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Supporting Information

Ultrafast IR Spectroscopy of Photo-induced Electron Transfer in Self-assembled Donor-Acceptor Coordination Cages

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Results of DFT calculations

Geometry optimizations and IR spectra of the ligands were calculated with the ORCA electronic structure program package as described in the main article.

Neutral phenothiazine ligand **D**

Figure SI-1: Geometry optimized structure of the neutral phenothiazine ligand **D**.

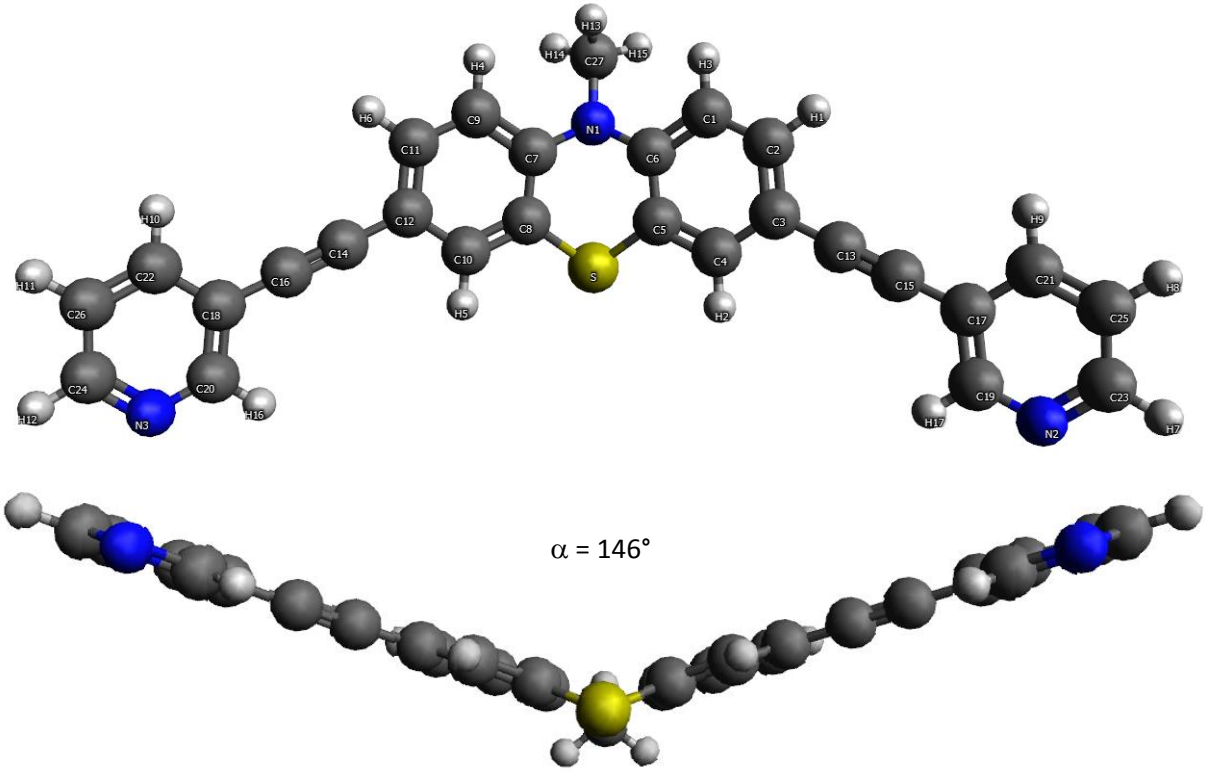

Table SI-1: Harmonic vibrational frequencies and intensities of **D.**

Freq / cm^{-1}	Int./km mol^{-1}
34.55	0.831661
39.29	1.211220
43.30	0.998120
47.04	0.911785
57.19	0.526784
90.26	0.101078
102.65	0.877015
113.75	0.076487
128.31	1.422830
140.42	1.672359
149.16	0.419161
163.75	0.288964
192.76	1.992761
212.26	0.042927
225.20	3.554161
247.76	0.041484
268.86	2.007094

270.43	0.582072
313.77	1.780745
338.38	0.207956
344.77	3.174807
366.37	2.137947
394.38	1.855725
397.06	4.002218
399.35	4.933753
424.49	0.847432
435.58	7.669744
437.21	13.208274
446.85	2.093959
447.02	0.531330
454.21	5.798922
478.16	12.915830
497.39	2.783598
529.61	8.038772
534.97	4.157249
538.87	1.604659
542.73	11.940448
563.78	0.179647
580.30	3.193436
588.40	2.745382
597.95	1.979512
607.18	3.630950
610.71	2.199818
641.87	9.678468
668.00	5.610443
679.85	2.234805
699.25	32.148984
701.12	33.603720
716.69	0.843787
733.84	0.717160
741.92	9.861223
764.73	0.809298
797.64	22.273891
798.00	21.521515
806.71	16.200397
811.85	51.732595
829.48	42.468475
885.22	2.101640
886.55	2.629159
888.62	24.132381
895.73	0.192047
915.27	0.537164
916.74	1.006296
928.77	0.248601
929.23	0.280809
941.94	0.775236
943.13	1.053502
973.86	0.323771
974.24	0.413366
996.18	9.018366
996.39	20.920818
1027.63	0.398176
1029.63	3.856858
1030.78	5.292731
1033.32	2.439617
1092.28	4.970827
1096.92	15.324377
1099.61	10.911191
1101.46	4.052077
1107.33	80.947421
1126.43	48.116548

1133.79	79.969641
1134.60	32.220601
1137.81	25.042583
1177.46	7.238171
1179.08	6.801046
1224.79	24.084227
1237.46	24.282899
1248.99	0.754920
1249.36	0.611613
1267.04	45.773691
1268.56	184.618972
1295.17	0.626302
1299.00	1.843269
1304.98	1.019736
1307.13	4.350809
1311.74	6.673289
1329.38	371.630836
1375.14	73.527000
1381.88	3.040609
1394.62	12.064812
1395.41	3.461325
1399.70	0.888381
1425.25	31.289505
1448.55	171.088098
1452.06	168.406069
1454.94	3.189162
1464.81	578.645626
1489.91	58.074819
1529.71	19.461669
1545.82	2.997944
1548.49	2.870952
1548.88	16.227741
1569.22	59.847762
1579.79	2.081918
1586.00	1.576181
1598.96	21.867305
2218.72	76.695360
2219.93	54.727525
2874.41	70.339627
2973.89	18.124371
3017.27	7.262588
3032.94	13.110115
3034.63	15.980487
3038.78	8.901293
3040.73	6.219728
3063.07	15.368475
3064.50	15.080667
3068.59	3.654859
3070.23	4.519005
3070.83	1.493124
3071.60	1.722411
3077.62	12.943995
3079.03	12.702155
3087.22	7.455267
3087.68	7.257505

Phenothiazine radical cation $\mathbf{D}^{\bullet+}$

Figure SI-2: Geometry optimized structure of the phenothiazine radical cation $\mathbf{D}^{\bullet+}$.

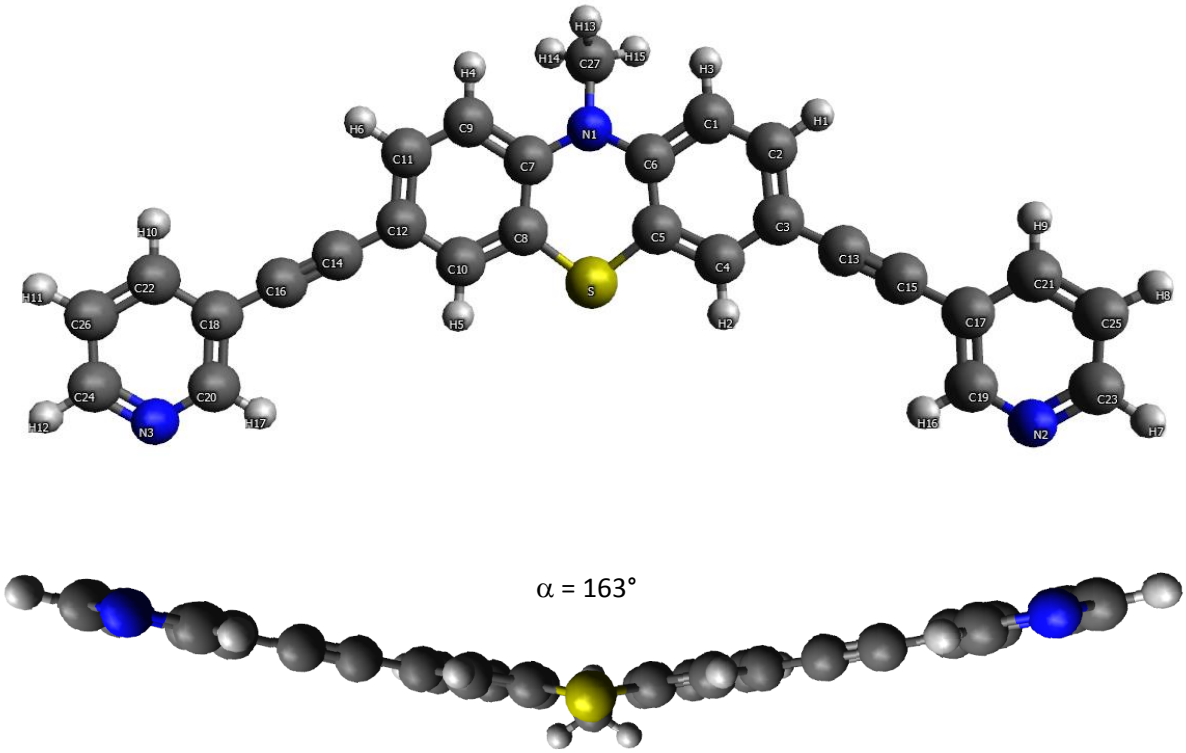

Table SI-2: Harmonic vibrational frequencies and intensities of $\mathbf{D}^{\bullet+}$.

Freq / cm^{-1}	Int./km mol^{-1}
37.36	0.058857
39.25	0.585598
41.88	0.961367
65.80	0.648431
92.44	0.720559
97.71	1.147219
118.09	0.158032
127.32	4.037895
140.70	1.611473
154.50	0.190085
163.20	0.181949
188.40	0.413993
215.08	29.974969
228.14	0.167080
232.42	0.642379
251.73	14.959850
274.30	3.256804
326.11	0.411668
348.70	0.214779
364.17	0.129478
374.73	3.080258
384.59	0.221815
390.32	6.739759

412.87	0.858909
419.67	1.874197
434.66	0.654249
438.60	20.174681
439.34	4.648538
452.24	3.507929
454.15	0.216972
479.92	3.730388
481.71	1.912853
529.41	2.094926
540.97	0.535812
544.74	2.070730
545.86	4.199129
560.42	10.887738
581.44	1.390058
586.62	5.281871
591.09	3.974882
604.37	1.938688
609.18	0.821560
645.48	15.127704
664.58	97.469654
672.30	1.980993
700.57	26.190287
707.64	23.241469
708.30	1.321266
721.47	0.734163
746.16	7.701804
764.86	4.309740
804.64	21.391111
807.82	22.354489
810.89	48.571931
812.33	4.174150
835.07	0.153158
879.72	27.268547
881.46	0.251524
893.58	3.712062
905.63	7.423535
921.56	1.769065
923.25	2.219746
953.88	0.013621
955.07	0.052811
960.70	0.329050
964.57	0.166562
994.27	94.010496
994.89	47.755962
995.97	9.052863
1011.68	0.646091
1021.36	10.479030
1027.85	47.851747
1029.97	21.212597
1041.01	32.356808
1082.38	2.824843
1084.62	16.860083
1088.48	697.565288
1098.71	5.652986
1108.75	48.130686
1130.24	495.976619
1136.57	63.847551
1142.69	7.363029
1153.97	10.010529
1181.43	68.213403
1183.29	52.392934
1225.23	10.740776
1239.67	13.744752

1255.37	3.020213
1256.43	5.307000
1262.26	13.714027
1288.05	199.325115
1302.86	43.026059
1307.39	119.321341
1311.02	37.585872
1312.77	574.734730
1318.77	61.759610
1336.60	0.089139
1370.56	818.332069
1385.40	4.809830
1394.01	21.542923
1396.62	17.113409
1398.27	5.045761
1427.98	38.863566
1440.49	28.822562
1445.72	86.594289
1452.94	0.294066
1463.22	1.815194
1484.09	50.490932
1497.93	0.071062
1522.84	12.682220
1542.83	47.386106
1544.05	62.919255
1558.98	2352.303807
1575.85	77.687061
1584.07	0.193565
1593.74	1.546542
2184.31	5737.092886
2194.58	281.898825
2932.76	8.180868
3025.26	2.280685
3036.61	3.118956
3040.64	3.628973
3046.03	6.309328
3046.81	4.506394
3055.19	0.667143
3070.59	1.186166
3071.20	1.298176
3072.03	1.093505
3072.16	1.130598
3084.11	0.003106
3084.27	0.306555
3085.63	13.635145
3086.43	9.511595
3104.33	1.048214
3105.72	0.547559

Neutral anthraquinone ligand **A**

Figure SI-3: Geometry optimized structure of the neutral anthraquinone ligand **A**.

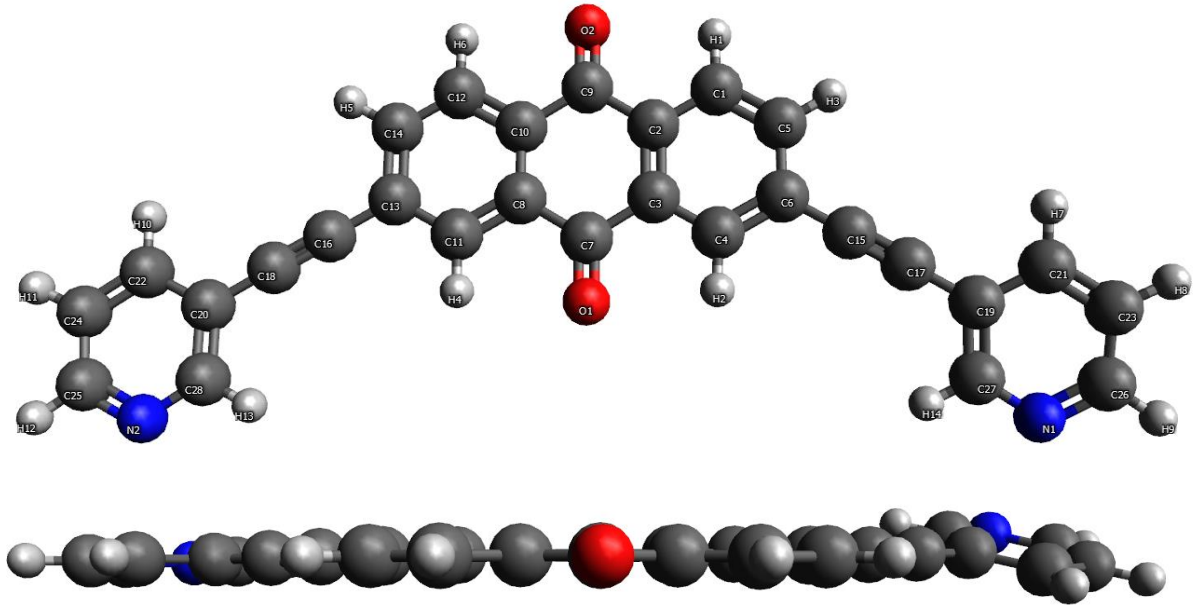

Table SI-3: Harmonic vibrational frequencies and intensities of **A**.

Freq / cm^{-1}	Int./km mol^{-1}
36.27	0.501827
43.97	1.848885
88.26	0.666779
88.70	4.599532
96.86	0.387836
124.26	1.121549
131.13	0.012173
138.52	0.311163
159.43	0.031369
170.05	0.194086
214.63	0.243107
219.20	0.011651
225.41	0.161380
274.94	1.399224
286.59	1.295363
308.33	0.106453
379.49	1.423137
382.89	56.962399
387.57	0.027612
388.61	0.426864
396.57	5.766616
402.57	2.049644
409.59	0.094440
413.83	7.536456
434.83	0.176812
454.27	7.740232
462.54	1.392309
469.21	8.827270
509.14	6.600715
533.94	0.061437

537.74	0.275058
556.22	0.115367
556.95	0.247103
574.86	0.306004
582.59	0.797925
589.08	0.359963
610.23	10.670878
614.35	0.344212
637.54	16.576131
660.18	28.324090
676.20	0.172232
688.95	0.718879
694.88	51.556438
697.40	38.583212
710.14	0.092613
718.40	0.218119
739.52	19.369510
772.78	1.816339
796.63	30.387554
798.02	17.087714
807.91	12.281992
818.40	5.180300
840.99	0.072446
863.55	47.748286
899.47	0.202000
914.39	74.072314
914.73	90.091867
918.94	1.232883
922.23	0.800293
933.84	3.622793
942.52	2.911785
945.76	0.818597
971.98	0.254504
976.12	0.652042
978.25	0.025458
981.03	0.174328
986.96	29.101781
996.44	15.979023
997.49	13.372360
1029.01	0.052294
1029.17	0.162767
1061.45	3.039700
1084.23	20.289023
1092.57	2.390760
1093.83	4.217375
1106.96	4.297309
1115.44	33.645004
1152.45	8.231669
1157.76	3.341056
1178.11	4.450483
1178.25	14.480094
1186.97	2.519762
1223.06	4.173175
1235.12	182.048819
1251.38	0.378993
1252.45	5.179682
1267.74	661.225590
1296.67	8.901335
1301.60	147.472203
1304.90	0.135130
1308.49	343.619950
1314.65	202.088074
1316.96	14.567097
1387.34	0.971627

1393.41	63.633747
1394.88	12.703919
1402.94	43.148590
1450.43	59.058739
1452.31	9.513491
1472.86	6.418678
1475.53	3.540456
1539.34	3.404007
1549.18	7.149785
1549.29	2.387838
1551.90	36.697036
1578.14	107.639136
1579.11	78.055143
1590.31	94.007793
1591.83	107.808066
1683.64	134.945369
1700.31	206.138840
2221.21	48.969948
2221.84	49.785213
3032.84	11.632061
3034.68	14.924315
3039.99	6.649404
3044.05	4.708222
3063.67	13.157796
3063.98	7.529400
3065.79	1.701037
3068.47	1.475659
3078.78	11.772357
3079.18	9.463025
3081.63	8.269919
3082.50	3.606930
3084.15	3.104823
3085.92	1.532512

Anthraquinone radical anion $\mathbf{A}^{\bullet-}$

Table SI-4: Harmonic vibrational frequencies and intensities of $\mathbf{A}^{\bullet-}$.

Freq / cm^{-1}	Int./km mol^{-1}
33.94	1.190558
36.59	0.705124
42.60	0.657386
60.37	1.652338
66.91	0.276701
92.98	0.026629
97.16	0.023510
113.58	4.914047
124.12	1.816972
151.59	0.081771
157.87	1.049863
159.60	1.000555
188.96	3.147259
216.95	0.549290
226.36	0.465707
231.26	0.581845
277.02	1.720973
284.11	0.681150
305.41	0.030123
371.83	7.472535
392.18	0.029793
396.05	0.725703
399.42	2.032311
407.76	4.254363
413.29	2.945451
416.59	28.831645
430.71	0.793070
453.22	13.595902
460.01	0.271178
467.79	3.676559
472.30	1.909026
499.08	2.145616
526.40	0.147080
534.13	1.827960
544.88	0.989819
557.26	2.636846
572.79	27.104670
583.17	2.409161
590.16	0.357204
609.86	15.511154
613.47	14.306278
633.38	0.254422
644.77	23.013882
674.95	1.209367
689.47	0.240321
698.47	32.988095
700.70	33.416991
706.67	10.410431
724.59	12.407084
729.46	3.076628
775.09	0.255699
789.34	23.756372
799.09	26.856236
801.70	7.430740
817.24	0.284142
824.71	2.717957
844.79	33.916066

894.00	2.548084
902.95	0.523226
904.20	0.049105
905.24	2.487036
928.82	0.958943
930.94	3.095193
931.92	2.944839
937.42	16.940534
958.96	0.720820
965.12	0.145230
967.95	0.339342
972.63	1.578601
976.60	55.566182
993.31	29.803973
993.78	26.692852
1026.58	126.834704
1026.88	15.289386
1055.96	19.499850
1077.94	767.124647
1088.68	8.919806
1088.92	7.248752
1098.76	7.800560
1108.43	216.615067
1152.42	17.897003
1161.03	1085.280672
1163.73	8.850947
1173.27	6.542455
1174.51	3.900755
1185.82	379.553425
1209.36	16.615717
1250.46	3.484009
1252.94	5.515115
1271.01	380.518659
1292.19	21.439935
1293.94	19.593006
1303.26	4.690596
1305.42	3.508020
1327.97	2.818015
1335.35	256.094370
1363.84	14.934430
1386.19	1.352296
1388.05	1.947385
1410.41	41.656994
1438.09	22.528592
1438.92	31.048516
1461.93	54.889469
1464.20	328.823969
1473.61	146.905578
1493.63	99.253362
1525.15	11.316304
1540.00	68.346256
1540.39	41.784321
1555.80	304.614596
1556.56	2065.352776
1579.83	6.938367
1583.82	1.247470
1619.18	30.829364
2180.91	4649.412330
2190.85	238.704322
3022.16	4.033915
3024.12	9.851500
3037.30	8.800230
3041.97	17.994582
3048.68	4.547679

3051.02	58.572997
3051.77	7.746130
3055.03	39.998060
3067.37	17.613843
3071.31	10.910490
3071.92	13.818978
3073.57	1.024356
3075.52	3.730184
3077.76	12.313827

Anthraquinone triplet $\mathbf{A}^{T}$

Table SI-5: Harmonic vibrational frequencies and intensities of $\mathbf{A}^{T}$.

Freq / cm^{-1}	Int./km mol^{-1}
33.81	0.702006
39.44	0.755915
56.37	1.212732
71.49	0.982827
87.75	0.020374
92.98	0.044856
104.51	5.100528
120.16	0.947502
140.04	0.247214
147.75	0.029987
158.82	1.651817
181.13	2.392429
215.03	0.667237
221.68	0.714891
225.93	0.443192
260.64	0.090761
276.82	0.666238
305.08	0.566062
370.36	0.765806
373.92	3.857263
384.52	26.198120
388.14	1.236019
393.47	5.673325
404.52	0.792782
409.70	6.355797
412.43	2.728601
436.86	0.156655
454.83	11.448205
462.70	2.805910
465.72	5.583678
470.54	6.162974
515.25	0.218092
528.31	2.930891
537.71	0.629243
549.13	4.053364
568.21	2.142553
576.82	3.602612
580.53	1.497050
602.72	8.499969
610.06	2.989771
620.05	8.126757
624.34	20.894798
665.25	7.244285
681.45	33.140717
683.21	10.060947
698.42	31.610591
703.68	0.171965
709.44	1.120754
725.74	17.333209
771.10	0.587511
790.90	23.360520
792.93	0.303482
797.55	20.070324
809.25	33.279014
836.00	0.959363
850.66	45.227925
873.45	25.314525

895.41	22.505189
910.63	0.291596
918.85	1.011664
925.29	0.869282
938.49	18.427890
940.53	2.600489
944.88	2.133097
957.59	92.799436
973.33	0.071622
974.65	0.103136
977.33	27.463180
978.83	0.916707
996.25	0.101637
997.53	15.906240
1014.95	66.842882
1029.15	0.770515
1041.39	226.656251
1079.24	42.632622
1087.03	12.835112
1093.23	10.120397
1101.37	22.461939
1114.31	93.613202
1144.71	26.305666
1160.86	15.457439
1169.54	19.169348
1173.41	22.299717
1177.84	8.840241
1197.70	8.365721
1222.10	46.992954
1251.00	4.896874
1251.97	2.825372
1265.64	19.188035
1286.30	97.141667
1299.50	5.612196
1301.81	23.646606
1305.87	9.098520
1322.12	62.759100
1331.96	95.383544
1340.57	27.052774
1369.16	100.793896
1393.24	35.445038
1397.20	126.403065
1403.57	327.659449
1447.14	11.178827
1464.08	273.310844
1468.51	154.528379
1483.22	33.482770
1488.24	564.011272
1515.58	99.667377
1528.95	211.888807
1539.76	555.635294
1549.19	13.603371
1570.01	612.037759
1577.05	50.135431
1590.00	35.673364
1660.66	111.972118
1981.25	457.316990
2217.48	13.423042
3034.41	14.593897
3041.04	2.979453
3041.22	2.703431
3044.50	0.749085
3064.39	5.676424
3064.89	10.072233

3066.98	2.024888
3071.56	4.517489
3075.29	2.437836
3078.95	14.181893
3081.79	14.282851
3082.48	0.383442
3085.58	9.198688
3089.12	1.120538