

Electronic Supplementary Information

Modelling the vibrationally mediated photo-dissociation of acetylene.

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The supplementary information consists of two parts. In the first, a set of figures (13-21) show the total flux for all states for the photodissociation of acetylene into the R_a dissociation channel 200fs after the excitation pulse has ended. Each figure is for a simulation with different IR+UV excitation pulses. Nomenclature is in Table 5 of the main text. The second part of the information is the operator file used in the Heidelberg MCTDH program for the dynamics simulations, with details of the acetylene coupled surfaces.

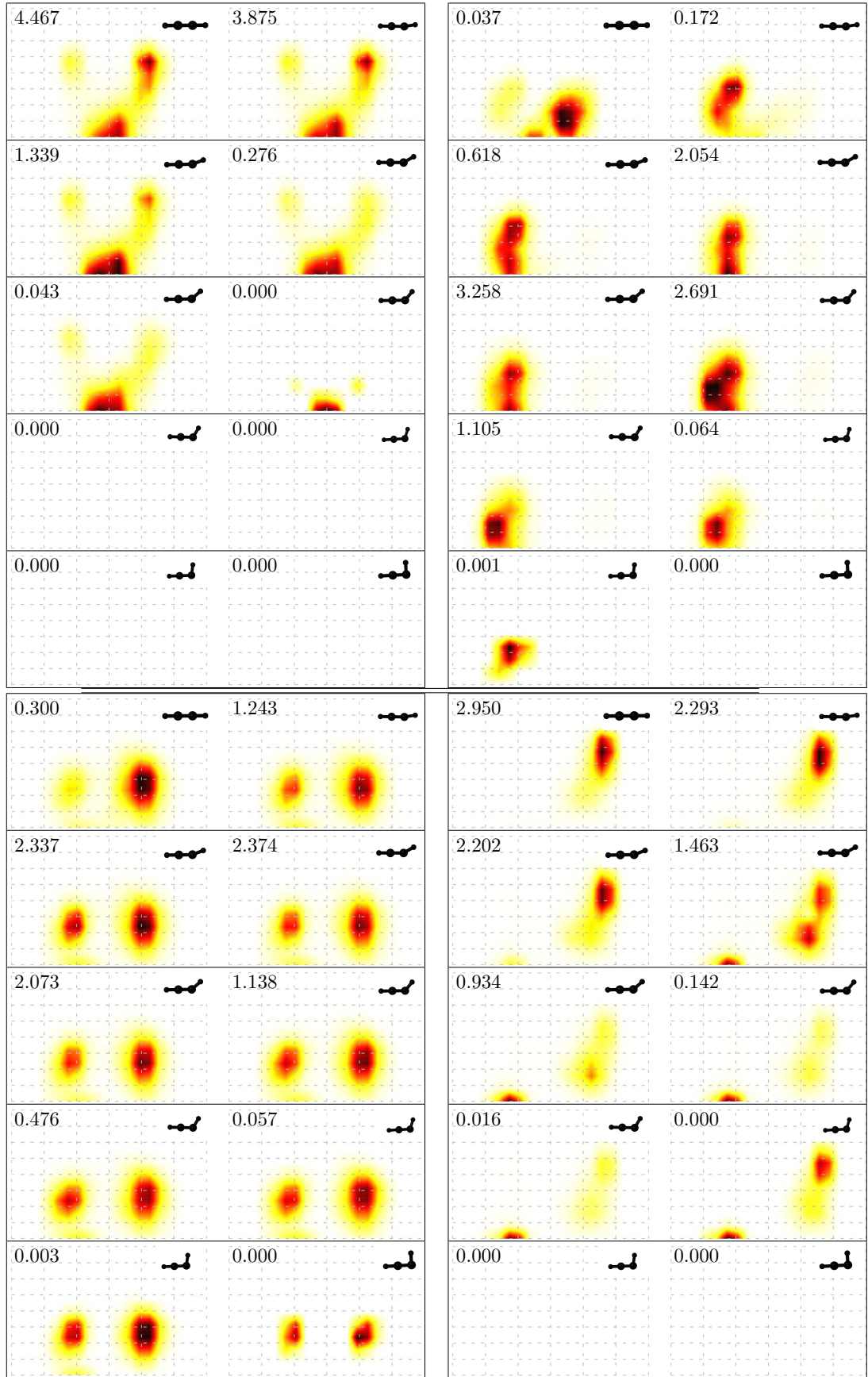


Figure 13: *top left*: uv0-ir0 (6.4,0), *top₁ right*: uv0-ir1 (6.4,1), *bot left*: uv0-ir2 (6.4,2), *bot right*: uv0-ir3 (6.4,3)

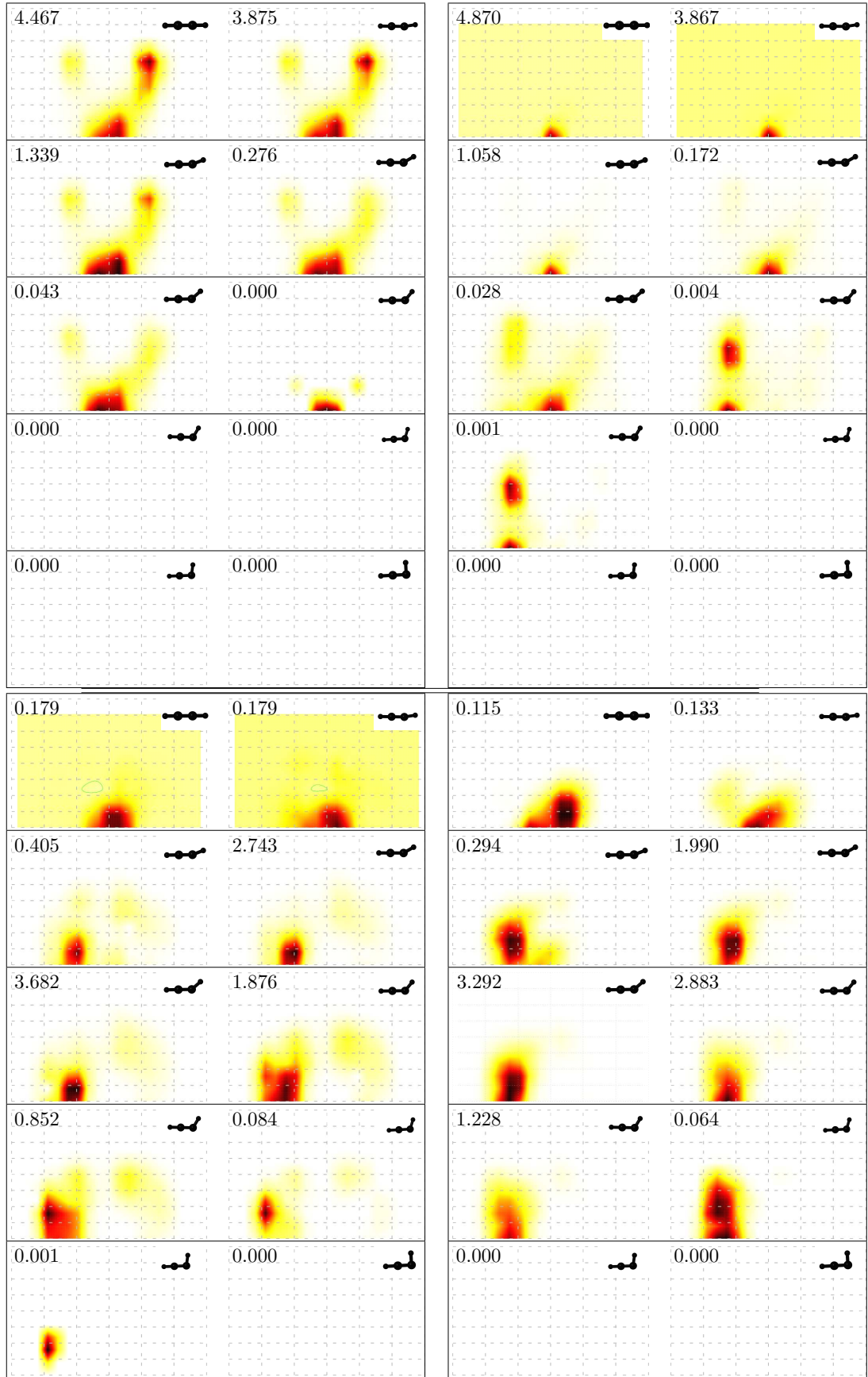


Figure 14: *top left*: uv0-ir4 (6.4,5), *top₂right*: uv0-ir5 (6.4,7), *bot left*: uv1-ir0 (6.68,0), *bot right*: uv1-ir1 (6.68,1)

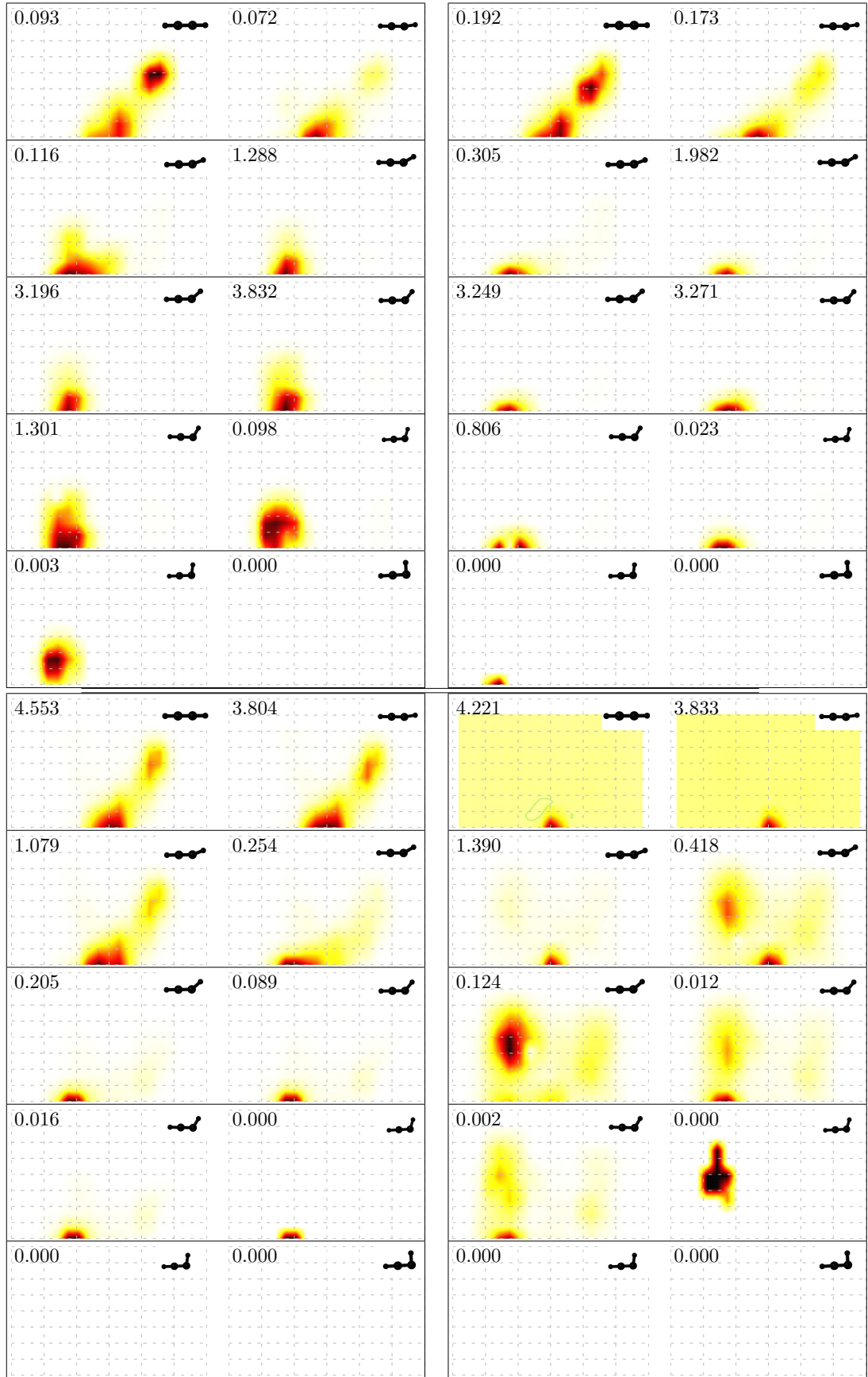


Figure 15: *top left*: uv1-ir2 (6.68,2), *top right*: uv1-ir3 (6.68,3), *bot left*: uv1-ir4 (6.68,5), *bot right*: uv1-ir5 (6.68,7)

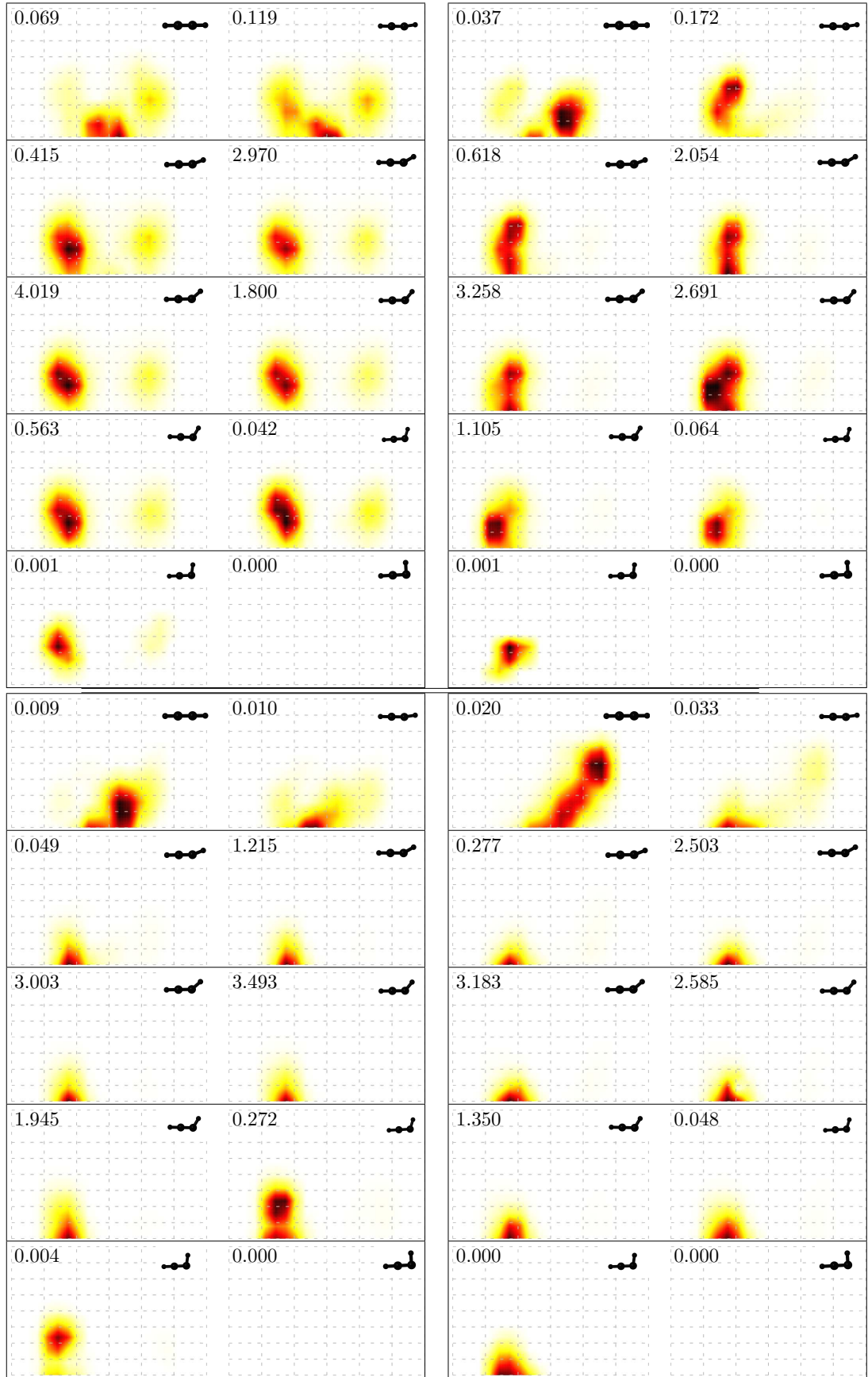


Figure 16: *top left*: uv2-ir0 (6.96,0), *top right*: uv2-ir1 (6.96,1), *bot left*: uv2-ir2 (6.96,2), *bot right*: uv2-ir3 (6.96,3)

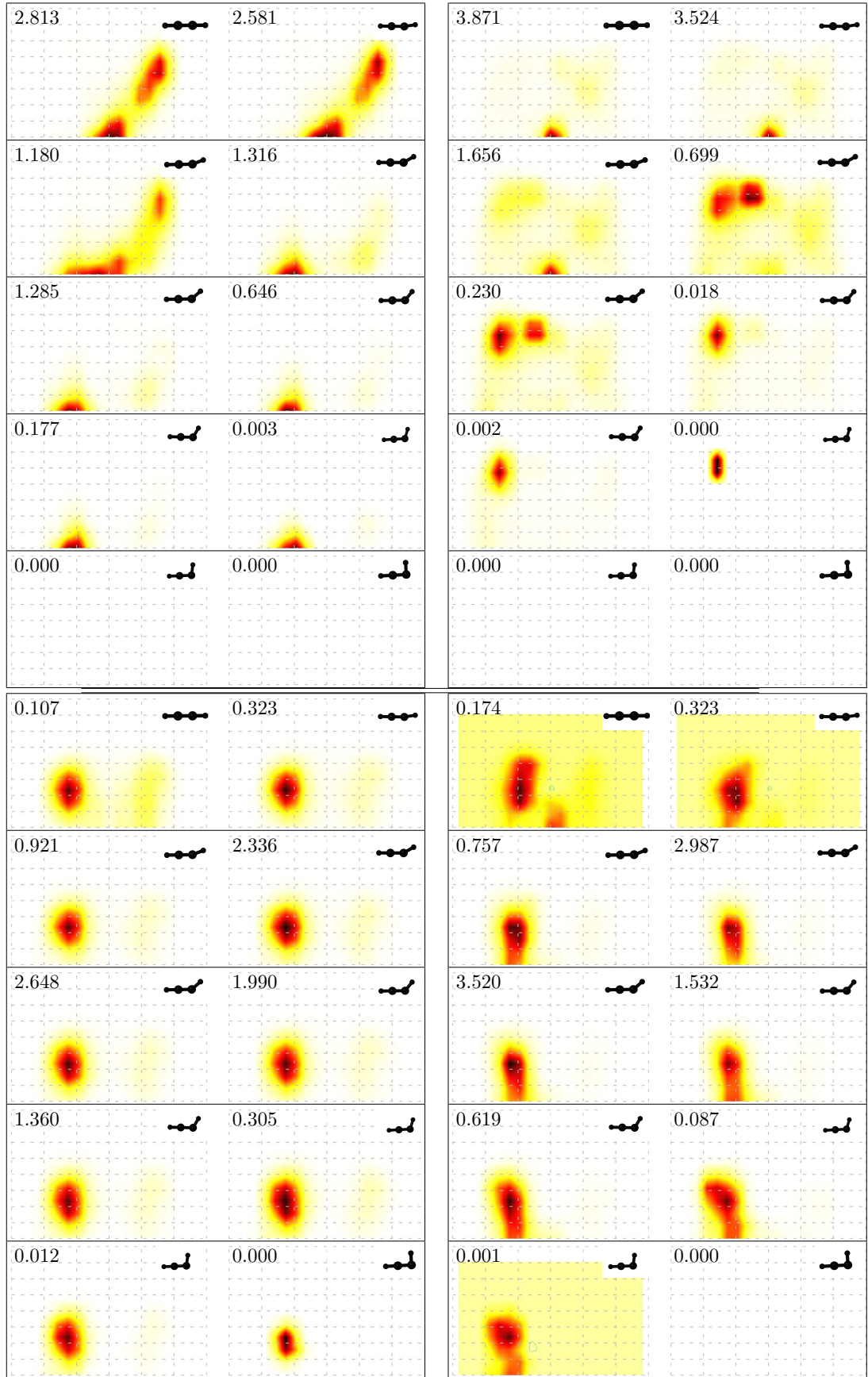


Figure 17: *top left*: uv2-ir4 (6.96,5), *top right*: uv2-ir5 (6.96,7), *bot left*: uv3-ir0 (7.24,0), *bot right*: uv3-ir1 (7.24,1)

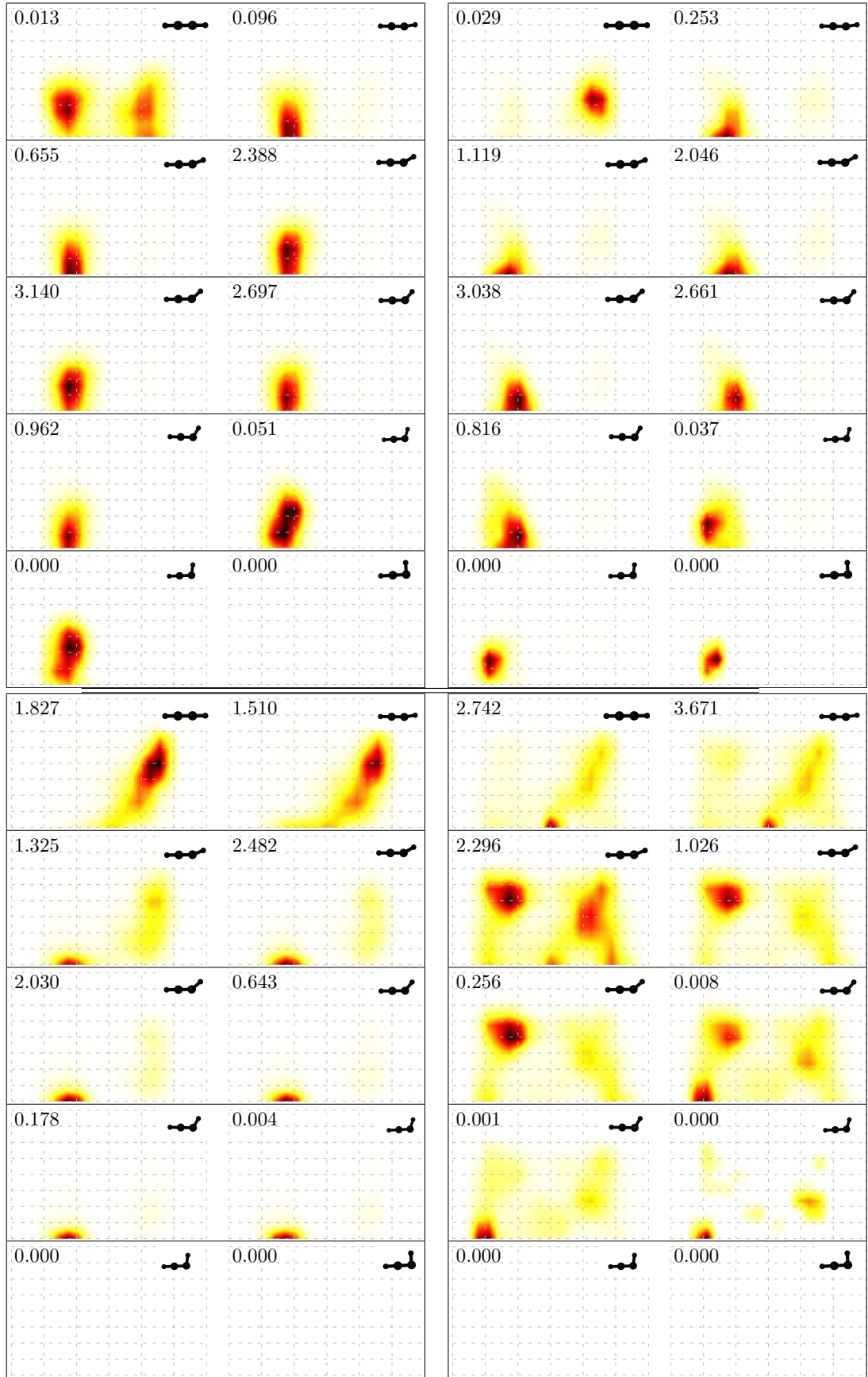


Figure 18: *top left*: uv3-ir2 (7.24,2), *top right*: uv3-ir3 (7.24,3), *bot left*: uv3-ir4 (7.24,5), *bot right*: uv3-ir5 (7.24,7)



Figure 19: *top left*: uv4-ir0 (7.52,0), *top right*: uv4-ir1 (7.52,1), *bot left*: uv4-ir2 (7.52,2), *bot right*: uv4-ir3 (7.52,3)

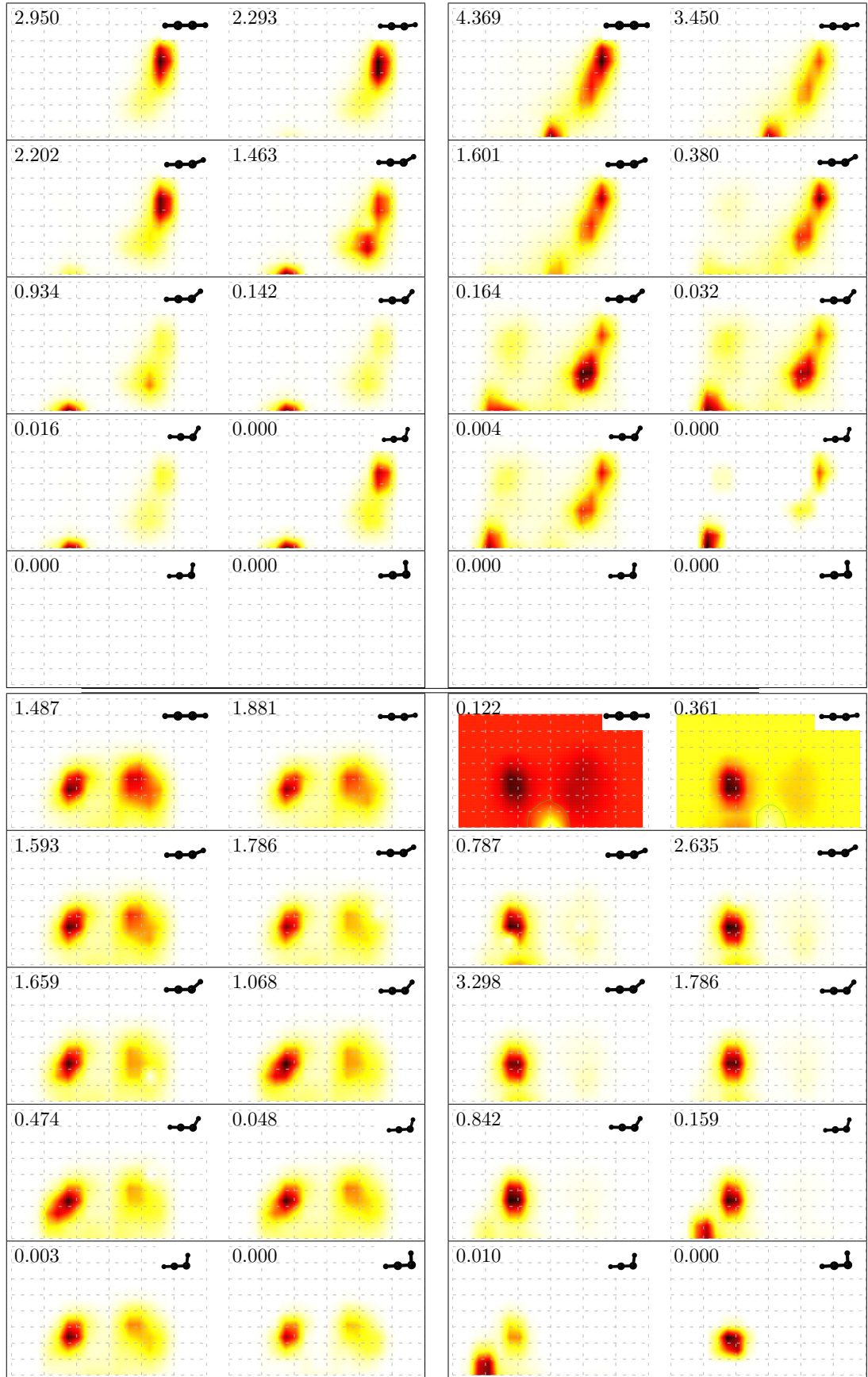


Figure 20: *top left*: uv4-ir4 (7.52,5), *top right*: uv4-ir5 (7.52,7), *bot left*: uv5-ir0 (7.8,0), *bot right*: uv5-ir1 (7.8,1)

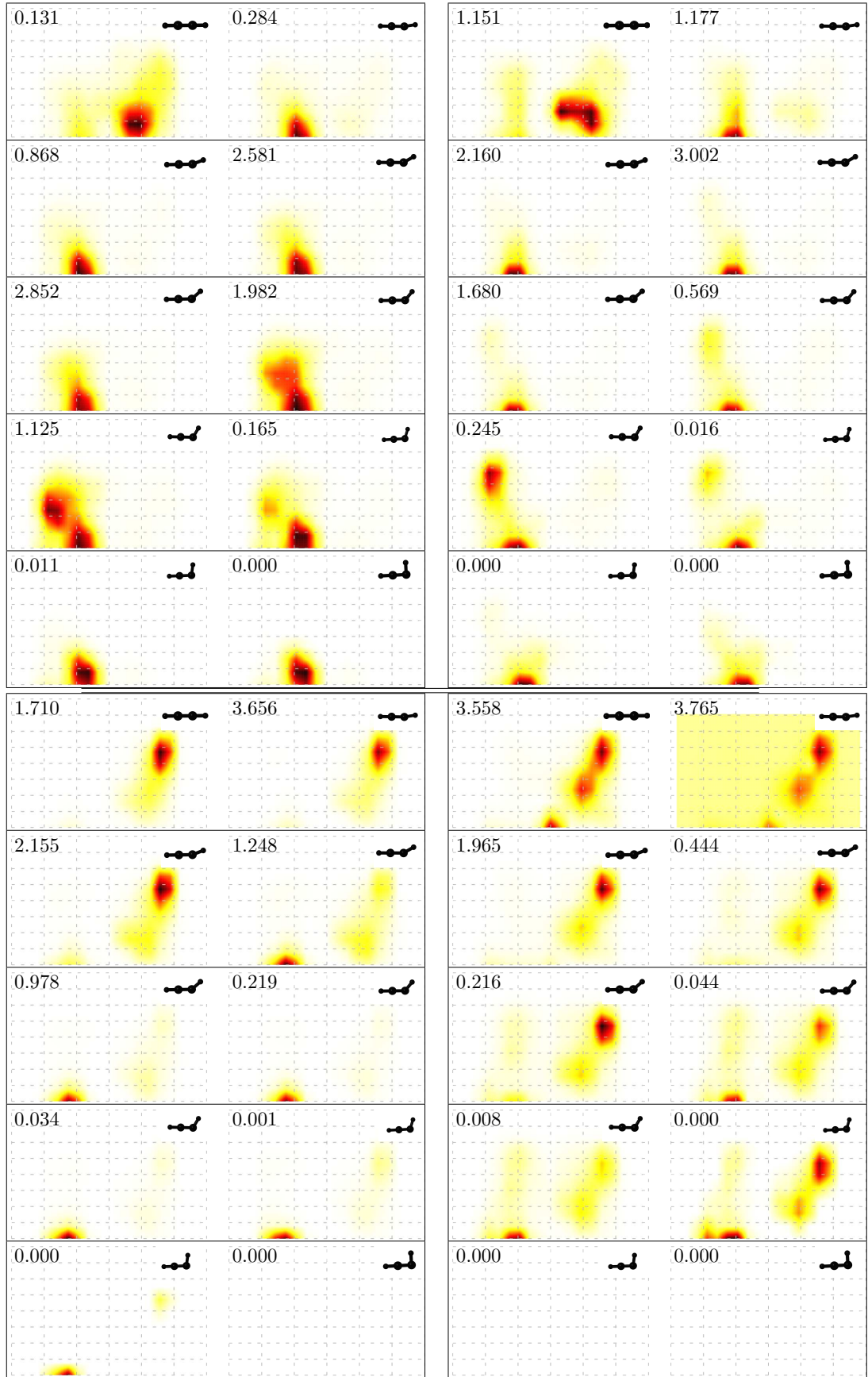


Figure 21: *top left*: uv5-ir2 (7.8,2), *top right*: uv5-ir3 (7.8,3), *bot left*: uv5-ir4 (7.8,5), *bot right*: uv5-ir5 (7.8,7)

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#####
## SUPPLEMENTARY INFORMATION B
#####
#####
## PARAMETERS AND LABELS
#####
```

```
OP_DEFINE-SECTION
TITLE
10-state 7-coordinate acetylene model
END-TITLE
END-OP_DEFINE-SECTION
PARAMETER-SECTION
```

#vertical energies

```
E1      = 0.00000 , ev
E2      = 6.91857 , ev
E3      = 7.26113 , ev
E4      = 7.26114 , ev
E5      = 8.26326 , ev
E6      = 8.26326 , ev
E7      = 8.57901 , ev
E8      = 8.57901 , ev
E9      = 9.37474 , ev
E10     = 9.37474 , ev
```

#Morse potential (radial coordinates (1, 4))

```
1D_1 = 6.466600000 , ev
1A_1 = 0.141069884
1X_1 = -0.077787000+16.668
1E_1 = -0.000770189 , ev
2D_1 = 8.705900000 , ev
2A_1 = 0.128314808
2X_1 = -0.478150000+16.668
2E_1 = -0.030830900 , ev
3D_1 = 8.972700000 , ev
3A_1 = 0.125538924
3X_1 = -0.424620000+16.668
3E_1 = -0.024178705 , ev
4D_1 = 8.972700000 , ev
4A_1 = 0.125538924
4X_1 = -0.424620000+16.668
4E_1 = -0.024178705 , ev
5D_1 = 7.846800000 , ev
5A_1 = 0.128590030
5X_1 = -0.068891000+16.668
5E_1 = -0.000610362 , ev
6D_1 = 7.846800000 , ev
6A_1 = 0.128590030
6X_1 = -0.068891000+16.668
6E_1 = -0.000610362 , ev
9D_1 = 7.539600000 , ev
9A_1 = 0.123402812
9X_1 = 0.190820000+16.668
9E_1 = -0.004280484 , ev
10D_1 = 7.539600000 , ev
10A_1 = 0.123402812
10X_1 = 0.190820000+16.668
10E_1 = -0.004280484 , ev
1D_4 = 6.466600000 , ev
1A_4 = 0.141069884
1X_4 = -0.077787000+16.668
1E_4 = -0.000770189 , ev
```

```
2D_4 = 8.705900000 , ev
2A_4 = 0.128314808
2X_4 = -0.478150000+16.668
2E_4 = -0.030830900 , ev
3D_4 = 8.972700000 , ev
3A_4 = 0.125538924
3X_4 = -0.424620000+16.668
3E_4 = -0.024178705 , ev
4D_4 = 8.972700000 , ev
4A_4 = 0.125538924
4X_4 = -0.424620000+16.668
4E_4 = -0.024178705 , ev
5D_4 = 7.846800000 , ev
5A_4 = 0.128590030
5X_4 = -0.068891000+16.668
5E_4 = -0.000610362 , ev
6D_4 = 7.846800000 , ev
6A_4 = 0.128590030
6X_4 = -0.068891000+16.668
6E_4 = -0.000610362 , ev
9D_4 = 7.539600000 , ev
9A_4 = 0.123402812
9X_4 = 0.190820000+16.668
9E_4 = -0.004280484 , ev
10D_4 = 7.539600000 , ev
10A_4 = 0.123402812
10X_4 = 0.190820000+16.668
10E_4 = -0.004280484 , ev
```

#morse potential (cc stretch)

```
1D_5 = 12.505000000 , ev
1A_5 = 0.052288683
1X_5 = -1.235300000
1E_5 = -0.048926363 , ev
2D_5 = 14.092000000 , ev
2A_5 = 0.039704236
2X_5 = 3.240500000
2E_5 = -0.265672377 , ev
3D_5 = 13.418000000 , ev
3A_5 = 0.040903859
3X_5 = 2.978600000
3E_5 = -0.225263422 , ev
4D_5 = 13.418000000 , ev
4A_5 = 0.040903859
4X_5 = 2.978600000
4E_5 = -0.225263422 , ev
5D_5 = 15.081000000 , ev
5A_5 = 0.043513700
5X_5 = 0.426480000
5E_5 = -0.005291167 , ev
6D_5 = 15.081000000 , ev
6A_5 = 0.043513700
6X_5 = 0.426480000
6E_5 = -0.005291167 , ev
7D_5 = 5.506200000 , ev
7A_5 = 0.059685408
7X_5 = 1.583100000
7E_5 = -0.054070913 , ev
8D_5 = 5.506200000 , ev
8A_5 = 0.059685408
8X_5 = 1.583100000
8E_5 = -0.054070913 , ev
```

```

9D_5 = 17.474000000 , ev
9A_5 = 0.040090461
9X_5 = 0.365540000
9E_5 = -0.003808171 , ev
10D_5 = 17.474000000 , ev
10A_5 = 0.040090461
10X_5 = 0.365540000
10E_5 = -0.003808171 , ev

```

```

#predissociation potential function (folded diabatic coupling between
n a state following a morse potential and a higher
#lying one following a decayling exponential.

```

```

7K1_1 = 2.9738, ev
7K2_1 = 0.15385000
7K3_1 = 0.36221000+16.668
7K4_1 = 0.07123, ev
7K5_1 = 2.56430000
7K6_1 = -0.58519000+16.668
7K7_1 = 3.6603, ev
7K8_1 = 7.0316, ev
7K9_1 = 0.11424000
7K1_4 = 2.9738, ev
7K2_4 = 0.15385000
7K3_4 = 0.36221000+16.668
7K4_4 = 0.07123, ev
7K5_4 = 2.56430000
7K6_4 = -0.58519000+16.668
7K7_4 = 3.6603, ev
7K8_4 = 7.0316, ev
7K9_4 = 0.11424000
8K1_1 = 2.9738, ev
8K2_1 = 0.15385000
8K3_1 = 0.36221000+16.668
8K4_1 = 0.07123, ev
8K5_1 = 2.56430000
8K6_1 = -0.58519000+16.668
8K7_1 = 3.6603, ev
8K8_1 = 7.0316, ev
8K9_1 = 0.11424000
8K1_4 = 2.9738, ev
8K2_4 = 0.15385000
8K3_4 = 0.36221000+16.668
8K4_4 = 0.07123, ev
8K5_4 = 2.56430000
8K6_4 = -0.58519000+16.668
8K7_4 = 3.6603, ev
8K8_4 = 7.0316, ev
8K9_4 = 0.11424000

```

```

#S0 model

```

```

p1_m1o1_m4o1_s0_0 = 0.0041, ev
p2_m2o4_s0_0 = 0.10114, ev
p3_m3o4_s0_0 = 0.10114, ev
p4_m6o4_s0_0 = 0.10114, ev
p5_m7o4_s0_0 = 0.10114, ev
p6_m2o2_s0_0 = 2.1261, ev
p8_m6o2_s0_0 = 2.1261, ev
p9_m7o2_s0_0 = 2.1261, ev
p10_m3o1_m2o3_s0_0 = 0.016238, ev
p11_m3o2_m2o2_s0_0 = 0.025286, ev
p12_m3o3_m2o1_s0_0 = 0.016238, ev
p13_m7o1_m6o3_s0_0 = 0.016238, ev

```

```

p14_m7o2_m6o2_s0_0 = 0.025286, ev
p15_m7o3_m6o1_s0_0 = 0.016238, ev
p17_m7o1_m6o1_s0_0 = 0.0668, ev
p16_m3o1_m2o1_s0_0 = 0.0668, ev

```

```

#parameters coupling radial coordinates (1,4) to Renner-Teller 4D s
ubspace

```

```

p1 = -1.9301000 , ev
p2 = -0.1189100
p3 = 0.55077000
p4 = 0.08799700 , ev
p5 = 2.94650000
p6 = 0.93562000
p7 = 0.33982000 , ev
p8 = -0.1113200
p9 = 3.93640000
p10 = -1.574800 , ev
p11 = 0.9224600
p12 = 0.3073200
p13 = 3.6992000 , ev
p14 = -0.254810
p15 = -0.364960
p16 = 3.8506000 , ev
p17 = 0.0525410
p18 = -1.004200
p19 = 1.6018000 , ev
p20 = 0.1001800
p21 = -1.554700
p22 = 2.4171000 , ev
p23 = -0.065758
p24 = -0.833810
p25 = 2.9423000
p26 = 0.1994400
p27 = 0.1765300
p28 = 3.8840000
p29 = 0.3721200
p30 = 8.9707000
p31 = 3.0463000
p32 = -5.326200
p33 = 1.5309000 , ev
p34 = -0.012014
p35 = -2.539400
p36 = 2.2920000
p37 = -3.235500 , ev
p38 = 0.1935600
p39 = -0.743790
p40 = -2.000000
p41 = 2.5913000 , ev
p42 = -0.050717
p43 = 1.2729000
p44 = 1.7451000
p45 = -2.535900 , ev
p46 = -0.305680
p47 = 0.3774700
p48 = -0.976620
p49 = -0.241630 , ev
p50 = 0.9150700
p51 = 2.9566000
p52 = 0.9001600
p53 = 3.1057000 , ev
p54 = 0.0168290
p55 = 0.4410400

```

p56 = -1.300200
p57 = -0.972500 ,ev
p58 = 0.0797090
p59 = -2.047100
p60 = -0.450400

#Renner-Teller 4D subspace model

p1_m1o1_m4o1_s1_1 = 0.0043, ev
p2_m1o1_m4o1_s2_2 = 0.0017, ev
p3_m1o1_m4o1_s3_3 = 0.0017, ev
p93_m2o2_s1_1 = 0.73176, ev
p33_m2o4_s1_1 = 24.665, ev
p94_m2o2_s2_2 = 0.49227, ev
p34_m2o4_s2_2 = 10.056, ev
p95_m2o2_s3_3 = 0.49227, ev
p35_m2o4_s3_3 = 3.4537, ev
p96_m2o2_s4_4 = 2.3484, ev
p36_m2o4_s4_4 = 4.6506, ev
p97_m2o2_s5_5 = 0.42884, ev
p37_m2o4_s5_5 = 5.5935, ev
p98_m2o2_s6_6 = 0.74085, ev
p38_m2o4_s6_6 = 4.7048, ev
p99_m2o2_s7_7 = 1.2521, ev
p39_m2o4_s7_7 = 3.1806, ev
p100_m2o2_s8_8 = 0.29211, ev
p40_m2o4_s8_8 = 1.2811, ev
p92_m2o2_s9_9 = 0.29211, ev
p32_m2o4_s9_9 = 2.2933, ev
p102_m3o2_s1_1 = 0.73176, ev
p42_m3o4_s1_1 = 24.665, ev
p103_m3o2_s2_2 = 0.49227, ev
p43_m3o4_s2_2 = 10.056, ev
p104_m3o2_s3_3 = 0.49227, ev
p44_m3o4_s3_3 = 3.4537, ev
p105_m3o2_s4_4 = 2.3484, ev
p45_m3o4_s4_4 = 4.6506, ev
p106_m3o2_s5_5 = 0.42884, ev
p46_m3o4_s5_5 = 5.5935, ev
p107_m3o2_s6_6 = 0.74085, ev
p47_m3o4_s6_6 = 4.7048, ev
p108_m3o2_s7_7 = 1.2521, ev
p48_m3o4_s7_7 = 3.1806, ev
p109_m3o2_s8_8 = 0.29211, ev
p49_m3o4_s8_8 = 1.2811, ev
p101_m3o2_s9_9 = 0.29211, ev
p41_m3o4_s9_9 = 2.2933, ev
p111_m6o2_s1_1 = 0.73176, ev
p51_m6o4_s1_1 = 24.665, ev
p112_m6o2_s2_2 = 0.49227, ev
p52_m6o4_s2_2 = 10.056, ev
p113_m6o2_s3_3 = 0.49227, ev
p53_m6o4_s3_3 = 3.4537, ev
p114_m6o2_s4_4 = 0.42884, ev
p54_m6o4_s4_4 = 5.5935, ev
p115_m6o2_s5_5 = 2.3484, ev
p55_m6o4_s5_5 = 4.6506, ev
p116_m6o2_s6_6 = 1.2521, ev
p56_m6o4_s6_6 = 3.1806, ev
p117_m6o2_s7_7 = 0.74085, ev
p57_m6o4_s7_7 = 4.7048, ev
p118_m6o2_s8_8 = 0.29211, ev
p58_m6o4_s8_8 = 1.2811, ev

p110_m6o2_s9_9 = 0.29211, ev
p50_m6o4_s9_9 = 2.2933, ev
p120_m7o2_s1_1 = 0.73176, ev
p60_m7o4_s1_1 = 24.665, ev
p121_m7o2_s2_2 = 0.49227, ev
p61_m7o4_s2_2 = 10.056, ev
p122_m7o2_s3_3 = 0.49227, ev
p62_m7o4_s3_3 = 3.4537, ev
p123_m7o2_s4_4 = 0.42884, ev
p63_m7o4_s4_4 = 5.5935, ev
p124_m7o2_s5_5 = 2.3484, ev
p64_m7o4_s5_5 = 4.6506, ev
p125_m7o2_s6_6 = 1.2521, ev
p65_m7o4_s6_6 = 3.1806, ev
p126_m7o2_s7_7 = 0.74085, ev
p66_m7o4_s7_7 = 4.7048, ev
p127_m7o2_s8_8 = 0.29211, ev
p67_m7o4_s8_8 = 1.2811, ev
p119_m7o2_s9_9 = 0.29211, ev
p59_m7o4_s9_9 = 2.2933, ev
p281_m2o1_s1_5 = -1.1168, ev
p282_m2o1_s1_6 = 1.2509, ev
p283_m2o1_s2_5 = 0.8052, ev
p284_m2o1_s2_6 = -0.8082, ev
p285_m2o1_s3_4 = 0.8052, ev
p286_m2o1_s3_7 = -0.8082, ev
p287_m2o1_s4_8 = 0.3317, ev
p288_m2o1_s5_9 = -0.3317, ev
p289_m2o1_s6_9 = -0.3681, ev
p290_m2o1_s7_8 = -0.3681, ev
p291_m3o1_s1_5 = -1.1168, ev
p292_m3o1_s1_6 = -1.2509, ev
p293_m3o1_s2_5 = 0.8052, ev
p294_m3o1_s2_6 = 0.8082, ev
p295_m3o1_s3_4 = 0.8052, ev
p296_m3o1_s3_7 = 0.8082, ev
p297_m3o1_s4_8 = -0.3317, ev
p298_m3o1_s5_9 = 0.3317, ev
p299_m3o1_s6_9 = -0.3681, ev
p300_m3o1_s7_8 = -0.3681, ev
p301_m6o1_s1_4 = 1.1168, ev
p302_m6o1_s1_7 = -1.2509, ev
p303_m6o1_s2_4 = 0.8052, ev
p304_m6o1_s2_7 = -0.8082, ev
p305_m6o1_s3_5 = -0.8052, ev
p306_m6o1_s3_6 = 0.8082, ev
p307_m6o1_s4_9 = -0.3317, ev
p308_m6o1_s5_8 = -0.3317, ev
p309_m6o1_s6_8 = 0.3681, ev
p310_m6o1_s7_9 = -0.3681, ev
p311_m7o1_s1_4 = 1.1168, ev
p312_m7o1_s1_7 = 1.2509, ev
p313_m7o1_s2_4 = 0.8052, ev
p314_m7o1_s2_7 = 0.8082, ev
p315_m7o1_s3_5 = -0.8052, ev
p316_m7o1_s3_6 = -0.8082, ev
p317_m7o1_s4_9 = 0.3317, ev
p318_m7o1_s5_8 = 0.3317, ev
p319_m7o1_s6_8 = 0.3681, ev
p320_m7o1_s7_9 = -0.3681, ev
p1_m1o1_m4o1_s1_1 = 0.0043, ev
p2_m1o1_m4o1_s2_2 = 0.0017, ev

p3_m1o1_m4o1_s3_3 = 0.0017, ev
p264_m3o1_m2o1_s1_1 = 1.3206, ev
p265_m3o1_m2o1_s2_2 = -0.0752, ev
p266_m3o1_m2o1_s3_3 = -0.0752, ev
p267_m3o1_m2o1_s4_4 = -1.0255, ev
p268_m3o1_m2o1_s5_5 = -1.7517, ev
p269_m3o1_m2o1_s6_6 = 1.5213, ev
p270_m3o1_m2o1_s7_7 = 0.4716, ev
p271_m3o1_m2o1_s8_8 = -0.0292, ev
p263_m3o1_m2o1_s9_9 = -0.0292, ev
p273_m7o1_m6o1_s1_1 = 1.3206, ev
p274_m7o1_m6o1_s2_2 = -0.0752, ev
p275_m7o1_m6o1_s3_3 = -0.0752, ev
p276_m7o1_m6o1_s4_4 = -1.7517, ev
p277_m7o1_m6o1_s5_5 = -1.0255, ev
p278_m7o1_m6o1_s6_6 = 0.4716, ev
p279_m7o1_m6o1_s7_7 = 1.5213, ev
p280_m7o1_m6o1_s8_8 = -0.0292, ev
p272_m7o1_m6o1_s9_9 = -0.0292, ev
p69_m2o2_s1_2 = 0.5939, ev
p68_m2o2_s1_9 = -0.2654, ev
p70_m2o2_s2_9 = 1.1446, ev
p71_m2o2_s3_8 = 1.1446, ev
p72_m2o2_s4_7 = -0.2441, ev
p73_m2o2_s5_6 = 0.7131, ev
p75_m3o2_s1_2 = 0.5939, ev
p74_m3o2_s1_9 = 0.2654, ev
p76_m3o2_s2_9 = -1.1446, ev
p77_m3o2_s3_8 = -1.1446, ev
p78_m3o2_s4_7 = 0.2441, ev
p79_m3o2_s5_6 = -0.7131, ev
p81_m6o2_s1_2 = -0.5939, ev
p80_m6o2_s1_9 = 0.2654, ev
p82_m6o2_s2_9 = 1.1446, ev
p83_m6o2_s3_8 = 1.1446, ev
p84_m6o2_s4_7 = 0.7131, ev
p85_m6o2_s5_6 = -0.2441, ev
p87_m7o2_s1_2 = -0.5939, ev
p86_m7o2_s1_9 = -0.2654, ev
p88_m7o2_s2_9 = -1.1446, ev
p89_m7o2_s3_8 = -1.1446, ev
p90_m7o2_s4_7 = -0.7131, ev
p91_m7o2_s5_6 = 0.2441, ev
p4_m3o1_m2o1_s1_2 = -0.4031, ev
p5_m2o1_m6o1_s1_3 = -1.1879, ev
p6_m2o1_m6o1_s1_8 = -0.2654, ev
p7_m2o1_m6o1_s4_5 = -0.1505, ev
p8_m2o1_m6o1_s4_6 = 0.0052, ev
p9_m2o1_m6o1_s5_7 = 0.0052, ev
p10_m2o1_m6o1_s6_7 = 0.4940, ev
p11_m2o1_m7o1_s1_3 = 0.8062, ev
p12_m2o1_m7o1_s2_8 = -1.3965, ev
p13_m2o1_m7o1_s3_9 = 1.3965, ev
p14_m2o1_m7o1_s4_5 = 1.0427, ev
p15_m2o1_m7o1_s4_6 = -0.3543, ev
p16_m2o1_m7o1_s5_7 = 0.3543, ev
p17_m2o1_m7o1_s6_7 = -1.0669, ev
p18_m3o1_m6o1_s1_3 = 0.8062, ev
p19_m3o1_m6o1_s2_8 = 1.3965, ev
p20_m3o1_m6o1_s3_9 = -1.3965, ev
p21_m3o1_m6o1_s4_5 = 1.0427, ev
p22_m3o1_m6o1_s4_6 = 0.3543, ev

p23_m3o1_m6o1_s5_7 = -0.3543, ev
p24_m3o1_m6o1_s6_7 = -1.0669, ev
p25_m3o1_m7o1_s1_3 = -1.1879, ev
p26_m3o1_m7o1_s1_8 = 0.2654, ev
p27_m3o1_m7o1_s4_5 = -0.1505, ev
p28_m3o1_m7o1_s4_6 = -0.0052, ev
p29_m3o1_m7o1_s5_7 = -0.0052, ev
p30_m3o1_m7o1_s6_7 = 0.4940, ev
p31_m7o1_m6o1_s1_2 = 0.4031, ev
p128_m3o1_m2o3_s9_9 = -0.00020958, ev
p177_m3o2_m2o2_s9_9 = 0.10586, ev
p186_m3o3_m2o1_s9_9 = -0.00020958, ev
p197_m2o2_m6o2_s9_9 = 0.68837, ev
p208_m3o1_m2o1_m6o2_s9_9 = 0.46064, ev
p219_m3o2_m6o2_s9_9 = 0.68837, ev
p230_m2o2_m7o1_m6o1_s9_9 = -0.46064, ev
p241_m3o1_m2o1_m7o1_m6o1_s9_9 = 2.7456, ev
p252_m3o2_m7o1_m6o1_s9_9 = -0.46064, ev
p129_m7o1_m6o3_s9_9 = -0.00020958, ev
p140_m2o2_m7o2_s9_9 = 0.68837, ev
p151_m3o1_m2o1_m7o2_s9_9 = -0.46064, ev
p162_m3o2_m7o2_s9_9 = 0.68837, ev
p173_m7o2_m6o2_s9_9 = -0.10586, ev
p176_m7o3_m6o1_s9_9 = -0.00020958, ev
p178_m3o1_m2o3_s1_1 = -0.54862, ev
p179_m3o2_m2o2_s1_1 = 0.61572, ev
p180_m3o3_m2o1_s1_1 = -0.54862, ev
p181_m2o2_m6o2_s1_1 = 2.5895, ev
p182_m3o1_m2o1_m6o2_s1_1 = -3.2087, ev
p183_m3o2_m6o2_s1_1 = 1.3162, ev
p184_m2o2_m7o1_m6o1_s1_1 = -3.2087, ev
p185_m3o1_m2o1_m7o1_m6o1_s1_1 = 5.1935, ev
p187_m3o2_m7o1_m6o1_s1_1 = -3.2087, ev
p188_m7o1_m6o3_s1_1 = -0.54862, ev
p189_m2o2_m7o2_s1_1 = 1.3162, ev
p190_m3o1_m2o1_m7o2_s1_1 = -3.2087, ev
p191_m3o2_m7o2_s1_1 = 2.5895, ev
p192_m7o2_m6o2_s1_1 = 0.61572, ev
p193_m7o3_m6o1_s1_1 = -0.54862, ev
p194_m3o1_m2o3_s2_2 = -0.49026, ev
p195_m3o2_m2o2_s2_2 = 0.20446, ev
p196_m3o3_m2o1_s2_2 = -0.49026, ev
p198_m2o2_m6o2_s2_2 = 0.048785, ev
p199_m3o1_m2o1_m6o2_s2_2 = 0.05975, ev
p200_m3o2_m6o2_s2_2 = 0.048785, ev
p201_m2o2_m7o1_m6o1_s2_2 = 0.05975, ev
p202_m3o1_m2o1_m7o1_m6o1_s2_2 = 0.19514, ev
p203_m3o2_m7o1_m6o1_s2_2 = 0.05975, ev
p204_m7o1_m6o3_s2_2 = -0.49026, ev
p205_m2o2_m7o2_s2_2 = 0.048785, ev
p206_m3o1_m2o1_m7o2_s2_2 = 0.05975, ev
p207_m3o2_m7o2_s2_2 = 0.048785, ev
p209_m7o2_m6o2_s2_2 = 0.20446, ev
p210_m7o3_m6o1_s2_2 = -0.49026, ev
p211_m3o1_m2o3_s3_3 = -0.37605, ev
p212_m3o2_m2o2_s3_3 = 0.52389, ev
p213_m3o3_m2o1_s3_3 = -0.37605, ev
p214_m2o2_m6o2_s3_3 = 0.16808, ev
p215_m3o1_m2o1_m6o2_s3_3 = 0.2313, ev
p216_m3o2_m6o2_s3_3 = 0.16808, ev
p217_m2o2_m7o1_m6o1_s3_3 = 0.2313, ev
p218_m3o1_m2o1_m7o1_m6o1_s3_3 = 0.55398, ev

p220_m3o2_m7o1_m6o1_s3_3 = 0.2313, ev
 p221_m7o1_m6o3_s3_3 = -0.37605, ev
 p222_m2o2_m7o2_s3_3 = 0.16808, ev
 p223_m3o1_m2o1_m7o2_s3_3 = 0.2313, ev
 p224_m3o2_m7o2_s3_3 = 0.16808, ev
 p225_m7o2_m6o2_s3_3 = 0.52389, ev
 p226_m7o3_m6o1_s3_3 = -0.37605, ev
 p227_m3o1_m2o3_s4_4 = 0.20941, ev
 p228_m3o2_m2o2_s4_4 = 1.101, ev
 p229_m3o3_m2o1_s4_4 = 0.20941, ev
 p231_m2o2_m6o2_s4_4 = 0.1863, ev
 p232_m3o1_m2o1_m6o2_s4_4 = 0.065764, ev
 p233_m3o2_m6o2_s4_4 = 0.1863, ev
 p234_m2o2_m7o1_m6o1_s4_4 = 0.063336, ev
 p235_m3o1_m2o1_m7o1_m6o1_s4_4 = 0.74035, ev
 p236_m3o2_m7o1_m6o1_s4_4 = 0.063336, ev
 p237_m7o1_m6o3_s4_4 = -0.057583, ev
 p238_m2o2_m7o2_s4_4 = 0.1863, ev
 p239_m3o1_m2o1_m7o2_s4_4 = 0.065764, ev
 p240_m3o2_m7o2_s4_4 = 0.1863, ev
 p242_m7o2_m6o2_s4_4 = 1.3849, ev
 p243_m7o3_m6o1_s4_4 = -0.057583, ev
 p244_m3o1_m2o3_s5_5 = -0.057583, ev
 p245_m3o2_m2o2_s5_5 = 1.3849, ev
 p246_m3o3_m2o1_s5_5 = -0.057583, ev
 p247_m2o2_m6o2_s5_5 = 0.033343, ev
 p248_m3o1_m2o1_m6o2_s5_5 = 0.035815, ev
 p249_m3o2_m6o2_s5_5 = 0.033343, ev
 p250_m2o2_m7o1_m6o1_s5_5 = 0.038243, ev
 p251_m3o1_m2o1_m7o1_m6o1_s5_5 = 0.12851, ev
 p253_m3o2_m7o1_m6o1_s5_5 = 0.038243, ev
 p254_m7o1_m6o3_s5_5 = 0.20941, ev
 p255_m2o2_m7o2_s5_5 = 0.033343, ev
 p256_m3o1_m2o1_m7o2_s5_5 = 0.035815, ev
 p257_m3o2_m7o2_s5_5 = 0.033343, ev
 p258_m7o2_m6o2_s5_5 = 1.101, ev
 p259_m7o3_m6o1_s5_5 = 0.20941, ev
 p260_m3o1_m2o3_s6_6 = 0.22487, ev
 p261_m3o2_m2o2_s6_6 = 0.89252, ev
 p262_m3o3_m2o1_s6_6 = 0.22487, ev
 p130_m2o2_m6o2_s6_6 = 0.60318, ev
 p131_m3o1_m2o1_m6o2_s6_6 = 1.2064, ev
 p132_m3o2_m6o2_s6_6 = 0.60318, ev
 p133_m2o2_m7o1_m6o1_s6_6 = 0.36563, ev
 p134_m3o1_m2o1_m7o1_m6o1_s6_6 = 0.73126, ev
 p135_m3o2_m7o1_m6o1_s6_6 = 0.36563, ev
 p136_m7o1_m6o3_s6_6 = -0.26556, ev
 p137_m2o2_m7o2_s6_6 = 0.60318, ev
 p138_m3o1_m2o1_m7o2_s6_6 = 1.2064, ev
 p139_m3o2_m7o2_s6_6 = 0.60318, ev
 p141_m7o2_m6o2_s6_6 = 0.37705, ev
 p142_m7o3_m6o1_s6_6 = -0.26556, ev
 p143_m3o1_m2o3_s7_7 = -0.26556, ev
 p144_m3o2_m2o2_s7_7 = 0.37705, ev
 p145_m3o3_m2o1_s7_7 = -0.26556, ev
 p146_m2o2_m6o2_s7_7 = 0.89819, ev
 p147_m3o1_m2o1_m6o2_s7_7 = -0.95807, ev
 p148_m3o2_m6o2_s7_7 = 0.89819, ev
 p149_m2o2_m7o1_m6o1_s7_7 = -0.11733, ev
 p150_m3o1_m2o1_m7o1_m6o1_s7_7 = 1.9113, ev
 p152_m3o2_m7o1_m6o1_s7_7 = -0.11733, ev
 p153_m7o1_m6o3_s7_7 = 0.22487, ev

p154_m2o2_m7o2_s7_7 = 0.89819, ev
 p155_m3o1_m2o1_m7o2_s7_7 = -0.95807, ev
 p156_m3o2_m7o2_s7_7 = 0.89819, ev
 p157_m7o2_m6o2_s7_7 = 0.89252, ev
 p158_m7o3_m6o1_s7_7 = 0.22487, ev
 p159_m3o1_m2o3_s8_8 = -0.015615, ev
 p160_m3o2_m2o2_s8_8 = -0.068021, ev
 p161_m3o3_m2o1_s8_8 = -0.015615, ev
 p163_m2o2_m6o2_s8_8 = 0.1917, ev
 p164_m3o1_m2o1_m6o2_s8_8 = -0.29839, ev
 p165_m3o2_m6o2_s8_8 = 0.1917, ev
 p166_m2o2_m7o1_m6o1_s8_8 = -0.29839, ev
 p167_m3o1_m2o1_m7o1_m6o1_s8_8 = 0.74834, ev
 p168_m3o2_m7o1_m6o1_s8_8 = -0.29839, ev
 p169_m7o1_m6o3_s8_8 = -0.015615, ev
 p170_m2o2_m7o2_s8_8 = 0.1917, ev
 p171_m3o1_m2o1_m7o2_s8_8 = -0.29839, ev
 p172_m3o2_m7o2_s8_8 = 0.1917, ev
 p174_m7o2_m6o2_s8_8 = -0.068021, ev
 p175_m7o3_m6o1_s8_8 = -0.015615, ev
 p128_m3o1_m2o3_s9_9 = 0.09583700, ev
 p321_m1o2_m2o2_s1_1 = 0.09583700, ev
 p322_m1o2_m2o2_s2_2 = 0.00028878, ev
 p177_m3o2_m2o2_s9_9 = 0.00028878, ev
 p186_m3o3_m2o1_s9_9 = 0.09583700, ev
 p323_m3o2_m4o2_s1_1 = 0.09583700, ev
 p197_m2o2_m6o2_s9_9 = 0.00028878, ev
 p324_m3o2_m4o2_s2_2 = 0.00028878, ev
 p208_m3o1_m2o1_m6o2_s9_9 = 0.09583700, ev
 p325_m1o2_m6o2_s1_1 = 0.09583700, ev
 p326_m1o2_m6o2_s2_2 = 0.00028878, ev
 p219_m3o2_m6o2_s9_9 = 0.00028878, ev
 p230_m2o2_m7o1_m6o1_s9_9 = 0.09583700, ev
 p327_m4o2_m7o2_s1_1 = 0.09583700, ev
 p241_m3o1_m2o1_m7o1_m6o1_s9_9 = 0.00028878, ev
 p328_m4o2_m7o2_s2_2 = 0.00028878, ev
 p252_m3o2_m7o1_m6o1_s9_9 = 0.00037217, ev
 p329_m1o2_m2o2_s3_3 = 0.00037217, ev
 p330_m3o2_m4o2_s3_3 = 0.00037217, ev
 p129_m7o1_m6o3_s9_9 = 0.00037217, ev
 p331_m1o2_m6o2_s3_3 = 0.00037217, ev
 p140_m2o2_m7o2_s9_9 = 0.00037217, ev
 p151_m3o1_m2o1_m7o2_s9_9 = 0.00037217, ev
 p332_m4o2_m7o2_s3_3 = 0.00037217, ev

#ad-hoc functions

7o8T1 = -5.7967, ev
 7o8T2 = -0.2260
 7o8T3 = -0.0250
 7o8T2_2 = -1.1500
 gam14_cd2 = -0.0168, ev
 gam14_cd1 = 0.0477, ev

#coordinate shifts:

r0 = 16.668
 pi2 = 1.57079
 pi = 3.141593

#pulse parameters

dip_s1 = 1.0
 A = 2.7726

```

B    = A/pi
C    = B^0.5
s1   = 60.0, ev
width1 = 21.2, fs
zz = 16.0
omega1 = PEN, eV
std   = 6.8, fs
hwidth = 30,fs
t1    = 30,fs
tdip_s2_x = 0.1060
tdip_s2_y = -0.1060
tdip_s34_x = 0.2227
tdip_s34_y = 0.2227
tdip_s34_y = 0.2227
tdip_s56_x = 0.0569
tdip_s56_y = 0.0569
tdip_md5_s56_x = -0.04502
tdip_md5_s56_0 = 0.17

kk = 1.0, ev
end-parameter-section
LABELS-SECTION
pcap = CAP[55,0.0012900,3,1]
rstp = step[40]

```

```

# predissiation potential model (coupling folded)

```

```

v7m1 = acpot2[7K1_1,7K2_1,7K3_1,7K4_1,7K5_1,7K6_1,7K7_1,
7K8_1,7K9_1]
v8m1 = acpot2[8K1_1,8K2_1,8K3_1,8K4_1,8K5_1,8K6_1,8K7_1,
8K8_1,8K9_1]
v7m4 = acpot2[7K1_4,7K2_4,7K3_4,7K4_4,7K5_4,7K6_4,7K7_4,
7K8_4,7K9_4]
v8m4 = acpot2[8K1_4,8K2_4,8K3_4,8K4_4,8K5_4,8K6_4,8K7_4,
8K8_4,8K9_4]

```

```

#morse potential

```

```

v1m1 =morse1[1D_1,1A_1,1X_1,1E_1]
v1m4 =morse1[1D_4,1A_4,1X_4,1E_4]
v1m5 =morse1[1D_5,1A_5,1X_5,1E_5]
v2m1 =morse1[2D_1,2A_1,2X_1,2E_1]
v3m1 =morse1[3D_1,3A_1,3X_1,3E_1]
v4m1 =morse1[4D_1,4A_1,4X_1,4E_1]
v5m1 =morse1[5D_1,5A_1,5X_1,5E_1]
v6m1 =morse1[6D_1,6A_1,6X_1,6E_1]
v9m1 =morse1[9D_1,9A_1,9X_1,9E_1]
v10m1=morse1[10D_1,10A_1,10X_1,10E_1]
v2m4 =morse1[2D_4,2A_4,2X_4,2E_4]
v3m4 =morse1[3D_4,3A_4,3X_4,3E_4]
v4m4 =morse1[4D_4,4A_4,4X_4,4E_4]
v5m4 =morse1[5D_4,5A_4,5X_4,5E_4]
v6m4 =morse1[6D_4,6A_4,6X_4,6E_4]
v9m4 =morse1[9D_4,9A_4,9X_4,9E_4]
v10m4=morse1[10D_4,10A_4,10X_4,10E_4]
v2m5 =morse1[2D_5,2A_5,2X_5,2E_5]
v3m5 =morse1[3D_5,3A_5,3X_5,3E_5]
v4m5 =morse1[4D_5,4A_5,4X_5,4E_5]
v5m5 =morse1[5D_5,5A_5,5X_5,5E_5]
v6m5 =morse1[6D_5,6A_5,6X_5,6E_5]
v7m5 =morse1[7D_5,7A_5,7X_5,7E_5]
v8m5 =morse1[8D_5,8A_5,8X_5,8E_5]
v9m5 =morse1[9D_5,9A_5,9X_5,9E_5]
v10m5=morse1[10D_5,10A_5,10X_5,10E_5]

```

```

7o8Ttnh14 = tanh[7o8T2, r0]^1.0
7o8Ttnh55 = tanh[7o8T3,0.0]^1.0
7o8Ttnh14_2 = tanh[7o8T2_2,r0]^1.0

```

```

qp1 = q[pi]
qp2 = q[pi]^2
qp3 = q[pi]^3
qp4 = q[pi]^4

```

```

qq1 = q[pi2]
qq2 = q[pi2]^2
qq3 = q[pi2]^3
qq4 = q[pi2]^4

```

```

pstp = step[r0]
nstp = rstep[r0]

```

```

rqc2 = q[0.0]^~2
rq1 = q[r0]^1
rq2 = q[r0]^2

```

```

#cosm are defined in text as G(x)

```

```

#cosp = 2.0d0*(1.0d0-cos(aa*(x-x0))), aa= first entry, x0 = second entry

```

```

#cosm= 0.25d0*(cos(aa*(x-x0))+3.0d0)*stpf((x-x0),aa,.false.)*stpf
((x-x0),-aa,.true.) + &
# 0.5d0*(stpf((x-x0),aa,.true.) + stpf((x-x0),-aa,.false.))
# where stpf(,,true./.false.) and forward/backward step functions. a
a= first entry, x0= second entry

```

```

cosm29_1 = cosm[p29,pi]
cosm29_2 = cosm[p29,pi2]
cosm30_1 = cosm[p30,pi]
cosm30_2 = cosm[p30,pi2]
cosm31_1 = cosm[p31,pi]
cosm31_2 = cosm[p31,pi2]
cosm32_1 = cosm[p32,pi]
cosm32_2 = cosm[p32,pi2]
cosm36_1 = cosm[p36,pi]
cosm36_2 = cosm[p36,pi2]
cosm40_1 = cosm[p40,pi]
cosm40_2 = cosm[p40,pi2]
cosm44_1 = cosm[p44,pi]
cosm44_2 = cosm[p44,pi2]
cosm25_1 = cosm[p25,pi]
cosm25_2 = cosm[p25,pi2]
cosm26_1 = cosm[p26,pi]
cosm26_2 = cosm[p26,pi2]
cosm27_2 = cosm[p27,pi2]
cosm27_1 = cosm[p27,pi]
cosm28_2 = cosm[p28,pi2]
cosm28_1 = cosm[p28,pi]
cosm48_1 = cosm[p48,pi]
cosm48_2 = cosm[p48,pi2]
cosm52_1 = cosm[p52,pi]
cosm52_2 = cosm[p52,pi2]
cosm56_1 = cosm[p56,pi]
cosm56_2 = cosm[p56,pi2]
cosm60_2 = cosm[p60,pi2]
cosm60_1 = cosm[p60,pi]

```

```

cosp3_1 = cosp[p3,pi]
cosp3_2 = cosp[p3,pi2]
cosp6_1 = cosp[p6,pi]
cosp6_2 = cosp[p6,pi2]
cosp9_1 = cosp[p9,pi]
cosp9_2 = cosp[p9,pi2]
cosp12_1 = cosp[p12,pi]
cosp12_2 = cosp[p12,pi2]
cosp35_1 = cosp[p35,pi]
cosp35_2 = cosp[p35,pi2]
cosp39_1 = cosp[p39,pi]
cosp39_2 = cosp[p39,pi2]
cosp43_1 = cosp[p43,pi]
cosp43_2 = cosp[p43,pi2]

```

```

sin15_2 = sin[p15,pi2]
sin15_1 = sin[p15,pi]
sin18_2 = sin[p18,pi2]
sin18_1 = sin[p18,pi]
sin21_2 = sin[p21,pi2]
sin21_1 = sin[p21,pi]
sin24_2 = sin[p24,pi2]
sin24_1 = sin[p24,pi]
sin47_2 = sin[p47,pi2]
sin47_1 = sin[p47,pi]
sin51_2 = sin[p51,pi2]
sin51_1 = sin[p51,pi]
sin55_2 = sin[p55,pi2]
sin55_1 = sin[p55,pi]
sin59_2 = sin[p59,pi2]
sin59_1 = sin[p59,pi]

```

```

tanh2 = tanh[p2 ,r0]
tanh5 = tanh[p5 ,r0]
tanh8 = tanh[p8 ,r0]
tanh11 = tanh[p11,r0]
tanh34 = tanh[p34,r0]
tanh14 = tanh[p14,r0]
tanh17 = tanh[p17,r0]
tanh20 = tanh[p20,r0]
tanh23 = tanh[p23,r0]
tanh38 = tanh[p38,r0]
tanh42 = tanh[p42,r0]
tanh46 = tanh[p46,r0]
tanh50 = tanh[p50,r0]
tanh54 = tanh[p54,r0]
tanh58 = tanh[p58,r0]

```

```

#pulse functions
pulse1 = gauss[A/width1^2,t1]
cosom1 = cos[omega1,t1]
step1 = step[-hwidth+t1]
rstep1 = rstep[hwidth+t1]

```

```

end-labels-section
end-parameter-section
LABELS-SECTION

```

```
#####
## SUPPLEMENTARY INFORMATION B
#####
#####
## HAMILTONIAN SECTION
#####
```

HAMILTONIAN-SECTION

```
-----
modes| v1 | v2 | v3 | v4 | v5 | v6 | v7 | el
-----
```

```
#pulse exciting the x-plane
-tdip_s2_x*s1*C/zz |2 qq1 |8 S1&2 |9 cosom1*pulse1*step1*rstep1
tdip_s2_x*s1*C/zz |3 qq1 |8 S1&2 |9 cosom1*pulse1*step1*rstep1
```

```
-tdip_s34_x*s1*C/zz |2 qq1 |8 S1&4 |9 cosom1*pulse1*step1*rstep1
tdip_s34_x*s1*C/zz |3 qq1 |8 S1&4 |9 cosom1*pulse1*step1*rstep1
-tdip_s34_x*s1*C/zz |6 qp1 |8 S1&3 |9 cosom1*pulse1*step1*rstep1
tdip_s34_x*s1*C/zz |7 qp1 |8 S1&3 |9 cosom1*pulse1*step1*rstep1
```

```
#kinetic energy
kk |5 KE
-kk*0.5 |1 dq^2
kk*0.5 |1 rqc2 |2 j^2
-kk*0.5 |4 dq^2
kk*0.5 |4 rqc2 |3 j^2
```

#S0:

E1 8 S1&1		
1.0 1 v1m1 8 S1&1		
1.0 4 v1m4 8 S1&1		
1.0 5 v1m5 8 S1&1		
1.000000*p1_m1o1_m4o1_s0_0	1 q^1 4 q^1	8 S1&1
0.041160*p2_m2o4_s0_0	2 q^4	8 S1&1
0.041160*p3_m3o4_s0_0	3 q^4	8 S1&1
0.041160*p4_m6o4_s0_0	6 q^4	8 S1&1
0.041160*p5_m7o4_s0_0	7 q^4	8 S1&1
0.500000*p6_m2o2_s0_0	2 q^2	8 S1&1
0.500000*p7_m3o2_s0_0	3 q^2	8 S1&1
0.500000*p8_m6o2_s0_0	6 q^2	8 S1&1
0.500000*p9_m7o2_s0_0	7 q^2	8 S1&1
1.000000*p10_m3o1_m2o3_s0_0	3 q^1 2 q^3	8 S1&1
1.000000*p11_m3o2_m2o2_s0_0	3 q^2 2 q^2	8 S1&1
1.000000*p12_m3o3_m2o1_s0_0	3 q^3 2 q^1	8 S1&1
1.000000*p13_m7o1_m6o3_s0_0	7 q^1 6 q^3	8 S1&1
1.000000*p14_m7o2_m6o2_s0_0	7 q^2 6 q^2	8 S1&1
1.000000*p15_m7o3_m6o1_s0_0	7 q^3 6 q^1	8 S1&1
1.000000*p16_m3o1_m2o1_s0_0	3 q^1 2 q^1	8 S1&1
1.000000*p17_m7o1_m6o1_s0_0	7 q^1 6 q^1	8 S1&1

#caps for dissociating coordinates

```
1.0 |1 pcap |8 S7&7
1.0 |4 pcap |8 S8&8
1.0 |4 pcap |8 S7&7
1.0 |1 pcap |8 S8&8
1.0 |1 pcap |8 S2&2
1.0 |4 pcap |8 S2&2
1.0 |4 pcap |8 S3&3
1.0 |1 pcap |8 S3&3
1.0 |4 pcap |8 S4&4
1.0 |1 pcap |8 S4&4
```

```

1.0 |4 pcap |8 S5&5
1.0 |1 pcap |8 S5&5
1.0 |4 pcap |8 S6&6
1.0 |1 pcap |8 S6&6
1.0 |4 pcap |8 S10&10
1.0 |1 pcap |8 S10&10
1.0 |4 pcap |8 S9&9
1.0 |1 pcap |8 S9&9

```

#vertical energies

```

E2 |8 S2&2
E3 |8 S3&3
E4 |8 S4&4
E5 |8 S5&5
E6 |8 S6&6
E7 |8 S7&7
E8 |8 S8&8
E9 |8 S9&9
E10 |8 S10&10

```

#morse potential for radial coordinates (1,4) and cc stretch

```

1.0 |1 v2m1 |8 S2&2
1.0 |1 v3m1 |8 S3&3
1.0 |1 v4m1 |8 S4&4
1.0 |1 v5m1 |8 S5&5
1.0 |1 v6m1 |8 S6&6
1.0 |1 v9m1 |8 S9&9
1.0 |1 v10m1 |8 S10&10
1.0 |4 v2m4 |8 S2&2
1.0 |4 v3m4 |8 S3&3
1.0 |4 v4m4 |8 S4&4
1.0 |4 v5m4 |8 S5&5
1.0 |4 v6m4 |8 S6&6
1.0 |4 v9m4 |8 S9&9
1.0 |4 v10m4 |8 S10&10
1.0 |5 v2m5 |8 S2&2
1.0 |5 v3m5 |8 S3&3
1.0 |5 v4m5 |8 S4&4
1.0 |5 v5m5 |8 S5&5
1.0 |5 v6m5 |8 S6&6
1.0 |5 v7m5 |8 S7&7
1.0 |5 v8m5 |8 S8&8
1.0 |5 v9m5 |8 S9&9
1.0 |5 v10m5 |8 S10&10
1.0 |1 v7m1 |8 S7&7
1.0 |1 v8m1 |8 S8&8
1.0 |4 v7m4 |8 S7&7
1.0 |4 v8m4 |8 S8&8

```

terms coupling radial dissociation coordinates

```

1.000000*p1_m1o1_m4o1_s1_1 |1 rq1 |4 rq1 |8 S2&2
1.000000*p2_m1o1_m4o1_s2_2 |1 rq1 |4 rq1 |8 S3&3
1.000000*p3_m1o1_m4o1_s3_3 |1 rq1 |4 rq1 |8 S4&4

```

#ad-hoc functions

```

1.000000*gam14_cd1 |1 pstp*rq1 |4 pstp*rq1 |8 S7&7
1.000000*gam14_cd1 |1 pstp*rq1 |4 pstp*rq1 |8 S8&8
1.000000*gam14_cd2 |1 nstp*rq1 |4 pstp*rq1 |8 S7&7
1.000000*gam14_cd2 |1 nstp*rq1 |4 pstp*rq1 |8 S8&8
1.000000*gam14_cd2 |1 pstp*rq1 |4 nstp*rq1 |8 S8&8
1.000000*gam14_cd2 |1 pstp*rq1 |4 nstp*rq1 |8 S7&7
1.000000*7o8T1 |1 7o8Ttnh14 |5 7o8Ttnh55 |4 nstp*7o8Ttnh14_2 |8 S6&6

```

```

1.000000*7o8T1 |4 7o8Ttnh14 |5 7o8Ttnh55 |1 nstp*7o8Ttnh14_2 |8 S6&6
1.000000*7o8T1 |4 7o8Ttnh14 |5 7o8Ttnh55 |1 nstp*7o8Ttnh14_2 |8 S7&7
1.000000*7o8T1 |1 7o8Ttnh14 |5 7o8Ttnh55 |4 nstp*7o8Ttnh14_2 |8 S7&7

```

```

#terms coupling dissociating radial coordinates to Renner-Teller 4D subspace
#cosp = 2.0d0*(1.0d0-cos(aa*(x-x0))), aa= first entry, x0 = second entry

```

```

#cosm= 0.25d0*(cos(aa*(x-x0))+3.0d0)*stp((x-x0),aa,.false.)*stp((x-x0),-aa,true.) + &
# 0.5d0*(stp((x-x0),aa,true.) + stp((x-x0),-aa,.false.))
# where stp(,true./.false.) and forward/backward step functions. aa= first entry, x0= second entry

```

```

+p1 |1 tanh2 |2 cosp3_2 |6 cosm29_1 |8 S7&7
+p1 |1 tanh2 |6 cosp3_1 |2 cosm29_2 |8 S8&8
+p1 |4 tanh2 |7 cosp3_1 |3 cosm29_2 |8 S8&8
+p1 |4 tanh2 |3 cosp3_2 |7 cosm29_1 |8 S7&7
+p4 |1 tanh5 |2 cosp6_2 |6 cosm30_1 |8 S8&8
+p4 |1 tanh5 |6 cosp6_1 |2 cosm30_2 |8 S7&7
+p4 |4 tanh5 |7 cosp6_1 |3 cosm30_2 |8 S7&7
+p4 |4 tanh5 |3 cosp6_2 |7 cosm30_1 |8 S8&8
+p7 |1 tanh8 |2 cosp9_2 |6 cosm31_1 |8 S2&2
+p7 |1 tanh8 |6 cosp9_1 |2 cosm31_2 |8 S2&2
+p7 |4 tanh8 |7 cosp9_1 |3 cosm31_2 |8 S2&2
+p7 |4 tanh8 |3 cosp9_2 |7 cosm31_1 |8 S2&2
+p10 |1 tanh11 |2 cosp12_2 |6 cosm32_1 |8 S4&4
+p10 |1 tanh11 |6 cosp12_1 |2 cosm32_2 |8 S4&4
+p10 |4 tanh11 |7 cosp12_1 |3 cosm32_2 |8 S4&4
+p10 |4 tanh11 |3 cosp12_2 |7 cosm32_1 |8 S4&4
+p33 |1 tanh34 |2 cosp35_2 |6 cosm36_1 |8 S3&3
+p33 |1 tanh34 |6 cosp35_1 |2 cosm36_2 |8 S3&3
+p33 |4 tanh34 |7 cosp35_1 |3 cosm36_2 |8 S3&3
+p33 |4 tanh34 |3 cosp35_2 |7 cosm36_1 |8 S3&3
+p37 |1 tanh38 |2 cosp39_2 |6 cosm40_1 |8 S5&5
+p37 |1 tanh38 |6 cosp39_1 |2 cosm40_2 |8 S6&6
+p37 |4 tanh38 |7 cosp39_1 |3 cosm40_2 |8 S6&6
+p37 |4 tanh38 |3 cosp39_2 |7 cosm40_1 |8 S5&5
+p41 |1 tanh42 |2 cosp43_2 |6 cosm44_1 |8 S6&6
+p41 |1 tanh42 |6 cosp43_1 |2 cosm44_2 |8 S5&5
+p41 |4 tanh42 |7 cosp43_1 |3 cosm44_2 |8 S5&5
+p41 |4 tanh42 |3 cosp43_2 |7 cosm44_1 |8 S6&6
+p13 |1 tanh14 |2 sin15_2 |6 cosm25_1 |8 S2&7
-p13 |4 tanh14 |3 sin15_2 |7 cosm25_1 |8 S2&7
-p13 |1 tanh14 |6 sin15_1 |2 cosm25_2 |8 S2&8
+p13 |4 tanh14 |7 sin15_1 |3 cosm25_2 |8 S2&8
-p16 |4 tanh17 |3 sin18_2 |7 cosm26_1 |8 S3&7
+p16 |1 tanh17 |2 sin18_2 |6 cosm26_1 |8 S3&7
+p16 |1 tanh17 |6 sin18_1 |2 cosm26_2 |8 S3&8
-p16 |4 tanh17 |7 sin18_1 |3 cosm26_2 |8 S3&8
-p16 |4 tanh17 |3 sin18_2 |7 cosm26_1 |8 S4&8
+p16 |1 tanh17 |2 sin18_2 |6 cosm26_1 |8 S4&8
+p16 |4 tanh17 |7 sin18_1 |3 cosm26_2 |8 S4&7
-p16 |1 tanh17 |6 sin18_1 |2 cosm26_2 |8 S4&7
+p19 |4 tanh20 |2 sin21_2 |6 cosm27_1 |8 S2&7
-p19 |1 tanh20 |3 sin21_2 |7 cosm27_1 |8 S2&7
-p19 |4 tanh20 |6 sin21_1 |2 cosm27_2 |8 S2&8
+p19 |1 tanh20 |7 sin21_1 |3 cosm27_2 |8 S2&8
-p22 |1 tanh23 |3 sin24_2 |7 cosm28_1 |8 S3&7
+p22 |4 tanh23 |2 sin24_2 |6 cosm28_1 |8 S3&7
+p22 |4 tanh23 |6 sin24_1 |2 cosm28_2 |8 S3&8
-p22 |1 tanh23 |7 sin24_1 |3 cosm28_2 |8 S3&8
-p22 |1 tanh23 |3 sin24_2 |7 cosm28_1 |8 S4&8
+p22 |4 tanh23 |2 sin24_2 |6 cosm28_1 |8 S4&8
+p22 |1 tanh23 |7 sin24_1 |3 cosm28_2 |8 S4&7

```

-p22	4 tanh23	6 sin24_1	2 cosm28_2	8	S4&7
+p45	4 tanh46	3 sin47_2	7 cosm48_1	8	S2&6
+p45	1 tanh46	2 sin47_2	6 cosm48_1	8	S2&6
-p45	1 tanh46	6 sin47_1	2 cosm48_2	8	S2&5
-p45	4 tanh46	7 sin47_1	3 cosm48_2	8	S2&5
+p49	1 tanh50	3 sin51_2	7 cosm52_1	8	S2&6
+p49	4 tanh50	2 sin51_2	6 cosm52_1	8	S2&6
-p49	4 tanh50	6 sin51_1	2 cosm52_2	8	S2&5
-p49	1 tanh50	7 sin51_1	3 cosm52_2	8	S2&5
+p53	4 tanh54	3 sin55_2	7 cosm56_1	8	S3&6
+p53	1 tanh54	2 sin55_2	6 cosm56_1	8	S3&6
+p53	1 tanh54	6 sin55_1	2 cosm56_2	8	S3&5
+p53	4 tanh54	7 sin55_1	3 cosm56_2	8	S3&5
+p53	4 tanh54	3 sin55_2	7 cosm56_1	8	S4&5
+p53	1 tanh54	2 sin55_2	6 cosm56_1	8	S4&5
-p53	4 tanh54	7 sin55_1	3 cosm56_2	8	S4&6
-p53	1 tanh54	6 sin55_1	2 cosm56_2	8	S4&6
+p57	1 tanh58	3 sin59_2	7 cosm60_1	8	S3&6
+p57	4 tanh58	2 sin59_2	6 cosm60_1	8	S3&6
+p57	4 tanh58	6 sin59_1	2 cosm60_2	8	S3&5
+p57	1 tanh58	7 sin59_1	3 cosm60_2	8	S3&5
+p57	1 tanh58	3 sin59_2	7 cosm60_1	8	S4&5
+p57	4 tanh58	2 sin59_2	6 cosm60_1	8	S4&5
-p57	1 tanh58	7 sin59_1	3 cosm60_2	8	S4&6
-p57	4 tanh58	6 sin59_1	2 cosm60_2	8	S4&6

bounded polynomial terms coupling radial dissociation coordinates (1,4) and 4D Renner–Teller subspace

1.000000*p321_m1o2_m2o2_s1_1	1 rq2	2 qq2	8	S2&2
1.000000*p322_m1o2_m2o2_s2_2	1 rq2	2 qq2	8	S3&3
1.000000*p323_m3o2_m4o2_s1_1	3 qq2	4 rq2	8	S2&2
1.000000*p324_m3o2_m4o2_s2_2	3 qq2	4 rq2	8	S3&3
1.000000*p325_m1o2_m6o2_s1_1	1 rq2	6 qp2	8	S2&2
1.000000*p326_m1o2_m6o2_s2_2	1 rq2	6 qp2	8	S3&3
1.000000*p327_m4o2_m7o2_s1_1	4 rq2	7 qp2	8	S2&2
1.000000*p328_m4o2_m7o2_s2_2	4 rq2	7 qp2	8	S3&3
1.000000*p329_m1o2_m2o2_s3_3	1 rq2	2 qq2	8	S4&4
1.000000*p330_m3o2_m4o2_s3_3	3 qq2	4 rq2	8	S4&4
1.000000*p331_m1o2_m6o2_s3_3	1 rq2	6 qp2	8	S4&4
1.000000*p332_m4o2_m7o2_s3_3	4 rq2	7 qp2	8	S4&4
1.000000*p1_m1o1_m4o1_s1_1	1 rq1	4 rq1	8	S2&2
1.000000*p2_m1o1_m4o1_s2_2	1 rq1	4 rq1	8	S3&3
1.000000*p3_m1o1_m4o1_s3_3	1 rq1	4 rq1	8	S4&4

4D Renner–Teller subspace model

1.000000*p4_m3o1_m2o1_s1_2	3 qq1	2 qq1	8	S2&3
1.000000*p5_m2o1_m6o1_s1_3	2 qq1	6 qp1	8	S2&4
1.000000*p6_m2o1_m6o1_s1_8	2 qq1	6 qp1	8	S2&9
1.000000*p7_m2o1_m6o1_s4_5	2 qq1	6 qp1	8	S5&6
1.000000*p8_m2o1_m6o1_s4_6	2 qq1	6 qp1	8	S5&7
1.000000*p9_m2o1_m6o1_s5_7	2 qq1	6 qp1	8	S6&8
1.000000*p10_m2o1_m6o1_s6_7	2 qq1	6 qp1	8	S7&8
1.000000*p11_m2o1_m7o1_s1_3	2 qq1	7 qp1	8	S2&4
1.000000*p12_m2o1_m7o1_s2_8	2 qq1	7 qp1	8	S3&9
1.000000*p13_m2o1_m7o1_s3_9	2 qq1	7 qp1	8	S4&10
1.000000*p14_m2o1_m7o1_s4_5	2 qq1	7 qp1	8	S5&6
1.000000*p15_m2o1_m7o1_s4_6	2 qq1	7 qp1	8	S5&7
1.000000*p16_m2o1_m7o1_s5_7	2 qq1	7 qp1	8	S6&8
1.000000*p17_m2o1_m7o1_s6_7	2 qq1	7 qp1	8	S7&8
1.000000*p18_m3o1_m6o1_s1_3	3 qq1	6 qp1	8	S2&4
1.000000*p19_m3o1_m6o1_s2_8	3 qq1	6 qp1	8	S3&9
1.000000*p20_m3o1_m6o1_s3_9	3 qq1	6 qp1	8	S4&10
1.000000*p21_m3o1_m6o1_s4_5	3 qq1	6 qp1	8	S5&6

1.000000*p22_m3o1_m6o1_s4_6	3 qq1 6 qp1	8 S5&7
1.000000*p23_m3o1_m6o1_s5_7	3 qq1 6 qp1	8 S6&8
1.000000*p24_m3o1_m6o1_s6_7	3 qq1 6 qp1	8 S7&8
1.000000*p25_m3o1_m7o1_s1_3	3 qq1 7 qp1	8 S2&4
1.000000*p26_m3o1_m7o1_s1_8	3 qq1 7 qp1	8 S2&9
1.000000*p27_m3o1_m7o1_s4_5	3 qq1 7 qp1	8 S5&6
1.000000*p28_m3o1_m7o1_s4_6	3 qq1 7 qp1	8 S5&7
1.000000*p29_m3o1_m7o1_s5_7	3 qq1 7 qp1	8 S6&8
1.000000*p30_m3o1_m7o1_s6_7	3 qq1 7 qp1	8 S7&8
1.000000*p31_m7o1_m6o1_s1_2	7 qp1 6 qp1	8 S2&3
0.041160*p32_m2o4_s9_9	2 qq4	8 S10&10
0.041160*p33_m2o4_s1_1	2 qq4	8 S2&2
0.041160*p34_m2o4_s2_2	2 qq4	8 S3&3
0.041160*p35_m2o4_s3_3	2 qq4	8 S4&4
0.041160*p36_m2o4_s4_4	2 qq4	8 S5&5
0.041160*p37_m2o4_s5_5	2 qq4	8 S6&6
0.041160*p38_m2o4_s6_6	2 qq4	8 S7&7
0.041160*p39_m2o4_s7_7	2 qq4	8 S8&8
0.041160*p40_m2o4_s8_8	2 qq4	8 S9&9
0.041160*p41_m3o4_s9_9	3 qq4	8 S10&10
0.041160*p42_m3o4_s1_1	3 qq4	8 S2&2
0.041160*p43_m3o4_s2_2	3 qq4	8 S3&3
0.041160*p44_m3o4_s3_3	3 qq4	8 S4&4
0.041160*p45_m3o4_s4_4	3 qq4	8 S5&5
0.041160*p46_m3o4_s5_5	3 qq4	8 S6&6
0.041160*p47_m3o4_s6_6	3 qq4	8 S7&7
0.041160*p48_m3o4_s7_7	3 qq4	8 S8&8
0.041160*p49_m3o4_s8_8	3 qq4	8 S9&9
0.041160*p50_m6o4_s9_9	6 qp4	8 S10&10
0.041160*p51_m6o4_s1_1	6 qp4	8 S2&2
0.041160*p52_m6o4_s2_2	6 qp4	8 S3&3
0.041160*p53_m6o4_s3_3	6 qp4	8 S4&4
0.041160*p54_m6o4_s4_4	6 qp4	8 S5&5
0.041160*p55_m6o4_s5_5	6 qp4	8 S6&6
0.041160*p56_m6o4_s6_6	6 qp4	8 S7&7
0.041160*p57_m6o4_s7_7	6 qp4	8 S8&8
0.041160*p58_m6o4_s8_8	6 qp4	8 S9&9
0.041160*p59_m7o4_s9_9	7 qp4	8 S10&10
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1.000000*p275_m7o1_m6o1_s3_3	7 qp1	6 qp1	8 S4&4
1.000000*p276_m7o1_m6o1_s4_4	7 qp1	6 qp1	8 S5&5
1.000000*p277_m7o1_m6o1_s5_5	7 qp1	6 qp1	8 S6&6
1.000000*p278_m7o1_m6o1_s6_6	7 qp1	6 qp1	8 S7&7
1.000000*p279_m7o1_m6o1_s7_7	7 qp1	6 qp1	8 S8&8
1.000000*p280_m7o1_m6o1_s8_8	7 qp1	6 qp1	8 S9&9
1.000000*p281_m2o1_s1_5	2 qq1		8 S2&6
1.000000*p282_m2o1_s1_6	2 qq1		8 S2&7
1.000000*p283_m2o1_s2_5	2 qq1		8 S3&6
1.000000*p284_m2o1_s2_6	2 qq1		8 S3&7
1.000000*p285_m2o1_s3_4	2 qq1		8 S4&5
1.000000*p286_m2o1_s3_7	2 qq1		8 S4&8
1.000000*p287_m2o1_s4_8	2 qq1		8 S5&9
1.000000*p288_m2o1_s5_9	2 qq1		8 S6&10
1.000000*p289_m2o1_s6_9	2 qq1		8 S7&10
1.000000*p290_m2o1_s7_8	2 qq1		8 S8&9
1.000000*p291_m3o1_s1_5	3 qq1		8 S2&6
1.000000*p292_m3o1_s1_6	3 qq1		8 S2&7
1.000000*p293_m3o1_s2_5	3 qq1		8 S3&6
1.000000*p294_m3o1_s2_6	3 qq1		8 S3&7
1.000000*p295_m3o1_s3_4	3 qq1		8 S4&5
1.000000*p296_m3o1_s3_7	3 qq1		8 S4&8
1.000000*p297_m3o1_s4_8	3 qq1		8 S5&9
1.000000*p298_m3o1_s5_9	3 qq1		8 S6&10
1.000000*p299_m3o1_s6_9	3 qq1		8 S7&10
1.000000*p300_m3o1_s7_8	3 qq1		8 S8&9
1.000000*p301_m6o1_s1_4	6 qp1		8 S2&5
1.000000*p302_m6o1_s1_7	6 qp1		8 S2&8
1.000000*p303_m6o1_s2_4	6 qp1		8 S3&5
1.000000*p304_m6o1_s2_7	6 qp1		8 S3&8
1.000000*p305_m6o1_s3_5	6 qp1		8 S4&6
1.000000*p306_m6o1_s3_6	6 qp1		8 S4&7
1.000000*p307_m6o1_s4_9	6 qp1		8 S5&10
1.000000*p308_m6o1_s5_8	6 qp1		8 S6&9
1.000000*p309_m6o1_s6_8	6 qp1		8 S7&9
1.000000*p310_m6o1_s7_9	6 qp1		8 S8&10
1.000000*p311_m7o1_s1_4	7 qp1		8 S2&5
1.000000*p312_m7o1_s1_7	7 qp1		8 S2&8
1.000000*p313_m7o1_s2_4	7 qp1		8 S3&5
1.000000*p314_m7o1_s2_7	7 qp1		8 S3&8
1.000000*p315_m7o1_s3_5	7 qp1		8 S4&6
1.000000*p316_m7o1_s3_6	7 qp1		8 S4&7
1.000000*p317_m7o1_s4_9	7 qp1		8 S5&10
1.000000*p318_m7o1_s5_8	7 qp1		8 S6&9
1.000000*p319_m7o1_s6_8	7 qp1		8 S7&9
1.000000*p320_m7o1_s7_9	7 qp1		8 S8&10

END-HAMILTONIAN-SECTION

END-OPERATOR

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