Electronic supplementary information (ESI)

Comparative computational study on the interactions of N719 and N749 dyes with iodine in dye-sensitized solar cells

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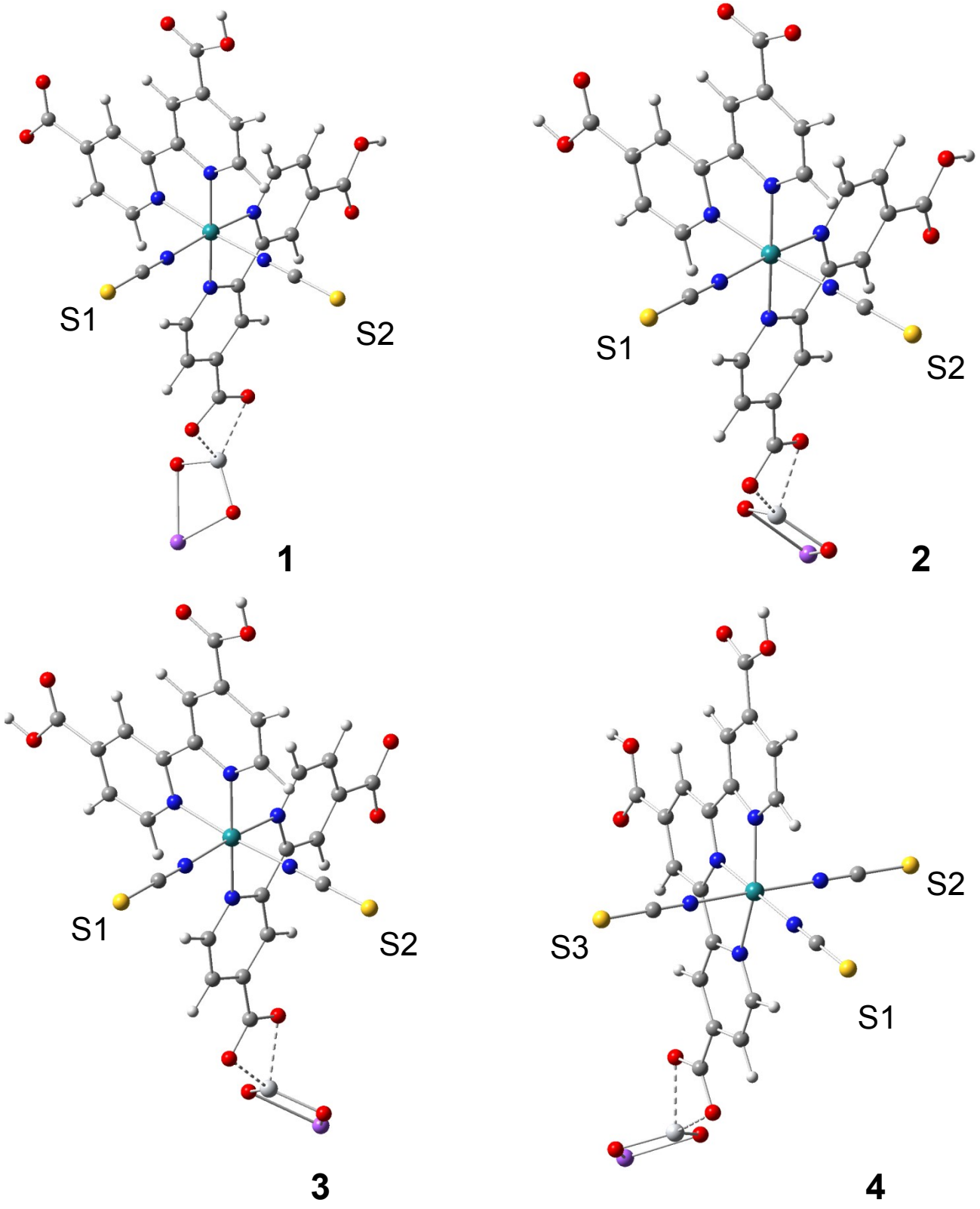


Fig. S1 Optimized geometries of the N719 and N749 species in the ground state. White, grey, blue, red, purple, yellow, ash, and teal indicate H, C, N, O, Na, S, Ti, and Ru atoms, respectively.

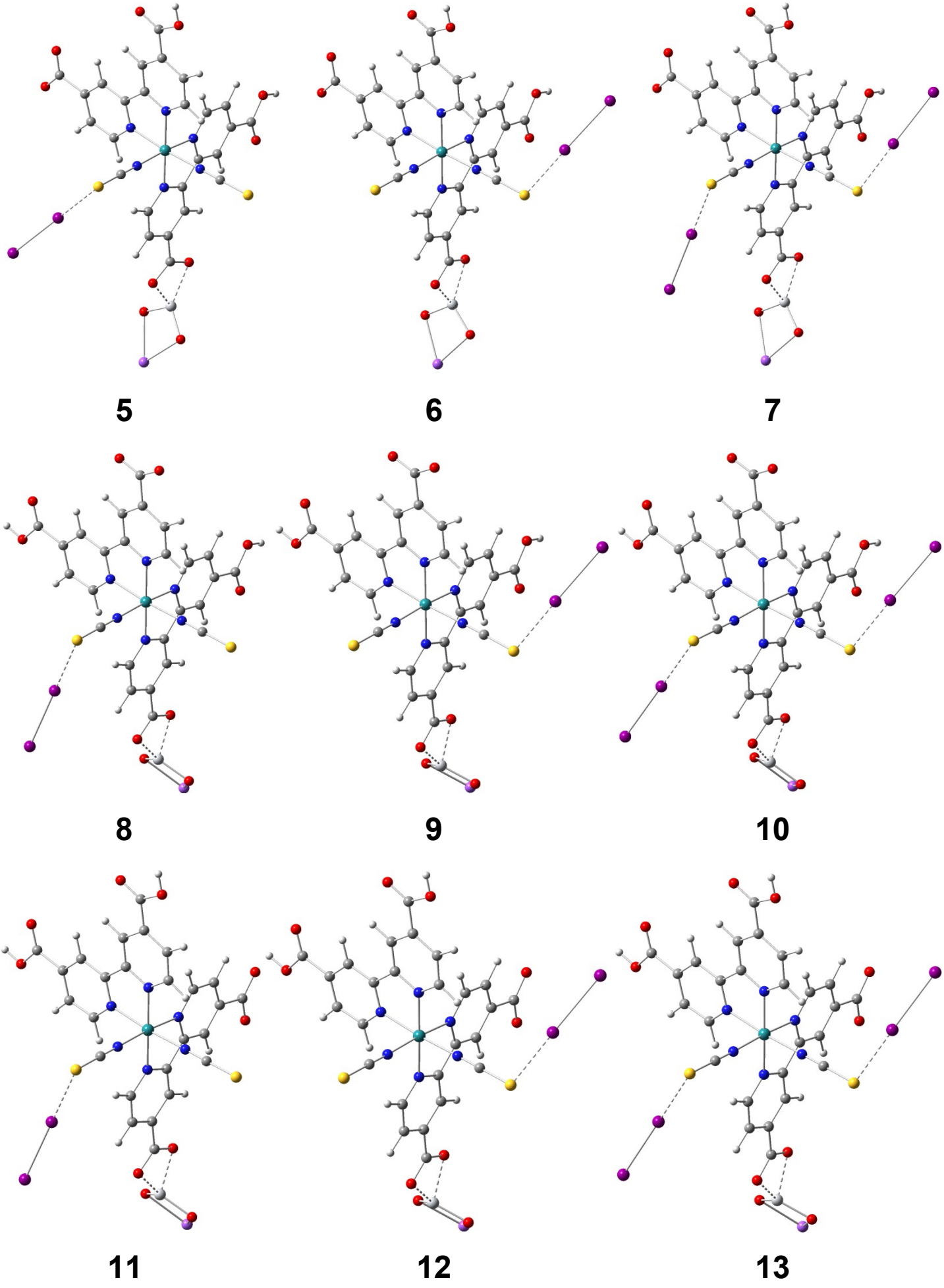


Fig. S2 Continued

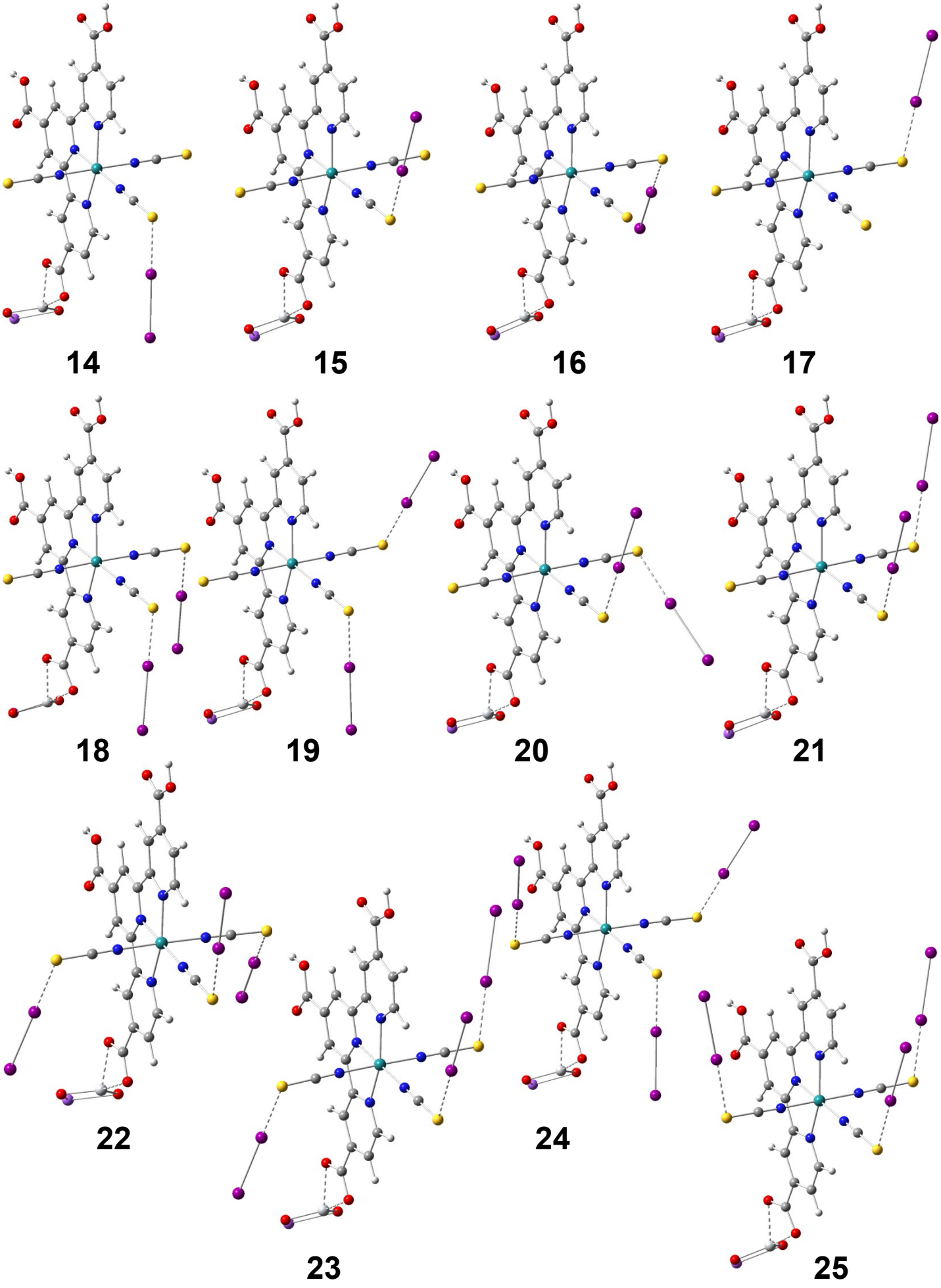


Fig. S2 Optimized geometries of the dye–I_2 species. White, grey, blue, red, purple, yellow, ash, teal, and violet indicate H, C, N, O, Na, S, Ti, Ru, and I atoms, respectively.

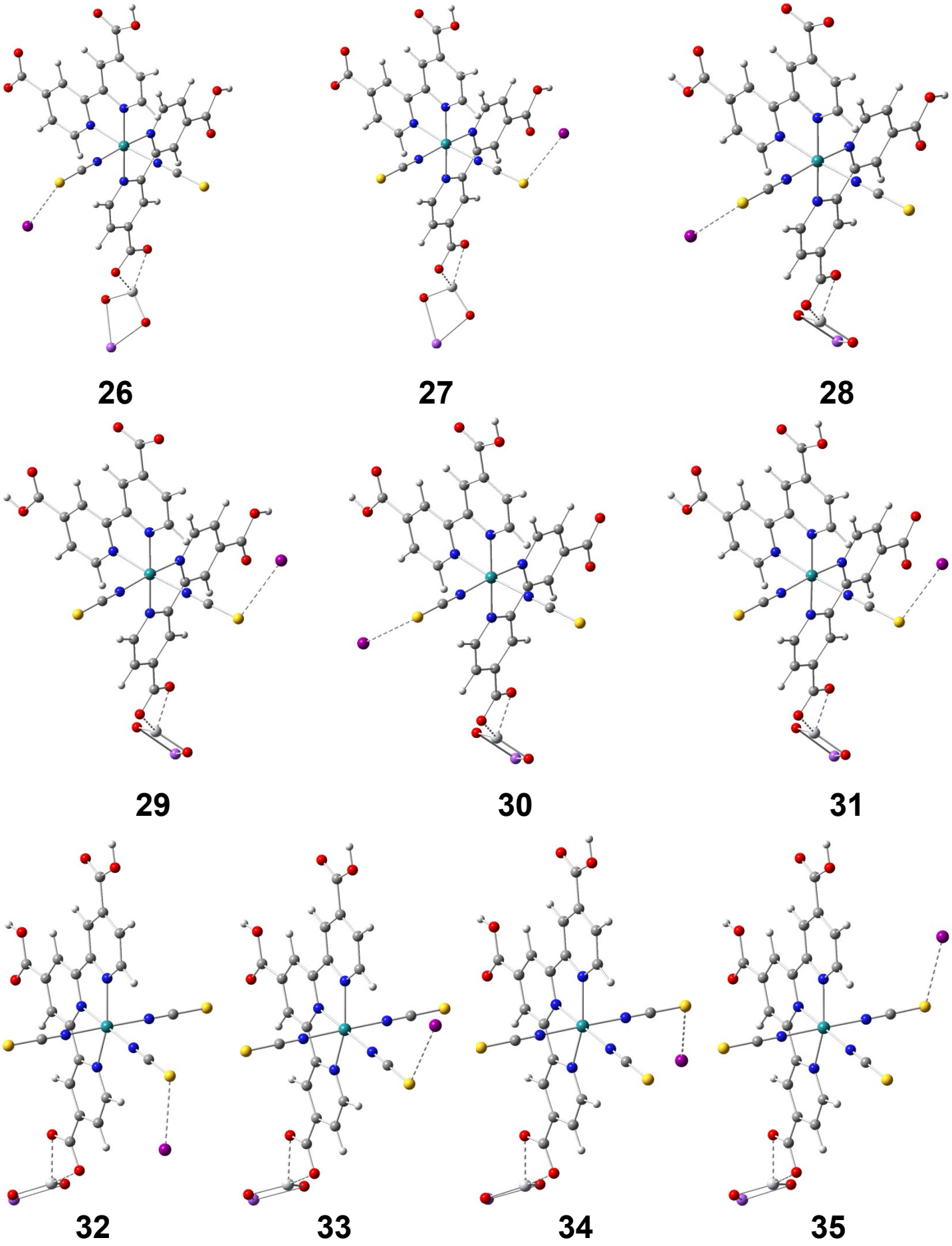


Fig. S3 Optimized geometries of the oxidized dye–I^- species. White, grey, blue, red, purple, yellow, ash, teal, and violet indicate H, C, N, O, Na, S, Ti, Ru, and I atoms, respectively.

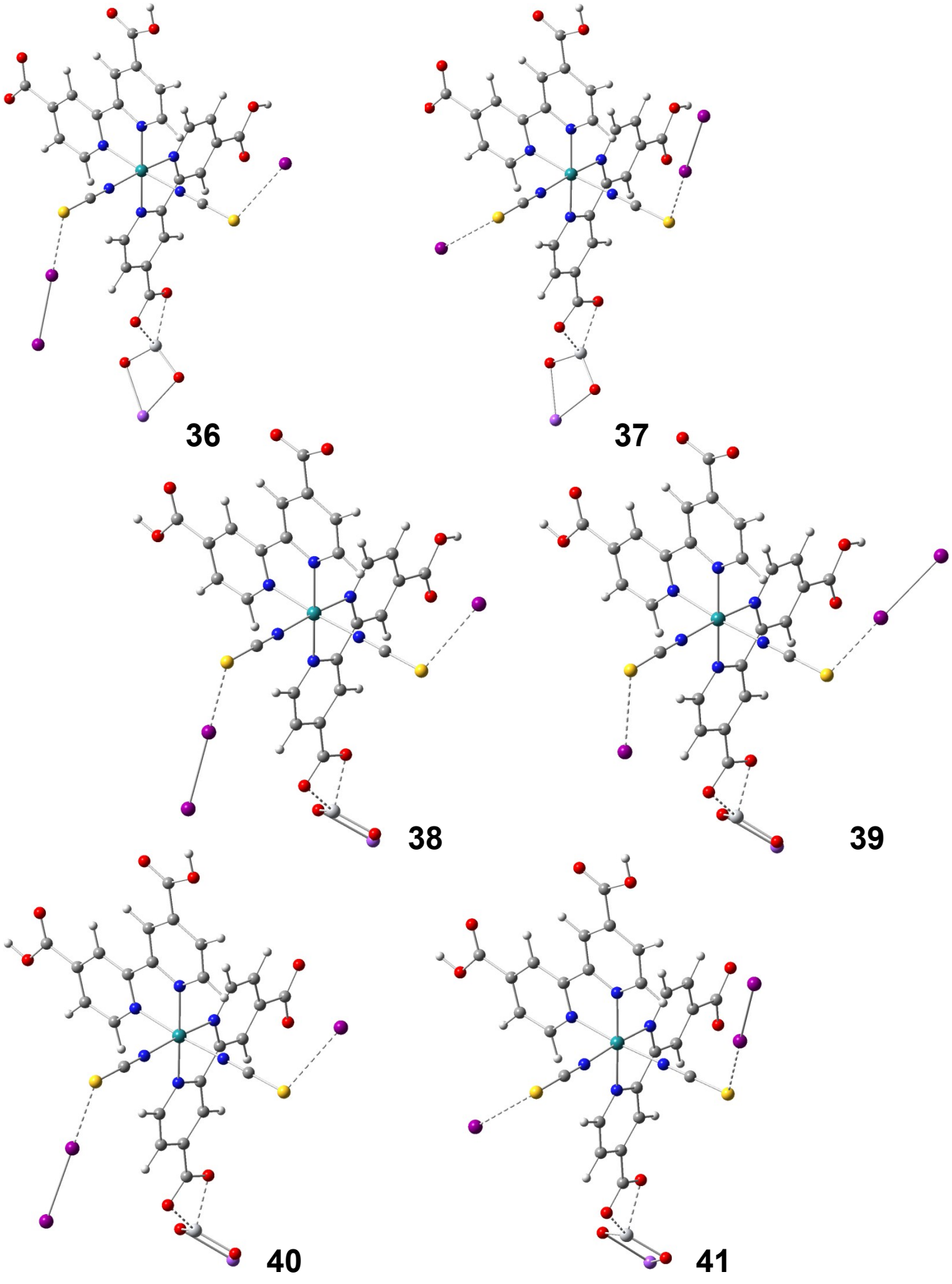
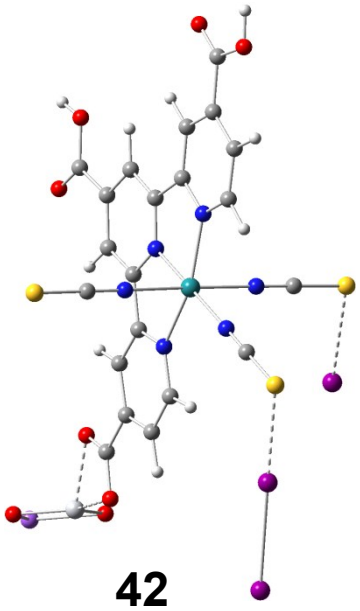


Fig. S4 Continued



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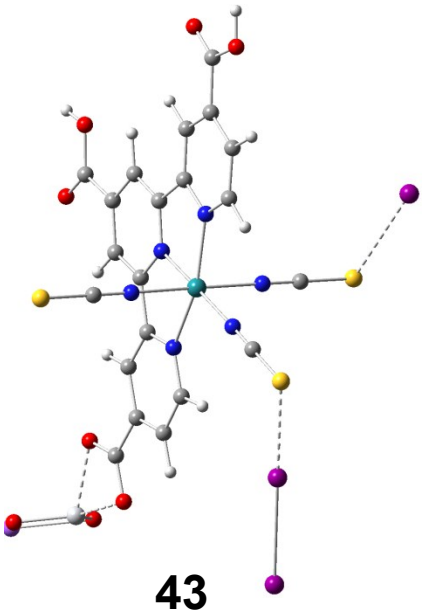

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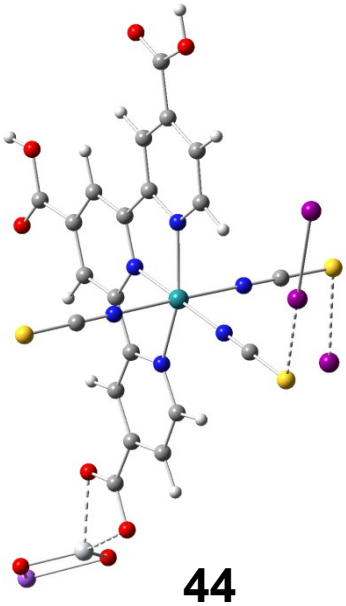

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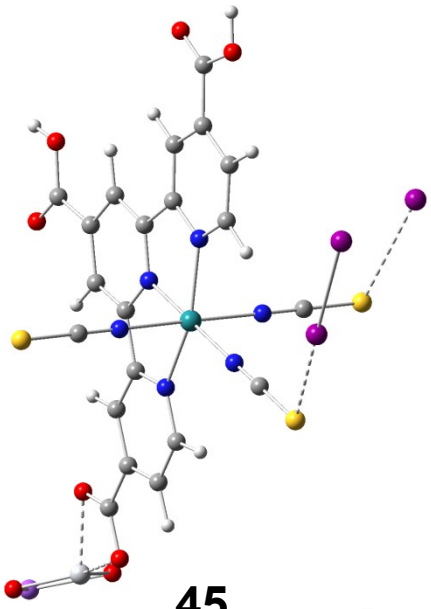

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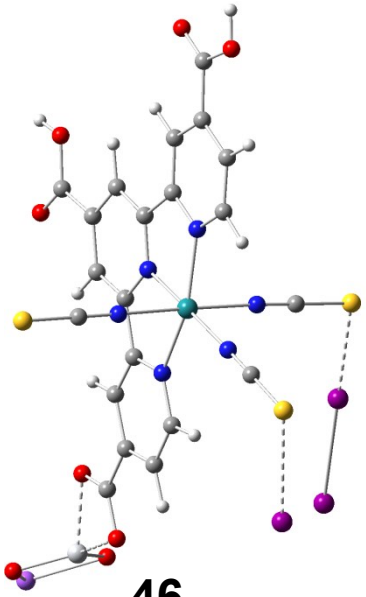

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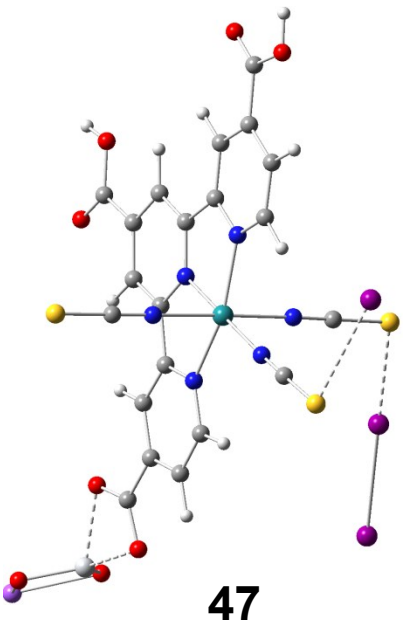

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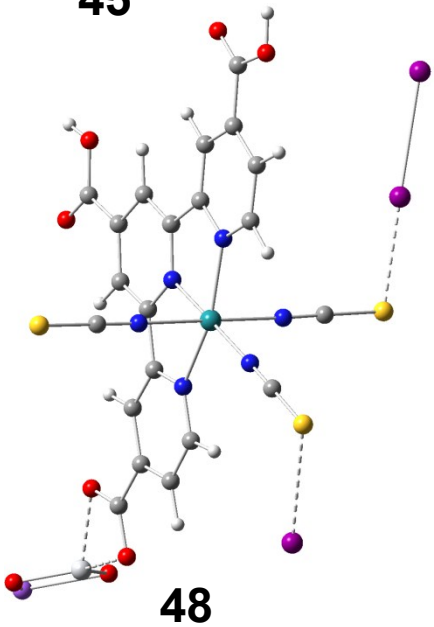

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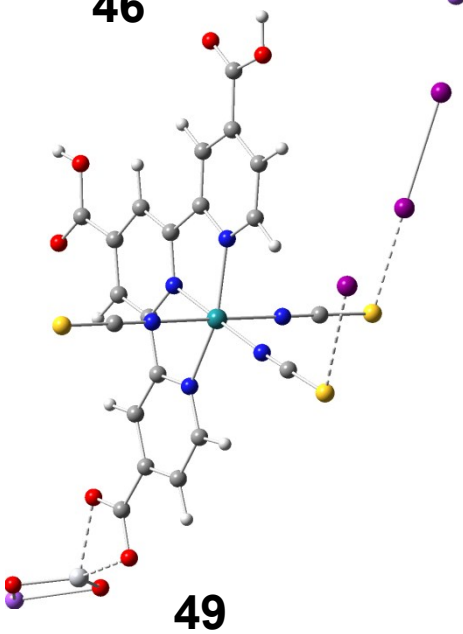

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Fig. S4 Continued

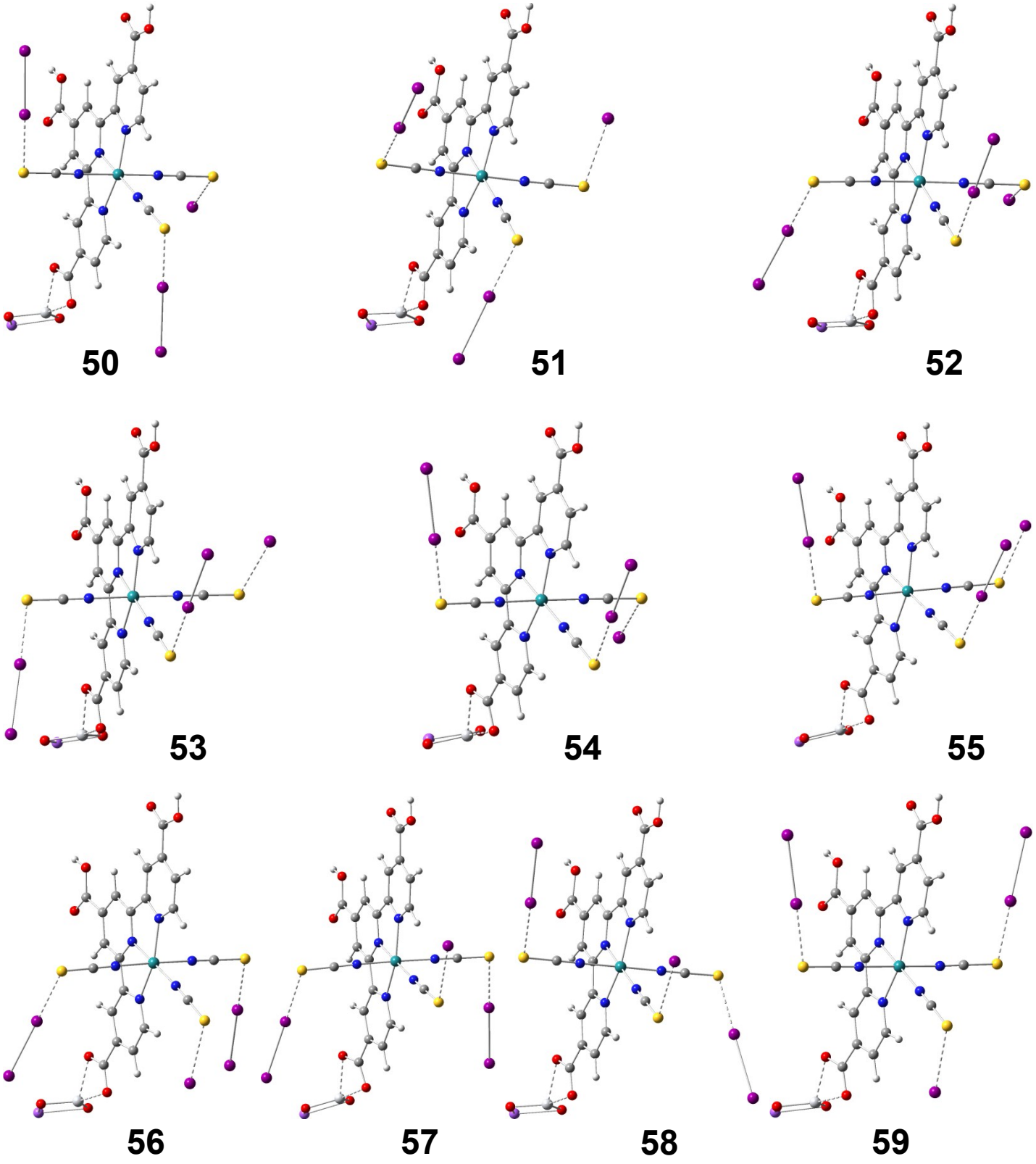

Fig. S4 Optimized geometries of the I_2–dye–I species. White, grey, blue, red, purple, yellow, ash, teal, and violet indicate H, C, N, O, Na, S, Ti, Ru, and I atoms, respectively.

Table S1 Atomic charges (e) on the S atom and the changes for the I_2–dye–I species

	S atom bonded to I_2 molecule				S atom bonded to I^-				Change in the S atom bonded to I_2				Change in the S atom bonded to I^-			
Species	ESP	Hirshfeld	Mulliken	NPA	ESP	Hirshfeld	Mulliken	NPA	ESP	Hirshfeld	Mulliken	NPA	ESP	Hirshfeld	Mulliken	NPA
36	–0.0777	–0.0597	–0.1363	–0.0633	–0.1246	–0.1123	–0.1320	–0.0539	0.1866	0.2017	0.1045	0.1007	0.1294	0.1498	0.1098	0.1108
37	–0.0821	–0.0607	–0.1378	–0.0646	–0.1174	–0.1126	–0.1330	–0.0551	0.1719	0.2013	0.1040	0.1002	0.1469	0.1487	0.1078	0.1090
38	–0.0815	–0.0582	–0.1349	–0.0615	–0.1143	–0.1123	–0.1328	–0.0549	0.1779	0.1995	0.1021	0.0981	0.1418	0.1482	0.1073	0.1082
39	–0.0835	–0.0597	–0.1389	–0.0637	–0.1195	–0.1098	–0.1285	–0.0513	0.1725	0.2008	0.1012	0.0993	0.1399	0.1480	0.1085	0.1084
40	–0.0932	–0.0602	–0.1379	–0.0643	–0.1134	–0.1126	–0.1330	–0.0552	0.1665	0.2019	0.1039	0.1006	0.1512	0.1484	0.1074	0.1082
41	–0.0844	–0.0596	–0.1363	–0.0633	–0.1193	–0.1121	–0.1317	–0.0534	0.1802	0.2013	0.1041	0.1002	0.1404	0.1499	0.1101	0.1115
42	–0.0686	–0.0590	–0.1379	–0.0639	–0.1029	–0.1162	–0.1340	–0.0568	0.2263	0.2521	0.1549	0.1612	0.1539	0.1728	0.1353	0.1402
43	–0.0655	–0.0572	–0.1359	–0.0621	–0.0907	–0.1157	–0.1330	–0.0560	0.2294	0.2539	0.1568	0.1630	0.1661	0.1733	0.1363	0.1410
44	–0.0707	–0.0574	–0.1369	–0.0627	–0.1122	–0.1155	–0.1330	–0.0558	0.2242	0.2537	0.1559	0.1624	0.1446	0.1735	0.1363	0.1413
45	–0.0836	–0.0578	–0.1370	–0.0630	–0.1070	–0.1160	–0.1339	–0.0567	0.2113	0.2532	0.1558	0.1621	0.1499	0.1730	0.1354	0.1403
46	–0.0698	–0.0600	–0.1386	–0.0634	–0.1138	–0.1133	–0.1315	–0.0547	0.1871	0.2290	0.1307	0.1336	0.1811	0.1977	0.1613	0.1704
47	–0.0786	–0.0589	–0.1382	–0.0629	–0.1160	–0.1117	–0.1290	–0.0523	0.1783	0.2301	0.1311	0.1341	0.1789	0.1994	0.1637	0.1727
48	–0.0750	–0.0594	–0.1386	–0.0637	–0.1168	–0.1127	–0.1306	–0.0539	0.1819	0.2295	0.1307	0.1333	0.1781	0.1983	0.1622	0.1712
49	–0.0677	–0.0596	–0.1396	–0.0641	–0.1140	–0.1123	–0.1298	–0.0532	0.1892	0.2294	0.1298	0.1330	0.1809	0.1987	0.1629	0.1719
50	–0.0721	–0.0580	–0.1359	–0.0630	–0.0951	–0.1117	–0.1320	–0.0561	0.2228	0.2531	0.1569	0.1621	0.1618	0.1773	0.1374	0.1409
	–0.0727	–0.0579	–0.1365	–0.0625					0.1842	0.2311	0.1328	0.1345				
51	–0.0951	–0.0579	–0.1340	–0.0620	–0.1180	–0.1112	–0.1311	–0.0552	0.1998	0.2531	0.1588	0.1631	0.1389	0.1778	0.1383	0.1419
	–0.0764	–0.0592	–0.1375	–0.0640					0.1805	0.2298	0.1318	0.1331				
52	–0.0644	–0.0573	–0.1358	–0.0625	–0.1251	–0.1118	–0.1324	–0.0567	0.2305	0.2537	0.1570	0.1626	0.1318	0.1771	0.1369	0.1403
	–0.0875	–0.0586	–0.1365	–0.0628					0.1694	0.2304	0.1328	0.1343				
53	–0.0709	–0.0574	–0.1354	–0.0621	–0.1197	–0.1122	–0.1325	–0.0565	0.2240	0.2536	0.1574	0.1630	0.1372	0.1768	0.1369	0.1405
	–0.0655	–0.0605	–0.1392	–0.0654					0.1914	0.2285	0.1302	0.1316				
54	–0.0744	–0.0576	–0.1363	–0.0629	–0.1001	–0.1108	–0.1310	–0.0550	0.2205	0.2535	0.1565	0.1622	0.1568	0.1782	0.1383	0.1420
	–0.0773	–0.0597	–0.1379	–0.0643					0.1796	0.2293	0.1314	0.1328				
55	–0.0793	–0.0582	–0.1372	–0.0637	–0.1212	–0.1121	–0.1330	–0.0571	0.2156	0.2528	0.1556	0.1614	0.1357	0.1769	0.1364	0.1400
	–0.0849	–0.0601	–0.1385	–0.0650					0.1720	0.2289	0.1308	0.1321				
56	–0.0733	–0.0598	–0.1380	–0.0646	–0.1127	–0.1108	–0.1295	–0.0534	0.1835	0.2292	0.1314	0.1324	0.1822	0.2002	0.1633	0.1717
	–0.0744	–0.0592	–0.1376	–0.0642					0.1824	0.2298	0.1317	0.1328				
57	–0.0798	–0.0590	–0.1373	–0.0640	–0.1064	–0.1095	–0.1276	–0.0515	0.1770	0.2300	0.1321	0.1330	0.1885	0.2016	0.1652	0.1736
	–0.0707	–0.0587	–0.1367	–0.0634					0.1862	0.2303	0.1326	0.1336				
58	–0.0670	–0.0614	–0.1402	–0.0668	–0.1035	–0.1108	–0.1290	–0.0529	0.1899	0.2276	0.1291	0.1302	0.1915	0.2002	0.1638	0.1722
	–0.0775	–0.0587	–0.1376	–0.0635					0.1794	0.2303	0.1317	0.1335				
59	–0.0867	–0.0592	–0.1373	–0.0642	–0.1258	–0.1106	–0.1297	–0.0534	0.1701	0.2297	0.1320	0.1328	0.1691	0.2004	0.1631	0.1717
	–0.0813	–0.0588	–0.1372	–0.0641					0.1756	0.2301	0.1321	0.1330				