_2$ . Detailed calculation results are also provided for the molecular systems considered in this work. See DOI: 00.0000/00000000.

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# 1 PES, Coriolis and dipole moment surface coefficients

## 1.1 C<sub>2</sub>H<sub>4</sub>O

**Listing 1** C<sub>2</sub>H<sub>4</sub>O: fourth order polynomial PES at the CCSD(T)/cc-pVTZ - b3lyp/6-31+G\*\* level of theory (in cm<sup>-1</sup>)<sup>1</sup>

PES C2H4O - ccb3 (ccsd(t)/cc-pVTZ - B3LYP/6-31+G\*\*) - (Sorted By energy)

line 1 : dimension numberOfElements

line x : index[dimension] coeff

```
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 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 425.08985
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 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 650.05405
 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 756.175
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 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 1598.28005
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 1605.63245
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0 0 2 0 0 1 0 0 0 0 0 0 1 0 0 1.02091  
0 0 2 0 0 1 0 0 0 0 1 0 0 0 0 -1.851375  
0 0 2 0 0 1 0 0 1 0 0 0 0 0 0 -5.779575  
0 0 0 0 0 0 0 0 0 0 1 0 1 2 0 -9.459015  
0 0 0 0 0 0 0 0 1 0 0 0 1 2 0 5.59968  
0 0 0 0 0 0 0 0 1 0 1 0 0 2 0 13.25928  
0 0 0 0 0 1 0 0 0 0 0 0 1 2 0 -0.585735  
0 0 0 0 0 1 0 0 0 0 1 0 0 2 0 -6.21874

0 0 0 0 0 1 0 0 1 0 0 0 0 2 0 -26.8905  
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0 0 1 0 0 0 0 0 0 0 1 0 0 2 0 0.388135  
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0 0 1 0 0 1 0 0 0 0 0 0 0 2 0 -18.41549  
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0 0 0 0 0 0 0 1 2 0 0 0 0 1 0 1.33695  
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0 0 0 0 0 0 0 2 1 0 1 0 0 0 0 -2.859605  
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0 0 0 0 0 1 0 2 0 0 1 0 0 0 0 8.362565  
0 0 0 0 0 1 0 2 1 0 0 0 0 0 0 2.7752  
0 0 1 0 0 0 0 2 0 0 0 0 1 0 0 -2.873705  
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0 0 1 0 0 0 0 2 1 0 0 0 0 0 0 1.96568  
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0 0 2 1 0 0 0 0 0 0 0 0 0 1 0 -0.853955  
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0 0 0 1 0 2 0 1 0 0 0 0 0 0 0 8.7671  
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0 0 0 2 0 0 0 0 1 0 0 0 1 0 0 2.416185  
0 0 0 2 0 0 0 0 1 0 1 0 0 0 0 -5.23831  
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0 0 0 2 0 1 0 0 0 0 1 0 0 0 0 -11.01553  
0 0 0 2 0 1 0 0 1 0 0 0 0 0 0 16.599305  
0 0 1 2 0 0 0 0 0 0 0 0 1 0 0 2.513205  
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0 0 0 0 0 1 0 0 0 0 0 0 1 0 2 0.587695  
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0 0 1 0 0 0 0 0 0 0 0 0 1 0 2 -2.595635  
0 0 1 0 0 0 0 0 0 0 1 0 0 0 2 0.37383  
0 0 1 0 0 0 0 0 1 0 0 0 0 0 2 -7.295215  
0 0 1 0 0 1 0 0 0 0 0 0 0 0 2 -18.62337  
0 0 0 0 0 0 0 1 0 0 0 0 0 1 2 11.2306  
0 0 0 1 0 0 0 0 0 0 0 0 0 1 2 -7.74697  
0 0 0 1 0 0 0 1 0 0 0 0 0 0 2 -0.37362  
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0 0 0 0 0 2 1 0 0 0 0 0 0 0 1 1.268655  
0 0 2 0 0 0 1 0 0 0 0 0 0 0 1 -1.233765  
0 0 0 0 0 0 1 0 0 0 0 0 0 2 1 -12.656175  
0 0 0 0 0 0 1 2 0 0 0 0 0 0 1 -2.30791  
0 0 0 2 0 0 1 0 0 0 0 0 0 0 1 -1.46938  
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0 0 0 0 0 0 2 0 1 0 0 0 1 0 0 2.41903  
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0 0 0 0 0 1 2 0 1 0 0 0 0 0 0 8.89064  
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1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 1 4.1962  
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0 0 0 2 0 0 0 0 0 1 0 1 0 0 0 2.159025  
0 0 0 0 0 0 0 0 0 1 0 1 0 0 2 10.77547  
0 0 0 0 0 0 2 0 0 1 0 1 0 0 0 1.98102

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0 0 0 0 1 0 0 0 2 1 0 0 0 0 0 0 -1.506235  
0 0 0 0 1 2 0 0 0 0 1 0 0 0 0 0 0.087065  
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0 0 0 0 2 1 0 0 1 0 0 0 0 0 0 0 18.236035  
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0 0 1 0 2 0 0 0 0 1 0 0 0 0 0 0 5.460375  
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0 0 0 1 2 0 0 1 0 0 0 0 0 0 0 0 10.65891  
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0 1 0 0 0 2 0 0 0 0 0 0 1 0 0 0 -5.188565  
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0 1 0 0 0 0 0 0 0 0 0 0 1 0 2 0 7.039265  
0 1 0 0 0 0 0 2 0 0 0 0 1 0 0 0 -2.9569  
0 1 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 -7.94524  
0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 2 7.24887  
0 1 0 0 0 0 2 0 0 0 0 0 1 0 0 0 -6.268485  
2 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -6.661155  
0 1 0 0 0 0 0 0 0 0 1 0 0 2 0 0 -7.851145

```

0 1 0 0 0 0 0 0 0 1 2 0 0 0 0 2.43384
0 1 0 0 0 0 0 0 2 1 0 0 0 0 0 0.641405
0 1 0 0 0 2 0 0 0 1 0 0 0 0 0 0.76277
0 1 2 0 0 0 0 0 0 1 0 0 0 0 0 0.98494
0 1 0 0 0 0 0 0 0 1 0 0 0 2 0 -9.904185
0 1 0 0 0 0 0 2 0 1 0 0 0 0 0 1.65266
0 1 0 2 0 0 0 0 0 1 0 0 0 0 0 5.160055
0 1 0 0 0 0 0 0 0 1 0 0 0 0 2 -9.81408
0 1 0 0 0 0 2 0 0 1 0 0 0 0 0 5.265435
2 1 0 0 0 0 0 0 0 1 0 0 0 0 0 -0.747245
0 1 0 0 0 0 0 0 0 1 0 2 0 0 0 -7.83967
0 1 0 0 0 0 0 0 0 2 0 1 0 0 0 -4.77056
0 1 0 0 1 0 0 0 0 0 0 0 2 0 0 21.08249
0 1 0 0 1 0 0 0 0 0 2 0 0 0 0 -2.225555
0 1 0 0 1 0 0 0 2 0 0 0 0 0 0 -0.12614
0 1 0 0 1 2 0 0 0 0 0 0 0 0 0 -15.074675
0 1 2 0 1 0 0 0 0 0 0 0 0 0 0 1.131915
0 1 0 0 1 0 0 0 0 0 0 0 0 2 0 23.128805
0 1 0 0 1 0 0 2 0 0 0 0 0 0 0 -2.875325
0 1 0 2 1 0 0 0 0 0 0 0 0 0 0 -16.274845
0 1 0 0 1 0 0 0 0 0 0 0 0 0 2 22.495895
0 1 0 0 1 0 2 0 0 0 0 0 0 0 0 -7.097315
2 1 0 0 1 0 0 0 0 0 0 0 0 0 0 -9.79327
0 1 0 0 1 0 0 0 0 0 0 2 0 0 0 20.708735
0 1 0 0 1 0 0 0 0 2 0 0 0 0 0 -3.073725
0 1 0 0 2 0 0 0 0 0 0 1 0 0 0 -6.939575
0 1 0 0 2 0 0 0 0 1 0 0 0 0 0 0.13003
0 2 0 0 0 0 0 0 0 0 1 0 1 0 0 2.00631
0 2 0 0 0 0 0 0 1 0 0 0 1 0 0 -0.581425
0 2 0 0 0 0 0 0 1 0 1 0 0 0 0 2.46956
0 2 0 0 0 1 0 0 0 0 0 0 0 1 0 0 -1.8088
0 2 0 0 0 1 0 0 0 0 0 1 0 0 0 0 -7.95294
0 2 0 0 0 1 0 0 1 0 0 0 0 0 0 -8.663885
0 2 1 0 0 0 0 0 0 0 0 0 0 1 0 0 -2.54274
0 2 1 0 0 0 0 0 0 0 0 1 0 0 0 0 11.98546
0 2 1 0 0 0 0 0 1 0 0 0 0 0 0 18.693195
0 2 1 0 0 1 0 0 0 0 0 0 0 0 0 -14.038835
0 2 0 0 0 0 0 1 0 0 0 0 0 0 1 0 1.34536
0 2 0 1 0 0 0 0 0 0 0 0 0 0 1 0 4.315975
0 2 0 1 0 0 0 1 0 0 0 0 0 0 0 0 -2.82314
0 2 0 0 0 0 1 0 0 0 0 0 0 0 0 1 2.7216
1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 1 2.50127
1 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0.19445
0 2 0 0 0 0 0 0 0 0 1 0 1 0 0 0 -1.39684
0 2 0 0 1 0 0 0 0 0 0 0 1 0 0 0 2.41141
0 2 0 0 1 0 0 0 0 0 1 0 0 0 0 0 -1.846775

```

**Listing 2** C<sub>2</sub>H<sub>4</sub>O: Coriolis coefficients at the b3lyp/6-31+G\*\* level of theory<sup>1</sup>

Coriolis coeffs C2H4O – B3LYP/6–31+G(d,p) – (Sorted By energy)

815.515 850.1797 899.5641 1052.2312 1156.8024 1157.9059 1174.993 1176.0453 1300.1081 1512.35

1549.0739 3109.4584 3117.8766 3196.5601 3211.2649

0.8502093948314251 0.7349746908278225 0.4693523020088895

29 54 54

```

0 11 12 0.001070
0 10 11 -0.036180
0 9 12 0.028820
0 9 10 -0.009820
0 8 11 0.196360
0 8 9 -0.285560
0 5 12 -0.516580
0 5 10 -0.811620
0 5 8 0.082160
0 4 11 0.484060
0 4 9 -0.747980
0 4 5 -0.039700
0 2 11 0.119180
0 2 9 -0.269670

```

0	2	5	0.253690
0	1	12	-0.141260
0	1	10	-0.230870
0	1	8	-0.265630
0	1	4	-0.195890
0	1	2	0.903590
0	13	14	-0.008520
0	7	14	-0.157230
0	6	13	0.315120
0	6	7	-0.654180
0	3	14	-0.474770
0	3	6	0.336460
0	0	13	-0.331830
0	0	7	0.274350
0	0	3	-0.792340
1	14	12	-0.014390
1	14	11	0.026770
1	14	10	-0.204250
1	14	9	-0.779810
1	14	8	0.185620
1	14	5	-0.324250
1	14	4	0.348360
1	14	2	0.074530
1	14	1	0.016590
1	13	12	0.043470
1	13	11	-0.007450
1	13	10	0.760140
1	13	9	0.208560
1	13	8	-0.040860
1	13	5	-0.380270
1	13	4	0.357620
1	13	2	0.060040
1	13	1	-0.114750
1	7	12	-0.762250
1	7	11	0.018270
1	7	10	0.033300
1	7	9	-0.072880
1	7	8	-0.354770
1	7	5	-0.174900
1	7	4	0.028710
1	7	2	-0.164330
1	7	1	-0.208730
1	6	12	0.378100
1	6	11	-0.353970
1	6	10	-0.135460
1	6	9	0.040420
1	6	8	0.053820
1	6	5	-0.201100
1	6	4	0.231770
1	6	2	-0.143110
1	6	1	0.222220
1	3	12	0.044240
1	3	11	-0.442390
1	3	10	0.139680
1	3	9	-0.236490
1	3	8	0.009240
1	3	5	-0.100630
1	3	4	0.067820
1	3	2	-0.003360
1	3	1	0.012180
1	0	12	-0.130620
1	0	11	-0.762440
1	0	10	0.167260
1	0	9	-0.121610
1	0	8	-0.126560
1	0	5	0.069490
1	0	4	-0.115270



0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0	0.0	-0.0108060767511	0.0
0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0	0.0	0.0	0.036733780577
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0	0.0	-0.0383472987167	0.0
0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0	0.0	0.0	0.0241543080259
1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.00492000496117	0.0	0.0
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.103356810916
0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0	-0.0193464355704	0.0	0.0
0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0	0.0	0.0	0.00129033957098
0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0	0.0	0.0	0.00195257048051
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2	0.0	0.0	0.00326125655798
0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00264687081535
0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00320476871589
0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0	0.0	0.0	0.00335925444643
0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00400504575693
0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0	0.0	0.0	0.000560700592716
0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0	0.0	0.0	0.00205796816113
0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0	0.0	0.0	0.00162436185962
0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0	0.0	0.0	0.00167111082166
2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00477471059091
0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00193612052245
0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00161905204412
0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00587093416056
0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0	-0.00333413472407	0.0	0.0
0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0	-0.00512344597261	0.0	0.0
0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0	0.0010462191767	0.0	0.0
1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0	0.0	-0.00151529405964	0.0
0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0	0.0	-0.0071457865928	0.0
0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0	0.0	-0.00115073602622	0.0
0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0	-0.0117864431804	0.0	0.0
0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1	0.0	0.0	0.000855679674636
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00857807003271
0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0	-0.00647954151561	0.0	0.0
0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0	0.0	0.0	0.0038775013098
0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0	0.0	0.00348087027729	0.0
0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0	0.0	0.0	-0.000626084480344
0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0	0.0	0.0	-0.00192770756467
0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0	0.0	0.00223986319154	0.0
0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0	0.0	0.0	0.00556914833465
1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0	0.0	-0.00365944509447	0.0
0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1	0.0	-0.00513777781571	0.0
0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0	-0.00803254299797	0.0	0.0
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1	-0.00279129666788	0.0	0.0
0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0	0.0	0.0	0.000844570728711
0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1	0.0	-0.0129726315593	0.0
0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0	0.0	0.0	-0.000305248342634
0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0	-0.00428386139094	0.0	0.0
1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0	0.0	-0.0060695763062	0.0
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1	0.0	-0.000118918860629	0.0
0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0	-0.00217639408584	0.0	0.0
0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0	0.00260786534719	0.0	0.0
0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0	0.0	0.0	-0.00441582638731
0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0	0.0	0.00842485444406	0.0
0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0	-0.00109302764605	0.0	0.0
0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0	0.0	-0.000972495280821	0.0
1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0	0.0	0.0	-0.00321754790796
0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0	0.0105983031844	0.0	0.0
0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0	0.0	0.0	0.000910040973248
0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0	0.0	-0.00201115381798	0.0
0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0	0.0	0.011853742171	0.0
0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0	0.0	0.00325702914547	0.0
0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0	-0.00914843751789	0.0	0.0
0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1	-0.00977672686204	0.0	0.0
0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0	0.0	0.0	-0.00153591485592
0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0	0.0	0.0	0.00444971906877
0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0	0.0	-0.0034809430435	0.0
0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0	-0.00315328930911	0.0	0.0
0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0	0.00554428187047	0.0	0.0











0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 1 0	120.252
0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0	49.617
0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0	-72.344
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 1	105.634
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 1 0 0 0 0	85.589
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 1 0 0 0 0 0 0 0 0	23.434
0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0	52.718
0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0	40.576
0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 1	-27.03
0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 1 0 0 0 0	-153.014
0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 1 0 0 0 0 0 0 0 0 0 0	-68.463
0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0	-30.89
0 0 1 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0	3.231
0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0	393.418
0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0	97.061
0 1 1 1 0	-998.478
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 1 0	6.248
0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 1 0	-5.1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 1 0 0	34.332
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 1 0 0 0	133.92
0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 1 0 0 0 0	-90.32
0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 1 0 0 0 0	46.924
0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 1 0 0	-30.913
0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 1 0 0 0 0	-56.624
0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 1 0 0 0	30.556
0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 1 0 0 0	-13.864
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 1 0 0	-2.576
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 1 0 0 0	105.384
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0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0	22.862
0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0	8.917
0 1 0 0 1 1 0	-24.843
0 1 1 0 0 0 1 0	-57.027
0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 1 0	44.963
0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 1 0	-12.259
0 1 0 1 0 0 1 0 0	-65.876
0 1 1 1 0 0 0 0 0	-13.932
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0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 1 0 0 0 0 0	48.938
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0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 1 0 0 0 0 0 0	66.766
0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 1 0 0 0 0 0 0	23.675
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0 1 0 1 0 0 1	-24.345
0 1 1 1 0 0 0	53.334
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 1 0 0 0	-50.492
0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0	-15.032
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0	35.842
0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0	8.594
0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0	-1.631
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 1 0	2.003
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0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 1 0	-112.841
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0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 1 0 0	150.991
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0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 1 0 0	132.805
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0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 1 0 0 0 0 0 0 0 0	-8.826
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0 0 0 1 1 0 1 0	6.005
0 0 0 1 0 1 1 0	1.241
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0	-35.335
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0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0	10.795
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0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0	-12.265
0 0 0 1 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0	20.009
0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0	-32.71
0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0	4.88
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0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0	-28.927
0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0	-15.468
0 0 1 1 0 1 0 0	13.178
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1	21.166
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0	12.146
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0	13.446
0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0	-33.326
0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0	9.249
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0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0	10.376
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0	-28.786
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0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0	7.541
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0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0	1.628
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0 0 0 0 1 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0	13.067
0 0 0 0 1 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	20.579
0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0	463.515
0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0	4.432
0 0 0 0 0 1 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0	16.815
0 0 0 0 0 1 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0	14.215
0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0	417.266
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0	322.975
0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0	18.09
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0	-15.621
0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0	6.383
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0	20.254
0 0 0 1 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	-7.294
1 0 0 1 0 1 0	21.18
0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0	-71.818
0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0	40.078











0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0	1.63075
0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0	6.143
0 0 2 0 0 2 0	2.0325
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2 0 0 0 0 2 0	25.86575
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0 0 0 0 0 2 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0	3.049
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0 0 0 0 0 2 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	50.023
0 0 0 0 2 2 0	2.07525
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0 1 0 0 0 3 0	-6.1003333333333325
0 2 0 2	-1.07925
0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0	-3.439
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2 2 0	5.37675
0 2 0 2 0 0 0	-1.0945
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0 2 0 0 2 0	2.263
0 2 0 2 0 0	-1.05825
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0 2 0 2 0	-1.105
0 2 0 0 0 2 0	3.4825
0 3 0 0 0 1 0	0.9006666666666666
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 2	26.9365
0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 2	8.9655
0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 2	-12.272
0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 2 0 0 0 0 0 0	3.242
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0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 2	19.8775
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0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0	-4.309
0 0 2 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0	3.1455
0 0 0 0 0 0 0 0 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1	2.078
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0 0 1 0 0 0 0 0 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0	-4.0925
0 0 1 0 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	-1.5485
1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2	-58.5315
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1 0 0 0 0 0 0 0 1 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0	5.536
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1 0 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1.576
2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0	-7.511

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2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 2.6875  
2 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 -2.434  
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0 1 0 2 0 1 5.2895  
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0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 -2.088
0 1 0 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -14.1455
2 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -7.604
0 1 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -15.0835
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 18.078
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 -2.836
0 1 0 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -16.0825
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 17.922
0 1 0 0 0 1 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 -2.5135
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 18.2905
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 -2.6935
0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 -1.5335
0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 -1.908
0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 5.605
0 2 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 3.892
1 2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.9365
0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 -3.6365
0 2 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 2.2875
0 2 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 2.076
0 2 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 4.8215
0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 -3.7665
0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -2.1055

```

**Listing 5** C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>: Coriolis coefficients at the b3lyp/6-31+G\*\* level of theory<sup>1</sup>

Coriolis coeffs C4H4N2 (pyrazine) – CCB3 – (Sorted By energy)

350.4917 422.4854 600.9536 707.7344 764.053 804.6875 942.503 980.9775 992.3867 1027.0025

1032.046 1082.5146 1156.452 1185.6626 1249.1209 1366.7569 1435.378 1511.3524 1565.9724

1623.8067 3172.9773 3174.1274 3190.2977 3195.2832

0.2132961965359373 0.1972604384699417 0.1024825504307146

29 30 36

```

0 6 23 -0.832870
0 6 19 -0.348160
0 6 14 0.277750
0 6 9 0.230410
0 6 2 0.234260
0 21 8 -0.796690
0 21 0 -0.319240
0 17 8 0.553130
0 17 0 -0.239790
0 12 8 0.059240
0 12 0 -0.867160
0 10 8 0.236270
0 10 0 -0.297680
0 20 7 -0.830700
0 20 4 -0.184390
0 18 7 -0.343780
0 18 4 0.826730
0 15 7 0.425260
0 15 4 0.395400
0 3 7 -0.104440
0 3 4 0.355220
0 5 22 -0.843480
0 5 16 0.373910
0 5 13 -0.198200
0 5 11 0.330840
0 1 22 0.088230
0 1 16 -0.517800
0 1 13 -0.778380
0 1 11 0.343840
1 7 23 0.519680
1 7 19 -0.658590
1 7 14 0.501520
1 7 9 0.079830

```

1	7	2	0.195710
1	4	23	0.091200
1	4	19	0.651850
1	4	14	0.542300
1	4	9	0.153450
1	4	2	0.499140
1	22	8	0.498640
1	22	0	0.179210
1	16	8	0.762150
1	16	0	-0.105870
1	13	8	-0.366350
1	13	0	0.469720
1	11	8	0.190460
1	11	0	0.857930
1	20	6	0.506370
1	18	6	-0.341760
1	15	6	0.763920
1	3	6	0.207910
1	5	21	0.510430
1	5	17	0.743520
1	5	12	-0.423250
1	5	10	0.086620
1	1	21	-0.053200
1	1	17	0.289360
1	1	12	0.255700
1	1	10	-0.920900
2	22	21	-0.019250
2	22	17	0.834450
2	22	12	-0.505430
2	22	10	0.218780
2	16	21	0.791800
2	16	17	-0.318770
2	16	12	0.427610
2	16	10	-0.297640
2	13	21	-0.201670
2	13	17	-0.057320
2	13	12	-0.313880
2	13	10	-0.926030
2	11	21	0.576210
2	11	17	0.445860
2	11	12	0.680570
2	11	10	0.077590
2	20	23	-0.015440
2	20	19	-0.583750
2	20	14	0.737350
2	20	9	0.217130
2	20	2	-0.261080
2	18	23	-0.364740
2	18	19	0.606620
2	18	14	-0.207190
2	18	9	-0.166200
2	18	2	0.654550
2	15	23	0.916140
2	15	19	0.204490
2	15	14	-0.054180
2	15	9	0.093180
2	15	2	0.327500
2	3	23	-0.077850
2	3	19	-0.498640
2	3	14	-0.601410
2	3	9	-0.036170
2	3	2	0.618300

**Listing 6** C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>: dipole moment surface coefficients at the b3lyp/6-31+G\*\* level of theory (in a.u.)<sup>1</sup>

DMS C4H4N2 (pyrazine) – CCB3 – (Sorted By energy)

line 1 : dimension numberOfElements

line x : index[dimension] C\_x C\_y C\_z







## 2 Full numerical results

### 2.1 C<sub>2</sub>H<sub>4</sub>O

**Table 1** Reference calculation for the PES operator with  $F = 200$  eigenvalues of C<sub>2</sub>H<sub>4</sub>O. The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$  and  $\epsilon = 0.005$ .

Number	Eigenvalue	Frequency	Intensity	Assignment
1	13254.34	792.73	0.12	$\omega_1(0.97), \omega_1 + \omega_9(0.14)$
2	13283.56	821.95	12.88	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
3	13339.91	878.30	79.00	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
4	13479.19	1017.58	0.00	$\omega_4(0.97), \omega_4 + \omega_9(0.14)$
5	13583.38	1121.76	0.79	$\omega_6(0.96), \omega_6 + \omega_9(0.14)$
6	13585.84	1124.23	0.05	$\omega_5(0.97), \omega_5 + \omega_9(0.14)$
7	13607.90	1146.29	3.81	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
8	13610.14	1148.53	0.00	$\omega_8(0.97), \omega_8 + \omega_9(0.14)$
9	13732.88	1271.27	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
10	13929.61	1468.00	0.11	$\omega_{10}(0.97), \omega_9 + \omega_{10}(0.13)$
11	13957.45	1495.83	3.80	$\omega_{11}(0.94), 2\omega_1(0.2)$
12	14049.62	1588.01	0.39	$2\omega_1(0.94), \omega_{11}(0.18)$
13	14073.30	1611.69	0.00	$\omega_1 + \omega_2(0.96), \omega_1 + \omega_2 + \omega_9(0.16)$
14	14103.11	1641.50	0.44	$2\omega_2(0.92), 2\omega_2 + \omega_9(0.18)$
15	14132.52	1670.91	0.00	$\omega_1 + \omega_3(0.96), \omega_1 + \omega_3 + \omega_9(0.18)$
16	14157.09	1695.48	0.34	$\omega_2 + \omega_3(0.94), \omega_2 + \omega_3 + \omega_9(0.19)$
17	14216.83	1755.22	0.06	$2\omega_3(0.94), 2\omega_3 + \omega_9(0.21)$
18	14267.85	1806.24	0.10	$\omega_1 + \omega_4(0.96), \omega_1 + \omega_4 + \omega_9(0.15)$
19	14294.49	1832.88	0.53	$\omega_2 + \omega_4(0.94), \omega_2 + \omega_4 + \omega_9(0.17)$
20	14351.27	1889.66	0.11	$\omega_3 + \omega_4(0.92), \omega_1 + \omega_5(0.27)$
21	14369.26	1907.65	1.36	$\omega_1 + \omega_5(0.9), \omega_3 + \omega_4(0.27)$
22	14371.20	1909.59	0.48	$\omega_1 + \omega_6(0.93), \omega_2 + \omega_4(0.14)$
23	14389.65	1928.04	0.28	$\omega_1 + \omega_8(0.82), \omega_2 + \omega_6(0.45)$
24	14399.77	1938.16	0.04	$\omega_1 + \omega_7(0.86), \omega_2 + \omega_5(0.43)$
25	14401.33	1939.72	0.47	$\omega_2 + \omega_6(0.81), \omega_1 + \omega_8(0.47)$
26	14405.54	1943.93	0.02	$\omega_2 + \omega_5(0.85), \omega_1 + \omega_7(0.44)$
27	14423.45	1961.84	0.01	$\omega_2 + \omega_7(0.94), \omega_2 + \omega_7 + \omega_9(0.17)$
28	14432.21	1970.60	0.01	$\omega_2 + \omega_8(0.96), \omega_2 + \omega_8 + \omega_9(0.17)$
29	14459.00	1997.39	1.24	$\omega_3 + \omega_6(0.95), \omega_3 + \omega_6 + \omega_9(0.18)$
30	14460.70	1999.09	0.17	$\omega_3 + \omega_5(0.96), \omega_3 + \omega_5 + \omega_9(0.18)$
31	14482.72	2021.11	0.21	$\omega_3 + \omega_7(0.96), \omega_3 + \omega_7 + \omega_9(0.19)$
32	14485.66	2024.05	0.00	$\omega_3 + \omega_8(0.96), \omega_3 + \omega_8 + \omega_9(0.18)$
33	14493.53	2031.92	0.00	$2\omega_4(0.96), 2\omega_4 + \omega_9(0.16)$
34	14522.17	2060.56	0.13	$\omega_1 + \omega_9(0.93), \omega_1 + 2\omega_9(0.23)$
35	14548.10	2086.49	0.07	$\omega_2 + \omega_9(0.91), \omega_2 + 2\omega_9(0.25)$
36	14589.45	2127.84	0.49	$\omega_4 + \omega_6(0.92), \omega_4 + \omega_6 + \omega_9(0.15)$
37	14595.87	2134.26	0.57	$\omega_4 + \omega_5(0.93), \omega_4 + \omega_5 + \omega_9(0.15)$
38	14602.41	2140.79	0.02	$\omega_3 + \omega_9(0.9), \omega_3 + 2\omega_9(0.27)$
39	14613.64	2152.03	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
40	14626.75	2165.14	0.13	$\omega_4 + \omega_8(0.96), \omega_4 + \omega_8 + \omega_9(0.15)$
41	14694.63	2233.01	0.04	$2\omega_6(0.83), 2\omega_5(0.41)$
42	14701.98	2240.37	1.29	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.24)$
43	14708.00	2246.39	0.00	$\omega_1 + \omega_{10}(0.83), \omega_6 + \omega_8(0.41)$
44	14709.65	2248.04	0.03	$2\omega_5(0.86), 2\omega_6(0.42)$
45	14725.44	2263.83	0.06	$\omega_5 + \omega_8(0.7), \omega_1 + \omega_{11}(0.56)$
46	14728.27	2266.66	0.12	$\omega_5 + \omega_7(0.85), \omega_4 + \omega_9(0.36)$
47	14728.27	2266.66	0.10	$\omega_6 + \omega_7(0.91), \omega_5 + \omega_8(0.2)$
48	14735.71	2274.09	0.17	$\omega_6 + \omega_8(0.85), \omega_1 + \omega_{10}(0.44)$
49	14743.95	2282.34	0.06	$\omega_1 + \omega_{11}(0.67), \omega_5 + \omega_8(0.63)$
50	14749.97	2288.36	0.01	$\omega_2 + \omega_{10}(0.88), 2\omega_7(0.35)$
51	14751.19	2289.58	0.00	$\omega_4 + \omega_9(0.84), \omega_5 + \omega_7(0.41)$
52	14751.53	2289.92	0.07	$2\omega_7(0.84), \omega_2 + \omega_{10}(0.36)$
53	14754.36	2292.75	0.14	$\omega_7 + \omega_8(0.96), \omega_7 + \omega_8 + \omega_9(0.16)$
54	14756.92	2295.31	0.02	$2\omega_8(0.91), 2\omega_7(0.31)$

Table 1 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
55	14772.47	2310.86	0.54	$\omega_2 + \omega_{11}(0.9), 3\omega_2(0.19)$
56	14807.28	2345.67	0.15	$\omega_3 + \omega_{10}(0.96), \omega_3 + \omega_9 + \omega_{10}(0.17)$
57	14832.07	2370.46	0.02	$\omega_3 + \omega_{11}(0.9), 2\omega_1 + \omega_3(0.18)$
58	14840.95	2379.34	0.00	$3\omega_1(0.88), \omega_1 + \omega_{11}(0.29)$
59	14850.38	2388.77	0.24	$\omega_6 + \omega_9(0.9), \omega_6 + 2\omega_9(0.23)$
60	14852.06	2390.45	0.15	$\omega_5 + \omega_9(0.92), \omega_5 + 2\omega_9(0.23)$
61	14863.46	2401.85	0.00	$2\omega_1 + \omega_2(0.92), 2\omega_1 + \omega_2 + \omega_9(0.16)$
62	14876.39	2414.78	0.37	$\omega_7 + \omega_9(0.92), \omega_7 + 2\omega_9(0.24)$
63	14877.26	2415.65	0.00	$\omega_8 + \omega_9(0.93), \omega_8 + 2\omega_9(0.23)$
64	14889.68	2428.07	0.01	$\omega_1 + 2\omega_2(0.9), \omega_1 + 2\omega_2 + \omega_9(0.18)$
65	14919.48	2457.87	0.04	$3\omega_2(0.85), \omega_2 + \omega_{11}(0.24)$
66	14926.27	2464.66	0.00	$2\omega_1 + \omega_3(0.93), 2\omega_1 + \omega_3 + \omega_9(0.18)$
67	14942.95	2481.34	0.07	$\omega_4 + \omega_{10}(0.96), \omega_4 + \omega_9 + \omega_{10}(0.14)$
68	14945.59	2483.98	0.00	$\omega_1 + \omega_2 + \omega_3(0.93), \omega_1 + \omega_2 + \omega_3 + \omega_9(0.2)$
69	14968.29	2506.68	0.00	$\omega_4 + \omega_{11}(0.92), 2\omega_1 + \omega_4(0.2)$
70	14971.62	2510.01	0.01	$2\omega_2 + \omega_3(0.86), 2\omega_2 + \omega_3 + \omega_9(0.2)$
71	14998.82	2537.21	0.00	$2\omega_9(0.88), 3\omega_9(0.3)$
72	15008.30	2546.69	0.00	$\omega_1 + 2\omega_3(0.94), \omega_1 + 2\omega_3 + \omega_9(0.21)$
73	15028.79	2567.18	0.00	$\omega_2 + 2\omega_3(0.9), \omega_2 + 2\omega_3 + \omega_9(0.22)$
74	15044.84	2583.23	0.36	$\omega_6 + \omega_{10}(0.93), \omega_5 + \omega_{11}(0.22)$
75	15048.72	2587.10	0.15	$\omega_5 + \omega_{10}(0.92), \omega_6 + \omega_{11}(0.27)$
76	15055.08	2593.47	0.00	$2\omega_1 + \omega_4(0.9), \omega_4 + \omega_{11}(0.18)$
77	15061.05	2599.43	0.00	$\omega_7 + \omega_{10}(0.85), \omega_8 + \omega_{11}(0.39)$
78	15063.11	2601.49	0.74	$\omega_8 + \omega_{10}(0.86), \omega_7 + \omega_{11}(0.38)$
79	15073.17	2611.56	0.02	$\omega_6 + \omega_{11}(0.76), \omega_1 + \omega_2 + \omega_4(0.41)$
80	15077.30	2615.69	0.20	$\omega_5 + \omega_{11}(0.89), \omega_6 + \omega_{10}(0.24)$
81	15077.48	2615.87	0.01	$\omega_1 + \omega_2 + \omega_4(0.81), \omega_6 + \omega_{11}(0.42)$
82	15091.45	2629.83	0.00	$3\omega_3(0.92), 3\omega_3 + \omega_9(0.24)$
83	15102.26	2640.65	0.00	$\omega_8 + \omega_{11}(0.82), \omega_7 + \omega_{10}(0.42)$
84	15102.58	2640.97	1.65	$\omega_7 + \omega_{11}(0.84), \omega_8 + \omega_{10}(0.41)$
85	15107.17	2645.56	0.01	$2\omega_2 + \omega_4(0.87), 2\omega_2 + \omega_4 + \omega_9(0.18)$
86	15136.54	2674.93	0.02	$\omega_1 + \omega_3 + \omega_4(0.83), 2\omega_1 + \omega_5(0.4)$
87	15153.19	2691.58	0.02	$2\omega_1 + \omega_5(0.78), \omega_1 + \omega_3 + \omega_4(0.44)$
88	15158.23	2696.62	0.00	$2\omega_1 + \omega_6(0.86), \omega_1 + \omega_2 + \omega_4(0.22)$
89	15161.58	2699.97	0.00	$\omega_2 + \omega_3 + \omega_4(0.89), \omega_1 + \omega_2 + \omega_5(0.21)$
90	15171.04	2709.43	0.00	$2\omega_1 + \omega_8(0.76), \omega_1 + \omega_2 + \omega_6(0.43)$
91	15181.04	2719.43	0.08	$\omega_1 + \omega_2 + \omega_5(0.84), 2\omega_1 + \omega_7(0.26)$
92	15188.43	2726.82	0.00	$\omega_1 + \omega_2 + \omega_6(0.77), 2\omega_1 + \omega_8(0.46)$
93	15195.35	2733.74	0.18	$2\omega_1 + \omega_7(0.89), \omega_1 + \omega_2 + \omega_5(0.27)$
94	15198.62	2737.01	0.02	$\omega_9 + \omega_{10}(0.93), 2\omega_9 + \omega_{10}(0.22)$
95	15204.06	2742.45	0.04	$\omega_1 + \omega_2 + \omega_8(0.66), 2\omega_2 + \omega_6(0.59)$
96	15212.07	2750.46	0.02	$\omega_1 + \omega_2 + \omega_7(0.87), 2\omega_2 + \omega_5(0.31)$
97	15217.73	2756.12	0.02	$\omega_1 + \omega_2 + \omega_8(0.65), 2\omega_2 + \omega_6(0.61)$
98	15220.98	2759.37	0.01	$2\omega_2 + \omega_5(0.85), \omega_1 + \omega_2 + \omega_7(0.33)$
99	15221.80	2760.19	0.00	$2\omega_3 + \omega_4(0.88), \omega_1 + \omega_3 + \omega_5(0.3)$
100	15224.44	2762.82	0.11	$\omega_9 + \omega_{11}(0.88), 2\omega_9 + \omega_{11}(0.22)$
101	15236.09	2774.48	0.18	$2\omega_2 + \omega_7(0.88), 2\omega_2 + \omega_7 + \omega_9(0.19)$
102	15244.37	2782.76	0.00	$\omega_1 + \omega_3 + \omega_5(0.87), 2\omega_3 + \omega_4(0.3)$
103	15245.80	2784.19	0.00	$\omega_1 + \omega_3 + \omega_6(0.91), \omega_1 + \omega_3 + \omega_6 + \omega_9(0.18)$
104	15251.02	2789.41	0.00	$2\omega_2 + \omega_8(0.91), 2\omega_2 + \omega_8 + \omega_9(0.19)$
105	15263.55	2801.94	0.00	$\omega_1 + \omega_3 + \omega_8(0.72), \omega_2 + \omega_3 + \omega_6(0.55)$
106	15271.91	2810.30	0.00	$\omega_2 + \omega_3 + \omega_5(0.73), \omega_1 + \omega_3 + \omega_7(0.58)$
107	15273.34	2811.73	0.00	$\omega_2 + \omega_3 + \omega_6(0.7), \omega_1 + \omega_3 + \omega_8(0.58)$
108	15275.59	2813.97	0.00	$\omega_1 + 2\omega_4(0.93), \omega_1 + 2\omega_4 + \omega_9(0.16)$
109	15276.86	2815.25	0.00	$\omega_1 + \omega_3 + \omega_7(0.75), \omega_2 + \omega_3 + \omega_5(0.56)$
110	15293.46	2831.85	0.00	$\omega_2 + \omega_3 + \omega_7(0.9), \omega_2 + \omega_3 + \omega_7 + \omega_9(0.2)$
111	15301.27	2839.66	0.11	$\omega_2 + 2\omega_4(0.91), \omega_2 + 2\omega_4 + \omega_9(0.17)$
112	15302.52	2840.91	0.00	$\omega_2 + \omega_3 + \omega_8(0.93), \omega_2 + \omega_3 + \omega_8 + \omega_9(0.2)$
113	15312.79	2851.18	0.04	$2\omega_1 + \omega_9(0.87), 2\omega_1 + 2\omega_9(0.22)$
114	15332.73	2871.12	0.01	$2\omega_3 + \omega_6(0.92), 2\omega_3 + \omega_6 + \omega_9(0.21)$

Table 1 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
115	15333.44	2871.83	0.00	$\omega_1 + \omega_2 + \omega_9(0.89), \omega_1 + \omega_2 + 2\omega_9(0.26)$
116	15333.70	2872.09	0.02	$2\omega_3 + \omega_5(0.93), 2\omega_3 + \omega_5 + \omega_9(0.21)$
117	15355.70	2894.09	0.02	$2\omega_3 + \omega_7(0.93), 2\omega_3 + \omega_7 + \omega_9(0.22)$
118	15358.94	2897.33	0.00	$\omega_3 + 2\omega_4(0.85), \omega_1 + \omega_4 + \omega_5(0.35)$
119	15359.23	2897.62	0.00	$2\omega_3 + \omega_8(0.93), 2\omega_3 + \omega_8 + \omega_9(0.22)$
120	15361.80	2900.19	0.12	$2\omega_2 + \omega_9(0.83), 2\omega_2 + 2\omega_9(0.27)$
121	15370.18	2908.57	17.10	$\omega_{12}(0.6), \omega_{10} + \omega_{11}(0.49)$
122	15373.63	2912.01	2.19	$\omega_1 + \omega_4 + \omega_5(0.65), \omega_{13}(0.34)$
123	15374.43	2912.82	6.27	$\omega_1 + \omega_4 + \omega_6(0.71), \omega_{10} + \omega_{11}(0.36)$
124	15379.79	2918.17	4.03	$2\omega_{10}(0.65), \omega_{13}(0.45)$
125	15391.07	2929.46	0.05	$\omega_1 + \omega_3 + \omega_9(0.88), \omega_1 + \omega_3 + 2\omega_9(0.27)$
126	15393.97	2932.36	0.36	$\omega_2 + \omega_4 + \omega_6(0.7), \omega_1 + \omega_4 + \omega_8(0.49)$
127	15399.36	2937.75	0.00	$\omega_1 + \omega_4 + \omega_7(0.74), \omega_2 + \omega_4 + \omega_5(0.46)$
128	15406.19	2944.58	0.26	$\omega_1 + \omega_4 + \omega_8(0.77), \omega_2 + \omega_4 + \omega_6(0.49)$
129	15409.04	2947.43	0.00	$\omega_2 + \omega_4 + \omega_5(0.76), \omega_1 + \omega_4 + \omega_7(0.51)$
130	15413.93	2952.31	0.00	$\omega_2 + \omega_3 + \omega_9(0.86), \omega_2 + \omega_3 + 2\omega_9(0.29)$
131	15415.97	2954.36	6.09	$2\omega_{10}(0.59), \omega_{13}(0.51)$
132	15425.96	2964.35	1.29	$\omega_2 + \omega_4 + \omega_7(0.78), \omega_{13}(0.26)$
133	15441.49	2979.88	0.05	$\omega_2 + \omega_4 + \omega_8(0.92), \omega_2 + \omega_4 + \omega_8 + \omega_9(0.18)$
134	15453.20	2991.59	18.32	$\omega_{10} + \omega_{11}(0.62), \omega_{12}(0.53)$
135	15457.72	2996.11	3.89	$2\omega_{11}(0.71), \omega_{13}(0.39)$
136	15459.01	2997.40	0.00	$\omega_3 + \omega_4 + \omega_6(0.88), \omega_1 + \omega_5 + \omega_6(0.18)$
137	15461.74	3000.13	0.28	$\omega_3 + \omega_4 + \omega_5(0.67), \omega_1 + 2\omega_5(0.48)$
138	15470.28	3008.67	0.00	$\omega_3 + \omega_4 + \omega_5(0.59), \omega_1 + 2\omega_6(0.51)$
139	15470.58	3008.97	0.06	$2\omega_3 + \omega_9(0.85), 2\omega_3 + 2\omega_9(0.31)$
140	15478.13	3016.52	0.00	$\omega_1 + \omega_5 + \omega_6(0.82), \omega_1 + \omega_4 + \omega_7(0.23)$
141	15483.62	3022.01	0.22	$\omega_3 + \omega_4 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_6(0.2)$
142	15489.69	3028.08	1.65	$\omega_1 + 2\omega_5(0.64), \omega_1 + 2\omega_6(0.62)$
143	15490.21	3028.60	0.03	$\omega_{14}(0.85), \omega_{13} + \omega_{14}(0.2)$
144	15493.81	3032.20	3.84	$\omega_1 + \omega_6 + \omega_8(0.54), 2\omega_1 + \omega_{10}(0.53)$
145	15494.04	3032.43	0.29	$\omega_3 + \omega_4 + \omega_8(0.75), \omega_1 + \omega_5 + \omega_8(0.5)$
146	15501.08	3039.47	0.04	$\omega_2 + 2\omega_6(0.72), 2\omega_1 + \omega_{10}(0.38)$
147	15501.71	3040.10	42.00	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.27)$
148	15501.74	3040.13	0.22	$\omega_1 + \omega_5 + \omega_8(0.62), \omega_3 + \omega_4 + \omega_8(0.55)$
149	15502.49	3040.88	0.00	$3\omega_4(0.93), 3\omega_4 + \omega_9(0.16)$
150	15509.55	3047.94	0.00	$\omega_1 + \omega_5 + \omega_7(0.8), \omega_1 + \omega_4 + \omega_9(0.28)$
151	15511.30	3049.69	0.00	$\omega_2 + \omega_5 + \omega_6(0.73), \omega_1 + \omega_6 + \omega_7(0.36)$
152	15514.67	3053.06	0.00	$\omega_1 + \omega_6 + \omega_7(0.83), \omega_2 + \omega_5 + \omega_6(0.26)$
153	15519.75	3058.14	0.16	$\omega_1 + \omega_6 + \omega_8(0.62), 2\omega_1 + \omega_{10}(0.51)$
154	15522.78	3061.17	0.21	$2\omega_1 + \omega_{11}(0.57), \omega_1 + \omega_5 + \omega_8(0.41)$
155	15524.00	3062.39	4.06	$\omega_1 + \omega_2 + \omega_{10}(0.69), \omega_2 + \omega_6 + \omega_8(0.44)$
156	15524.20	3062.59	0.01	$\omega_2 + 2\omega_5(0.85), \omega_2 + 2\omega_6(0.33)$
157	15528.21	3066.60	0.00	$\omega_1 + \omega_7 + \omega_8(0.66), \omega_2 + \omega_6 + \omega_7(0.59)$
158	15528.85	3067.24	1.88	$\omega_1 + 2\omega_8(0.76), \omega_1 + \omega_2 + \omega_{10}(0.37)$
159	15534.76	3073.15	0.00	$\omega_1 + \omega_4 + \omega_9(0.83), \omega_1 + \omega_5 + \omega_7(0.34)$
160	15539.22	3077.60	0.00	$\omega_1 + \omega_2 + \omega_{11}(0.56), \omega_2 + \omega_5 + \omega_8(0.5)$
161	15540.29	3078.68	1.98	$\omega_2 + \omega_5 + \omega_7(0.69), \omega_1 + 2\omega_7(0.39)$
162	15544.11	3082.50	0.00	$\omega_1 + \omega_7 + \omega_8(0.61), \omega_2 + \omega_6 + \omega_7(0.5)$
163	15545.14	3083.53	0.00	$\omega_1 + 2\omega_7(0.85), \omega_2 + \omega_5 + \omega_7(0.28)$
164	15552.76	3091.15	0.17	$\omega_2 + \omega_6 + \omega_8(0.79), \omega_1 + \omega_2 + \omega_{10}(0.41)$
165	15559.09	3097.48	0.00	$\omega_2 + \omega_5 + \omega_8(0.74), \omega_1 + \omega_2 + \omega_{11}(0.53)$
166	15560.65	3099.03	0.02	$\omega_2 + 2\omega_7(0.9), \omega_2 + 2\omega_7 + \omega_9(0.18)$
167	15561.18	3099.57	0.00	$\omega_2 + \omega_4 + \omega_9(0.76), \omega_2 + \omega_5 + \omega_7(0.46)$
168	15567.02	3105.40	0.00	$\omega_3 + 2\omega_6(0.79), \omega_3 + 2\omega_5(0.43)$
169	15568.30	3106.69	0.13	$2\omega_2 + \omega_{10}(0.9), 2\omega_2 + \omega_9 + \omega_{10}(0.17)$
170	15569.60	3107.99	0.00	$\omega_2 + \omega_7 + \omega_8(0.92), \omega_2 + \omega_7 + \omega_8 + \omega_9(0.18)$
171	15573.51	3111.90	0.00	$\omega_3 + \omega_5 + \omega_6(0.88), \omega_3 + \omega_4 + \omega_7(0.23)$
172	15578.37	3116.76	0.01	$\omega_2 + 2\omega_8(0.93), \omega_2 + 2\omega_8 + \omega_9(0.18)$
173	15580.97	3119.36	0.00	$\omega_3 + 2\omega_5(0.83), \omega_3 + 2\omega_6(0.45)$
174	15583.97	3122.36	0.00	$\omega_1 + \omega_3 + \omega_{10}(0.76), \omega_3 + \omega_6 + \omega_8(0.44)$

Table 1 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
175	15586.45	3124.84	0.02	$2\omega_2 + \omega_{11}(0.82), 4\omega_2(0.24)$
176	15590.30	3128.69	0.01	$2\omega_4 + \omega_6(0.87), \omega_1 + \omega_4 + \omega_5(0.18)$
177	15597.91	3136.30	0.00	$\omega_3 + \omega_5 + \omega_7(0.76), \omega_3 + \omega_4 + \omega_9(0.43)$
178	15598.79	3137.17	0.00	$\omega_3 + \omega_5 + \omega_8(0.7), \omega_1 + \omega_3 + \omega_{11}(0.5)$
179	15600.41	3138.80	0.05	$\omega_3 + \omega_6 + \omega_7(0.87), \omega_3 + \omega_5 + \omega_8(0.25)$
180	15600.83	3139.22	0.00	$2\omega_4 + \omega_5(0.88), \omega_4 + \omega_6 + \omega_7(0.17)$
181	15609.05	3147.44	0.00	$\omega_3 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_3 + \omega_{10}(0.49)$
182	15615.83	3154.22	0.01	$2\omega_4 + \omega_7(0.85), \omega_4 + \omega_5 + \omega_6(0.25)$
183	15616.22	3154.61	0.00	$\omega_3 + \omega_4 + \omega_9(0.69), \omega_3 + \omega_5 + \omega_7(0.5)$
184	15617.40	3155.78	0.03	$\omega_1 + \omega_3 + \omega_{11}(0.68), \omega_3 + \omega_5 + \omega_8(0.56)$
185	15622.38	3160.77	0.00	$\omega_3 + 2\omega_7(0.71), \omega_2 + \omega_3 + \omega_{10}(0.57)$
186	15622.91	3161.30	0.00	$\omega_2 + \omega_3 + \omega_{10}(0.72), \omega_3 + 2\omega_7(0.56)$
187	15625.31	3163.70	0.06	$4\omega_1(0.77), 2\omega_1 + \omega_{11}(0.39)$
188	15626.30	3164.69	0.01	$\omega_3 + \omega_7 + \omega_8(0.93), \omega_3 + \omega_7 + \omega_8 + \omega_9(0.2)$
189	15629.28	3167.67	0.00	$\omega_3 + 2\omega_8(0.91), \omega_3 + 2\omega_7(0.23)$
190	15631.22	3169.61	0.00	$\omega_1 + \omega_5 + \omega_9(0.84), \omega_3 + \omega_4 + \omega_9(0.23)$
191	15634.74	3173.13	0.00	$\omega_1 + \omega_6 + \omega_9(0.86), \omega_1 + \omega_6 + 2\omega_9(0.22)$
192	15639.08	3177.47	0.00	$2\omega_4 + \omega_8(0.94), 2\omega_4 + \omega_8 + \omega_9(0.17)$
193	15642.90	3181.29	0.00	$\omega_2 + \omega_3 + \omega_{11}(0.85), \omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.18)$
194	15649.07	3187.46	0.00	$3\omega_1 + \omega_2(0.84), \omega_1 + \omega_2 + \omega_{11}(0.24)$
195	15652.68	3191.07	0.00	$\omega_1 + \omega_8 + \omega_9(0.71), \omega_2 + \omega_6 + \omega_9(0.5)$
196	15661.39	3199.78	0.00	$\omega_2 + \omega_5 + \omega_9(0.75), \omega_1 + \omega_7 + \omega_9(0.47)$
197	15662.05	3200.44	0.00	$\omega_2 + \omega_6 + \omega_9(0.68), \omega_1 + \omega_8 + \omega_9(0.54)$
198	15667.19	3205.58	0.00	$\omega_1 + \omega_7 + \omega_9(0.76), \omega_2 + \omega_5 + \omega_9(0.46)$
199	15676.29	3214.68	0.00	$2\omega_1 + 2\omega_2(0.84), 2\omega_1 + \omega_{11}(0.2)$

**Table 2** Reference calculation for the PES + diagonal Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$  and  $\epsilon = 0.005$ .

Number	Eigenvalue	Frequency	Intensity	Assignment
1	13258.09	794.93	0.12	$\omega_1(0.97), \omega_1 + \omega_9(0.14)$
2	13286.27	823.11	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
3	13342.46	879.29	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
4	13482.60	1019.44	0.00	$\omega_4(0.97), \omega_4 + \omega_9(0.14)$
5	13586.72	1123.56	0.79	$\omega_6(0.96), \omega_6 + \omega_9(0.14)$
6	13588.99	1125.82	0.05	$\omega_5(0.97), \omega_5 + \omega_9(0.14)$
7	13610.99	1147.82	3.81	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
8	13613.32	1150.16	0.00	$\omega_8(0.97), \omega_8 + \omega_9(0.14)$
9	13734.94	1271.77	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
10	13932.82	1469.66	0.11	$\omega_{10}(0.97), \omega_9 + \omega_{10}(0.13)$
11	13960.72	1497.56	3.82	$\omega_{11}(0.94), 2\omega_1(0.19)$
12	14055.47	1592.31	0.38	$2\omega_1(0.94), \omega_{11}(0.18)$
13	14078.23	1615.07	0.00	$\omega_1 + \omega_2(0.96), \omega_1 + \omega_2 + \omega_9(0.16)$
14	14107.03	1643.87	0.44	$2\omega_2(0.92), 2\omega_2 + \omega_9(0.18)$
15	14137.31	1674.15	0.00	$\omega_1 + \omega_3(0.96), \omega_1 + \omega_3 + \omega_9(0.18)$
16	14162.20	1699.03	0.34	$\omega_2 + \omega_3(0.94), \omega_2 + \omega_3 + \omega_9(0.19)$
17	14220.38	1757.22	0.06	$2\omega_3(0.94), 2\omega_3 + \omega_9(0.21)$
18	14274.56	1811.40	0.10	$\omega_1 + \omega_4(0.96), \omega_1 + \omega_4 + \omega_9(0.15)$
19	14299.09	1835.93	0.53	$\omega_2 + \omega_4(0.94), \omega_2 + \omega_4 + \omega_9(0.17)$
20	14355.75	1892.59	0.10	$\omega_3 + \omega_4(0.92), \omega_1 + \omega_5(0.25)$
21	14374.60	1911.43	1.38	$\omega_1 + \omega_5(0.91), \omega_3 + \omega_4(0.26)$
22	14376.74	1913.58	0.48	$\omega_1 + \omega_6(0.93), \omega_1 + \omega_6 + \omega_9(0.14)$
23	14394.94	1931.77	0.29	$\omega_1 + \omega_8(0.8), \omega_2 + \omega_6(0.48)$
24	14404.86	1941.69	0.04	$\omega_1 + \omega_7(0.83), \omega_2 + \omega_5(0.49)$
25	14406.12	1942.96	0.46	$\omega_2 + \omega_6(0.79), \omega_1 + \omega_8(0.5)$
26	14410.13	1946.96	0.02	$\omega_2 + \omega_5(0.82), \omega_1 + \omega_7(0.5)$
27	14427.83	1964.66	0.01	$\omega_2 + \omega_7(0.94), \omega_2 + \omega_7 + \omega_9(0.17)$
28	14436.74	1973.58	0.01	$\omega_2 + \omega_8(0.96), \omega_2 + \omega_8 + \omega_9(0.17)$
29	14463.47	2000.31	1.24	$\omega_3 + \omega_6(0.95), \omega_3 + \omega_6 + \omega_9(0.18)$
30	14464.86	2001.69	0.17	$\omega_3 + \omega_5(0.96), \omega_3 + \omega_5 + \omega_9(0.18)$
31	14486.90	2023.73	0.21	$\omega_3 + \omega_7(0.96), \omega_3 + \omega_7 + \omega_9(0.19)$

Table 2 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
32	14489.89	2026.73	0.00	$\omega_3 + \omega_8(0.96), \omega_3 + \omega_8 + \omega_9(0.18)$
33	14498.80	2035.63	0.00	$2\omega_4(0.96), 2\omega_4 + \omega_9(0.16)$
34	14526.52	2063.36	0.13	$\omega_1 + \omega_9(0.93), \omega_1 + 2\omega_9(0.23)$
35	14551.49	2088.32	0.07	$\omega_2 + \omega_9(0.91), \omega_2 + 2\omega_9(0.25)$
36	14594.68	2131.52	0.49	$\omega_4 + \omega_6(0.92), \omega_4 + \omega_6 + \omega_9(0.15)$
37	14600.89	2137.72	0.57	$\omega_4 + \omega_5(0.93), \omega_4 + \omega_5 + \omega_9(0.15)$
38	14605.51	2142.34	0.02	$\omega_3 + \omega_9(0.9), \omega_3 + 2\omega_9(0.27)$
39	14618.77	2155.60	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
40	14631.79	2168.63	0.13	$\omega_4 + \omega_8(0.96), \omega_4 + \omega_8 + \omega_9(0.15)$
41	14699.68	2236.51	0.04	$2\omega_6(0.83), 2\omega_5(0.42)$
42	14706.96	2243.79	1.29	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.24)$
43	14713.33	2250.17	0.00	$\omega_1 + \omega_{10}(0.82), \omega_6 + \omega_8(0.42)$
44	14714.47	2251.31	0.03	$2\omega_5(0.86), 2\omega_6(0.43)$
45	14730.60	2267.43	0.07	$\omega_5 + \omega_8(0.71), \omega_1 + \omega_{11}(0.54)$
46	14733.06	2269.89	0.12	$\omega_5 + \omega_7(0.84), \omega_4 + \omega_9(0.37)$
47	14733.25	2270.08	0.10	$\omega_6 + \omega_7(0.91), \omega_5 + \omega_8(0.22)$
48	14740.87	2277.70	0.17	$\omega_6 + \omega_8(0.85), \omega_1 + \omega_{10}(0.44)$
49	14749.35	2286.18	0.05	$\omega_1 + \omega_{11}(0.69), \omega_5 + \omega_8(0.61)$
50	14754.39	2291.22	0.02	$\omega_2 + \omega_{10}(0.9), 2\omega_7(0.31)$
51	14755.30	2292.13	0.00	$\omega_4 + \omega_9(0.83), \omega_5 + \omega_7(0.42)$
52	14756.14	2292.97	0.07	$2\omega_7(0.86), \omega_2 + \omega_{10}(0.31)$
53	14759.78	2296.62	0.14	$\omega_7 + \omega_8(0.95), \omega_7 + \omega_8 + \omega_9(0.16)$
54	14761.71	2298.55	0.02	$2\omega_8(0.91), 2\omega_7(0.3)$
55	14777.06	2313.90	0.54	$\omega_2 + \omega_{11}(0.9), 3\omega_2(0.19)$
56	14811.63	2348.47	0.15	$\omega_3 + \omega_{10}(0.96), \omega_3 + \omega_9 + \omega_{10}(0.17)$
57	14836.38	2373.22	0.02	$\omega_3 + \omega_{11}(0.9), \omega_6 + \omega_9(0.18)$
58	14848.85	2385.68	0.00	$3\omega_1(0.88), \omega_1 + \omega_{11}(0.28)$
59	14854.28	2391.11	0.24	$\omega_6 + \omega_9(0.9), \omega_6 + 2\omega_9(0.22)$
60	14855.75	2392.58	0.15	$\omega_5 + \omega_9(0.92), \omega_5 + 2\omega_9(0.23)$
61	14870.53	2407.36	0.00	$2\omega_1 + \omega_2(0.92), 2\omega_1 + \omega_2 + \omega_9(0.16)$
62	14880.02	2416.86	0.37	$\omega_7 + \omega_9(0.92), \omega_7 + 2\omega_9(0.24)$
63	14881.18	2418.01	0.00	$\omega_8 + \omega_9(0.93), \omega_8 + 2\omega_9(0.23)$
64	14895.87	2432.71	0.01	$\omega_1 + 2\omega_2(0.9), \omega_1 + 2\omega_2 + \omega_9(0.18)$
65	14924.72	2461.56	0.04	$3\omega_2(0.85), \omega_2 + \omega_{11}(0.23)$
66	14933.23	2470.07	0.00	$2\omega_1 + \omega_3(0.93), 2\omega_1 + \omega_3 + \omega_9(0.18)$
67	14948.27	2485.10	0.07	$\omega_4 + \omega_{10}(0.96), \omega_4 + \omega_9 + \omega_{10}(0.14)$
68	14952.97	2489.81	0.00	$\omega_1 + \omega_2 + \omega_3(0.93), \omega_1 + \omega_2 + \omega_3 + \omega_9(0.2)$
69	14973.58	2510.42	0.00	$\omega_4 + \omega_{11}(0.92), 2\omega_1 + \omega_4(0.19)$
70	14979.20	2516.03	0.01	$2\omega_2 + \omega_3(0.87), 2\omega_2 + \omega_3 + \omega_9(0.2)$
71	15001.40	2538.23	0.00	$2\omega_9(0.88), 3\omega_9(0.3)$
72	15014.14	2550.97	0.00	$\omega_1 + 2\omega_3(0.94), \omega_1 + 2\omega_3 + \omega_9(0.21)$
73	15036.31	2573.15	0.00	$\omega_2 + 2\omega_3(0.9), \omega_2 + 2\omega_3 + \omega_9(0.22)$
74	15049.89	2586.72	0.36	$\omega_6 + \omega_{10}(0.93), \omega_5 + \omega_{11}(0.22)$
75	15054.56	2591.39	0.15	$\omega_5 + \omega_{10}(0.92), \omega_6 + \omega_{11}(0.27)$
76	15064.76	2601.59	0.01	$2\omega_1 + \omega_4(0.88), \omega_7 + \omega_{10}(0.19)$
77	15065.84	2602.67	0.00	$\omega_7 + \omega_{10}(0.83), \omega_8 + \omega_{11}(0.38)$
78	15067.95	2604.79	0.74	$\omega_8 + \omega_{10}(0.86), \omega_7 + \omega_{11}(0.38)$
79	15079.61	2616.44	0.02	$\omega_6 + \omega_{11}(0.82), \omega_5 + \omega_{10}(0.29)$
80	15082.26	2619.09	0.20	$\omega_5 + \omega_{11}(0.89), \omega_6 + \omega_{10}(0.24)$
81	15085.07	2621.91	0.01	$\omega_1 + \omega_2 + \omega_4(0.86), \omega_6 + \omega_{11}(0.31)$
82	15096.02	2632.86	0.00	$3\omega_3(0.92), 3\omega_3 + \omega_9(0.24)$
83	15107.20	2644.03	0.00	$\omega_8 + \omega_{11}(0.82), \omega_7 + \omega_{10}(0.42)$
84	15107.48	2644.31	1.66	$\omega_7 + \omega_{11}(0.84), \omega_8 + \omega_{10}(0.41)$
85	15113.07	2649.91	0.01	$2\omega_2 + \omega_4(0.87), 2\omega_2 + \omega_4 + \omega_9(0.18)$
86	15144.24	2681.08	0.02	$\omega_1 + \omega_3 + \omega_4(0.82), 2\omega_1 + \omega_5(0.41)$
87	15160.81	2697.65	0.02	$2\omega_1 + \omega_5(0.77), \omega_1 + \omega_3 + \omega_4(0.44)$
88	15166.00	2702.83	0.00	$2\omega_1 + \omega_6(0.86), \omega_1 + \omega_2 + \omega_4(0.22)$
89	15168.55	2705.39	0.00	$\omega_2 + \omega_3 + \omega_4(0.89), \omega_1 + \omega_2 + \omega_5(0.21)$
90	15178.65	2715.49	0.00	$2\omega_1 + \omega_8(0.75), \omega_1 + \omega_2 + \omega_6(0.45)$
91	15187.79	2724.62	0.09	$\omega_1 + \omega_2 + \omega_5(0.85), 2\omega_1 + \omega_7(0.25)$

Table 2 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
92	15195.45	2732.29	0.00	$\omega_1 + \omega_2 + \omega_6(0.76), 2\omega_1 + \omega_8(0.48)$
93	15202.49	2739.32	0.02	$\omega_9 + \omega_{10}(0.93), 2\omega_9 + \omega_{10}(0.22)$
94	15202.74	2739.57	0.17	$2\omega_1 + \omega_7(0.89), \omega_1 + \omega_2 + \omega_5(0.26)$
95	15210.43	2747.27	0.04	$\omega_1 + \omega_2 + \omega_8(0.63), 2\omega_2 + \omega_6(0.61)$
96	15218.60	2755.43	0.02	$\omega_1 + \omega_2 + \omega_7(0.85), 2\omega_2 + \omega_5(0.34)$
97	15224.05	2760.89	0.02	$\omega_1 + \omega_2 + \omega_8(0.67), 2\omega_2 + \omega_6(0.58)$
98	15226.76	2763.59	0.01	$2\omega_2 + \omega_5(0.84), \omega_1 + \omega_2 + \omega_7(0.37)$
99	15227.35	2764.18	0.00	$2\omega_3 + \omega_4(0.88), \omega_1 + \omega_3 + \omega_5(0.29)$
100	15228.30	2765.13	0.11	$\omega_9 + \omega_{11}(0.88), 2\omega_9 + \omega_{11}(0.22)$
101	15241.82	2778.65	0.18	$2\omega_2 + \omega_7(0.88), 2\omega_2 + \omega_7 + \omega_9(0.19)$
102	15250.76	2787.59	0.00	$\omega_1 + \omega_3 + \omega_5(0.88), 2\omega_3 + \omega_4(0.29)$
103	15252.54	2789.37	0.00	$\omega_1 + \omega_3 + \omega_6(0.91), \omega_1 + \omega_3 + \omega_6 + \omega_9(0.18)$
104	15256.93	2793.76	0.00	$2\omega_2 + \omega_8(0.91), 2\omega_2 + \omega_8 + \omega_9(0.19)$
105	15270.36	2807.20	0.00	$\omega_1 + \omega_3 + \omega_8(0.74), \omega_2 + \omega_3 + \omega_6(0.53)$
106	15278.57	2815.40	0.00	$\omega_2 + \omega_3 + \omega_5(0.71), \omega_1 + \omega_3 + \omega_7(0.6)$
107	15280.26	2817.09	0.00	$\omega_2 + \omega_3 + \omega_6(0.72), \omega_1 + \omega_3 + \omega_8(0.56)$
108	15283.43	2820.26	0.00	$\omega_1 + \omega_3 + \omega_7(0.73), \omega_2 + \omega_3 + \omega_5(0.59)$
109	15285.21	2822.05	0.00	$\omega_1 + 2\omega_4(0.93), \omega_1 + 2\omega_4 + \omega_9(0.16)$
110	15300.29	2837.12	0.00	$\omega_2 + \omega_3 + \omega_7(0.91), \omega_2 + \omega_3 + \omega_7 + \omega_9(0.2)$
111	15307.84	2844.67	0.12	$\omega_2 + 2\omega_4(0.91), \omega_2 + 2\omega_4 + \omega_9(0.17)$
112	15309.50	2846.34	0.00	$\omega_2 + \omega_3 + \omega_8(0.93), \omega_2 + \omega_3 + \omega_8 + \omega_9(0.2)$
113	15319.37	2856.21	0.04	$2\omega_1 + \omega_9(0.88), 2\omega_1 + 2\omega_9(0.22)$
114	15338.35	2875.18	0.01	$2\omega_3 + \omega_6(0.92), 2\omega_3 + \omega_6 + \omega_9(0.21)$
115	15338.89	2875.73	0.02	$2\omega_3 + \omega_5(0.93), 2\omega_3 + \omega_5 + \omega_9(0.21)$
116	15339.16	2876.00	0.00	$\omega_1 + \omega_2 + \omega_9(0.89), \omega_1 + \omega_2 + 2\omega_9(0.26)$
117	15360.98	2897.82	0.02	$2\omega_3 + \omega_7(0.93), 2\omega_3 + \omega_7 + \omega_9(0.22)$
118	15364.53	2901.36	0.00	$2\omega_3 + \omega_8(0.93), 2\omega_3 + \omega_8 + \omega_9(0.22)$
119	15365.50	2902.34	0.00	$\omega_3 + 2\omega_4(0.86), \omega_1 + \omega_4 + \omega_5(0.31)$
120	15366.59	2903.42	0.13	$2\omega_2 + \omega_9(0.82), 2\omega_2 + 2\omega_9(0.26)$
121	15375.24	2912.08	21.94	$\omega_{12}(0.68), \omega_{10} + \omega_{11}(0.56)$
122	15379.95	2916.79	4.22	$\omega_1 + \omega_4 + \omega_5(0.51), 2\omega_{10}(0.49)$
123	15382.12	2918.96	1.66	$\omega_1 + \omega_4 + \omega_6(0.81), \omega_{10} + \omega_{11}(0.22)$
124	15385.64	2922.48	2.23	$\omega_1 + \omega_4 + \omega_5(0.6), 2\omega_{10}(0.52)$
125	15396.52	2933.36	0.04	$\omega_1 + \omega_3 + \omega_9(0.89), \omega_1 + \omega_3 + 2\omega_9(0.27)$
126	15401.03	2937.86	0.43	$\omega_2 + \omega_4 + \omega_6(0.74), \omega_1 + \omega_4 + \omega_8(0.43)$
127	15407.00	2943.83	0.00	$\omega_1 + \omega_4 + \omega_7(0.68), \omega_2 + \omega_4 + \omega_5(0.54)$
128	15414.11	2950.94	0.23	$\omega_1 + \omega_4 + \omega_8(0.8), \omega_2 + \omega_4 + \omega_6(0.44)$
129	15416.06	2952.90	0.00	$\omega_2 + \omega_4 + \omega_5(0.71), \omega_1 + \omega_4 + \omega_7(0.59)$
130	15419.81	2956.64	0.00	$\omega_2 + \omega_3 + \omega_9(0.86), \omega_2 + \omega_3 + 2\omega_9(0.29)$
131	15420.74	2957.57	6.44	$2\omega_{10}(0.61), \omega_{13}(0.52)$
132	15432.07	2968.91	0.88	$\omega_2 + \omega_4 + \omega_7(0.81), 2\omega_{11}(0.22)$
133	15447.96	2984.79	0.06	$\omega_2 + \omega_4 + \omega_8(0.92), \omega_2 + \omega_4 + \omega_8 + \omega_9(0.18)$
134	15458.43	2995.26	18.61	$\omega_{10} + \omega_{11}(0.63), \omega_{12}(0.53)$
135	15462.97	2999.80	3.81	$2\omega_{11}(0.72), \omega_{13}(0.38)$
136	15465.41	3002.25	0.00	$\omega_3 + \omega_4 + \omega_6(0.88), \omega_3 + \omega_4 + \omega_6 + \omega_9(0.18)$
137	15468.30	3005.14	0.31	$\omega_3 + \omega_4 + \omega_5(0.71), \omega_1 + 2\omega_5(0.45)$
138	15474.74	3011.57	0.06	$2\omega_3 + \omega_9(0.85), 2\omega_3 + 2\omega_9(0.31)$
139	15477.07	3013.90	0.01	$\omega_3 + \omega_4 + \omega_5(0.55), \omega_1 + 2\omega_6(0.53)$
140	15485.42	3022.25	0.01	$\omega_1 + \omega_5 + \omega_6(0.82), \omega_1 + \omega_4 + \omega_7(0.23)$
141	15489.89	3026.73	0.24	$\omega_3 + \omega_4 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_6(0.2)$
142	15494.25	3031.08	0.03	$\omega_{14}(0.85), \omega_{13} + \omega_{14}(0.2)$
143	15496.75	3033.58	2.81	$\omega_1 + 2\omega_5(0.63), \omega_1 + 2\omega_6(0.62)$
144	15500.46	3037.30	0.23	$\omega_3 + \omega_4 + \omega_8(0.78), \omega_1 + \omega_5 + \omega_8(0.46)$
145	15500.83	3037.66	3.34	$\omega_1 + \omega_6 + \omega_8(0.55), 2\omega_1 + \omega_{10}(0.54)$
146	15506.08	3042.91	42.22	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.24)$
147	15507.68	3044.51	0.04	$\omega_2 + 2\omega_6(0.73), 2\omega_1 + \omega_{10}(0.38)$
148	15508.57	3045.41	0.22	$\omega_1 + \omega_5 + \omega_8(0.65), \omega_3 + \omega_4 + \omega_8(0.51)$
149	15509.57	3046.41	0.00	$3\omega_4(0.93), 3\omega_4 + \omega_9(0.16)$
150	15516.71	3053.54	0.00	$\omega_1 + \omega_5 + \omega_7(0.8), \omega_1 + \omega_4 + \omega_9(0.28)$
151	15517.94	3054.78	0.00	$\omega_2 + \omega_5 + \omega_6(0.75), \omega_1 + \omega_6 + \omega_7(0.32)$



Table 2 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
152	15521.85	3058.69	0.00	$\omega_1 + \omega_6 + \omega_7(0.85), \omega_2 + \omega_5 + \omega_6(0.24)$
153	15526.98	3063.81	0.14	$\omega_1 + \omega_6 + \omega_8(0.62), 2\omega_1 + \omega_{10}(0.52)$
154	15530.31	3067.15	0.19	$2\omega_1 + \omega_{11}(0.6), \omega_1 + \omega_5 + \omega_8(0.41)$
155	15530.38	3067.22	0.00	$\omega_2 + 2\omega_5(0.83), \omega_2 + 2\omega_6(0.34)$
156	15530.46	3067.29	3.18	$\omega_1 + \omega_2 + \omega_{10}(0.69), \omega_2 + \omega_6 + \omega_8(0.45)$
157	15535.24	3072.08	0.00	$\omega_1 + \omega_7 + \omega_8(0.63), \omega_2 + \omega_6 + \omega_7(0.62)$
158	15535.85	3072.68	1.58	$\omega_1 + 2\omega_8(0.77), \omega_1 + \omega_2 + \omega_{10}(0.35)$
159	15542.03	3078.86	0.00	$\omega_1 + \omega_4 + \omega_9(0.83), \omega_1 + \omega_5 + \omega_7(0.34)$
160	15545.90	3082.73	0.00	$\omega_1 + \omega_2 + \omega_{11}(0.56), \omega_2 + \omega_5 + \omega_8(0.52)$
161	15546.50	3083.33	1.76	$\omega_2 + \omega_5 + \omega_7(0.69), \omega_1 + 2\omega_7(0.35)$
162	15551.09	3087.93	0.00	$\omega_1 + \omega_7 + \omega_8(0.63), \omega_2 + \omega_6 + \omega_7(0.47)$
163	15551.86	3088.69	0.00	$\omega_1 + 2\omega_7(0.87), \omega_2 + \omega_5 + \omega_7(0.23)$
164	15559.31	3096.14	0.15	$\omega_2 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_2 + \omega_{10}(0.41)$
165	15565.69	3102.53	0.00	$\omega_2 + \omega_5 + \omega_8(0.73), \omega_1 + \omega_2 + \omega_{11}(0.55)$
166	15566.71	3103.55	0.02	$\omega_2 + 2\omega_7(0.9), \omega_1 + \omega_5 + \omega_7(0.18)$
167	15566.74	3103.58	0.00	$\omega_2 + \omega_4 + \omega_9(0.75), \omega_2 + \omega_5 + \omega_7(0.48)$
168	15573.28	3110.11	0.00	$\omega_3 + 2\omega_6(0.78), \omega_3 + 2\omega_5(0.45)$
169	15573.91	3110.74	0.12	$2\omega_2 + \omega_{10}(0.9), 2\omega_2 + \omega_9 + \omega_{10}(0.17)$
170	15576.47	3113.31	0.00	$\omega_2 + \omega_7 + \omega_8(0.92), \omega_2 + \omega_7 + \omega_8 + \omega_9(0.18)$
171	15579.64	3116.47	0.00	$\omega_3 + \omega_5 + \omega_6(0.88), \omega_3 + \omega_4 + \omega_7(0.23)$
172	15584.71	3121.55	0.01	$\omega_2 + 2\omega_8(0.93), \omega_2 + 2\omega_8 + \omega_9(0.18)$
173	15586.89	3123.72	0.00	$\omega_3 + 2\omega_5(0.82), \omega_3 + 2\omega_6(0.46)$
174	15590.40	3127.23	0.00	$\omega_1 + \omega_3 + \omega_{10}(0.76), \omega_3 + \omega_6 + \omega_8(0.44)$
175	15592.40	3129.23	0.02	$2\omega_2 + \omega_{11}(0.82), 4\omega_2(0.24)$
176	15597.51	3134.34	0.01	$2\omega_4 + \omega_6(0.87), \omega_1 + \omega_4 + \omega_5(0.18)$
177	15603.73	3140.56	0.00	$\omega_3 + \omega_5 + \omega_7(0.74), \omega_3 + \omega_4 + \omega_9(0.44)$
178	15604.97	3141.80	0.00	$\omega_3 + \omega_5 + \omega_8(0.71), \omega_1 + \omega_3 + \omega_{11}(0.48)$
179	15606.59	3143.43	0.05	$\omega_3 + \omega_6 + \omega_7(0.87), \omega_3 + \omega_5 + \omega_8(0.26)$
180	15607.82	3144.66	0.00	$2\omega_4 + \omega_5(0.88), \omega_4 + \omega_6 + \omega_7(0.17)$
181	15615.39	3152.22	0.00	$\omega_3 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_3 + \omega_{10}(0.5)$
182	15621.62	3158.45	0.00	$\omega_3 + \omega_4 + \omega_9(0.68), \omega_3 + \omega_5 + \omega_7(0.52)$
183	15622.99	3159.83	0.01	$2\omega_4 + \omega_7(0.82), \omega_4 + \omega_5 + \omega_6(0.24)$
184	15623.98	3160.82	0.04	$\omega_1 + \omega_3 + \omega_{11}(0.68), \omega_3 + \omega_5 + \omega_8(0.51)$
185	15628.36	3165.19	0.00	$\omega_3 + 2\omega_7(0.89), \omega_3 + 2\omega_8(0.21)$
186	15629.70	3166.53	0.00	$\omega_2 + \omega_3 + \omega_{10}(0.9), \omega_2 + \omega_3 + \omega_9 + \omega_{10}(0.19)$
187	15632.88	3169.71	0.01	$\omega_3 + \omega_7 + \omega_8(0.93), \omega_3 + \omega_7 + \omega_8 + \omega_9(0.2)$
188	15635.06	3171.90	0.04	$4\omega_1(0.65), \omega_3 + 2\omega_8(0.51)$
189	15635.24	3172.08	0.02	$\omega_3 + 2\omega_8(0.76), 4\omega_1(0.43)$
190	15637.22	3174.05	0.00	$\omega_1 + \omega_5 + \omega_9(0.85), \omega_3 + \omega_4 + \omega_9(0.22)$
191	15640.94	3177.77	0.00	$\omega_1 + \omega_6 + \omega_9(0.86), \omega_1 + \omega_6 + 2\omega_9(0.22)$
192	15646.03	3182.86	0.00	$2\omega_4 + \omega_8(0.94), 2\omega_4 + \omega_8 + \omega_9(0.17)$
193	15649.94	3186.77	0.00	$\omega_2 + \omega_3 + \omega_{11}(0.85), \omega_2 + \omega_6 + \omega_9(0.19)$
194	15658.19	3195.03	0.00	$3\omega_1 + \omega_2(0.85), \omega_1 + \omega_2 + \omega_{11}(0.23)$
195	15658.69	3195.53	0.00	$\omega_1 + \omega_8 + \omega_9(0.67), \omega_2 + \omega_6 + \omega_9(0.53)$
196	15666.73	3203.57	0.00	$\omega_2 + \omega_5 + \omega_9(0.77), \omega_1 + \omega_7 + \omega_9(0.42)$
197	15667.76	3204.60	0.00	$\omega_2 + \omega_6 + \omega_9(0.66), \omega_1 + \omega_8 + \omega_9(0.58)$
198	15672.96	3209.80	0.00	$\omega_1 + \omega_7 + \omega_9(0.79), \omega_2 + \omega_5 + \omega_9(0.42)$
199	15684.63	3221.46	0.00	$2\omega_1 + 2\omega_2(0.84), 2\omega_1 + \omega_{11}(0.2)$

**Table 3** Reference calculation for the PES + full Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000 \text{ cm}^{-1}$  and  $\epsilon = 0.005$ .

Number	Eigenvalue	Frequency	Intensity	Assignment
1	13257.90	794.85	0.12	$\omega_1(0.97), \omega_1 + \omega_9(0.14)$
2	13286.16	823.11	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
3	13342.37	879.32	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
4	13482.44	1019.39	0.00	$\omega_4(0.97), \omega_4 + \omega_9(0.14)$
5	13586.57	1123.51	0.81	$\omega_6(0.96), \omega_6 + \omega_9(0.14)$
6	13588.83	1125.78	0.04	$\omega_5(0.97), \omega_5 + \omega_9(0.14)$
7	13610.82	1147.76	3.79	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
8	13613.16	1150.10	0.02	$\omega_8(0.97), \omega_8 + \omega_9(0.14)$
9	13734.79	1271.74	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
10	13932.66	1469.61	0.11	$\omega_{10}(0.97), \omega_9 + \omega_{10}(0.13)$

Table 3 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
11	13960.52	1497.47	3.80	$\omega_{11}(0.94), 2\omega_1(0.19)$
12	14055.18	1592.13	0.37	$2\omega_1(0.94), \omega_{11}(0.18)$
13	14078.05	1614.99	0.00	$\omega_1 + \omega_2(0.96), \omega_1 + \omega_2 + \omega_9(0.16)$
14	14106.89	1643.84	0.44	$2\omega_2(0.92), 2\omega_2 + \omega_9(0.18)$
15	14137.15	1674.10	0.00	$\omega_1 + \omega_3(0.96), \omega_1 + \omega_3 + \omega_9(0.18)$
16	14162.08	1699.03	0.33	$\omega_2 + \omega_3(0.94), \omega_2 + \omega_3 + \omega_9(0.19)$
17	14220.40	1757.35	0.06	$2\omega_3(0.94), 2\omega_3 + \omega_9(0.21)$
18	14274.30	1811.25	0.10	$\omega_1 + \omega_4(0.96), \omega_1 + \omega_4 + \omega_9(0.15)$
19	14298.90	1835.85	0.53	$\omega_2 + \omega_4(0.94), \omega_2 + \omega_4 + \omega_9(0.17)$
20	14355.57	1892.52	0.10	$\omega_3 + \omega_4(0.92), \omega_1 + \omega_5(0.25)$
21	14374.30	1911.25	1.13	$\omega_1 + \omega_5(0.9), \omega_3 + \omega_4(0.25)$
22	14376.52	1913.47	0.71	$\omega_1 + \omega_6(0.92), \omega_1 + \omega_6 + \omega_9(0.14)$
23	14394.93	1931.88	0.29	$\omega_1 + \omega_8(0.8), \omega_2 + \omega_6(0.49)$
24	14404.56	1941.51	0.06	$\omega_1 + \omega_7(0.83), \omega_2 + \omega_5(0.48)$
25	14405.92	1942.87	0.43	$\omega_2 + \omega_6(0.79), \omega_1 + \omega_8(0.5)$
26	14409.94	1946.88	0.03	$\omega_2 + \omega_5(0.82), \omega_1 + \omega_7(0.49)$
27	14427.72	1964.67	0.01	$\omega_2 + \omega_7(0.94), \omega_2 + \omega_7 + \omega_9(0.17)$
28	14436.47	1973.42	0.02	$\omega_2 + \omega_8(0.95), \omega_2 + \omega_8 + \omega_9(0.17)$
29	14463.31	2000.26	1.22	$\omega_3 + \omega_6(0.94), \omega_3 + \omega_6 + \omega_9(0.18)$
30	14464.71	2001.66	0.18	$\omega_3 + \omega_5(0.95), \omega_3 + \omega_5 + \omega_9(0.18)$
31	14486.81	2023.76	0.21	$\omega_3 + \omega_7(0.95), \omega_3 + \omega_7 + \omega_9(0.19)$
32	14489.70	2026.65	0.00	$\omega_3 + \omega_8(0.96), \omega_3 + \omega_8 + \omega_9(0.18)$
33	14498.60	2035.55	0.00	$2\omega_4(0.96), 2\omega_4 + \omega_9(0.16)$
34	14526.27	2063.22	0.13	$\omega_1 + \omega_9(0.93), \omega_1 + 2\omega_9(0.23)$
35	14551.32	2088.27	0.07	$\omega_2 + \omega_9(0.91), \omega_2 + 2\omega_9(0.25)$
36	14594.46	2131.41	0.47	$\omega_4 + \omega_6(0.92), \omega_4 + \omega_6 + \omega_9(0.15)$
37	14600.69	2137.63	0.60	$\omega_4 + \omega_5(0.93), \omega_4 + \omega_5 + \omega_9(0.15)$
38	14605.32	2142.27	0.02	$\omega_3 + \omega_9(0.9), \omega_3 + 2\omega_9(0.27)$
39	14618.25	2155.20	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
40	14631.59	2168.53	0.13	$\omega_4 + \omega_8(0.96), \omega_4 + \omega_8 + \omega_9(0.15)$
41	14699.47	2236.41	0.04	$2\omega_6(0.83), 2\omega_5(0.42)$
42	14706.90	2243.84	1.30	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.25)$
43	14712.89	2249.84	0.00	$\omega_1 + \omega_{10}(0.82), \omega_6 + \omega_8(0.41)$
44	14714.21	2251.16	0.03	$2\omega_5(0.86), 2\omega_6(0.43)$
45	14730.35	2267.30	0.06	$\omega_5 + \omega_8(0.71), \omega_1 + \omega_{11}(0.55)$
46	14732.68	2269.63	0.24	$\omega_5 + \omega_7(0.64), \omega_6 + \omega_7(0.6)$
47	14733.17	2270.12	0.00	$\omega_6 + \omega_7(0.69), \omega_5 + \omega_7(0.55)$
48	14740.60	2277.55	0.15	$\omega_6 + \omega_8(0.85), \omega_1 + \omega_{10}(0.44)$
49	14749.06	2286.01	0.06	$\omega_1 + \omega_{11}(0.69), \omega_5 + \omega_8(0.61)$
50	14754.18	2291.12	0.01	$\omega_2 + \omega_{10}(0.89), 2\omega_7(0.33)$
51	14755.12	2292.07	0.00	$\omega_4 + \omega_9(0.83), \omega_5 + \omega_7(0.42)$
52	14755.56	2292.51	0.08	$2\omega_7(0.82), \omega_2 + \omega_{10}(0.34)$
53	14759.47	2296.42	0.14	$\omega_7 + \omega_8(0.95), \omega_7 + \omega_8 + \omega_9(0.16)$
54	14761.93	2298.88	0.01	$2\omega_8(0.89), 2\omega_7(0.37)$
55	14776.81	2313.76	0.55	$\omega_2 + \omega_{11}(0.9), 3\omega_2(0.19)$
56	14811.48	2348.43	0.15	$\omega_3 + \omega_{10}(0.96), \omega_3 + \omega_9 + \omega_{10}(0.17)$
57	14836.13	2373.08	0.02	$\omega_3 + \omega_{11}(0.9), \omega_6 + \omega_9(0.18)$
58	14848.44	2385.39	0.00	$3\omega_1(0.88), \omega_1 + \omega_{11}(0.28)$
59	14854.07	2391.02	0.20	$\omega_6 + \omega_9(0.89), \omega_6 + 2\omega_9(0.22)$
60	14855.53	2392.48	0.19	$\omega_5 + \omega_9(0.92), \omega_5 + 2\omega_9(0.23)$
61	14870.21	2407.15	0.00	$2\omega_1 + \omega_2(0.92), 2\omega_1 + \omega_2 + \omega_9(0.16)$
62	14879.77	2416.72	0.36	$\omega_7 + \omega_9(0.91), \omega_7 + 2\omega_9(0.24)$
63	14880.93	2417.88	0.01	$\omega_8 + \omega_9(0.92), \omega_8 + 2\omega_9(0.23)$
64	14895.65	2432.60	0.01	$\omega_1 + 2\omega_2(0.9), \omega_1 + 2\omega_2 + \omega_9(0.18)$
65	14924.47	2461.41	0.04	$3\omega_2(0.85), \omega_2 + \omega_{11}(0.24)$
66	14932.95	2469.90	0.00	$2\omega_1 + \omega_3(0.93), 2\omega_1 + \omega_3 + \omega_9(0.18)$
67	14948.04	2484.99	0.07	$\omega_4 + \omega_{10}(0.96), \omega_4 + \omega_9 + \omega_{10}(0.14)$
68	14952.76	2489.71	0.00	$\omega_1 + \omega_2 + \omega_3(0.93), \omega_1 + \omega_2 + \omega_3 + \omega_9(0.2)$
69	14973.24	2510.19	0.00	$\omega_4 + \omega_{11}(0.92), 2\omega_1 + \omega_4(0.19)$
70	14978.97	2515.92	0.01	$2\omega_2 + \omega_3(0.86), 2\omega_2 + \omega_3 + \omega_9(0.2)$

Table 3 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
71	15001.19	2538.14	0.00	$2\omega_9(0.88), 3\omega_9(0.3)$
72	15014.07	2551.01	0.00	$\omega_1 + 2\omega_3(0.94), \omega_1 + 2\omega_3 + \omega_9(0.21)$
73	15036.43	2573.38	0.00	$\omega_2 + 2\omega_3(0.9), \omega_2 + 2\omega_3 + \omega_9(0.22)$
74	15050.07	2587.02	0.35	$\omega_6 + \omega_{10}(0.93), \omega_5 + \omega_{11}(0.19)$
75	15054.33	2591.27	0.16	$\omega_5 + \omega_{10}(0.92), \omega_6 + \omega_{11}(0.27)$
76	15064.28	2601.22	0.01	$2\omega_1 + \omega_4(0.88), \omega_7 + \omega_{10}(0.21)$
77	15065.65	2602.60	0.01	$\omega_7 + \omega_{10}(0.82), \omega_8 + \omega_{11}(0.38)$
78	15067.62	2604.57	0.74	$\omega_8 + \omega_{10}(0.86), \omega_7 + \omega_{11}(0.38)$
79	15079.32	2616.27	0.02	$\omega_6 + \omega_{11}(0.82), \omega_5 + \omega_{10}(0.29)$
80	15081.54	2618.48	0.22	$\omega_5 + \omega_{11}(0.9), 2\omega_1 + \omega_5(0.21)$
81	15084.74	2621.69	0.01	$\omega_1 + \omega_2 + \omega_4(0.86), \omega_6 + \omega_{11}(0.31)$
82	15096.19	2633.14	0.00	$3\omega_3(0.92), 3\omega_3 + \omega_9(0.24)$
83	15106.78	2643.73	0.30	$\omega_8 + \omega_{11}(0.75), \omega_7 + \omega_{10}(0.39)$
84	15107.31	2644.26	1.34	$\omega_7 + \omega_{11}(0.76), \omega_8 + \omega_{10}(0.37)$
85	15112.77	2649.71	0.00	$2\omega_2 + \omega_4(0.87), 2\omega_2 + \omega_4 + \omega_9(0.18)$
86	15143.86	2680.81	0.02	$\omega_1 + \omega_3 + \omega_4(0.82), 2\omega_1 + \omega_5(0.41)$
87	15160.44	2697.38	0.02	$2\omega_1 + \omega_5(0.77), \omega_1 + \omega_3 + \omega_4(0.45)$
88	15165.60	2702.55	0.00	$2\omega_1 + \omega_6(0.86), \omega_1 + \omega_2 + \omega_4(0.22)$
89	15168.28	2705.23	0.00	$\omega_2 + \omega_3 + \omega_4(0.88), \omega_1 + \omega_2 + \omega_5(0.21)$
90	15178.66	2715.61	0.00	$2\omega_1 + \omega_8(0.74), \omega_1 + \omega_2 + \omega_6(0.46)$
91	15187.45	2724.40	0.08	$\omega_1 + \omega_2 + \omega_5(0.84), 2\omega_1 + \omega_7(0.25)$
92	15195.14	2732.08	0.00	$\omega_1 + \omega_2 + \omega_6(0.75), 2\omega_1 + \omega_8(0.48)$
93	15202.26	2739.20	0.17	$2\omega_1 + \omega_7(0.89), \omega_1 + \omega_2 + \omega_5(0.27)$
94	15202.27	2739.22	0.02	$\omega_9 + \omega_{10}(0.93), 2\omega_9 + \omega_{10}(0.22)$
95	15210.37	2747.31	0.04	$\omega_1 + \omega_2 + \omega_8(0.63), 2\omega_2 + \omega_6(0.61)$
96	15218.31	2755.25	0.02	$\omega_1 + \omega_2 + \omega_7(0.85), 2\omega_2 + \omega_5(0.34)$
97	15223.78	2760.73	0.02	$\omega_1 + \omega_2 + \omega_8(0.68), 2\omega_2 + \omega_6(0.58)$
98	15226.55	2763.50	0.01	$2\omega_2 + \omega_5(0.84), \omega_1 + \omega_2 + \omega_7(0.37)$
99	15227.24	2764.18	0.00	$2\omega_3 + \omega_4(0.88), \omega_1 + \omega_3 + \omega_5(0.29)$
100	15228.04	2764.98	0.11	$\omega_9 + \omega_{11}(0.88), 2\omega_9 + \omega_{11}(0.22)$
101	15241.70	2778.65	0.18	$2\omega_2 + \omega_7(0.88), 2\omega_2 + \omega_7 + \omega_9(0.19)$
102	15250.41	2787.35	0.00	$\omega_1 + \omega_3 + \omega_5(0.86), 2\omega_3 + \omega_4(0.28)$
103	15252.32	2789.27	0.00	$\omega_1 + \omega_3 + \omega_6(0.89), \omega_1 + \omega_3 + \omega_6 + \omega_9(0.17)$
104	15256.48	2793.43	0.00	$2\omega_2 + \omega_8(0.91), 2\omega_2 + \omega_8 + \omega_9(0.19)$
105	15270.24	2807.19	0.00	$\omega_1 + \omega_3 + \omega_8(0.73), \omega_2 + \omega_3 + \omega_6(0.54)$
106	15278.35	2815.30	0.00	$\omega_2 + \omega_3 + \omega_5(0.7), \omega_1 + \omega_3 + \omega_7(0.6)$
107	15280.05	2816.99	0.00	$\omega_2 + \omega_3 + \omega_6(0.71), \omega_1 + \omega_3 + \omega_8(0.57)$
108	15283.18	2820.12	0.00	$\omega_1 + \omega_3 + \omega_7(0.73), \omega_2 + \omega_3 + \omega_5(0.59)$
109	15285.00	2821.95	0.00	$\omega_1 + 2\omega_4(0.93), \omega_1 + 2\omega_4 + \omega_9(0.16)$
110	15300.36	2837.31	0.00	$\omega_2 + \omega_3 + \omega_7(0.9), \omega_2 + \omega_3 + \omega_7 + \omega_9(0.2)$
111	15307.60	2844.55	0.12	$\omega_2 + 2\omega_4(0.91), \omega_2 + 2\omega_4 + \omega_9(0.17)$
112	15309.05	2845.99	0.00	$\omega_2 + \omega_3 + \omega_8(0.93), \omega_2 + \omega_3 + \omega_8 + \omega_9(0.2)$
113	15318.97	2855.92	0.04	$2\omega_1 + \omega_9(0.88), 2\omega_1 + 2\omega_9(0.22)$
114	15338.22	2875.16	0.00	$2\omega_3 + \omega_6(0.91), 2\omega_3 + \omega_6 + \omega_9(0.21)$
115	15338.81	2875.76	0.02	$2\omega_3 + \omega_5(0.92), 2\omega_3 + \omega_5 + \omega_9(0.21)$
116	15338.85	2875.80	0.00	$\omega_1 + \omega_2 + \omega_9(0.89), \omega_1 + \omega_2 + 2\omega_9(0.26)$
117	15361.02	2897.97	0.01	$2\omega_3 + \omega_7(0.93), 2\omega_3 + \omega_7 + \omega_9(0.22)$
118	15364.37	2901.32	0.00	$2\omega_3 + \omega_8(0.93), 2\omega_3 + \omega_8 + \omega_9(0.22)$
119	15365.27	2902.22	0.00	$\omega_3 + 2\omega_4(0.86), \omega_1 + \omega_4 + \omega_5(0.31)$
120	15366.46	2903.40	0.13	$2\omega_2 + \omega_9(0.82), 2\omega_2 + 2\omega_9(0.26)$
121	15375.17	2912.12	21.80	$\omega_{12}(0.68), \omega_{10} + \omega_{11}(0.56)$
122	15379.70	2916.65	3.96	$\omega_1 + \omega_4 + \omega_5(0.52), 2\omega_{10}(0.47)$
123	15381.74	2918.68	2.07	$\omega_1 + \omega_4 + \omega_6(0.79), \omega_{10} + \omega_{11}(0.23)$
124	15385.52	2922.47	2.32	$\omega_1 + \omega_4 + \omega_5(0.59), 2\omega_{10}(0.53)$
125	15396.22	2933.17	0.04	$\omega_1 + \omega_3 + \omega_9(0.89), \omega_1 + \omega_3 + 2\omega_9(0.27)$
126	15400.85	2937.80	0.44	$\omega_2 + \omega_4 + \omega_6(0.75), \omega_1 + \omega_4 + \omega_8(0.42)$
127	15406.31	2943.26	0.00	$\omega_1 + \omega_4 + \omega_7(0.7), \omega_2 + \omega_4 + \omega_5(0.51)$
128	15413.87	2950.81	0.22	$\omega_1 + \omega_4 + \omega_8(0.8), \omega_2 + \omega_4 + \omega_6(0.43)$
129	15415.60	2952.54	0.00	$\omega_2 + \omega_4 + \omega_5(0.72), \omega_1 + \omega_4 + \omega_7(0.56)$
130	15419.49	2956.44	0.01	$\omega_2 + \omega_3 + \omega_9(0.86), \omega_2 + \omega_3 + 2\omega_9(0.29)$

Table 3 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
131	15420.33	2957.27	6.48	$2\omega_{10}(0.61), \omega_{13}(0.52)$
132	15431.64	2968.59	0.89	$\omega_2 + \omega_4 + \omega_7(0.81), \omega_{13}(0.22)$
133	15447.61	2984.56	0.05	$\omega_2 + \omega_4 + \omega_8(0.92), \omega_2 + \omega_4 + \omega_8 + \omega_9(0.18)$
134	15457.86	2994.80	18.56	$\omega_{10} + \omega_{11}(0.63), \omega_{12}(0.53)$
135	15462.42	2999.36	3.79	$2\omega_{11}(0.72), \omega_{13}(0.38)$
136	15465.11	3002.06	0.00	$\omega_3 + \omega_4 + \omega_6(0.88), \omega_3 + \omega_4 + \omega_6 + \omega_9(0.18)$
137	15467.96	3004.91	0.31	$\omega_3 + \omega_4 + \omega_5(0.7), \omega_1 + 2\omega_5(0.46)$
138	15474.58	3011.52	0.06	$2\omega_3 + \omega_9(0.85), 2\omega_3 + 2\omega_9(0.31)$
139	15476.79	3013.73	0.01	$\omega_3 + \omega_4 + \omega_5(0.55), \omega_1 + 2\omega_6(0.52)$
140	15485.19	3022.14	0.01	$\omega_1 + \omega_5 + \omega_6(0.82), \omega_1 + \omega_4 + \omega_7(0.23)$
141	15489.38	3026.33	0.28	$\omega_3 + \omega_4 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_6(0.2)$
142	15494.06	3031.00	0.02	$\omega_{14}(0.85), \omega_{13} + \omega_{14}(0.2)$
143	15496.33	3033.27	2.73	$\omega_1 + 2\omega_5(0.63), \omega_1 + 2\omega_6(0.62)$
144	15499.89	3036.84	1.48	$\omega_3 + \omega_4 + \omega_8(0.6), \omega_1 + \omega_5 + \omega_8(0.37)$
145	15500.64	3037.58	2.07	$\omega_3 + \omega_4 + \omega_8(0.5), 2\omega_1 + \omega_{10}(0.43)$
146	15505.88	3042.82	42.42	$\omega_{15}(0.81), \omega_1 + 2\omega_8(0.24)$
147	15507.34	3044.28	0.03	$\omega_2 + 2\omega_6(0.71), 2\omega_1 + \omega_{10}(0.35)$
148	15508.45	3045.39	0.21	$\omega_1 + \omega_5 + \omega_8(0.63), \omega_3 + \omega_4 + \omega_8(0.49)$
149	15509.31	3046.26	0.01	$3\omega_4(0.93), 3\omega_4 + \omega_9(0.16)$
150	15516.22	3053.17	0.00	$\omega_1 + \omega_5 + \omega_7(0.79), \omega_1 + \omega_4 + \omega_9(0.27)$
151	15517.77	3054.72	0.00	$\omega_2 + \omega_5 + \omega_6(0.74), \omega_1 + \omega_6 + \omega_7(0.35)$
152	15521.52	3058.47	0.00	$\omega_1 + \omega_6 + \omega_7(0.84), \omega_2 + \omega_5 + \omega_6(0.26)$
153	15526.61	3063.56	0.13	$\omega_1 + \omega_6 + \omega_8(0.62), 2\omega_1 + \omega_{10}(0.51)$
154	15529.89	3066.83	0.16	$2\omega_1 + \omega_{11}(0.57), \omega_1 + \omega_5 + \omega_8(0.4)$
155	15530.07	3067.01	2.93	$\omega_1 + \omega_2 + \omega_{10}(0.71), \omega_2 + \omega_6 + \omega_8(0.44)$
156	15530.09	3067.04	0.02	$\omega_2 + 2\omega_5(0.8), \omega_2 + 2\omega_6(0.33)$
157	15535.06	3072.01	0.00	$\omega_1 + \omega_7 + \omega_8(0.63), \omega_2 + \omega_6 + \omega_7(0.61)$
158	15535.65	3072.60	1.82	$\omega_1 + 2\omega_8(0.78), \omega_1 + \omega_2 + \omega_{10}(0.31)$
159	15541.80	3078.75	0.00	$\omega_1 + \omega_4 + \omega_9(0.83), \omega_1 + \omega_5 + \omega_7(0.34)$
160	15545.36	3082.30	0.10	$\omega_1 + \omega_2 + \omega_{11}(0.54), \omega_2 + \omega_5 + \omega_8(0.5)$
161	15546.29	3083.23	1.58	$\omega_2 + \omega_5 + \omega_7(0.67), \omega_1 + 2\omega_7(0.36)$
162	15550.81	3087.76	0.00	$\omega_1 + \omega_7 + \omega_8(0.63), \omega_2 + \omega_6 + \omega_7(0.47)$
163	15551.70	3088.64	0.00	$\omega_1 + 2\omega_7(0.85), \omega_2 + \omega_5 + \omega_7(0.24)$
164	15558.96	3095.91	0.16	$\omega_2 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_2 + \omega_{10}(0.4)$
165	15565.30	3102.25	0.00	$\omega_2 + \omega_5 + \omega_8(0.73), \omega_1 + \omega_2 + \omega_{11}(0.54)$
166	15566.46	3103.41	0.02	$\omega_2 + 2\omega_7(0.89), \omega_1 + \omega_5 + \omega_7(0.18)$
167	15566.47	3103.42	0.00	$\omega_2 + \omega_4 + \omega_9(0.75), \omega_2 + \omega_5 + \omega_7(0.48)$
168	15573.01	3109.96	0.00	$\omega_3 + 2\omega_6(0.78), \omega_3 + 2\omega_5(0.45)$
169	15573.58	3110.53	0.12	$2\omega_2 + \omega_{10}(0.9), 2\omega_2 + \omega_9 + \omega_{10}(0.17)$
170	15576.04	3112.99	0.00	$\omega_2 + \omega_7 + \omega_8(0.91), \omega_2 + \omega_7 + \omega_8 + \omega_9(0.18)$
171	15579.57	3116.52	0.00	$\omega_3 + \omega_5 + \omega_6(0.87), \omega_3 + \omega_4 + \omega_7(0.23)$
172	15584.45	3121.40	0.01	$\omega_2 + 2\omega_8(0.93), \omega_2 + 2\omega_8 + \omega_9(0.18)$
173	15586.61	3123.56	0.00	$\omega_3 + 2\omega_5(0.82), \omega_3 + 2\omega_6(0.46)$
174	15589.87	3126.82	0.00	$\omega_1 + \omega_3 + \omega_{10}(0.75), \omega_3 + \omega_6 + \omega_8(0.43)$
175	15592.12	3129.07	0.02	$2\omega_2 + \omega_{11}(0.82), 4\omega_2(0.24)$
176	15597.12	3134.06	0.01	$2\omega_4 + \omega_6(0.87), \omega_1 + \omega_4 + \omega_5(0.18)$
177	15603.55	3140.49	0.00	$\omega_3 + \omega_5 + \omega_7(0.74), \omega_3 + \omega_4 + \omega_9(0.43)$
178	15604.65	3141.60	0.00	$\omega_3 + \omega_5 + \omega_8(0.72), \omega_1 + \omega_3 + \omega_{11}(0.49)$
179	15606.36	3143.30	0.05	$\omega_3 + \omega_6 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_8(0.24)$
180	15607.44	3144.39	0.00	$2\omega_4 + \omega_5(0.88), \omega_4 + \omega_6 + \omega_7(0.17)$
181	15615.12	3152.07	0.00	$\omega_3 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_3 + \omega_{10}(0.5)$
182	15621.35	3158.30	0.00	$\omega_3 + \omega_4 + \omega_9(0.68), \omega_3 + \omega_5 + \omega_7(0.52)$
183	15622.09	3159.04	0.01	$2\omega_4 + \omega_7(0.83), \omega_4 + \omega_5 + \omega_6(0.25)$
184	15623.64	3160.59	0.04	$\omega_1 + \omega_3 + \omega_{11}(0.69), \omega_3 + \omega_5 + \omega_8(0.53)$
185	15627.97	3164.92	0.00	$\omega_3 + 2\omega_7(0.88), \omega_3 + 2\omega_8(0.29)$
186	15629.44	3166.38	0.00	$\omega_2 + \omega_3 + \omega_{10}(0.92), \omega_2 + \omega_3 + \omega_9 + \omega_{10}(0.19)$
187	15632.63	3169.58	0.01	$\omega_3 + \omega_7 + \omega_8(0.93), \omega_3 + \omega_7 + \omega_8 + \omega_9(0.2)$
188	15634.61	3171.56	0.05	$4\omega_1(0.77), 2\omega_1 + \omega_{11}(0.37)$
189	15635.30	3172.24	0.00	$\omega_3 + 2\omega_8(0.88), \omega_3 + 2\omega_7(0.3)$
190	15636.81	3173.76	0.00	$\omega_1 + \omega_5 + \omega_9(0.84), \omega_3 + \omega_4 + \omega_9(0.22)$

Table 3 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
191	15640.60	3177.55	0.00	$\omega_1 + \omega_6 + \omega_9(0.86), \omega_1 + \omega_6 + 2\omega_9(0.22)$
192	15645.77	3182.72	0.00	$2\omega_4 + \omega_8(0.94), 2\omega_4 + \omega_8 + \omega_9(0.17)$
193	15649.47	3186.42	0.00	$\omega_2 + \omega_3 + \omega_{11}(0.85), \omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.18)$
194	15657.69	3194.64	0.00	$3\omega_1 + \omega_2(0.85), \omega_1 + \omega_2 + \omega_{11}(0.23)$
195	15658.55	3195.50	0.00	$\omega_1 + \omega_8 + \omega_9(0.67), \omega_2 + \omega_6 + \omega_9(0.53)$
196	15666.36	3203.31	0.00	$\omega_2 + \omega_5 + \omega_9(0.76), \omega_1 + \omega_7 + \omega_9(0.43)$
197	15667.45	3204.40	0.00	$\omega_2 + \omega_6 + \omega_9(0.65), \omega_1 + \omega_8 + \omega_9(0.58)$
198	15672.60	3209.54	0.00	$\omega_1 + \omega_7 + \omega_9(0.79), \omega_2 + \omega_5 + \omega_9(0.43)$
199	15684.27	3221.21	0.00	$2\omega_1 + 2\omega_2(0.84), 2\omega_1 + \omega_{11}(0.2)$

**Table 4** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$ ,  $\epsilon = 0.005$  and  $\epsilon_f = 0.01\text{ km/mol}$ .

Number	Eigenvalue	Frequency	Intensity	Assignment
1(1)	13257.91	794.87	0.12	$\omega_1(0.97), \omega_1 + \omega_9(0.14)$
2(2)	13286.12	823.08	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
3(3)	13342.32	879.28	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
4(5)	13586.04	1122.99	0.79	$\omega_6(0.96), \omega_6 + \omega_9(0.14)$
5(6)	13588.30	1125.25	0.05	$\omega_5(0.97), \omega_5 + \omega_9(0.14)$
6(7)	13610.32	1147.28	3.81	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
7(9)	13734.34	1271.30	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
8(10)	13932.07	1469.03	0.11	$\omega_{10}(0.97), \omega_9 + \omega_{10}(0.13)$
9(11)	13959.96	1496.92	3.82	$\omega_{11}(0.94), 2\omega_1(0.19)$
10(12)	14054.52	1591.48	0.38	$2\omega_1(0.94), \omega_{11}(0.18)$
11(14)	14106.35	1643.30	0.44	$2\omega_2(0.92), 2\omega_2 + \omega_9(0.18)$
12(16)	14161.54	1698.50	0.34	$\omega_2 + \omega_3(0.94), \omega_2 + \omega_3 + \omega_9(0.19)$
13(17)	14219.73	1756.69	0.06	$2\omega_3(0.94), 2\omega_3 + \omega_9(0.21)$
14(18)	14273.54	1810.50	0.10	$\omega_1 + \omega_4(0.96), \omega_1 + \omega_4 + \omega_9(0.15)$
15(19)	14298.23	1835.19	0.53	$\omega_2 + \omega_4(0.94), \omega_2 + \omega_4 + \omega_9(0.17)$
16(20)	14355.09	1892.05	0.10	$\omega_3 + \omega_4(0.92), \omega_1 + \omega_5(0.26)$
17(21)	14373.68	1910.63	1.37	$\omega_1 + \omega_5(0.91), \omega_3 + \omega_4(0.26)$
18(22)	14375.64	1912.59	0.48	$\omega_1 + \omega_6(0.93), \omega_1 + \omega_6 + \omega_9(0.14)$
19(23)	14393.91	1930.86	0.29	$\omega_1 + \omega_8(0.81), \omega_2 + \omega_6(0.48)$
20(24)	14403.92	1940.88	0.04	$\omega_1 + \omega_7(0.83), \omega_2 + \omega_5(0.48)$
21(25)	14405.23	1942.18	0.46	$\omega_2 + \omega_6(0.8), \omega_1 + \omega_8(0.5)$
22(26)	14409.26	1946.22	0.02	$\omega_2 + \omega_5(0.82), \omega_1 + \omega_7(0.49)$
23(28)	14435.91	1972.87	0.01	$\omega_2 + \omega_8(0.96), \omega_2 + \omega_8 + \omega_9(0.17)$
24(29)	14462.67	1999.62	1.24	$\omega_3 + \omega_6(0.95), \omega_3 + \omega_6 + \omega_9(0.18)$
25(30)	14464.03	2000.99	0.17	$\omega_3 + \omega_5(0.96), \omega_3 + \omega_5 + \omega_9(0.18)$
26(31)	14486.10	2023.06	0.21	$\omega_3 + \omega_7(0.96), \omega_3 + \omega_7 + \omega_9(0.19)$
27(34)	14525.66	2062.62	0.13	$\omega_1 + \omega_9(0.93), \omega_1 + 2\omega_9(0.23)$
28(35)	14550.78	2087.73	0.07	$\omega_2 + \omega_9(0.91), \omega_2 + 2\omega_9(0.25)$
29(36)	14593.75	2130.71	0.49	$\omega_4 + \omega_6(0.92), \omega_4 + \omega_6 + \omega_9(0.15)$
30(37)	14599.77	2136.73	0.57	$\omega_4 + \omega_5(0.93), \omega_4 + \omega_5 + \omega_9(0.15)$
31(38)	14604.82	2141.78	0.02	$\omega_3 + \omega_9(0.9), \omega_3 + 2\omega_9(0.27)$
32(39)	14617.70	2154.66	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
33(40)	14630.81	2167.77	0.13	$\omega_4 + \omega_8(0.96), \omega_4 + \omega_8 + \omega_9(0.15)$
34(41)	14698.62	2235.57	0.04	$2\omega_6(0.83), 2\omega_5(0.42)$
35(42)	14705.88	2242.84	1.28	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.24)$
36(44)	14713.48	2250.44	0.03	$2\omega_5(0.86), 2\omega_6(0.43)$
37(45)	14729.49	2266.45	0.07	$\omega_5 + \omega_8(0.71), \omega_1 + \omega_{11}(0.55)$
38(46)	14732.25	2269.21	0.10	$\omega_6 + \omega_7(0.91), \omega_5 + \omega_8(0.21)$
39(47)	14732.27	2269.22	0.12	$\omega_5 + \omega_7(0.85), \omega_4 + \omega_9(0.37)$
40(48)	14740.11	2277.07	0.17	$\omega_6 + \omega_8(0.85), \omega_1 + \omega_{10}(0.44)$
41(49)	14748.26	2285.22	0.05	$\omega_1 + \omega_{11}(0.68), \omega_5 + \omega_8(0.62)$
42(50)	14753.51	2290.47	0.01	$\omega_2 + \omega_{10}(0.9), 2\omega_7(0.31)$
43(52)	14755.22	2292.17	0.07	$2\omega_7(0.85), \omega_2 + \omega_{10}(0.32)$
44(53)	14758.82	2295.77	0.14	$\omega_7 + \omega_8(0.95), \omega_7 + \omega_8 + \omega_9(0.16)$
45(54)	14760.78	2297.73	0.02	$2\omega_8(0.91), 2\omega_7(0.3)$

Table 4 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
46(55)	14776.18	2313.13	0.54	$\omega_2 + \omega_{11}(0.9), 3\omega_2(0.19)$
47(56)	14810.78	2347.73	0.15	$\omega_3 + \omega_{10}(0.96), \omega_3 + \omega_9 + \omega_{10}(0.17)$
48(57)	14835.54	2372.50	0.02	$\omega_3 + \omega_{11}(0.9), \omega_6 + \omega_9(0.18)$
49(59)	14853.41	2390.37	0.24	$\omega_6 + \omega_9(0.9), \omega_6 + 2\omega_9(0.22)$
50(60)	14854.85	2391.81	0.15	$\omega_5 + \omega_9(0.92), \omega_5 + 2\omega_9(0.23)$
51(62)	14879.16	2416.12	0.37	$\omega_7 + \omega_9(0.92), \omega_7 + 2\omega_9(0.24)$
52(64)	14894.83	2431.78	0.01	$\omega_1 + 2\omega_2(0.9), \omega_1 + 2\omega_2 + \omega_9(0.18)$
53(65)	14923.89	2460.85	0.04	$3\omega_2(0.85), \omega_2 + \omega_{11}(0.23)$
54(67)	14947.17	2484.13	0.07	$\omega_4 + \omega_{10}(0.96), \omega_4 + \omega_9 + \omega_{10}(0.14)$
55(74)	15048.77	2585.73	0.36	$\omega_6 + \omega_{10}(0.93), \omega_5 + \omega_{11}(0.22)$
56(75)	15053.44	2590.40	0.15	$\omega_5 + \omega_{10}(0.92), \omega_6 + \omega_{11}(0.27)$
57(78)	15066.79	2603.75	0.75	$\omega_8 + \omega_{10}(0.86), \omega_7 + \omega_{11}(0.38)$
58(79)	15078.44	2615.39	0.02	$\omega_6 + \omega_{11}(0.81), \omega_1 + \omega_2 + \omega_4(0.31)$
59(80)	15081.13	2618.09	0.20	$\omega_5 + \omega_{11}(0.89), \omega_6 + \omega_{10}(0.24)$
60(81)	15083.74	2620.69	0.01	$\omega_1 + \omega_2 + \omega_4(0.85), \omega_6 + \omega_{11}(0.33)$
61(83)	15106.43	2643.39	1.66	$\omega_7 + \omega_{11}(0.84), \omega_8 + \omega_{10}(0.41)$
62(86)	15142.79	2679.75	0.02	$\omega_1 + \omega_3 + \omega_4(0.82), 2\omega_1 + \omega_5(0.42)$
63(87)	15159.16	2696.12	0.02	$2\omega_1 + \omega_5(0.76), \omega_1 + \omega_3 + \omega_4(0.46)$
64(91)	15186.35	2723.31	0.09	$\omega_1 + \omega_2 + \omega_5(0.84), 2\omega_1 + \omega_7(0.25)$
65(93)	15201.37	2738.33	0.17	$2\omega_1 + \omega_7(0.89), \omega_1 + \omega_2 + \omega_5(0.26)$
66(94)	15201.56	2738.52	0.02	$\omega_9 + \omega_{10}(0.93), 2\omega_9 + \omega_{10}(0.22)$
67(95)	15209.21	2746.17	0.04	$\omega_1 + \omega_2 + \omega_8(0.64), 2\omega_2 + \omega_6(0.6)$
68(96)	15217.42	2754.38	0.02	$\omega_1 + \omega_2 + \omega_7(0.86), 2\omega_2 + \omega_5(0.33)$
69(97)	15222.92	2759.88	0.02	$\omega_1 + \omega_2 + \omega_8(0.67), 2\omega_2 + \omega_6(0.59)$
70(99)	15227.39	2764.35	0.11	$\omega_9 + \omega_{11}(0.88), 2\omega_9 + \omega_{11}(0.22)$
71(101)	15240.81	2777.77	0.18	$2\omega_2 + \omega_7(0.88), 2\omega_2 + \omega_7 + \omega_9(0.19)$
72(111)	15306.54	2843.49	0.12	$\omega_2 + 2\omega_4(0.91), \omega_2 + 2\omega_4 + \omega_9(0.17)$
73(113)	15318.13	2855.09	0.05	$2\omega_1 + \omega_9(0.87), 2\omega_1 + 2\omega_9(0.22)$
74(115)	15337.97	2874.92	0.02	$2\omega_3 + \omega_5(0.93), 2\omega_3 + \omega_5 + \omega_9(0.21)$
75(117)	15360.08	2897.04	0.02	$2\omega_3 + \omega_7(0.93), 2\omega_3 + \omega_7 + \omega_9(0.22)$
76(119)	15365.72	2902.68	0.15	$2\omega_2 + \omega_9(0.83), 2\omega_2 + 2\omega_9(0.26)$
77(121)	15373.38	2910.33	22.28	$\omega_{12}(0.68), \omega_{10} + \omega_{11}(0.56)$
78(122)	15378.36	2915.31	4.28	$\omega_1 + \omega_4 + \omega_5(0.51), \omega_{13}(0.47)$
79(123)	15380.44	2917.40	1.70	$\omega_1 + \omega_4 + \omega_6(0.81), \omega_{10} + \omega_{11}(0.22)$
80(124)	15384.20	2921.15	2.42	$\omega_1 + \omega_4 + \omega_5(0.59), 2\omega_{10}(0.52)$
81(125)	15395.51	2932.47	0.04	$\omega_1 + \omega_3 + \omega_9(0.88), \omega_1 + \omega_3 + 2\omega_9(0.27)$
82(126)	15399.55	2936.51	0.43	$\omega_2 + \omega_4 + \omega_6(0.73), \omega_1 + \omega_4 + \omega_8(0.44)$
83(128)	15412.59	2949.55	0.24	$\omega_1 + \omega_4 + \omega_8(0.79), \omega_2 + \omega_4 + \omega_6(0.45)$
84(130)	15418.97	2955.93	6.48	$2\omega_{10}(0.63), \omega_{13}(0.52)$
85(132)	15430.79	2967.75	0.82	$\omega_2 + \omega_4 + \omega_7(0.81), \omega_{13}(0.21)$
86(133)	15446.74	2983.70	0.08	$\omega_2 + \omega_4 + \omega_8(0.92), \omega_2 + \omega_4 + \omega_8 + \omega_9(0.18)$
87(134)	15456.53	2993.48	18.20	$\omega_{10} + \omega_{11}(0.64), \omega_{12}(0.53)$
88(135)	15461.08	2998.04	3.57	$2\omega_{11}(0.73), \omega_{13}(0.37)$
89(137)	15466.77	3003.73	0.36	$\omega_3 + \omega_4 + \omega_5(0.68), \omega_1 + 2\omega_5(0.47)$
90(138)	15473.97	3010.92	0.05	$2\omega_3 + \omega_9(0.85), 2\omega_3 + 2\omega_9(0.31)$
91(141)	15488.74	3025.69	0.23	$\omega_3 + \omega_4 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_6(0.2)$
92(142)	15492.09	3029.04	0.03	$\omega_{14}(0.85), \omega_{13} + \omega_{14}(0.2)$
93(143)	15495.05	3032.01	3.51	$\omega_1 + 2\omega_5(0.63), \omega_1 + 2\omega_6(0.61)$
94(144)	15499.15	3036.11	0.24	$\omega_3 + \omega_4 + \omega_8(0.76), \omega_1 + \omega_5 + \omega_8(0.49)$
95(145)	15499.17	3036.12	3.37	$\omega_1 + \omega_6 + \omega_8(0.55), 2\omega_1 + \omega_{10}(0.54)$
96(146)	15503.65	3040.60	41.70	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.23)$
97(147)	15506.24	3043.20	0.05	$\omega_2 + 2\omega_6(0.72), 2\omega_1 + \omega_{10}(0.38)$
98(148)	15507.08	3044.04	0.20	$\omega_1 + \omega_5 + \omega_8(0.63), \omega_3 + \omega_4 + \omega_8(0.54)$
99(153)	15525.49	3062.44	0.14	$\omega_1 + \omega_6 + \omega_8(0.62), 2\omega_1 + \omega_{10}(0.52)$
100(154)	15528.55	3065.51	0.19	$2\omega_1 + \omega_{11}(0.58), \omega_1 + \omega_5 + \omega_8(0.41)$
101(155)	15528.99	3065.95	3.11	$\omega_1 + \omega_2 + \omega_{10}(0.69), \omega_2 + \omega_6 + \omega_8(0.44)$
102(157)	15534.30	3071.26	1.48	$\omega_1 + 2\omega_8(0.76), \omega_1 + \omega_2 + \omega_{10}(0.37)$
103(160)	15545.26	3082.22	1.64	$\omega_2 + \omega_5 + \omega_7(0.69), \omega_1 + 2\omega_7(0.35)$
104(164)	15558.12	3095.07	0.14	$\omega_2 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_2 + \omega_{10}(0.41)$
105(165)	15565.66	3102.62	0.02	$\omega_2 + 2\omega_7(0.9), \omega_1 + \omega_5 + \omega_7(0.18)$

Table 4 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
106(169)	15572.90	3109.86	0.12	$2\omega_2 + \omega_{10}(0.9), 2\omega_2 + \omega_9 + \omega_{10}(0.17)$
107(174)	15591.37	3128.33	0.01	$2\omega_2 + \omega_{11}(0.82), 4\omega_2(0.24)$
108(178)	15605.51	3142.46	0.05	$\omega_3 + \omega_6 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_8(0.24)$
109(183)	15622.74	3159.69	0.04	$\omega_1 + \omega_3 + \omega_{11}(0.69), \omega_3 + \omega_5 + \omega_8(0.53)$
110(188)	15632.84	3169.80	0.05	$4\omega_1(0.77), 2\omega_1 + \omega_{11}(0.38)$

**Table 5** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$ ,  $\varepsilon = 0.005$  and  $\varepsilon_f = 0.1$  km/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(1)	13257.91	794.87	0.12	$\omega_1(0.97), \omega_1 + \omega_9(0.14)$
2(2)	13286.12	823.08	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
3(3)	13342.33	879.29	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
4(5)	13586.04	1123.00	0.79	$\omega_6(0.96), \omega_6 + \omega_9(0.14)$
5(7)	13610.33	1147.28	3.81	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
6(9)	13734.35	1271.30	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
7(10)	13932.07	1469.03	0.11	$\omega_{10}(0.97), \omega_9 + \omega_{10}(0.13)$
8(11)	13959.97	1496.92	3.82	$\omega_{11}(0.94), 2\omega_1(0.19)$
9(12)	14054.54	1591.49	0.38	$2\omega_1(0.94), \omega_{11}(0.18)$
10(14)	14106.37	1643.32	0.44	$2\omega_2(0.92), 2\omega_2 + \omega_9(0.18)$
11(16)	14161.56	1698.51	0.34	$\omega_2 + \omega_3(0.94), \omega_2 + \omega_3 + \omega_9(0.19)$
12(18)	14273.55	1810.51	0.10	$\omega_1 + \omega_4(0.96), \omega_1 + \omega_4 + \omega_9(0.15)$
13(19)	14298.24	1835.19	0.53	$\omega_2 + \omega_4(0.94), \omega_2 + \omega_4 + \omega_9(0.17)$
14(20)	14355.09	1892.05	0.10	$\omega_3 + \omega_4(0.92), \omega_1 + \omega_5(0.26)$
15(21)	14373.69	1910.64	1.37	$\omega_1 + \omega_5(0.91), \omega_3 + \omega_4(0.26)$
16(22)	14375.65	1912.60	0.48	$\omega_1 + \omega_6(0.93), \omega_1 + \omega_6 + \omega_9(0.14)$
17(23)	14393.92	1930.87	0.29	$\omega_1 + \omega_8(0.81), \omega_2 + \omega_6(0.48)$
18(25)	14405.24	1942.20	0.46	$\omega_2 + \omega_6(0.8), \omega_1 + \omega_8(0.5)$
19(29)	14462.70	1999.66	1.24	$\omega_3 + \omega_6(0.95), \omega_3 + \omega_6 + \omega_9(0.18)$
20(30)	14464.05	2001.00	0.17	$\omega_3 + \omega_5(0.96), \omega_3 + \omega_5 + \omega_9(0.18)$
21(31)	14486.13	2023.08	0.21	$\omega_3 + \omega_7(0.96), \omega_3 + \omega_7 + \omega_9(0.19)$
22(34)	14525.68	2062.63	0.13	$\omega_1 + \omega_9(0.93), \omega_1 + 2\omega_9(0.23)$
23(36)	14593.76	2130.72	0.49	$\omega_4 + \omega_6(0.92), \omega_4 + \omega_6 + \omega_9(0.15)$
24(37)	14599.78	2136.74	0.57	$\omega_4 + \omega_5(0.93), \omega_4 + \omega_5 + \omega_9(0.15)$
25(39)	14617.71	2154.66	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
26(40)	14630.84	2167.79	0.13	$\omega_4 + \omega_8(0.96), \omega_4 + \omega_8 + \omega_9(0.15)$
27(42)	14705.89	2242.85	1.28	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.24)$
28(46)	14732.26	2269.22	0.10	$\omega_6 + \omega_7(0.91), \omega_5 + \omega_8(0.21)$
29(47)	14732.28	2269.23	0.12	$\omega_5 + \omega_7(0.85), \omega_4 + \omega_9(0.37)$
30(48)	14740.12	2277.07	0.17	$\omega_6 + \omega_8(0.85), \omega_1 + \omega_{10}(0.44)$
31(53)	14758.83	2295.78	0.14	$\omega_7 + \omega_8(0.95), \omega_7 + \omega_8 + \omega_9(0.16)$
32(55)	14776.20	2313.16	0.54	$\omega_2 + \omega_{11}(0.9), 3\omega_2(0.19)$
33(56)	14810.79	2347.74	0.15	$\omega_3 + \omega_{10}(0.96), \omega_3 + \omega_9 + \omega_{10}(0.17)$
34(59)	14853.44	2390.40	0.24	$\omega_6 + \omega_9(0.9), \omega_6 + 2\omega_9(0.22)$
35(60)	14854.87	2391.83	0.15	$\omega_5 + \omega_9(0.92), \omega_5 + 2\omega_9(0.23)$
36(62)	14879.17	2416.13	0.37	$\omega_7 + \omega_9(0.92), \omega_7 + 2\omega_9(0.24)$
37(74)	15048.79	2585.74	0.36	$\omega_6 + \omega_{10}(0.93), \omega_5 + \omega_{11}(0.22)$
38(75)	15053.48	2590.44	0.15	$\omega_5 + \omega_{10}(0.92), \omega_6 + \omega_{11}(0.27)$
39(78)	15066.80	2603.76	0.75	$\omega_8 + \omega_{10}(0.86), \omega_7 + \omega_{11}(0.38)$
40(80)	15081.15	2618.11	0.20	$\omega_5 + \omega_{11}(0.89), \omega_6 + \omega_{10}(0.24)$
41(83)	15106.45	2643.40	1.66	$\omega_7 + \omega_{11}(0.84), \omega_8 + \omega_{10}(0.41)$
42(93)	15201.40	2738.35	0.17	$2\omega_1 + \omega_7(0.89), \omega_1 + \omega_2 + \omega_5(0.27)$
43(99)	15227.43	2764.39	0.11	$\omega_9 + \omega_{11}(0.88), 2\omega_9 + \omega_{11}(0.22)$
44(101)	15240.84	2777.79	0.18	$2\omega_2 + \omega_7(0.88), 2\omega_2 + \omega_7 + \omega_9(0.19)$
45(111)	15306.59	2843.54	0.12	$\omega_2 + 2\omega_4(0.91), \omega_2 + 2\omega_4 + \omega_9(0.17)$
46(119)	15365.80	2902.75	0.15	$2\omega_2 + \omega_9(0.83), 2\omega_2 + 2\omega_9(0.26)$
47(121)	15373.39	2910.34	22.31	$\omega_{12}(0.68), \omega_{10} + \omega_{11}(0.56)$
48(122)	15378.40	2915.36	4.32	$\omega_1 + \omega_4 + \omega_5(0.51), \omega_{13}(0.48)$
49(123)	15380.49	2917.44	1.68	$\omega_1 + \omega_4 + \omega_6(0.81), \omega_{10} + \omega_{11}(0.22)$

Table 5 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
50(124)	15384.25	2921.20	2.39	$\omega_1 + \omega_4 + \omega_5(0.59), 2\omega_{10}(0.52)$
51(126)	15399.59	2936.54	0.43	$\omega_2 + \omega_4 + \omega_6(0.73), \omega_1 + \omega_4 + \omega_8(0.44)$
52(128)	15412.62	2949.57	0.24	$\omega_1 + \omega_4 + \omega_8(0.79), \omega_2 + \omega_4 + \omega_6(0.45)$
53(130)	15419.00	2955.95	6.48	$2\omega_{10}(0.63), \omega_{13}(0.52)$
54(132)	15430.87	2967.83	0.81	$\omega_2 + \omega_4 + \omega_7(0.81), \omega_{13}(0.21)$
55(134)	15456.55	2993.50	18.20	$\omega_{10} + \omega_{11}(0.64), \omega_{12}(0.53)$
56(135)	15461.13	2998.09	3.57	$2\omega_{11}(0.73), \omega_{13}(0.37)$
57(137)	15466.84	3003.80	0.36	$\omega_3 + \omega_4 + \omega_5(0.68), \omega_1 + 2\omega_5(0.47)$
58(141)	15488.79	3025.75	0.23	$\omega_3 + \omega_4 + \omega_7(0.88), \omega_3 + \omega_5 + \omega_6(0.2)$
59(143)	15495.07	3032.03	3.52	$\omega_1 + 2\omega_5(0.63), \omega_1 + 2\omega_6(0.61)$
60(144)	15499.22	3036.17	3.36	$\omega_1 + \omega_6 + \omega_8(0.55), 2\omega_1 + \omega_{10}(0.54)$
61(145)	15499.22	3036.18	0.24	$\omega_3 + \omega_4 + \omega_8(0.76), \omega_1 + \omega_5 + \omega_8(0.49)$
62(146)	15503.66	3040.61	41.70	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.23)$
63(148)	15507.15	3044.11	0.20	$\omega_1 + \omega_5 + \omega_8(0.63), \omega_3 + \omega_4 + \omega_8(0.54)$
64(153)	15525.54	3062.49	0.14	$\omega_1 + \omega_6 + \omega_8(0.62), 2\omega_1 + \omega_{10}(0.52)$
65(154)	15528.65	3065.60	0.19	$2\omega_1 + \omega_{11}(0.58), \omega_1 + \omega_5 + \omega_8(0.41)$
66(155)	15529.02	3065.97	3.11	$\omega_1 + \omega_2 + \omega_{10}(0.69), \omega_2 + \omega_6 + \omega_8(0.44)$
67(157)	15534.32	3071.28	1.48	$\omega_1 + 2\omega_8(0.76), \omega_1 + \omega_2 + \omega_{10}(0.37)$
68(160)	15545.29	3082.24	1.64	$\omega_2 + \omega_5 + \omega_7(0.69), \omega_1 + 2\omega_7(0.35)$
69(164)	15558.15	3095.10	0.14	$\omega_2 + \omega_6 + \omega_8(0.78), \omega_1 + \omega_2 + \omega_{10}(0.41)$
70(169)	15572.95	3109.90	0.12	$2\omega_2 + \omega_{10}(0.9), 2\omega_2 + \omega_9 + \omega_{10}(0.17)$

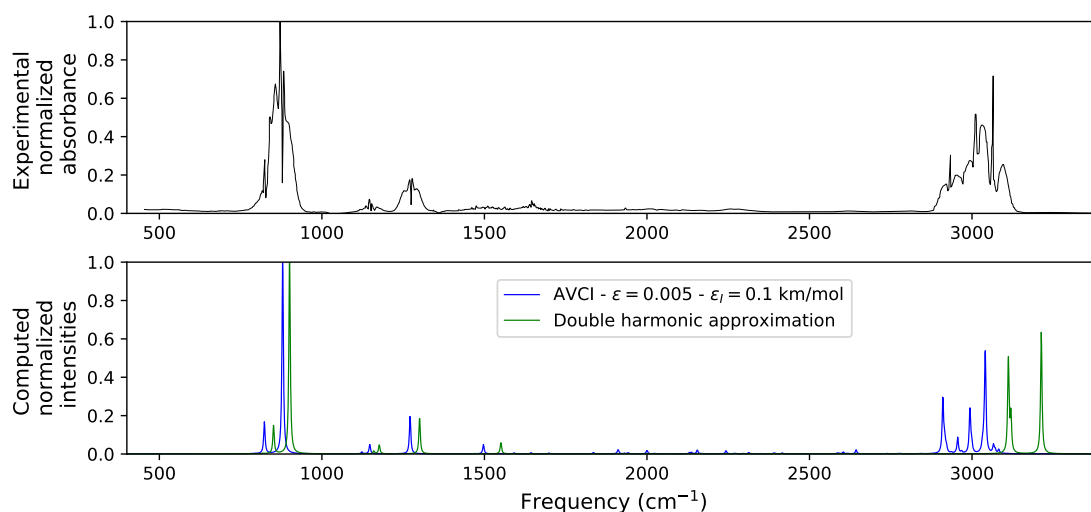
**Table 6** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$ ,  $\varepsilon = 0.005$  and  $\varepsilon_I = 1.0$  km/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	13286.14	823.10	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
2(3)	13342.34	879.30	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
3(7)	13610.34	1147.29	3.81	$\omega_7(0.97), \omega_7 + \omega_9(0.15)$
4(9)	13734.36	1271.31	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
5(11)	13959.98	1496.94	3.82	$\omega_{11}(0.94), 2\omega_{11}(0.19)$
6(21)	14373.87	1910.82	1.37	$\omega_1 + \omega_5(0.91), \omega_3 + \omega_4(0.26)$
7(29)	14462.72	1999.68	1.24	$\omega_3 + \omega_6(0.95), \omega_3 + \omega_6 + \omega_9(0.18)$
8(39)	14617.75	2154.70	1.53	$\omega_4 + \omega_7(0.92), \omega_5 + \omega_6(0.22)$
9(42)	14705.94	2242.89	1.29	$\omega_5 + \omega_6(0.91), \omega_4 + \omega_7(0.24)$
10(83)	15106.52	2643.47	1.66	$\omega_7 + \omega_{11}(0.84), \omega_8 + \omega_{10}(0.41)$
11(121)	15373.43	2910.38	22.36	$\omega_{12}(0.68), \omega_{10} + \omega_{11}(0.56)$
12(122)	15378.48	2915.44	4.37	$\omega_1 + \omega_4 + \omega_5(0.5), 2\omega_{10}(0.48)$
13(123)	15380.61	2917.56	1.63	$\omega_1 + \omega_4 + \omega_6(0.81), \omega_{10} + \omega_{11}(0.21)$
14(124)	15384.32	2921.28	2.33	$\omega_1 + \omega_4 + \omega_5(0.6), 2\omega_{10}(0.52)$
15(129)	15419.05	2956.01	6.52	$2\omega_{10}(0.63), \omega_{13}(0.52)$
16(134)	15456.63	2993.58	18.21	$\omega_{10} + \omega_{11}(0.64), \omega_{12}(0.53)$
17(135)	15461.25	2998.20	3.58	$2\omega_{11}(0.73), \omega_{13}(0.37)$
18(143)	15495.19	3032.14	3.57	$\omega_1 + 2\omega_5(0.62), \omega_1 + 2\omega_6(0.61)$
19(144)	15499.38	3036.33	3.36	$2\omega_1 + \omega_{10}(0.54), \omega_1 + \omega_6 + \omega_8(0.54)$
20(146)	15503.72	3040.68	41.67	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.23)$
21(155)	15529.13	3066.08	3.09	$\omega_1 + \omega_2 + \omega_{10}(0.69), \omega_2 + \omega_6 + \omega_8(0.44)$
22(157)	15534.40	3071.36	1.48	$\omega_1 + 2\omega_8(0.77), \omega_1 + \omega_2 + \omega_{10}(0.37)$
23(160)	15545.39	3082.35	1.63	$\omega_2 + \omega_5 + \omega_7(0.69), \omega_1 + 2\omega_7(0.35)$

**Table 7** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 200$  eigenvalues of  $C_2H_4O$ . The parameters are  $p = 8$ ,  $E_{max} = 25000\text{cm}^{-1}$ ,  $\varepsilon = 0.005$  and  $\varepsilon_I = 10.0$  km/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	13286.15	823.09	12.89	$\omega_2(0.96), \omega_2 + \omega_9(0.16)$
2(3)	13342.36	879.30	79.08	$\omega_3(0.97), \omega_3 + \omega_9(0.17)$
3(9)	13734.39	1271.33	15.41	$\omega_9(0.94), 2\omega_9(0.22)$
4(121)	15373.48	2910.42	22.59	$\omega_{12}(0.69), \omega_{10} + \omega_{11}(0.56)$
5(134)	15456.70	2993.64	18.26	$\omega_{10} + \omega_{11}(0.64), \omega_{12}(0.53)$
6(146)	15504.00	3040.94	41.85	$\omega_{15}(0.8), \omega_1 + 2\omega_8(0.23)$





**Fig. 1** Comparison between experimental data<sup>2,3</sup> for  $C_2H_4O$  and an A-VCI computation using SI ( $\epsilon_I = 0.1$  km/mol) with the following parameters:  $F = 200$ ,  $p = 8$ ,  $\epsilon = 0.005$  and  $E_{max} = 25,000$   $cm^{-1}$ . The bandshapes have been created using a Lorentzian profile with a width at half height of  $15$   $cm^{-1}$  and normalized.

**Table 8** Calculation in double harmonic approximation for vibrational states of  $C_2H_4O$  with non-zero intensity.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(1)	13459.05	817.66	0.16	$\omega_1(1)$
2(2)	13492.67	851.27	11.10	$\omega_2(1)$
3(3)	13541.92	900.52	77.89	$\omega_3(1)$
4(6)	13801.04	1159.64	1.10	$\omega_6(1)$
5(7)	13817.88	1176.48	3.57	$\omega_7(1)$
6(9)	13941.95	1300.56	14.21	$\omega_9(1)$
7(11)	14192.01	1550.62	4.45	$\omega_{11}(1)$
8(135)	15753.13	3111.74	37.05	$\omega_{12}(1)$
9(138)	15760.97	3119.57	14.74	$\omega_{13}(1)$
10(168)	15854.50	3213.11	47.68	$\omega_{15}(1)$

## 2.2 $C_4H_4N_2$

**Table 9** Calculation in double harmonic approximation for vibrational states of  $C_4H_4N_2$  with non-zero intensity.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	17191.50	423.13	25.50	$\omega_2(1)$
2(8)	17573.72	805.35	31.31	$\omega_6(1)$
3(16)	17800.80	1032.44	30.03	$\omega_{11}(1)$
4(19)	17851.32	1082.96	11.18	$\omega_{12}(1)$
5(24)	17925.28	1156.92	8.45	$\omega_{13}(1)$
6(25)	17954.45	1186.09	3.63	$\omega_{14}(1)$
7(50)	18204.14	1435.77	31.44	$\omega_{17}(1)$
8(61)	18280.10	1511.74	0.23	$\omega_{18}(1)$
9(2496)	19943.09	3174.72	3.24	$\omega_{22}(1)$
10(2557)	19959.25	3190.88	65.91	$\omega_{23}(1)$

**Table 10** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 2400$  eigenvalues of  $C_4H_4N_2$ . The parameters are  $p = 8$ ,  $E_{max} = 22000$   $cm^{-1}$ ,  $\epsilon = 0.05$  and  $\epsilon_I = 0.1$  km/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	16984.35	418.18	26.47	$\omega_2(0.97), \omega_2 + \omega_{10}(0.15)$
2(8)	17354.45	788.28	31.73	$\omega_6(0.96), \omega_6 + \omega_{10}(0.17)$

Table 10 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
3(17)	17600.15	1033.97	31.15	$\omega_{11}(0.97), \omega_{10} + \omega_{11}(0.18)$
4(18)	17628.41	1062.23	0.20	$\omega_1 + \omega_4(0.97), \omega_1 + \omega_4 + \omega_{10}(0.15)$
5(19)	17634.31	1068.13	9.58	$\omega_{12}(0.92), \omega_1 + \omega_5(0.28)$
6(20)	17675.36	1109.18	1.60	$\omega_1 + \omega_5(0.93), \omega_{12}(0.27)$
7(23)	17710.52	1144.34	7.16	$\omega_{13}(0.91), \omega_2 + \omega_5(0.31)$
8(25)	17726.40	1160.22	4.12	$\omega_{14}(0.94), \omega_{10} + \omega_{14}(0.24)$
9(26)	17758.93	1192.75	0.48	$\omega_2 + \omega_5(0.92), \omega_{13}(0.31)$
10(37)	17912.36	1346.19	1.01	$\omega_2 + \omega_7(0.94), \omega_{17}(0.15)$
11(43)	17954.54	1388.36	0.23	$\omega_2 + \omega_8(0.96), \omega_2 + \omega_8 + \omega_{10}(0.15)$
12(48)	17985.35	1419.17	30.09	$\omega_{17}(0.95), \omega_{10} + \omega_{17}(0.19)$
13(57)	18063.02	1496.85	0.21	$\omega_{18}(0.95), \omega_{10} + \omega_{18}(0.19)$
14(85)	18201.65	1635.48	0.18	$\omega_3 + \omega_{11}(0.96), \omega_3 + \omega_{10} + \omega_{11}(0.18)$
15(93)	18247.03	1680.86	0.81	$\omega_6 + \omega_7(0.7), \omega_3 + \omega_{12}(0.56)$
16(94)	18253.87	1687.70	0.96	$\omega_3 + \omega_{12}(0.65), \omega_6 + \omega_7(0.55)$
17(107)	18300.50	1734.32	1.78	$\omega_6 + \omega_8(0.89), \omega_7 + \omega_9(0.24)$
18(111)	18312.39	1746.21	0.26	$\omega_5 + \omega_9(0.93), \omega_6 + \omega_7(0.2)$
19(118)	18331.10	1764.93	0.20	$\omega_3 + \omega_{14}(0.83), \omega_4 + \omega_{11}(0.44)$
20(135)	18387.85	1821.67	0.17	$\omega_6 + \omega_{10}(0.92), \omega_6 + 2\omega_{10}(0.25)$
21(161)	18463.46	1897.28	0.28	$\omega_1 + \omega_{19}(0.94), \omega_1 + \omega_{10} + \omega_{19}(0.19)$
22(167)	18479.84	1913.66	0.69	$\omega_7 + \omega_9(0.89), \omega_6 + \omega_8(0.26)$
23(181)	18511.01	1944.83	2.32	$\omega_8 + \omega_9(0.92), \omega_6 + \omega_7(0.19)$
24(259)	18664.62	2098.44	0.27	$\omega_{10} + \omega_{12}(0.89), 2\omega_{10} + \omega_{12}(0.28)$
25(266)	18675.80	2109.62	0.40	$\omega_7 + \omega_{14}(0.93), \omega_7 + \omega_{10} + \omega_{14}(0.22)$
26(432)	18890.76	2324.58	0.17	$\omega_{12} + \omega_{15}(0.79), \omega_3 + \omega_6 + \omega_7(0.33)$
27(702)	19115.62	2549.44	0.12	$\omega_9 + \omega_{19}(0.95), \omega_9 + \omega_{10} + \omega_{19}(0.2)$
28(912)	19240.20	2674.02	0.26	$\omega_{15} + \omega_{17}(0.72), \omega_{12} + \omega_{20}(0.44)$
29(960)	19260.52	2694.34	0.12	$\omega_{13} + \omega_{19}(0.87), \omega_{12} + \omega_{20}(0.34)$
30(991)	19277.50	2711.32	0.11	$\omega_{14} + \omega_{19}(0.71), \omega_2 + \omega_6 + \omega_{18}(0.49)$
31(1159)	19351.88	2785.70	0.12	$\omega_{16} + \omega_{17}(0.67), \omega_6 + \omega_8 + \omega_{10}(0.46)$
32(1285)	19403.23	2837.05	2.59	$\omega_{16} + \omega_{18}(0.87), \omega_2 + \omega_8 + \omega_{16}(0.23)$
33(1364)	19436.00	2869.82	0.29	$\omega_1 + 2\omega_6 + \omega_8(0.8), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.27)$
34(1645)	19530.13	2963.95	0.27	$\omega_2 + \omega_7 + \omega_{20}(0.84), \omega_{17} + \omega_{20}(0.24)$
35(1656)	19533.44	2967.27	0.46	$\omega_{17} + \omega_{19}(0.86), \omega_{22}(0.25)$
36(1659)	19534.42	2968.24	0.25	$\omega_6 + \omega_7 + \omega_{15}(0.56), \omega_1 + \omega_3 + \omega_5 + \omega_{15}(0.37)$
37(1677)	19539.76	2973.59	0.19	$\omega_1 + \omega_3 + \omega_5 + \omega_{15}(0.55), \omega_1 + \omega_5 + 2\omega_7(0.39)$
38(1690)	19543.86	2977.68	0.83	$\omega_6 + \omega_7 + \omega_{15}(0.51), 2\omega_7 + \omega_{12}(0.48)$
39(1719)	19551.33	2985.15	0.12	$2\omega_5 + \omega_{17}(0.95), 2\omega_5 + \omega_{10} + \omega_{17}(0.16)$
40(1728)	19553.17	2986.99	15.01	$\omega_{17} + \omega_{20}(0.65), \omega_{23}(0.44)$
41(1733)	19554.33	2988.15	0.49	$2\omega_2 + \omega_{10} + \omega_{12}(0.86), \omega_1 + \omega_2 + \omega_{10} + \omega_{13}(0.26)$
42(1798)	19573.86	3007.68	0.18	$2\omega_6 + \omega_{17}(0.85), \omega_5 + \omega_9 + \omega_{15}(0.32)$
43(1840)	19587.73	3021.56	0.37	$2\omega_7 + \omega_{13}(0.56), \omega_1 + \omega_5 + \omega_7 + \omega_8(0.53)$
44(1845)	19588.74	3022.57	0.74	$\omega_{18} + \omega_{19}(0.84), \omega_{17} + \omega_{20}(0.37)$
45(1861)	19593.41	3027.23	3.95	$\omega_{22}(0.63), 2\omega_7 + \omega_{13}(0.41)$
46(1867)	19596.66	3030.48	0.20	$\omega_6 + \omega_8 + \omega_{15}(0.83), \omega_1 + \omega_5 + \omega_7 + \omega_8(0.24)$
47(1877)	19599.24	3033.06	0.67	$\omega_1 + \omega_5 + \omega_7 + \omega_8(0.57), 2\omega_7 + \omega_{13}(0.44)$
48(1884)	19601.92	3035.75	0.75	$2\omega_9 + \omega_{12}(0.56), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.5)$
49(1910)	19610.01	3043.83	1.45	$2\omega_9 + \omega_{12}(0.68), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.47)$
50(1933)	19618.93	3052.75	0.21	$\omega_1 + \omega_5 + 2\omega_8(0.72), 2\omega_8 + \omega_{12}(0.34)$
51(1937)	19619.66	3053.48	0.10	$\omega_1 + \omega_2 + 2\omega_3 + \omega_{11}(0.83), \omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.38)$
52(1943)	19620.13	3053.96	0.81	$3\omega_1 + \omega_2 + \omega_5 + \omega_6(0.65), 3\omega_1 + \omega_5 + \omega_{15}(0.28)$
53(1946)	19620.49	3054.31	1.63	$2\omega_1 + \omega_3 + \omega_5 + \omega_9(0.63), 3\omega_1 + \omega_2 + \omega_5 + \omega_6(0.32)$
54(1964)	19624.94	3058.76	1.76	$\omega_3 + \omega_{10} + \omega_{17}(0.82), \omega_3 + 2\omega_{10} + \omega_{17}(0.25)$
55(1999)	19635.69	3069.52	0.18	$\omega_7 + \omega_8 + \omega_{13}(0.82), \omega_2 + \omega_5 + \omega_7 + \omega_8(0.31)$
56(2005)	19639.77	3073.59	22.96	$\omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.64), \omega_{23}(0.44)$
57(2008)	19640.31	3074.13	26.15	$\omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.6), \omega_{23}(0.47)$
58(2026)	19645.12	3078.95	0.92	$3\omega_1 + \omega_5 + \omega_{15}(0.71), 2\omega_1 + \omega_{12} + \omega_{15}(0.34)$
59(2041)	19648.35	3082.17	4.47	$\omega_1 + \omega_5 + 2\omega_9(0.74), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.28)$
60(2047)	19649.87	3083.69	0.22	$\omega_2 + \omega_4 + \omega_6 + \omega_{13}(0.75), \omega_4 + \omega_{13} + \omega_{15}(0.39)$
61(2102)	19667.84	3101.67	0.12	$2\omega_6 + \omega_{18}(0.79), \omega_{18} + \omega_{20}(0.38)$
62(2110)	19671.25	3105.07	0.23	$\omega_{18} + \omega_{20}(0.55), 2\omega_6 + \omega_{18}(0.52)$

Table 10 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
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**Table 11** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 2400$  eigenvalues of  $C_4H_4N_2$ . The parameters are  $\rho = 8$ ,  $E_{max} = 22000\text{cm}^{-1}$ ,  $\varepsilon = 0.04$  and  $\varepsilon_l = 0.1$  km/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	16977.54	416.17	26.44	$\omega_2(0.97), \omega_2 + \omega_{10}(0.15)$
2(8)	17344.93	783.56	31.67	$\omega_6(0.96), \omega_6 + \omega_{10}(0.17)$
3(17)	17593.46	1032.09	31.25	$\omega_{11}(0.97), \omega_{10} + \omega_{11}(0.19)$
4(18)	17619.63	1058.26	0.20	$\omega_1 + \omega_4(0.97), \omega_1 + \omega_4 + \omega_{10}(0.16)$
5(19)	17625.96	1064.60	9.38	$\omega_{12}(0.92), \omega_1 + \omega_5(0.29)$
6(20)	17665.19	1103.82	1.70	$\omega_1 + \omega_5(0.92), \omega_{12}(0.29)$
7(24)	17701.11	1139.74	7.06	$\omega_{13}(0.91), \omega_2 + \omega_5(0.31)$
8(25)	17717.03	1155.66	4.21	$\omega_{14}(0.94), \omega_{10} + \omega_{14}(0.25)$
9(27)	17750.22	1188.85	0.47	$\omega_2 + \omega_5(0.92), \omega_{13}(0.31)$
10(37)	17899.87	1338.50	0.90	$\omega_2 + \omega_7(0.93), \omega_1 + \omega_8(0.15)$
11(44)	17943.88	1382.51	0.23	$\omega_2 + \omega_8(0.95), \omega_2 + \omega_8 + \omega_{10}(0.16)$
12(49)	17977.93	1416.56	30.22	$\omega_{17}(0.95), \omega_{10} + \omega_{17}(0.19)$
13(60)	18053.38	1492.02	0.21	$\omega_{18}(0.95), \omega_{10} + \omega_{18}(0.2)$
14(88)	18193.70	1632.33	0.17	$\omega_3 + \omega_{11}(0.96), \omega_3 + \omega_{10} + \omega_{11}(0.18)$
15(92)	18229.10	1667.74	0.20	$\omega_3 + \omega_{12}(0.8), \omega_6 + \omega_7(0.45)$
16(94)	18237.65	1676.29	1.60	$\omega_6 + \omega_7(0.76), \omega_3 + \omega_{12}(0.43)$
17(108)	18285.56	1724.19	1.79	$\omega_6 + \omega_8(0.87), \omega_7 + \omega_9(0.24)$
18(112)	18301.42	1740.05	0.25	$\omega_5 + \omega_9(0.93), \omega_6 + \omega_7(0.2)$
19(119)	18318.20	1756.84	0.17	$\omega_3 + \omega_{14}(0.93), \omega_3 + \omega_{10} + \omega_{14}(0.25)$
20(137)	18371.80	1810.44	0.16	$\omega_6 + \omega_{10}(0.92), \omega_6 + 2\omega_{10}(0.26)$
21(157)	18434.08	1872.71	0.11	$\omega_4 + \omega_{14}(0.94), \omega_4 + \omega_{10} + \omega_{14}(0.25)$
22(164)	18448.35	1886.99	0.27	$\omega_1 + \omega_{19}(0.94), \omega_1 + \omega_{10} + \omega_{19}(0.2)$
23(169)	18467.85	1906.48	0.61	$\omega_7 + \omega_9(0.91), \omega_6 + \omega_8(0.27)$
24(186)	18500.20	1938.83	2.33	$\omega_8 + \omega_9(0.92), \omega_6 + \omega_7(0.19)$
25(262)	18648.31	2086.95	0.27	$\omega_{10} + \omega_{12}(0.88), 2\omega_{10} + \omega_{12}(0.29)$
26(267)	18655.86	2094.49	0.40	$\omega_7 + \omega_{14}(0.93), \omega_7 + \omega_{10} + \omega_{14}(0.22)$
27(281)	18679.96	2118.60	0.13	$\omega_8 + \omega_{13}(0.89), \omega_2 + \omega_5 + \omega_8(0.34)$
28(444)	18873.29	2311.92	0.20	$\omega_{12} + \omega_{15}(0.84), \omega_1 + \omega_2 + \omega_5 + \omega_6(0.32)$
29(919)	19210.49	2649.12	0.12	$\omega_{12} + \omega_{20}(0.58), \omega_{15} + \omega_{17}(0.5)$
30(985)	19243.59	2682.23	0.21	$\omega_{13} + \omega_{19}(0.92), \omega_{10} + \omega_{13} + \omega_{19}(0.22)$
31(1029)	19260.33	2698.97	0.17	$\omega_{14} + \omega_{19}(0.81), \omega_2 + \omega_7 + \omega_{16}(0.28)$
32(1166)	19324.95	2763.58	0.11	$\omega_{16} + \omega_{17}(0.82), \omega_{15} + \omega_{18}(0.25)$
33(1268)	19363.38	2802.01	0.60	$\omega_1 + 2\omega_6 + \omega_8(0.63), 2\omega_1 + \omega_2 + \omega_4 + \omega_8(0.36)$
34(1326)	19386.24	2824.87	0.56	$\omega_3 + \omega_4 + \omega_{18}(0.8), \omega_{16} + \omega_{18}(0.48)$
35(1339)	19391.02	2829.66	1.52	$\omega_{16} + \omega_{18}(0.74), \omega_3 + \omega_4 + \omega_{18}(0.52)$
36(1550)	19462.28	2900.92	0.15	$\omega_1 + \omega_8 + \omega_{20}(0.73), \omega_2 + \omega_9 + \omega_{18}(0.5)$
37(1643)	19492.38	2931.02	0.12	$\omega_1 + \omega_5 + 2\omega_7(0.47), \omega_6 + \omega_7 + \omega_{15}(0.46)$
38(1687)	19504.99	2943.63	0.19	$\omega_2 + \omega_7 + \omega_{20}(0.73), \omega_1 + \omega_2 + \omega_{10} + \omega_{13}(0.37)$
39(1725)	19515.33	2953.97	0.56	$\omega_{17} + \omega_{19}(0.84), \omega_{22}(0.26)$
40(1784)	19531.72	2970.35	6.99	$\omega_1 + \omega_6 + \omega_7 + \omega_9(0.48), \omega_1 + \omega_5 + 2\omega_7(0.4)$
41(1798)	19536.48	2975.11	0.19	$\omega_8 + \omega_9 + \omega_{10}(0.75), \omega_2 + \omega_3 + \omega_6 + \omega_{14}(0.36)$
42(1799)	19536.80	2975.43	0.15	$\omega_2 + \omega_3 + \omega_6 + \omega_{14}(0.72), \omega_8 + \omega_9 + \omega_{10}(0.4)$
43(1814)	19540.37	2979.00	6.85	$\omega_{17} + \omega_{20}(0.6), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.41)$
44(1841)	19552.07	2990.70	0.18	$\omega_2 + \omega_8 + \omega_{20}(0.86), \omega_2 + \omega_3 + \omega_8 + \omega_{10}(0.2)$
45(1846)	19553.02	2991.66	0.14	$2\omega_6 + \omega_{17}(0.52), \omega_1 + \omega_3 + \omega_9 + \omega_{12}(0.5)$
46(1849)	19553.21	2991.84	0.18	$2\omega_6 + \omega_{17}(0.76), \omega_1 + \omega_3 + \omega_9 + \omega_{12}(0.34)$
47(1870)	19558.85	2997.48	0.39	$\omega_1 + \omega_8 + \omega_{19}(0.66), \omega_2 + \omega_7 + \omega_{19}(0.39)$
48(1901)	19567.21	3005.84	0.23	$3\omega_1 + \omega_6 + \omega_{14}(0.65), \omega_1 + \omega_5 + \omega_7 + \omega_8(0.39)$
49(1902)	19567.41	3006.05	0.25	$3\omega_1 + \omega_6 + \omega_{14}(0.66), \omega_1 + \omega_5 + \omega_7 + \omega_8(0.39)$
50(1907)	19567.91	3006.54	0.11	$\omega_3 + \omega_{14} + \omega_{15}(0.84), \omega_2 + \omega_3 + \omega_6 + \omega_{14}(0.34)$
51(1943)	19577.22	3015.86	1.88	$\omega_{18} + \omega_{19}(0.83), \omega_{17} + \omega_{20}(0.32)$
52(1948)	19578.00	3016.64	3.66	$\omega_{22}(0.63), \omega_{18} + \omega_{20}(0.33)$
53(1973)	19586.63	3025.27	0.11	$\omega_3 + \omega_{12} + \omega_{16}(0.59), \omega_2 + \omega_3 + \omega_8 + \omega_{10}(0.59)$

Table 11 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
54(2031)	19603.09	3041.72	0.65	$2\omega_1 + \omega_3 + \omega_4 + \omega_{11}(0.76), \omega_3 + \omega_{10} + \omega_{17}(0.48)$
55(2034)	19603.18	3041.81	1.38	$\omega_3 + \omega_{10} + \omega_{17}(0.71), 2\omega_1 + \omega_3 + \omega_4 + \omega_{11}(0.52)$
56(2088)	19619.50	3058.13	4.88	$\omega_1 + \omega_5 + 2\omega_9(0.72), 2\omega_9 + \omega_{12}(0.4)$
57(2106)	19624.48	3063.12	1.54	$\omega_2 + \omega_4 + \omega_6 + \omega_{13}(0.82), 2\omega_2 + \omega_4 + \omega_5 + \omega_6(0.3)$
58(2110)	19625.60	3064.23	53.93	$\omega_{23}(0.68), \omega_{17} + \omega_{20}(0.39)$
59(2234)	19662.97	3101.61	0.36	$\omega_{18} + \omega_{20}(0.69), 2\omega_3 + \omega_4 + \omega_{14}(0.38)$
60(2386)	19715.94	3154.58	0.27	$\omega_1 + 2\omega_7 + \omega_8(0.85), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.27)$

**Table 12** Intensity selection calculation for the PES + diagonal Coriolis operator with  $F = 2400$  eigenvalues of  $C_4H_4N_2$ . The parameters are  $p = 8$ ,  $E_{max} = 22000\text{cm}^{-1}$ ,  $\varepsilon = 0.03$  and  $\varepsilon_l = 0.1$  mk/mol.

Number	Eigenvalue	Frequency	Intensity	Assignment
1(2)	16975.76	415.50	26.45	$\omega_2(0.97), \omega_2 + \omega_{10}(0.15)$
2(8)	17334.19	773.93	31.32	$\omega_6(0.96), \omega_6 + \omega_{10}(0.17)$
3(15)	17576.97	1016.72	31.15	$\omega_{11}(0.96), \omega_{10} + \omega_{11}(0.18)$
4(18)	17604.36	1044.11	0.20	$\omega_1 + \omega_4(0.97), \omega_1 + \omega_4 + \omega_{10}(0.16)$
5(19)	17616.72	1056.47	8.98	$\omega_{12}(0.91), \omega_1 + \omega_5(0.32)$
6(20)	17652.32	1092.07	1.96	$\omega_1 + \omega_5(0.91), \omega_{12}(0.32)$
7(23)	17688.99	1128.74	6.70	$\omega_{13}(0.91), \omega_2 + \omega_5(0.31)$
8(25)	17705.47	1145.22	4.23	$\omega_{14}(0.93), \omega_{10} + \omega_{14}(0.25)$
9(26)	17736.95	1176.70	0.48	$\omega_2 + \omega_5(0.92), \omega_{13}(0.31)$
10(34)	17834.58	1274.32	0.10	$\omega_1 + \omega_8(0.92), \omega_2 + \omega_7(0.16)$
11(37)	17883.46	1323.21	0.83	$\omega_2 + \omega_7(0.93), \omega_1 + \omega_8(0.15)$
12(41)	17924.34	1364.09	0.22	$\omega_2 + \omega_8(0.95), \omega_2 + \omega_8 + \omega_{10}(0.15)$
13(48)	17965.66	1405.41	30.07	$\omega_{17}(0.95), \omega_{10} + \omega_{17}(0.2)$
14(57)	18037.66	1477.41	0.21	$\omega_{18}(0.95), \omega_{10} + \omega_{18}(0.2)$
15(82)	18170.11	1609.86	0.16	$\omega_3 + \omega_{11}(0.96), \omega_3 + \omega_{10} + \omega_{11}(0.18)$
16(91)	18208.04	1647.79	0.30	$\omega_3 + \omega_{12}(0.75), \omega_6 + \omega_7(0.5)$
17(93)	18216.37	1656.12	1.54	$\omega_6 + \omega_7(0.71), \omega_3 + \omega_{12}(0.49)$
18(103)	18257.48	1697.23	1.85	$\omega_6 + \omega_8(0.88), \omega_7 + \omega_9(0.26)$
19(109)	18281.59	1721.34	0.26	$\omega_5 + \omega_9(0.92), \omega_6 + \omega_7(0.22)$
20(115)	18296.89	1736.63	0.16	$\omega_3 + \omega_{14}(0.87), 2\omega_1 + \omega_{12}(0.3)$
21(130)	18349.51	1789.26	0.15	$\omega_6 + \omega_{10}(0.91), \omega_6 + 2\omega_{10}(0.26)$
22(152)	18413.73	1853.48	0.11	$\omega_4 + \omega_{14}(0.93), \omega_4 + \omega_{10} + \omega_{14}(0.25)$
23(158)	18425.86	1865.61	0.27	$\omega_1 + \omega_{19}(0.94), \omega_1 + \omega_{10} + \omega_{19}(0.2)$
24(165)	18441.14	1880.88	0.56	$\omega_7 + \omega_9(0.88), \omega_6 + \omega_8(0.28)$
25(176)	18475.03	1914.77	2.29	$\omega_8 + \omega_9(0.9), \omega_6 + \omega_7(0.2)$
26(253)	18621.45	2061.19	0.35	$\omega_7 + \omega_{14}(0.89), \omega_1 + \omega_6 + \omega_9(0.24)$
27(259)	18629.25	2069.00	0.28	$\omega_{10} + \omega_{12}(0.86), 2\omega_{10} + \omega_{12}(0.29)$
28(272)	18652.90	2092.65	0.14	$\omega_8 + \omega_{13}(0.92), \omega_2 + \omega_5 + \omega_8(0.23)$
29(425)	18850.54	2290.29	0.21	$\omega_{12} + \omega_{15}(0.84), \omega_2 + \omega_6 + \omega_{12}(0.29)$
30(676)	19063.18	2502.93	0.13	$\omega_9 + \omega_{19}(0.84), \omega_1 + \omega_3 + \omega_{19}(0.29)$
31(899)	19189.22	2628.97	0.11	$\omega_{12} + \omega_{20}(0.67), \omega_{15} + \omega_{17}(0.37)$
32(943)	19211.15	2650.90	0.17	$\omega_{13} + \omega_{19}(0.89), \omega_{10} + \omega_{13} + \omega_{19}(0.23)$
33(979)	19228.71	2668.46	0.18	$\omega_{14} + \omega_{19}(0.86), \omega_{10} + \omega_{14} + \omega_{19}(0.27)$
34(1131)	19297.18	2736.93	0.32	$\omega_1 + 2\omega_6 + \omega_8(0.61), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.28)$
35(1302)	19364.74	2804.49	2.03	$\omega_{16} + \omega_{18}(0.89), \omega_{23}(0.2)$
36(1540)	19447.30	2887.05	0.12	$\omega_2 + \omega_9 + \omega_{18}(0.7), 2\omega_7 + \omega_{12}(0.34)$
37(1669)	19485.76	2925.51	0.49	$\omega_1 + \omega_5 + 2\omega_7(0.44), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.44)$
38(1682)	19489.06	2928.80	0.51	$\omega_{17} + \omega_{19}(0.79), \omega_{22}(0.24)$
39(1761)	19510.20	2949.95	0.26	$2\omega_6 + \omega_{17}(0.88), 2\omega_6 + \omega_{10} + \omega_{17}(0.17)$
40(1765)	19511.10	2950.84	0.10	$\omega_2 + \omega_8 + \omega_{20}(0.87), \omega_2 + \omega_8 + \omega_{10} + \omega_{20}(0.19)$
41(1769)	19513.17	2952.91	0.12	$4\omega_1 + \omega_6 + \omega_7(0.52), \omega_2 + \omega_4 + \omega_6 + \omega_{11}(0.37)$
42(1790)	19517.27	2957.01	0.19	$3\omega_1 + 2\omega_3 + \omega_5(0.53), \omega_1 + 3\omega_3 + \omega_5(0.31)$
43(1799)	19519.83	2959.58	0.29	$2\omega_1 + 2\omega_2 + \omega_{17}(0.72), 3\omega_1 + \omega_2 + \omega_{18}(0.48)$
44(1802)	19520.96	2960.71	11.82	$\omega_{17} + \omega_{20}(0.7), \omega_{23}(0.39)$
45(1820)	19526.92	2966.67	0.32	$\omega_3 + \omega_{14} + \omega_{15}(0.84), \omega_2 + \omega_3 + \omega_6 + \omega_{14}(0.24)$
46(1917)	19553.27	2993.02	0.34	$\omega_3 + \omega_{12} + \omega_{16}(0.78), \omega_1 + 2\omega_3 + \omega_4 + \omega_5(0.25)$
47(1922)	19554.14	2993.89	0.94	$\omega_{18} + \omega_{19}(0.75), \omega_4 + \omega_{11} + \omega_{15}(0.29)$

Table 12 (continued)

Number	Eigenvalue	Frequency	Intensity	Assignment
48(1923)	19554.44	2994.19	0.19	$\omega_4 + \omega_{11} + \omega_{15}(0.54), \omega_2 + \omega_3 + \omega_9 + \omega_{11}(0.44)$
49(1943)	19559.81	2999.56	4.07	$\omega_{22}(0.64), \omega_{18} + \omega_{20}(0.41)$
50(1991)	19572.58	3012.33	1.34	$\omega_3 + \omega_{10} + \omega_{17}(0.8), \omega_3 + 2\omega_{10} + \omega_{17}(0.26)$
51(2066)	19594.74	3034.49	2.67	$\omega_2 + \omega_6 + \omega_8 + \omega_9(0.51), \omega_2 + \omega_5 + \omega_7 + \omega_8(0.39)$
52(2116)	19608.72	3048.47	51.73	$\omega_{23}(0.67), \omega_{17} + \omega_{20}(0.37)$
53(2130)	19613.52	3053.27	6.16	$\omega_2 + \omega_5 + \omega_7 + \omega_8(0.54), \omega_2 + \omega_6 + \omega_8 + \omega_9(0.4)$
54(2178)	19626.31	3066.06	2.51	$\omega_1 + 2\omega_7 + \omega_8(0.68), \omega_1 + \omega_6 + \omega_7 + \omega_9(0.34)$
55(2194)	19632.35	3072.10	0.29	$\omega_6 + \omega_8 + \omega_{16}(0.78), \omega_2 + \omega_6 + \omega_8 + \omega_9(0.29)$
56(2206)	19634.99	3074.74	0.34	$\omega_{18} + \omega_{20}(0.64), \omega_{22}(0.33)$
57(2209)	19636.35	3076.09	0.27	$\omega_6 + \omega_7 + \omega_{16}(0.43), \omega_{18} + \omega_{20}(0.42)$

## Notes and references

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