

**Studies on the stereochemical assignment of 3-acylidene 2-oxindoles**  
**Electronic Supplementary Information 2**  
**Theoretical Studies**

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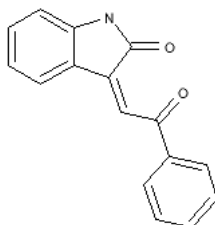
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**S1.** 3-phenacylidene-1H-indol-2-one

**General Information**

Log file : T2110-01-B-OPT-H-Zisomer.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3ccccc3NC2=O
Formula	:	C <sub>16</sub> H <sub>11</sub> NO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	6.0634 Debye
Energy	:	-821.74826633 a.u.
Number of imaginary frequencies	:	0

**Cartesian Co-ordinates (XYZ format)**

30

C	-0.20572527	0.54951090	-0.00036246
C	-1.53535497	0.64481246	-0.38080150
C	-2.14948821	1.88713372	-0.63838840
C	-1.41466248	3.06040287	-0.51034117
C	-0.07318053	2.98018003	-0.12703553
C	0.51861417	1.74029374	0.12321275
H	0.25763935	-0.41005796	0.19439387
H	-1.87117052	4.02430868	-0.70472455
H	0.51175070	3.88607216	-0.02374462
H	1.56023955	1.69467175	0.41932866
C	-3.69973350	0.11025839	-0.95868182
C	-3.54066086	1.61234593	-1.00949597
N	-2.47195363	-0.37953067	-0.57531202
H	-2.28621984	-1.36547542	-0.46481413
O	-4.69646502	-0.54629070	-1.20485985
C	-4.52958965	2.44960451	-1.34581399
H	-4.34440327	3.52057505	-1.38120234
C	-5.90583086	2.04486370	-1.81130862
O	-6.11344624	2.00262690	-3.01246190
C	-6.98284340	1.82201540	-0.80871278
C	-6.74808598	1.93263650	0.56763917
C	-8.27179241	1.51074898	-1.26585758
C	-7.78671455	1.73287177	1.47323143

H	-5.75664377	2.17461443	0.93056798
C	-9.30548286	1.30865169	-0.36123660
H	-8.44088554	1.43082941	-2.33248377
C	-9.06403828	1.42003310	1.01059246
H	-7.60011005	1.82028294	2.53706455
H	-10.29916954	1.06566954	-0.71915156
H	-9.87169170	1.26328266	1.71645927

### TD-DFT Calculations

No.	Energy (cm <sup>-1</sup> )	Wavelength (nm)	Osc. Strength	Major contribs
1	26245	381.03	0.04	HOMO→LUMO (96%)
2	28791	347.33	0.01	HOMO→L+1 (83%)
3	31229	320.21	0.03	H-4→LUMO (26%), H-4→L+1 (15%), H-1→LUMO (18%), HOMO→L+1 (14%)
4	32875	304.19	0.05	H-5→LUMO (14%), H-4→L+1 (24%), H-3→LUMO (21%), H-1→L+1 (14%)
5	33432	299.12	0.17	H-4→LUMO (14%), H-1→LUMO (61%)
6	34968	285.98	0.01	H-5→LUMO (13%), H-4→LUMO (26%), H-1→L+1 (40%)
7	35156	284.45	0.01	H-3→LUMO (20%), H-2→LUMO (76%)
8	35639	280.59	0.03	H-4→LUMO (16%), H-4→L+1 (18%), H-3→LUMO (21%), H-1→L+1 (22%)
9	36582	273.36	0.01	H-5→LUMO (52%), H-4→L+1 (17%)
10	37182	268.95	0.02	H-3→L+1 (40%), H-2→L+1 (44%)
11	38632	258.85	0.33	H-5→L+1 (21%), H-3→L+1 (35%), H-2→L+1 (30%)
12	40991	243.96	0.33	HOMO→L+3 (72%)
13	41161	242.95	0.00	HOMO→L+2 (96%)
14	41344	241.87	0.10	H-5→L+1 (55%), H-4→L+1 (11%), H-2→L+1 (11%)
15	44155	226.47	0.00	HOMO→L+4 (84%), HOMO→L+5 (10%)
16	45764	218.51	0.04	H-6→LUMO (10%), H-1→L+3 (25%), HOMO→L+5 (14%), HOMO→L+6 (42%)
17	46445	215.31	0.02	H-1→L+2 (73%)
18	46563	214.76	0.04	H-6→LUMO (46%), H-1→L+2 (15%), H-1→L+3 (22%)
19	47123	212.21	0.00	HOMO→L+5 (56%), HOMO→L+6 (17%), HOMO→L+8 (16%)
20	47304	211.40	0.00	HOMO→L+7 (90%)
21	47598	210.09	0.01	H-7→LUMO (34%), H-6→L+1 (39%)
22	48570	205.89	0.03	H-4→L+2 (57%), H-3→L+2 (23%)
23	48945	204.31	0.00	H-5→L+3 (11%), H-4→L+3 (34%), H-3→L+3 (33%)
24	49002	204.07	0.10	H-7→LUMO (20%), H-6→L+1 (42%)
25	49237	203.10	0.13	H-4→L+2 (22%), H-3→L+2 (17%), H-2→L+2 (24%)
26	49414	202.37	0.00	HOMO→L+8 (68%)
27	49728	201.10	0.01	H-1→L+4 (77%), H-1→L+5 (10%)
28	50445	198.24	0.10	H-7→LUMO (14%), H-7→L+1 (24%), H-1→L+3 (14%), HOMO→L+6 (12%)
29	50639	197.48	0.00	HOMO→L+10 (77%)
30	50875	196.56	0.01	H-2→L+3 (46%), HOMO→L+9 (38%)
31	50894	196.49	0.02	H-7→L+1 (14%), H-2→L+3 (35%), HOMO→L+9 (31%)
32	51194	195.34	0.06	H-7→L+1 (24%), H-4→L+3 (28%), H-3→L+3 (30%)
33	51596	193.81	0.10	H-8→LUMO (32%), H-8→L+1 (30%)

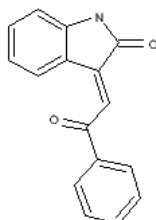
34	51666	193.55	0.22	H-8→LUMO (14%), H-8→L+1 (12%), H-3→L+2 (11%), H-2→L+2 (10%)
35	52019	192.24	0.20	H-7→L+1 (13%), H-3→L+2 (20%), H-2→L+2 (21%)
36	52369	190.95	0.03	H-9→LUMO (48%), H-1→L+5 (21%)
37	52413	190.79	0.01	H-9→LUMO (25%), H-1→L+5 (22%), HOMO→L+11 (10%)
38	52538	190.34	0.01	H-2→L+4 (62%), H-2→L+5 (16%)
39	52615	190.06	0.22	H-5→L+2 (23%), H-5→L+3 (21%), H-1→L+6 (20%)
40	52735	189.63	0.02	H-5→L+2 (45%), HOMO→L+11 (15%)
41	52779	189.47	0.02	H-5→L+2 (12%), H-1→L+6 (10%), HOMO→L+11 (47%)
42	52893	189.06	0.01	H-1→L+7 (47%), HOMO→L+12 (17%), HOMO→L+14 (15%)
43	53064	188.45	0.02	H-3→L+4 (62%), H-3→L+5 (15%)
44	53353	187.43	0.00	H-1→L+7 (37%), HOMO→L+12 (39%), HOMO→L+14 (16%)
45	53576	186.65	0.25	H-5→L+3 (26%), H-1→L+6 (16%)
46	54023	185.11	0.01	HOMO→L+12 (20%), HOMO→L+14 (52%)
47	54190	184.53	0.03	H-4→L+4 (42%), H-4→L+8 (10%)
48	54528	183.39	0.01	H-4→L+4 (26%), H-1→L+8 (37%)
49	54626	183.06	0.00	HOMO→L+13 (82%)
50	54763	182.61	0.00	H-9→LUMO (13%), H-8→LUMO (39%), H-8→L+1 (36%)
51	55012	181.78	0.03	H-4→L+6 (24%), H-3→L+6 (27%)
52	55213	181.12	0.01	H-10→LUMO (17%), H-10→L+1 (19%), H-1→L+8 (28%)
53	55757	179.35	0.00	H-10→LUMO (18%), H-10→L+1 (16%), H-1→L+10 (33%)
54	55983	178.63	0.01	H-2→L+4 (16%), H-2→L+5 (43%), H-2→L+8 (10%)
55	56058	178.39	0.03	H-3→L+5 (30%), H-1→L+9 (13%)
56	56383	177.36	0.01	H-1→L+9 (54%)
57	56524	176.92	0.00	H-11→LUMO (16%), H-2→L+5 (16%), H-2→L+6 (48%)
58	56648	176.53	0.01	H-11→LUMO (37%), H-10→LUMO (11%), H-2→L+6 (19%)
59	56802	176.05	0.00	H-3→L+7 (11%), H-1→L+10 (20%)
60	56878	175.82	0.00	HOMO→L+15 (74%)
61	56974	175.52	0.01	H-4→L+6 (31%), H-3→L+6 (26%)
62	57118	175.08	0.01	H-4→L+5 (18%), H-1→L+9 (10%)
63	57400	174.22	0.03	H-2→L+9 (78%)
64	57478	173.98	0.01	H-12→LUMO (55%)
65	57527	173.83	0.01	H-12→LUMO (18%), H-4→L+5 (39%)
66	57667	173.41	0.02	HOMO→L+16 (63%)
67	57843	172.88	0.02	H-3→L+9 (13%), H-2→L+7 (36%)
68	58013	172.37	0.01	H-9→L+1 (12%), H-5→L+4 (19%), H-1→L+11 (13%), HOMO→L+17 (22%)
69	58100	172.12	0.02	H-3→L+7 (26%), H-2→L+7 (31%)
70	58170	171.91	0.01	H-9→L+1 (16%), H-3→L+9 (19%), HOMO→L+17 (20%)
71	58192	171.84	0.00	H-9→L+1 (10%), H-3→L+9 (36%), HOMO→L+17 (12%)
72	58231	171.73	0.00	H-9→L+1 (22%), H-1→L+11 (32%), HOMO→L+16 (17%)
73	58379	171.30	0.09	H-10→LUMO (19%), H-10→L+1 (22%), H-2→L+8 (12%)
74	58529	170.86	0.03	H-4→L+7 (25%), H-1→L+11 (14%)
75	58633	170.55	0.01	H-5→L+6 (17%), H-1→L+12 (30%)

76	58743	170.23	0.01	H-5→L+5 (10%), H-5→L+6 (35%), H-2→L+8 (11%)
77	58750	170.21	0.02	H-4→L+7 (12%), H-3→L+8 (13%), H-2→L+8 (19%)
78	58919	169.72	0.03	H-3→L+8 (32%), H-2→L+10 (13%)
79	59047	169.36	0.02	H-11→L+1 (25%), H-4→L+7 (10%), H-2→L+10 (21%)
80	59243	168.80	0.11	H-4→L+8 (10%), H-4→L+9 (16%), H-3→L+10 (23%), H-1→L+14 (12%)
81	59314	168.60	0.02	HOMO→L+18 (53%), HOMO→L+19 (23%)
82	59480	168.12	0.10	H-4→L+9 (10%), H-3→L+10 (16%), H-1→L+14 (19%)
83	59733	167.41	0.01	H-13→LUMO (14%), H-4→L+9 (21%), H-1→L+14 (11%)
84	59844	167.10	0.03	H-13→LUMO (22%), H-1→L+13 (14%), H-1→L+14 (13%)
85	59950	166.81	0.02	H-13→LUMO (12%), H-4→L+8 (16%), H-4→L+9 (20%), H-4→L+10 (10%), H-1→L+13 (16%)
86	60189	166.14	0.02	H-13→LUMO (21%), H-7→L+3 (10%), HOMO→L+18 (14%), HOMO→L+19 (35%)
87	60405	165.55	0.01	H-6→L+2 (30%), H-4→L+8 (11%), H-1→L+13 (25%)
88	60422	165.50	0.01	H-6→L+2 (59%), H-1→L+13 (10%)
89	60569	165.10	0.03	H-6→L+3 (21%), H-5→L+5 (22%), H-5→L+6 (11%), H-5→L+7 (15%)
90	60768	164.56	0.02	H-6→L+3 (14%), H-5→L+5 (38%)
91	60945	164.08	0.03	H-6→L+3 (11%), H-5→L+7 (23%), H-5→L+8 (10%), H-5→L+10 (11%)
92	61232	163.31	0.04	H-5→L+7 (31%)
93	61610	162.31	0.01	HOMO→L+20 (61%)
94	61768	161.90	0.04	H-7→L+3 (28%), HOMO→L+21 (22%)
95	61778	161.87	0.01	H-2→L+12 (55%)
96	61984	161.33	0.05	H-5→L+8 (24%), H-3→L+12 (22%)
97	62071	161.11	0.00	H-14→LUMO (28%), H-8→L+2 (31%)
98	62129	160.96	0.00	H-8→L+2 (41%), H-3→L+12 (10%)
99	62179	160.83	0.00	H-14→LUMO (22%), H-3→L+11 (17%), H-2→L+11 (13%)
100	62347	160.39	0.01	H-1→L+15 (67%)

## S2. 3-phenacylidene-1H-indol-2-one

## General Information

Log file : T2110-02-OPT-H-Eisomer.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3ccccc3NC2=O
Formula	:	C <sub>16</sub> H <sub>11</sub> NO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	1.6682 Debye
Energy	:	-821.75390949 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	0.71683812	-0.15687326	-0.00845505
C	1.95855939	0.44754970	0.08906075
C	3.16514254	-0.29568306	0.09586682
C	3.10058689	-1.68884981	0.00490967
C	1.85387099	-2.30828142	-0.09656142
C	0.68062389	-1.55212379	-0.10278746
H	-0.19401956	0.42920813	-0.01156258
H	4.01367140	-2.26389456	0.02063494
H	1.79741931	-3.38777471	-0.16758622
H	-0.27910754	-2.05011845	-0.17963043
C	3.59410644	2.04092050	0.27069128
C	4.25759888	0.66597700	0.20282382
N	2.24410820	1.81168234	0.19294576
H	1.55682909	2.55054832	0.21333560
O	4.14055872	3.12290764	0.37145582
C	5.60851145	0.63970834	0.23565617
H	6.06818533	1.61775982	0.31640497
C	6.50655079	-0.53112131	0.19899337
O	6.08241415	-1.68200207	0.25792250
C	7.98332977	-0.28427854	0.11694219
C	8.84084034	-1.35894728	0.40084460
C	8.54199505	0.94751066	-0.25596130
C	10.21873760	-1.20414698	0.32917640
H	8.40377998	-2.30934596	0.67947459

C 9.92410564 1.09766948 -0.34028077  
H 7.91106606 1.79094207 -0.50382507  
C 10.76431751 0.02659165 -0.04275067  
H 10.86972237 -2.03904390 0.56105518  
H 10.34327793 2.05147958 -0.63821739  
H 11.83981419 0.14831387 -0.10160708

### TD-DFT Calculations

No.	Energy (cm <sup>-1</sup> )	Wavelength (nm)	Osc. Strength	Major contribs
1	20605	485.31	0.08	HOMO→LUMO (97%) H-4→LUMO (36%), H-3→LUMO (25%), H-2→LUMO (35%)
2	24065	415.55	0.00	H-1→LUMO (94%) H-3→LUMO (44%), H-2→LUMO (51%)
3	27509	363.51	0.52	H-5→LUMO (92%) H-4→LUMO (53%), H-3→LUMO (26%), H-2→LUMO (12%)
4	28771	347.57	0.00	HOMO→L+1 (97%) H-6→LUMO (41%)
5	29639	337.39	0.00	HOMO→L+3 (44%) H-4→L+1 (32%), H-3→L+1 (18%), H-2→L+1 (44%)
6	30831	324.35	0.02	H-7→LUMO (11%), H-6→LUMO (37%), H-1→L+1 (33%)
7	36126	276.81	0.00	H-3→L+1 (34%), H-2→L+1 (16%), HOMO→L+2 (24%)
8	39537	252.93	0.20	H-7→LUMO (65%), H-1→L+1 (13%), HOMO→L+2 (15%)
9	40409	247.47	0.00	H-3→L+1 (15%), HOMO→L+2 (56%)
10	41364	241.76	0.05	H-6→LUMO (10%), H-1→L+1 (40%), HOMO→L+3 (30%)
11	41723	239.67	0.03	HOMO→L+4 (77%)
12	42055	237.78	0.15	HOMO→L+6 (19%) H-4→L+1 (51%), H-3→L+1 (11%), H-2→L+1 (16%), H-2→L+2 (10%)
13	42735	234.00	0.00	H-9→LUMO (84%), H-8→LUMO (12%)
14	43608	229.31	0.17	H-9→LUMO (11%), H-8→LUMO (81%)
15	44730	223.56	0.00	H-1→L+3 (37%), HOMO→L+5 (53%)
16	45325	220.63	0.14	H-5→L+1 (87%) H-4→L+2 (36%), H-3→L+2 (31%), H-2→L+2 (27%)
17	45868	218.02	0.01	HOMO→L+4 (10%), HOMO→L+6 (59%)
18	46014	217.32	0.00	HOMO→L+7 (21%) H-1→L+2 (86%)
19	46643	214.40	0.04	HOMO→L+6 (10%)
20	46993	212.80	0.00	HOMO→L+7 (67%) H-4→L+3 (23%), H-3→L+3 (22%), H-2→L+3 (49%)
21	47452	210.74	0.01	H-10→LUMO (93%)
22	47715	209.58	0.00	
23	48077	208.00	0.03	
24	48135	207.75	0.01	
25	48905	204.48	0.00	
26	49489	202.07	0.00	



27	50330	198.69	0.04	H-12→LUMO (40%), H-5→L+3 (22%), H-2→L+3 (10%)
28	50469	198.14	0.00	H-1→L+4 (28%), HOMO→L+8 (39%)
29	50519	197.95	0.03	H-4→L+2 (10%), H-3→L+3 (14%), H-1→L+3 (24%), HOMO→L+5 (16%)
30	50656	197.41	0.19	H-12→LUMO (20%), H-4→L+2 (12%), H-1→L+3 (14%), HOMO→L+5 (10%)
31	50742	197.07	0.00	H-1→L+4 (51%), HOMO→L+8 (35%)
32	51212	195.27	0.17	H-11→LUMO (34%), H-3→L+2 (14%), H-2→L+3 (16%)
33	51332	194.81	0.11	H-4→L+3 (23%), H-2→L+2 (13%)
34	51747	193.25	0.00	HOMO→L+9 (76%)
35	51805	193.03	0.02	H-12→LUMO (16%), H-5→L+3 (47%)
36	52027	192.21	0.06	H-4→L+3 (20%), H-3→L+3 (27%), H-2→L+4 (11%)
37	52106	191.92	0.04	H-2→L+4 (59%), H-2→L+6 (14%)
38	52633	190.00	0.03	H-3→L+4 (31%), H-1→L+6 (36%)
39	52695	189.77	0.43	H-6→L+1 (10%), H-1→L+5 (41%), HOMO→L+10 (26%)
40	53051	188.50	0.19	H-11→LUMO (12%), H-1→L+5 (22%), HOMO→L+10 (32%)
41	53339	187.48	0.09	H-11→LUMO (16%), H-6→L+1 (10%), H-3→L+2 (16%), H-2→L+2 (11%), HOMO→L+10 (16%)
42	53469	187.02	0.01	H-4→L+4 (13%), H-3→L+4 (37%), H-1→L+6 (16%)
43	53727	186.12	0.00	HOMO→L+11 (32%), HOMO→L+13 (50%)
44	53915	185.48	0.04	H-4→L+5 (25%), H-3→L+5 (18%), H-2→L+5 (31%)
45	53973	185.28	0.01	H-4→L+4 (32%), H-1→L+7 (27%)
46	54236	184.38	0.01	H-13→LUMO (21%), H-1→L+7 (30%)
47	54254	184.32	0.01	H-13→LUMO (19%), H-1→L+7 (26%), HOMO→L+11 (14%)
48	54365	183.94	0.00	H-5→L+2 (95%)
49	54468	183.59	0.01	H-13→LUMO (12%), HOMO→L+11 (35%), HOMO→L+13 (10%)
50	54971	181.91	0.00	H-14→LUMO (85%)
51	55070	181.59	0.02	H-6→L+1 (20%), HOMO→L+12 (51%)
52	55420	180.44	0.05	H-13→LUMO (11%), H-6→L+1 (31%), HOMO→L+12 (19%)
53	55571	179.95	0.01	H-2→L+6 (43%), HOMO→L+14 (16%)
54	55602	179.85	0.02	H-13→LUMO (11%), H-2→L+6 (17%), HOMO→L+14 (37%)
55	56022	178.50	0.01	H-1→L+8 (53%)
56	56330	177.52	0.04	H-5→L+4 (10%), H-2→L+7 (44%), H-2→L+9 (16%)
57	56411	177.27	0.02	H-3→L+6 (40%), H-2→L+7 (11%)

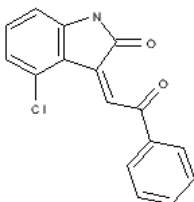
58	56491	177.02	0.06	H-4→L+5 (11%), H-3→L+5 (23%), H-2→L+5 (42%)
59	56729	176.28	0.02	H-5→L+4 (23%), H-4→L+6 (19%), H-1→L+9 (11%)
60	56914	175.70	0.05	H-4→L+5 (22%), H-3→L+5 (27%)
61	56983	175.49	0.04	H-3→L+6 (10%), H-3→L+7 (15%), H-1→L+9 (10%)
62	57098	175.14	0.00	H-5→L+5 (47%)
63	57195	174.84	0.01	H-4→L+6 (29%), H-1→L+9 (27%)
64	57518	173.86	0.03	H-7→L+1 (25%), H-3→L+7 (20%)
65	57635	173.51	0.04	H-7→L+1 (41%), H-5→L+4 (11%)
66	57839	172.89	0.05	HOMO→L+15 (54%), HOMO→L+18 (15%)
67	58090	172.15	0.00	H-2→L+8 (53%)
68	58143	171.99	0.00	H-5→L+5 (15%), H-4→L+5 (11%), H-4→L+10 (14%), H-3→L+10 (12%), H-2→L+10 (19%)
69	58257	171.65	0.02	H-4→L+7 (38%), H-1→L+10 (15%)
70	58444	171.10	0.02	H-1→L+10 (54%)
71	58476	171.01	0.00	H-8→L+1 (89%)
72	58784	170.12	0.00	H-1→L+10 (14%), HOMO→L+15 (13%), HOMO→L+16 (22%), HOMO→L+18 (27%)
73	58893	169.80	0.00	H-3→L+8 (37%), H-1→L+11 (10%), HOMO→L+18 (13%)
74	58990	169.52	0.00	H-2→L+7 (17%), H-2→L+9 (48%)
75	59064	169.31	0.00	H-3→L+8 (15%), HOMO→L+16 (49%), HOMO→L+18 (17%)
76	59374	168.42	0.01	H-4→L+8 (40%), H-3→L+8 (14%), H-1→L+11 (17%)
77	59686	167.54	0.01	H-4→L+8 (16%), H-1→L+11 (13%), H-1→L+13 (33%)
78	59764	167.32	0.03	H-3→L+7 (13%), H-3→L+9 (40%), H-1→L+13 (14%)
79	59835	167.13	0.00	HOMO→L+17 (64%)
80	59881	167.00	0.06	H-7→L+3 (14%), H-6→L+3 (38%)
81	60148	166.26	0.00	H-5→L+6 (13%), H-4→L+9 (23%), H-1→L+11 (14%), H-1→L+13 (13%)
82	60248	165.98	0.00	H-4→L+9 (23%), H-1→L+11 (21%), H-1→L+12 (10%)
83	60363	165.66	0.05	H-16→LUMO (15%), H-15→LUMO (37%)
84	60567	165.11	0.01	H-5→L+6 (52%), H-4→L+9 (15%)
85	60615	164.97	0.01	H-6→L+2 (75%)
86	60762	164.58	0.02	H-1→L+12 (24%), H-1→L+14 (24%), HOMO→L+19 (14%)
87	61047	163.81	0.01	H-7→L+3 (10%), H-1→L+12 (20%), HOMO→L+19 (44%)
88	61118	163.62	0.13	H-3→L+10 (28%), H-2→L+10 (21%)
89	61311	163.10	0.03	H-1→L+12 (12%), H-1→L+14 (26%)

90	61324	163.07	0.04	H-5→L+4 (12%), H-5→L+7 (61%)
91	61571	162.41	0.00	H-4→L+10 (12%), H-2→L+10 (10%), H-2→L+14 (12%), H-1→L+14 (24%)
92	61679	162.13	0.00	H-10→L+1 (13%), H-9→L+1 (62%)
93	61866	161.64	0.00	H-2→L+11 (59%), H-2→L+13 (25%)
94	62063	161.13	0.00	H-8→L+2 (89%)
95	62183	160.82	0.01	H-16→LUMO (14%), H-2→L+12 (10%)
96	62277	160.57	0.00	H-2→L+11 (20%), H-2→L+13 (30%), H-2→L+15 (24%)
97	62349	160.39	0.03	H-10→L+1 (12%), H-7→L+3 (33%), H-6→L+3 (11%)
98	62387	160.29	0.01	H-10→L+1 (24%), H-4→L+10 (13%)
99	62444	160.14	0.01	H-15→LUMO (10%), H-10→L+1 (36%), H-9→L+1 (10%)
100	62650	159.62	0.01	H-5→L+10 (16%), H-3→L+11 (12%), H-3→L+13 (13%), H-1→L+15 (13%)

## S3. 4-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : T2010-01-OPT-Z-isomer-Chlorine-MeOH.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3c(cccc3Cl)NC2=O
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	6.5232 Debye
Energy	:	-1281.36802408 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

```

C  1.16052270 -1.29697239  0.04353309
C  -0.16645576 -1.63972270  0.24250893
C  -0.77292269 -2.75231767 -0.38801295
C   0.01390628 -3.51990914 -1.24047542
C   1.35390198 -3.20058346 -1.46083343
C   1.91283071 -2.09707069 -0.82003284
H   1.59941280 -0.44024122  0.53866744
H   1.94824922 -3.81107116 -2.12709785
H   2.95408654 -1.85696387 -0.99784613
C  -2.33636069 -1.62548137  1.00386357
C  -2.16831684 -2.79341078  0.05981505
N  -1.11117446 -1.00192571  1.04940438
H  -0.93134958 -0.18554416  1.61542690
O  -3.34032393 -1.29310060  1.60689354
C  -3.17290831 -3.63369107 -0.22555164
H  -3.01340079 -4.46936083 -0.89794940
C  -4.54227352 -3.60355735  0.40799567
O  -4.74197817 -4.33396721  1.36378419
C  -5.62045431 -2.79233980 -0.21815898
C  -6.90758085 -2.84344816  0.33654794
C  -5.38748789 -1.99761546 -1.34765136
C  -7.94169903 -2.10780025 -0.22661991
H  -7.07516003 -3.46383286  1.20815134
C  -6.42650414 -1.26292157 -1.91270399

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H -4.39737988 -1.95259380 -1.78475976  
 C -7.70219183 -1.31621695 -1.35294378  
 H -8.93416405 -2.14835262 0.20681755  
 H -6.24148703 -0.64978498 -2.78675938  
 H -8.51016426 -0.74274927 -1.79273212  
 Cl -0.65548187 -4.92076445 -2.06960750

### TD-DFT Calculations

No.	Energy (cm <sup>-1</sup> )	Wavelength (nm)	Osc. Strength	Major contribs
1	27087	369.18	0.04	HOMO→LUMO (95%)
2	29744	336.20	0.02	H-4→L+1 (10%), H-1→L+1 (10%), HOMO→L+1 (64%)
3	31609	316.36	0.05	H-4→LUMO (24%), H-1→LUMO (22%), HOMO→L+1 (28%)
4	32559	307.13	0.10	H-4→L+1 (34%), H-1→LUMO (27%), H-1→L+1 (16%)
5	33150	301.66	0.06	H-5→LUMO (12%), H-4→LUMO (26%), H-3→LUMO (19%), H-1→LUMO (32%)
6	34590	289.10	0.00	H-4→LUMO (32%), H-3→LUMO (18%), H-2→LUMO (26%), H-1→L+1 (14%)
7	34814	287.24	0.00	H-3→LUMO (23%), H-2→LUMO (67%)
8	35313	283.18	0.02	H-4→L+1 (23%), H-3→LUMO (12%), H-1→L+1 (46%)
9	36250	275.86	0.00	H-5→LUMO (64%), H-4→L+1 (10%), H-3→LUMO (10%)
10	36882	271.14	0.02	H-3→L+1 (32%), H-2→L+1 (54%)
11	38793	257.78	0.41	H-5→L+1 (16%), H-3→L+1 (46%), H-2→L+1 (27%)
12	41058	243.56	0.28	HOMO→L+2 (72%)
13	41674	239.96	0.08	H-5→L+1 (71%)
14	42537	235.09	0.01	HOMO→L+3 (98%)
15	44966	222.39	0.04	H-1→L+2 (62%), HOMO→L+5 (26%)
16	45214	221.17	0.00	HOMO→L+4 (73%), HOMO→L+6 (10%)
17	45453	220.01	0.11	HOMO→L+7 (11%), H-6→LUMO (74%)
18	45746	218.60	0.00	HOMO→L+5 (16%), HOMO→L+4 (10%)
19	45861	218.05	0.00	HOMO→L+6 (84%), H-8→LUMO (70%), H-7→LUMO (21%)
20	46397	215.53	0.02	H-1→L+3 (88%)
21	47472	210.65	0.15	H-8→LUMO (14%), H-7→LUMO (39%), H-7→L+1 (11%), H-1→L+5 (12%)
22	47965	208.49	0.01	H-4→L+2 (38%), H-3→L+2 (30%)
23	48249	207.26	0.00	H-1→L+4 (33%), H-1→L+6 (45%), H-1→L+7 (10%)
24	48532	206.05	0.12	H-7→L+1 (28%), H-6→L+1 (29%), H-1→L+5 (11%)
25	48664	205.49	0.01	H-4→L+3 (61%), H-3→L+3 (13%)

26	49049	203.88	0.01	HOMO→L+7 (43%), HOMO→L+8 (10%)
27	49228	203.13	0.08	H-2→L+2 (32%), HOMO→L+7 (10%)
28	49232	203.12	0.20	H-3→L+3 (16%), H-2→L+3 (14%), HOMO→L+5 (12%)
29	49354	202.62	0.01	HOMO→L+7 (12%), HOMO→L+8 (82%)
30	49451	202.22	0.05	H-3→L+2 (18%), H-2→L+2 (55%)
31	49798	200.81	0.01	H-7→L+1 (19%), H-6→L+1 (30%), H-4→L+2 (19%), H- 3→L+2 (20%)
32	49845	200.62	0.01	H-1→L+4 (46%), H-1→L+6 (32%)
33	50034	199.86	0.13	H-6→L+1 (18%), H-4→L+2 (25%), H-3→L+2 (16%)
34	50968	196.20	0.01	H-8→L+1 (65%), H-7→L+1 (14%)
35	51431	194.43	0.17	H-7→LUMO (11%), H-5→L+2 (22%), H-1→L+5 (25%)
36	51512	194.13	0.06	HOMO→L+10 (55%)
37	51787	193.10	0.03	H-9→LUMO (18%), H-9→L+1 (33%), HOMO→L+9 (10%), HOMO→L+11 (10%)
38	51897	192.69	0.34	H-5→L+2 (16%), H-3→L+3 (17%), H-2→L+3 (25%)
39	51907	192.65	0.07	H-9→L+1 (15%), H-8→L+1 (10%), H-5→L+2 (24%)
40	52079	192.02	0.03	HOMO→L+9 (14%), HOMO→L+10 (21%), HOMO→L+11 (29%)
41	52507	190.45	0.04	HOMO→L+9 (50%), HOMO→L+11 (27%)
42	52551	190.29	0.00	H-2→L+4 (71%), H-2→L+7 (21%)
43	52954	188.84	0.00	H-3→L+4 (14%), H-1→L+7 (47%)
44	53106	188.30	0.01	H-3→L+4 (60%), H-3→L+7 (14%), H-1→L+7 (10%)
45	53235	187.85	0.00	H-5→L+3 (91%)
46	53626	186.48	0.00	H-1→L+8 (86%)
47	53744	186.07	0.01	H-4→L+5 (34%), H-3→L+5 (31%)
48	54010	185.15	0.00	H-9→LUMO (60%), H-9→L+1 (31%)
49	54094	184.86	0.02	H-4→L+4 (51%)
50	54291	184.19	0.00	HOMO→L+12 (73%)
51	54686	182.86	0.00	H-10→LUMO (42%), H- 1→L+10 (13%)
52	54847	182.33	0.03	H-10→LUMO (34%), H- 1→L+10 (16%)
53	54862	182.27	0.00	H-2→L+5 (87%)
54	55167	181.27	0.00	H-4→L+5 (18%), H-3→L+5 (32%), HOMO→L+14 (20%)
55	55240	181.03	0.00	H-4→L+5 (17%), H-3→L+5 (17%), HOMO→L+14 (24%), HOMO→L+15 (18%)
56	55489	180.22	0.00	H-11→LUMO (12%), H- 11→L+1 (20%), H-1→L+10 (12%), H-1→L+11 (10%), HOMO→L+13 (15%)

57	55553	180.01	0.00	H-11→LUMO (10%), HOMO→L+13 (36%)
58	55665	179.65	0.01	H-13→LUMO (24%), H-12→LUMO (26%), HOMO→L+13 (11%)
59	55703	179.52	0.01	H-2→L+4 (14%), H-2→L+6 (10%), H-2→L+7 (56%)
60	55859	179.02	0.00	H-11→L+1 (10%), H-1→L+9 (17%), H-1→L+11 (26%)
61	55903	178.88	0.02	H-3→L+6 (24%), H-3→L+7 (39%)
62	56088	178.29	0.02	H-4→L+6 (26%), H-3→L+6 (16%), H-3→L+7 (16%)
63	56191	177.97	0.00	HOMO→L+13 (10%), HOMO→L+14 (20%), HOMO→L+15 (51%)
64	56304	177.61	0.01	H-1→L+9 (46%), H-1→L+11 (12%)
65	56376	177.38	0.00	H-2→L+6 (69%)
66	56650	176.52	0.00	H-13→LUMO (47%), H- 12→LUMO (33%)
67	56765	176.17	0.00	H-4→L+6 (27%), H-3→L+6 (41%)
68	57100	175.13	0.01	H-5→L+5 (11%), H-4→L+10 (31%), H-1→L+10 (14%)
69	57186	174.87	0.02	H-6→L+2 (11%), H-5→L+5 (42%)
70	57309	174.49	0.01	H-7→L+2 (10%), H-6→L+2 (54%), H-5→L+5 (19%)
71	57426	174.14	0.01	H-5→L+4 (26%), H-4→L+7 (31%)
72	57468	174.01	0.03	H-2→L+9 (83%)
73	57798	173.02	0.02	H-11→LUMO (23%), H- 11→L+1 (11%), H-5→L+4 (13%), H-4→L+7 (13%)
74	57899	172.71	0.00	H-11→LUMO (17%), H- 11→L+1 (13%), H-5→L+4 (14%), H-4→L+7 (16%)
75	57984	172.46	0.00	H-8→L+2 (74%), H-7→L+2 (10%)
76	58158	171.95	0.00	H-1→L+12 (75%)
77	58239	171.71	0.00	H-3→L+9 (79%)
78	58343	171.40	0.03	H-10→L+1 (61%), H-2→L+10 (15%)
79	58450	171.09	0.01	HOMO→L+16 (70%)
80	58554	170.78	0.07	H-2→L+8 (51%)
81	58730	170.27	0.04	H-5→L+4 (15%), H-3→L+8 (45%)
82	58886	169.82	0.05	H-12→L+1 (11%), HOMO→L+17 (25%)
83	59043	169.37	0.01	H-12→L+1 (16%), HOMO→L+17 (19%)
84	59271	168.72	0.05	H-1→L+13 (16%), H-1→L+15 (21%)
85	59279	168.69	0.03	H-1→L+14 (35%), H-1→L+15 (11%)
86	59457	168.19	0.02	H-4→L+8 (39%), H-4→L+9 (10%), H-1→L+13 (13%)
87	59536	167.96	0.13	H-3→L+8 (15%), H-3→L+10 (13%), H-1→L+13 (18%)
88	59598	167.79	0.00	H-2→L+11 (70%)
89	59758	167.34	0.04	H-4→L+9 (30%), HOMO→L+18 (11%)

90	59840	167.11	0.01	H-3→L+11 (66%)
91	59996	166.68	0.01	H-7→L+2 (10%), H-5→L+6 (14%), H-1→L+13 (13%), HOMO→L+18 (30%)
92	60073	166.47	0.01	H-5→L+6 (59%), HOMO→L+18 (23%)
93	60232	166.02	0.01	H-1→L+14 (21%), H-1→L+15 (38%)
94	60450	165.43	0.00	H-14→LUMO (90%)
95	60615	164.97	0.04	H-7→L+2 (17%), HOMO→L+18 (15%), HOMO→L+20 (23%)
96	60763	164.57	0.01	H-7→L+3 (25%), H-6→L+3 (53%)
97	61028	163.86	0.02	H-7→L+2 (11%), HOMO→L+17 (11%), HOMO→L+20 (33%)
98	61097	163.67	0.00	H-4→L+11 (51%)
99	61251	163.26	0.02	H-5→L+7 (59%)
100	61449	162.74	0.05	H-12→L+1 (17%), H-5→L+7 (11%), H-5→L+10 (11%), H-3→L+10 (10%), HOMO→L+19 (12%)

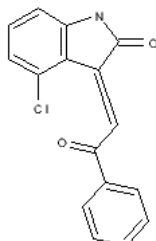
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## S4. 4-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : T2010-02-OPT-E-isomer-Chlorine-MeOH.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3c(cccc3Cl)NC2=O
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	4.1442 Debye
Energy	:	-1281.36432731 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	-0.35428497	-0.61643422	0.18292153
C	-1.52710772	0.02227397	-0.18056856
C	-2.79907346	-0.60632235	-0.13627197
C	-2.84885120	-1.89902246	0.38615209
C	-1.68135059	-2.56811142	0.75802135
C	-0.44893676	-1.93223143	0.64030939
H	0.60012943	-0.10901614	0.12481727
H	-1.74644029	-3.57325029	1.15182340
H	0.44916135	-2.46315932	0.93182778
C	-2.99198651	1.66560721	-0.82855254
C	-3.77326965	0.37830603	-0.61717564
N	-1.67571318	1.34191835	-0.60734266
H	-0.92445374	2.01287913	-0.67576927
O	-3.42332077	2.75162053	-1.16448700
C	-5.06766558	0.38611865	-0.97426045
H	-5.45324230	1.36384487	-1.26240468
C	-6.01897717	-0.74686712	-1.19164693
O	-5.72774887	-1.62302458	-1.99023163
C	-7.33677769	-0.70443225	-0.50147295
C	-8.30868816	-1.65762353	-0.83928096
C	-7.62172651	0.25202152	0.48201764
C	-9.54497242	-1.65015602	-0.20735160
H	-8.07513332	-2.39286399	-1.59926975

C	-8.86107349	0.25657472	1.11623538
H	-6.87528563	0.98724425	0.75929654
C	-9.82269955	-0.69213611	0.77121031
H	-10.29406929	-2.38676429	-0.47316575
H	-9.07591152	0.99693799	1.87761927
H	-10.78814602	-0.68693578	1.26409435
Cl	-4.37495422	-2.71306872	0.67960650

### TD-DFT Calculations

No.	Energy (cm <sup>-1</sup> )	Wavelength (nm)	Osc. Strength	Major contribs
1	24700	404.86	0.06	HOMO→LUMO (97%)
2	28347	352.78	0.03	H-4→LUMO (66%), H-1→LUMO (16%)
3	29569	338.19	0.15	H-4→LUMO (15%), H-1→LUMO (74%)
4	32364	308.99	0.01	H-3→LUMO (12%), H-2→LUMO (86%)
5	32691	305.90	0.02	HOMO→L+1 (88%)
6	33171	301.47	0.07	H-5→LUMO (38%), H-4→LUMO (12%), H-3→LUMO (36%)
7	33829	295.61	0.01	H-5→LUMO (42%), H-3→LUMO (37%)
8	36102	277.00	0.02	H-4→L+1 (14%), H-1→L+1 (68%)
9	37425	267.20	0.01	H-4→L+1 (53%), H-3→L+1 (10%), H-1→L+1 (17%)
10	39130	255.56	0.02	H-3→L+1 (20%), H-2→L+1 (68%)
11	40949	244.21	0.48	H-3→L+1 (12%), HOMO→L+2 (51%)
12	41428	241.38	0.21	H-6→LUMO (10%), H-3→L+1 (38%), H-2→L+1 (14%), HOMO→L+2 (15%)
13	42557	234.98	0.03	H-8→LUMO (17%), H-7→LUMO (17%), H-6→LUMO (45%)
14	42756	233.89	0.00	HOMO→L+3 (88%)
15	43011	232.50	0.02	H-8→LUMO (24%), H-7→LUMO (24%), H-6→LUMO (30%), H-5→L+1 (11%)
16	43558	229.58	0.01	H-8→LUMO (16%), H-5→L+1 (69%)
17	44779	223.32	0.10	H-8→LUMO (30%), H-7→LUMO (40%)
18	45009	222.18	0.12	H-1→L+2 (51%), HOMO→L+4 (18%), HOMO→L+5 (20%)
19	45505	219.75	0.01	HOMO→L+4 (56%), HOMO→L+5 (12%), HOMO→L+6 (20%)
20	46134	216.76	0.00	H-1→L+3 (47%), HOMO→L+6 (26%), HOMO→L+7 (16%)
21	46277	216.09	0.01	H-1→L+3 (47%), HOMO→L+6 (23%), HOMO→L+7 (14%)
22	48150	207.68	0.00	H-4→L+2 (21%), H-4→L+3 (51%), H-3→L+3 (10%)
23	48377	206.71	0.09	H-4→L+2 (19%), H-4→L+3 (19%), H-1→L+2 (11%), HOMO→L+5 (15%)

24	48585	205.83	0.05	H-4→L+2 (30%)
25	49065	203.81	0.00	H-1→L+4 (12%), HOMO→L+7 (37%), HOMO→L+9 (13%)
26	49313	202.79	0.02	H-2→L+2 (22%), HOMO→L+8 (27%)
27	49336	202.69	0.03	H-2→L+2 (20%), H-1→L+6 (11%), HOMO→L+8 (22%)
28	49401	202.43	0.01	H-1→L+6 (11%), H-1→L+7 (13%), HOMO→L+8 (18%)
29	49466	202.16	0.02	H-9→LUMO (48%), H-2→L+2 (29%)
30	49689	201.25	0.14	H-6→L+1 (19%), H-3→L+3 (10%), H-2→L+2 (17%)
31	49874	200.51	0.07	H-9→LUMO (14%), H-6→L+1 (24%), H-3→L+2 (20%), H-2→L+3 (10%)
32	49935	200.26	0.03	H-3→L+2 (20%), H-1→L+4 (34%), HOMO→L+8 (11%)
33	50016	199.94	0.07	H-3→L+2 (36%), H-1→L+4 (20%)
34	50237	199.05	0.08	H-7→L+1 (39%), H-5→L+2 (11%), H-1→L+5 (12%), H-1→L+6 (11%)
35	50754	197.03	0.06	H-8→L+1 (38%), H-7→L+1 (16%), H-1→L+5 (12%)
36	51217	195.25	0.10	H-5→L+2 (46%), H-4→L+2 (10%)
37	51545	194.01	0.01	HOMO→L+7 (10%), HOMO→L+9 (71%)
38	51825	192.96	0.42	H-10→LUMO (20%), H-3→L+3 (18%), H-2→L+3 (35%)
39	52044	192.14	0.01	H-10→LUMO (24%), HOMO→L+10 (25%), HOMO→L+11 (20%)
40	52246	191.40	0.08	H-8→L+1 (18%), HOMO→L+10 (27%)
41	52547	190.31	0.00	H-2→L+4 (59%), H-2→L+5 (16%), H-2→L+6 (15%)
42	52694	189.77	0.01	H-13→LUMO (11%), H-11→LUMO (51%)
43	52916	188.98	0.05	H-12→LUMO (12%), H-10→LUMO (23%), HOMO→L+10 (12%)
44	52942	188.89	0.02	H-1→L+6 (14%), H-1→L+7 (23%), H-1→L+8 (15%)
45	53311	187.58	0.02	H-12→LUMO (37%), H-11→LUMO (17%)
46	53335	187.49	0.05	HOMO→L+10 (13%), HOMO→L+11 (47%)
47	53416	187.21	0.00	H-3→L+4 (43%), H-3→L+6 (10%), H-1→L+8 (16%)
48	53701	186.22	0.00	H-1→L+7 (26%), H-1→L+8 (47%)
49	53996	185.20	0.01	H-4→L+4 (17%), H-4→L+5 (47%)
50	54302	184.15	0.00	H-4→L+4 (58%), H-4→L+5 (15%)
51	54368	183.93	0.00	HOMO→L+12 (69%)
52	54512	183.45	0.00	H-5→L+3 (95%)
53	54709	182.79	0.00	HOMO→L+13 (12%), HOMO→L+14 (48%), HOMO→L+15 (27%)

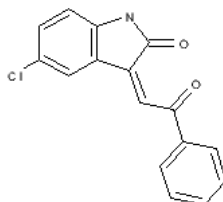
54	55016	181.76	0.01	H-2→L+4 (18%), H-2→L+5 (53%)
55	55222	181.09	0.01	H-1→L+9 (40%)
56	55486	180.22	0.01	H-13→LUMO (22%), H-3→L+5 (21%)
57	55579	179.92	0.00	H-13→LUMO (18%), H-3→L+4 (12%), H-3→L+5 (27%)
58	55632	179.75	0.03	H-3→L+5 (10%), H-1→L+9 (14%)
59	55717	179.48	0.00	H-1→L+9 (10%), HOMO→L+13 (38%)
60	55898	178.90	0.00	H-9→L+1 (50%)
61	55926	178.81	0.01	H-9→L+1 (24%), H-1→L+10 (32%), H-1→L+11 (15%)
62	56217	177.88	0.01	H-2→L+6 (36%)
63	56284	177.67	0.01	H-5→L+5 (21%), H-2→L+7 (13%)
64	56340	177.49	0.01	H-5→L+5 (10%), H-4→L+6 (10%), H-2→L+7 (34%)
65	56441	177.17	0.00	H-6→L+2 (40%), HOMO→L+15 (15%)
66	56550	176.83	0.00	H-6→L+2 (12%), HOMO→L+14 (16%), HOMO→L+15 (33%)
67	56635	176.57	0.04	H-6→L+2 (12%), H-3→L+6 (31%), H-2→L+7 (14%)
68	56864	175.86	0.01	H-1→L+10 (17%), H-1→L+11 (39%)
69	57033	175.34	0.01	H-3→L+7 (66%)
70	57042	175.31	0.05	H-5→L+4 (33%)
71	57204	174.81	0.00	H-8→L+2 (27%), H-7→L+2 (47%)
72	57377	174.29	0.02	H-14→LUMO (22%), H-5→L+4 (10%), H-5→L+5 (11%), H-4→L+7 (18%)
73	57651	173.46	0.01	H-2→L+6 (11%), H-2→L+7 (10%), H-2→L+8 (31%), H-2→L+10 (36%)
74	57821	172.95	0.01	HOMO→L+13 (10%), HOMO→L+16 (54%)
75	57932	172.62	0.01	H-14→LUMO (51%), H-5→L+5 (10%)
76	58067	172.22	0.00	H-4→L+6 (18%), H-4→L+7 (36%), H-4→L+8 (13%)
77	58269	171.62	0.01	H-1→L+12 (50%)
78	58436	171.13	0.00	H-3→L+8 (39%), H-3→L+10 (23%)
79	58724	170.29	0.03	H-2→L+8 (18%), H-2→L+9 (15%), H-2→L+10 (17%), H-2→L+11 (19%)
80	58989	169.52	0.02	H-1→L+14 (28%), H-1→L+15 (15%), HOMO→L+17 (22%)
81	59096	169.22	0.01	H-4→L+8 (19%), HOMO→L+17 (21%)
82	59122	169.14	0.02	H-10→L+1 (25%), H-8→L+2 (13%)
83	59232	168.83	0.01	H-10→L+1 (18%), H-4→L+8 (18%), HOMO→L+17 (11%)
84	59287	168.67	0.01	H-3→L+9 (16%), H-3→L+10 (21%)
85	59417	168.30	0.10	H-6→L+3 (10%), H-3→L+11 (11%), H-2→L+11 (23%)
86	59556	167.91	0.00	H-2→L+7 (10%), H-2→L+9 (54%), H-2→L+10 (16%)

87	59660	167.62	0.00	H-11→L+1 (33%), H-6→L+3 (28%)
88	59788	167.26	0.00	H-1→L+13 (46%)
89	59952	166.80	0.02	H-6→L+3 (10%), H-4→L+9 (12%), H-4→L+10 (12%), H-4→L+11 (15%)
90	60011	166.64	0.09	H-6→L+3 (19%), H-3→L+9 (25%)
91	60138	166.28	0.04	H-3→L+9 (21%), H-3→L+10 (12%)
92	60236	166.02	0.00	H-5→L+6 (49%)
93	60396	165.57	0.00	HOMO→L+18 (66%)
94	60478	165.35	0.01	H-5→L+6 (18%), H-4→L+10 (11%), H-1→L+15 (13%)
95	60617	164.97	0.04	H-16→LUMO (17%), H-3→L+11 (12%), H-1→L+15 (10%)
96	60702	164.74	0.00	H-8→L+3 (20%), H-7→L+3 (59%)
97	60753	164.60	0.00	H-16→LUMO (18%), H-15→LUMO (10%), H-12→L+1 (16%)
98	60778	164.53	0.00	H-16→LUMO (10%), H-4→L+9 (19%), H-4→L+10 (15%), H-1→L+15 (12%)
99	60917	164.16	0.06	H-10→L+1 (17%)
100	61238	163.30	0.00	HOMO→L+19 (72%)

## S5. 5-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : V2711-01-Z-Cl5.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3cc(ccc3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	4.9477 Debye
Energy	:	-1281.36888058 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	0.04157984	-0.18501930	0.00523506
C	-1.27003479	0.06415867	-0.36732301
C	-1.75016356	1.37584043	-0.55493379
C	-0.90562063	2.46241522	-0.36653227
C	0.41167653	2.20495129	0.00888890
C	0.88919908	0.91020292	0.19458461
H	0.40915745	-1.19328582	0.14796434
H	1.91907787	0.75122362	0.48583630
C	-3.47459936	-0.20822096	-0.97071677
C	-3.16071677	1.26943648	-0.93922853
N	-2.30430245	-0.84371144	-0.61643660
H	-2.22212863	-1.84819794	-0.55887169
O	-4.53235960	-0.74279088	-1.24917746
C	-4.05417252	2.22385645	-1.22521019
H	-3.76017928	3.27030873	-1.19630277
C	-5.46098375	1.98920023	-1.71828270
O	-5.65306044	2.02373219	-2.92186999
C	-6.56599569	1.83576465	-0.73541290
C	-7.87589169	1.69022667	-1.21549439
C	-6.33525562	1.84953690	0.64607286
C	-8.93504143	1.55557346	-0.32809055
H	-8.04096127	1.68410754	-2.28572655
C	-7.39923239	1.71737766	1.53432405
H	-5.32762289	1.96327758	1.02694476

C -8.69767666 1.56924105 1.04893112  
 H -9.94524956 1.44091952 -0.70331609  
 H -7.21605110 1.72899568 2.60223508  
 H -9.52517128 1.46500933 1.74137366  
 H -1.24986351 3.47911119 -0.50557232  
 Cl 1.51006043 3.56772685 0.25615034

### TD-DFT Calculations

No.	Energy ( $\text{cm}^{-1}$ )	Wavelength (nm)	Osc. Strength	Major contribs
1	25625	390.24	0.03	HOMO→LUMO (97%)
2	28901	346.00	0.01	HOMO→L+1 (86%)
3	31223	320.28	0.03	H-4→LUMO (25%), H-4→L+1 (17%), H-1→LUMO (20%), H-1→L+1 (13%), HOMO→L+1 (11%)
4	32594	306.81	0.03	H-5→LUMO (12%), H-4→LUMO (15%), H-4→L+1 (22%), H-3→LUMO (20%), H-1→L+1 (16%)
5	33932	294.71	0.16	H-5→LUMO (12%), H-3→LUMO (13%), H-1→LUMO (51%)
6	34534	289.57	0.01	H-2→LUMO (92%)
7	34731	287.92	0.03	H-4→LUMO (41%), H-3→LUMO (44%)
8	35824	279.14	0.01	H-5→LUMO (49%), H-3→LUMO (11%), H-1→L+1 (23%)
9	36711	272.40	0.01	H-5→LUMO (17%), H-4→L+1 (32%), H-1→L+1 (30%)
10	36794	271.79	0.02	H-3→L+1 (31%), H-2→L+1 (56%)
11	38551	259.40	0.52	H-5→L+1 (14%), H-3→L+1 (40%), H-2→L+1 (20%), HOMO→L+2 (18%)
12	39915	250.53	0.25	HOMO→L+2 (57%)
13	41365	241.75	0.01	HOMO→L+3 (86%)
14	41419	241.43	0.08	H-5→L+1 (56%), HOMO→L+3 (13%)
15	43301	230.94	0.06	H-6→LUMO (82%)
16	44041	227.06	0.00	HOMO→L+4 (27%), HOMO→L+5 (35%)
17	44747	223.48	0.03	HOMO→L+6 (31%), H-1→L+2 (33%), HOMO→L+4 (34%), HOMO→L+5 (19%)
18	45031	222.07	0.00	HOMO→L+5 (19%), HOMO→L+6 (15%), HOMO→L+7 (48%)
19	46255	216.19	0.00	H-7→LUMO (95%)
20	46832	213.53	0.00	H-6→L+1 (86%)
21	47167	212.01	0.01	H-4→L+3 (16%), H-1→L+3 (79%)
22	47492	210.56	0.02	H-4→L+2 (18%), H-1→L+2 (19%), HOMO→L+8 (19%)
23	47533	210.38	0.01	HOMO→L+6 (11%), HOMO→L+8 (55%)

24	47726	209.53	0.00	HOMO→L+6 (26%), HOMO→L+7 (36%), HOMO→L+9 (20%)
25	48161	207.64	0.04	H-8→LUMO (33%), H-3→L+2 (17%)
26	48944	204.31	0.14	H-8→LUMO (22%), H-2→L+2 (23%), H-1→L+2 (11%)
27	49107	203.64	0.19	H-3→L+3 (37%), H-2→L+3 (14%)
28	49225	203.15	0.02	H-3→L+2 (12%), H-2→L+2 (67%)
29	49533	201.88	0.02	H-4→L+3 (70%), H-1→L+3 (14%)
30	49712	201.16	0.01	HOMO→L+9 (72%)
31	49842	200.63	0.04	H-4→L+2 (41%), H-3→L+2 (38%)
32	50335	198.67	0.14	H-8→L+1 (70%)
33	50902	196.46	0.00	H-1→L+4 (25%), H-1→L+5 (34%), H-1→L+6 (14%), HOMO→L+11 (10%)
34	50953	196.26	0.01	HOMO→L+11 (67%)
35	51180	195.39	0.01	H-7→L+1 (88%)
36	51196	195.33	0.02	HOMO→L+10 (78%)
37	51487	194.22	0.07	H-5→L+2 (53%)
38	51577	193.88	0.01	H-9→LUMO (32%), H-9→L+1 (49%)
39	51907	192.65	0.27	H-3→L+3 (28%), H-2→L+3 (41%)
40	51978	192.39	0.02	H-1→L+5 (11%), H-1→L+6 (25%), H-1→L+7 (43%)
41	52613	190.07	0.29	H-1→L+4 (21%), H-1→L+5 (13%)
42	52655	189.92	0.07	H-2→L+4 (31%), H-2→L+5 (25%), H-2→L+6 (15%)
43	53158	188.12	0.01	H-5→L+3 (87%)
44	53215	187.92	0.01	H-3→L+4 (38%), H-3→L+5 (30%), H-3→L+6 (14%)
45	53499	186.92	0.00	HOMO→L+13 (48%), HOMO→L+14 (12%), HOMO→L+15 (12%)
46	53627	186.47	0.01	HOMO→L+12 (62%)
47	53776	185.96	0.01	H-9→LUMO (41%), H-9→L+1 (27%)
48	53894	185.55	0.03	H-9→LUMO (10%), H-4→L+4 (18%), H-3→L+4 (12%), H-3→L+5 (13%)
49	53948	185.36	0.02	H-4→L+5 (15%), H-1→L+6 (16%), H-1→L+7 (12%), H-1→L+8 (11%)
50	54466	183.60	0.04	H-1→L+7 (12%), H-1→L+8 (23%), HOMO→L+15 (29%)
51	54552	183.31	0.04	H-10→LUMO (41%), H-1→L+8 (18%)
52	54646	183.00	0.02	HOMO→L+15 (21%)
53	54744	182.67	0.00	H-13→LUMO (20%), H-12→LUMO (19%), H-11→LUMO (11%), HOMO→L+15 (13%)
54	54809	182.45	0.00	H-2→L+4 (19%), H-2→L+5 (16%), H-1→L+8 (11%)
55	54915	182.10	0.01	H-2→L+4 (26%), H-2→L+5 (23%), HOMO→L+14 (10%)



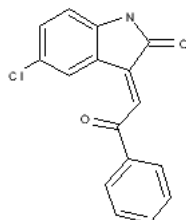
56	55007	181.79	0.00	HOMO→L+13 (12%), HOMO→L+14 (55%)
57	55206	181.14	0.01	H-4→L+4 (26%), H-4→L+5 (11%), H-3→L+5 (10%)
58	55386	180.55	0.04	H-4→L+4 (11%), H-4→L+5 (29%), H-3→L+4 (19%), H- 3→L+5 (13%)
59	55635	179.74	0.01	H-11→LUMO (12%), H- 11→L+1 (15%), H-1→L+9 (26%)
60	55948	178.74	0.05	H-6→L+2 (65%)
61	56091	178.28	0.01	H-2→L+5 (15%), H-2→L+6 (46%), H-2→L+7 (16%)
62	56295	177.64	0.04	H-3→L+5 (10%), H-3→L+6 (40%), H-3→L+7 (12%)
63	56461	177.11	0.01	H-13→LUMO (42%), H- 12→LUMO (17%), H- 11→LUMO (17%)
64	56768	176.16	0.01	H-1→L+9 (38%), H-1→L+11 (16%)
65	56962	175.55	0.00	H-7→L+2 (86%)
66	57168	174.92	0.00	H-4→L+6 (10%), H-1→L+10 (25%)
67	57338	174.41	0.01	HOMO→L+16 (76%)
68	57365	174.32	0.03	H-5→L+4 (43%), H-5→L+5 (22%)
69	57479	173.98	0.03	H-2→L+10 (76%)
70	57617	173.56	0.04	H-3→L+8 (13%), H-2→L+7 (11%), H-1→L+10 (25%)
71	57663	173.42	0.01	H-12→LUMO (13%), H- 11→LUMO (17%), H-11→L+1 (11%), H-1→L+11 (10%)
72	57702	173.30	0.03	H-12→L+1 (10%), H-3→L+6 (10%)
73	57846	172.87	0.00	H-4→L+6 (17%), H-3→L+7 (14%), H-2→L+7 (14%)
74	58033	172.32	0.01	H-1→L+11 (13%),
75	58109	172.09	0.02	HOMO→L+17 (19%)
76	58169	171.91	0.01	HOMO→L+17 (47%)
77	58228	171.74	0.03	H-10→L+1 (11%), H-4→L+6 (17%), H-3→L+8 (10%)
78	58247	171.68	0.00	H-2→L+8 (40%), H-2→L+9 (12%), H-2→L+11 (11%)
79	58318	171.47	0.00	H-4→L+6 (15%), H-3→L+7 (14%), H-3→L+10 (22%)
80	58549	170.80	0.02	H-10→L+1 (38%), H-3→L+10 (32%)
81	58628	170.57	0.01	H-10→L+1 (13%), H-3→L+10 (18%)
82	58811	170.04	0.01	H-5→L+5 (13%),
83	58873	169.86	0.05	HOMO→L+18 (30%)
84	58929	169.70	0.04	H-4→L+8 (14%),
85	59068	169.30	0.02	HOMO→L+18 (20%)
86	59133	169.11	0.02	H-6→L+3 (53%), H-4→L+7 (21%)
87	59231	168.83	0.14	H-6→L+3 (21%), H-4→L+7 (41%)
				H-4→L+8 (32%)
				HOMO→L+18 (14%),
				HOMO→L+19 (51%)
				H-3→L+9 (12%), H-3→L+11 (20%), H-2→L+9 (12%)

88	59377	168.41	0.05	H-2→L+9 (25%), H-2→L+11 (33%)
89	59578	167.85	0.01	H-3→L+7 (11%), H-3→L+9 (32%), H-3→L+11 (23%)
90	59816	167.18	0.06	H-8→L+2 (35%), H-4→L+10 (11%), H-1→L+12 (14%)
91	59991	166.69	0.04	H-8→L+2 (12%), HOMO→L+19 (12%), HOMO→L+20 (40%)
92	60027	166.59	0.06	H-8→L+2 (31%), H-4→L+10 (16%), H-1→L+12 (10%)
93	60247	165.98	0.01	H-1→L+13 (46%)
94	60569	165.10	0.01	H-4→L+10 (26%), H-1→L+12 (44%), H-1→L+15 (10%)
95	60852	164.33	0.01	H-5→L+6 (47%), H-4→L+9 (12%)
96	61018	163.89	0.01	H-16→LUMO (12%), H-14→LUMO (41%), H-5→L+6 (10%)
97	61080	163.72	0.01	H-14→LUMO (15%), H-5→L+6 (12%), H-4→L+10 (10%)
98	61153	163.52	0.04	H-14→LUMO (10%), H-4→L+10 (11%), H-4→L+11 (11%)
99	61351	163.00	0.00	H-13→L+1 (12%), H-6→L+4 (20%), H-6→L+5 (23%), H-5→L+8 (13%)
100	61453	162.73	0.02	H-13→L+1 (33%), H-5→L+8 (10%)

## S6. 5-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : V2711-02-E-Cl5.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3cc(ccc3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	3.0084 Debye
Energy	:	-1281.37448718 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	1.09890509	0.46393159	0.33268195
C	0.04457384	1.28343868	-0.03394722
C	-1.21035290	0.76176769	-0.43136215
C	-1.39729714	-0.62087733	-0.46309310
C	-0.33221716	-1.43549454	-0.09067181
C	0.89915007	-0.91839749	0.30203533
H	2.05419087	0.87354255	0.63493413
H	1.70357299	-1.58611023	0.58149707
C	-1.21212459	3.14179230	-0.49326634
C	-2.07146668	1.90231240	-0.73309833
N	0.01297769	2.67744327	-0.08139762
H	0.78415591	3.28627896	0.15043895
O	-1.53567898	4.30472422	-0.63311273
C	-3.34845233	2.10555053	-1.12148917
H	-3.61770558	3.14976645	-1.22935963
C	-4.38574743	1.09771478	-1.42813885
O	-4.12705231	-0.10085252	-1.48817897
C	-5.77877331	1.57675195	-1.69751883
C	-6.68051529	0.66761810	-2.27364635
C	-6.22858667	2.86650944	-1.37642956
C	-7.99175692	1.04057205	-2.53531671
H	-6.32965565	-0.32843915	-2.51143980
C	-7.54788208	3.23485851	-1.62788200

H -5.56771708 3.58605838 -0.91147524  
 C -8.42914772 2.32707191 -2.21178770  
 H -8.67517662 0.33267042 -2.98951459  
 H -7.88601255 4.23082924 -1.36752057  
 H -9.45345116 2.61883473 -2.41327906  
 H -2.34407711 -1.03164530 -0.77588671  
 Cl -0.55147296 -3.18982458 -0.12423487

### TD-DFT Calculations

No.	Energy ( $\text{cm}^{-1}$ )	Wavelength (nm)	Osc. Strength	Major contribs
1	19912	502.22	0.07	HOMO→LUMO (98%) H-4→LUMO (48%), H-3→LUMO (28%), H-2→LUMO (20%)
2	23963	417.31	0.00	
3	27914	358.24	0.55	H-1→LUMO (93%)
4	28167	355.02	0.00	H-3→LUMO (26%), H-2→LUMO (71%)
5	29548	338.43	0.00	H-5→LUMO (93%)
6	30657	326.19	0.00	H-4→LUMO (41%), H-3→LUMO (43%)
7	35416	282.36	0.01	HOMO→L+1 (93%)
8	37462	266.94	0.01	H-6→LUMO (87%)
9	39183	255.21	0.32	H-8→LUMO (21%), HOMO→L+2 (61%)
10	39963	250.23	0.00	H-7→LUMO (90%)
11	40326	247.98	0.01	H-4→L+1 (38%), H-3→L+1 (20%), H-2→L+1 (29%)
12	41499	240.97	0.03	H-3→L+1 (25%), H-2→L+1 (35%), HOMO→L+3 (10%)
13	42072	237.69	0.10	H-8→LUMO (47%), H-1→L+1 (12%), HOMO→L+3 (23%)
14	42603	234.72	0.01	H-8→LUMO (14%), HOMO→L+3 (66%)
15	43514	229.81	0.10	H-1→L+1 (69%), HOMO→L+2 (11%)
16	44528	224.58	0.00	HOMO→L+5 (62%), HOMO→L+6 (30%)
17	45101	221.72	0.16	H-4→L+1 (41%), H-3→L+1 (24%), H-2→L+1 (13%)
18	45351	220.50	0.11	H-1→L+2 (20%), HOMO→L+4 (67%)
19	45526	219.65	0.00	H-9→LUMO (65%), HOMO→L+7 (22%)
20	45538	219.59	0.00	H-9→LUMO (29%), HOMO→L+5 (12%), HOMO→L+7 (48%)
21	47094	212.34	0.00	H-5→L+1 (88%)
22	47738	209.48	0.00	H-4→L+2 (24%), H-3→L+2 (20%), H-2→L+2 (29%)
23	47927	208.65	0.00	H-4→L+3 (32%), H-3→L+3 (22%), H-2→L+3 (14%)
24	47998	208.34	0.00	HOMO→L+5 (13%), HOMO→L+6 (48%), HOMO→L+7 (12%)
25	48055	208.10	0.00	H-12→LUMO (36%), H-11→LUMO (35%)
26	48201	207.47	0.08	H-10→LUMO (53%), H-1→L+2 (26%)

27	48296	207.06	0.00	HOMO→L+8 (80%)
28	49040	203.92	0.05	H-12→LUMO (12%), H-2→L+2 (16%), H-1→L+3 (37%)
29	49123	203.57	0.01	H-12→LUMO (33%), H-11→LUMO (39%), H-1→L+3 (10%)
30	49414	202.37	0.02	H-4→L+2 (10%), H-2→L+2 (30%), H-1→L+3 (35%)
31	49526	201.91	0.05	H-10→LUMO (22%), H-4→L+2 (15%), H-3→L+2 (14%), H-1→L+2 (27%)
32	50276	198.90	0.04	H-5→L+2 (64%)
33	50600	197.63	0.10	H-5→L+2 (11%), H-4→L+2 (29%), H-3→L+2 (17%)
34	50789	196.89	0.13	H-13→LUMO (46%), H-4→L+3 (15%), H-3→L+3 (18%)
35	50822	196.76	0.00	HOMO→L+9 (71%)
36	51341	194.78	0.13	H-13→LUMO (15%), H-4→L+3 (12%), H-3→L+2 (12%), H-2→L+3 (24%)
37	51795	193.07	0.00	H-1→L+5 (45%), HOMO→L+10 (35%)
38	51965	192.44	0.00	H-1→L+5 (34%), HOMO→L+10 (46%)
39	52000	192.31	0.24	H-6→L+1 (54%), H-1→L+4 (27%)
40	52300	191.21	0.00	H-2→L+5 (70%), H-2→L+6 (20%)
41	52717	189.69	0.10	H-13→LUMO (14%), H-2→L+4 (10%), HOMO→L+11 (25%)
42	52844	189.24	0.01	H-3→L+5 (13%), H-1→L+6 (29%), H-1→L+7 (20%)
43	52889	189.07	0.07	H-1→L+4 (11%), HOMO→L+11 (55%)
44	53160	188.11	0.15	H-6→L+1 (14%), H-4→L+4 (20%), H-3→L+4 (21%), H-2→L+4 (15%), H-1→L+4 (12%)
45	53327	187.52	0.02	H-3→L+5 (32%), H-1→L+7 (38%)
46	53444	187.11	0.00	H-16→LUMO (11%), H-14→LUMO (69%)
47	53523	186.83	0.35	H-13→LUMO (11%), H-6→L+1 (14%), H-4→L+4 (14%), H-3→L+3 (10%), H-2→L+3 (13%), H-1→L+4 (11%)
48	54156	184.65	0.00	H-4→L+5 (53%), H-3→L+5 (18%)
49	54323	184.09	0.00	HOMO→L+12 (59%)
50	54850	182.32	0.00	HOMO→L+12 (13%), HOMO→L+13 (36%), HOMO→L+15 (36%)
51	54870	182.25	0.00	H-5→L+3 (96%)
52	55114	181.44	0.01	H-7→L+1 (82%)
53	55128	181.40	0.10	H-4→L+4 (15%), H-2→L+4 (45%)
54	55200	181.16	0.00	HOMO→L+13 (22%), HOMO→L+14 (22%), HOMO→L+15 (20%)
55	55397	180.52	0.00	H-4→L+5 (18%), H-1→L+6 (25%)

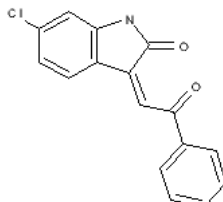
56	55549	180.02	0.01	H-8→L+1 (23%), H-6→L+2 (22%), H-4→L+4 (11%), H-3→L+4 (25%)
57	55729	179.44	0.00	H-1→L+8 (15%), HOMO→L+13 (13%), HOMO→L+14 (41%), HOMO→L+15 (11%)
58	55803	179.20	0.00	H-2→L+5 (13%), H-2→L+6 (43%), H-1→L+8 (14%)
59	55874	178.98	0.00	H-2→L+6 (12%), H-1→L+8 (52%)
60	55941	178.76	0.05	H-8→L+1 (16%), H-6→L+2 (19%), H-4→L+4 (14%), H-3→L+4 (18%)
61	56195	177.95	0.01	H-5→L+4 (63%)
62	56555	176.82	0.03	H-3→L+6 (39%), H-1→L+9 (14%)
63	56629	176.59	0.03	H-8→L+1 (25%), H-6→L+2 (21%)
64	56749	176.22	0.02	H-8→L+1 (11%), H-2→L+7 (12%), H-2→L+8 (27%), H-2→L+10 (14%)
65	56853	175.89	0.00	H-4→L+6 (15%), H-3→L+7 (14%), H-2→L+7 (22%), H-2→L+8 (17%)
66	57127	175.05	0.03	H-16→LUMO (33%), H-5→L+5 (11%)
67	57138	175.01	0.04	H-16→LUMO (30%), H-5→L+5 (13%), H-4→L+6 (11%)
68	57409	174.19	0.00	H-16→LUMO (13%), H-7→L+2 (66%)
69	57540	173.79	0.02	H-5→L+5 (12%), H-4→L+6 (10%), H-3→L+6 (12%), H-3→L+8 (26%)
70	57654	173.45	0.01	H-5→L+5 (18%), H-3→L+8 (15%), H-1→L+9 (17%), H-1→L+10 (18%)
71	57882	172.77	0.01	H-4→L+6 (13%), H-4→L+11 (14%)
72	57985	172.46	0.00	H-4→L+6 (15%), H-1→L+9 (19%)
73	58039	172.30	0.01	H-9→L+1 (18%), H-3→L+7 (18%)
74	58134	172.02	0.03	H-15→LUMO (38%), H-9→L+1 (19%), HOMO→L+16 (15%)
75	58147	171.98	0.00	H-15→LUMO (14%), H-9→L+1 (46%)
76	58213	171.78	0.01	H-15→LUMO (18%), HOMO→L+16 (49%)
77	58333	171.43	0.01	H-5→L+5 (11%), H-4→L+8 (33%), H-3→L+8 (11%), H-1→L+10 (18%)
78	58606	170.63	0.00	H-4→L+7 (40%), H-3→L+7 (26%)
79	58751	170.21	0.00	H-4→L+7 (17%), H-2→L+9 (58%)
80	58909	169.75	0.02	HOMO→L+16 (12%), HOMO→L+17 (22%), HOMO→L+18 (40%)
81	59226	168.85	0.02	H-4→L+8 (24%), H-1→L+10 (30%), HOMO→L+17 (12%)
82	59383	168.40	0.01	HOMO→L+17 (35%), HOMO→L+18 (19%)

83	59462	168.17	0.04	H-8→L+2 (47%), H-6→L+3 (20%)
84	59487	168.10	0.02	H-2→L+8 (17%), H-2→L+10 (43%), H-1→L+11 (11%)
85	59506	168.05	0.01	H-8→L+2 (13%), H-6→L+3 (70%)
86	59567	167.88	0.02	H-1→L+11 (51%)
87	59643	167.67	0.00	H-3→L+9 (50%), HOMO→L+17 (10%)
88	60098	166.39	0.00	H-4→L+9 (18%), HOMO→L+19 (31%)
89	60240	166.00	0.00	H-4→L+9 (31%), HOMO→L+19 (37%)
90	60278	165.90	0.00	H-4→L+9 (15%), HOMO→L+20 (50%)
91	60408	165.54	0.02	H-3→L+10 (43%), HOMO→L+19 (12%)
92	60416	165.52	0.03	H-17→LUMO (25%), H-3→L+10 (15%), H-2→L+11 (10%), HOMO→L+20 (10%)
93	60796	164.48	0.00	H-5→L+6 (48%), H-4→L+10 (25%)
94	60865	164.30	0.15	H-3→L+11 (24%), H-2→L+11 (32%)
95	61090	163.69	0.01	H-5→L+6 (28%), H-4→L+10 (43%)
96	61445	162.75	0.00	H-1→L+12 (51%)
97	61524	162.54	0.06	H-4→L+11 (20%), H-3→L+11 (14%), H-1→L+14 (18%)
98	61648	162.21	0.01	H-6→L+4 (61%), HOMO→L+21 (13%)
99	61682	162.12	0.03	H-5→L+7 (39%), H-5→L+8 (16%)
100	61775	161.88	0.00	H-6→L+5 (24%), H-6→L+6 (27%), H-6→L+7 (29%)

## S7. 6-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : V2711-03-Z-Cl6.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3ccc(cc3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	4.4781 Debye
Energy	:	-1281.36947453 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	0.03373035	-0.19507575	0.01105960
C	-1.27388060	0.06496447	-0.36770654
C	-1.75315380	1.37737226	-0.55882102
C	-0.89929426	2.45521355	-0.36594573
C	0.42430627	2.22360086	0.01599461
C	0.86143255	0.91390401	0.19594592
H	0.40042907	-1.20189261	0.15713090
C	-3.47458744	-0.20741977	-0.98066795
C	-3.16138887	1.26982903	-0.94681722
N	-2.30434728	-0.84353900	-0.62019444
H	-2.22200632	-1.84804308	-0.56219256
O	-4.52853966	-0.74534571	-1.26499784
C	-4.05562782	2.22425151	-1.23257613
H	-3.76062989	3.27040172	-1.20222640
C	-5.46319818	1.99193132	-1.72305739
O	-5.66061735	2.03024173	-2.92578864
C	-6.56552172	1.83539844	-0.73687929
C	-7.87635136	1.68577182	-1.21316385
C	-6.33126020	1.85185635	0.64396626
C	-8.93287945	1.55032837	-0.32274160
H	-8.04414463	1.67701399	-2.28293824
C	-7.39264917	1.71938968	1.53531313
H	-5.32276154	1.96839607	1.02169263
C	-8.69205475	1.56771326	1.05365694



H -9.94378948 1.43243670 -0.69510669  
H -7.20671129 1.73393798 2.60271335  
H -9.51758957 1.46347451 1.74843705  
H -1.24410868 3.47245693 -0.50874990  
H 1.10512507 3.04938316 0.17077059  
Cl 2.53454161 0.63455224 0.67836642

### TD-DFT Calculations

No.	Energy (cm <sup>-1</sup> )	Wavelength (nm)	Osc. Strength	Major contribs
1	26721	374.24	0.07	HOMO→LUMO (94%)
2	29082	343.85	0.00	HOMO→L+1 (81%)
3	31514	317.32	0.05	H-4→LUMO (31%), H-4→L+1 (16%), H-1→LUMO (16%), HOMO→L+1 (14%)
4	32800	304.87	0.09	H-5→LUMO (10%), H-4→L+1 (33%), H-3→LUMO (14%), H-1→LUMO (15%), H-1→L+1 (12%)
5	33288	300.41	0.16	H-5→LUMO (10%), H-4→LUMO (14%), H-3→LUMO (13%), H-1→LUMO (50%)
6	34707	288.13	0.01	H-2→LUMO (89%)
7	34832	287.09	0.01	H-4→LUMO (36%), H-3→LUMO (44%)
8	35793	279.39	0.01	H-5→LUMO (42%), H-3→LUMO (12%), H-1→L+1 (34%)
9	36349	275.11	0.00	H-5→LUMO (29%), H-4→L+1 (22%), H-1→L+1 (35%)
10	36873	271.20	0.02	H-3→L+1 (28%), H-2→L+1 (58%)
11	38658	258.68	0.49	H-5→L+1 (14%), H-3→L+1 (39%), H-2→L+1 (20%)
12	39987	250.08	0.23	HOMO→L+2 (18%)
13	41399	241.55	0.08	HOMO→L+2 (61%)
14	41780	239.35	0.00	H-5→L+1 (67%)
15	44098	226.77	0.03	HOMO→L+3 (98%)
16	44675	223.84	0.00	H-6→LUMO (74%), HOMO→L+5 (12%)
17	45052	221.97	0.02	HOMO→L+4 (64%), HOMO→L+6 (26%)
18	45592	219.33	0.00	H-1→L+2 (47%), HOMO→L+5 (40%), HOMO→L+4 (14%), HOMO→L+6 (26%)
19	46037	217.22	0.00	HOMO→L+7 (50%)
20	46931	213.08	0.00	H-6→L+1 (84%)
21	47247	211.66	0.02	H-7→LUMO (95%)
22	47674	209.76	0.01	H-4→L+3 (19%), H-1→L+3 (78%), H-4→L+2 (39%), H-3→L+2 (32%)
23	47995	208.35	0.00	HOMO→L+6 (17%), HOMO→L+7 (38%), HOMO→L+8 (31%)
24	48398	206.62	0.01	H-8→LUMO (26%), H-1→L+2 (18%), HOMO→L+5 (13%)

25	48456	206.37	0.00	HOMO→L+6 (18%), HOMO→L+8 (53%), HOMO→L+9 (14%)
26	48840	204.75	0.08	H-4→L+3 (41%), H-3→L+3 (27%), H-1→L+3 (16%)
27	49031	203.95	0.07	H-2→L+2 (69%)
28	49233	203.11	0.17	H-8→LUMO (15%), H-3→L+2 (20%), H-2→L+2 (22%)
29	49342	202.67	0.20	H-8→LUMO (12%), H-4→L+3 (26%), H-3→L+3 (15%), H-2→L+3 (12%)
30	49816	200.74	0.23	H-4→L+2 (37%), H-3→L+2 (28%)
31	49974	200.11	0.00	H-1→L+4 (34%), H-1→L+6 (42%)
32	50159	199.37	0.00	HOMO→L+9 (75%)
33	50955	196.25	0.00	H-1→L+4 (36%), H-1→L+7 (41%)
34	51012	196.03	0.11	H-5→L+2 (52%), H-1→L+5 (14%)
35	51286	194.99	0.04	H-9→L+1 (17%), H-8→L+1 (43%), H-5→L+2 (15%)
36	51479	194.25	0.02	HOMO→L+10 (13%), HOMO→L+11 (58%)
37	51591	193.83	0.02	HOMO→L+10 (72%), HOMO→L+11 (12%)
38	51721	193.35	0.08	H-9→LUMO (21%), H-9→L+1 (32%), H-8→L+1 (15%)
39	51936	192.54	0.12	H-7→L+1 (45%), H-3→L+3 (14%), H-2→L+3 (19%)
40	51993	192.33	0.08	H-7→L+1 (51%), H-3→L+3 (10%), H-2→L+3 (14%)
41	52612	190.07	0.01	H-2→L+4 (63%), H-2→L+6 (18%)
42	52714	189.70	0.29	H-8→LUMO (10%), H-8→L+1 (15%), H-1→L+5 (31%)
43	53165	188.09	0.01	H-5→L+3 (74%), H-3→L+4 (11%)
44	53198	187.98	0.01	H-5→L+3 (17%), H-3→L+4 (55%), H-3→L+6 (12%)
45	53304	187.60	0.01	H-1→L+6 (11%), H-1→L+7 (34%), H-1→L+8 (20%)
46	53710	186.19	0.00	HOMO→L+12 (66%)
47	53790	185.91	0.01	H-4→L+5 (30%), H-3→L+5 (30%)
48	53907	185.50	0.00	H-4→L+4 (10%), H-1→L+6 (11%), H-1→L+8 (24%), HOMO→L+12 (11%), HOMO→L+13 (15%)
49	53988	185.23	0.00	H-9→LUMO (51%), H-9→L+1 (33%)
50	54382	183.88	0.00	H-1→L+8 (31%), HOMO→L+13 (29%), HOMO→L+15 (15%)
51	54516	183.43	0.00	H-4→L+4 (30%), H-4→L+9 (10%)
52	54751	182.65	0.04	HOMO→L+13 (32%), HOMO→L+15 (41%)
53	54871	182.25	0.00	H-2→L+5 (67%)
54	54972	181.91	0.01	H-12→L+1 (11%), H-11→LUMO (13%), H-11→L+1 (10%), H-4→L+4 (22%)

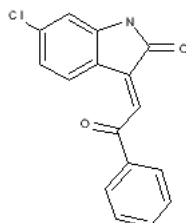
55	55009	181.79	0.01	H-13→LUMO (23%), H-12→LUMO (17%), H-11→LUMO (14%), H-2→L+5 (15%)
56	55184	181.21	0.05	H-10→LUMO (44%), H-3→L+5 (24%)
57	55365	180.62	0.03	H-10→LUMO (27%), H-4→L+5 (21%), H-3→L+5 (17%)
58	55664	179.65	0.01	H-12→L+1 (11%), H-11→L+1 (11%), H-1→L+9 (31%)
59	55817	179.16	0.01	H-6→L+2 (19%), HOMO→L+14 (50%)
60	55858	179.02	0.02	H-6→L+2 (49%), HOMO→L+14 (22%)
61	56027	178.49	0.01	H-2→L+4 (18%), H-2→L+6 (49%), H-2→L+7 (13%)
62	56247	177.79	0.04	H-3→L+4 (12%), H-3→L+6 (45%), H-3→L+7 (14%)
63	56425	177.23	0.00	H-4→L+11 (10%), H-1→L+9 (31%), H-1→L+11 (14%)
64	56633	176.58	0.00	H-13→LUMO (47%), H-12→LUMO (16%), H-11→LUMO (22%)
65	56967	175.54	0.01	H-5→L+4 (12%), H-4→L+7 (11%), H-1→L+10 (20%)
66	57181	174.88	0.02	H-5→L+5 (68%)
67	57221	174.76	0.02	H-4→L+6 (21%), H-1→L+10 (32%)
68	57342	174.39	0.02	H-2→L+7 (17%), H-2→L+10 (48%)
69	57585	173.66	0.00	H-4→L+6 (37%), H-1→L+10 (27%)
70	57646	173.47	0.01	H-2→L+7 (37%), H-2→L+10 (30%)
71	57703	173.30	0.01	H-7→L+2 (67%), H-1→L+11 (13%)
72	57729	173.22	0.00	H-7→L+2 (28%), H-1→L+11 (28%)
73	57756	173.14	0.04	HOMO→L+16 (48%)
74	57933	172.61	0.01	H-12→LUMO (12%), H-3→L+7 (13%), HOMO→L+16 (17%)
75	57977	172.48	0.02	H-4→L+7 (10%)
76	58269	171.62	0.00	H-3→L+7 (14%), H-3→L+10 (21%), H-2→L+8 (19%)
77	58301	171.52	0.00	H-5→L+4 (11%), H-4→L+7 (17%), HOMO→L+17 (21%)
78	58362	171.34	0.02	H-6→L+3 (11%), H-4→L+7 (21%), H-3→L+10 (17%), HOMO→L+17 (13%)
79	58372	171.31	0.03	H-10→L+1 (25%), H-3→L+10 (17%)
80	58382	171.29	0.00	H-6→L+3 (67%)
81	58520	170.88	0.01	H-10→L+1 (15%), H-3→L+10 (14%), H-2→L+8 (27%), H-2→L+11 (13%)
82	58595	170.66	0.01	H-3→L+8 (42%)
83	58700	170.36	0.01	HOMO→L+17 (12%), HOMO→L+18 (40%)
84	58818	170.01	0.06	H-10→L+1 (18%), H-2→L+9 (24%)
85	58993	169.51	0.05	H-4→L+8 (18%), H-1→L+12 (16%), HOMO→L+18 (20%)

86	59213	168.88	0.13	H-11→L+1 (12%), H-3→L+9 (11%), H-3→L+11 (14%), H-1→L+12 (20%)
87	59364	168.45	0.02	H-4→L+8 (16%), H-3→L+9 (12%), H-3→L+11 (12%), H-1→L+12 (18%)
88	59440	168.24	0.02	H-2→L+8 (19%), H-2→L+9 (19%), H-2→L+11 (24%)
89	59610	167.76	0.02	H-4→L+8 (11%), H-4→L+10 (21%), H-1→L+12 (17%), H-1→L+13 (12%)
90	59751	167.36	0.04	H-3→L+8 (13%), H-3→L+9 (12%), H-3→L+11 (18%), H-1→L+13 (14%)
91	59948	166.81	0.02	H-1→L+15 (42%)
92	60106	166.37	0.01	H-14→LUMO (22%), H-8→L+2 (22%)
93	60213	166.08	0.01	H-14→LUMO (59%), H-8→L+2 (10%)
94	60361	165.67	0.03	HOMO→L+19 (47%), HOMO→L+20 (24%)
95	60657	164.86	0.01	H-4→L+9 (20%), H-4→L+10 (24%), H-4→L+11 (25%)
96	60790	164.50	0.02	H-5→L+6 (63%)
97	60902	164.20	0.00	H-8→L+2 (18%), H-6→L+5 (10%), H-5→L+7 (10%), H-1→L+13 (15%)
98	61082	163.71	0.05	H-5→L+7 (15%), H-5→L+8 (12%)
99	61117	163.62	0.03	H-6→L+5 (15%), HOMO→L+20 (30%)
100	61220	163.34	0.02	H-6→L+5 (11%), H-5→L+7 (13%), HOMO→L+20 (19%)

## S8. 6-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : V2711-04-E-Cl6.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3ccc(cc3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	1.7017 Debye
Energy	:	-1281.37530478 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	1.11671495	0.48853150	0.30611321
C	0.05453622	1.27983999	-0.09584110
C	-1.22178531	0.74531192	-0.40345243
C	-1.41469800	-0.63334388	-0.30347279
C	-0.36040905	-1.45242870	0.10127298
C	0.87523377	-0.88347584	0.39668262
H	2.08642054	0.90609306	0.53971016
C	-1.19317186	3.10958076	-0.67217493
C	-2.07592201	1.86825478	-0.77311110
N	0.04120665	2.66296721	-0.26273108
H	0.82873398	3.27666521	-0.11359486
O	-1.50299156	4.26163816	-0.90115666
C	-3.36404562	2.05938959	-1.13361907
H	-3.62379169	3.09450173	-1.32193780
C	-4.42364597	1.04681039	-1.31686723
O	-4.18390989	-0.15712073	-1.28893530
C	-5.82055712	1.52479935	-1.57149029
C	-6.75339794	0.58983082	-2.04771543
C	-6.24327087	2.84030771	-1.32796013
C	-8.06908512	0.96183699	-2.28833723
H	-6.42330933	-0.42573255	-2.22536111
C	-7.56665421	3.20861697	-1.55739188
H	-5.55698586	3.58116937	-0.93935287

C -8.47938728 2.27415538 -2.04258823  
H -8.77696133 0.23307519 -2.66565537  
H -7.88344908 4.22527218 -1.35689843  
H -9.50700760 2.56530929 -2.22744894  
H -2.37732697 -1.05597997 -0.54662502  
H -0.49784938 -2.52205586 0.18209860  
Cl 2.19666815 -1.92990851 0.90284014

### TD-DFT Calculations

No.	Energy ( $\text{cm}^{-1}$ )	Wavelength (nm)	Osc. Strength	Major contribs
1	21242	470.76	0.14	HOMO→LUMO (95%)
2	23987	416.89	0.00	H-4→LUMO (51%), H-3→LUMO (19%), H-2→LUMO (27%)
3	27406	364.88	0.53	H-1→LUMO (93%)
4	28382	352.34	0.00	H-3→LUMO (34%), H-2→LUMO (60%)
5	29798	335.60	0.00	H-5→LUMO (87%)
6	30404	328.90	0.02	H-5→LUMO (10%), H-4→LUMO (35%), H-3→LUMO (40%), H-2→LUMO (12%)
7	36582	273.36	0.01	HOMO→L+1 (95%)
8	38058	262.76	0.09	H-6→LUMO (81%), HOMO→L+2 (14%)
9	39570	252.72	0.21	H-8→LUMO (14%), H-6→LUMO (12%), H-1→L+1 (10%), HOMO→L+2 (57%)
10	40213	248.67	0.01	H-4→L+1 (44%), H-3→L+1 (13%), H-2→L+1 (36%)
11	41335	241.93	0.01	H-7→LUMO (91%)
12	41567	240.58	0.03	H-3→L+1 (31%), H-2→L+1 (25%)
13	42174	237.11	0.14	H-8→LUMO (45%), H-1→L+1 (36%)
14	43236	231.29	0.00	HOMO→L+3 (83%)
15	43512	229.82	0.13	H-8→LUMO (24%), H-1→L+1 (42%), HOMO→L+2 (16%)
16	45055	221.95	0.14	H-4→L+1 (38%), H-3→L+1 (22%), H-2→L+1 (17%)
17	45463	219.96	0.00	HOMO→L+5 (71%), HOMO→L+6 (19%)
18	45719	218.73	0.01	H-9→LUMO (94%)
19	45864	218.03	0.04	H-1→L+2 (37%), HOMO→L+4 (53%)
20	46329	215.85	0.00	HOMO→L+7 (88%)
21	47259	211.60	0.00	H-5→L+1 (74%)
22	47485	210.59	0.00	H-5→L+1 (12%), H-4→L+2 (25%), H-3→L+2 (15%), H-2→L+2 (38%)
23	47698	209.65	0.01	H-4→L+3 (46%), H-3→L+3 (21%), H-2→L+3 (22%)
24	48271	207.16	0.00	H-12→LUMO (44%), H-11→LUMO (45%)
25	48689	205.39	0.00	HOMO→L+5 (16%), HOMO→L+6 (67%)
26	48719	205.26	0.11	H-10→LUMO (31%), H-1→L+2 (30%), HOMO→L+4 (15%)

27	48819	204.84	0.08	H-1→L+3 (71%)
28	49166	203.39	0.00	H-4→L+2 (20%), H-3→L+2 (15%), H-2→L+2 (40%)
29	49270	202.97	0.00	HOMO→L+8 (89%)
30	49319	202.76	0.00	H-12→LUMO (43%), H-11→LUMO (45%)
31	49622	201.52	0.01	H-10→LUMO (20%), H-4→L+2 (23%), H-3→L+2 (39%)
32	50134	199.46	0.09	H-10→LUMO (31%), H-5→L+2 (22%), HOMO→L+4 (13%)
33	50279	198.89	0.03	H-5→L+2 (53%), H-4→L+2 (14%)
34	50702	197.23	0.00	H-1→L+5 (30%), H-1→L+6 (13%), H-1→L+7 (44%)
35	50800	196.85	0.13	H-13→LUMO (34%), H-4→L+3 (16%), H-3→L+3 (22%)
36	51269	195.05	0.17	H-13→LUMO (24%), H-4→L+3 (10%), H-2→L+3 (23%)
37	51516	194.12	0.00	H-1→L+5 (36%), H-1→L+7 (42%)
38	51609	193.76	0.00	HOMO→L+9 (73%)
39	51832	192.93	0.52	H-6→L+1 (23%), H-1→L+4 (43%)
40	52178	191.65	0.02	H-2→L+5 (65%), H-2→L+6 (17%)
41	52310	191.17	0.08	H-6→L+1 (40%), H-1→L+4 (21%)
42	52681	189.82	0.02	H-14→LUMO (15%), H-2→L+4 (14%), HOMO→L+10 (36%)
43	52768	189.51	0.02	H-14→LUMO (29%), HOMO→L+10 (40%)
44	52795	189.41	0.03	H-14→LUMO (39%), H-4→L+4 (11%), H-3→L+4 (10%), H-2→L+4 (18%)
45	52959	188.83	0.00	H-3→L+5 (53%), H-3→L+6 (11%), H-1→L+6 (19%)
46	53297	187.63	0.23	H-13→LUMO (22%), H-4→L+4 (17%), H-3→L+3 (12%), HOMO→L+11 (19%)
47	53827	185.78	0.01	H-4→L+5 (39%), HOMO→L+11 (18%)
48	53910	185.50	0.03	H-4→L+5 (15%), HOMO→L+11 (41%)
49	54600	183.15	0.00	H-4→L+5 (18%), H-1→L+6 (32%), H-1→L+9 (10%)
50	54650	182.98	0.00	H-1→L+8 (11%), HOMO→L+13 (61%)
51	54970	181.92	0.00	H-5→L+3 (97%)
52	55073	181.58	0.01	H-1→L+8 (70%), HOMO→L+13 (13%)
53	55124	181.41	0.12	H-4→L+4 (16%), H-3→L+4 (13%), H-2→L+4 (46%)
54	55373	180.59	0.01	HOMO→L+12 (65%)
55	55399	180.51	0.10	H-6→L+2 (44%), H-3→L+4 (22%)
56	55691	179.56	0.02	H-2→L+6 (21%), HOMO→L+14 (37%)
57	55705	179.52	0.01	H-2→L+6 (39%), HOMO→L+14 (11%)
58	55815	179.16	0.02	H-6→L+2 (27%), H-4→L+4 (12%), H-3→L+4 (17%), HOMO→L+14 (20%)

59	56139	178.13	0.00	H-7→L+1 (59%), H-5→L+4 (21%)
60	56294	177.64	0.02	H-3→L+6 (28%), H-2→L+7 (13%), H-2→L+8 (13%), H-1→L+9 (10%)
61	56302	177.61	0.00	H-7→L+1 (20%), H-5→L+4 (56%)
62	56361	177.43	0.01	H-3→L+6 (12%), H-2→L+7 (25%), H-2→L+8 (20%)
63	56762	176.18	0.00	H-3→L+6 (11%), HOMO→L+15 (59%)
64	56889	175.78	0.02	H-5→L+5 (10%), H-4→L+6 (41%), H-1→L+9 (12%)
65	57010	175.41	0.02	H-4→L+7 (11%), H-3→L+7 (22%), H-3→L+8 (13%), H-2→L+10 (17%)
66	57299	174.52	0.00	H-5→L+5 (16%), H-1→L+9 (30%)
67	57471	174.00	0.03	H-8→L+1 (10%), H-3→L+8 (15%), H-2→L+7 (11%), H-1→L+10 (18%)
68	57500	173.91	0.01	H-8→L+1 (18%), H-4→L+6 (23%), H-1→L+9 (12%)
69	57642	173.49	0.01	H-16→LUMO (67%)
70	57686	173.35	0.06	H-16→LUMO (11%), H-8→L+1 (24%), H-5→L+5 (11%), H-2→L+7 (13%)
71	57869	172.80	0.00	H-4→L+11 (25%), H-2→L+11 (16%)
72	58030	172.32	0.01	H-5→L+5 (14%), H-4→L+7 (14%), H-2→L+7 (16%)
73	58222	171.76	0.00	H-9→L+1 (79%)
74	58362	171.34	0.03	H-2→L+9 (11%), HOMO→L+16 (25%), HOMO→L+17 (19%)
75	58418	171.18	0.01	H-2→L+9 (54%)
76	58460	171.06	0.01	H-4→L+7 (10%), H-3→L+7 (40%), H-1→L+10 (17%)
77	58534	170.84	0.02	H-4→L+7 (16%), H-3→L+8 (15%), H-1→L+10 (22%)
78	58673	170.44	0.00	H-7→L+1 (12%), H-7→L+2 (78%)
79	58701	170.36	0.00	H-6→L+3 (71%), H-1→L+11 (10%)
80	58829	169.98	0.02	H-15→LUMO (21%), H-6→L+3 (21%), H-1→L+11 (25%)
81	59047	169.36	0.00	H-15→LUMO (13%), H-4→L+7 (10%), H-4→L+8 (17%)
82	59189	168.95	0.00	H-3→L+9 (56%)
83	59210	168.89	0.01	H-15→LUMO (10%), H-1→L+11 (10%), HOMO→L+16 (19%), HOMO→L+17 (34%)
84	59260	168.75	0.00	H-15→LUMO (16%), H-1→L+11 (30%), HOMO→L+16 (15%), HOMO→L+17 (16%)
85	59373	168.43	0.00	H-4→L+8 (19%), H-2→L+8 (22%), H-2→L+10 (36%)
86	59887	166.98	0.01	H-4→L+9 (58%)
87	60110	166.36	0.00	H-3→L+8 (26%), H-3→L+10 (53%)
88	60182	166.16	0.01	H-4→L+9 (11%), H-1→L+13 (17%), HOMO→L+18 (48%)

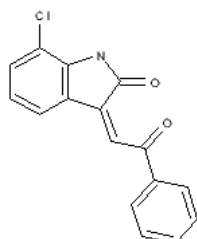


89	60367	165.65	0.00	H-1→L+13 (50%), HOMO→L+18 (27%)
90	60411	165.53	0.02	H-17→LUMO (22%), H-8→L+2 (17%), H-6→L+4 (10%), H- 2→L+11 (10%)
91	60498	165.30	0.04	H-17→LUMO (17%), H-8→L+2 (20%), H-6→L+4 (17%)
92	60640	164.91	0.00	H-4→L+10 (57%)
93	60884	164.25	0.09	H-3→L+11 (22%), H-2→L+11 (14%)
94	60991	163.96	0.02	H-1→L+12 (48%)
95	61019	163.88	0.08	H-6→L+4 (14%), H-5→L+6 (31%)
96	61213	163.36	0.02	H-6→L+4 (26%), H-5→L+6 (25%), H-1→L+14 (21%)
97	61362	162.97	0.05	H-5→L+7 (63%)
98	61504	162.59	0.05	H-4→L+11 (15%), H-2→L+14 (14%)
99	61568	162.42	0.01	H-6→L+7 (12%), HOMO→L+19 (51%)
100	61766	161.90	0.01	H-6→L+5 (12%), H-1→L+14 (32%)

## S9. 7-chloro-3-phenacylidene-1H-indol-2-one

## General Information

Log file : V2711-05-Z-Cl7.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3cccc(c3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	5.7710 Debye
Energy	:	-1281.36754233 a.u.
Number of imaginary frequencies :		0

## Cartesian Co-ordinates (XYZ format)

30

C	0.03438716	-0.16961837	0.00327386
C	-1.27880192	0.05769306	-0.37432337
C	-1.75299895	1.37335348	-0.55749589
C	-0.90631258	2.45620966	-0.35979268
C	0.41706452	2.21855927	0.02078270
C	0.88614923	0.91793281	0.20151378
C	-3.47609878	-0.21534431	-0.98217797
C	-3.16294312	1.26107478	-0.94576174
N	-2.30329490	-0.85276353	-0.62762052
H	-2.21512628	-1.85693693	-0.57183295
O	-4.52976799	-0.75413221	-1.26333356
C	-4.05584383	2.21624851	-1.23183095
H	-3.75988865	3.26206231	-1.20137489
C	-5.46364212	1.98439646	-1.72306538
O	-5.65802288	2.01653337	-2.92628980
C	-6.56672430	1.83515739	-0.73716027
C	-7.87805319	1.68916857	-1.21330440
C	-6.33227205	1.85289538	0.64371049
C	-8.93478680	1.55783510	-0.32257101
H	-8.04626465	1.67976749	-2.28299713
C	-7.39390707	1.72435868	1.53526032
H	-5.32351303	1.96684074	1.02156675
C	-8.69372559	1.57568967	1.05379009

H -9.94606495 1.44248152 -0.69467449  
H -7.20777512 1.73929083 2.60260725  
H -9.51946545 1.47411644 1.74871314  
H -1.26125789 3.47050118 -0.49753091  
H 1.09242821 3.04995227 0.17900881  
H 1.91227221 0.74031419 0.49645939  
Cl 0.61365837 -1.81537843 0.22869709

### TD-DFT Calculations

No.	Energy ( $\text{cm}^{-1}$ )	Wavelength (nm)	Osc. Strength	Major contribs
1	26638	375.40	0.04	HOMO→LUMO (95%)
2	29526	338.69	0.02	HOMO→L+1 (66%)
3	31374	318.74	0.06	H-4→LUMO (24%), H-4→L+1 (10%), H-1→LUMO (24%), HOMO→L+1 (28%)
4	32418	308.47	0.14	H-4→L+1 (33%), H-1→LUMO (37%), H-1→L+1 (15%)
5	32882	304.12	0.03	H-5→LUMO (14%), H-4→LUMO (31%), H-3→LUMO (20%), H-1→LUMO (21%)
6	34390	290.78	0.00	H-4→LUMO (24%), H-3→LUMO (17%), H-2→LUMO (34%), H-1→L+1 (16%)
7	34529	289.61	0.01	H-3→LUMO (25%), H-2→LUMO (60%)
8	35064	285.19	0.01	H-4→L+1 (22%), H-3→LUMO (16%), H-1→L+1 (41%)
9	36031	277.54	0.00	H-5→LUMO (62%), H-4→L+1 (13%)
10	36754	272.08	0.03	H-3→L+1 (26%), H-2→L+1 (62%)
11	38816	257.63	0.40	H-5→L+1 (15%), H-3→L+1 (51%), H-2→L+1 (21%)
12	40878	244.63	0.27	HOMO→L+2 (73%)
13	41517	240.87	0.08	H-5→L+1 (72%)
14	42417	235.75	0.01	HOMO→L+3 (98%)
15	44593	224.25	0.00	HOMO→L+4 (36%), HOMO→L+6 (53%)
16	44969	222.38	0.08	H-1→L+2 (57%), HOMO→L+5 (33%)
17	45617	219.21	0.01	HOMO→L+4 (43%), HOMO→L+6 (34%), HOMO→L+7 (12%)
18	45871	218.00	0.13	H-6→LUMO (71%)
19	46345	215.77	0.01	H-1→L+3 (89%)
20	47035	212.61	0.05	H-8→LUMO (32%), H-6→L+1 (33%), H-1→L+2 (12%), HOMO→L+5 (15%)
21	47613	210.03	0.02	H-7→LUMO (77%), H-6→L+1 (13%)
22	47722	209.55	0.10	H-7→LUMO (18%), H-6→L+1 (40%)
23	48286	207.10	0.00	H-4→L+2 (27%), H-3→L+2 (20%), H-1→L+6 (20%)
24	48376	206.71	0.00	H-4→L+2 (14%), H-3→L+2 (11%), H-1→L+4 (13%), H-1→L+6 (38%)

25	48673	205.45	0.01	H-1→L+6 (13%), HOMO→L+7 (43%), HOMO→L+8 (17%)
26	48769	205.05	0.01	H-4→L+3 (72%), H-3→L+3 (12%)
27	49208	203.22	0.11	H-4→L+3 (14%), H-3→L+3 (32%), H-2→L+3 (23%)
28	49453	202.21	0.00	H-1→L+4 (42%), HOMO→L+7 (21%)
29	49612	201.57	0.01	H-2→L+2 (91%)
30	49817	200.73	0.00	H-1→L+4 (13%), H-1→L+6 (10%), HOMO→L+8 (40%), HOMO→L+10 (25%)
31	49968	200.13	0.04	H-8→LUMO (10%), H-4→L+2 (25%), H-3→L+2 (49%)
32	50392	198.44	0.14	H-8→LUMO (12%), H-5→L+2 (10%), H-4→L+2 (12%), H-3→L+2 (10%), H-1→L+5 (22%)
33	50812	196.80	0.42	H-8→LUMO (16%), H-1→L+5 (34%)
34	51125	195.60	0.03	HOMO→L+8 (27%), HOMO→L+10 (33%), HOMO→L+11 (19%)
35	51463	194.31	0.02	H-9→LUMO (31%), H-9→L+1 (47%)
36	51760	193.20	0.19	H-8→L+1 (23%), H-3→L+3 (16%), H-2→L+3 (26%)
37	51935	192.55	0.07	H-5→L+2 (42%), H-2→L+3 (12%)
38	52019	192.24	0.02	HOMO→L+9 (17%), HOMO→L+11 (46%)
39	52188	191.61	0.03	HOMO→L+9 (55%), HOMO→L+11 (15%)
40	52389	190.88	0.09	H-8→L+1 (49%), H-5→L+2 (10%)
41	52551	190.29	0.01	H-1→L+7 (46%), H-1→L+8 (17%), HOMO→L+9 (10%)
42	52655	189.92	0.01	H-2→L+4 (64%), H-2→L+7 (22%)
43	52688	189.80	0.01	H-7→L+1 (91%)
44	53252	187.79	0.01	H-3→L+4 (67%), H-3→L+7 (18%)
45	53399	187.27	0.01	H-5→L+3 (91%)
46	53561	186.70	0.00	H-1→L+7 (15%), H-1→L+8 (44%), H-1→L+10 (24%)
47	53704	186.21	0.04	H-9→LUMO (56%), H-9→L+1 (26%)
48	53944	185.38	0.06	H-10→LUMO (38%), H-4→L+5 (19%), H-3→L+5 (12%)
49	54119	184.78	0.03	H-10→LUMO (14%), H-4→L+4 (20%), H-4→L+5 (10%), H-3→L+5 (18%)
50	54379	183.89	0.08	H-10→LUMO (19%), H-4→L+4 (14%), H-1→L+11 (10%)
51	54424	183.74	0.00	HOMO→L+12 (53%), HOMO→L+14 (15%), HOMO→L+15 (17%)
52	54761	182.61	0.01	H-13→LUMO (24%), H-11→LUMO (39%)
53	54806	182.46	0.01	H-4→L+4 (31%)
54	54937	182.03	0.00	H-2→L+5 (78%)
55	55142	181.35	0.00	HOMO→L+12 (18%), HOMO→L+13 (14%), HOMO→L+15 (33%)

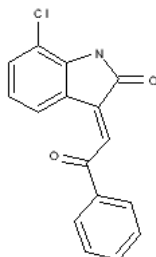
56	55253	180.98	0.00	H-12→LUMO (11%), H-12→L+1 (16%), H-1→L+8 (12%), H-1→L+10 (27%)
57	55330	180.73	0.01	H-4→L+5 (29%), H-3→L+5 (43%), HOMO→L+13 (12%)
58	55446	180.36	0.00	HOMO→L+13 (48%)
59	55789	179.25	0.00	H-1→L+10 (18%), H-1→L+11 (32%)
60	55887	178.93	0.01	H-2→L+4 (18%), H-2→L+6 (24%), H-2→L+7 (33%)
61	55970	178.67	0.02	H-3→L+6 (23%), H-3→L+7 (14%), H-1→L+9 (13%)
62	56200	177.94	0.01	HOMO→L+14 (39%), HOMO→L+15 (13%)
63	56265	177.73	0.00	H-1→L+9 (51%), HOMO→L+14 (13%)
64	56383	177.36	0.00	H-13→LUMO (43%), H-11→LUMO (21%), H-2→L+6 (10%)
65	56469	177.09	0.00	H-2→L+6 (49%), H-2→L+7 (22%)
66	56571	176.77	0.01	H-4→L+6 (17%), H-3→L+6 (18%), H-3→L+7 (33%)
67	56879	175.81	0.00	H-4→L+8 (17%), H-4→L+11 (22%), H-1→L+11 (26%)
68	56987	175.48	0.01	H-4→L+6 (47%), H-3→L+6 (33%)
69	57297	174.53	0.05	H-6→L+2 (27%), H-5→L+5 (46%)
70	57494	173.93	0.01	H-2→L+9 (61%)
71	57538	173.80	0.01	H-10→L+1 (37%), H-2→L+9 (19%)
72	57657	173.44	0.02	H-12→LUMO (16%), H-12→L+1 (14%), H-6→L+2 (27%), H-5→L+5 (13%)
73	57731	173.22	0.02	H-5→L+4 (13%), H-4→L+7 (43%)
74	57831	172.92	0.03	H-12→LUMO (10%), H-12→L+1 (14%), H-10→L+1 (34%), H-6→L+2 (15%)
75	58229	171.74	0.01	H-5→L+4 (29%), H-3→L+9 (30%)
76	58242	171.70	0.03	H-5→L+4 (23%), H-4→L+7 (17%), H-3→L+9 (18%)
77	58333	171.43	0.00	H-7→L+2 (20%), H-1→L+12 (46%)
78	58371	171.32	0.00	H-7→L+2 (73%), H-1→L+12 (14%)
79	58510	170.91	0.01	HOMO→L+16 (48%)
80	58561	170.76	0.04	H-3→L+9 (22%), H-2→L+8 (13%), HOMO→L+16 (18%)
81	58847	169.93	0.00	H-3→L+8 (12%), H-2→L+8 (26%), H-2→L+11 (31%)
82	58898	169.78	0.06	H-3→L+8 (16%), H-2→L+11 (17%), H-1→L+13 (10%), H-1→L+15 (13%)
83	59012	169.46	0.06	H-3→L+8 (18%), H-1→L+15 (32%)
84	59202	168.91	0.14	H-11→L+1 (10%), H-3→L+11 (43%)
85	59293	168.65	0.01	H-1→L+13 (30%), H-1→L+15 (17%)
86	59326	168.56	0.01	H-14→LUMO (79%)

87	59562	167.89	0.04	H-4→L+8 (20%), H-4→L+9 (14%), H-4→L+11 (16%)
88	59744	167.38	0.03	H-1→L+14 (16%), HOMO→L+17 (12%), HOMO→L+18 (27%)
89	59858	167.06	0.01	H-6→L+3 (10%), HOMO→L+17 (63%)
90	59902	166.94	0.00	H-6→L+3 (82%)
91	59950	166.81	0.01	H-3→L+10 (11%), H-2→L+10 (45%)
92	60040	166.56	0.01	H-4→L+9 (10%), H-3→L+10 (20%), H-2→L+10 (19%), HOMO→L+18 (14%)
93	60084	166.43	0.03	H-5→L+6 (68%)
94	60191	166.14	0.01	H-1→L+14 (30%), H-1→L+15 (12%), HOMO→L+18 (15%)
95	60361	165.67	0.00	H-4→L+9 (28%), H-3→L+10 (26%)
96	60612	164.98	0.02	HOMO→L+19 (63%), HOMO→L+20 (17%)
97	61134	163.58	0.03	H-4→L+10 (50%)
98	61249	163.27	0.02	H-13→L+1 (39%), H-11→L+1 (12%), H-4→L+10 (10%)
99	61446	162.74	0.04	H-8→L+2 (55%)
100	61551	162.47	0.00	H-5→L+7 (75%)

**S10.** 7-chloro-3-phenacylidene-1H-indol-2-one

**General Information**

Log file : V2711-06-E-Cl7.log



SMILES	:	c1ccc(cc1)C(=O)C=C2c3cccc(c3NC2=O)Cl
Formula	:	C <sub>16</sub> H <sub>10</sub> ClNO <sub>2</sub>
Charge	:	0
Multiplicity	:	1
Dipole	:	1.5606 Debye
Energy	:	-1281.37266045 a.u.
Number of imaginary frequencies :		0

**Cartesian Co-ordinates (XYZ format)**

30

C	1.09934938	0.47816724	0.29921222
C	0.05285746	1.28965366	-0.10222767
C	-1.22108066	0.74277860	-0.39937460
C	-1.41725802	-0.63411379	-0.28875560
C	-0.35506269	-1.44283187	0.12033366
C	0.89327723	-0.89737928	0.41250271
C	-1.19685662	3.10962033	-0.68808091
C	-2.07675695	1.86623323	-0.77683359
N	0.04057624	2.66877484	-0.27848923
H	0.83005470	3.28120708	-0.13407362
O	-1.50844908	4.25911236	-0.92469221
C	-3.36465240	2.05360484	-1.13704813
H	-3.62271762	3.08777881	-1.33327889
C	-4.42856264	1.04182768	-1.31318963
O	-4.19149256	-0.16178723	-1.27926350
C	-5.82347298	1.52342069	-1.56939626
C	-6.75983953	0.58882684	-2.03969145
C	-6.24113512	2.84209943	-1.33413565
C	-8.07397747	0.96431202	-2.28279161
H	-6.43348980	-0.42901447	-2.21111250
C	-7.56310129	3.21382499	-1.56590188
H	-5.55239487	3.58317280	-0.95042264

C -8.47920513 2.27979112 -2.04543304  
 H -8.78459263 0.23599544 -2.65570331  
 H -7.87603378 4.23292971 -1.37194610  
 H -9.50562000 2.57372236 -2.23252892  
 H -2.38202357 -1.05386305 -0.52676713  
 H -0.49685511 -2.51255608 0.20995866  
 H 1.71231472 -1.53191113 0.72612846  
 Cl 2.67066526 1.18126833 0.65995914

### TD-DFT Calculations

No.	Energy ( $\text{cm}^{-1}$ )	Wavelength (nm)	Osc. Strength	Major contribs
1	20970	476.88	0.06	HOMO→LUMO (98%) H-4→LUMO (55%), H-3→LUMO (17%), H-2→LUMO (24%)
2	23843	419.42	0.00	H-1→LUMO (95%) H-3→LUMO (32%), H-2→LUMO (63%)
3	26637	375.41	0.48	H-5→LUMO (76%), H-3→LUMO (10%)
4	28146	355.29	0.00	H-5→LUMO (20%), H-4→LUMO (26%), H-3→LUMO (39%), H-2→LUMO (11%)
5	29723	336.44	0.00	HOMO→L+1 (97%) H-6→LUMO (64%), HOMO→L+2 (24%)
6	30175	331.40	0.04	H-4→L+1 (48%), H-3→L+1 (12%), H-2→L+1 (34%)
7	36696	272.51	0.01	H-6→LUMO (25%), H-1→L+1 (47%), HOMO→L+2 (17%)
8	38995	256.44	0.31	H-3→L+1 (36%), H-2→L+1 (30%)
9	40238	248.52	0.01	H-7→LUMO (99%) H-8→LUMO (54%), H-1→L+1 (20%), HOMO→L+2 (10%)
10	40661	245.94	0.02	H-8→LUMO (36%), H-1→L+1 (22%), HOMO→L+2 (26%)
11	41615	240.30	0.02	HOMO→L+3 (92%) HOMO→L+5 (24%), HOMO→L+6 (64%)
12	41967	238.28	0.00	H-4→L+1 (35%), H-3→L+1 (27%), H-2→L+1 (17%)
13	42587	234.81	0.22	H-9→LUMO (92%) H-1→L+2 (49%), HOMO→L+4 (33%)
14	42715	234.11	0.04	HOMO→L+5 (55%), HOMO→L+6 (12%), HOMO→L+7 (26%)
15	43624	229.23	0.00	H-10→LUMO (27%), H-5→L+1 (50%)
16	44861	222.91	0.00	H-10→LUMO (37%), H-5→L+1 (34%), H-1→L+3 (11%)
17	44885	222.79	0.12	H-4→L+3 (11%), H-3→L+3 (13%), H-1→L+3 (53%)
18	45517	219.70	0.01	H-10→LUMO (13%), H-4→L+3 (35%), H-1→L+3 (20%)
19	45726	218.69	0.07	
20	46054	217.14	0.01	
21	47317	211.34	0.01	
22	47456	210.72	0.00	
23	47754	209.41	0.01	
24	47832	209.06	0.03	



25	48048	208.13	0.00	H-12→LUMO (19%), H-11→LUMO (31%), H-4→L+2 (13%), H-2→L+2 (16%)
26	48209	207.43	0.00	H-12→LUMO (18%), H-11→LUMO (22%), H-4→L+2 (17%), H-3→L+2 (10%), H-2→L+2 (26%)
27	49049	203.88	0.00	H-1→L+5 (13%), HOMO→L+5 (10%), HOMO→L+7 (50%)
28	49120	203.58	0.00	H-12→LUMO (38%), H-11→LUMO (29%), H-1→L+6 (15%)
29	49161	203.41	0.00	H-12→LUMO (16%), H-1→L+6 (42%)
30	49518	201.95	0.24	H-1→L+2 (32%), HOMO→L+4 (37%)
31	49639	201.45	0.02	H-4→L+2 (25%), H-3→L+2 (12%), H-2→L+2 (44%)
32	50335	198.67	0.02	H-1→L+5 (20%), HOMO→L+8 (38%), HOMO→L+10 (15%)
33	50356	198.59	0.11	H-5→L+2 (11%), H-4→L+2 (12%), H-3→L+2 (29%)
34	50454	198.20	0.00	H-1→L+5 (40%), H-1→L+7 (17%), HOMO→L+8 (16%)
35	50716	197.17	0.04	H-13→LUMO (19%), H-5→L+2 (34%), H-4→L+2 (10%), H-3→L+3 (10%)
36	50754	197.03	0.16	H-13→LUMO (23%), H-5→L+2 (22%), H-3→L+3 (11%)
37	51226	195.21	0.04	H-13→LUMO (16%), H-3→L+2 (12%), H-2→L+3 (10%), H-1→L+4 (33%)
38	51443	194.39	0.56	H-4→L+3 (10%), H-2→L+3 (15%), H-1→L+4 (30%)
39	52136	191.81	0.00	H-2→L+5 (14%), HOMO→L+9 (41%)
40	52281	191.27	0.00	H-2→L+5 (45%), H-2→L+6 (13%), H-2→L+7 (10%), HOMO→L+9 (14%)
41	52394	190.86	0.00	H-14→LUMO (74%), H-5→L+2 (10%)
42	52676	189.84	0.07	H-3→L+5 (13%), H-1→L+7 (21%)
43	52752	189.57	0.07	H-3→L+4 (10%), H-2→L+4 (12%), H-1→L+7 (16%)
44	53097	188.33	0.12	H-6→L+1 (13%), H-4→L+4 (35%), H-2→L+4 (15%)
45	53265	187.74	0.00	HOMO→L+8 (15%), HOMO→L+9 (17%), HOMO→L+10 (49%)
46	53685	186.27	0.00	H-3→L+5 (38%), H-1→L+7 (16%)
47	53845	185.72	0.04	H-6→L+1 (35%), HOMO→L+11 (36%)
48	54196	184.52	0.01	H-6→L+1 (14%), H-4→L+5 (31%), HOMO→L+11 (21%)
49	54283	184.22	0.01	H-4→L+5 (25%), HOMO→L+11 (27%)
50	54772	182.58	0.00	H-1→L+8 (56%), H-1→L+10 (15%)
51	54976	181.90	0.00	HOMO→L+13 (71%)
52	55186	181.21	0.01	H-5→L+3 (95%)

53	55218	181.10	0.10	H-4→L+4 (11%), H-3→L+4 (17%), H-2→L+4 (49%)
54	55462	180.30	0.01	H-2→L+5 (22%), H-2→L+6 (53%)
55	55701	179.53	0.06	H-4→L+4 (20%), H-3→L+4 (43%)
56	55771	179.30	0.03	H-3→L+4 (10%), HOMO→L+12 (36%), HOMO→L+14 (13%)
57	55959	178.70	0.00	H-2→L+7 (42%), HOMO→L+14 (12%)
58	55993	178.59	0.00	H-1→L+9 (12%), HOMO→L+14 (40%)
59	56098	178.26	0.00	H-16→LUMO (73%)
60	56256	177.76	0.00	H-1→L+9 (11%), HOMO→L+12 (32%), HOMO→L+14 (12%)
61	56460	177.12	0.01	H-3→L+6 (28%), H-2→L+7 (13%), H-1→L+9 (16%)
62	56702	176.36	0.00	H-5→L+4 (66%)
63	56743	176.23	0.01	H-4→L+6 (36%)
64	56917	175.70	0.01	H-2→L+8 (50%), H-2→L+9 (14%)
65	57052	175.28	0.05	H-6→L+2 (76%)
66	57087	175.17	0.01	H-3→L+6 (27%), H-3→L+7 (30%)
67	57142	175.00	0.00	H-3→L+7 (11%), H-1→L+10 (25%), HOMO→L+15 (15%)
68	57241	174.70	0.00	H-7→L+1 (72%), H-7→L+2 (20%)
69	57446	174.08	0.00	H-4→L+7 (50%), HOMO→L+15 (17%)
70	57513	173.88	0.01	H-4→L+7 (11%), H-1→L+10 (15%), HOMO→L+15 (47%)
71	57734	173.21	0.02	H-5→L+5 (53%)
72	57802	173.00	0.03	H-4→L+11 (25%), H-3→L+11 (10%), H-2→L+11 (16%), H-1→L+11 (11%)
73	58005	172.40	0.03	H-3→L+8 (10%), H-1→L+11 (54%)
74	58126	172.04	0.00	H-9→L+1 (80%)
75	58312	171.49	0.02	H-3→L+8 (36%), H-1→L+11 (20%)
76	58459	171.06	0.10	H-8→L+1 (62%)
77	58507	170.92	0.00	H-2→L+8 (12%), H-2→L+9 (57%)
78	58651	170.50	0.03	H-15→LUMO (74%), H-8→L+1 (11%)
79	58901	169.78	0.00	H-4→L+8 (59%)
80	59115	169.16	0.01	H-1→L+13 (14%), HOMO→L+16 (56%)
81	59211	168.89	0.00	H-7→L+1 (21%), H-7→L+2 (73%)
82	59269	168.72	0.00	H-3→L+9 (47%), H-1→L+12 (21%)
83	59477	168.13	0.00	H-1→L+13 (42%), H-1→L+14 (24%), HOMO→L+17 (15%)
84	59805	167.21	0.01	H-1→L+12 (10%), H-1→L+13 (25%), H-1→L+14 (15%), HOMO→L+16 (14%)
85	59944	166.82	0.00	H-5→L+6 (34%), H-4→L+9 (12%), HOMO→L+17 (10%)

86	59960	166.78	0.00	H-5→L+6 (47%), H-4→L+9 (15%)
87	60035	166.57	0.00	H-6→L+3 (81%)
88	60283	165.88	0.01	H-4→L+9 (19%), H-1→L+14 (18%), HOMO→L+17 (23%)
89	60299	165.84	0.00	H-2→L+10 (59%)
90	60378	165.62	0.02	H-17→LUMO (18%), H-4→L+9 (16%), H-1→L+12 (19%)
91	60549	165.15	0.02	H-17→LUMO (25%), H-1→L+14 (20%)
92	60876	164.27	0.12	H-3→L+11 (20%), H-2→L+11 (20%)
93	60960	164.04	0.04	H-3→L+10 (35%), H-1→L+15 (14%)
94	61146	163.54	0.01	HOMO→L+18 (80%)
95	61410	162.84	0.00	H-4→L+10 (22%), H-3→L+10 (19%), H-1→L+15 (18%), HOMO→L+19 (14%)
96	61478	162.66	0.04	H-4→L+10 (13%), H-4→L+11 (13%), H-3→L+11 (14%), H-2→L+11 (11%)
97	61678	162.13	0.02	H-5→L+7 (32%), HOMO→L+19 (32%)
98	61790	161.84	0.01	H-8→L+2 (12%), H-5→L+7 (26%), HOMO→L+19 (18%)
99	61806	161.80	0.00	H-11→L+1 (47%), HOMO→L+20 (15%)
100	61862	161.65	0.01	H-11→L+1 (26%), H-5→L+7 (14%), HOMO→L+20 (19%)