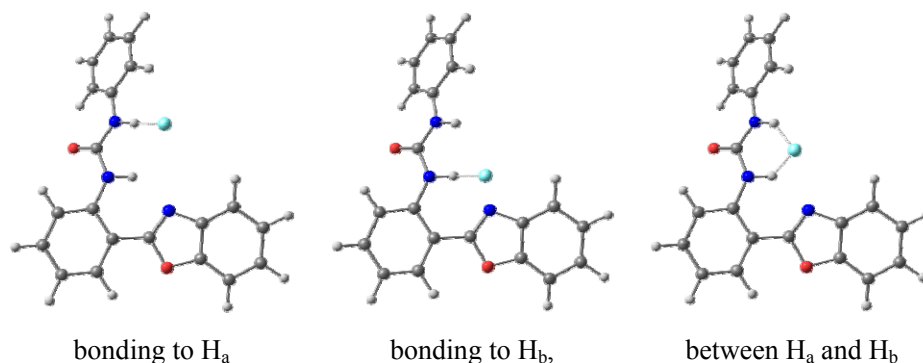


Supporting Information

## Fluoride-Sensing Mechanism of 2-(2'-phenylureaphenyl)benzoxazole

Guang-Yue Li, Tian-Shu Chu\*

### 1. Initial Configurations for PUBO-F



**Fig. S1** A set of initial configurations with different fluoride position for PUBO-F optimization.  
gray: C; white: H; red: O; blue: N; cyan: F.

### 2. XYZ coordinates (angstrom) and SCF energies (AU)

Calculated using **Gaussian 09** program

**Note:** upper case letters before the atomic coordinates indicate the atomic symbol of the atoms involved in the calculations.

#### PUBO in the S<sub>0</sub> state

E = -1089.36816866

C	-1.855683	2.340705	-0.004356
C	-0.648381	1.656250	-0.006411
C	-0.595566	0.257091	-0.007623
C	-1.750122	-0.518379	-0.006816
C	-2.935768	0.184093	-0.004776
C	-3.015512	1.574957	-0.003540
N	-4.355364	1.928774	-0.001595
C	-5.011608	0.805133	-0.001589
O	-4.213098	-0.303211	-0.003555
C	-6.445078	0.602535	-0.000156
C	-6.936967	-0.707975	-0.000347
C	-8.292116	-0.967399	0.000813
C	-9.181790	0.101119	0.002200
C	-8.728428	1.408222	0.002433
C	-7.357635	1.691677	0.001276

N	-6.847925	2.980511	0.001520
C	-7.534313	4.174668	0.002523
N	-6.683263	5.249772	0.003221
C	-6.997825	6.613395	0.003807
C	-8.298757	7.122646	0.003552
C	-8.498029	8.497933	0.004097
C	-7.428358	9.381839	0.004889
C	-6.134407	8.872261	0.005130
C	-5.918570	7.505161	0.004594
O	-8.755290	4.272395	0.002942
H	-1.896657	3.422600	-0.003432
H	0.278759	2.216392	-0.007121
H	0.368890	-0.235726	-0.009242
H	-1.719011	-1.600002	-0.007733
H	-6.230420	-1.527205	-0.001446
H	-8.651724	-1.988418	0.000641
H	-10.250007	-0.081712	0.003121
H	-9.427162	2.228838	0.003500
H	-5.824324	3.014765	0.000749
H	-5.692775	5.051479	0.003376
H	-9.139681	6.447707	0.002949
H	-9.513677	8.876867	0.003888
H	-7.597750	10.451653	0.005308
H	-5.283039	9.542916	0.005736
H	-4.905772	7.116273	0.004771

**PUBO in the S<sub>1</sub> state**

E = -1089.24856942

C	-1.942718	2.470468	-0.003906
C	-0.712698	1.824567	-0.005427
C	-0.606551	0.429769	-0.006271
C	-1.746640	-0.385729	-0.005601
C	-2.955357	0.265080	-0.004098
C	-3.094124	1.670866	-0.003217
N	-4.413518	1.983088	-0.001741
C	-5.073742	0.808387	-0.001719
O	-4.202943	-0.281804	-0.003150
C	-6.453969	0.571783	-0.000676
C	-6.969140	-0.747364	-0.000898
C	-8.327244	-0.990488	0.000223
C	-9.254088	0.063191	0.001669
C	-8.797616	1.374842	0.001938
C	-7.431010	1.657714	0.000801
N	-6.914281	2.932272	0.000811

C	-7.581913	4.129973	0.002719
N	-6.680633	5.182615	0.001568
C	-6.942060	6.534974	0.003000
C	-8.235887	7.087378	0.006658
C	-8.383655	8.461829	0.007923
C	-7.276185	9.305252	0.005621
C	-5.993434	8.757795	0.001996
C	-5.822557	7.391289	0.000698
O	-8.795758	4.267015	0.004992
H	-2.015685	3.550787	-0.003265
H	0.194342	2.418026	-0.005990
H	0.373494	-0.031074	-0.007461
H	-1.677882	-1.466021	-0.006231
H	-6.273670	-1.575622	-0.001977
H	-8.679146	-2.015712	-0.000004
H	-10.317104	-0.138491	0.002535
H	-9.492755	2.199704	0.003017
H	-5.872878	2.945017	-0.000407
H	-5.696348	4.943504	-0.000773
H	-9.095438	6.436865	0.008449
H	-9.381779	8.882556	0.010768
H	-7.409416	10.379817	0.006641
H	-5.124971	9.404796	0.000185
H	-4.827242	6.961683	-0.002099

**ESIPT structure of PUBO in the S<sub>1</sub> state**

E = -1089.27523695

C	-1.825374	2.399344	0.097003
C	-0.620578	1.698449	0.106415
C	-0.576505	0.305684	0.089254
C	-1.747572	-0.460162	0.061194
C	-2.927426	0.242324	0.051512
C	-2.986977	1.639312	0.069251
N	-4.319758	1.949007	0.062780
C	-5.060143	0.811758	0.022113
O	-4.203780	-0.257727	0.025837
C	-6.457293	0.621002	-0.029706
C	-6.969799	-0.683958	-0.011715
C	-8.342466	-0.926732	-0.080329
C	-9.237383	0.127681	-0.152262
C	-8.755441	1.443051	-0.149741
C	-7.388678	1.732624	-0.082623
N	-6.829308	2.984467	-0.118601
C	-7.549440	4.109759	0.083606

N	-6.716230	5.215999	-0.123598
C	-6.996820	6.557667	-0.052735
C	-8.255857	7.081527	0.295311
C	-8.432596	8.452933	0.343961
C	-7.388240	9.325379	0.054119
C	-6.140169	8.808838	-0.292086
C	-5.942062	7.446051	-0.346959
O	-8.733919	4.249791	0.410431
H	-1.857006	3.480552	0.110645
H	0.308388	2.255319	0.127786
H	0.381821	-0.198098	0.097793
H	-1.728478	-1.541797	0.046389
H	-6.285028	-1.519278	0.053845
H	-8.697742	-1.950475	-0.072052
H	-10.303313	-0.053771	-0.207623
H	-9.446216	2.270257	-0.202948
H	-4.797297	2.846195	0.028470
H	-5.774349	4.975431	-0.400910
H	-9.065374	6.405265	0.519057
H	-9.405199	8.847587	0.613067
H	-7.542919	10.396371	0.096201
H	-5.318754	9.477155	-0.520429
H	-4.972180	7.042516	-0.615487

**PUBO-a1 in the S<sub>0</sub> state**

E = -1088.87430011

C	-1.695538	1.971686	0.838828
C	-0.529877	1.257062	0.595111
C	-0.555382	-0.006985	-0.005630
C	-1.751167	-0.609645	-0.385025
C	-2.893844	0.119481	-0.131995
C	-2.896924	1.379971	0.463286
N	-4.207403	1.818036	0.568214
C	-4.930509	0.866316	0.060746
O	-4.189114	-0.209875	-0.393191
C	-6.370011	0.722396	-0.047343
C	-6.887859	-0.582506	-0.050558
C	-8.244492	-0.825546	-0.107064
C	-9.115373	0.263560	-0.177581
C	-8.631827	1.554119	-0.189512
C	-7.245428	1.846656	-0.140313
N	-6.739417	3.099161	-0.293303
C	-7.395540	4.184005	0.128064
N	-6.823503	5.346614	-0.405506

C	-7.148953	6.679493	-0.219430
C	-8.197283	7.134578	0.592740
C	-8.446289	8.496143	0.709440
C	-7.676869	9.435227	0.034963
C	-6.635591	8.987086	-0.772236
C	-6.373834	7.634310	-0.899403
O	-8.353512	4.267835	0.925587
H	-1.673858	2.949813	1.303444
H	0.424534	1.686632	0.875085
H	0.376987	-0.530612	-0.178621
H	-1.780682	-1.587241	-0.848720
H	-6.197970	-1.414405	0.015953
H	-8.621668	-1.840575	-0.096150
H	-10.186334	0.097590	-0.229922
H	-9.321081	2.383841	-0.263085
H	-6.044061	5.162484	-1.019347
H	-8.801366	6.413918	1.121663
H	-9.263059	8.823043	1.343822
H	-7.882027	10.494139	0.134756
H	-6.018363	9.697689	-1.310538
H	-5.558810	7.298408	-1.532030

**PUBO-a2 in the  $S_0$  state**

E = -1088.87881054

C	-1.829800	2.301966	-0.003821
C	-0.629673	1.603508	-0.006432
C	-0.593299	0.204379	-0.008316
C	-1.758544	-0.556331	-0.007638
C	-2.935949	0.159758	-0.005038
C	-2.999831	1.551673	-0.003133
N	-4.333943	1.925379	-0.000713
C	-5.007674	0.810348	-0.001202
O	-4.217536	-0.311721	-0.003789
C	-6.438552	0.613499	0.000403
C	-6.930399	-0.700120	0.000094
C	-8.282146	-0.967447	0.001335
C	-9.175488	0.103253	0.002938
C	-8.728645	1.408504	0.003315
C	-7.352796	1.710427	0.002077
N	-6.868997	2.989089	0.002479
C	-7.545127	4.234408	0.003425
N	-6.654740	5.223485	0.003827
C	-7.015821	6.553809	0.004501
C	-8.321246	7.097247	0.003822

C	-8.525354	8.471967	0.004460
C	-7.460584	9.364562	0.005835
C	-6.165466	8.850152	0.006528
C	-5.951088	7.483665	0.005877
O	-8.794325	4.264928	0.003873
H	-1.857576	3.384413	-0.002370
H	0.303835	2.153160	-0.007052
H	0.364935	-0.300578	-0.010355
H	-1.740455	-1.638385	-0.009065
H	-6.220809	-1.516968	-0.001162
H	-8.638644	-1.989644	0.001078
H	-10.243584	-0.083826	0.003938
H	-9.423465	2.233369	0.004534
H	-5.855868	3.072725	0.001848
H	-9.165282	6.424735	0.002800
H	-9.543154	8.849440	0.003878
H	-7.632441	10.434486	0.006335
H	-5.314065	9.522872	0.007592
H	-4.939605	7.091413	0.006396

**PUBO-a2 in the S<sub>1</sub> state**

E = -1088.79238652

C	-2.251933	2.914608	-0.130835
C	-1.009068	2.386079	0.222039
C	-0.866656	1.077937	0.676624
C	-1.982697	0.232975	0.796521
C	-3.196525	0.769917	0.445668
C	-3.370823	2.085826	-0.016433
N	-4.695430	2.298885	-0.275675
C	-5.320328	1.144137	0.020250
O	-4.421576	0.165519	0.472118
C	-6.681166	0.810230	-0.060609
C	-7.136312	-0.491876	0.302824
C	-8.465336	-0.842578	0.232162
C	-9.423538	0.078380	-0.202908
C	-9.015555	1.366165	-0.565656
C	-7.685648	1.744956	-0.505829
N	-7.232808	3.027916	-0.860028
C	-7.922563	4.094238	-1.300823
N	-7.106468	5.176849	-1.660414
C	-6.870666	6.137310	-0.767914
C	-7.331878	6.116151	0.582464
C	-7.025112	7.148108	1.437549
C	-6.257785	8.229173	0.998061

C	-5.794652	8.273201	-0.320084
C	-6.093315	7.254984	-1.191364
O	-9.141214	4.158884	-1.477772
H	-2.347297	3.934330	-0.483647
H	-0.129111	3.014290	0.139960
H	0.114219	0.702640	0.941237
H	-1.890252	-0.787053	1.148385
H	-6.406656	-1.215739	0.641462
H	-8.765037	-1.844968	0.518428
H	-10.470099	-0.191720	-0.260658
H	-9.741494	2.091490	-0.901941
H	-6.213184	3.143403	-0.768656
H	-7.926382	5.279856	0.928250
H	-7.380371	7.122801	2.460367
H	-6.022001	9.035429	1.680527
H	-5.200399	9.114684	-0.653957
H	-5.746086	7.270184	-2.216590

**ESIPT structure of PUBO-a2 in the S<sub>1</sub> state**

E = -1088.77781834

C	-2.257446	2.935275	-0.141148
C	-1.010306	2.415610	0.215764
C	-0.862134	1.111509	0.672861
C	-1.967806	0.257255	0.794944
C	-3.185998	0.780519	0.441667
C	-3.351228	2.090703	-0.020017
N	-4.690778	2.234525	-0.265496
C	-5.340412	1.069611	0.028102
O	-4.407487	0.152033	0.471206
C	-6.699815	0.777462	-0.062413
C	-7.174564	-0.510478	0.308296
C	-8.513912	-0.827850	0.236727
C	-9.434103	0.123036	-0.206835
C	-8.995923	1.397665	-0.575512
C	-7.650727	1.769609	-0.525454
N	-7.127178	3.005090	-0.884656
C	-7.844959	4.036588	-1.278287
N	-7.054779	5.153647	-1.665647
C	-6.844940	6.123496	-0.772456
C	-7.290906	6.088888	0.581628
C	-7.010477	7.129483	1.438293
C	-6.281676	8.236414	0.999050
C	-5.832030	8.294618	-0.322119
C	-6.106135	7.266397	-1.193422

O	-9.082371	4.174009	-1.425382
H	-2.366260	3.951313	-0.496889
H	-0.136371	3.050652	0.132466
H	0.120712	0.743999	0.939956
H	-1.868985	-0.760657	1.149051
H	-6.461042	-1.248708	0.652770
H	-8.845616	-1.819085	0.525542
H	-10.488391	-0.119486	-0.268551
H	-9.707034	2.134979	-0.917685
H	-5.290683	2.997818	-0.613860
H	-7.854703	5.232921	0.930404
H	-7.357107	7.088745	2.464137
H	-6.066096	9.048339	1.681821
H	-5.266480	9.154169	-0.661309
H	-5.766529	7.297509	-2.221409

**PUBO-F in the  $S_0$  state**

E = -1189.58578863

C	-1.785578	2.220610	-0.083038
C	-0.607690	1.512130	-0.275736
C	-0.605908	0.124277	-0.461419
C	-1.784165	-0.615371	-0.460359
C	-2.939772	0.110309	-0.266517
C	-2.968491	1.491028	-0.080945
N	-4.288501	1.878477	0.080504
C	-4.983440	0.784156	-0.003719
O	-4.229287	-0.339186	-0.216738
C	-6.416325	0.618802	0.105412
C	-6.942703	-0.679939	0.086143
C	-8.298949	-0.909490	0.181242
C	-9.157029	0.178810	0.309685
C	-8.667502	1.470629	0.338709
C	-7.293721	1.729104	0.228299
N	-6.780892	3.012687	0.281901
C	-7.462413	4.198259	0.019543
N	-6.702174	5.283743	0.302781
C	-7.039922	6.613569	0.057056
C	-8.133902	7.042271	-0.706144
C	-8.356797	8.399918	-0.901631
C	-7.510644	9.355978	-0.356222
C	-6.420109	8.933584	0.397709
C	-6.184988	7.584941	0.601966
O	-8.611692	4.217868	-0.422718
H	-1.789380	3.293079	0.065452



H	0.336047	2.043898	-0.283368
H	0.336772	-0.388364	-0.608795
H	-1.791779	-1.688129	-0.602463
H	-6.259596	-1.514026	-0.004442
H	-8.684305	-1.920973	0.162626
H	-10.225426	0.020433	0.400066
H	-9.344322	2.303564	0.442140
H	-5.766433	3.075232	0.378104
H	-5.768202	5.133955	0.856387
H	-8.804771	6.313938	-1.133702
H	-9.210130	8.709034	-1.495255
H	-7.695944	10.411563	-0.514811
H	-5.743994	9.661511	0.832103
H	-5.334252	7.252304	1.185592
F	-4.572915	4.986664	1.572105

### 3. Vibrational Frequencies

#### PUBO in the $S_0$ state

mode	wave number $\text{cm}^{-1}$	IR intensity $\text{km/mol}$	selection rules IR
1	3.0082	5.1805	YES
2	22.8655	0.1395	YES
3	40.0857	0.5667	YES
4	41.6316	0.5813	YES
5	54.3335	12.1249	YES
6	60.9191	1.2466	YES
7	78.4151	1.0315	YES
8	112.7978	0.685	YES
9	152.0119	2.2297	YES
10	180.6448	12.8878	YES
11	216.532	4.006	YES
12	234.8153	2.3065	YES
13	244.933	0.1166	YES
14	254.0576	0.2413	YES
15	285.2296	5.584	YES
16	325.0289	0.3038	YES
17	332.3896	2.538	YES
18	372.7321	13.9826	YES
19	413.5821	0.0522	YES
20	418.89	4.3498	YES
21	418.9718	5.9429	YES
22	452.8112	5.2988	YES

23	496.2591	53.1359	YES
24	515.537	0.2048	YES
25	527.978	51.5421	YES
26	533.69	13.4685	YES
27	535.2076	0.1408	YES
28	566.6309	2.4826	YES
29	576.2883	3.7524	YES
30	622.8521	4.0739	YES
31	630.1178	1.9532	YES
32	632.9129	0.3203	YES
33	641.433	2.8442	YES
34	648.3683	7.0686	YES
35	666.76	0.0153	YES
36	698.6382	1.6561	YES
37	704.7993	76.2081	YES
38	722.7412	119.0752	YES
39	750.2096	152.367	YES
40	754.4345	234.8994	YES
41	758.6404	99.0285	YES
42	771.6219	9.12	YES
43	802.7114	18.8535	YES
44	820.9454	8.4166	YES
45	845.0628	0.1333	YES
46	845.1895	40.3975	YES
47	849.7865	0.0991	YES
48	872.101	2.6769	YES
49	898.2118	11.9091	YES
50	911.7391	15.1461	YES
51	912.7624	0.6628	YES
52	942.59	4.9261	YES
53	953.6559	0.1846	YES
54	959.7135	17.5298	YES
55	960.6292	3.2396	YES
56	961.4798	0.0091	YES
57	974.7815	0.0332	YES
58	975.067	1.0086	YES
59	1014.329	3.2164	YES
60	1027.866	20.7382	YES
61	1046.21	12.7643	YES
62	1058.658	54.4133	YES
63	1069.79	30.7316	YES
64	1080.972	37.6065	YES
65	1114.772	24.4779	YES
66	1127.498	15.8309	YES

67	1155.637	8.847	YES
68	1164.464	3.3357	YES
69	1172.611	1.5521	YES
70	1178.161	61.0218	YES
71	1199.364	36.723	YES
72	1218.276	50.4574	YES
73	1239.336	570.9495	YES
74	1261.964	542.3667	YES
75	1278.895	112.0256	YES
76	1288.348	239.7607	YES
77	1302.417	159.5153	YES
78	1315.538	92.297	YES
79	1335.261	639.9441	YES
80	1349.483	85.5242	YES
81	1369.339	14.4688	YES
82	1371.823	48.1703	YES
83	1397.177	4.9108	YES
84	1470.056	276.6635	YES
85	1474.262	219.3594	YES
86	1482.727	78.1885	YES
87	1509.023	187.0808	YES
88	1511.531	127.8675	YES
89	1530.922	205.4125	YES
90	1570.235	685.2495	YES
91	1578.387	561.1927	YES
92	1592.266	243.5525	YES
93	1639.007	605.9729	YES
94	1647.148	52.8616	YES
95	1649.715	123.3917	YES
96	1653.447	28.9116	YES
97	1664.998	32.3086	YES
98	1671.357	266.1402	YES
99	1731.84	344.5315	YES
100	3184.699	6.7397	YES
101	3190.775	3.4928	YES
102	3196.702	5.0787	YES
103	3198.016	2.4131	YES
104	3198.837	18.7864	YES
105	3209.199	5.0812	YES
106	3211.421	14.2474	YES
107	3212.094	7.9156	YES
108	3218.284	6.6981	YES
109	3225.625	4.6891	YES
110	3225.755	4.43	YES

111	3258.875	5.9135	YES
112	3266.123	12.9813	YES
113	3302.333	738.6529	YES
114	3614.946	87.3295	YES

**PUBO in the S<sub>1</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
1	16.9274	2.4285	YES
2	30.2917	1.8191	YES
3	40.6864	0.8707	YES
4	46.9367	1.0589	YES
5	55.9168	1.7527	YES
6	80.8972	15.9793	YES
7	93.9443	0.4191	YES
8	114.0071	1.6558	YES
9	140.5845	3.7224	YES
10	176.6203	99.6533	YES
11	210.3818	88.6764	YES
12	216.9521	3.6545	YES
13	240.838	1.2748	YES
14	258.6501	1.2581	YES
15	286.6152	96.5594	YES
16	302.6432	0.3181	YES
17	331.4618	13.5528	YES
18	369.0316	38.8706	YES
19	399.3139	0.0169	YES
20	402.1132	0.1872	YES
21	413.8698	6.94	YES
22	417.9137	6.4277	YES
23	466.704	0.1323	YES
24	475.7177	6.6306	YES
25	486.179	13.5639	YES
26	508.7427	4266.25	YES
27	542.4118	2.5762	YES
28	552.8516	11.365	YES
29	561.174	206.0087	YES
30	571.7923	40.1433	YES
31	592.5343	74.6277	YES
32	620.6394	61.3922	YES
33	622.3167	41.1115	YES
34	626.5274	896.4185	YES
35	632.8294	0.9231	YES
36	638.6667	74.0096	YES

37	669.2359	1361.913	YES
38	713.0603	59.6784	YES
39	725.8057	70.2893	YES
40	727.4326	201.7093	YES
41	747.6413	179.9781	YES
42	785.403	1404.513	YES
43	804.327	0.4635	YES
44	812.5292	0.1058	YES
45	813.728	241.2081	YES
46	833.7631	0.4857	YES
47	838.9526	643.6463	YES
48	869.2307	122.3948	YES
49	879.639	1016.877	YES
50	885.1736	2.7791	YES
51	904.65	0.353	YES
52	908.5589	837.63	YES
53	913.4977	5.1438	YES
54	917.2126	42.3757	YES
55	923.1679	0.316	YES
56	941.5446	1.4711	YES
57	963.2206	1.2533	YES
58	972.5527	20985.05	YES
59	983.3648	0.004	YES
60	1017.512	1888.308	YES
61	1024.436	708.9024	YES
62	1033.45	203.5651	YES
63	1044.57	1126.983	YES
64	1048.97	452.1518	YES
65	1060.794	6351.275	YES
66	1116.318	65.8649	YES
67	1118.578	59.8184	YES
68	1140.155	39.5668	YES
69	1158.803	197.299	YES
70	1167.369	298.164	YES
71	1174.485	2.4824	YES
72	1200.306	168.4559	YES
73	1202.472	25.5019	YES
74	1239.267	1150.749	YES
75	1261.89	1770.038	YES
76	1283.137	50.7763	YES
77	1295.512	233.8609	YES
78	1316.238	1925.536	YES
79	1317.277	212.8144	YES
80	1352.894	1591.888	YES

81	1359.441	1369.368	YES
82	1382.086	25.7458	YES
83	1403.939	337.4869	YES
84	1438.812	513.3578	YES
85	1446.03	3112.996	YES
86	1470.354	30.2813	YES
87	1483.187	1069.299	YES
88	1499.271	54.7888	YES
89	1512.312	10.917	YES
90	1527.39	131.7134	YES
91	1548.885	1094.337	YES
92	1571.103	204.5667	YES
93	1590.484	69.3706	YES
94	1601.122	747.2299	YES
95	1612.845	2291.02	YES
96	1631.636	813.0244	YES
97	1638.425	409.841	YES
98	1672.904	95.5391	YES
99	1741.469	716.1084	YES
100	3009.135	652.4145	YES
101	3189.506	25.0754	YES
102	3194.016	54.227	YES
103	3197.202	1.3789	YES
104	3202.906	88.1388	YES
105	3204.619	8.4221	YES
106	3210.718	10.6178	YES
107	3212.188	12.0564	YES
108	3216.389	17.9333	YES
109	3219.036	79.3022	YES
110	3220.269	308.4371	YES
111	3224.48	47.611	YES
112	3257.902	26.5356	YES
113	3265.354	56.0889	YES
114	3586.785	504.6081	YES

**PUBO-e in the S<sub>1</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
1	13.8228	4.0112	YES
2	21.3759	0.7801	YES
3	29.4488	2.4608	YES
4	48.7911	2.4637	YES
5	52.5777	2.6203	YES
6	62.597	5.9771	YES

7	94.0133	3.3625	YES
8	106.7666	8.721	YES
9	150.3116	4.106	YES
10	176.6122	1.8961	YES
11	210.2694	0.6195	YES
12	225.0701	0.5991	YES
13	233.916	2.5822	YES
14	254.3603	6.7444	YES
15	283.8423	19.6336	YES
16	310.3703	1.2378	YES
17	326.1877	70.4649	YES
18	364.8893	0.6654	YES
19	389.0158	4.209	YES
20	404.0491	0.1824	YES
21	411.991	84.1313	YES
22	420.2835	40.0433	YES
23	473.2719	14.641	YES
24	481.6881	5.4352	YES
25	484.6431	5.5024	YES
26	497.9946	77.8718	YES
27	520.6476	689.335	YES
28	543.9025	312.2958	YES
29	571.6792	15.6453	YES
30	590.4165	58.6001	YES
31	598.2803	7.7136	YES
32	605.2366	13.4737	YES
33	622.7303	8.9054	YES
34	629.3752	55.7928	YES
35	633.2486	42.375	YES
36	635.8255	11.3844	YES
37	657.1567	151.5681	YES
38	679.6291	45.6945	YES
39	725.69	104.7438	YES
40	734.5681	125.648	YES
41	739.0745	207.7215	YES
42	749.8167	278.2451	YES
43	798.6677	393.9523	YES
44	813.6607	60.8127	YES
45	821.3471	0.2809	YES
46	827.438	57.6462	YES
47	834.7272	2.048	YES
48	834.9587	132.1581	YES
49	889.4072	97.5216	YES
50	891.0694	23.3025	YES

51	901.6053	4.754	YES
52	901.6597	313.6208	YES
53	905.5524	6.5614	YES
54	912.0624	21.3373	YES
55	932.9559	0.5679	YES
56	936.3281	5.4156	YES
57	960.3535	1.6256	YES
58	978.5585	15.8536	YES
59	991.3044	4236.53	YES
60	1011.639	471.197	YES
61	1028.173	67.857	YES
62	1037.296	77.0045	YES
63	1049.14	0.2151	YES
64	1065.746	1035.346	YES
65	1082.532	3750.43	YES
66	1112.823	73.4339	YES
67	1117.546	8.9194	YES
68	1122.324	95.7683	YES
69	1163.877	337.6974	YES
70	1168.589	78.5561	YES
71	1172.214	2.9076	YES
72	1185.254	625.1041	YES
73	1199.843	84.7175	YES
74	1218.402	343.3372	YES
75	1250.877	481.842	YES
76	1267.511	291.3936	YES
77	1280.925	87.916	YES
78	1298.548	292.4843	YES
79	1328.986	2.1504	YES
80	1335.2	153.8904	YES
81	1351.777	145.892	YES
82	1363.507	987.9518	YES
83	1381.952	14.1393	YES
84	1426.147	40.777	YES
85	1448.152	195.8002	YES
86	1449.151	364.4388	YES
87	1465.741	6.3775	YES
88	1490.004	102.8109	YES
89	1505.216	88.1324	YES
90	1516.784	252.8094	YES
91	1530.878	281.8679	YES
92	1553.009	516.6165	YES
93	1563.108	142.8783	YES
94	1591.101	508.2744	YES



95	1606.945	45.5638	YES
96	1633.657	633.8251	YES
97	1642.812	181.5483	YES
98	1650.167	233.7941	YES
99	1659.34	97.0331	YES
100	3193.21	2.2603	YES
101	3194.105	12.7859	YES
102	3197.982	30.1907	YES
103	3198.953	6.4247	YES
104	3206.603	14.3096	YES
105	3209.396	49.4353	YES
106	3212.255	14.791	YES
107	3217.158	157.0498	YES
108	3219.156	27.5004	YES
109	3224.985	1.1876	YES
110	3227.533	0.7722	YES
111	3250.057	9.1594	YES
112	3260.175	33.9724	YES
113	3495.888	871.5219	YES
114	3604.444	240.0646	YES

**PUBO-a1 in the  $S_0$  state**

mode	wave number $\text{cm}^{-1}$	IR intensity $\text{km/mol}$	selection rules IR
1	18.3589	2.8346	YES
2	22.7814	1.2594	YES
3	26.6476	0.8142	YES
4	46.6233	1.5961	YES
5	58.1963	2.2717	YES
6	64.0266	2.4902	YES
7	77.5076	12.0241	YES
8	120.3759	6.3761	YES
9	156.9029	7.097	YES
10	168.1192	1.4467	YES
11	211.2679	2.9643	YES
12	223.2804	1.4146	YES
13	253.0631	0.7822	YES
14	260.8348	3.0689	YES
15	272.4675	20.7279	YES
16	329.3516	1.5261	YES
17	347.8336	3.9574	YES
18	356.5103	0.3099	YES
19	412.7103	0.0363	YES
20	422.9732	10.0312	YES

21	439.1994	28.9023	YES
22	478.2838	39.3815	YES
23	499.3948	15.704	YES
24	528.0408	8.1066	YES
25	536.654	14.9044	YES
26	541.4636	0.4361	YES
27	565.092	132.6596	YES
28	572.1026	6.8594	YES
29	575.516	6.4076	YES
30	603.4147	23.7417	YES
31	629.6893	2.0647	YES
32	637.3453	4.2029	YES
33	644.5583	21.8209	YES
34	685.7173	14.7764	YES
35	698.9608	4.1796	YES
36	713.3625	5.4789	YES
37	737.5617	64.1646	YES
38	743.7475	160.9213	YES
39	750.918	158.0249	YES
40	761.5355	255.718	YES
41	770.7154	6.4195	YES
42	800.0766	16.4424	YES
43	816.3736	47.7246	YES
44	840.1269	0.4637	YES
45	846.4482	25.8814	YES
46	849.3667	0.0365	YES
47	861.5521	11.6621	YES
48	884.1724	12.5822	YES
49	899.6252	5.4632	YES
50	908.9105	6.943	YES
51	933.6749	91.7819	YES
52	936.9465	5.6623	YES
53	947.4295	0.1587	YES
54	948.9197	0.0828	YES
55	955.0088	3.9464	YES
56	964.92	1.6274	YES
57	966.8268	0.3453	YES
58	1008.048	3.0602	YES
59	1025.765	197.659	YES
60	1028.082	19.2492	YES
61	1034.484	116.0799	YES
62	1051.689	80.8583	YES
63	1068.561	22.3781	YES
64	1103.816	30.3363	YES

65	1126.021	4.7256	YES
66	1150.145	47.15	YES
67	1163.106	7.1508	YES
68	1167.713	6.6879	YES
69	1173.045	92.902	YES
70	1189.446	66.6306	YES
71	1215.698	252.6065	YES
72	1233.049	668.0994	YES
73	1256.11	882.7812	YES
74	1273.393	66.8682	YES
75	1274.716	11.7687	YES
76	1293.514	41.8958	YES
77	1312.054	21.1444	YES
78	1330.826	792.9854	YES
79	1360.217	172.715	YES
80	1364.879	409.1014	YES
81	1395.85	881.3354	YES
82	1398.195	515.7668	YES
83	1445.234	399.1047	YES
84	1464.643	363.6039	YES
85	1483.878	127.8628	YES
86	1501.121	719.2801	YES
87	1509.056	5.0795	YES
88	1524.609	41.7117	YES
89	1534.585	131.0044	YES
90	1571.265	788.4377	YES
91	1595.909	203.4478	YES
92	1607.322	885.1739	YES
93	1628.497	111.2364	YES
94	1643.946	119.7162	YES
95	1651.439	236.8333	YES
96	1656.213	130.9243	YES
97	1663.552	23.4427	YES
98	3176.089	14.3159	YES
99	3178.118	15.154	YES
100	3182.393	5.0779	YES
101	3191.722	26.5263	YES
102	3193.299	2.5522	YES
103	3199.559	7.5872	YES
104	3204.615	7.1673	YES
105	3207.325	19.2989	YES
106	3213.585	23.6648	YES
107	3213.673	6.3766	YES
108	3221.679	5.574	YES

109	3224.572	9.2984	YES
110	3248.825	7.3946	YES
111	3616.525	62.76	YES

**PUBO-a2 in the S<sub>0</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
1	18.7119	0.1693	YES
2	24.1439	1.0629	YES
3	41.0581	0.8997	YES
4	44.7523	5.0401	YES
5	61.8892	0.3186	YES
6	71.2344	4.2006	YES
7	100.281	1.3951	YES
8	112.2235	2.1735	YES
9	149.2225	1.609	YES
10	179.5923	10.1195	YES
11	219.6881	7.5798	YES
12	232.6552	0.0642	YES
13	253.0069	0.3742	YES
14	263.8026	2.1028	YES
15	284.0719	1.1896	YES
16	325.7547	0.4802	YES
17	333.568	3.1366	YES
18	381.2898	38.4263	YES
19	415.0608	3.4411	YES
20	419.0792	4.1334	YES
21	422.0993	0.048	YES
22	452.53	7.2307	YES
23	510.7511	17.4983	YES
24	517.0276	7.103	YES
25	531.773	11.0465	YES
26	534.0757	0.2193	YES
27	565.1031	0.666	YES
28	576.323	8.0903	YES
29	626.4759	3.3722	YES
30	627.2558	3.111	YES
31	632.1575	11.5663	YES
32	640.9408	2.6655	YES
33	645.196	10.2819	YES
34	666.3576	0.2804	YES
35	698.418	1.779	YES
36	710.2314	6.172	YES
37	741.3079	240.1664	YES

38	749.8883	48.4609	YES
39	753.307	256.1805	YES
40	765.3177	5.929	YES
41	774.4617	57.2806	YES
42	798.6441	50.8101	YES
43	814.0445	2.5408	YES
44	843.8129	0.0188	YES
45	844.6272	29.271	YES
46	849.5509	0.098	YES
47	867.2763	3.5051	YES
48	887.5857	20.0008	YES
49	901.4026	10.1042	YES
50	911.0098	19.1331	YES
51	939.5491	5.2893	YES
52	946.6795	0.157	YES
53	949.7914	27.1788	YES
54	950.576	0.5962	YES
55	953.2901	2.2003	YES
56	967.9633	1.1559	YES
57	968.7872	0.4867	YES
58	998.5518	206.2611	YES
59	1021.505	153.0341	YES
60	1027.904	23.6275	YES
61	1045.971	10.6668	YES
62	1056.637	78.8481	YES
63	1069.728	78.0442	YES
64	1093.357	47.4922	YES
65	1126.279	22.9909	YES
66	1149.526	48.5734	YES
67	1163.487	5.1236	YES
68	1164.276	1.9465	YES
69	1172.518	135.2751	YES
70	1175.763	34.3551	YES
71	1217.065	148.0449	YES
72	1225.378	485.5675	YES
73	1262.948	110.762	YES
74	1274.556	784.6861	YES
75	1291.215	734.8433	YES
76	1308.27	523.5166	YES
77	1312.419	130.2566	YES
78	1318.959	632.8074	YES
79	1346.951	0.3592	YES
80	1371.727	37.663	YES
81	1391.652	970.3152	YES

82	1398.31	155.9223	YES
83	1468.134	93.7625	YES
84	1478.057	23.2618	YES
85	1481.734	96.7757	YES
86	1491.277	159.6066	YES
87	1507.357	541.2326	YES
88	1511.549	99.8966	YES
89	1547.478	147.5931	YES
90	1575.527	804.1772	YES
91	1595.782	259.7478	YES
92	1601.185	427.2258	YES
93	1620.421	886.0665	YES
94	1646.948	11.22	YES
95	1654.021	340.7231	YES
96	1661.558	78.251	YES
97	1666.125	30.83	YES
98	3167.619	21.6306	YES
99	3171.904	12.5148	YES
100	3185.456	40.3155	YES
101	3188.339	10.5765	YES
102	3196.242	2.5257	YES
103	3200.074	28.7193	YES
104	3207.535	5.4462	YES
105	3207.65	9.2937	YES
106	3216.594	7.8187	YES
107	3222.501	9.4075	YES
108	3223.715	4.2197	YES
109	3242.942	4.0246	YES
110	3255.15	21.7319	YES
111	3447.675	393.6521	YES

**PUBO-a2 in the S<sub>1</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
1	17.4165	3.8786	YES
2	27.7067	4.1252	YES
3	35.579	0.3559	YES
4	53.4871	0.6591	YES
5	56.4945	2.0666	YES
6	86.3573	1.2023	YES
7	91.1773	3.595	YES
8	123.4555	7.7097	YES
9	152.3619	2.6906	YES
10	158.9538	1.012	YES

11	199.5117	4.1061	YES
12	229.3085	1.1913	YES
13	249.9286	0.1099	YES
14	256.9764	0.4082	YES
15	273.4851	10.6015	YES
16	306.9327	1.4348	YES
17	329.2663	2.3443	YES
18	394.786	13.9292	YES
19	401.5295	0.0977	YES
20	410.7414	15.7735	YES
21	420.4141	9.4212	YES
22	449.6264	9.0074	YES
23	481.3349	0.4715	YES
24	482.8028	4.5253	YES
25	514.3635	2.8513	YES
26	538.0637	16.7775	YES
27	556.7701	0.4046	YES
28	562.4805	2.2213	YES
29	571.5299	4.1303	YES
30	590.301	33.8844	YES
31	609.9982	6.07	YES
32	618.8051	19.0614	YES
33	620.6788	28.278	YES
34	635.2756	1.4866	YES
35	640.5257	0.0068	YES
36	666.2383	16.2916	YES
37	703.2948	19.7747	YES
38	709.0523	132.8894	YES
39	726.2267	172.8564	YES
40	743.1405	167.7709	YES
41	791.6299	36.0778	YES
42	796.1975	2.0312	YES
43	810.4334	0.4825	YES
44	820.579	12.2097	YES
45	823.527	76.9228	YES
46	831.0142	36.8643	YES
47	858.4079	43.4989	YES
48	874.8519	96.8745	YES
49	876.7532	10.4958	YES
50	882.8618	11.5226	YES
51	911.0495	11.3748	YES
52	911.7231	7.8421	YES
53	911.9435	16.0075	YES
54	918.6826	0.1415	YES

55	937.1005	0.2846	YES
56	974.6315	5.5483	YES
57	988.386	25.8968	YES
58	989.571	18.4761	YES
59	1021.286	91.5427	YES
60	1024.657	62.3399	YES
61	1028.298	477.6457	YES
62	1038.128	18.4654	YES
63	1049.918	71.7674	YES
64	1110.944	33.8677	YES
65	1111.724	35.2348	YES
66	1128.083	83.9879	YES
67	1160.61	21.8683	YES
68	1162.483	6.2485	YES
69	1169.123	2.9625	YES
70	1181.895	24.7851	YES
71	1196.758	221.328	YES
72	1210.507	155.9826	YES
73	1253.213	161.682	YES
74	1272.428	310.977	YES
75	1284.238	574.4389	YES
76	1314.167	528.0527	YES
77	1319.458	190.7867	YES
78	1329.819	636.6684	YES
79	1359.483	16.8476	YES
80	1365.7	20.0441	YES
81	1395.842	130.1924	YES
82	1410.972	99.9867	YES
83	1441.456	333.8363	YES
84	1475.831	13.6058	YES
85	1482.114	490.5373	YES
86	1487.143	19.4404	YES
87	1493	20.364	YES
88	1493.56	28.3241	YES
89	1532.34	284.5981	YES
90	1569.906	518.0976	YES
91	1576.009	1.6362	YES
92	1599.783	1155.929	YES
93	1615.558	127.2765	YES
94	1624.078	342.6248	YES
95	1643.288	280.0746	YES
96	1651.759	242.2155	YES
97	1666.807	393.9179	YES
98	3177.648	31.4811	YES



99	3181.946	27.5192	YES
100	3198.472	4.5623	YES
101	3200.963	57.2832	YES
102	3202.124	760.594	YES
103	3204.741	27.9811	YES
104	3205.573	82.8303	YES
105	3205.785	21.9176	YES
106	3213.1	0.0762	YES
107	3213.573	16.5884	YES
108	3215.319	3.0408	YES
109	3219.349	7.8206	YES
110	3225.418	11.5525	YES
111	3239.677	1.0884	YES

**PUBO-a2e in the S<sub>1</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
1	17.4902	2.7383	YES
2	28.2362	2.6643	YES
3	43.2632	1.5254	YES
4	48.2463	0.6059	YES
5	60.5793	3.0724	YES
6	81.883	13.9534	YES
7	103.307	4.3989	YES
8	121.4018	2.0566	YES
9	148.8253	6.9991	YES
10	167.0013	7.0214	YES
11	207.9587	2.721	YES
12	225.9604	1.7186	YES
13	253.2249	1.6075	YES
14	256.7394	39.1036	YES
15	272.9213	14.3943	YES
16	317.3885	4.5155	YES
17	327.7057	8.461	YES
18	390.3717	0.4253	YES
19	399.9876	21.413	YES
20	407.2053	12.9877	YES
21	422.9471	5.4431	YES
22	453.0684	2.3007	YES
23	477.7227	1.3819	YES
24	480.1667	5.1138	YES
25	496.1854	4.6693	YES
26	525.7042	19.4738	YES
27	541.9213	61.7775	YES

28	554.4828	18.8099	YES
29	571.4686	10.7234	YES
30	589.9334	17.825	YES
31	595.1578	13.9145	YES
32	614.2471	2.0033	YES
33	629.4829	35.5298	YES
34	634.2944	7.4725	YES
35	646.8533	15.7458	YES
36	661.8564	24.3174	YES
37	705.5394	39.1676	YES
38	724.366	22.3073	YES
39	729.8112	391.1164	YES
40	740.0775	42.4758	YES
41	745.1453	159.0131	YES
42	800.8242	26.2958	YES
43	812.897	2.6746	YES
44	817.7494	0.2939	YES
45	820.0025	10.6622	YES
46	822.5202	4.9428	YES
47	853.4273	35.0072	YES
48	875.8951	21.0202	YES
49	882.2544	6.9247	YES
50	885.5167	73.9133	YES
51	892.7214	4.0877	YES
52	900.4148	0.7318	YES
53	913.2867	19.5448	YES
54	926.2563	0.4906	YES
55	931.7485	0.2338	YES
56	968.9446	8.3875	YES
57	981.4361	0.5413	YES
58	986.5698	56.7458	YES
59	1010.174	62.937	YES
60	1023.155	37.6238	YES
61	1031.525	171.3771	YES
62	1038.538	14.6326	YES
63	1056.213	50.8659	YES
64	1107.04	26.1539	YES
65	1110.949	24.063	YES
66	1122.213	109.7816	YES
67	1149.852	181.3924	YES
68	1163.358	46.3904	YES
69	1166.784	2.9825	YES
70	1169.189	84.6059	YES
71	1177.43	11.0114	YES

72	1213.684	107.5181	YES
73	1219.004	92.1559	YES
74	1264.978	21.6005	YES
75	1276.414	263.7348	YES
76	1317.487	32.8148	YES
77	1318.637	100.95	YES
78	1334.196	342.3325	YES
79	1347.973	305.0836	YES
80	1350.175	252.4003	YES
81	1364.263	57.1986	YES
82	1388.589	1072.631	YES
83	1428.039	14.8915	YES
84	1446.907	356.9529	YES
85	1475.987	10.4884	YES
86	1480.123	262.8557	YES
87	1490.324	30.8898	YES
88	1495.927	146.8221	YES
89	1501.174	260.7104	YES
90	1544.558	304.2855	YES
91	1563.739	2397.101	YES
92	1578.83	5.5406	YES
93	1598.417	499.4397	YES
94	1611.339	69.7187	YES
95	1614.382	47.2637	YES
96	1649.883	455.0862	YES
97	1661.625	0.8407	YES
98	3177.499	10.5433	YES
99	3193.747	23.626	YES
100	3193.79	11.6004	YES
101	3193.948	10.8151	YES
102	3198.126	4.184	YES
103	3206.204	21.2194	YES
104	3208.45	17.3969	YES
105	3210.579	8.2284	YES
106	3213.896	11.3948	YES
107	3220.249	18.3944	YES
108	3221.734	7.6025	YES
109	3229.033	0.5293	YES
110	3236.292	10.7936	YES
111	3241.53	1272.194	YES

**PUBO-F in the S<sub>0</sub> state**

mode	wave number cm <sup>-1</sup>	IR intensity km/mol	selection rules IR
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1	18.8288	3.9469	YES
2	27.5576	1.4928	YES
3	32.0756	2.1054	YES
4	47.5516	2.2879	YES
5	56.4703	2.5383	YES
6	64.9937	3.5212	YES
7	81.7503	7.2044	YES
8	97.2324	13.5045	YES
9	115.5846	40.1762	YES
10	120.6522	7.0761	YES
11	143.5865	4.6284	YES
12	188.4395	8.4863	YES
13	209.5416	8.368	YES
14	243.987	3.4909	YES
15	254.6224	0.212	YES
16	256.3229	3.7309	YES
17	276.8413	162.7294	YES
18	289.2209	14.0094	YES
19	327.9017	1.5692	YES
20	337.2989	3.7854	YES
21	382.0057	41.2306	YES
22	414.4755	0.1327	YES
23	420.0421	3.9346	YES
24	424.5993	15.7284	YES
25	459.1303	12.1176	YES
26	509.4783	15.3909	YES
27	521.7436	12.0966	YES
28	534.7077	18.4824	YES
29	539.7857	0.1615	YES
30	565.9395	6.4867	YES
31	575.5299	1.6967	YES
32	628.8248	8.9773	YES
33	633.8614	2.2589	YES
34	638.4147	53.5032	YES
35	643.9672	16.1644	YES
36	649.8376	121.7835	YES
37	658.7921	2.5818	YES
38	676.227	5.7402	YES
39	698.4455	8.701	YES
40	719.6916	4.5206	YES
41	747.3025	75.8581	YES
42	756.021	148.8671	YES
43	757.8966	225.937	YES
44	765.6561	75.0801	YES

45	794.8315	21.2798	YES
46	822.2021	71.2605	YES
47	845.6107	20.6498	YES
48	852.9784	0.0528	YES
49	852.9846	0.4087	YES
50	861.2754	3.9564	YES
51	902.1066	18.5433	YES
52	905.3224	32.1786	YES
53	911.0308	14.39	YES
54	944.2398	4.4174	YES
55	955.5165	25.7078	YES
56	957.7305	1.2218	YES
57	958.9976	0.2768	YES
58	960.2208	3.2261	YES
59	968.5396	0.4106	YES
60	975.8949	1.1806	YES
61	1011.582	24.5762	YES
62	1027.265	25.3194	YES
63	1038.562	91.7599	YES
64	1054.337	42.0351	YES
65	1063.532	77.9695	YES
66	1064.803	117.3476	YES
67	1077.875	54.804	YES
68	1104.445	13.5635	YES
69	1126.799	20.7179	YES
70	1156.36	22.0825	YES
71	1163.841	3.1006	YES
72	1169.986	2.1735	YES
73	1178.772	62.2459	YES
74	1187.968	20.8925	YES
75	1219.058	51.259	YES
76	1255.359	159.9016	YES
77	1264.856	606.9392	YES
78	1280.319	176.9832	YES
79	1297.411	1223.014	YES
80	1301.132	130.8865	YES
81	1314.742	29.6817	YES
82	1328.089	329.2259	YES
83	1348.277	69.9075	YES
84	1369.651	17.6185	YES
85	1372.778	239.991	YES
86	1397.401	8.594	YES
87	1471.83	232.0473	YES
88	1476.274	56.4818	YES

89	1482.274	89.3701	YES
90	1508.479	19.8478	YES
91	1511.219	131.2029	YES
92	1526.928	379.4759	YES
93	1559.142	534.9582	YES
94	1589.005	358.6994	YES
95	1610.82	218.9566	YES
96	1624.797	302.6494	YES
97	1644.698	332.7141	YES
98	1648.832	23.3943	YES
99	1662.94	46.5916	YES
100	1667.553	125.988	YES
101	1682.456	751.8104	YES
102	1730.349	116.4969	YES
103	2157.563	2842.457	YES
104	3180.506	2.1604	YES
105	3186.075	20.327	YES
106	3194.501	5.3506	YES
107	3196.958	2.4827	YES
108	3197.461	3.8619	YES
109	3206.68	25.203	YES
110	3208.186	6.3708	YES
111	3210.501	8.854	YES
112	3218.507	6.6428	YES
113	3224.659	7.1659	YES
114	3224.881	3.2888	YES
115	3254.576	2.711	YES
116	3256.901	3.5124	YES
117	3387.824	545.9638	YES