

## Supplementary Material

# Excited States of Bromopyrimidines Probed by VUV Photoabsorption Spectroscopy and Theoretical Calculations

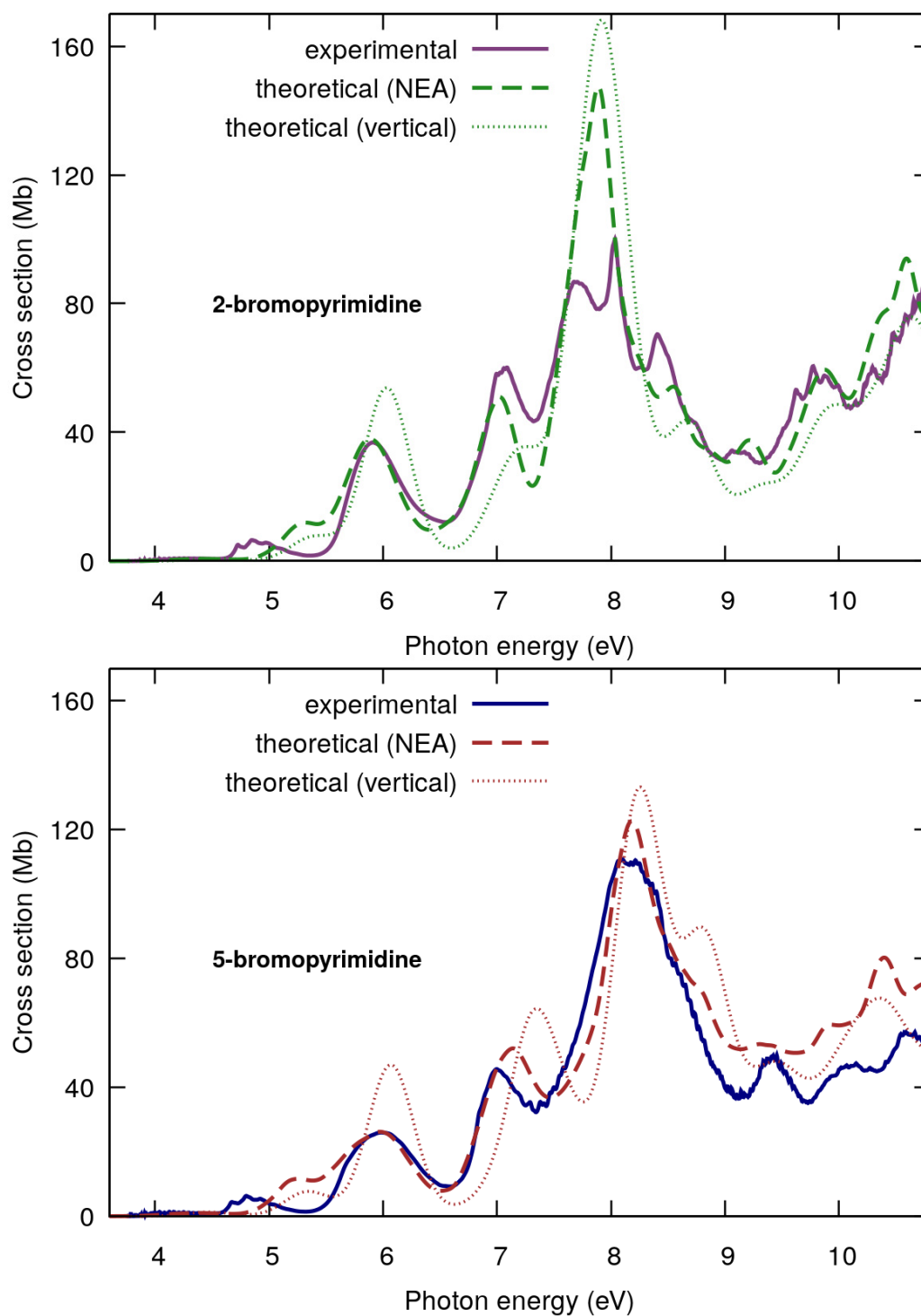
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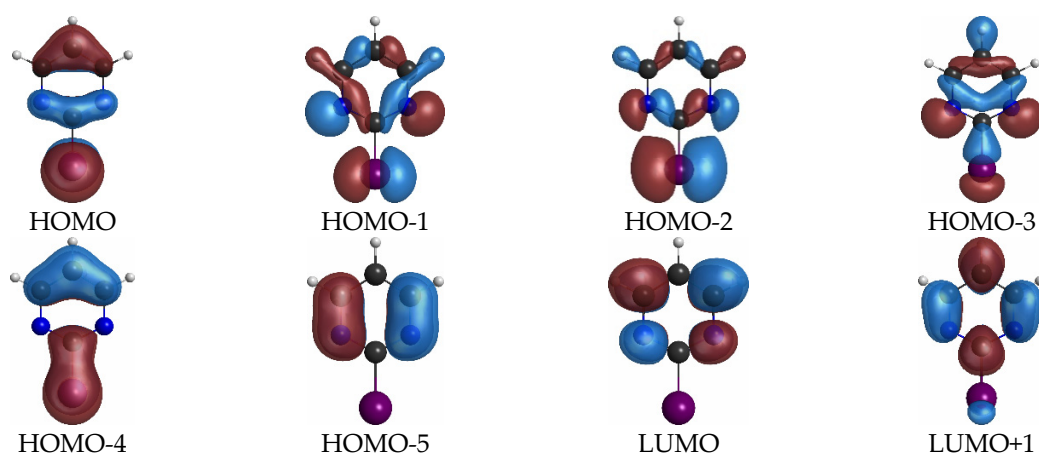
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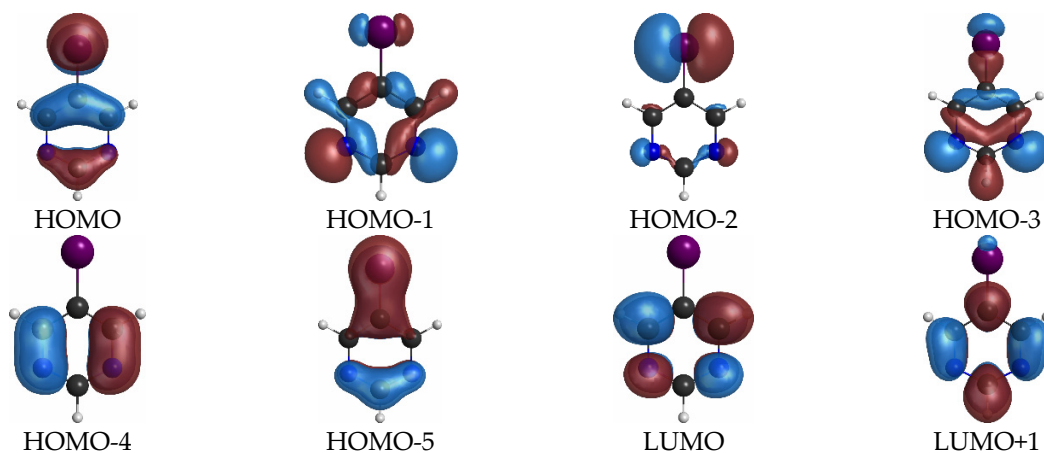
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**Figure S1.** Comparison between measured and theoretical absorption cross sections for 2-bromopyrimidine (top) and 5-bromopyrimidine (bottom), the latter computed with the vertical approximation (for an arbitrary linewidth of 0.4 eV) and with the nuclear ensemble approach (NEA).



**Figure S2.** The frontier canonical orbitals for 2-bromopyrimidine.



**Figure S3.** The frontier canonical orbitals for 5-bromopyrimidine.

Set of geometries optimized at the CAM-B3LYP/aug-cc-pVDZ+2s2p2d level of theory:

Ground state ( $S_0$ ) geometry (in angstrom) of 2-bromopyrimidine

```

C  0.000000  0.000000 -0.144547
N  0.000000  1.189023 -0.724716
N  0.000000 -1.189023 -0.724716
C  0.000000  1.180041 -2.058947
C  0.000000 -1.180041 -2.058947
C  0.000000  0.000000 -2.791483
H  0.000000  2.155443 -2.548233
H  0.000000 -2.155443 -2.548233
H  0.000000  0.000000 -3.879105

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Br 0.000000 0.000000 1.755575

First excited state ( $S_1$ ) geometry (in angstrom) of 2-bromopyrimidine

C 0.000000 0.000000 -0.086024

N 0.000000 1.119786 -0.750749

N 0.000000 -1.119786 -0.750749

C 0.000000 1.192639 -2.129466

C 0.000000 -1.192639 -2.129466

C 0.000000 0.000000 -2.844207

H 0.000000 2.178314 -2.583072

H 0.000000 -2.178314 -2.583072

H 0.000000 0.000000 -3.933463

Br 0.000000 0.000000 1.792716

Ground state ( $S_0$ ) geometry (in angstrom) of 5-bromopyrimidine

C 0.000000 0.000000 -2.764489

N 0.000000 1.189493 -2.166023

N 0.000000 -1.189493 -2.166023

C 0.000000 1.189164 -0.834710

C 0.000000 -1.189164 -0.834710

C 0.000000 0.000000 -0.115937

H 0.000000 2.155526 -0.328742

H 0.000000 -2.155526 -0.328742

Br 0.000000 0.000000 1.775297

H 0.000000 0.000000 -3.854496

First excited state ( $S_1$ ) geometry (in angstrom) of 5-bromopyrimidine

C 0.196112 2.857635 0.000000

N 1.241155 2.085856 0.000000

N -0.997666 2.259002 0.000000

C 1.269757 0.721378 0.000000

C -1.124591 0.886310 0.000000

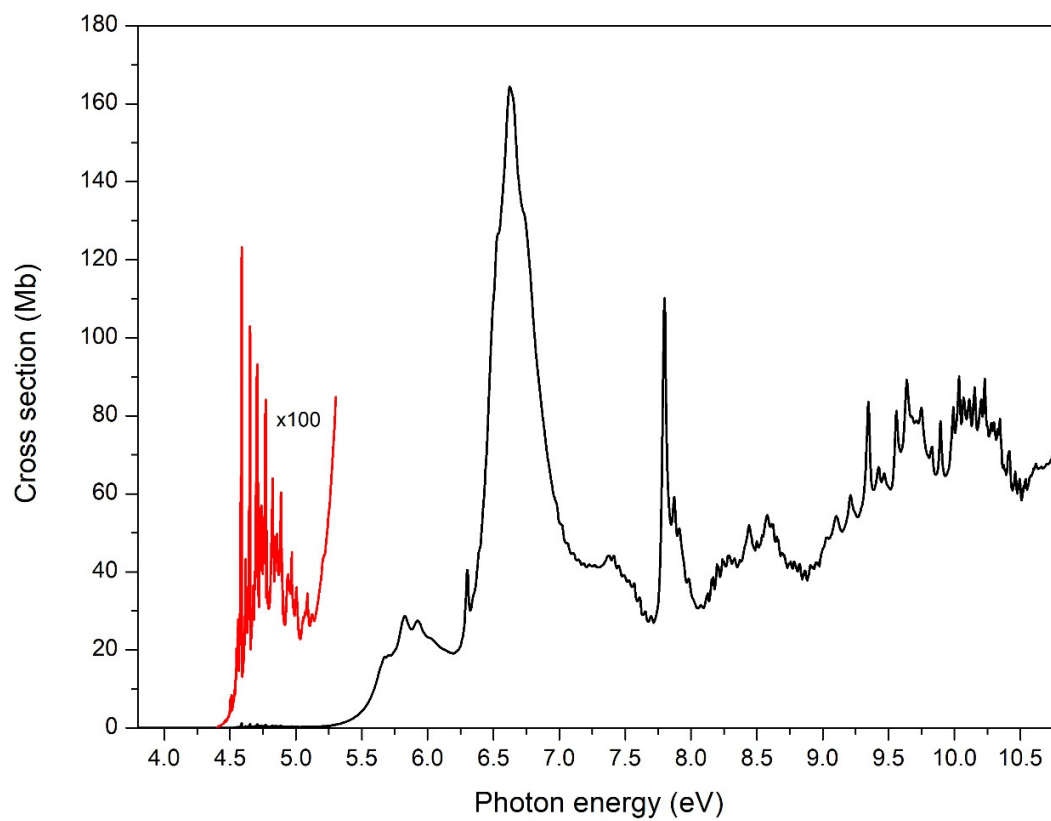
C 0.000000 0.099947 0.000000

H 2.219114 0.201108 0.000000

H -2.130184 0.475844 0.000000

Br -0.117817 -1.783517 0.000000

H 0.282577 3.940519 0.000000



**Figure S4.** High-resolution VUV photoabsorption spectrum of bromobenzene in the 3.7–10.8 eV photon energy range. The original data was kindly provided by Palmer et al. [47] and can also be found online in the MPI-Mainz UV/VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest ([www.uv-vis-spectral-atlas-mainz.org](http://www.uv-vis-spectral-atlas-mainz.org)).

**Table S1.** Ground state ( $S_0$ ) frequencies (in  $\text{cm}^{-1}$ ) of 2-bromopyrimidine.

	Symmetry	Harmonic freq.	Anharmonic freq.	Character
1	a <sub>1</sub>	3243.7	3114.9	H's stretching
2		3196.2	3065.5	H's stretching
3		1645.4	1606.5	ring stretching
4		1439.1	1413.1	ring stretching / H's symmetric rocking
5		1196.5	1178.0	ring stretching / H's symmetric rocking
6		1104.5	1090.0	ring stretching
7		1019.3	1005.9	ring stretching
8		756.9	748.9	ring stretching
9		336.7	336.6	C-Br stretching
10	a <sub>2</sub>	1019.6	992.5	H's twisting
11		419.5	410.2	ring deformation
12	b <sub>1</sub>	1024.3	998.4	H's wagging/twisting
13		823.8	810.5	H's wagging
14		803.8	787.5	ring deformation
15		486.3	476.1	ring deformation
16		150.9	150.9	Br wagging (out-of-plane)
17	b <sub>2</sub>	3199.3	3083.5	H's stretching
18		1638.2	1596.1	ring stretching
19		1467.8	1442.8	ring stretching / H's symmetric rocking
20		1299.7	1282.4	H's asymmetric rocking
21		1244.1	1200.9	ring stretching
22		1115.4	1101.7	H rocking
23		637.6	633.0	ring deformation
24		274.5	273.4	Br rocking (in-plane)

**Table S2.** First excited state ( $S_0$ ) frequencies (in  $\text{cm}^{-1}$ ) of 2-bromopyrimidine.

	Symmetry	Harmonic freq.	Anharmonic freq.	Character
1	a <sub>1</sub>	3267.9	3135.3	H's stretching
2		3225.8	3096.7	H's stretching
3		1530.7	1497.1	ring stretching
4		1439.3	1411.8	ring stretching / H's symmetric rocking
5		1163.9	1145.3	ring stretching / H's symmetric rocking
6		1071.6	1057.4	ring stretching
7		968.1	955.3	ring stretching
8		728.6	720.9	ring stretching
9		330.5	330.3	C-Br stretching
10	a <sub>2</sub>	598.4	582.5	H's twisting
11		232.4	227.0	ring deformation
12	b <sub>1</sub>	934.9	914.8	H wagging
13		709.3	695.2	H's wagging / ring deformation
14		549.1	538.0	ring deformation
15		481.3	471.5	ring deformation
16		168.9	168.8	Br wagging (out-of-plane)
17	b <sub>2</sub>	3254.4	3136.7	H's stretching
18		1384.6	1350.8	ring stretching
19		1341.9	1311.6	ring stretching / H's symmetric rocking
20		1240.5	1217.2	H's asymmetric rocking
21		1035.4	1018.9	H rocking
22		873.2	856.9	ring stretching
23		370.8	367.6	ring deformation
24		194.1	193.0	Br rocking (in-plane)

**Table S3.** Ground state ( $S_0$ ) frequencies (in  $\text{cm}^{-1}$ ) of 5-bromopyrimidine.

	Symmetry	Harmonic freq.	Anharmonic freq.	Character
1	a <sub>1</sub>	3212.0	3089.6	H's stretching
2		3204.7	3060.7	H's stretching
3		1640.0	1599.2	ring stretching
4		1458.6	1424.7	ring stretching / H's symmetric rocking
5		1180.0	1168.3	H's rocking / ring stretching
6		1128.7	1111.8	ring breathing
7		1045.6	1027.7	ring stretching
8		756.2	746.4	ring stretching
9		333.4	325.1	C-Br stretching
10	a <sub>2</sub>	1006.3	975.4	H's twisting / ring deformation
11		423.7	415.8	ring deformation
12	b <sub>1</sub>	1034.6	1004.1	H's wagging/twisting
13		948.4	921.4	H's wagging / ring deformation
14		745.2	728.9	ring deformation
15		436.3	427.6	ring deformation
16		171.0	166.1	Br wagging (out-of-plane)
17	b <sub>2</sub>	3205.0	3069.2	H's stretching
18		1635.8	1597.2	ring stretching
19		1467.3	1440.6	H rocking / ring stretching
20		1365.3	1331.8	H's symmetric rocking
21		1238.1	1208.7	ring stretching
22		1221.3	1198.5	ring stretching / H's rocking
23		635.5	628.1	ring stretching
24		247.4	244.3	Br rocking (in-plane)

**Table S4.** First excited state ( $S_1$ ) frequencies (in  $\text{cm}^{-1}$ ) of 5-bromopyrimidine.

	Symmetry	Harmonic freq.	Anharmonic freq.	Character
1	$a'$	3287.1	3155.7	H stretching
2		3252.6	3109.6	H stretching
3		3246.2	3114.9	H stretching
4		1595.2	1557.2	ring stretching
5		1470.7	1436.9	ring stretching / H's rocking
6		1382.3	1356.1	H rocking
7		1319.0	1289.3	ring stretching
8		1288.8	1257.5	H's rocking
9		1165.6	1150.4	ring stretching / H's rocking
10		1095.5	1078.4	ring stretching
11		1058.7	1039.8	ring stretching
12		989.4	972.6	ring stretching
13		726.1	713.0	ring stretching
14		715.3	705.1	ring stretching
15		327.5	319.6	C-Br stretching
16		251.2	248.1	Br rocking (in-plane)
17		225.7	222.3	ring stretching
18	$a''$	933.7	906.8	H wagging
19		769.7	747.2	H wagging
20		574.5	560.4	ring deformation
21		513.1	501.5	ring deformation
22		447.8	436.0	H wagging
23		264.7	259.1	ring deformation
24		162.6	157.8	Br wagging (out-of-plane)

**Table S5.** Vibrational progression assignments for the low-energy tail (3.75 - 4.15 eV) of the absorption band I of 2-bromopyrimidine. From left to right, energies (in eV) of the experimental peak, and computed energies (in eV), intensities (in arbitrary units), and characters of the most important vibronic transitions between  $S_0$  and  $S_1$  electronic states. Several more transitions take place, however here we only show those with intensities larger than 0.5.

3.828	3.827	1.3	$9^1 \rightarrow 0$
	3.829	0.6	$9^1;16^1 \rightarrow 16^1$
3.845	3.846	0.7	$11^1 \rightarrow 11^1$
3.863	3.859	1.0	$24^1 \rightarrow 24^1$
3.868	3.868	5.7	$0 \rightarrow 0$
	3.871	2.6	$16^1 \rightarrow 16^1$
	3.873	1.2	$16^2 \rightarrow 16^2$
	3.875	0.5	$16^3 \rightarrow 16^3$
3.885	3.887	1.1	$11^1 \rightarrow 9^1;11^1$
3.902	3.899	1.6	$24^1 \rightarrow 9^1;24^1$
3.909	3.902	0.7	$24^1;16^1 \rightarrow 9^1;24^1;16^1$
	3.909	8.5	$0 \rightarrow 9^1$
	3.912	3.9	$16^1 \rightarrow 9^1;16^1$
	3.914	1.8	$16^2 \rightarrow 9^1;16^2$
	3.916	0.8	$16^3 \rightarrow 9^1;16^3$
	3.916	0.8	$9^1 \rightarrow 8^1$
	3.921	0.7	$24^1 \rightarrow 23^1;9^1$
3.924	3.928	0.8	$11^1 \rightarrow 9^2;11^1$
3.943	3.940	1.2	$24^1 \rightarrow 9^2;24^1$
	3.943	0.5	$24^1;16^1 \rightarrow 9^2;24^1;16^1$
3.949	3.945	1.0	$9^1 \rightarrow 7^1$
	3.948	0.6	$24^1 \rightarrow 8^1;24^1$
	3.950	1.2	$9^1 \rightarrow 9^3$
	3.950	6.3	$0 \rightarrow 9^2$
	3.952	0.6	$9^1;16^1 \rightarrow 9^3;16^1$
	3.953	2.9	$16^1 \rightarrow 9^2;16^1$

3.956	3.955	1.3	$16^2 \rightarrow 9^2; 16^2$
	3.957	0.6	$16^3 \rightarrow 9^2; 16^3$
	3.958	0.9	$9^1 \rightarrow 6^1$
	3.958	3.3	$0 \rightarrow 8^1$
	3.960	1.5	$16^1 \rightarrow 8^1; 16^1$
	3.962	0.7	$16^2 \rightarrow 8^1; 16^2$
	3.964	0.5	$11^1 \rightarrow 7^1; 11^1$
3.965	3.969	1.4	$9^1 \rightarrow 5^1$
	3.971	0.6	$9^1; 16^1 \rightarrow 5^1; 16^1$
3.974	3.976	0.6	$11^1 \rightarrow 8^1; 9^1; 11^1$
	3.977	0.7	$24^1 \rightarrow 7^1; 24^1$
	3.981	0.6	$24^1 \rightarrow 9^3; 24^1$
3.988	3.987	4.1	$0 \rightarrow 7^1$
	3.988	0.7	$11^1 \rightarrow 5^1; 11^1$
	3.989	0.9	$24^1 \rightarrow 8^1; 9^1; 24^1$
	3.989	1.9	$16^1 \rightarrow 7^1; 16^1$
	3.990	0.7	$24^1 \rightarrow 6^1; 24^1$
	3.991	1.1	$9^1 \rightarrow 9^4$
	3.991	3.1	$0 \rightarrow 9^3$
	3.991	0.9	$16^2 \rightarrow 7^1; 16^2$
	3.993	0.5	$9^1; 16^1 \rightarrow 9^4; 16^1$
	3.994	1.4	$16^1 \rightarrow 9^3; 16^1$
3.998	3.996	0.6	$16^2 \rightarrow 9^3; 16^2$
	3.999	4.7	$0 \rightarrow 8^1; 9^1$
	4.000	3.9	$0 \rightarrow 6^1$
	4.001	1.1	$24^1 \rightarrow 5^1; 24^1$
	4.001	2.2	$16^1 \rightarrow 8^1; 9^1; 16^1$
	4.002	1.8	$16^1 \rightarrow 6^1; 16^1$
	4.003	1.0	$16^2 \rightarrow 8^1; 9^1; 16^2$
	4.004	0.8	$16^2 \rightarrow 6^1; 16^2$
	4.005	0.8	$11^1 \rightarrow 7^1; 9^1; 11^1$
4.006	4.010	5.8	$0 \rightarrow 5^1$
	4.013	2.7	$16^1 \rightarrow 5^1; 16^1$
	4.015	1.2	$16^2 \rightarrow 5^1; 16^2$
4.014	4.017	0.6	$16^3 \rightarrow 5^1; 16^3$

	4.018	0.7	$11^1 \rightarrow 6^1; 9^1; 11^1$
	4.018	1.1	$24^1 \rightarrow 7^1; 9^1; 24^1$
	4.020	0.5	$24^1; 16^1 \rightarrow 7^1; 9^1; 24^1; 16^1$
4.024	4.028	6.1	$0 \rightarrow 7^1; 9^1$
	4.029	1.1	$11^1 \rightarrow 5^1; 9^1; 11^1$
	4.030	0.6	$24^1 \rightarrow 8^1; 9^2; 24^1$
	4.030	2.8	$16^1 \rightarrow 7^1; 9^1; 16^1$
	4.031	1.0	$24^1 \rightarrow 6^1; 9^1; 24^1$
	4.032	0.6	$9^1 \rightarrow 9^5$
	4.032	1.1	$0 \rightarrow 9^4$
	4.032	1.3	$16^2 \rightarrow 7^1; 9^1; 16^2$
	4.035	0.5	$16^1 \rightarrow 9^4; 16^1$
	4.035	0.6	$16^3 \rightarrow 7^1; 9^1; 16^3$
	4.035	0.6	$9^1 \rightarrow 7^1; 8^1$
4.037	4.039	0.6	$9^1 \rightarrow 8^1; 9^3$
	4.040	3.3	$0 \rightarrow 8^1; 9^2$
	4.041	5.7	$0 \rightarrow 6^1; 9^1$
	4.041	1.6	$24^1 \rightarrow 5^1; 9^1; 24^1$
	4.042	1.5	$16^1 \rightarrow 8^1; 9^2; 16^1$
	4.043	2.6	$16^1 \rightarrow 6^1; 9^1; 16^1$
	4.044	0.7	$24^1; 16^1 \rightarrow 5^1; 9^1; 24^1; 16^1$
	4.044	0.7	$16^2 \rightarrow 8^1; 9^2; 16^2$
	4.045	1.2	$16^2 \rightarrow 6^1; 9^1; 16^2$
	4.046	0.6	$11^1 \rightarrow 7^1; 9^2; 11^1$
4.045	4.047	0.6	$16^3 \rightarrow 6^1; 9^1; 16^3$
	4.047	0.6	$9^1 \rightarrow 6^1; 8^1$
	4.047	0.9	$0 \rightarrow 8^2$
	4.051	8.5	$0 \rightarrow 5^1; 9^1$
	4.054	3.9	$16^1 \rightarrow 5^1; 9^1; 16^1$
	4.054	1.0	$0 \rightarrow 3^1$
4.053	4.056	1.8	$16^2 \rightarrow 5^1; 9^1; 16^2$
	4.058	0.8	$16^3 \rightarrow 5^1; 9^1; 16^3$
	4.058	0.9	$9^1 \rightarrow 5^1; 8^1$
	4.059	0.5	$11^1 \rightarrow 6^1; 9^2; 11^1$
	4.059	0.8	$24^1 \rightarrow 7^1; 9^2; 24^1$
	4.063	0.7	$24^1 \rightarrow 5^1; 23^1; 9^1$

4.063	4.068	0.8	$9^1 \rightarrow 7^1; 9^3$
	4.069	4.5	$0 \rightarrow 7^1; 9^2$
	4.070	0.8	$11^1 \rightarrow 5^1; 9^2; 11^1$
	4.071	2.1	$16^1 \rightarrow 7^1; 9^2; 16^1$
	4.072	0.8	$24^1 \rightarrow 6^1; 9^2; 24^1$
	4.073	0.9	$16^2 \rightarrow 7^1; 9^2; 16^2$
4.077	4.076	0.7	$9^1 \rightarrow 6^1; 7^1$
	4.076	2.3	$0 \rightarrow 7^1; 8^1$
	4.079	1.1	$16^1 \rightarrow 7^1; 8^1; 16^1$
	4.080	0.5	$9^1 \rightarrow 8^1; 9^4$
	4.081	0.8	$9^1 \rightarrow 6^1; 9^3$
	4.081	1.5	$0 \rightarrow 8^1; 9^3$
	4.081	4.1	$0 \rightarrow 6^1; 9^2$
	4.082	1.1	$24^1 \rightarrow 5^1; 9^2; 24^1$
	4.083	0.7	$16^1 \rightarrow 8^1; 9^3; 16^1$
	4.084	1.9	$16^1 \rightarrow 6^1; 9^2; 16^1$
	4.085	0.5	$24^1; 16^1 \rightarrow 5^1; 9^2; 24^1; 16^1$
	4.086	0.9	$16^2 \rightarrow 6^1; 9^2; 16^2$
4.085	4.087	1.0	$9^1 \rightarrow 5^1; 7^1$
	4.088	1.2	$0 \rightarrow 8^2; 9^1$
	4.089	2.2	$0 \rightarrow 6^1; 8^1$
	4.090	0.6	$24^1 \rightarrow 5^1; 8^1; 24^1$
	4.090	0.6	$16^1 \rightarrow 8^2; 9^1; 16^1$
	4.091	1.0	$16^1 \rightarrow 6^1; 8^1; 16^1$
	4.092	1.1	$9^1 \rightarrow 5^1; 9^3$
	4.092	6.2	$0 \rightarrow 5^1; 9^2$
	4.094	0.5	$9^1; 16^1 \rightarrow 5^1; 9^3; 16^1$
	4.095	2.8	$16^1 \rightarrow 5^1; 9^2; 16^1$
	4.095	1.5	$0 \rightarrow 3^1; 9^1$
	4.097	1.3	$16^2 \rightarrow 5^1; 9^2; 16^2$
	4.097	0.7	$16^1 \rightarrow 3^1; 9^1; 16^1$
4.092	4.099	0.6	$16^3 \rightarrow 5^1; 9^2; 16^3$
	4.100	1.0	$9^1 \rightarrow 5^1; 6^1$
	4.100	3.4	$0 \rightarrow 5^1; 8^1$
	4.102	1.5	$16^1 \rightarrow 5^1; 8^1; 16^1$
	4.104	0.7	$16^2 \rightarrow 5^1; 8^1; 16^2$
4.102	4.105	1.4	$0 \rightarrow 7^2$

	4.106	0.5	$11^1 \rightarrow 5^1; 7^1; 11^1$
	4.107	0.6	$24^1 \rightarrow 7^1; 8^1; 9^1; 24^1$
	4.108	0.6	$16^1 \rightarrow 7^2; 16^1$
	4.108	0.5	$24^1 \rightarrow 6^1; 7^1; 24^1$
	4.109	0.8	$9^1 \rightarrow 7^1; 9^4$
	4.110	2.1	$0 \rightarrow 7^1; 9^3$
	4.111	0.7	$9^1 \rightarrow 5^2$
	4.112	1.0	$16^1 \rightarrow 7^1; 9^3; 16^1$
4.116	4.117	3.3	$0 \rightarrow 7^1; 8^1; 9^1$
	4.118	2.8	$0 \rightarrow 6^1; 7^1$
	4.118	0.6	$11^1 \rightarrow 5^1; 8^1; 9^1; 11^1$
	4.119	0.8	$24^1 \rightarrow 5^1; 7^1; 24^1$
	4.120	0.6	$24^1 \rightarrow 6^1; 8^1; 9^1; 24^1$
	4.120	1.3	$16^1 \rightarrow 6^1; 7^1; 16^1$
	4.122	0.7	$9^1 \rightarrow 6^1; 9^4$
	4.122	0.5	$0 \rightarrow 8^1; 9^4$
	4.122	2.0	$0 \rightarrow 6^1; 9^3$
	4.122	0.6	$16^2 \rightarrow 6^1; 7^1; 16^2$
	4.123	0.5	$24^1 \rightarrow 5^1; 9^3; 24^1$
	4.125	0.9	$16^1 \rightarrow 6^1; 9^3; 16^1$
4.125	4.129	4.3	$0 \rightarrow 5^1; 7^1$
	4.129	0.8	$0 \rightarrow 8^2; 9^2$
	4.130	3.1	$0 \rightarrow 6^1; 8^1; 9^1$
	4.131	1.3	$0 \rightarrow 6^2$
	4.131	0.9	$24^1 \rightarrow 5^1; 8^1; 9^1; 24^1$
	4.131	2.0	$16^1 \rightarrow 5^1; 7^1; 16^1$
	4.132	0.7	$24^1 \rightarrow 5^1; 6^1; 24^1$
	4.132	1.4	$16^1 \rightarrow 6^1; 8^1; 9^1; 16^1$
	4.133	1.0	$9^1 \rightarrow 5^1; 9^4$
	4.133	0.6	$16^1 \rightarrow 6^2; 16^1$
	4.133	2.9	$0 \rightarrow 5^1; 9^3$
	4.133	0.9	$16^2 \rightarrow 5^1; 7^1; 16^2$
	4.134	0.7	$16^2 \rightarrow 6^1; 8^1; 9^1; 16^2$
	4.136	1.3	$16^1 \rightarrow 5^1; 9^3; 16^1$
	4.136	1.1	$0 \rightarrow 3^1; 9^2$
	4.136	0.5	$11^1 \rightarrow 6^1; 7^1; 9^1; 11^1$
4.135	4.138	0.6	$16^2 \rightarrow 5^1; 9^3; 16^2$
	4.138	0.5	$16^1 \rightarrow 3^1; 9^2; 16^1$

4.141	4.7	$0 \rightarrow 5^1; 8^1; 9^1$
4.142	3.9	$0 \rightarrow 5^1; 6^1$
4.143	0.5	$24^1 \rightarrow 5^2; 24^1$
4.143	0.6	$0 \rightarrow 3^1; 8^1$
4.144	1.8	$16^1 \rightarrow 5^1; 6^1; 16^1$
4.146	0.8	$16^2 \rightarrow 5^1; 6^1; 16^2$
4.146	2.0	$0 \rightarrow 7^2; 9^1$
4.147	0.8	$11^1 \rightarrow 5^1; 7^1; 9^1; 11^1$

**Table S6.** Vibrational progression assignments for the absorption band I (3.7 - 4.6 eV) of 2-bromopyrimidine. From left to right, energies (in eV) of the experimental peak, and computed energies (in eV), intensities (in arbitrary units), and characters of the most important vibronic transitions between  $S_0$  and  $S_1$  electronic states. Several more transitions take place, however here we only show those with intensities larger than 1.0.

3.87	3.827	1.3	$9^1 \rightarrow 0$
	3.859	1.0	$24^1 \rightarrow 24^1$
	3.868	5.7	$0 \rightarrow 0$
	3.871	2.6	$16^1 \rightarrow 16^1$
	3.873	1.2	$16^2 \rightarrow 16^2$
	3.887	1.1	$11^1 \rightarrow 9^1; 11^1$
3.91	3.899	1.6	$24^1 \rightarrow 9^1; 24^1$
	3.909	8.5	$0 \rightarrow 9^1$
	3.912	3.9	$16^1 \rightarrow 9^1; 16^1$
	3.914	1.8	$16^2 \rightarrow 9^1; 16^2$
	3.940	1.2	$24^1 \rightarrow 9^2; 24^1$
3.96	3.945	1.0	$9^1 \rightarrow 7^1$
	3.950	1.2	$9^1 \rightarrow 9^3$
	3.950	6.3	$0 \rightarrow 9^2$
	3.953	2.9	$16^1 \rightarrow 9^2; 16^1$
	3.955	1.3	$16^2 \rightarrow 9^2; 16^2$
	3.958	3.3	$0 \rightarrow 8^1$
	3.960	1.5	$16^1 \rightarrow 8^1; 16^1$
	3.969	1.4	$9^1 \rightarrow 5^1$
4.00	3.987	4.1	$0 \rightarrow 7^1$
	3.989	1.9	$16^1 \rightarrow 7^1; 16^1$
	3.991	1.1	$9^1 \rightarrow 9^4$
	3.991	3.1	$0 \rightarrow 9^3$
	3.994	1.4	$16^1 \rightarrow 9^3; 16^1$
	3.999	4.7	$0 \rightarrow 8^1; 9^1$
	4.000	3.9	$0 \rightarrow 6^1$
	4.001	1.1	$24^1 \rightarrow 5^1; 24^1$
	4.001	2.2	$16^1 \rightarrow 8^1; 9^1; 16^1$
	4.002	1.8	$16^1 \rightarrow 6^1; 16^1$
	4.003	1.0	$16^2 \rightarrow 8^1; 9^1; 16^2$
	4.010	5.8	$0 \rightarrow 5^1$
	4.013	2.7	$16^1 \rightarrow 5^1; 16^1$
	4.015	1.2	$16^2 \rightarrow 5^1; 16^2$

	4.018	1.1	$24^1 \rightarrow 7^1; 9^1; 24^1$
4.04	4.028	6.1	$0 \rightarrow 7^1; 9^1$
	4.029	1.1	$11^1 \rightarrow 5^1; 9^1; 11^1$
	4.030	2.8	$16^1 \rightarrow 7^1; 9^1; 16^1$
	4.031	1.0	$24^1 \rightarrow 6^1; 9^1; 24^1$
	4.032	1.1	$0 \rightarrow 9^4$
	4.032	1.3	$16^2 \rightarrow 7^1; 9^1; 16^2$
	4.040	3.3	$0 \rightarrow 8^1; 9^2$
	4.041	5.7	$0 \rightarrow 6^1; 9^1$
	4.041	1.6	$24^1 \rightarrow 5^1; 9^1; 24^1$
	4.042	1.5	$16^1 \rightarrow 8^1; 9^2; 16^1$
	4.043	2.6	$16^1 \rightarrow 6^1; 9^1; 16^1$
	4.045	1.2	$16^2 \rightarrow 6^1; 9^1; 16^2$
	4.051	8.5	$0 \rightarrow 5^1; 9^1$
	4.054	3.9	$16^1 \rightarrow 5^1; 9^1; 16^1$
	4.054	1.0	$0 \rightarrow 3^1$
	4.056	1.8	$16^2 \rightarrow 5^1; 9^1; 16^2$
4.08	4.069	4.5	$0 \rightarrow 7^1; 9^2$
	4.071	2.1	$16^1 \rightarrow 7^1; 9^2; 16^1$
	4.076	2.3	$0 \rightarrow 7^1; 8^1$
	4.079	1.1	$16^1 \rightarrow 7^1; 8^1; 16^1$
	4.081	1.5	$0 \rightarrow 8^1; 9^3$
	4.081	4.1	$0 \rightarrow 6^1; 9^2$
	4.082	1.1	$24^1 \rightarrow 5^1; 9^2; 24^1$
	4.084	1.9	$16^1 \rightarrow 6^1; 9^2; 16^1$
	4.087	1.0	$9^1 \rightarrow 5^1; 7^1$
	4.088	1.2	$0 \rightarrow 8^2; 9^1$
	4.089	2.2	$0 \rightarrow 6^1; 8^1$
	4.091	1.0	$16^1 \rightarrow 6^1; 8^1; 16^1$
	4.092	1.1	$9^1 \rightarrow 5^1; 9^3$
	4.092	6.2	$0 \rightarrow 5^1; 9^2$
	4.095	2.8	$16^1 \rightarrow 5^1; 9^2; 16^1$
	4.095	1.5	$0 \rightarrow 3^1; 9^1$
	4.097	1.3	$16^2 \rightarrow 5^1; 9^2; 16^2$
	4.100	1.0	$9^1 \rightarrow 5^1; 6^1$
	4.100	3.4	$0 \rightarrow 5^1; 8^1$
	4.102	1.5	$16^1 \rightarrow 5^1; 8^1; 16^1$
	4.105	1.4	$0 \rightarrow 7^2$
	4.110	2.1	$0 \rightarrow 7^1; 9^3$

	4.112	1.0	$16^1 \rightarrow 7^1; 9^3; 16^1$
4.12	4.117	3.3	$0 \rightarrow 7^1; 8^1; 9^1$
	4.118	2.8	$0 \rightarrow 6^1; 7^1$
	4.120	1.3	$16^1 \rightarrow 6^1; 7^1; 16^1$
	4.122	2.0	$0 \rightarrow 6^1; 9^3$
	4.129	4.3	$0 \rightarrow 5^1; 7^1$
	4.130	3.1	$0 \rightarrow 6^1; 8^1; 9^1$
	4.131	1.3	$0 \rightarrow 6^2$
	4.131	2.0	$16^1 \rightarrow 5^1; 7^1; 16^1$
	4.132	1.4	$16^1 \rightarrow 6^1; 8^1; 9^1; 16^1$
	4.133	1.0	$9^1 \rightarrow 5^1; 9^4$
	4.133	2.9	$0 \rightarrow 5^1; 9^3$
	4.136	1.3	$16^1 \rightarrow 5^1; 9^3; 16^1$
	4.136	1.1	$0 \rightarrow 3^1; 9^2$
	4.141	4.7	$0 \rightarrow 5^1; 8^1; 9^1$
	4.142	3.9	$0 \rightarrow 5^1; 6^1$
	4.144	1.8	$16^1 \rightarrow 5^1; 6^1; 16^1$
	4.146	2.0	$0 \rightarrow 7^2; 9^1$
	4.152	2.8	$0 \rightarrow 5^2$
	4.155	1.3	$16^1 \rightarrow 5^2; 16^1$
	4.158	2.3	$0 \rightarrow 7^1; 8^1; 9^2$
4.17	4.159	4.1	$0 \rightarrow 6^1; 7^1; 9^1$
	4.160	1.1	$24^1 \rightarrow 5^1; 7^1; 9^1; 24^1$
	4.170	6.2	$0 \rightarrow 5^1; 7^1; 9^1$
	4.171	2.1	$0 \rightarrow 6^1; 8^1; 9^2$
	4.172	1.8	$0 \rightarrow 6^2; 9^1$
	4.173	1.0	$24^1 \rightarrow 5^1; 6^1; 9^1; 24^1$
	4.174	1.0	$0 \rightarrow 5^1; 9^4$
	4.182	3.3	$0 \rightarrow 5^1; 8^1; 9^2$
	4.183	5.6	$0 \rightarrow 5^1; 6^1; 9^1$
	4.187	1.5	$0 \rightarrow 7^2; 9^2$
	4.193	4.0	$0 \rightarrow 5^2; 9^1$
	4.196	1.8	$16^1 \rightarrow 5^2; 9^1; 16^1$
	4.199	1.1	$0 \rightarrow 7^1; 8^1; 9^3$
	4.200	2.9	$0 \rightarrow 6^1; 7^1; 9^2$
4.21	4.207	1.6	$0 \rightarrow 6^1; 7^1; 8^1$
	4.211	4.4	$0 \rightarrow 5^1; 7^1; 9^2$
	4.213	1.3	$0 \rightarrow 6^2; 9^2$

	4.213	1.2	$0 \rightarrow 3^1; 7^1; 9^1$
	4.218	2.4	$0 \rightarrow 5^1; 7^1; 8^1$
	4.223	1.5	$0 \rightarrow 5^1; 8^1; 9^3$
	4.224	4.0	$0 \rightarrow 5^1; 6^1; 9^2$
	4.230	1.2	$0 \rightarrow 5^1; 8^2; 9^1$
	4.231	2.2	$0 \rightarrow 5^1; 6^1; 8^1$
	4.234	2.8	$0 \rightarrow 5^2; 9^2$
	4.236	1.1	$0 \rightarrow 7^2; 8^1; 9^1$
	4.237	1.3	$16^1 \rightarrow 5^2; 9^2; 16^1$
	4.237	1.3	$0 \rightarrow 3^1; 5^1; 9^1$
	4.241	1.4	$0 \rightarrow 6^1; 7^1; 9^3$
	4.242	1.6	$0 \rightarrow 5^2; 8^1$
4.25	4.247	1.4	$0 \rightarrow 5^1; 7^2$
	4.248	2.2	$0 \rightarrow 6^1; 7^1; 8^1; 9^1$
	4.252	2.1	$0 \rightarrow 5^1; 7^1; 9^3$
	4.259	3.3	$0 \rightarrow 5^1; 7^1; 8^1; 9^1$
	4.260	2.9	$0 \rightarrow 5^1; 6^1; 7^1$
	4.264	1.8	$0 \rightarrow 5^1; 6^1; 9^3$
	4.271	2.1	$0 \rightarrow 5^2; 7^1$
	4.272	3.1	$0 \rightarrow 5^1; 6^1; 8^1; 9^1$
	4.273	1.3	$0 \rightarrow 5^1; 6^2$
	4.275	1.3	$0 \rightarrow 5^2; 9^3$
	4.277	1.3	$0 \rightarrow 6^1; 7^2; 9^1$
	4.283	2.2	$0 \rightarrow 5^2; 8^1; 9^1$
	4.284	1.9	$0 \rightarrow 5^2; 6^1$
	4.288	2.1	$0 \rightarrow 5^1; 7^2; 9^1$
	4.289	1.5	$0 \rightarrow 6^1; 7^1; 8^1; 9^2$
	4.290	1.3	$0 \rightarrow 6^2; 7^1; 9^1$
4.29	4.300	2.3	$0 \rightarrow 5^1; 7^1; 8^1; 9^2$
	4.301	4.0	$0 \rightarrow 5^1; 6^1; 7^1; 9^1$
	4.312	2.9	$0 \rightarrow 5^2; 7^1; 9^1$
	4.313	2.1	$0 \rightarrow 5^1; 6^1; 8^1; 9^2$
	4.314	1.8	$0 \rightarrow 5^1; 6^2; 9^1$
	4.324	1.5	$0 \rightarrow 5^2; 8^1; 9^2$
	4.325	2.6	$0 \rightarrow 5^2; 6^1; 9^1$
	4.329	1.4	$0 \rightarrow 5^1; 7^2; 9^2$
4.34	4.335	1.2	$0 \rightarrow 5^3; 9^1$
	4.341	1.0	$0 \rightarrow 5^1; 7^1; 8^1; 9^3$

	4.342	2.8	$0 \rightarrow 5^1; 6^1; 7^1; 9^2$
	4.349	1.6	$0 \rightarrow 5^1; 6^1; 7^1; 8^1$
	4.353	2.0	$0 \rightarrow 5^2; 7^1; 9^2$
	4.355	1.2	$0 \rightarrow 5^1; 6^2; 9^2$
	4.356	1.0	$0 \rightarrow 3^1; 5^1; 7^1; 9^1$
	4.360	1.2	$0 \rightarrow 5^2; 7^1; 8^1$
	4.366	1.8	$0 \rightarrow 5^2; 6^1; 9^2$
	4.373	1.1	$0 \rightarrow 5^2; 6^1; 8^1$
	4.378	1.1	$0 \rightarrow 5^1; 7^2; 8^1; 9^1$
4.39	4.383	1.3	$0 \rightarrow 5^1; 6^1; 7^1; 9^3$
	4.390	2.2	$0 \rightarrow 5^1; 6^1; 7^1; 8^1; 9^1$
	4.401	1.6	$0 \rightarrow 5^2; 7^1; 8^1; 9^1$
	4.402	1.4	$0 \rightarrow 5^2; 6^1; 7^1$
	4.414	1.4	$0 \rightarrow 5^2; 6^1; 8^1; 9^1$
	4.419	1.3	$0 \rightarrow 5^1; 6^1; 7^2; 9^1$

**Table S7.** Vibrational progression assignments for the absorption band I (3.7 - 4.6 eV) of 5-bromopyrimidine. From left to right, energies (in eV) of the experimental peak, and computed energies (in eV), intensities (in arbitrary units), and characters of the most important vibronic transitions between  $S_0$  and  $S_1$  electronic states. Several more transitions take place, however here we only show those with intensities larger than 2.0.

3.79	3.768	2.3	$11^1 \rightarrow 23^1$
	3.785	3.1	$16^2 \rightarrow 24^2$
	3.786	7.9	$16^1 \rightarrow 24^1$
	3.787	2.7	$9^1 \rightarrow 15^1$
	3.787	2.4	$24^1;16^1 \rightarrow 16^1;24^1$
	3.787	20.1	$0 \rightarrow 0$
	3.788	6.0	$24^1 \rightarrow 16^1$
3.83	3.827	4.5	$0 \rightarrow 15^1$
	3.843	2.4	$0 \rightarrow 17^2$
	3.855	2.7	$11^1 \rightarrow 14^1;23^1$
3.87	3.873	3.7	$16^2 \rightarrow 14^1;24^2$
	3.874	9.3	$16^1 \rightarrow 14^1;24^1$
	3.874	3.1	$9^1 \rightarrow 14^1;15^1$
	3.874	2.8	$24^1;16^1 \rightarrow 14^1;16^1;24^1$
	3.875	3.2	$16^1 \rightarrow 13^1;24^1$
	3.875	23.7	$0 \rightarrow 14^1$
	3.875	7.0	$24^1 \rightarrow 14^1;16^1$
	3.876	2.1	$24^2 \rightarrow 14^1;16^2$
	3.876	8.0	$0 \rightarrow 13^1$
	3.876	2.4	$24^1 \rightarrow 13^1;16^1$
	3.889	2.3	$11^1 \rightarrow 12^1;23^1$
3.91	3.903	2.2	$0 \rightarrow 13^1;17^1$
	3.906	3.2	$16^2 \rightarrow 12^1;24^2$
	3.907	8.1	$16^1 \rightarrow 12^1;24^1$
	3.907	2.8	$9^1 \rightarrow 12^1;15^1$
	3.908	2.4	$24^1;16^1 \rightarrow 12^1;16^1;24^1$
	3.908	20.5	$0 \rightarrow 12^1$
	3.909	6.1	$24^1 \rightarrow 12^1;16^1$
	3.915	5.0	$0 \rightarrow 14^1;15^1$
	3.915	4.1	$16^1 \rightarrow 11^1;24^1$
	3.916	2.1	$0 \rightarrow 13^1;15^1$
	3.916	10.3	$0 \rightarrow 11^1$
	3.917	3.1	$24^1 \rightarrow 11^1;16^1$
	3.920	3.5	$16^1 \rightarrow 10^1;24^1$
	3.921	8.9	$0 \rightarrow 10^1$

	3.922	2.7	$24^1 \rightarrow 10^1; 16^1$
	3.929	2.7	$16^1 \rightarrow 9^1; 24^1$
	3.930	3.2	$0 \rightarrow 14^1; 17^2$
	3.930	7.0	$0 \rightarrow 9^1$
	3.931	2.1	$24^1 \rightarrow 9^1; 16^1$
	3.948	4.7	$0 \rightarrow 12^1; 15^1$
3.96	3.956	2.3	$0 \rightarrow 11^1; 15^1$
	3.961	4.9	$16^1 \rightarrow 14^2; 24^1$
	3.962	4.5	$16^1 \rightarrow 13^1; 14^1; 24^1$
	3.962	12.5	$0 \rightarrow 14^2$
	3.963	3.7	$24^1 \rightarrow 14^2; 16^1$
	3.963	2.4	$0 \rightarrow 12^1; 17^2$
	3.963	11.5	$0 \rightarrow 13^1; 14^1$
	3.964	3.4	$24^1 \rightarrow 13^1; 14^1; 16^1$
	3.976	2.7	$11^1 \rightarrow 12^1; 14^1; 23^1$
	3.981	4.2	$0 \rightarrow 4^1$
4.00	3.991	2.4	$0 \rightarrow 13^1; 14^1; 17^1$
	3.993	3.7	$16^2 \rightarrow 12^1; 14^1; 24^2$
	3.994	9.3	$16^1 \rightarrow 12^1; 14^1; 24^1$
	3.995	3.1	$9^1 \rightarrow 12^1; 14^1; 15^1$
	3.995	2.8	$24^1; 16^1 \rightarrow 12^1; 14^1; 16^1; 24^1$
	3.995	3.2	$16^1 \rightarrow 12^1; 13^1; 24^1$
	3.995	23.5	$0 \rightarrow 12^1; 14^1$
	3.996	7.0	$24^1 \rightarrow 12^1; 14^1; 16^1$
	3.996	2.1	$24^2 \rightarrow 12^1; 14^1; 16^2$
	3.996	8.1	$0 \rightarrow 12^1; 13^1$
	3.997	2.4	$24^1 \rightarrow 12^1; 13^1; 16^1$
	4.002	2.4	$0 \rightarrow 14^2; 15^1$
	4.003	4.8	$16^1 \rightarrow 11^1; 14^1; 24^1$
	4.003	2.7	$0 \rightarrow 13^1; 14^1; 15^1$
	4.004	12.1	$0 \rightarrow 11^1; 14^1$
	4.004	3.6	$24^1 \rightarrow 11^1; 14^1; 16^1$
	4.005	3.8	$0 \rightarrow 11^1; 13^1$
	4.008	4.1	$16^1 \rightarrow 10^1; 14^1; 24^1$
	4.009	10.4	$0 \rightarrow 10^1; 14^1$
	4.009	3.1	$24^1 \rightarrow 10^1; 14^1; 16^1$
	4.010	3.7	$0 \rightarrow 10^1; 13^1$
	4.017	3.2	$16^1 \rightarrow 9^1; 14^1; 24^1$
	4.018	8.0	$0 \rightarrow 9^1; 14^1$
	4.018	2.4	$24^1 \rightarrow 9^1; 14^1; 16^1$
	4.019	3.1	$0 \rightarrow 9^1; 13^1$
	4.024	2.3	$0 \rightarrow 12^1; 13^1; 17^1$

	4.028	3.9	$16^1 \rightarrow 12^2; 24^1$
	4.029	9.9	$0 \rightarrow 12^2$
	4.029	2.9	$24^1 \rightarrow 12^2; 16^1$
4.04	4.035	4.9	$0 \rightarrow 12^1; 14^1; 15^1$
	4.036	4.2	$16^1 \rightarrow 11^1; 12^1; 24^1$
	4.036	2.1	$0 \rightarrow 12^1; 13^1; 15^1$
	4.037	10.6	$0 \rightarrow 11^1; 12^1$
	4.037	3.2	$24^1 \rightarrow 11^1; 12^1; 16^1$
	4.041	3.6	$16^1 \rightarrow 10^1; 12^1; 24^1$
	4.042	9.1	$0 \rightarrow 10^1; 12^1$
	4.042	2.7	$24^1 \rightarrow 10^1; 12^1; 16^1$
	4.043	2.5	$0 \rightarrow 11^1; 14^1; 15^1$
	4.048	2.1	$0 \rightarrow 10^1; 14^1; 15^1$
	4.050	2.8	$16^1 \rightarrow 9^1; 12^1; 24^1$
	4.050	2.9	$16^1 \rightarrow 13^1; 14^2; 24^1$
	4.050	3.8	$0 \rightarrow 14^3$
	4.050	4.9	$0 \rightarrow 10^1; 11^1$
	4.051	3.2	$0 \rightarrow 12^1; 14^1; 17^2$
	4.051	7.1	$0 \rightarrow 9^1; 12^1$
	4.051	7.3	$0 \rightarrow 13^1; 14^2$
	4.051	2.1	$24^1 \rightarrow 9^1; 12^1; 16^1$
	4.051	2.2	$24^1 \rightarrow 13^1; 14^2; 16^1$
	4.059	3.8	$0 \rightarrow 9^1; 11^1$
	4.064	2.9	$0 \rightarrow 9^1; 10^1$
	4.068	5.0	$0 \rightarrow 4^1; 14^1$
	4.068	2.2	$0 \rightarrow 12^2; 15^1$
	4.077	2.4	$0 \rightarrow 11^1; 12^1; 15^1$
4.08	4.081	2.0	$0 \rightarrow 10^1; 12^1; 15^1$
	4.082	4.7	$16^1 \rightarrow 12^1; 14^2; 24^1$
	4.083	4.4	$16^1 \rightarrow 12^1; 13^1; 14^1; 24^1$
	4.083	12.0	$0 \rightarrow 12^1; 14^2$
	4.083	3.6	$24^1 \rightarrow 12^1; 14^2; 16^1$
	4.084	11.3	$0 \rightarrow 12^1; 13^1; 14^1$
	4.084	3.4	$24^1 \rightarrow 12^1; 13^1; 14^1; 16^1$
	4.090	2.5	$16^1 \rightarrow 11^1; 14^2; 24^1$
	4.091	2.2	$16^1 \rightarrow 11^1; 13^1; 14^1; 24^1$
	4.091	6.3	$0 \rightarrow 11^1; 14^2$
	4.092	5.5	$0 \rightarrow 11^1; 13^1; 14^1$
	4.095	2.2	$16^1 \rightarrow 10^1; 14^2; 24^1$
	4.096	2.1	$16^1 \rightarrow 10^1; 13^1; 14^1; 24^1$
	4.096	5.5	$0 \rightarrow 10^1; 14^2$
	4.097	5.3	$0 \rightarrow 10^1; 13^1; 14^1$

4.101	4.4	$0 \rightarrow 4^1; 12^1$
4.105	4.1	$0 \rightarrow 9^1; 14^2$
4.106	4.4	$0 \rightarrow 9^1; 13^1; 14^1$
4.111	2.3	$0 \rightarrow 12^1; 13^1; 14^1; 17^1$
4.115	4.4	$16^1 \rightarrow 12^2; 14^1; 24^1$
4.116	11.1	$0 \rightarrow 12^2; 14^1$
4.117	3.3	$24^1 \rightarrow 12^2; 14^1; 16^1$
4.117	3.8	$0 \rightarrow 12^2; 13^1$
4.12	4.123	2.3 $0 \rightarrow 12^1; 14^2; 15^1$
	4.123	4.8 $16^1 \rightarrow 11^1; 12^1; 14^1; 24^1$
	4.124	2.7 $0 \rightarrow 12^1; 13^1; 14^1; 15^1$
	4.124	12.1 $0 \rightarrow 11^1; 12^1; 14^1$
	4.125	3.6 $24^1 \rightarrow 11^1; 12^1; 14^1; 16^1$
	4.125	3.9 $0 \rightarrow 11^1; 12^1; 13^1$
	4.128	4.1 $16^1 \rightarrow 10^1; 12^1; 14^1; 24^1$
	4.129	10.3 $0 \rightarrow 10^1; 12^1; 14^1$
	4.130	3.1 $24^1 \rightarrow 10^1; 12^1; 14^1; 16^1$
	4.130	3.7 $0 \rightarrow 10^1; 12^1; 13^1$
	4.133	2.2 $0 \rightarrow 11^2; 14^1$
	4.137	2.3 $16^1 \rightarrow 10^1; 11^1; 14^1; 24^1$
	4.137	3.1 $16^1 \rightarrow 9^1; 12^1; 14^1; 24^1$
	4.138	5.7 $0 \rightarrow 10^1; 11^1; 14^1$
	4.138	8.0 $0 \rightarrow 9^1; 12^1; 14^1$
	4.138	2.8 $0 \rightarrow 13^1; 14^3$
	4.139	2.4 $24^1 \rightarrow 9^1; 12^1; 14^1; 16^1$
	4.139	3.2 $0 \rightarrow 9^1; 12^1; 13^1$
	4.142	2.0 $0 \rightarrow 10^2; 14^1$
	4.146	4.4 $0 \rightarrow 9^1; 11^1; 14^1$
	4.149	3.0 $0 \rightarrow 12^3$
	4.151	3.4 $0 \rightarrow 9^1; 10^1; 14^1$
	4.155	2.7 $0 \rightarrow 4^1; 14^2$
	4.156	2.3 $0 \rightarrow 12^2; 14^1; 15^1$
	4.156	2.2 $0 \rightarrow 4^1; 13^1; 14^1$
	4.157	2.0 $16^1 \rightarrow 11^1; 12^2; 24^1$
	4.158	5.2 $0 \rightarrow 11^1; 12^2$
	4.162	4.3 $0 \rightarrow 10^1; 12^2$
	4.164	2.5 $0 \rightarrow 11^1; 12^1; 14^1; 15^1$
4.17	4.169	2.1 $0 \rightarrow 10^1; 12^1; 14^1; 15^1$
	4.170	2.8 $16^1 \rightarrow 12^1; 13^1; 14^2; 24^1$
	4.170	3.6 $0 \rightarrow 12^1; 14^3$
	4.171	5.1 $0 \rightarrow 10^1; 11^1; 12^1$
	4.171	3.4 $0 \rightarrow 9^1; 12^2$

4.171	7.0	$0 \rightarrow 12^1; 13^1; 14^2$
4.172	2.1	$24^1 \rightarrow 12^1; 13^1; 14^2; 16^1$
4.180	3.9	$0 \rightarrow 9^1; 11^1; 12^1$
4.180	3.5	$0 \rightarrow 11^1; 13^1; 14^2$
4.184	3.0	$0 \rightarrow 9^1; 10^1; 12^1$
4.184	3.3	$0 \rightarrow 10^1; 13^1; 14^2$
4.188	2.0	$16^1 \rightarrow 4^1; 12^1; 14^1; 24^1$
4.189	5.1	$0 \rightarrow 4^1; 12^1; 14^1$
4.193	2.7	$0 \rightarrow 9^1; 13^1; 14^2$
4.197	2.2	$0 \rightarrow 4^1; 11^1; 14^1$
4.202	2.2	$16^1 \rightarrow 12^2; 14^2; 24^1$
4.203	2.1	$16^1 \rightarrow 12^2; 13^1; 14^1; 24^1$
4.204	5.5	$0 \rightarrow 12^2; 14^2$
4.204	5.3	$0 \rightarrow 12^2; 13^1; 14^1$
4.21	4.211	2.4 $16^1 \rightarrow 11^1; 12^1; 14^2; 24^1$
	4.212	2.1 $16^1 \rightarrow 11^1; 12^1; 13^1; 14^1; 24^1$
	4.212	6.2 $0 \rightarrow 11^1; 12^1; 14^2$
	4.213	5.4 $0 \rightarrow 11^1; 12^1; 13^1; 14^1$
	4.216	2.1 $16^1 \rightarrow 10^1; 12^1; 14^2; 24^1$
	4.217	2.0 $16^1 \rightarrow 10^1; 12^1; 13^1; 14^1; 24^1$
	4.217	5.3 $0 \rightarrow 10^1; 12^1; 14^2$
	4.218	5.1 $0 \rightarrow 10^1; 12^1; 13^1; 14^1$
	4.222	2.2 $0 \rightarrow 4^1; 12^2$
	4.225	3.0 $0 \rightarrow 10^1; 11^1; 14^2$
	4.226	4.0 $0 \rightarrow 9^1; 12^1; 14^2$
	4.226	2.7 $0 \rightarrow 10^1; 11^1; 13^1; 14^1$
	4.227	4.3 $0 \rightarrow 9^1; 12^1; 13^1; 14^1$
	4.234	2.2 $0 \rightarrow 9^1; 11^1; 14^2$
	4.235	2.2 $0 \rightarrow 9^1; 11^1; 13^1; 14^1$
	4.237	3.2 $0 \rightarrow 12^3; 14^1$
	4.244	2.3 $16^1 \rightarrow 11^1; 12^2; 14^1; 24^1$
	4.245	5.8 $0 \rightarrow 11^1; 12^2; 14^1$
4.25	4.250	4.8 $0 \rightarrow 10^1; 12^2; 14^1$
	4.253	2.2 $0 \rightarrow 11^2; 12^1; 14^1$
	4.257	2.3 $16^1 \rightarrow 10^1; 11^1; 12^1; 14^1; 24^1$
	4.258	5.7 $0 \rightarrow 10^1; 11^1; 12^1; 14^1$
	4.259	3.8 $0 \rightarrow 9^1; 12^2; 14^1$
	4.259	2.6 $0 \rightarrow 12^1; 13^1; 14^3$
	4.267	4.4 $0 \rightarrow 9^1; 11^1; 12^1; 14^1$
	4.272	3.3 $0 \rightarrow 9^1; 10^1; 12^1; 14^1$
	4.276	2.7 $0 \rightarrow 4^1; 12^1; 14^2$
	4.277	2.2 $0 \rightarrow 4^1; 12^1; 13^1; 14^1$

	4.291	2.4	$0 \rightarrow 10^1; 11^1; 12^2$
	4.292	3.2	$0 \rightarrow 12^2; 13^1; 14^2$
4.29	4.300	3.4	$0 \rightarrow 11^1; 12^1; 13^1; 14^2$
	4.305	3.2	$0 \rightarrow 10^1; 12^1; 13^1; 14^2$
	4.309	2.5	$0 \rightarrow 4^1; 12^2; 14^1$
	4.314	2.6	$0 \rightarrow 9^1; 12^1; 13^1; 14^2$
	4.317	2.3	$0 \rightarrow 4^1; 11^1; 12^1; 14^1$
	4.332	2.9	$0 \rightarrow 11^1; 12^2; 14^2$
	4.333	2.6	$0 \rightarrow 11^1; 12^2; 13^1; 14^1$
	4.337	2.4	$0 \rightarrow 10^1; 12^2; 14^2$
	4.338	2.4	$0 \rightarrow 10^1; 12^2; 13^1; 14^1$
4.33	4.346	2.9	$0 \rightarrow 10^1; 11^1; 12^1; 14^2$
	4.347	2.7	$0 \rightarrow 10^1; 11^1; 12^1; 13^1; 14^1$
	4.354	2.2	$0 \rightarrow 9^1; 11^1; 12^1; 14^2$
	4.355	2.2	$0 \rightarrow 9^1; 11^1; 12^1; 13^1; 14^1$
	4.379	2.7	$0 \rightarrow 10^1; 11^1; 12^2; 14^1$
4.38	4.388	2.1	$0 \rightarrow 9^1; 11^1; 12^2; 14^1$