

Supporting Information

Electronic structure and spectral properties of aurones as visible range fluorescent probes: a DFT/TDDFT study

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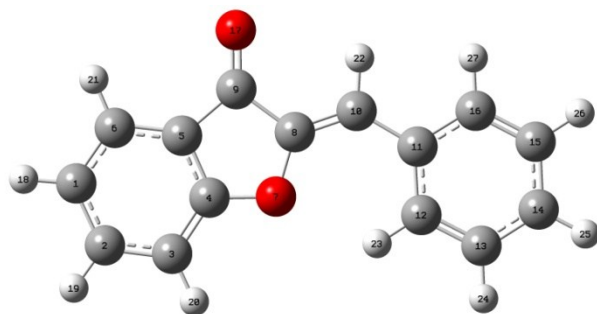
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Table S1. Comparison of the key geometric parameters between the experiment and computation for Z-2-p-methoxyaurone.

parameters	Exp.	PBE0	parameters	Exp.	PBE0
R(1-2)	1.38	1.384	A(2-1-6)	122.9	122.4
R(1-6)	1.39	1.390	A(1-2-3)	116.1	116.5
R(1-9)	1.38	1.366	A(6-1-9)	112.9	113.0
R(2-3)	1.38	1.391	A(1-6-5)	120.2	120.5
R(3-4)	1.40	1.400	A(1-6-7)	106.7	106.7
R(4-5)	1.38	1.386	A(1-9-8)	107.0	107.2
R(5-6)	1.39	1.390	A(2-3-4)	122.3	122.0
R(6-7)	1.46	1.469	A(3-4-5)	120.7	120.4
R(7-8)	1.48	1.487	A(4-5-6)	117.8	118.2
R(7-10)	1.23	1.213	A(6-7-8)	104.5	103.2
R(8-9)	1.40	1.380	A(6-7-10)	130.0	130.0
R(8-11)	1.33	1.342	A(7-8-9)	109.0	110.0
R(11-12)	1.45	1.444	A(7-8-11)	125.7	125.0
R(12-13)	1.40	1.400	A(8-11-12)	131.8	130.8
R(12-17)	1.40	1.409	A(13-12-17)	117.3	117.6
R(13-14)	1.38	1.387	A(12-13-14)	122.7	122.0
R(14-15)	1.39	1.395	A(12-17-16)	120.4	120.9
R(15-16)	1.39	1.400	A(14-15-16)	119.9	119.5
R(15-18)	1.36	1.348	A(15-16-17)	120.9	120.6
R(16-17)	1.37	1.377			
R(18-19)	1.43	1.411			

Table S2. Comparison of the calculated key geometric parameters at gas phase and solvent (ethanol) for Z-aurone.



parameters	gas	ethanol	parameters	gas	ethanol
R(1,2)	1.3997	1.4013	A(5,4,7)	112.9823	112.8559
R(1,6)	1.3865	1.386	A(4,5,6)	120.5047	120.4448
R(2,3)	1.3906	1.391	A(4,5,9)	106.6736	106.6373
R(3,4)	1.3832	1.3832	A(6,5,9)	132.8217	132.9179
R(4,7)	1.3674	1.3677	A(1,6,5)	118.157	118.0923
R(5,6)	1.3902	1.3926	A(4,7,8)	107.2631	107.2412
R(5,9)	1.4678	1.463	A(7,8,9)	109.8979	109.8679
R(7,8)	1.3773	1.3762	A(7,8,10)	125.2617	125.0612
R(8,10)	1.3403	1.3417	A(9,8,10)	124.8404	125.0709
R(9,17)	1.2115	1.2173	A(5,9,8)	103.1831	103.3976
R(10,11)	1.4494	1.4494	A(5,9,17)	130.1321	130.0501
R(11,12)	1.4042	1.4053	A(8,9,17)	126.6848	126.5523
R(11,16)	1.4029	1.4041	A(8,10,11)	130.7491	130.6754
R(13,14)	1.3918	1.3929	A(10,11,12)	123.5673	123.6406
R(14,15)	1.3902	1.3913	A(10,11,16)	118.0495	117.8751
R(15,16)	1.3856	1.3864	A(12,11,16)	118.3832	118.4843
A(1,2,3)	122.0178	122.0786	A(11,12,13)	120.3455	120.3094
A(2,3,4)	116.4863	116.3837	A(12,13,14)	120.5704	120.5259
A(3,4,5)	122.4584	122.5765	A(13,14,15)	119.7212	119.7844
A(3,4,7)	124.5594	124.5675	A(14,15,16)	119.9209	119.9253
			A(11,16,15)	121.0588	120.9707

Table S3. Comparison of the key geometric parameters between the two isomers of aurone.

parameters	<i>E</i> -aurone	<i>Z</i> -aurone	parameters	<i>E</i> -aurone	<i>Z</i> -aurone
R(1,2)	1.4014	1.3997	A(2,1,6)	120.4	120.4
R(1,6)	1.3851	1.3865	A(1,2,3)	122.1	122.0
R(2,3)	1.3892	1.3906	A(2,3,4)	116.5	116.5
R(3,4)	1.3857	1.3832	A(3,4,5)	122.3	122.5
R(4,5)	1.3889	1.3899	A(3,4,7)	125.0	124.6
R(4,7)	1.3555	1.3674	A(5,4,7)	112.7	113.0
R(5,6)	1.3915	1.3902	A(4,5,6)	120.7	120.5
R(5,9)	1.4626	1.4678	A(4,5,9)	107.0	106.7
R(7,8)	1.3922	1.3773	A(6,5,9)	132.2	132.8
R(8,9)	1.4943	1.4917	A(1,6,5)	118.0	118.2
R(8,10)	1.3477	1.3403	A(4,7,8)	108.0	107.3
R(9,11)	1.2158	1.2115	A(7,8,9)	108.7	109.9
R(10,12)	1.4499	1.4494	A(5,9,8)	103.5	103.2
R(12,13)	1.4059	1.4042	A(5,9,11)	128.0	130.1
R(12,17)	1.4046	1.4029	A(8,9,11)	128.4	126.7
R(13,14)	1.3845	1.3855	A(13,12,17)	118.3	118.4
R(14,15)	1.3906	1.3918	A(12,13,14)	121.2	120.3
R(15,16)	1.3912	1.3902	A(13,14,15)	119.8	120.6
R(16,17)	1.3861	1.3856	A(14,15,16)	119.7	119.7
			A(15,16,17)	120.9	119.9
			A(12,17,16)	120.1	121.1

Table S4. Comparison of the key geometric parameters between the studied Z-aurones in ground state (S_0).

parameters	aurone	1	2	3	4
R(1,2)	1.3997	1.3996	1.3998	1.3999	1.3999
R(1,6)	1.3865	1.3866	1.3866	1.3867	1.3869
R(2,3)	1.3906	1.3906	1.3904	1.3902	1.3902
R(3,4)	1.3832	1.3835	1.3842	1.3846	1.3848
R(4,5)	1.3899	1.3901	1.3905	1.3908	1.3906
R(4,7)	1.3674	1.3666	1.3646	1.3628	1.3619
R(5,6)	1.3902	1.3901	1.3901	1.39	1.3899
R(5,9)	1.4678	1.4686	1.4692	1.4699	1.4708
R(7,8)	1.3773	1.3796	1.3822	1.3845	1.3867
R(8,9)	1.4917	1.4884	1.484	1.4803	1.4795
R(8,10)	1.3403	1.3417	1.3433	1.3455	1.3462
R(9,17)	1.2115	1.2123	1.214	1.2155	1.2155
R(10,11)	1.4494	1.4451	1.4413	1.4375	1.4352
R(11,12)	1.4042	1.4049	1.4064	1.4052	1.4043
R(11,16)	1.4029	1.4021	1.4044	1.4034	1.4106
R(12,13)	1.3855	1.379	1.3789	1.3794	1.3761
R(13,14)	1.3918	1.4013	1.4041	1.4168	1.4171
R(14,15)	1.3902	1.3983	1.4022	1.4149	1.4123
R(15,16)	1.3856	1.3835	1.3795	1.3798	1.3921
A(2,1,6)	120.4	120.4	118.2	120.4	120.4
A(1,2,3)	122.0	122.0	116.6	122.0	121.9
A(3,4,5)	122.5	122.4	120.5	122.3	122.3
A(3,4,7)	124.6	124.6	106.7	124.7	124.8
A(5,4,7)	113.0	113.0	107.1	112.9	112.9
A(4,5,6)	120.5	120.5	132.8	120.5	120.5
A(4,5,9)	106.7	106.7	119.9	106.7	106.7
A(4,7,8)	107.3	107.2	125.2	107.1	107.2
A(7,8,9)	109.9	110.0	127	110.1	110.0
A(7,8,10)	125.3	124.9	131	124.6	124.6
A(5,9,17)	130.1	130.0	124	129.7	129.4
A(8,10,11)	130.7	126.8	117.3	131.2	130.6
A(10,11,12)	123.6	123.8	121.9	124.2	124.2
A(10,11,16)	118.0	118.7	118.9	118.8	119.3
A(12,11,16)	118.4	117.5	119.4	117.0	116.5
A(11,12,13)	120.3	120.6	121	122.0	123.1
A(12,13,14)	120.6	121.1	118.2	119.9	119.3
A(13,14,15)	119.7	119.1	120.4	118.9	119.3
A(14,15,16)	119.9	119.2	116.8	119.4	119.3
A(11,16,15)	121.1	122.4	113.8	122.7	122.3

Table S5. The calculated key geometric parameters of the excited state (S_1) of aurones.

aurone		1		2	
parameters		parameters		parameters	
R(1,2)	1.3995	R(1,2)	1.4012	R(1,2)	1.4023
R(1,6)	1.4011	R(1,6)	1.396	R(1,6)	1.394
R(2,3)	1.4073	R(2,3)	1.4073	R(2,3)	1.4096
R(3,4)	1.3766	R(3,4)	1.3746	R(3,4)	1.3729
R(4,5)	1.4039	R(4,5)	1.4028	R(4,5)	1.4054
R(4,7)	1.3789	R(4,7)	1.3839	R(4,7)	1.3854
R(5,6)	1.399	R(5,6)	1.4031	R(5,6)	1.4074
R(5,9)	1.4467	R(5,9)	1.4445	R(5,9)	1.4386
R(7,8)	1.3468	R(7,8)	1.3508	R(7,8)	1.3566
R(8,9)	1.4744	R(8,9)	1.476	R(8,9)	1.4819
R(8,10)	1.3969	R(8,10)	1.3922	R(8,10)	1.382
R(9,17)	1.2512	R(9,17)	1.2518	R(9,17)	1.2535
R(10,11)	1.4137	R(10,11)	1.4135	R(10,11)	1.4261
R(11,12)	1.4307	R(11,12)	1.4321	R(11,12)	1.4282
R(11,16)	1.4319	R(11,16)	1.4316	R(11,16)	1.4283
R(12,13)	1.3816	R(12,13)	1.3716	R(12,13)	1.3747
R(13,14)	1.4039	R(13,14)	1.4189	R(13,14)	1.4209
R(14,15)	1.4042	R(14,15)	1.418	R(14,15)	1.4223
R(15,16)	1.3795	R(15,16)	1.3732	R(15,16)	1.372
A(2,1,6)	121.6	R(18,19)	1.3851	A(2,1,6)	121.4
A(1,2,3)	120.8	R(19,20)	1.2238	A(1,2,3)	120.9
A(2,3,4)	116.2	R(19,21)	1.5042	A(2,3,4)	116.4
A(3,4,5)	124.8	A(2,1,6)	121.4	A(3,4,5)	124.4
A(3,4,7)	124.5	A(1,2,3)	121.0	A(3,4,7)	124.6
A(5,4,7)	110.7	A(2,3,4)	116.3	A(5,4,7)	111.0
A(4,5,6)	118.2	A(3,4,5)	124.5	A(4,5,6)	118.4
A(4,5,9)	106.9	A(3,4,7)	124.6	A(4,5,9)	107.2
A(6,5,9)	134.8	A(5,4,7)	110.9	A(6,5,9)	134.4
A(1,6,5)	118.4	A(4,5,6)	118.5	A(1,6,5)	118.5
A(4,7,8)	108.4	A(4,5,9)	107.0	A(4,7,8)	107.7
A(7,8,9)	110.1	A(6,5,9)	134.5	A(7,8,9)	110.1
A(7,8,10)	123.2	A(1,6,5)	118.4	A(7,8,10)	123.7
A(9,8,10)	126.6	A(4,7,8)	107.9	A(9,8,10)	126.2
A(5,9,8)	103.9	A(7,8,9)	110.3	A(5,9,8)	104.0
A(5,9,17)	131.2	A(7,8,10)	123.5	A(5,9,17)	131.3
A(8,9,17)	124.9	A(9,8,10)	126.2	A(8,9,17)	124.7
A(8,10,11)	130.4	A(5,9,8)	103.9	A(8,10,11)	129.6
A(10,11,12)	124.7	A(5,9,17)	131.1	A(10,11,12)	124.6
A(10,11,16)	117.9	A(8,9,17)	125.0	A(10,11,16)	118.5

A(12,11,16)	117.5	A(8,10,11)	129.8	A(12,11,16)	116.9
A(11,12,13)	120.5	A(10,11,12)	124.7	A(11,12,13)	121.4
A(12,13,14)	120.8	A(10,11,16)	118.6	A(12,13,14)	120.8
A(13,14,15)	119.8	A(12,11,16)	116.7	A(13,14,15)	118.5
A(14,15,16)	120.1	A(11,12,13)	120.9	A(13,14,18)	120.8
A(11,16,15)	121.3	A(12,13,14)	121.3	A(15,14,18)	120.7
		A(13,14,15)	118.9	A(14,15,16)	120.2
		A(13,14,18)	117.1		
		A(15,14,18)	124.0		
		A(14,15,16)	119.6		
		A(11,16,15)	122.6		
		A(14,18,19)	129.7		

3		4	
parameters		parameters	
R(1,2)	1.4033	R(1,2)	1.4033
R(1,6)	1.3929	R(1,6)	1.3929
R(2,3)	1.4087	R(2,3)	1.4088
R(3,4)	1.3744	R(3,4)	1.3743
R(4,5)	1.4061	R(4,5)	1.4059
R(4,7)	1.3813	R(4,7)	1.3814
R(5,6)	1.4083	R(5,6)	1.4083
R(5,9)	1.4383	R(5,9)	1.4386
R(7,8)	1.366	R(7,8)	1.3653
R(8,9)	1.4819	R(8,9)	1.4809
R(8,10)	1.3722	R(8,10)	1.3749
R(9,17)	1.254	R(9,17)	1.2539
R(10,11)	1.439	R(10,11)	1.4341
R(11,12)	1.4192	R(11,12)	1.4137
R(11,16)	1.419	R(11,16)	1.4334
R(12,13)	1.3804	R(12,13)	1.3797
R(13,14)	1.4306	R(13,14)	1.4332
R(14,15)	1.4323	R(14,15)	1.4268
R(15,16)	1.3778	R(15,16)	1.3843
R(18,19)	1.5221	R(18,19)	1.5215
R(19,20)	1.5158	R(19,20)	1.5153
R(20,21)	1.4558	R(20,21)	1.4571
R(21,22)	1.4557	R(21,22)	1.4537
R(22,23)	1.516	R(22,23)	1.5136
R(23,24)	1.5221	R(23,24)	1.5226
A(2,1,6)	121.3	A(2,1,6)	121.3
A(1,2,3)	121.0	A(1,2,3)	120.9
A(2,3,4)	116.6	A(2,3,4)	116.6
A(3,4,5)	124.1	A(3,4,5)	124.1

A(3,4,7)	124.7	A(3,4,7)	124.7
A(5,4,7)	111.3	A(5,4,7)	111.2
A(4,5,6)	118.6	A(4,5,6)	118.6
A(4,5,9)	107.2	A(4,5,9)	107.1
A(6,5,9)	134.2	A(6,5,9)	134.3
A(1,6,5)	118.5	A(1,6,5)	118.5
A(4,7,8)	107.5	A(4,7,8)	107.6
A(7,8,9)	109.9	A(7,8,9)	109.9
A(7,8,10)	123.8	A(7,8,10)	123.9
A(9,8,10)	126.3	A(9,8,10)	126.2
A(5,9,8)	104.1	A(5,9,8)	104.1
A(5,9,17)	130.9	A(5,9,17)	130.9
A(8,9,17)	125.0	A(8,9,17)	125.0
A(8,10,11)	129.7	A(8,10,11)	129.1
A(10,11,12)	124.5	A(10,11,12)	124.7
A(10,11,16)	118.5	A(10,11,16)	118.9
A(12,11,16)	117.0	A(12,11,16)	116.4
A(11,12,13)	122.2	A(11,12,13)	122.9
A(12,13,14)	119.6	A(12,13,14)	119.3
A(12,13,18)	121.4	A(12,13,18)	121.3
A(14,13,18)	119.0	A(14,13,18)	119.4
A(13,14,15)	119.2	A(13,14,15)	119.7
A(13,14,21)	120.5	A(13,14,21)	119.8
A(15,14,21)	120.3	A(15,14,21)	120.5
A(14,15,16)	119.1	A(14,15,16)	118.8
A(14,15,24)	119.1	A(14,15,24)	119.9
A(16,15,24)	121.8	A(16,15,24)	121.3
A(11,16,15)	122.8	A(11,16,15)	122.9

Table S6. Calculated absorption and emission maxima (nm, eV) and oscillator strengths (f) for studied *E*-aurones at the PCM-TD-PBE0/6-31+G* level.

Molecule	absorption	E	f	emission	E	f
<i>E</i> -aurone	384.03	3.2285	0.3559	454.53	2.7277	0.6476
<i>E</i> -1	406.28	3.0517	0.7500	486.47	2.5486	1.0473
<i>E</i> -2	421.80	2.9394	0.7409	525.60	2.3589	0.8346
<i>E</i> -3	473.22	2.6200	0.8953	550.71	2.2514	1.0696
<i>E</i> -4	470.33	2.6361	0.8905	548.92	2.2587	1.0584

Figure S1 Electron density plots of the frontier molecular orbital HOMO-4 for S_0 state of the title compounds (isocontour value 0.02 au).

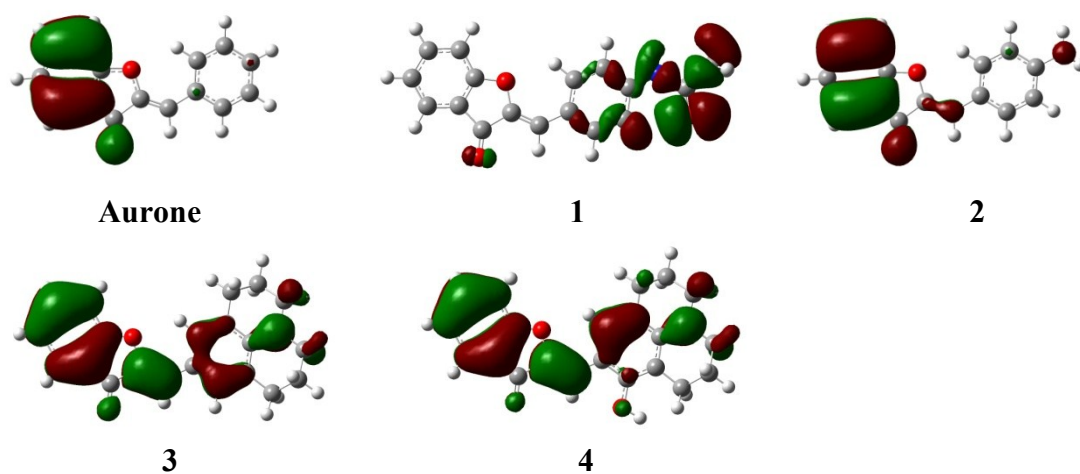
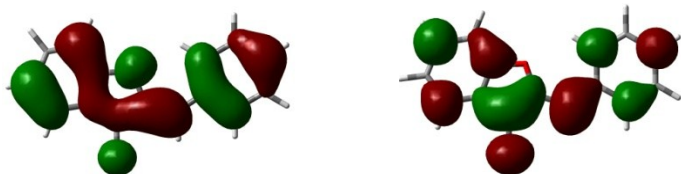
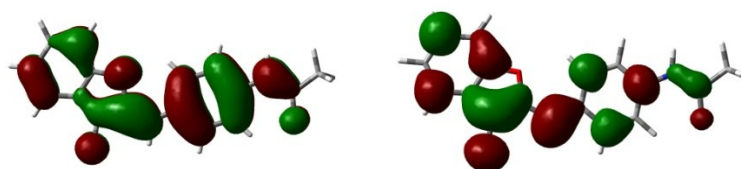


Figure S2 Calculated natural transition orbitals (NTOs) that characterize the electron (left) and hole (right) of the electronic excited state responsible for the lowest energy absorption band. Values list in parenthesis are the largest natural transition orbital eigenvalue.

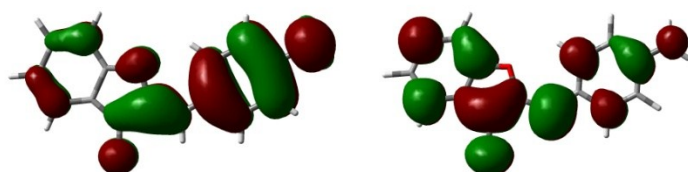
Aurone (0.99812)



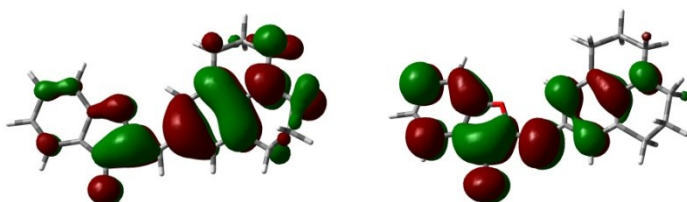
Aurone-1 (0.99803)



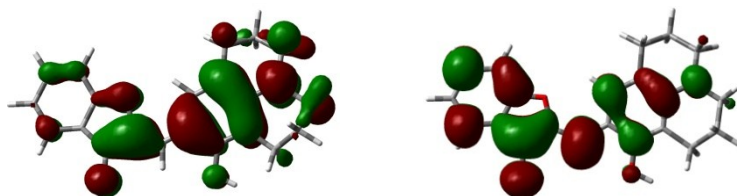
Aurone-2 (1.00147)



Aurone-3 (1.00322)



Aurone-4 (1.00319)



Aurone- S_0

6	0	-4.564731	0.312423	0.819307
6	0	-4.163015	-1.012122	1.027402
6	0	-2.833042	-1.404433	0.921964
6	0	-1.921733	-0.415067	0.599412
6	0	-2.298447	0.906100	0.388541
6	0	-3.631400	1.285712	0.496912
8	0	-0.577080	-0.616544	0.454026
6	0	-0.013841	0.599027	0.134645
6	0	-1.072341	1.648208	0.071843
6	0	1.290461	0.812952	-0.087699
6	0	2.416728	-0.099004	-0.061468
6	0	2.300496	-1.468248	0.227539
6	0	3.423315	-2.279999	0.234356
6	0	4.680397	-1.751744	-0.044496
6	0	4.810728	-0.397908	-0.332364
6	0	3.690791	0.417928	-0.340371
8	0	-0.913866	2.821817	-0.183544
1	0	-5.613106	0.572365	0.912189
1	0	-4.910360	-1.757576	1.278810
1	0	-2.520818	-2.429238	1.082812
1	0	-3.915674	2.319178	0.330528
1	0	1.501752	1.853635	-0.324148
1	0	1.326815	-1.887025	0.445489
1	0	3.318452	-3.336246	0.459343
1	0	5.554770	-2.393971	-0.037167
1	0	5.786877	0.021946	-0.550744
1	0	3.792360	1.475287	-0.565222

Aurone-1- S_0

6	0	-6.119260	-0.819955	-0.000103
6	0	-5.390255	-2.014689	-0.000111
6	0	-3.999686	-2.029486	-0.000063
6	0	-3.368760	-0.798228	-0.000009
6	0	-4.073048	0.400262	-0.000003
6	0	-5.463174	0.401576	-0.000049
8	0	-2.013845	-0.620210	0.000047
6	0	-1.780942	0.739565	0.000081
6	0	-3.073995	1.476710	0.000042
6	0	-0.567162	1.311350	0.000098
6	0	0.751597	0.720544	0.000086

6	0	0.987608	-0.664429	0.000083
6	0	2.275684	-1.156929	0.000055
6	0	3.380846	-0.295375	0.000014
6	0	3.165562	1.086229	0.000020
6	0	1.868656	1.567889	0.000064
8	0	-3.224171	2.679684	0.000091
7	0	4.649926	-0.879171	0.000010
6	0	5.880995	-0.266513	-0.000183
8	0	6.039883	0.934055	-0.000508
6	0	7.051350	-1.222582	0.000230
1	0	-7.202795	-0.856487	-0.000142
1	0	-5.923977	-2.959490	-0.000156
1	0	-3.434653	-2.953875	-0.000069
1	0	-6.003817	1.341972	-0.000045
1	0	-0.623472	2.397819	0.000112
1	0	0.151698	-1.351419	0.000112
1	0	2.435594	-2.232107	0.000068
1	0	4.012509	1.756445	-0.000032
1	0	1.711593	2.642290	0.000083
1	0	4.655206	-1.886215	0.000174
1	0	7.665486	-1.013376	-0.878103
1	0	6.773660	-2.278791	-0.002049
1	0	7.662453	-1.016420	0.881420

Aurone-2- S_0

6	0	-5.202592	-0.111162	-0.079527
6	0	-4.684049	-1.407087	0.025791
6	0	-3.315796	-1.653931	0.038082
6	0	-2.486553	-0.549965	-0.059413
6	0	-2.980662	0.745500	-0.164899
6	0	-4.350952	0.978813	-0.176036
8	0	-1.122929	-0.600958	-0.063496
6	0	-0.667111	0.699110	-0.175649
6	0	-1.815379	1.636539	-0.246807
6	0	0.627227	1.056492	-0.214392
6	0	1.828783	0.262636	-0.155774
6	0	1.840526	-1.138636	-0.036841
6	0	3.026066	-1.840881	0.015953
6	0	4.262867	-1.179115	-0.046064
6	0	4.261878	0.217903	-0.166709
6	0	3.071667	0.913463	-0.219031
8	0	-1.766376	2.845270	-0.348061
7	0	5.441950	-1.887821	-0.042770

1	0	-6.276983	0.034408	-0.085240
1	0	-5.368407	-2.245992	0.100074
1	0	-2.913281	-2.656567	0.119308
1	0	-4.726496	1.993162	-0.258787
1	0	0.749918	2.133906	-0.306148
1	0	0.901871	-1.675114	0.015389
1	0	3.006929	-2.923426	0.103714
1	0	5.206025	0.751699	-0.221966
1	0	3.093944	1.995347	-0.310497
1	0	6.276458	-1.380623	0.201198
1	0	5.409704	-2.821475	0.331903

Aurone-3- S_0

6	0	-6.462357	0.751299	0.061967
6	0	-5.718583	1.935600	0.124613
6	0	-4.328347	1.932349	0.121415
6	0	-3.711100	0.694874	0.052610
6	0	-4.431120	-0.493381	-0.010609
6	0	-5.821048	-0.476285	-0.006279
8	0	-2.362412	0.499695	0.038567
6	0	-2.149768	-0.866189	-0.038509
6	0	-3.445189	-1.581763	-0.073690
6	0	-0.938153	-1.449895	-0.077884
6	0	0.384390	-0.887236	-0.051407
6	0	0.654853	0.488666	0.039247
6	0	1.943063	0.980342	0.079270
6	0	3.042549	0.090895	-0.006124
6	0	2.791618	-1.297359	-0.114092
6	0	1.488542	-1.750969	-0.117879
8	0	-3.618924	-2.782950	-0.139542
6	0	2.211744	2.454045	0.200235
6	0	3.481328	2.809744	-0.558749
6	0	4.637839	1.983880	-0.030179
7	0	4.328604	0.567823	0.017003
6	0	5.482752	-0.307526	0.083967
6	0	5.128294	-1.692279	0.590376
6	0	3.955491	-2.243038	-0.207171
1	0	-7.545514	0.800983	0.067104
1	0	-6.240502	2.885633	0.177446
1	0	-3.751532	2.848311	0.170078
1	0	-6.373255	-1.408766	-0.055878
1	0	-1.013077	-2.533963	-0.140380
1	0	-0.170933	1.188515	0.091083

1	0	1.312760	-2.821906	-0.185894
1	0	2.333179	2.728703	1.257206
1	0	1.355195	3.020397	-0.175374
1	0	3.724201	3.871387	-0.459196
1	0	3.339183	2.602639	-1.625142
1	0	4.924091	2.337629	0.973481
1	0	5.517509	2.116490	-0.672795
1	0	6.220782	0.156999	0.750122
1	0	5.955318	-0.380272	-0.908943
1	0	4.854961	-1.636753	1.649846
1	0	6.006588	-2.338918	0.510335
1	0	4.257861	-2.367884	-1.256085
1	0	3.662848	-3.232573	0.155006

Aurone-4- S_0

6	0	-6.516362	0.815991	0.039908
6	0	-5.780105	2.004109	0.116863
6	0	-4.389957	2.008204	0.129698
6	0	-3.764887	0.774312	0.061920
6	0	-4.477393	-0.417402	-0.015336
6	0	-5.867175	-0.407716	-0.026873
8	0	-2.416058	0.586028	0.061710
6	0	-2.193641	-0.780188	-0.021013
6	0	-3.484541	-1.501041	-0.073263
6	0	-0.977154	-1.355794	-0.053112
6	0	0.333314	-0.772021	-0.011702
6	0	0.580329	0.607337	0.079692
6	0	1.846990	1.144258	0.108480
6	0	2.968582	0.282232	0.023748
6	0	2.764625	-1.113558	-0.045418
6	0	1.465073	-1.611864	-0.072248
8	0	-3.655755	-2.702143	-0.147366
6	0	2.070066	2.625952	0.210904
6	0	3.305277	3.011295	-0.587981
6	0	4.500462	2.229962	-0.078942
7	0	4.237526	0.804543	0.015659
6	0	5.412359	-0.038902	-0.021958
6	0	5.148699	-1.395025	0.597891
6	0	3.946310	-2.046874	-0.069222
8	0	1.230135	-2.944035	-0.163809
1	0	-7.599816	0.859607	0.032710
1	0	-6.307850	2.951047	0.168199
1	0	-3.818794	2.927125	0.189391

1	0	-6.413429	-1.343100	-0.087464
1	0	-1.034679	-2.438116	-0.122584
1	0	-0.268565	1.278587	0.127717
1	0	2.213108	2.919606	1.260284
1	0	1.186148	3.160317	-0.147726
1	0	3.518877	4.081147	-0.510159
1	0	3.140041	2.783307	-1.646756
1	0	4.809543	2.616498	0.905015
1	0	5.352897	2.370628	-0.755076
1	0	6.212114	0.471587	0.526952
1	0	5.765672	-0.158914	-1.059711
1	0	4.946884	-1.270443	1.667066
1	0	6.039228	-2.021732	0.499559
1	0	4.206345	-2.332662	-1.098538
1	0	3.717281	-2.976201	0.469493
1	0	2.060508	-3.408500	-0.284471

Aurone- S_1

6	0	-4.632668	-0.466130	0.000080
6	0	-4.034787	-1.731514	0.000005
6	0	-2.633869	-1.865782	-0.000061
6	0	-1.911528	-0.693930	-0.000049
6	0	-2.472684	0.592964	0.000023
6	0	-3.867014	0.707238	0.000091
8	0	-0.534370	-0.624346	-0.000102
6	0	-0.174347	0.673463	-0.000056
6	0	-1.372614	1.532559	0.000008
6	0	1.156134	1.099112	-0.000096
6	0	2.357113	0.353285	-0.000036
6	0	2.428072	-1.075642	0.000163
6	0	3.651581	-1.717286	0.000204
6	0	4.848686	-0.983890	0.000057
6	0	4.806759	0.419644	-0.000131
6	0	3.593325	1.075777	-0.000172
8	0	-1.356423	2.783697	0.000059
1	0	-5.716732	-0.391490	0.000127
1	0	-4.654109	-2.623190	-0.000004
1	0	-2.148449	-2.836805	-0.000116
1	0	-4.344427	1.683269	0.000146
1	0	1.240196	2.184290	-0.000166
1	0	1.514337	-1.658581	0.000289
1	0	3.686590	-2.803520	0.000357
1	0	5.804379	-1.501001	0.000094

1	0	5.731347	0.990410	-0.000242
1	0	3.560258	2.162602	-0.000321

Aurone-1- S_1				
6	0	-6.101478	-0.885923	-0.000017
6	0	-5.356134	-2.072486	-0.000016
6	0	-3.949092	-2.043929	-0.000013
6	0	-3.365737	-0.799260	-0.000010
6	0	-4.076040	0.410436	-0.000010
6	0	-5.478321	0.363270	-0.000014
8	0	-2.000919	-0.570046	-0.000005
6	0	-1.804340	0.766332	-0.000003
6	0	-3.099313	1.474682	-0.000004
6	0	-0.543819	1.357268	0.000005
6	0	0.736601	0.758449	0.000000
6	0	0.976766	-0.653323	-0.000031
6	0	2.254980	-1.150750	-0.000037
6	0	3.381353	-0.287876	-0.000004
6	0	3.171155	1.114450	0.000028
6	0	1.889400	1.607287	0.000028
8	0	-3.236932	2.718868	-0.000007
7	0	4.623897	-0.880083	-0.000005
6	0	5.881191	-0.298930	0.000045
8	0	6.045859	0.913725	-0.000302
6	0	7.029757	-1.270284	0.000260
1	0	-7.186932	-0.940950	-0.000019
1	0	-5.866810	-3.031015	-0.000018
1	0	-3.356629	-2.953852	-0.000012
1	0	-6.062375	1.279743	-0.000014
1	0	-0.590662	2.444234	0.000017
1	0	0.139827	-1.341211	-0.000055
1	0	2.411149	-2.227261	-0.000062
1	0	4.021980	1.782216	0.000049
1	0	1.739260	2.683897	0.000054
1	0	4.613643	-1.893237	0.000009
1	0	7.650373	-1.077679	-0.880600
1	0	6.727243	-2.319978	-0.002315
1	0	7.647020	-1.081189	0.884275

Aurone-2- S_1				
6	0	-4.998148	-0.684978	0.000154
6	0	-4.314728	-1.909414	-0.000163

6	0	-2.905769	-1.952068	-0.000347
6	0	-2.257501	-0.741849	-0.000206
6	0	-2.905765	0.505080	0.000099
6	0	-4.312935	0.529013	0.000289
8	0	-0.880952	-0.585811	-0.000338
6	0	-0.616370	0.744719	-0.000121
6	0	-1.881889	1.515703	0.000164
6	0	0.660745	1.272749	-0.000194
6	0	1.920937	0.605060	-0.000160
6	0	2.087107	-0.813485	0.000264
6	0	3.335587	-1.388959	0.000394
6	0	4.507589	-0.585664	0.000106
6	0	4.361294	0.829071	-0.000342
6	0	3.111226	1.394565	-0.000460
8	0	-1.955468	2.767007	0.000417
7	0	5.729872	-1.150160	0.000291
1	0	-6.085321	-0.684695	0.000297
1	0	-4.873858	-2.840695	-0.000273
1	0	-2.361420	-2.891818	-0.000585
1	0	-4.848892	1.474554	0.000535
1	0	0.671223	2.360306	-0.000203
1	0	1.212027	-1.452631	0.000521
1	0	3.435198	-2.471527	0.000764
1	0	5.248242	1.457328	-0.000599
1	0	3.017995	2.477740	-0.000785
1	0	6.571196	-0.590534	0.000210
1	0	5.847581	-2.153741	0.000589

Aurone-3- S_1

6	0	-6.442906	0.807350	0.066041
6	0	-5.681082	1.984808	0.116880
6	0	-4.273172	1.937875	0.105933
6	0	-3.699852	0.690361	0.043619
6	0	-4.429709	-0.510303	-0.008485
6	0	-5.836486	-0.445005	0.003273
8	0	-2.339621	0.450803	0.024218
6	0	-2.160577	-0.901909	-0.040030
6	0	-3.475395	-1.584989	-0.064768
6	0	-0.929642	-1.507222	-0.075796
6	0	0.383737	-0.919837	-0.050936
6	0	0.639302	0.473327	0.037768

6	0	1.920869	0.985084	0.073427
6	0	3.039840	0.097279	-0.005480
6	0	2.807470	-1.312281	-0.109147
6	0	1.511177	-1.778986	-0.117201
8	0	-3.640038	-2.826809	-0.121540
6	0	2.169645	2.461505	0.189689
6	0	3.450528	2.831667	-0.544581
6	0	4.601765	2.009681	0.000019
7	0	4.308603	0.583832	0.017789
6	0	5.479466	-0.280123	0.060176
6	0	5.158341	-1.668759	0.576701
6	0	3.982624	-2.241874	-0.201809
1	0	-7.527935	0.876939	0.075956
1	0	-6.179707	2.948829	0.165468
1	0	-3.670474	2.840652	0.144823
1	0	-6.430466	-1.354451	-0.036292
1	0	-0.986554	-2.592098	-0.131392
1	0	-0.194564	1.165187	0.088074
1	0	1.346164	-2.852735	-0.184376
1	0	2.265732	2.738696	1.250509
1	0	1.311240	3.016372	-0.203240
1	0	3.685088	3.893524	-0.420135
1	0	3.335593	2.642543	-1.619369
1	0	4.851324	2.327281	1.025541
1	0	5.505207	2.149035	-0.605765
1	0	6.224867	0.212473	0.696054
1	0	5.909306	-0.335629	-0.953166
1	0	4.913052	-1.619550	1.645116
1	0	6.047019	-2.298905	0.471082
1	0	4.271934	-2.368981	-1.256032
1	0	3.704578	-3.233857	0.169443

Aurone-4- S_1

6	0	-6.506523	0.858490	0.058829
6	0	-5.757775	2.044013	0.115947
6	0	-4.349378	2.012293	0.112372
6	0	-3.762803	0.771018	0.050620
6	0	-4.479072	-0.437346	-0.007728
6	0	-5.886513	-0.387277	-0.003264
8	0	-2.399979	0.545507	0.037781
6	0	-2.205748	-0.804213	-0.029515
6	0	-3.512050	-1.501092	-0.062300

6	0	-0.967135	-1.400143	-0.060724
6	0	0.330572	-0.790751	-0.024543
6	0	0.563080	0.600689	0.067483
6	0	1.828661	1.149301	0.095593
6	0	2.969435	0.284945	0.019994
6	0	2.782391	-1.128147	-0.041813
6	0	1.492247	-1.628198	-0.085322
8	0	-3.662501	-2.744453	-0.122724
6	0	2.034205	2.632186	0.192771
6	0	3.284872	3.032095	-0.575918
6	0	4.470359	2.250804	-0.046373
7	0	4.220154	0.816159	0.000817
6	0	5.413494	-0.013778	-0.016813
6	0	5.169081	-1.370026	0.609253
6	0	3.977343	-2.044902	-0.055992
8	0	1.239904	-2.956056	-0.192443
1	0	-7.592270	0.916521	0.063238
1	0	-6.267043	3.002492	0.163748
1	0	-3.756604	2.921392	0.156133
1	0	-6.470696	-1.302817	-0.047695
1	0	-1.012197	-2.482703	-0.120066
1	0	-0.289588	1.268608	0.114217
1	0	2.149001	2.925340	1.247914
1	0	1.149608	3.156503	-0.183939
1	0	3.490351	4.102048	-0.469692
1	0	3.150879	2.825117	-1.645219
1	0	4.735529	2.593995	0.966687
1	0	5.352617	2.405733	-0.678368
1	0	6.197465	0.527360	0.524924
1	0	5.756895	-0.122428	-1.058665
1	0	4.976112	-1.248921	1.682297
1	0	6.069593	-1.982429	0.502199
1	0	4.238619	-2.327629	-1.086652
1	0	3.763156	-2.976973	0.483999
1	0	2.065630	-3.454074	-0.277027
