Supplementary Information: Insights into localization, energy ordering, and substituent effect in excited states of azobenzenes from coupled cluster calculations of nuclear spin-induced circular dichroism

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S1. PHYSICAL CONSTANTS

NSCD prefactors

For carbon ($\mathcal{L}_C$) and hydrogen ($\mathcal{L}_H$) (in $\mu\text{rad} \cdot \text{mol}^{-1} \cdot \text{dm}^3 \cdot \text{cm}^{-1}$):

$\mathcal{L}_C = 1.3125973044$

$\mathcal{L}_H = 5.2189931889$

The general expression for the prefactor is

$$\mathcal{L}_K = -\frac{10^7}{48\pi}\gamma_K I_K \frac{c_0 N_A e^3 \hbar \mu_0^2}{m_e a_0 E_H} \tag{S1}$$

Solvents

TABLE S1. Dielectric constants ϵ_r and refractive indices η_D for the three solvents.

Solvent	ϵ_r	η_D
DMSO	46.45	1.479
C_6H_{12}[1]	2.023	1.4264
$CHCl_3$[2]	4.8069	1.4459

S2. TRANSITION STRENGTHS

TABLE S2. AZO-1. aug-cc-pwCVDZ. Transition strength components $S_{0f}^{\alpha\alpha} = T_{0f}^{\alpha} T_{f0}^{\alpha}$ for $\alpha \in x, y, z$. The molecule lies (roughly) on the xy plane, with the long axis along y.

State n	E_n	f	S_{0f}^{xx}	S_{0f}^{yy}	S_{0f}^{zz}
1	2.959	0.000	0.0000	0.0000	0.0000
2	3.796	0.868	0.0366	9.2925	0.0000
3	4.508	0.008	0.0698	0.0010	0.0000
4	4.549	0.018	0.0087	0.1515	0.0000

S3. NSCD INTENSITIES

TABLE S3. AZO-2. aug-cc-pwCVDZ. Transition strength components $S_{0f}^{\alpha\alpha} = T_{0f}^{\alpha} T_{f0}^{\alpha}$ for $\alpha \in x, y, z$. The molecule lies (roughly) on the xz plane, with the long axis along z.

State n	E_n	f	S_{0f}^{xx}	S_{0f}^{yy}	S_{0f}^{zz}
1	2.964	0.000	0.0000	0.0000	0.0000
2	3.589	0.919	0.0298	0.0001	10.4251
3	4.437	0.028	0.0141	0.0000	0.2459
4	4.528	0.008	0.0637	0.0000	0.0065

TABLE S4. AZO-3. aug-cc-pwCVDZ. Transition strength components $S_{0f}^{\alpha\alpha} = T_{0f}^{\alpha} T_{f0}^{\alpha}$ for $\alpha \in x, y, z$. The molecule lies (roughly) on the xz plane, with the long axis along z.

State n	E_n	f	S_{0f}^{xx}	S_{0f}^{yy}	S_{0f}^{zz}
1	2.866	$1.12 \cdot 10^{-6}$	0.0000	0.0000	0.0000
2	3.339	1.043	0.0252	0.0001	12.7198
3	3.854	$3.05 \cdot 10^{-10}$	0.0000	0.0000	0.0000
4	4.352	0.004	0.0000	0.0000	0.0407
5	4.430	0.011	0.0941	0.0000	0.0049
6	4.441	0.001	0.0002	0.0057	0.0000

TABLE S5. AZO-1. aug-cc-pwCVDZ.

	RI-CC2				DFT/BH+HLYP			
Atom	ES1	ES2	ES3	ES4	ES1	ES2	ES3	ES4
E (eV)	2.959	3.796	4.508	4.549	3.015	3.790	4.748	4.838
ω (a.u.)	0.109	0.140	0.166	0.167	0.111	0.139	0.175	0.178
f	0.000	0.868	0.008	0.018	0.000	0.822	0.012	0.003
Atom#	NSCD ($\mathcal{L}_K\mathcal{B}_K \times 1000$)							
C1	−2.57	235.83	−75.99	148.82	−0.38	139.88	−28.42	51.03
C2	51.02	−318.52	−109.29	201.89	5.74	−139.57	−35.97	56.83
C3	4.71	50.43	−95.07	259.93	0.55	71.24	−40.82	99.75
C4	−0.57	58.04	−67.64	151.45	−0.04	62.88	−29.86	51.19
C5	−3.26	14.97	−37.41	53.91	−0.35	109.02	−11.36	19.72
C6	−4.38	68.22	−80.65	146.64	−0.46	9.62	−34.48	64.00
C7	−40.25	−111.27	−27.46	−71.77	−4.82	−50.78	−131.43	−8.27
C8	4.09	245.35	−41.59	−58.78	0.51	180.70	−112.76	−6.99
C9	2.39	117.22	−76.92	−63.95	0.28	80.70	−183.47	−10.35
C10	3.13	66.04	−14.09	−66.29	0.37	73.77	−98.53	−8.26
C11	0.36	155.70	−58.70	−61.68	0.03	139.55	−151.54	−7.94
C12	−4.79	92.05	−114.41	−80.22	−0.57	106.55	−259.41	−15.13
H1	−0.95	−23.53	85.51	−144.19	−0.09	−11.67	37.87	−47.25
H2	−0.33	226.24	94.42	−179.60	−0.06	161.96	46.65	−63.37
H3	−0.16	40.33	80.73	−176.71	−0.01	23.65	38.31	−56.56
H4	−0.41	−53.08	109.84	−126.35	0.08	−150.61	40.45	−39.59
H5	−1.08	−250.94	53.20	37.11	−0.15	−217.89	124.26	0.76
H6	0.07	−168.79	64.75	61.27	0.00	−135.76	158.23	5.23
H7	0.31	−89.18	70.36	67.57	0.05	−24.17	172.59	7.25
H8	0.62	−127.98	51.92	64.05	0.06	−106.13	146.90	3.96
H9	0.63	46.40	72.67	58.19	0.12	54.28	192.75	3.60
H10	−0.62	92.10	60.08	−103.19	−0.06	89.39	24.90	−36.35

TABLE S6. AZO-2. aug-cc-pwCVDZ.

	RI-CC2				DFT/BH+HLYP			
Atom	ES1	ES2	ES3	ES4	ES1	ES2	ES3	ES4
E (eV)	2.964	3.589	4.437	4.528	3.031	3.657	4.720	4.781
ω (a.u.)	0.109	0.132	0.163	0.166	0.111	0.134	0.173	0.176
f	0.000	0.919	0.028	0.008	0.000	0.894	0.010	0.014
Atom#				NSCD ($\mathcal{L}_K\mathcal{B}_K \times 1000$)				
C1	−3.25	311.97	−12.27	35.86	0.03	197.83	7.09	48.20
C2	86.44	−305.82	136.18	38.27	0.14	−139.39	79.59	42.52
C3	7.74	91.72	344.45	44.08	0.02	89.07	196.44	92.41
C4	−0.94	−122.20	258.29	42.86	0.00	−83.76	146.87	79.42
C5	−6.02	−113.85	−19.57	6.46	0.01	−0.57	3.62	12.37
C6	−8.21	88.08	−11.17	35.24	0.00	−4.20	31.64	69.04
C7	−57.34	−108.88	37.37	−33.59	−0.20	−67.20	42.86	−109.98
C8	5.77	175.98	33.26	−53.22	0.02	143.69	30.86	−101.41
C9	3.46	63.23	31.77	−80.66	0.01	51.04	40.84	−171.49
C10	4.78	6.01	27.28	−19.15	0.01	24.31	30.56	−82.05
C11	0.44	102.04	30.86	−62.77	0.00	110.72	34.21	−137.05
C12	−7.18	49.84	38.67	−136.85	−0.03	74.24	56.38	−251.69
H1	−1.86	−12.39	−36.40	−29.32	0.00	6.37	−35.92	−41.57
H2	−0.39	272.84	−142.58	−28.76	0.00	207.37	−97.35	−43.66
H3	−0.35	115.35	−225.26	−36.09	0.00	86.22	−128.26	−56.74
H4	0.11	−147.41	−32.98	−26.89	0.00	−148.73	−37.49	−18.86
H5	−2.07	−187.65	−40.59	30.71	−0.01	−185.37	−36.05	94.99
H6	0.06	−106.36	−44.88	59.22	0.00	−99.59	−44.49	133.50
H7	0.54	−33.85	−35.67	65.22	0.00	11.87	−39.51	151.34
H8	0.88	−68.78	−41.11	51.13	0.00	−70.38	−43.54	122.62
H9	1.72	79.74	−36.84	55.91	0.00	83.95	−49.55	160.50
H10	−0.83	90.06	−42.85	−15.92	0.04	115.47	−38.07	−27.91
H11	−0.99	115.40	−66.82	−26.12	0.00	110.54	−40.90	−26.91

TABLE S7. AZO-3. aug-cc-pwCVDZ.

	RI-CC2						DFT/BH+HLYP					
	ES1	ES2	ES3	ES4	ES5	ES6	ES1	ES2	ES3	ES4	ES5	ES6
E (eV)	2.866	3.339	3.854	4.352	4.430	4.441	2.956	3.426	4.155	4.535	4.587	4.607
ω (a.u.)	0.105	0.123	0.142	0.160	0.163	0.163	0.109	0.126	0.153	0.167	0.169	0.169
f	0.000	1.043	0.000	0.004	0.011	0.000	0.000	1.067	0.000	0.017	0.000	0.000
Atom#	NSCD ($\mathcal{L}_K\mathcal{B}_K \times 1000$)											
C1	1.30	323.72	0.00	−30.64	81.12	−45.71	12.14	227.75	0.02	−63.31	−7.78	60.06
C2	−33.90	−144.08	0.00	−15.02	51.61	1.14	−208.71	73.98	−0.08	−84.01	6.27	76.33
C3	−2.86	206.39	0.00	51.90	59.84	−0.34	−17.52	204.19	0.00	−85.72	1.51	89.77
C4	0.30	−20.31	0.00	27.55	41.48	2.66	1.06	7.16	0.01	−66.63	0.49	62.80
C5	2.42	−35.48	0.00	−4.47	−5.95	6.57	13.10	62.80	0.00	−8.02	3.50	8.69
C6	3.31	129.92	0.00	−36.96	41.22	1.18	19.82	53.57	0.02	−64.70	−3.61	67.29
C7	18.66	−16.36	0.00	25.58	94.16	28.11	118.68	51.32	0.03	22.71	20.17	2.30
C8	−2.02	204.87	0.00	39.29	−631.14	663.89	−13.38	229.81	0.17	−202.03	127.96	17.57
C9	−1.08	125.98	0.00	−0.36	2454.17	−2372.76	−5.79	189.49	0.11	463.36	−379.53	−98.41
C10	−2.25	−242.08	0.00	−40.75	120.38	−781.70	−13.69	−205.94	−0.02	18.89	−430.57	11.68
C11	−0.10	146.01	0.00	22.90	2235.44	−2184.57	−0.62	210.13	−0.18	564.01	−559.69	−59.05
C12	2.62	146.28	0.00	6.46	−231.58	240.60	16.44	205.83	−0.15	−189.23	61.01	0.41
H1	0.70	−45.34	0.00	20.17	−40.92	−2.44	4.01	−40.30	0.00	62.84	−0.48	−59.26
H2	−0.09	201.63	0.00	−14.17	−47.84	6.35	0.46	119.59	0.00	71.63	−0.03	−73.13
H3	0.11	31.83	0.00	−25.53	−47.51	0.13	0.56	12.98	0.00	65.12	0.14	−63.44
H4	−0.03	−157.05	0.00	17.57	−41.05	−3.43	−0.92	−166.58	0.00	57.35	−1.76	−52.31
H5	1.09	−154.32	0.00	−17.05	100.84	−149.35	6.83	−205.99	−0.03	72.00	−23.31	−13.73
H6	0.02	−47.26	0.00	−6.84	−44.14	5.22	0.11	−70.79	0.06	76.85	−2.80	−1.00
H7	−0.27	−38.52	0.00	−20.10	77.96	−111.16	−1.21	−73.38	−0.04	92.02	−5.32	−7.92
H8	−0.68	38.42	0.00	−3.78	59.43	−105.90	−7.39	−0.62	0.03	107.38	−32.83	−8.72
H9	0.39	40.37	0.00	6.39	−25.17	0.44	1.56	61.49	0.00	33.69	0.23	−34.68
H10	0.32	57.99	0.00	−1.99	−24.85	0.17	1.84	59.33	0.00	36.11	−0.07	−35.02

TABLE S8. AZO-3. Excited state 2. COSMO-RI-CC2/aug-cc-pVDZ.

	DMSO	C_6H_{12}	$CHCl_3$
E (eV)	2.918	3.110	3.019
ω (a.u.)	0.107	0.114	0.111
f	1.134	1.134	1.134
Atom#		NSCD ($\mathcal{L}_K\mathcal{B}_K$ values)	
C1	350.02	392.98	388.71
C2	1,752.74	-41.93	98.17
C3	429.66	278.82	304.37
C4	42.04	25.32	44.30
C5	-46.51	31.86	54.86
C6	9.34	179.03	176.89
C7	-610.94	-32.52	-69.60
C8	278.74	227.72	223.27
C9	177.03	151.74	149.31
C10	-67.72	-176.31	-159.86
C11	163.43	171.20	167.29
C12	35.00	146.38	132.83
H1	-137.25	-80.72	-91.58
H2	173.76	201.58	191.73
H3	-62.10	-22.35	-37.87
H4	-247.00	-223.36	-230.24
H5	-224.79	-177.28	-176.97
H6	-23.25	-34.73	-28.56
H7	3.88	-16.65	-9.50
H8	123.77	53.29	59.35
H9	-28.95	15.68	2.29
H10	-15.58	32.91	17.61

S4. NATURAL TRANSITION ORBITALS

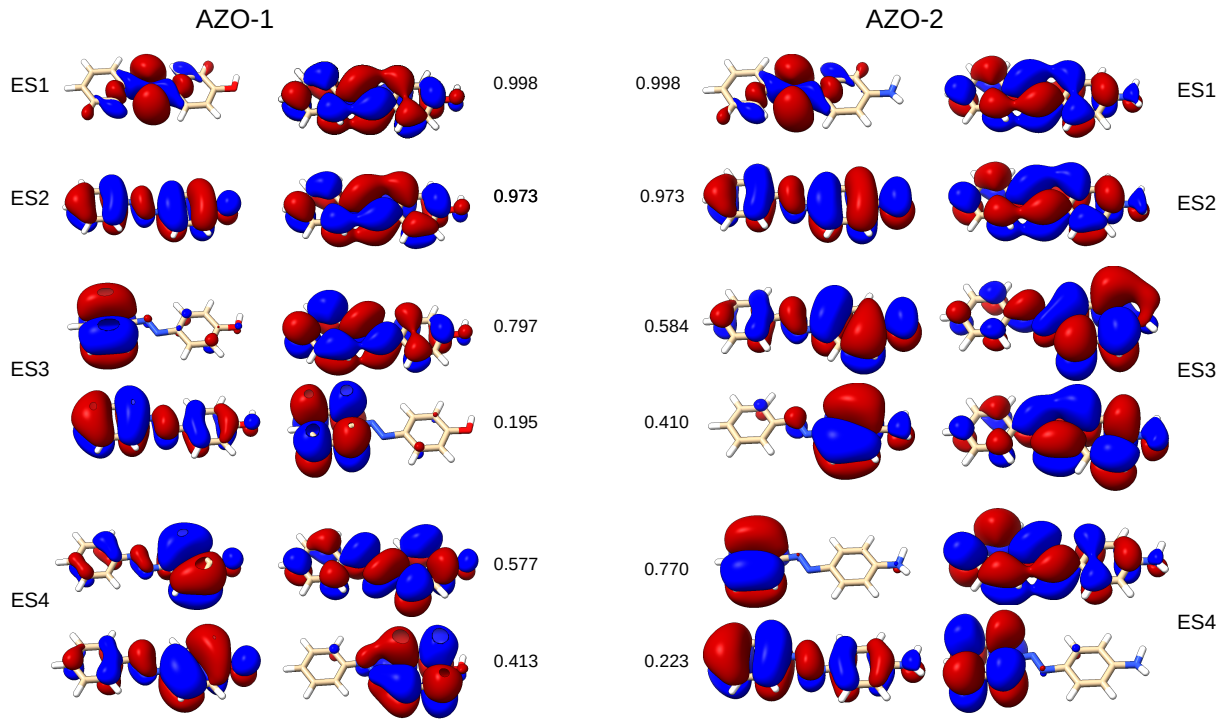

FIG. S1. RI-CC2/aug-cc-pwCVDZ. Natural transition orbitals for the first four electronic transitions of AZO-1 (left) and AZO-2 (right). Isosurface value 0.015.

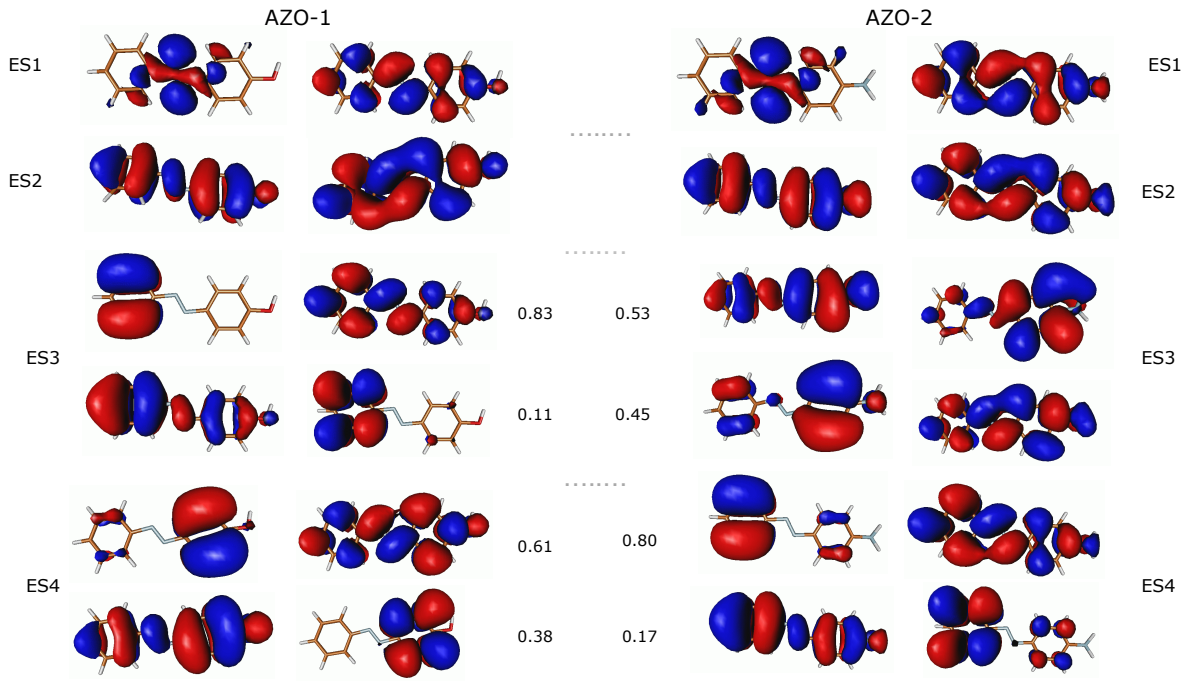

FIG. S2. TD-DFT/BH+HLYP/aug-cc-pwCVDZ. Natural transition orbitals for the first four electronic transitions of AZO-1 (left) and AZO-2 (right). Isosurface value 0.015.

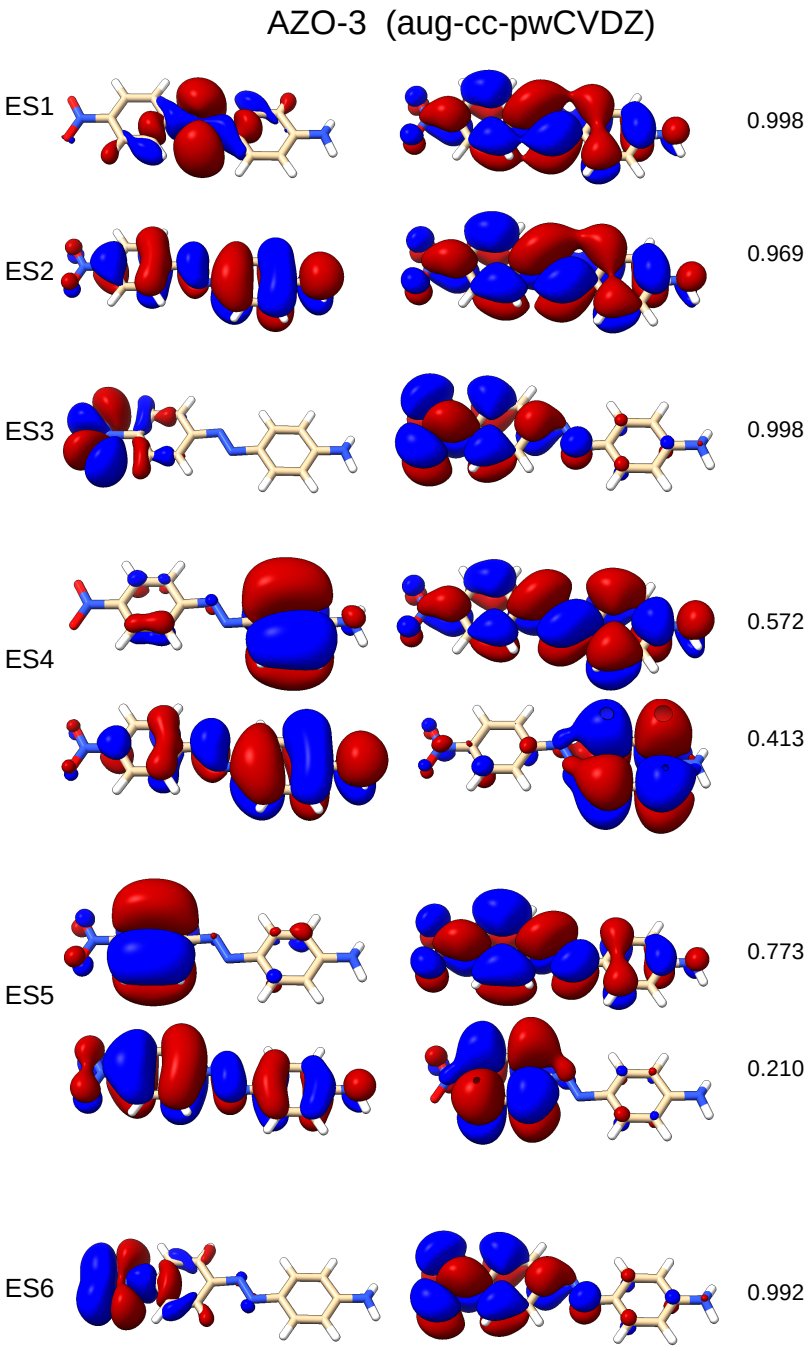

FIG. S3. RI-CC2/aug-cc-pwCVDZ. Natural transition orbitals for the first six electronic transitions of AZO-3. Isosurface value 0.015.

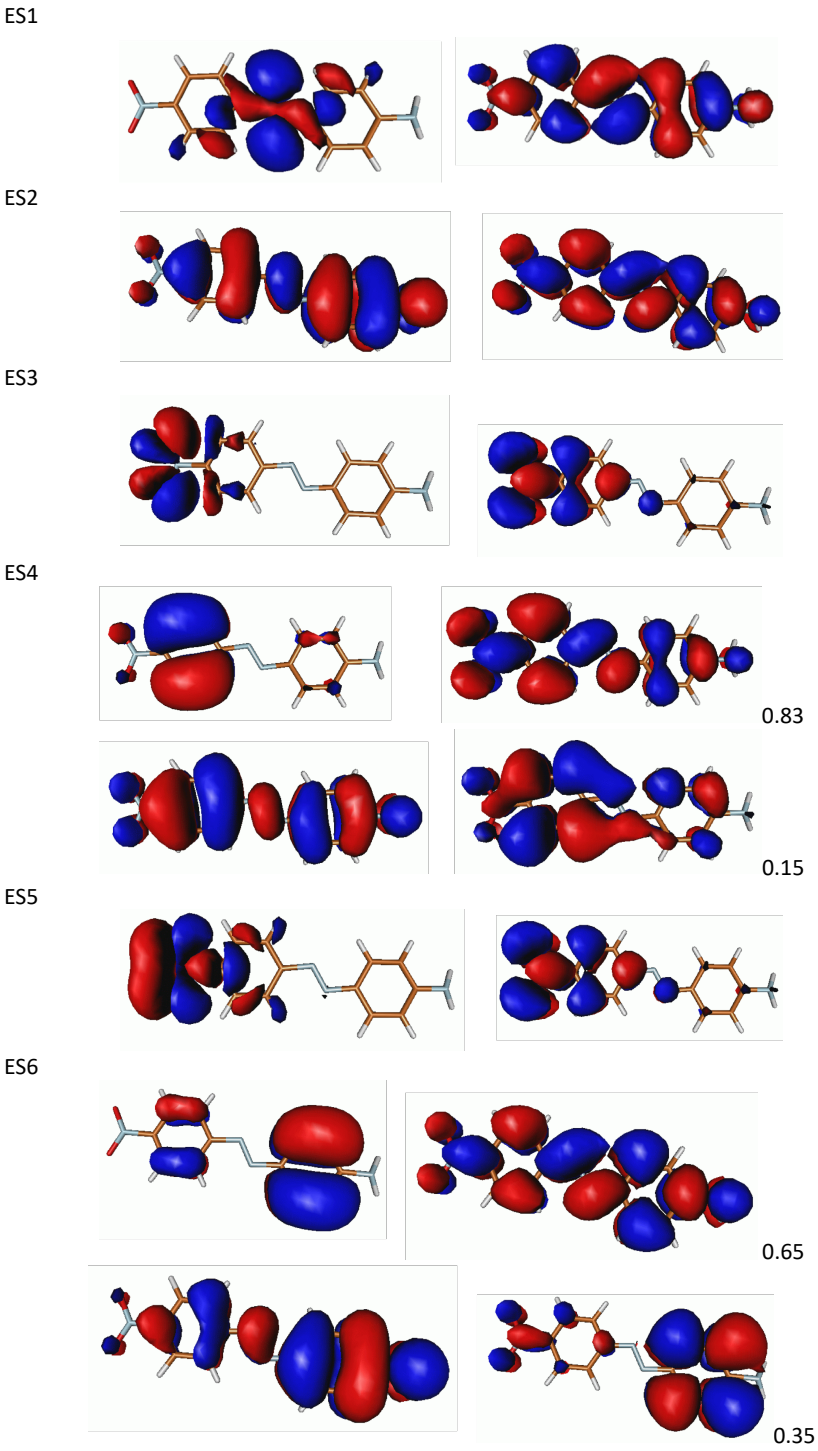

FIG. S4. TD-DFT/BH+HLYP/aug-cc-pwCVDZ. Natural transition orbitals for the first six electronic transitions of AZO-3. Isosurface value 0.015.

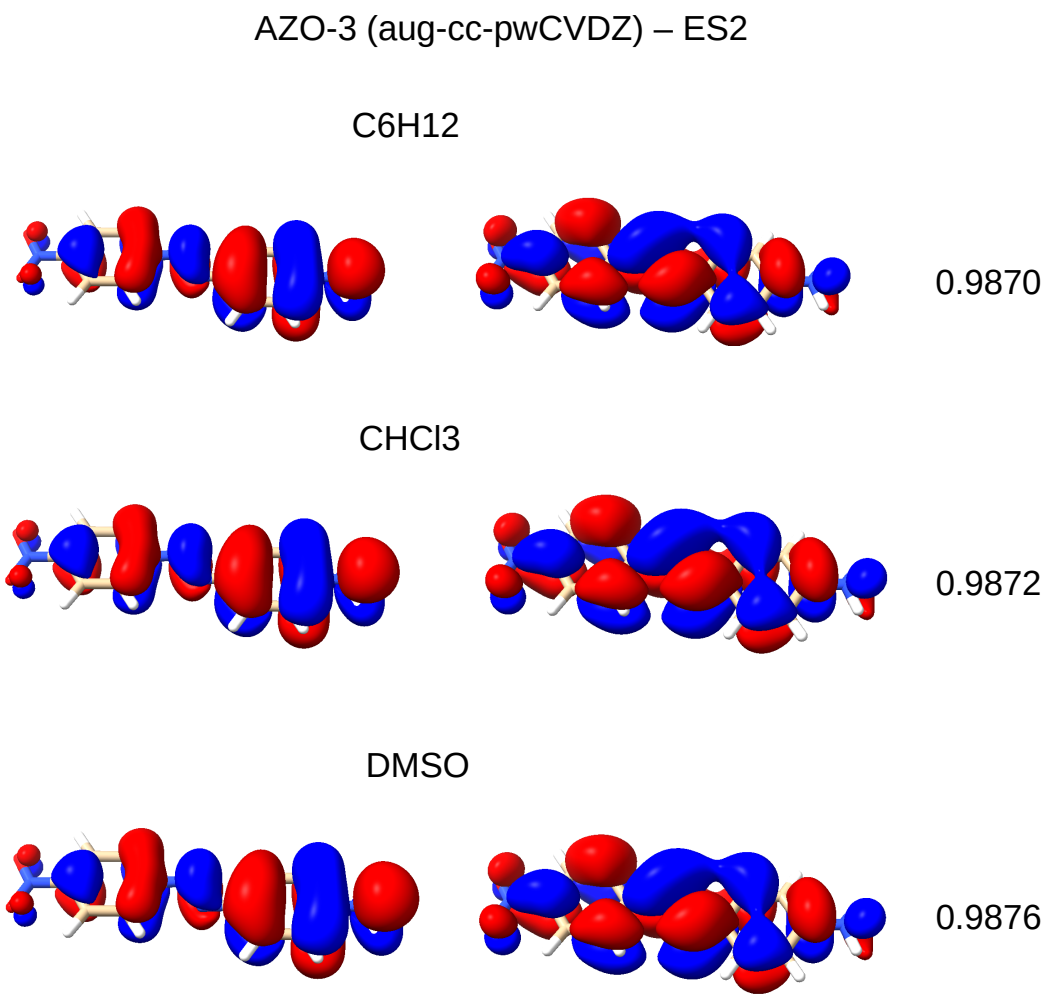

FIG. S5. COSMO-CC2/aug-cc-pwCVDZ. Natural transition orbitals for the second electronic transitions of AZO-3. Isosurface value 0.015.

S5. SUM-OVER-STATES ANALYSIS

The CC sum-over-states expression for the $\mathcal{B}_K$ term is

$$\mathcal{B}_K \propto -\frac{1}{2}\epsilon_{\alpha\beta\gamma}\left[\left\{\sum_{k\neq m}\frac{\langle 0|\hat{\mu}_\alpha|k\rangle\langle k|\hat{h}^{\mathrm{pso}}_\gamma|m\rangle}{E_m-E_k}-\sum_{k\neq 0}\frac{\langle 0|\hat{h}^{\mathrm{pso}}_\gamma|k\rangle\langle k|\hat{\mu}_\alpha|m\rangle}{E_k-E_0}\right\}\langle m|\hat{\mu}_\beta|0\rangle \right. \tag{S2}$$

$$\left. -\langle 0|\hat{\mu}_\beta|m\rangle\left\{\sum_{k\neq m}\frac{\langle m|\hat{h}^{\mathrm{pso}}_\gamma|k\rangle\langle k|\hat{\mu}_\alpha|0\rangle}{E_m-E_k}-\sum_{k\neq 0}\frac{\langle m|\hat{\mu}_\alpha|k\rangle\langle k|\hat{h}^{\mathrm{pso}}_\gamma|0\rangle}{E_k-E_0}\right\}\right] . \tag{S3}$$

We split the SOS expression into dispersive and absorptive components[3]

$$\mathcal{B}_{K,d} = -\frac{1}{2}\epsilon_{\alpha\beta\gamma}\sum_{k\neq m}\left\{\frac{\langle 0|\hat{\mu}_\alpha|k\rangle\langle k|\hat{h}^{\mathrm{pso}}_\gamma|m\rangle}{E_m-E_k}\langle m|\hat{\mu}_\beta|0\rangle-\langle 0|\hat{\mu}_\beta|m\rangle\frac{\langle m|\hat{h}^{\mathrm{pso}}_\gamma|k\rangle\langle k|\hat{\mu}_\alpha|0\rangle}{E_m-E_k}\right\} \tag{S4}$$

$$\mathcal{B}_{K,a} = -\frac{1}{2}\epsilon_{\alpha\beta\gamma}\sum_{k\neq 0}\left\{\frac{\langle 0|\hat{h}^{\mathrm{pso}}_\gamma|k\rangle\langle k|\hat{\mu}_\alpha|m\rangle}{E_k-E_0}\langle m|\hat{\mu}_\beta|0\rangle-\langle 0|\hat{\mu}_\beta|m\rangle\frac{\langle m|\hat{\mu}_\alpha|k\rangle\langle k|\hat{h}^{\mathrm{pso}}_\gamma|0\rangle}{E_k-E_0}\right\} . \tag{S5}$$

The atoms selected for the SOS study are C2, C5, C9, and C12. The number of states included in the sum is twice the number of states under investigation (as specified in captions). Tables S9, S10, and S11 show the exact (analytic) and SOS NSCD values for AZO-1, AZO-2 and AZO-3, respectively. The values of the $\mathcal{B}_{K,d}$ and $\mathcal{B}_{K,a}$ terms are plotted separately as bar plots in Figures S6 (AZO-1), S7 (AZO-2), and S8 (AZO-3). Note that the numbers are scaled by 1000 but not multiplied by the unit prefactor $\mathcal{L}_C$.

AZO-1

TABLE S9. AZO-1. RI-CC2/aug-cc-pwCVDZ. Exact and sum-over-states ($n_k = 8$) $\mathcal{B}_K \times 1000$ of C2, C5, C9, and C12..

	ES#	1	2	3	4
C2	Exact	38.87	−242.66	−83.27	153.81
	SOS	34.01	−105.17	−79.82	145.61
C5	Exact	−4.59	−86.73	−14.91	4.92
	SOS	−2.59	6.66	−31.07	70.40
C9	Exact	1.82	89.31	−58.60	−48.72
	SOS	1.54	118.68	−22.22	−47.46
C12	Exact	−3.65	70.13	−87.17	−61.12
	SOS	−2.76	90.44	−18.83	−47.06

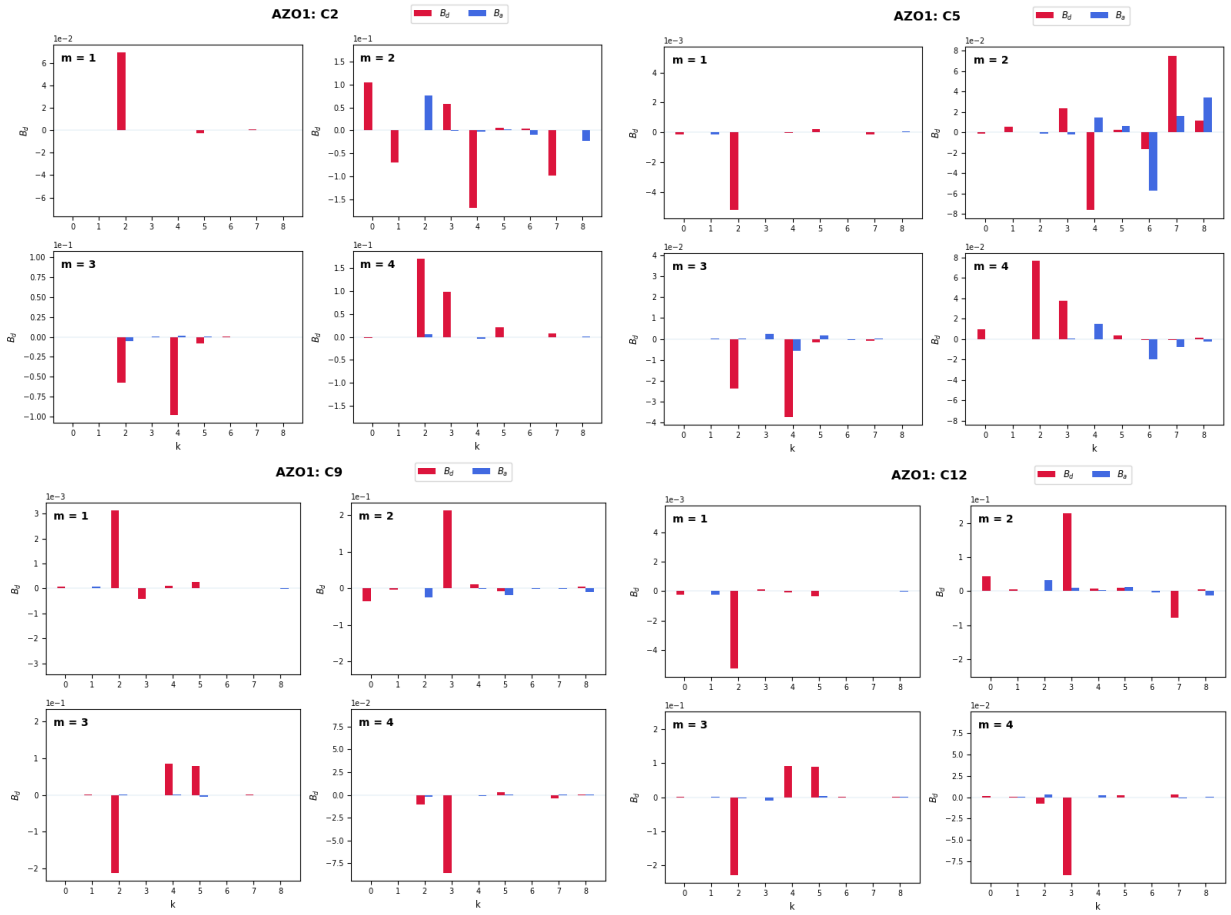

FIG. S6. AZO-1. RI-CC2/aug-cc-pwCVDZ. Bar plots of $\mathcal{B}_{C,d}(k \to m)$ (red) and $\mathcal{B}_{C,a}(k \to m)$ (blue) of C2, C5, C9, and C12 for the four lowest excited states. Number of intermediate states $n_k = 8$. Note the offset of the y-values given above the axes.

AZO-2

TABLE S10. AZO-2. RI-CC2/aug-cc-pwCVDZ. Exact and sum-over-states ($n_k = 8$) $\mathcal{B}_K \times 1000$ of C2, C5, C9, and C12.

	ES#	1	2	3	4
C2	Exact	65.86	−232.98	103.75	29.15
	SOS	59.74	−107.89	99.82	33.12
C5	Exact	−4.59	−86.73	−14.91	4.92
	SOS	−4.84	−86.67	23.05	11.15
C9	Exact	2.63	48.17	24.20	−61.45
	SOS	2.24	70.27	22.26	−24.55
C12	Exact	−5.47	37.97	29.46	−104.26
	SOS	−4.34	52.19	27.21	−23.12

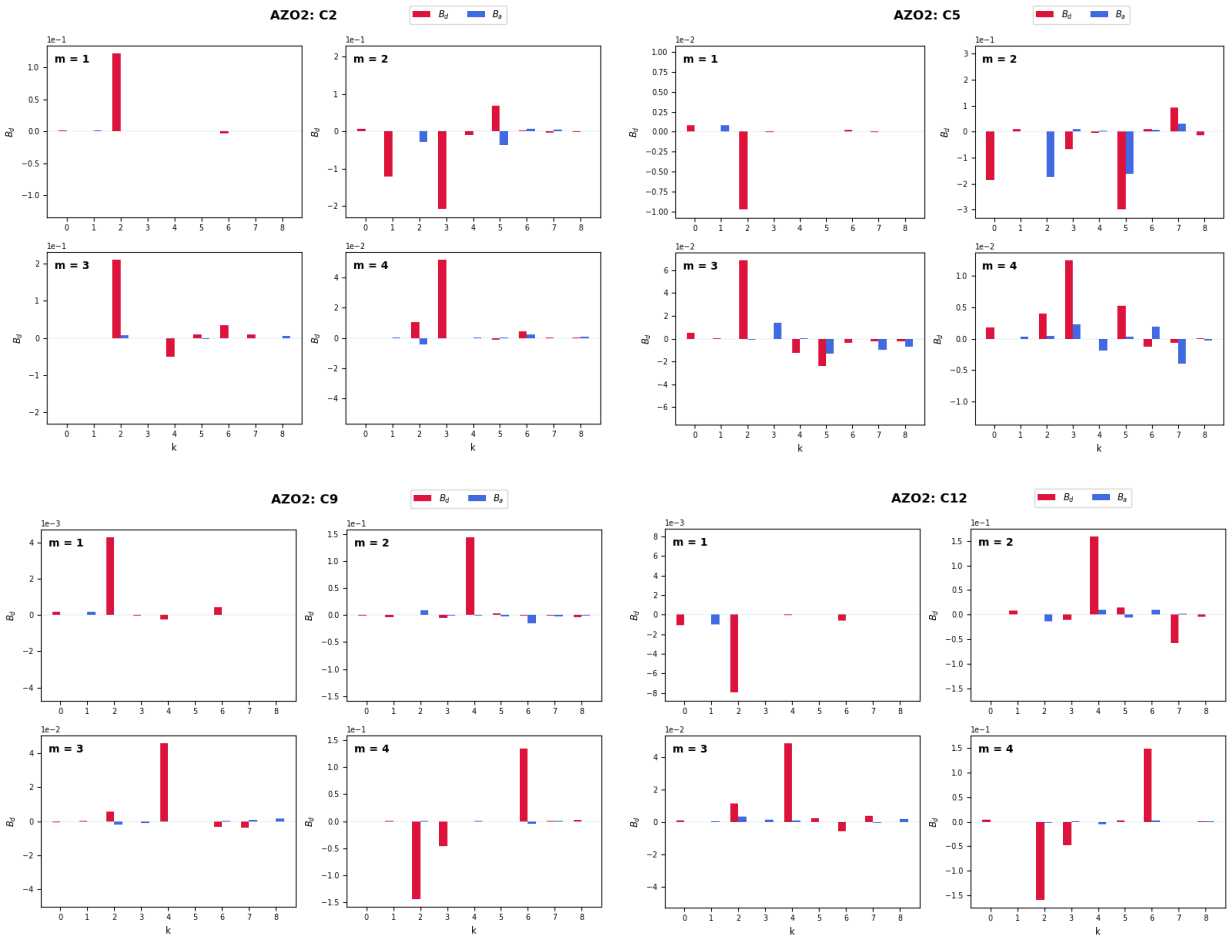

FIG. S7. AZO-2. RI-CC2/aug-cc-pwCVDZ. Bar plots of $\mathcal{B}_{C,d}(k \to m)$ (red) and $\mathcal{B}_{C,a}(k \to m)$ (blue) of C2, C5, C9, and C12 for the four lowest excited states. Number of intermediate states $n_k = 8$. Note the offset of the y-values given above the axes.

AZO-3

TABLE S11. AZO-3. RI-CC2/aug-cc-pwCVDZ. Exact and sum-over-states ($n_k = 12$) $\mathcal{B}_K \times 1000$ of C2, C5, C9, and C12.

	ES#	1	2	3	4	5	6
C2	Exact	−25.83	−109.76	0.00	−11.44	39.32	0.87
	SOS	−24.75	27.09	−0.00	−19.13	40.90	−11.71
C5	Exact	2.85	−27.03	0.00	−3.41	−4.54	5.01
	SOS	1.86	−53.28	0.00	−2.08	6.17	4.88
C9	Exact	−0.82	95.97	0.00	−0.28	1869.70	−1807.68
	SOS	−1.06	107.66	0.00	−0.15	1920.39	−1844.30
C12	Exact	1.99	111.45	0.00	4.92	−176.43	183.30
	SOS	1.62	107.98	0.00	6.06	−100.84	170.87

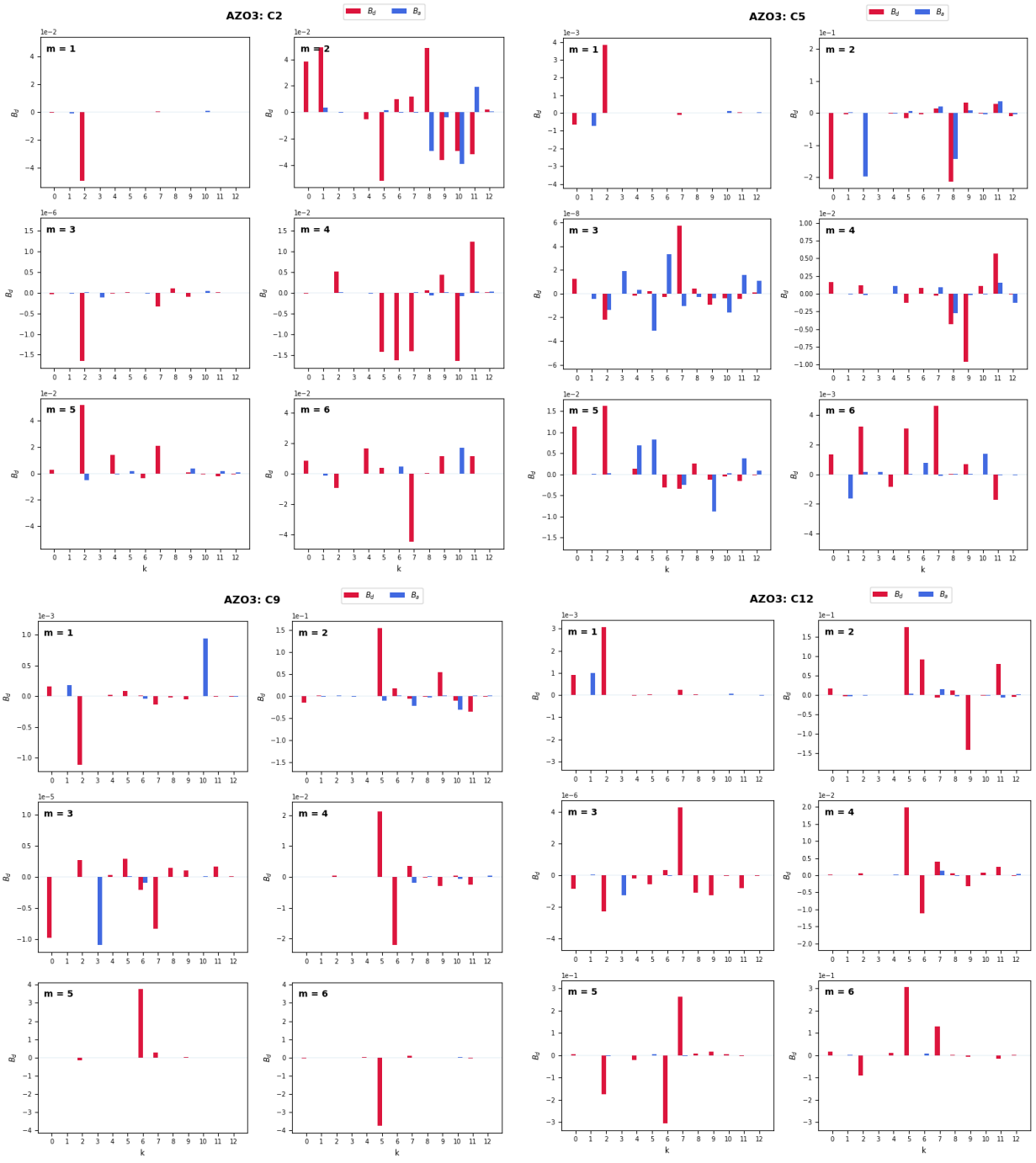

FIG. S8. AZO-3. RI-CC2/aug-cc-pwCVDZ. Bar plots of $\mathcal{B}_{C,d}(k \to m)$ (red) and $\mathcal{B}_{C,a}(k \to m)$ (blue) of C2, C5, C9, and C12 for the six lowest excited states. Number of intermediate states $n_k = 12$. Note the offset of the y-values given above the axes.

S6. CARTESIAN COORDINATES

The coordinates are provided in Angstrom and `.xyz` format.

AZO-1

```
C     1.0357887   -2.0353758    0.0006766
C    -0.2565927   -1.4965821    0.0002726
C    -1.3626410   -2.3515573   -0.0003573
C    -1.1934234   -3.7282563   -0.0005237
C     0.0947305   -4.2615577   -0.0002036
C     1.2055258   -3.4107999    0.0004448
N    -0.5548141   -0.1172454    0.0003184
N     0.4705064    0.6310168    0.0004193
C     0.1659645    2.0145128    0.0003292
C    -1.1304066    2.5443198    0.0006897
C    -1.3020669    3.9220753    0.0003706
C    -0.1953763    4.7755535   -0.0002874
C     1.0931160    4.2454362   -0.0006321
C     1.2732546    2.8658121   -0.0002831
O     0.2118701   -5.6195230   -0.0005667
H     2.2035091   -3.8333257    0.0007386
H     1.8852879   -1.3687292    0.0011038
H    -2.0390292   -4.4008634   -0.0008599
H    -2.3508346   -1.9127315   -0.0008502
H     2.2600432    2.4235006   -0.0005380
H     1.9512518    4.9031105   -0.0012208
H    -0.3401306    5.8472298   -0.0005037
H    -2.3008539    4.3370765    0.0005835
H    -1.9734575    1.8697411    0.0011645
H     1.1487778   -5.8428373   -0.0002853
```

AZO-2

```
C     1.0527302    0.0325583    1.8403427
C    -0.2366122    0.0222357    1.2903279
C    -1.3445158    0.0230522    2.1420936
C    -1.1777059    0.0341979    3.5187191
C     0.1060409    0.0479658    4.0764812
C     1.2149219    0.0428400    3.2141678
N    -0.5282765    0.0124603   -0.0870202
N     0.4996235    0.0111704   -0.8339255
C     0.1964631    0.0015885   -2.2174378
C    -1.0991601    0.0010802   -2.7494077
```

C	-1.2697246	-0.0084430	-4.1273553
C	-0.1624559	-0.0176988	-4.9799709
C	1.1254203	-0.0171661	-4.4482717
C	1.3040921	-0.0072797	-3.0684584
N	0.2859971	-0.0071984	5.4555693
H	2.2117720	0.0455223	3.6379429
H	1.9068110	0.0325888	1.1793613
H	-2.0421990	0.0306114	4.1704887
H	-2.3318231	0.0156988	1.7007928
H	2.2905099	-0.0065954	-2.6252640
H	1.9843511	-0.0243526	-5.1049532
H	-0.3061530	-0.0252178	-6.0517891
H	-2.2682373	-0.0087672	-4.5431717
H	-1.9426921	0.0081521	-2.0754755
H	1.1626942	0.3725353	5.7753286
H	-0.4872619	0.3551849	5.9901982

AZO-3

C	1.0578959	0.0033142	1.8459808
C	-0.2289174	-0.0045857	1.2885601
C	-1.3429169	-0.0137353	2.1333649
C	-1.1843443	-0.0151715	3.5101324
C	0.0965083	-0.0106374	4.0760544
C	1.2112028	0.0026930	3.2199706
C	0.2077954	0.0017575	-2.2148239
C	-1.0907427	-0.0082698	-2.7401938
C	-1.2798329	-0.0086591	-4.1138518
C	-0.1623482	0.0012050	-4.9442103
C	1.1349826	0.0115116	-4.4502403
C	1.3107029	0.0116291	-3.0720006
H	2.2052834	0.0140889	3.6498178
H	1.9170276	0.0097096	1.1915797
H	-2.0528152	-0.0183976	4.1564187
H	-2.3275405	-0.0205797	1.6862017
H	2.3000522	0.0194317	-2.6364233
H	1.9684946	0.0191423	-5.1346279
H	-2.2657581	-0.0162560	-4.5516676
H	-1.9304564	-0.0155677	-2.0619480
H	1.1493368	-0.2992726	5.7863350
H	-0.5064157	-0.2993101	5.9919319
N	-0.5127848	-0.0056434	-0.0869416
N	0.5161518	0.0027739	-0.8321503
N	0.2672165	0.0535821	5.4522322
N	-0.3640701	0.0006728	-6.3995285
O	-1.5219277	-0.0111654	-6.8107910

```
O      0.6381130     0.0120177    -7.1103172
```

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