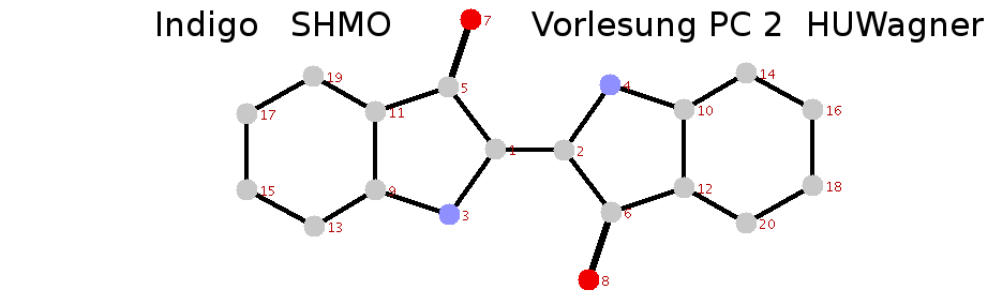
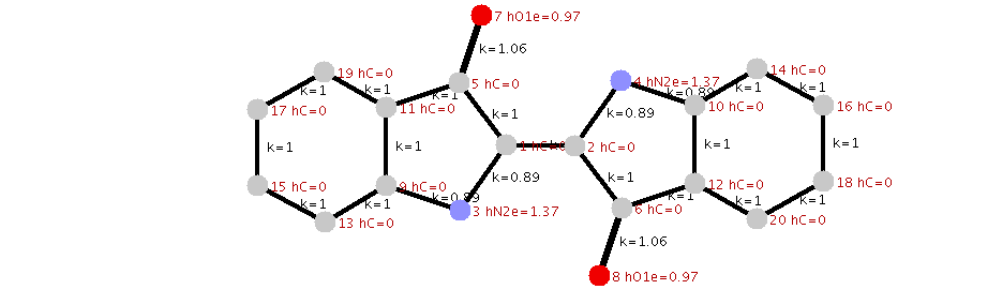
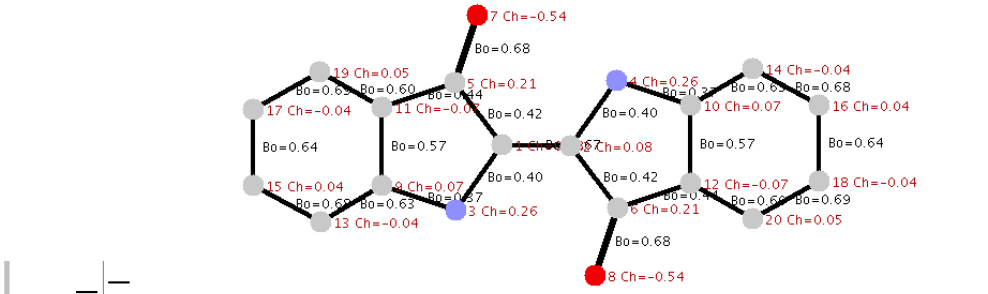
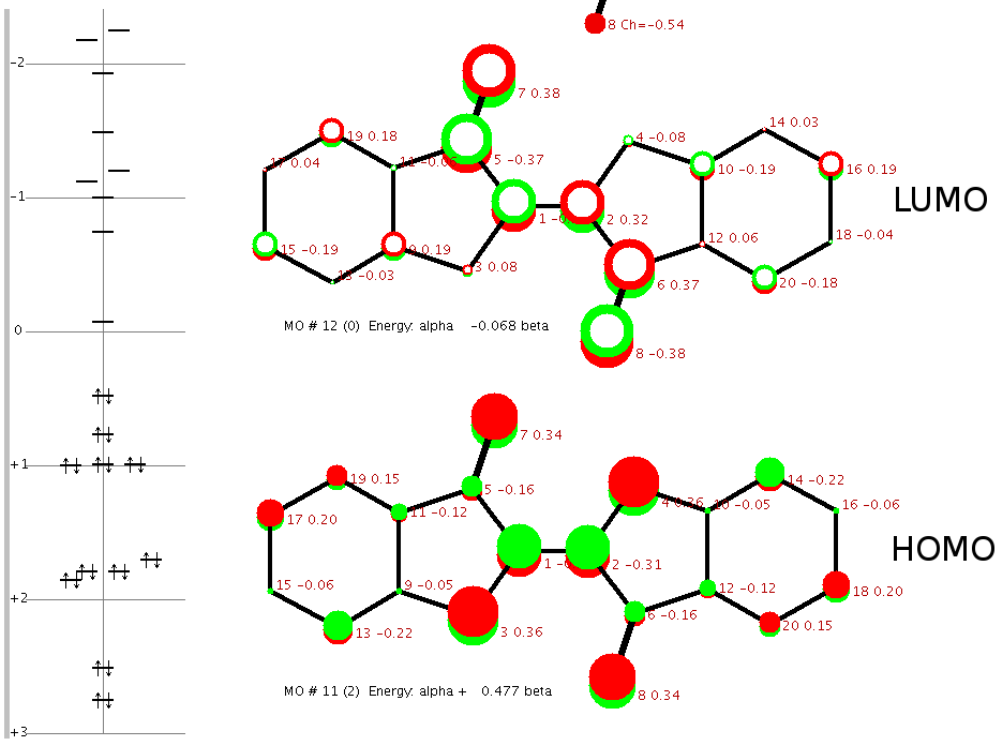

Indigo SHMO
Vorlesung PC 2 HUWagner






LUMO
MO # 12 (0) Energy: alpha -0.068 beta
HOMO
MO # 11 (2) Energy: alpha + 0.477 beta

```
Simple Hueckel Molecular Orbital Calculation -  Data Table           Indigo
SHMO Version 20100131   R.Cannings & H-U.Wagner

Number of Electrons = 22    Net Charge = 0
Total energy =  22 alpha  +   33.308 beta

Lowest Unoccupied MO = LUMO #  12   Energy: alpha    -0.068 beta
Highest Occupied  MO = HOMO #  11   Energy: alpha +   0.477 beta

Orbital Energies / Coefficents Table
```

MO number		1	2	3	4	5	6	7	8
Occupancy		(2)	(2)	(2)	(2)	(2)	(2)	(2)	(2)
Energy		2.753	2.515	1.859	1.793	1.790	1.706	1.000	0.995
#									
1	C	-0.345	-0.164	0.248	-0.018	0.040	-0.138	0.316	0.002
2	C	-0.345	0.164	0.248	0.018	0.040	0.138	0.316	-0.002
3	N2e	-0.379	-0.366	0.111	0.329	0.389	-0.333	0.000	-0.004
4	N2e	-0.379	0.366	0.111	-0.329	0.389	0.333	0.000	0.004
5	C	-0.268	-0.250	0.114	-0.342	-0.315	-0.077	0.000	0.007
6	C	-0.268	0.250	0.114	0.342	-0.315	0.077	0.000	-0.007
7	O1e	-0.159	-0.171	0.136	-0.440	-0.407	-0.111	0.000	0.304
8	O1e	-0.159	0.171	0.136	0.440	-0.407	0.111	0.000	-0.304
9	C	-0.244	-0.308	-0.187	0.174	0.144	0.012	-0.316	0.000
10	C	-0.244	0.308	-0.187	-0.174	0.144	-0.012	-0.316	0.000
11	C	-0.223	-0.283	-0.180	-0.129	-0.172	0.124	-0.316	-0.317
12	C	-0.223	0.283	-0.180	0.129	-0.172	-0.124	-0.316	0.317
13	C	-0.111	-0.165	-0.266	0.148	0.084	0.193	0.000	0.320
14	C	-0.111	0.165	-0.266	-0.148	0.084	-0.193	0.000	-0.320
15	C	-0.062	-0.107	-0.308	0.091	0.006	0.317	0.316	0.318
16	C	-0.062	0.107	-0.308	-0.091	0.006	-0.317	0.316	-0.318
17	C	-0.060	-0.103	-0.306	0.016	-0.074	0.348	0.316	-0.003
18	C	-0.060	0.103	-0.306	-0.016	-0.074	-0.348	0.316	0.003
19	C	-0.103	-0.154	-0.261	-0.063	-0.137	0.277	0.000	-0.322
20	C	-0.103	0.154	-0.261	0.063	-0.137	-0.277	0.000	0.322

MO number		9	10	11	12	13	14	15	16
Occupancy		(2)	(2)	(2)	(0)	(0)	(0)	(0)	(0)
Energy		0.993	0.772	0.477	-0.068	-0.744	-1.000	-1.120	-1.201
#									
1	C	0.136	0.133	-0.313	-0.320	-0.233	0.196	-0.089	0.178
2	C	0.136	-0.133	-0.313	0.320	-0.233	-0.196	-0.089	-0.178
3	N2e	0.007	0.282	0.362	0.081	0.145	0.000	0.173	-0.164
4	N2e	0.007	-0.282	0.362	-0.081	0.145	0.000	0.173	0.164
5	C	-0.007	-0.016	-0.158	-0.370	0.279	0.000	0.034	0.110
6	C	-0.007	0.016	-0.158	0.370	0.279	0.000	0.034	-0.110
7	O1e	-0.330	0.085	0.341	0.378	-0.172	0.000	-0.017	-0.054
8	O1e	-0.330	-0.085	0.341	-0.378	-0.172	0.000	-0.017	0.054
9	C	-0.139	-0.323	-0.050	0.190	-0.110	-0.196	-0.395	0.295
10	C	-0.139	0.323	-0.050	-0.190	-0.110	0.196	-0.395	-0.295
11	C	0.207	-0.235	-0.124	-0.055	0.209	-0.196	0.069	-0.254
12	C	0.207	0.235	-0.124	0.055	0.209	0.196	0.069	0.254
13	C	-0.351	-0.265	-0.222	-0.030	-0.256	0.392	0.220	0.045
14	C	-0.351	0.265	-0.222	0.030	-0.256	-0.392	0.220	-0.045
15	C	-0.210	0.118	-0.056	-0.187	0.300	-0.196	0.149	-0.349
16	C	-0.210	-0.118	-0.056	0.187	0.300	0.196	0.149	0.349
17	C	0.142	0.356	0.195	0.043	0.032	-0.196	-0.386	0.375
18	C	0.142	-0.356	0.195	-0.043	0.032	0.196	-0.386	-0.375
19	C	0.351	0.157	0.149	0.185	-0.324	0.392	0.284	-0.101
20	C	0.351	-0.157	0.149	-0.185	-0.324	-0.392	0.284	0.101

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Unoccupied MOs number 17 to 20 not printed
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Population Tables
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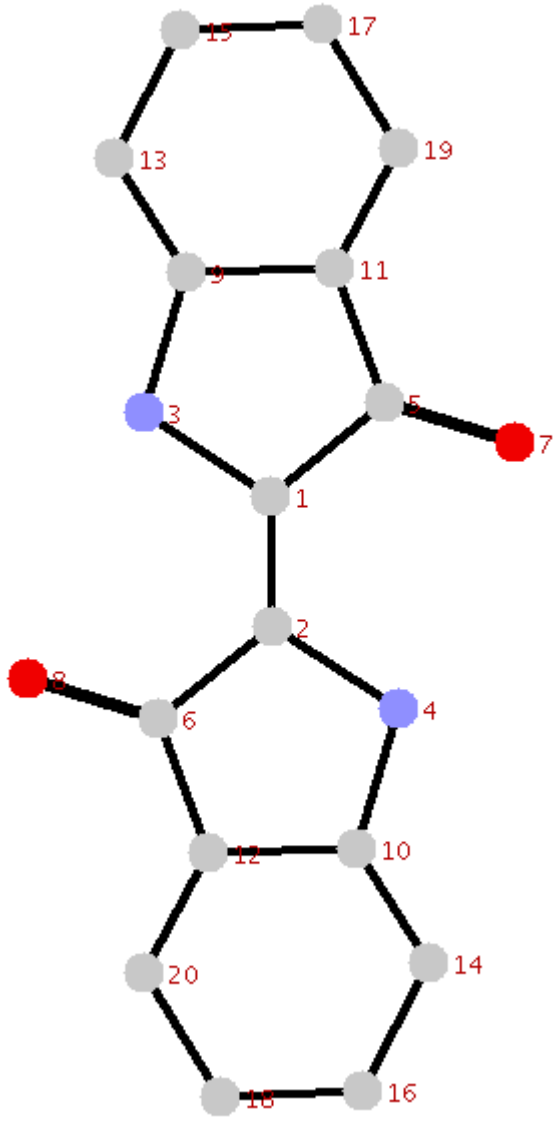
Atoms

#	Symbol	hX	ElectronPop.	NetCharge
1	C	0.00	0.924	0.076
2	C	0.00	0.924	0.076
3	N2e	1.37	1.743	0.257
4	N2e	1.37	1.743	0.257
5	C	0.00	0.789	0.211
6	C	0.00	0.789	0.211
7	O1e	0.97	1.538	-0.538
8	O1e	0.97	1.538	-0.538
9	C	0.00	0.932	0.068
10	C	0.00	0.932	0.068
11	C	0.00	1.074	-0.074
12	C	0.00	1.074	-0.074
13	C	0.00	1.043	-0.043
14	C	0.00	1.043	-0.043
15	C	0.00	0.963	0.037
16	C	0.00	0.963	0.037
17	C	0.00	1.041	-0.041
18	C	0.00	1.041	-0.041
19	C	0.00	0.952	0.048
20	C	0.00	0.952	0.048



Bonds

i	j	X	--Y	kXY	BondOrder
1	2	C	--C	1.00	0.669
1	3	C	--N2e	0.89	0.399
2	4	C	--N2e	0.89	0.399
1	5	C	--C	1.00	0.424
2	6	C	--C	1.00	0.424
5	7	C	--O1e	1.06	0.675
6	8	C	--O1e	1.06	0.675
3	9	N2e	--C	0.89	0.367
4	10	N2e	--C	0.89	0.367
9	11	C	--C	1.00	0.565
10	12	C	--C	1.00	0.565
11	5	C	--C	1.00	0.436
6	12	C	--C	1.00	0.436
9	13	C	--C	1.00	0.626
10	14	C	--C	1.00	0.626
13	15	C	--C	1.00	0.677
14	16	C	--C	1.00	0.677
15	17	C	--C	1.00	0.641
16	18	C	--C	1.00	0.641
17	19	C	--C	1.00	0.688
18	20	C	--C	1.00	0.688
19	11	C	--C	1.00	0.597
12	20	C	--C	1.00	0.597
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