

## Supporting Information

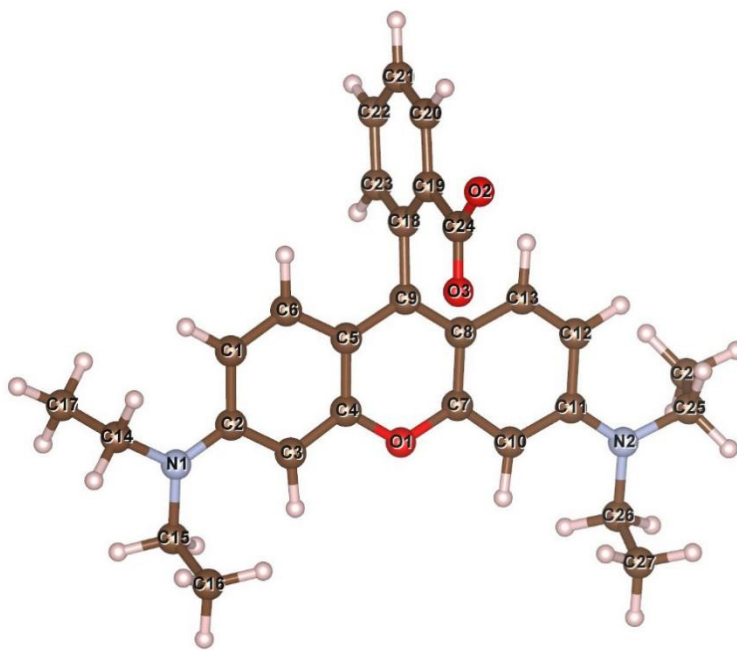
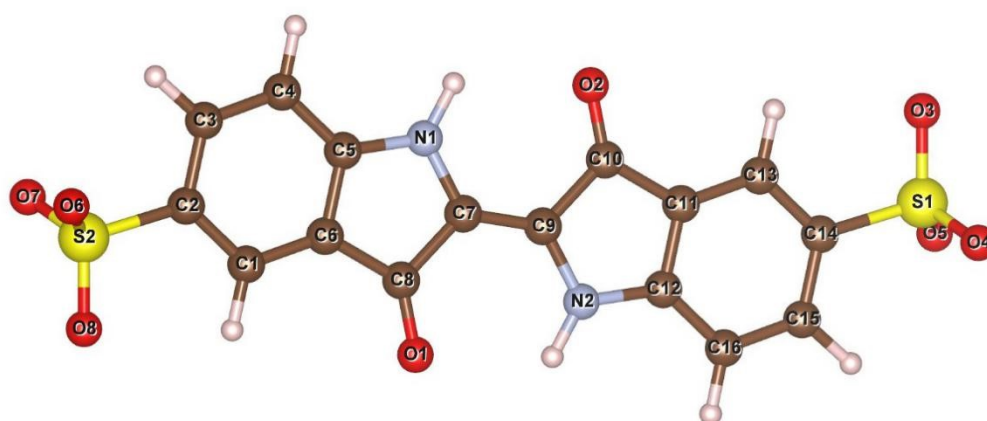


Figure S1. Optimized geometries of RhB

Table S1. Hirshfeld charges and condensed orbital-weighted Fukui indices of RhB

Atom	Hirshfeld charge	$f^+$	$f^-$	$f^0$
C1	-0.0572	0.0361	0.0295	0.0328
C2	0.0774	0.0518	0.0193	0.0355
C3	-0.0880	0.0216	0.0402	0.0309
C4	0.1008	0.0493	0.0180	0.0337
C5	-0.0357	0.0400	0.0352	0.0376
C6	-0.0180	0.0566	0.0171	0.0369
C7	0.1008	0.0493	0.0180	0.0337
C8	-0.0357	0.0400	0.0352	0.0376
C9	0.0825	0.1540	0.0180	0.0860
C10	-0.0880	0.0216	0.0402	0.0309
C11	0.0774	0.0518	0.0193	0.0355
C12	-0.0572	0.0361	0.0295	0.0328
C13	-0.0180	0.0566	0.0171	0.0369
C14	0.0129	0.0038	0.0069	0.0053
C15	0.0126	0.0037	0.0068	0.0052
C16	-0.0855	0.0024	0.0057	0.0040
C17	-0.0855	0.0023	0.0057	0.0040

C18	-0.0025	0.0328	0.0234	0.0281
C19	-0.0263	0.0241	0.0375	0.0308
C20	-0.0461	0.0183	0.0246	0.0214
C21	-0.0438	0.0173	0.0214	0.0193
C22	-0.0417	0.0204	0.0213	0.0209
C23	-0.0434	0.0233	0.0216	0.0225
C24	0.1163	0.0088	0.0324	0.0206
C25	0.0129	0.0038	0.0069	0.0053
C26	0.0126	0.0037	0.0068	0.0052
C27	-0.0855	0.0024	0.0057	0.0040
C28	-0.0855	0.0023	0.0057	0.0040
N1	-0.0248	0.0306	0.0544	0.0425
N2	-0.0248	0.0306	0.0544	0.0425
O1	-0.0745	0.0333	0.0150	0.0242
O2	-0.4569	0.0050	0.1293	0.0671
O3	-0.4254	0.0197	0.1325	0.0761

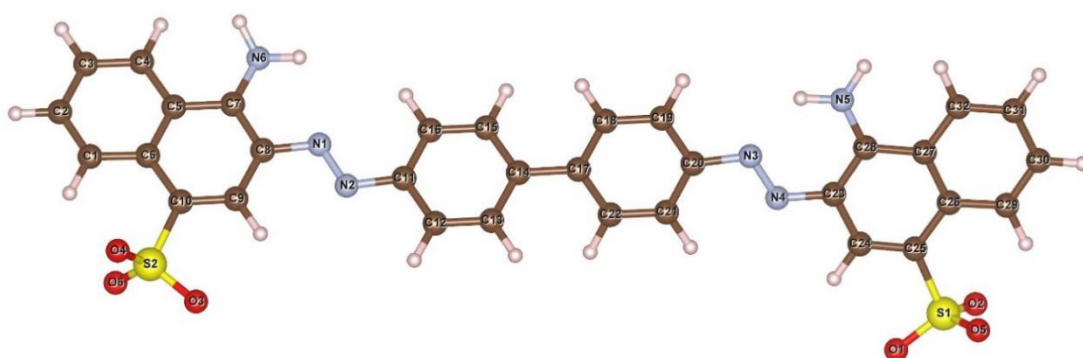


**Figure S2.** Optimized geometries of IC

**Table S2.** Hirshfeld charges and condensed orbital-weighted Fukui indices of IC

Atom	Hirshfeld charge	$f^+$	$f^-$	$f^0$
C1	-0.0226	0.0262	0.0239	0.0250
C2	-0.0520	0.0131	0.0413	0.0272
C3	-0.0209	0.0287	0.0226	0.0257
C4	-0.0448	0.0185	0.0320	0.0252
C5	0.0596	0.0260	0.0270	0.0265
C6	-0.0491	0.0206	0.0358	0.0282
C7	0.0294	0.0426	0.0437	0.0431
C8	0.1306	0.0564	0.0187	0.0376
C9	0.0293	0.0426	0.0437	0.0431
C10	0.1306	0.0564	0.0187	0.0376
C11	-0.0491	0.0206	0.0358	0.0282

C12	0.0596	0.0260	0.0270	0.0265
C13	-0.0226	0.0262	0.0239	0.0250
C14	-0.0520	0.0131	0.0413	0.0272
C15	-0.0209	0.0287	0.0226	0.0257
C16	-0.0448	0.0185	0.0320	0.0252
N1	-0.0657	0.0124	0.0634	0.0379
N2	-0.0657	0.0124	0.0634	0.0379
O1	-0.2890	0.0527	0.0394	0.0461
O2	-0.2890	0.0527	0.0394	0.0461
O3	-0.4465	0.0038	0.0359	0.0198
O4	-0.4672	0.0042	0.0425	0.0234
O5	-0.4694	0.0043	0.0434	0.0238
O6	-0.4694	0.0043	0.0434	0.0238
O7	-0.4672	0.0042	0.0425	0.0233
O8	-0.4465	0.0038	0.0359	0.0199
S1	0.4002	0.0106	0.0175	0.0140
S2	0.4002	0.0106	0.0175	0.0140

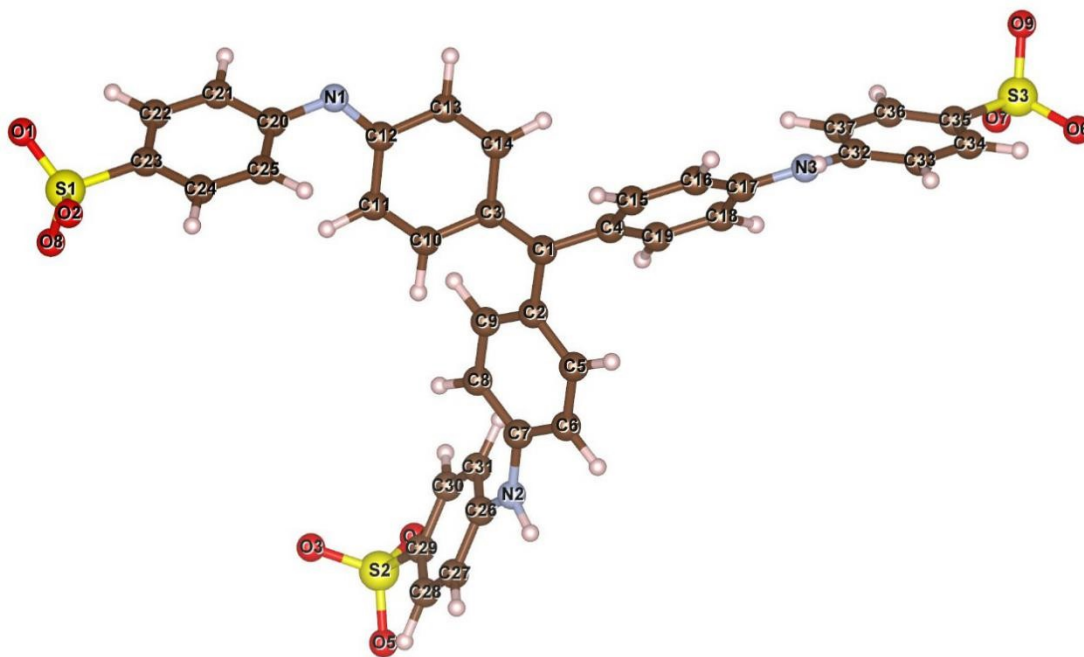


**Figure S3.** Optimized geometries of CR

**Table S3.** Hirshfeld charges and condensed orbital-weighted Fukui indices of CR

Atom	Hirshfeld charge	$f^+$	$f^-$	$f^0$
C1	-0.0494	0.0099	0.0184	0.0142
C2	-0.0361	0.0116	0.0148	0.0132
C3	-0.0414	0.0100	0.0169	0.0135
C4	-0.0413	0.0117	0.0172	0.0145
C5	-0.0198	0.0090	0.0164	0.0127
C6	-0.0061	0.0100	0.0154	0.0127
C7	0.0642	0.0163	0.0229	0.0196
C8	-0.0211	0.0107	0.0365	0.0236
C9	-0.0539	0.0126	0.0210	0.0168
C10	-0.0588	0.0080	0.0321	0.0200

C11	0.0093	0.0125	0.0206	0.0166
C12	-0.0433	0.0122	0.0156	0.0139
C13	-0.0408	0.0102	0.0152	0.0127
C14	-0.0019	0.0127	0.0180	0.0153
C15	-0.0391	0.0098	0.0149	0.0124
C16	-0.0464	0.0132	0.0163	0.0148
C17	-0.0042	0.0121	0.0188	0.0155
C18	-0.0410	0.0101	0.0154	0.0128
C19	-0.0451	0.0116	0.0163	0.0140
C20	0.0110	0.0120	0.0212	0.0166
C21	-0.0488	0.0126	0.0171	0.0148
C22	-0.0391	0.0097	0.0152	0.0124
C23	-0.0207	0.0098	0.0365	0.0232
C24	-0.0509	0.0114	0.0208	0.0161
C25	-0.0672	0.0068	0.0348	0.0208
C26	-0.0055	0.0098	0.0153	0.0125
C27	-0.0209	0.0090	0.0176	0.0133
C28	0.0719	0.0165	0.0217	0.0191
C29	-0.0504	0.0096	0.0187	0.0142
C30	-0.0355	0.0115	0.0143	0.0129
C31	-0.0424	0.0097	0.0175	0.0136
C32	-0.0408	0.0117	0.0169	0.0143
N1	-0.0540	0.0264	0.0272	0.0268
N2	-0.0772	0.0255	0.0337	0.0296
N3	-0.0646	0.0215	0.0352	0.0284
N4	-0.0635	0.0242	0.0285	0.0263
N5	-0.1241	0.0097	0.0305	0.0201
N6	-0.1485	0.0068	0.0320	0.0194
O1	-0.4456	0.0025	0.0173	0.0099
O2	-0.4605	0.0026	0.0215	0.0121
O3	-0.4443	0.0027	0.0171	0.0099
O4	-0.4591	0.0027	0.0212	0.0119
O5	-0.4614	0.0026	0.0216	0.0121
O6	-0.4597	0.0027	0.0212	0.0119
S1	0.4054	0.0066	0.0101	0.0083
S2	0.4062	0.0068	0.0099	0.0084



**Figure S4.** Optimized geometries of MB

**Table S4.** Hirshfeld charges and condensed orbital-weighted Fukui indices of MB

Atom	Hirshfeld charge	$f^+$	$f^-$	$f^0$
C1	0.0339	0.0334	0.0240	0.0287
C2	-0.0206	0.0106	0.0243	0.0175
C3	-0.0228	0.0150	0.0272	0.0211
C4	-0.0204	0.0107	0.0241	0.0174
C5	-0.0327	0.0130	0.0139	0.0134
C6	-0.0592	0.0109	0.0196	0.0153
C7	0.0535	0.0123	0.0178	0.0150
C8	-0.0604	0.0100	0.0203	0.0152
C9	-0.0286	0.0130	0.0141	0.0135
C10	-0.0264	0.0174	0.0129	0.0151
C11	-0.0620	0.0144	0.0230	0.0187
C12	0.0597	0.0176	0.0135	0.0156
C13	-0.0620	0.0143	0.0227	0.0185
C14	-0.0334	0.0154	0.0134	0.0144
C15	-0.0294	0.0128	0.0136	0.0132
C16	-0.0594	0.0109	0.0199	0.0154
C17	0.0537	0.0125	0.0177	0.0151
C18	-0.0593	0.0103	0.0196	0.0149
C19	-0.0315	0.0135	0.0142	0.0139
C20	0.0302	0.0102	0.0197	0.0149
C21	-0.0588	0.0104	0.0189	0.0146

C22	-0.0467	0.0092	0.0129	0.0111
C23	-0.0541	0.0079	0.0208	0.0143
C24	-0.0461	0.0092	0.0131	0.0111
C25	-0.0533	0.0097	0.0191	0.0144
C26	0.0483	0.0093	0.0162	0.0127
C27	-0.0562	0.0101	0.0184	0.0143
C28	-0.0426	0.0096	0.0117	0.0106
C29	-0.0549	0.0079	0.0211	0.0145
C30	-0.0417	0.0098	0.0119	0.0108
C31	-0.0543	0.0094	0.0182	0.0138
C32	0.0485	0.0093	0.0162	0.0128
C33	-0.0569	0.0102	0.0188	0.0145
C34	-0.0429	0.0095	0.0117	0.0106
C35	-0.0553	0.0079	0.0213	0.0146
C36	-0.0412	0.0099	0.0119	0.0109
C37	-0.0546	0.0095	0.0181	0.0138
N1	-0.2055	0.0216	0.0533	0.0374
N2	-0.0814	0.0053	0.0393	0.0223
N3	-0.0811	0.0053	0.0392	0.0223
O1	-0.4609	0.0034	0.0158	0.0096
O2	-0.4577	0.0033	0.0154	0.0093
O3	-0.4774	0.0040	0.0185	0.0112
O4	-0.4601	0.0034	0.0155	0.0094
O5	-0.4569	0.0034	0.0149	0.0092
O6	-0.4546	0.0034	0.0145	0.0090
O7	-0.4639	0.0035	0.0160	0.0098
O8	-0.4783	0.0040	0.0188	0.0114
O9	-0.4770	0.0039	0.0183	0.0111
S1	0.3972	0.0091	0.0073	0.0082
S2	0.3978	0.0091	0.0073	0.0082
S3	0.3979	0.0092	0.0073	0.0082