

**Supporting Information**

**for**

**The electronic structure of cyanine dyes: ring currents and valence bond calculations**

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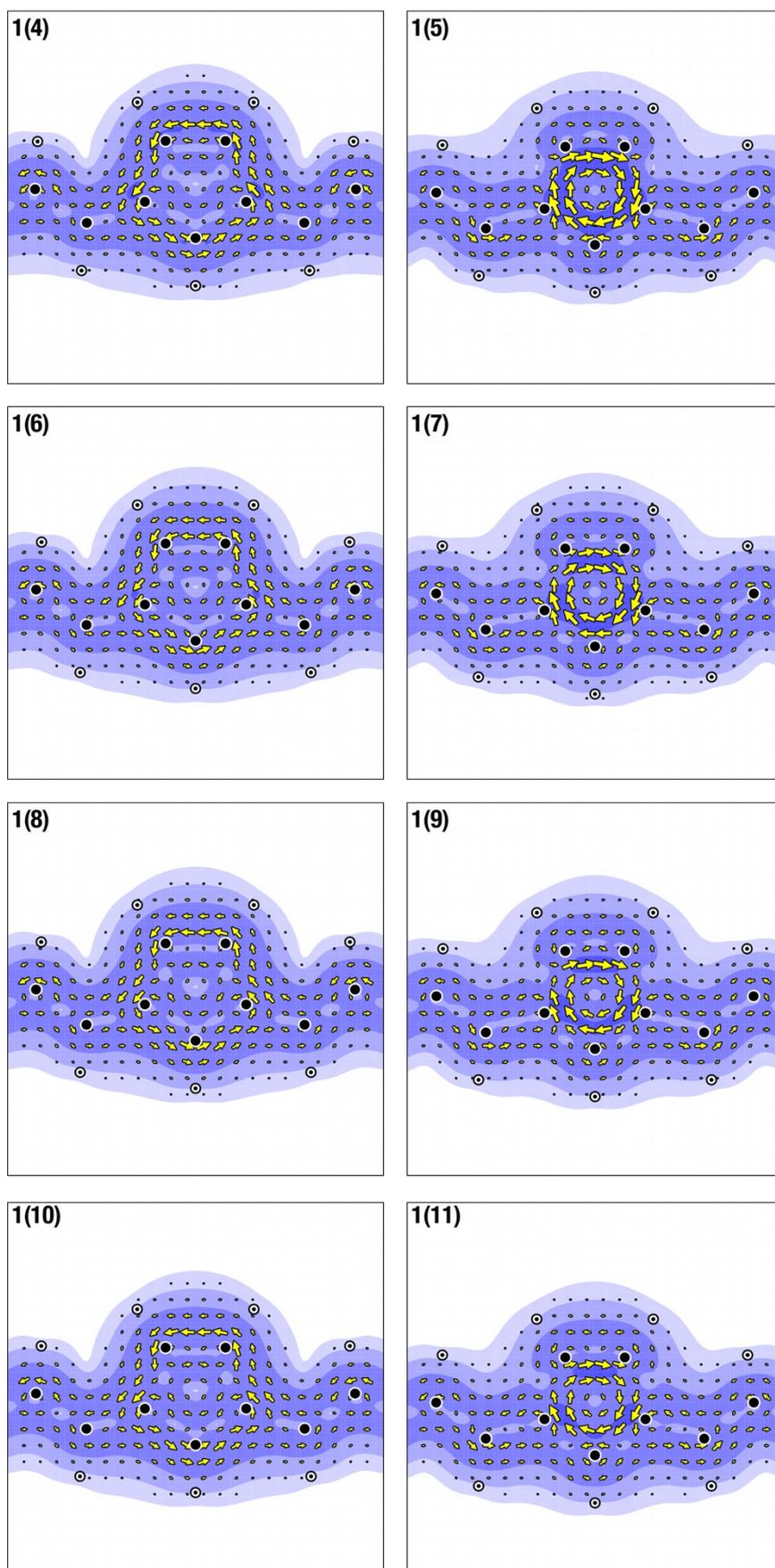
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Figure S1. The induced  $\pi$  current density for the molecules **1(4)**-**1(11)**.



**Table S1.** The Cartesian coordinates (atomic units) of **1(2)**.

ATOM	X	Y	Z
N	0.000000	-6.680681	0.125655
N	0.000000	6.680681	0.125655
C	0.000000	-4.589665	-1.216569
C	0.000000	4.589665	-1.216569
C	0.000000	-2.141309	-0.262060
C	0.000000	2.141309	-0.262060
C	0.000000	-1.280366	2.344943
C	0.000000	1.280366	2.344943
C	0.000000	0.000000	-1.829546
H	0.000000	-6.641424	2.032885
H	0.000000	6.641424	2.032885
H	0.000000	-8.393927	-0.708239
H	0.000000	8.393927	-0.708239
H	0.000000	-4.847858	-3.253997
H	0.000000	4.847858	-3.253997
H	0.000000	-2.462847	4.012597
H	0.000000	2.462847	4.012597
H	0.000000	0.000000	-3.874944

**Table S2.** The Cartesian coordinates (atomic units) of **1(3)**.

ATOM	X	Y	Z
N	0.000000	-9.086789	-0.350244
N	0.000000	9.086789	-0.350244
C	0.000000	-6.706336	0.423660
C	0.000000	6.706336	0.423660
C	0.000000	-4.637313	-1.166759
C	0.000000	4.637313	-1.166759
C	0.000000	-2.143401	-0.320706
C	0.000000	2.143401	-0.320706
C	0.000000	-1.262912	2.363686
C	0.000000	1.262912	2.363686
C	0.000000	0.000000	-1.857681
H	0.000000	-6.453130	2.458753
H	0.000000	6.453130	2.458753
H	0.000000	-4.961750	-3.195577
H	0.000000	4.961750	-3.195577
H	0.000000	-2.465560	4.016906
H	0.000000	2.465560	4.016906
H	0.000000	0.000000	-3.899122
H	0.000000	-9.526644	-2.205290
H	0.000000	9.526644	-2.205290
H	0.000000	-10.530678	0.886650
H	0.000000	10.530678	0.886650

**Table S3.** The Cartesian coordinates (atomic units) of **1(4)**.

ATOM	X	Y	Z
C	0.000000	-2.158017	-0.193784
C	0.000000	2.158017	-0.193784
C	0.000000	0.000000	-1.750245
C	0.000000	1.277736	2.419386
C	0.000000	-1.277736	2.419386
H	0.000000	0.000000	-3.796942
H	0.000000	2.474916	4.074971
H	0.000000	-2.474916	4.074971
C	0.000000	-4.630247	-1.096849
C	0.000000	4.630247	-1.096849
C	0.000000	-6.832562	0.344889
C	0.000000	6.832562	0.344889
C	0.000000	-9.169687	-0.814993
C	0.000000	9.169687	-0.814993
N	0.000000	-11.385664	0.353595
N	0.000000	11.385664	0.353595
H	0.000000	-4.854811	-3.144580
H	0.000000	4.854811	-3.144580
H	0.000000	-6.727476	2.395420
H	0.000000	6.727476	2.395420
H	0.000000	-9.276424	-2.866919
H	0.000000	9.276424	-2.866919
H	0.000000	-11.505801	2.255458
H	0.000000	11.505801	2.255458
H	0.000000	13.016339	-0.626006
H	0.000000	-13.016339	-0.626006

**Table S4.** The Cartesian coordinates (atomic units) of **1(5)**.

ATOM	X	Y	Z
C	0.000000	-2.146072	-0.498922
C	0.000000	2.146072	-0.498922
C	0.000000	0.000000	-2.040449
C	0.000000	1.264977	2.170346
C	0.000000	-1.264977	2.170346
H	0.000000	0.000000	-4.084244
H	0.000000	2.477310	3.814436
H	0.000000	-2.477310	3.814436
C	0.000000	-4.644147	-1.338004
C	0.000000	4.644147	-1.338004
C	0.000000	-6.757974	0.200114
C	0.000000	6.757974	0.200114
C	0.000000	-9.234789	-0.717877
C	0.000000	9.234789	-0.717877
C	0.000000	-11.285978	0.880269
C	0.000000	11.285978	0.880269
H	0.000000	-4.939660	-3.370690
H	0.000000	4.939660	-3.370690
H	0.000000	-6.496177	2.239834
H	0.000000	6.496177	2.239834
H	0.000000	-9.541955	-2.749392
H	0.000000	9.541955	-2.749392
H	0.000000	-10.985391	2.911765
H	0.000000	10.985391	2.911765
N	0.000000	13.694980	0.163789
N	0.000000	-13.694980	0.163789
H	0.000000	15.103468	1.438488
H	0.000000	-15.103468	1.438488
H	0.000000	14.185276	-1.676320
H	0.000000	-14.185276	-1.676320

**Table S5.** The Cartesian coordinates (atomic units) of **1(6)**.

ATOM	X	Y	Z
C	0.000000	-2.157575	-0.497627
C	0.000000	2.157575	-0.497627
C	0.000000	0.000000	-2.052543
C	0.000000	1.276489	2.119295
C	0.000000	-1.276489	2.119295
H	0.000000	0.000000	-4.099926
H	0.000000	2.474057	3.773840
H	0.000000	-2.474057	3.773840
C	0.000000	-4.640482	-1.372737
C	0.000000	4.640482	-1.372737
C	0.000000	-6.788429	0.143675
C	0.000000	6.788429	0.143675
C	0.000000	-9.214575	-0.823043
C	0.000000	9.214575	-0.823043
C	0.000000	-11.402331	0.661675
C	0.000000	11.402331	0.661675
H	0.000000	-4.914700	-3.413356
H	0.000000	4.914700	-3.413356
H	0.000000	-6.557561	2.183252
H	0.000000	6.557561	2.183252
H	0.000000	-9.440427	-2.870982
H	0.000000	9.440427	-2.870982
H	0.000000	-11.203746	2.706570
H	0.000000	11.203746	2.706570
C	0.000000	13.781448	-0.378282
C	0.000000	-13.781448	-0.378282
N	0.000000	15.939337	0.915860
N	0.000000	-15.939337	0.915860
H	0.000000	13.999633	-2.420800
H	0.000000	-13.999633	-2.420800
H	0.000000	-17.618314	0.027910
H	0.000000	17.618314	0.027910
H	0.000000	-15.952790	2.820473
H	0.000000	15.952790	2.820473

**Table S6.** The Cartesian coordinates (atomic units) of **1(7)**.

ATOM	X	Y	Z
C	0.000000	2.148208	0.750445
C	0.000000	-2.148208	0.750445
C	0.000000	0.000000	2.293490
C	0.000000	-1.266443	-1.911995
C	0.000000	1.266443	-1.911995
H	0.000000	0.000000	4.336301
H	0.000000	-2.478615	-3.557347
H	0.000000	2.478615	-3.557347
C	0.000000	4.652029	1.574261
C	0.000000	-4.652029	1.574261
C	0.000000	6.762633	0.024541
C	0.000000	-6.762633	0.024541
C	0.000000	9.237047	0.947432
C	0.000000	-9.237047	0.947432
C	0.000000	11.352665	-0.578026
C	0.000000	-11.352665	-0.578026
H	0.000000	4.966384	3.605364
H	0.000000	-4.966384	3.605364
H	0.000000	6.500850	-2.015293
H	0.000000	-6.500850	-2.015293
H	0.000000	9.501436	2.986709
H	0.000000	-9.501436	2.986709
H	0.000000	11.072602	-2.619415
H	0.000000	-11.072602	-2.619415
C	0.000000	-13.846178	0.315821
C	0.000000	13.846178	0.315821
C	0.000000	-15.871907	-1.304046
C	0.000000	15.871907	-1.304046
H	0.000000	-14.173217	2.344389
H	0.000000	14.173217	2.344389
N	0.000000	18.298786	-0.622991
N	0.000000	-18.298786	-0.622991
H	0.000000	15.534065	-3.329922
H	0.000000	-15.534065	-3.329922
H	0.000000	-19.685454	-1.920355
H	0.000000	19.685454	-1.920355
H	0.000000	-18.808689	1.211171
H	0.000000	18.808689	1.211171

**Table S7.** The Cartesian coordinates (atomic units) of **1(8)**.

ATOM	X	Y	Z
C	0.000000	2.156928	0.662414
C	0.000000	-2.156928	0.662414
C	0.000000	0.000000	2.216466
C	0.000000	-1.276733	-1.955493
C	0.000000	1.276733	-1.955493
H	0.000000	0.000000	4.262740
H	0.000000	-2.482436	-3.604821
H	0.000000	2.482436	-3.604821
C	0.000000	4.642579	1.532590
C	0.000000	-4.642579	1.532590
C	0.000000	6.793551	0.021864
C	0.000000	-6.793551	0.021864
C	0.000000	9.221523	0.996271
C	0.000000	-9.221523	0.996271
C	0.000000	11.406244	-0.490136
C	0.000000	-11.406244	-0.490136
H	0.000000	4.914653	3.573205
H	0.000000	-4.914653	3.573205
H	0.000000	6.572098	-2.020910
H	0.000000	-6.572098	-2.020910
H	0.000000	9.448623	3.044422
H	0.000000	-9.448623	3.044422
H	0.000000	11.181710	-2.533275
H	0.000000	-11.181710	-2.533275
C	0.000000	-13.819836	0.484860
C	0.000000	13.819836	0.484860
C	0.000000	-16.030700	-0.980168
C	0.000000	16.030700	-0.980168
H	0.000000	-14.034848	2.533698
H	0.000000	14.034848	2.533698
C	0.000000	18.385470	0.099288
C	0.000000	-18.385470	0.099288
H	0.000000	15.860347	-3.028218
H	0.000000	-15.860347	-3.028218
N	0.000000	-20.577149	-1.149797
N	0.000000	20.577149	-1.149797
H	0.000000	-18.559946	2.145653
H	0.000000	18.559946	2.145653
H	0.000000	-20.633438	-3.051379
H	0.000000	20.633438	-3.051379

H	0.000000	-22.237485	-0.230967
H	0.000000	22.237485	-0.230967

**Table S8.** The Cartesian coordinates (atomic units) of **1(9)**.

ATOM	X	Y	Z
C	0.000000	2.148275	1.029919
C	0.000000	-2.148275	1.029919
C	0.000000	0.000000	2.573388
C	0.000000	-1.267378	-1.629982
C	0.000000	1.267378	-1.629982
H	0.000000	0.000000	4.618035
H	0.000000	-2.476358	-3.277386
H	0.000000	2.476358	-3.277386
C	0.000000	4.648378	1.862726
C	0.000000	-4.648378	1.862726
C	0.000000	6.753155	0.307015
C	0.000000	-6.753155	0.307015
C	0.000000	9.229194	1.210188
C	0.000000	-9.229194	1.210188
C	0.000000	11.333866	-0.335637
C	0.000000	-11.333866	-0.335637
H	0.000000	4.959674	3.895823
H	0.000000	-4.959674	3.895823
H	0.000000	6.474446	-1.729212
H	0.000000	-6.474446	-1.729212
H	0.000000	9.510119	3.247164
H	0.000000	-9.510119	3.247164
H	0.000000	11.036997	-2.373459
H	0.000000	-11.036997	-2.373459
C	0.000000	-13.823560	0.555357
C	0.000000	13.823560	0.555357
C	0.000000	-15.915337	-0.993962
C	0.000000	15.915337	-0.993962
H	0.000000	-14.115085	2.591611
H	0.000000	14.115085	2.591611
C	0.000000	18.419568	-0.113388
C	0.000000	-18.419568	-0.113388
H	0.000000	15.613347	-3.032673
H	0.000000	-15.613347	-3.032673
C	0.000000	-20.457809	-1.710600
C	0.000000	20.457809	-1.710600
H	0.000000	-18.740658	1.916968

H	0.000000	18.740658	1.916968
H	0.000000	-20.161741	-3.743631
H	0.000000	20.161741	-3.743631
N	0.000000	-22.881432	-0.995859
N	0.000000	22.881432	-0.995859
H	0.000000	-24.280782	-2.277595
H	0.000000	24.280782	-2.277595
H	0.000000	-23.370194	0.843262
H	0.000000	23.370194	0.843262

**Table S9.** The Cartesian coordinates (atomic units) of **1(10)**.

ATOM	X	Y	Z
C	0.000000	2.157867	0.850997
C	0.000000	-2.157867	0.850997
C	0.000000	0.000000	2.404549
C	0.000000	-1.276771	-1.766487
C	0.000000	1.276771	-1.766487
H	0.000000	0.000000	4.451084
H	0.000000	-2.483920	-3.414668
H	0.000000	2.483920	-3.414668
C	0.000000	4.646767	1.715999
C	0.000000	-4.646767	1.715999
C	0.000000	6.794553	0.203499
C	0.000000	-6.794553	0.203499
C	0.000000	9.225066	1.174242
C	0.000000	-9.225066	1.174242
C	0.000000	11.409007	-0.305096
C	0.000000	-11.409007	-0.305096
H	0.000000	4.920535	3.756433
H	0.000000	-4.920535	3.756433
H	0.000000	6.569370	-1.837614
H	0.000000	-6.569370	-1.837614
H	0.000000	9.449735	3.220679
H	0.000000	-9.449735	3.220679
H	0.000000	11.190916	-2.349467
H	0.000000	-11.190916	-2.349467
C	0.000000	-13.822424	0.683253
C	0.000000	13.822424	0.683253
C	0.000000	-16.026357	-0.786870
C	0.000000	16.026357	-0.786870
H	0.000000	-14.030125	2.732789
H	0.000000	14.030125	2.732789

C	0.000000	18.428062	0.205069
C	0.000000	-18.428062	0.205069
H	0.000000	15.815070	-2.832159
H	0.000000	-15.815070	-2.832159
C	0.000000	-20.659094	-1.240166
C	0.000000	20.659094	-1.240166
H	0.000000	-18.630314	2.255787
H	0.000000	18.630314	2.255787
H	0.000000	-20.510864	-3.290449
H	0.000000	20.510864	-3.290449
C	0.000000	-22.998014	-0.135545
C	0.000000	22.998014	-0.135545
N	0.000000	-25.210805	-1.358737
N	0.000000	25.210805	-1.358737
H	0.000000	-23.142330	1.913743
H	0.000000	23.142330	1.913743
H	0.000000	-25.288080	-3.259041
H	0.000000	25.288080	-3.259041
H	0.000000	-26.858091	-0.417435
H	0.000000	26.858091	-0.417435

**Table S10.** The Cartesian coordinates (atomic units) of **1(11)**.

ATOM	X	Y	Z
C	0.000000	2.149448	1.308274
C	0.000000	-2.149448	1.308274
C	0.000000	0.000000	2.852323
C	0.000000	-1.268282	-1.346138
C	0.000000	1.268282	-1.346138
H	0.000000	0.000000	4.896258
H	0.000000	-2.482587	-2.989076
H	0.000000	2.482587	-2.989076
C	0.000000	4.650870	2.137927
C	0.000000	-4.650870	2.137927
C	0.000000	6.763447	0.589770
C	0.000000	-6.763447	0.589770
C	0.000000	9.235913	1.499792
C	0.000000	-9.235913	1.499792
C	0.000000	11.346544	-0.041893
C	0.000000	-11.346544	-0.041893
H	0.000000	4.954869	4.171772
H	0.000000	-4.954869	4.171772
H	0.000000	6.498812	-1.448737

H	0.000000	-6.498812	-1.448737
H	0.000000	9.514389	3.537128
H	0.000000	-9.514389	3.537128
H	0.000000	11.053483	-2.079242
H	0.000000	-11.053483	-2.079242
C	0.000000	-13.831166	0.850864
C	0.000000	13.831166	0.850864
C	0.000000	-15.931044	-0.695265
C	0.000000	15.931044	-0.695265
H	0.000000	-14.120517	2.887199
H	0.000000	14.120517	2.887199
C	0.000000	18.425523	0.201239
C	0.000000	-18.425523	0.201239
H	0.000000	15.635023	-2.734312
H	0.000000	-15.635023	-2.734312
C	0.000000	-20.521185	-1.334645
C	0.000000	20.521185	-1.334645
H	0.000000	-18.709245	2.238625
H	0.000000	18.709245	2.238625
H	0.000000	-20.229681	-3.374691
H	0.000000	20.229681	-3.374691
C	0.000000	-23.032584	-0.459495
C	0.000000	23.032584	-0.459495
C	0.000000	-25.046530	-2.081380
C	0.000000	25.046530	-2.081380
H	0.000000	-23.372445	1.568028
H	0.000000	23.372445	1.568028
H	0.000000	-24.706737	-4.107351
H	0.000000	24.706737	-4.107351
N	0.000000	-27.486532	-1.409855
N	0.000000	27.486532	-1.409855
H	0.000000	28.005626	0.419751
H	0.000000	-28.005626	0.419751
H	0.000000	28.867842	-2.710243
H	0.000000	-28.867842	-2.710243

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