Supplementary Material

Thiourea organocatalysts as emerging chiral pollutants: en route to porphyrin-based (chir)optical sensing

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Contents

1. Spectroscopic UV-Vis titrations and CD spectra

The details of UV-Vis spectroscopic titrations and characterization of UV-Vis and CD spectra for the complexes of zinc porphyrins **P1**–**P9** and thioureas **1a**–**d**. Complexation of **1a**–**c** with ZnTPP (**P3**) has been previously described [1].

Spectroscopic data of system **1a** + **P1**

Table S1. Absorptions (AU) of **P1** (2.0×10^{-6} M) derived from the UV-Vis titration of **P1** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 419.4 nm	AU 430.4 nm	$C_{\mathbf{1a}}$, M
1	1.086	0.167	0,00
2	1.063	0.188	$3.02\cdot10^{-5}$
3	1.046	0.213	$6.02\cdot10^{-5}$
4	1.024	0.230	$9.02\cdot10^{-5}$
5	1.005	0.252	$1.20\cdot10^{-4}$
6	0.968	0.283	$1.80\cdot10^{-4}$
7	0.933	0.326	$2.39\cdot10^{-4}$
8	0.898	0.363	$2.98\cdot10^{-4}$
9	0.867	0.395	$3.57\cdot10^{-4}$
10	0.835	0.431	$4.16\cdot10^{-4}$
11	0.807	0.459	$4.74\cdot10^{-4}$
12	0.780	0.486	$5.32\cdot10^{-4}$
13	0.759	0.511	$5.90\cdot10^{-4}$
14	0.736	0.534	$6.47\cdot10^{-4}$
15	0.724	0.547	$7.04\cdot10^{-4}$

16	0.700	0.574	$7.61 \cdot 10^{-4}$
17	0.680	0.594	$8.18 \cdot 10^{-4}$
18	0.663	0.612	$8.74 \cdot 10^{-4}$
19	0.648	0.628	$9.31 \cdot 10^{-4}$
20	0.618	0.661	$1.04 \cdot 10^{-3}$
21	0.593	0.689	$1.15 \cdot 10^{-3}$
22	0.563	0.721	$1.32 \cdot 10^{-3}$
23	0.535	0.753	$1.48 \cdot 10^{-3}$
24	0.504	0.786	$1.69 \cdot 10^{-3}$
25	0.480	0.814	$1.90 \cdot 10^{-3}$
26	0.459	0.838	$2.10 \cdot 10^{-3}$
27	0.439	0.861	$2.31 \cdot 10^{-3}$
28	0.412	0.893	$2.70 \cdot 10^{-3}$
29	0.381	0.926	$3.26 \cdot 10^{-3}$
30	0.357	0.958	$3.89 \cdot 10^{-3}$
31	0.334	0.988	$4.64 \cdot 10^{-3}$
32	0.319	1.007	$5.34 \cdot 10^{-3}$
33	0.307	1.024	$5.99 \cdot 10^{-3}$
34	0.299	1.037	$6.61 \cdot 10^{-3}$
35	0.293	1.047	$7.18 \cdot 10^{-3}$
36	0.287	1.060	$7.72 \cdot 10^{-3}$
37	0.898	0.363	$7.72 \cdot 10^{-3}$

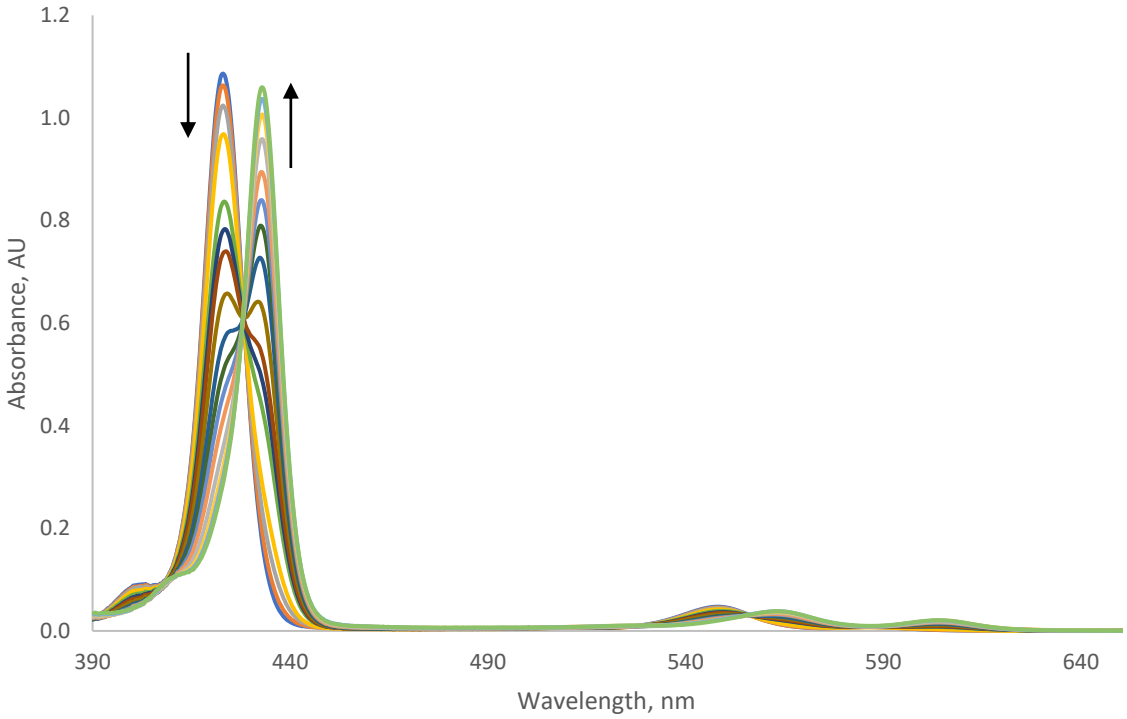


Figure S1. Changes in UV-Vis spectrum of **P1** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$7.72\cdot10^{-3}$ M).

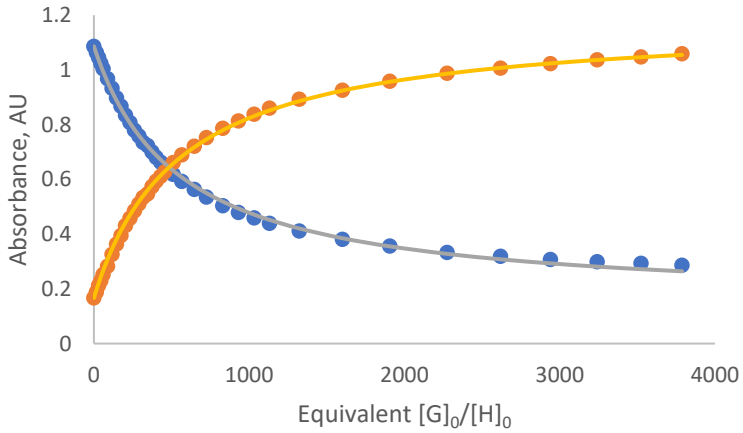


Figure S2. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P1** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P1** host. Blue points – absorption at 419.4 nm, orange points – absorption at 430.4 nm.

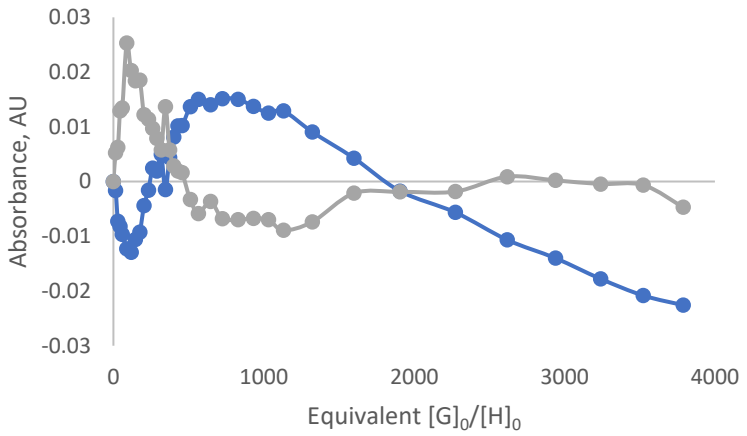


Figure S3. Residual analysis of UV-Vis titration between **P1** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P1** host. Blue points – absorption at 419.4 nm, grey points – absorption at 430.4 nm.

K_a (**1a** + **P1**) = (9.0 ± 0.1) × 10^2 M^{-1}

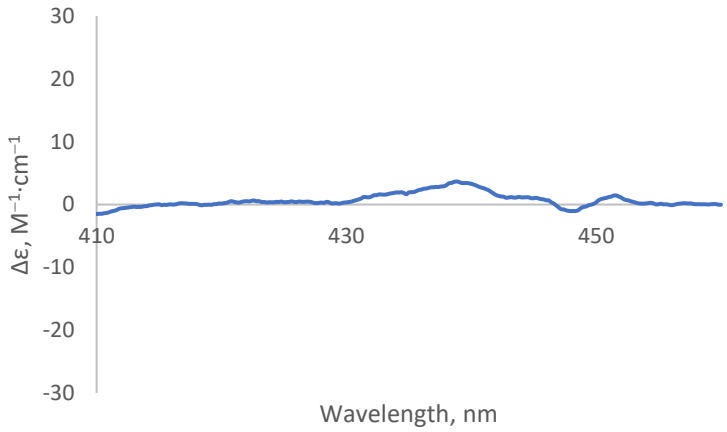


Figure S4. Experimental CD spectrum generated by mixing **P1** ($2.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($7.6 \cdot 10^{-3}$ M), 91% conversion to complex.

Spectroscopic data of system **1a** + **P2**

Table S2. Absorptions (AU) of **P2** (2.0×10^{-6} M) derived from the UV-Vis titration of **P2** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 422.6 nm	AU 432.4 nm	$C_{\mathbf{1a}}$, M
1	1.110	0.160	0.00
2	1.025	0.250	$5.34E{\cdot}10^{-5}$
3	0.953	0.328	$1.07{\cdot}10^{-4}$
4	0.888	0.395	$1.60{\cdot}10^{-4}$
5	0.835	0.452	$2.12{\cdot}10^{-4}$
6	0.790	0.498	$2.65{\cdot}10^{-4}$
7	0.751	0.540	$3.17{\cdot}10^{-4}$
8	0.717	0.578	$3.69{\cdot}10^{-4}$
9	0.685	0.608	$4.20{\cdot}10^{-4}$
10	0.658	0.635	$4.72{\cdot}10^{-4}$
11	0.634	0.659	$5.23{\cdot}10^{-4}$
12	0.611	0.680	$5.74{\cdot}10^{-4}$
13	0.591	0.701	$6.25{\cdot}10^{-4}$
14	0.574	0.720	$6.75{\cdot}10^{-4}$
15	0.556	0.739	$7.26{\cdot}10^{-4}$
16	0.541	0.754	$7.76{\cdot}10^{-4}$
17	0.528	0.765	$8.25{\cdot}10^{-4}$
18	0.504	0.790	$9.24{\cdot}10^{-4}$
19	0.483	0.809	$1.02{\cdot}10^{-3}$

20	0.465	0.830	$1.12 \cdot 10^{-3}$
21	0.443	0.854	$1.26 \cdot 10^{-3}$
22	0.420	0.879	$1.45 \cdot 10^{-3}$
23	0.399	0.901	$1.64 \cdot 10^{-3}$
24	0.376	0.927	$1.91 \cdot 10^{-3}$
25	0.353	0.953	$2.26 \cdot 10^{-3}$
26	0.335	0.973	$2.65 \cdot 10^{-3}$
27	0.319	0.992	$3.05 \cdot 10^{-3}$
28	0.308	1.005	$3.45 \cdot 10^{-3}$
29	0.299	1.017	$3.82 \cdot 10^{-3}$
30	0.292	1.027	$4.19 \cdot 10^{-3}$
31	0.284	1.042	$4.80 \cdot 10^{-3}$

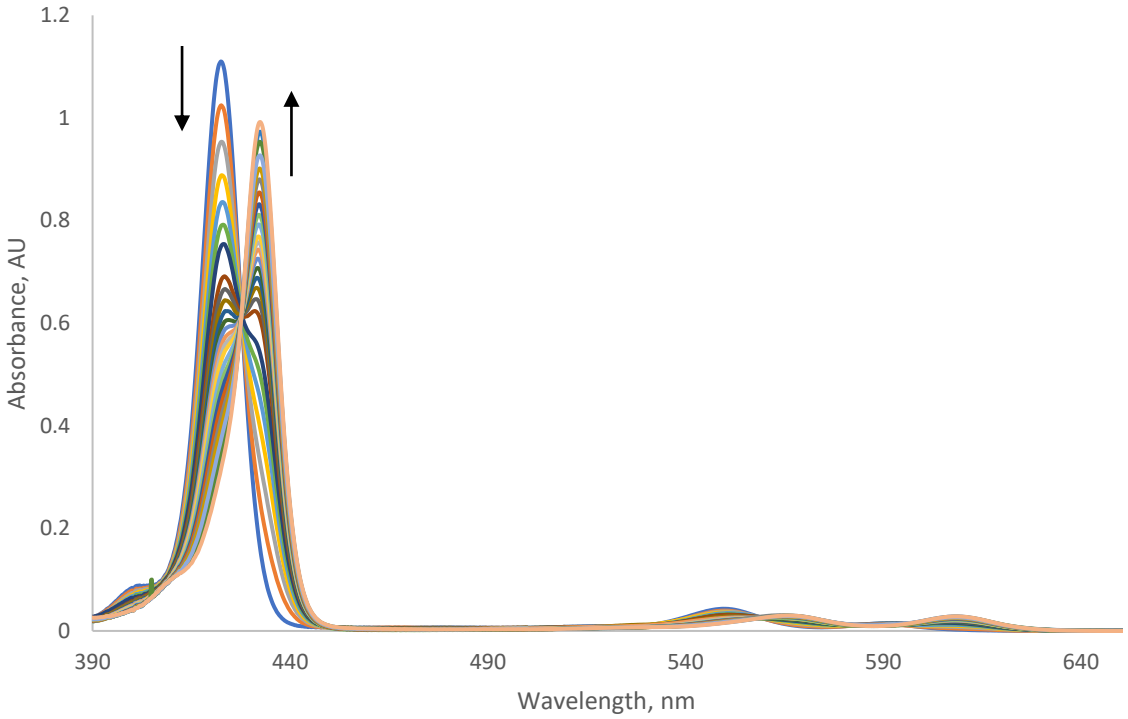


Figure S5. Changes in UV-Vis spectrum of **P2** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$4.80\cdot10^{-3}$ M).

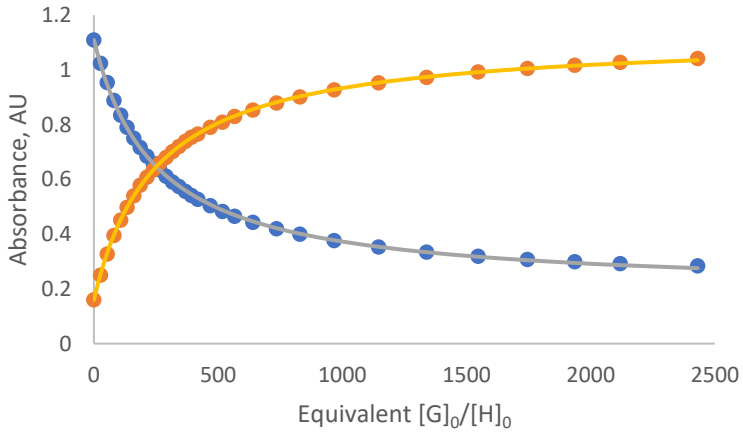


Figure S6. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P2** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P2** host. Blue points – absorption at 422.6 nm, orange points – absorption at 432.4 nm.

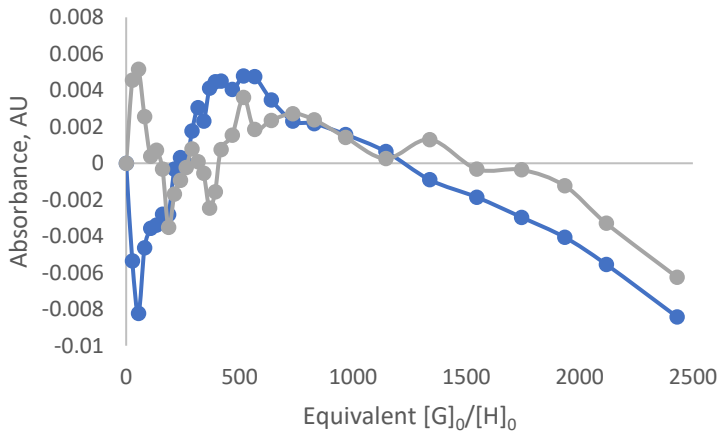


Figure S7. Residual analysis of UV-Vis titration between **P2** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P2** host. Blue points – absorption at 422.6 nm, grey points – absorption at 432.4 nm.

K_a (**1a** + **P2**) = (2.05 ± 0.01) × 10^3 M^{-1}

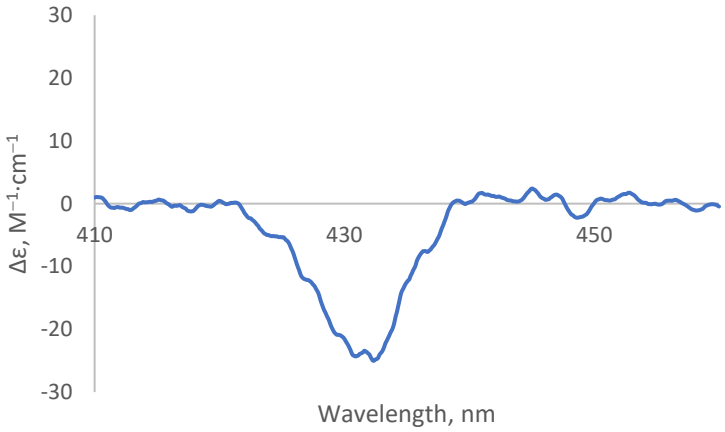


Figure S8. Experimental CD spectrum generated by mixing **P2** ($2.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($4.8 \cdot 10^{-3}$ M), 91% conversion to complex.

Spectroscopic data of system **1a** + **P4**

Table S3. Absorptions (AU) of **P4** (2.2×10^{-6} M) derived from the UV-Vis titration of **P4** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 418.0 nm	AU 428.6 nm	C_{1a}, M
1	1.080	0.090	0.00
2	0.847	0.336	$1.20\cdot10^{-4}$
3	0.781	0.403	$1.79\cdot10^{-4}$
4	0.704	0.479	$2.38\cdot10^{-4}$
5	0.647	0.541	$2.97\cdot10^{-4}$
6	0.592	0.585	$3.55\cdot10^{-4}$
7	0.561	0.627	$4.14\cdot10^{-4}$
8	0.533	0.657	$4.72\cdot10^{-4}$
9	0.507	0.684	$5.29\cdot10^{-4}$
10	0.485	0.705	$5.87\cdot10^{-4}$
11	0.467	0.724	$6.44\cdot10^{-4}$
12	0.450	0.741	$7.01\cdot10^{-4}$
13	0.436	0.754	$7.58\cdot10^{-4}$
14	0.424	0.766	$8.14\cdot10^{-4}$
15	0.413	0.778	$8.70\cdot10^{-4}$
16	0.395	0.796	$9.82\cdot10^{-4}$
17	0.380	0.811	$1.09\cdot10^{-3}$
18	0.359	0.834	$1.31\cdot10^{-3}$
19	0.336	0.859	$1.63\cdot10^{-3}$

20	0.317	0.883	$2.04 \cdot 10^{-3}$
21	0.304	0.900	$2.49 \cdot 10^{-3}$
22	0.290	0.922	$3.34 \cdot 10^{-3}$
23	0.280	0.925	$4.12 \cdot 10^{-3}$

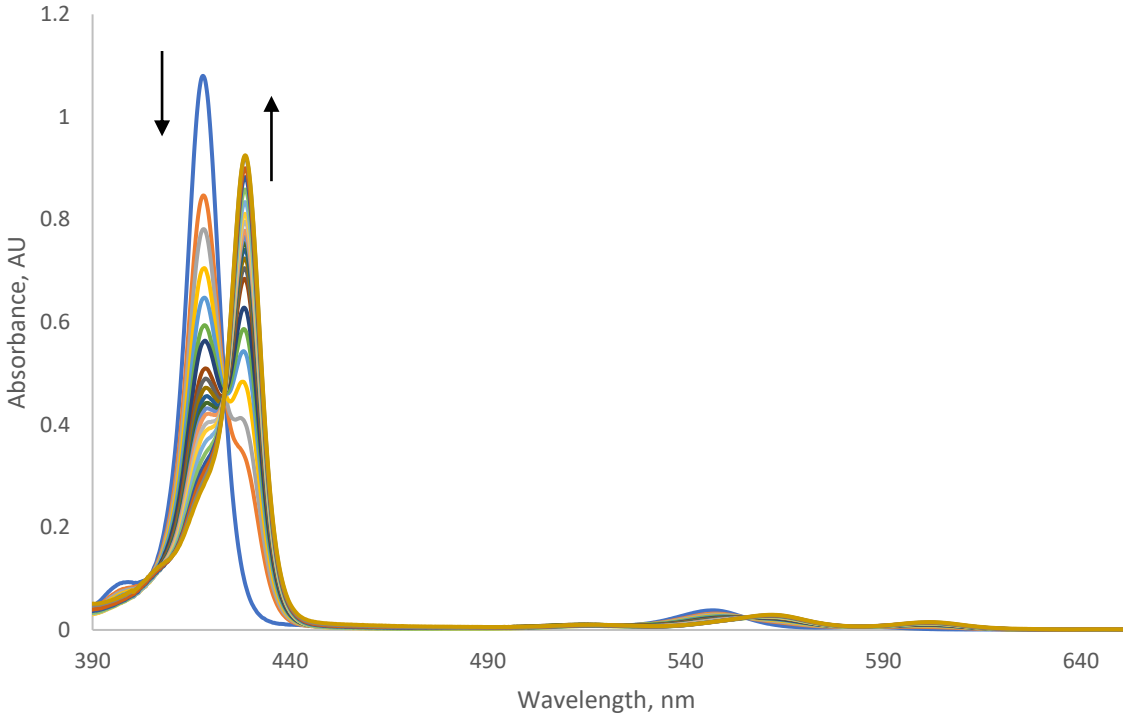


Figure S9. Changes in UV-Vis spectrum of **P4** (2.2×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$4.12 \cdot 10^{-3}$ M).

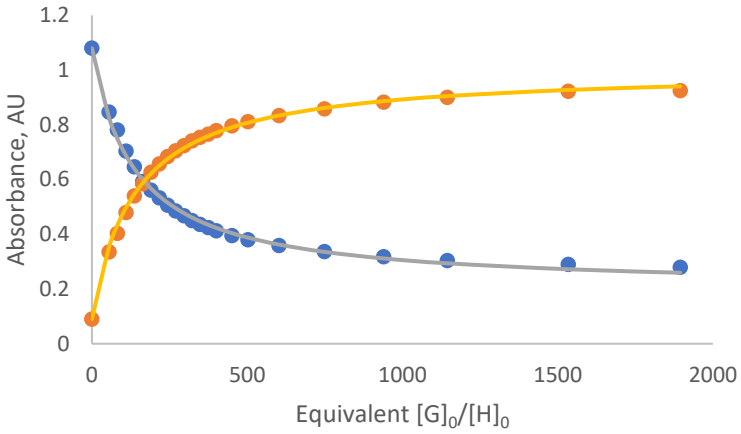


Figure S10. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P4** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P4** host. Blue points – absorption at 418.0 nm, orange points – absorption at 428.6 nm.

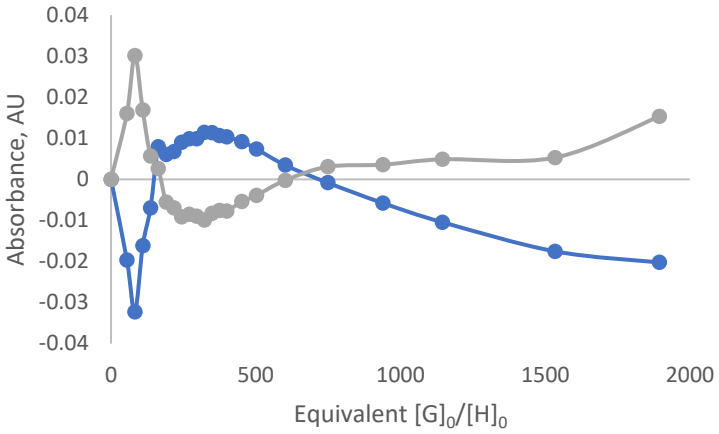


Figure S11. Residual analysis of UV-Vis titration between **P4** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P4** host. Blue points – absorption at 418.0 nm, grey points – absorption at 428.6 nm.

K_a (**1a** + **P4**) = (2.30 ± 0.04) × 10^3 M^{-1}

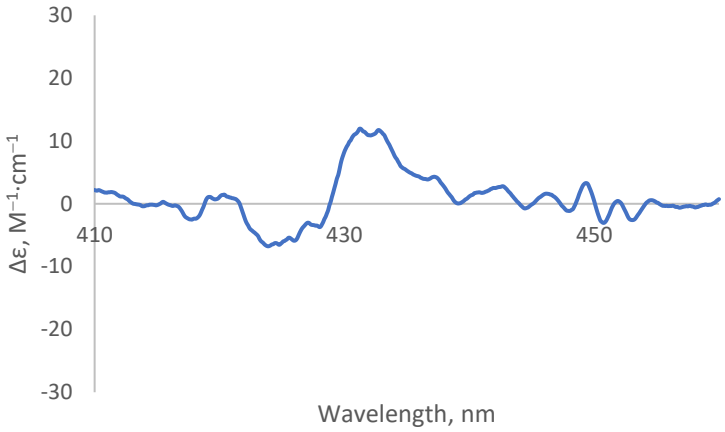


Figure S12. Experimental CD spectrum generated by mixing **P4** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($4.3 \cdot 10^{-3}$ M), 94% conversion to complex.

Spectroscopic data of system **1a** + **P5**

Table S4. Absorptions (AU) of **P5** (2.2×10^{-6} M) derived from the UV-Vis titration of **P5** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 419.4 nm	AU 430.0 nm	C_{1a}, M
1	1.299	0.120	0.00
2	1.097	0.334	$5.45 \cdot 10^{-5}$
3	0.943	0.492	$1.09 \cdot 10^{-4}$
4	0.831	0.608	$1.63 \cdot 10^{-4}$
5	0.742	0.699	$2.17 \cdot 10^{-4}$
6	0.674	0.767	$2.70 \cdot 10^{-4}$
7	0.618	0.824	$3.23 \cdot 10^{-4}$
8	0.573	0.869	$3.76 \cdot 10^{-4}$
9	0.536	0.906	$4.29 \cdot 10^{-4}$
10	0.504	0.938	$4.81 \cdot 10^{-4}$

11	0.477	0.966	$5.34 \cdot 10^{-4}$
12	0.454	0.989	$5.86 \cdot 10^{-4}$
13	0.433	1.011	$6.37 \cdot 10^{-4}$
14	0.416	1.029	$6.89 \cdot 10^{-4}$
15	0.399	1.045	$7.40 \cdot 10^{-4}$
16	0.384	1.060	$7.91 \cdot 10^{-4}$
17	0.360	1.084	$8.93 \cdot 10^{-4}$
18	0.342	1.105	$9.93 \cdot 10^{-4}$
19	0.314	1.137	$1.19 \cdot 10^{-3}$
20	0.287	1.171	$1.48 \cdot 10^{-3}$
21	0.264	1.209	$1.95 \cdot 10^{-3}$
22	0.242	1.258	$2.83 \cdot 10^{-3}$

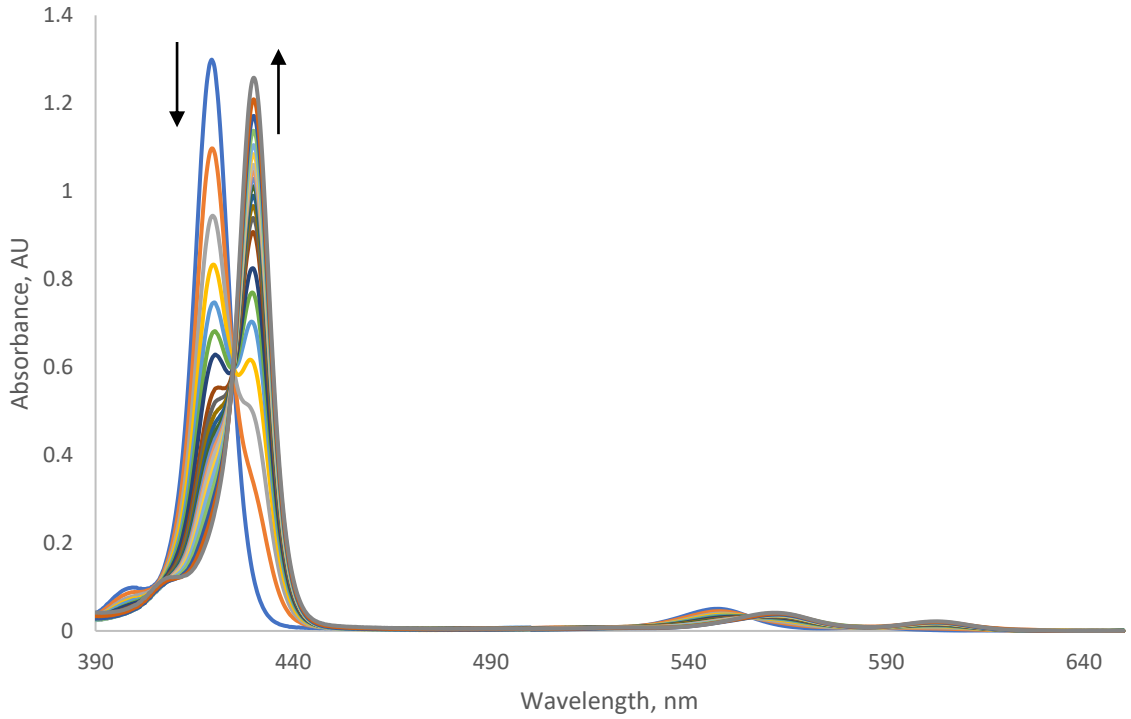


Figure S13. Changes in UV-Vis spectrum of **P5** (2.2×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$2.83\cdot10^{-3}$ M).

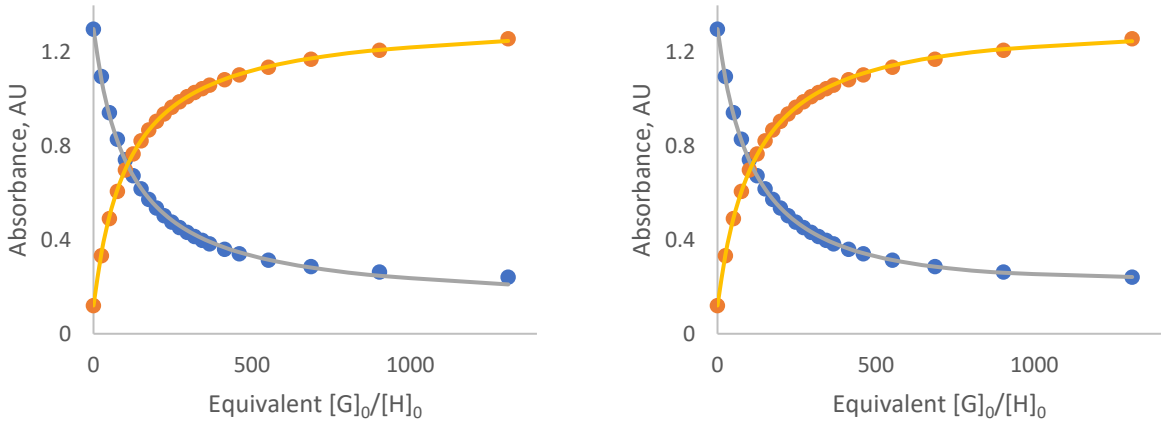


Figure S14. UV-Vis experimental (points) and 1:1 (left) and 1:2 (right) fitted (line) titration curves of **P5** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P5** host. Blue points – absorption at 419.4 nm, orange points – absorption at 430.0 nm.

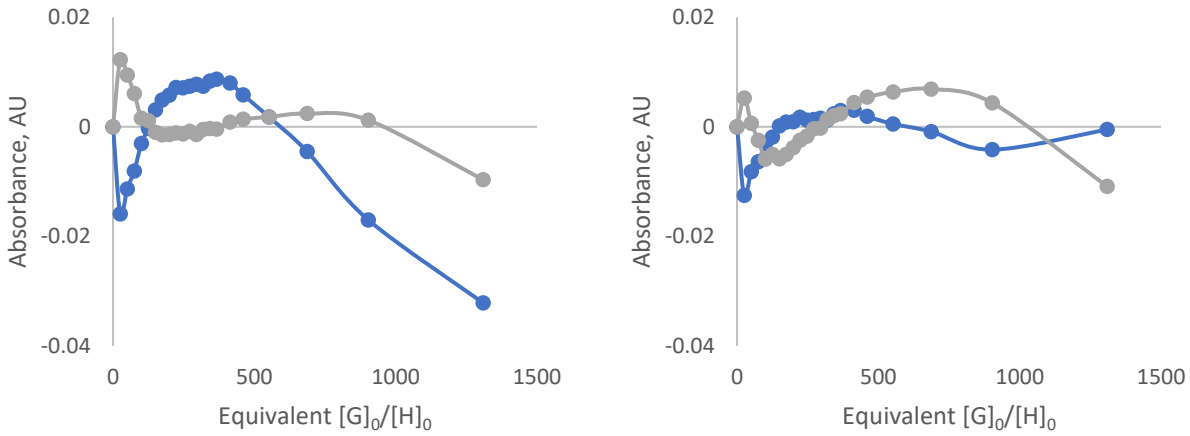


Figure S15. Residual analysis of UV-Vis titration between **P5** and **1a** in CH_2Cl_2 using 1:1 (left) and 1:2 (right) model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P5** host. Blue points – absorption at 419.4 nm, grey points – absorption at 430.0 nm.

Table S5. 1:1 and 1:2 model fitting data comparison derived from the UV-Vis titration of **P5** with **1a** in CH_2Cl_2 at 293 K.

Fitting model	K_a, M^{-1}	SSR fitting error
1:1	$K_1 = (4.18 \pm 0.05) \times 10^3$	$2.8 \cdot 10^{-3}$
1:2	$K_1 = (3.94 \pm 0.02) \times 10^3$ $K_2 = 50 \pm 10$	$0.8 \cdot 10^{-3}$

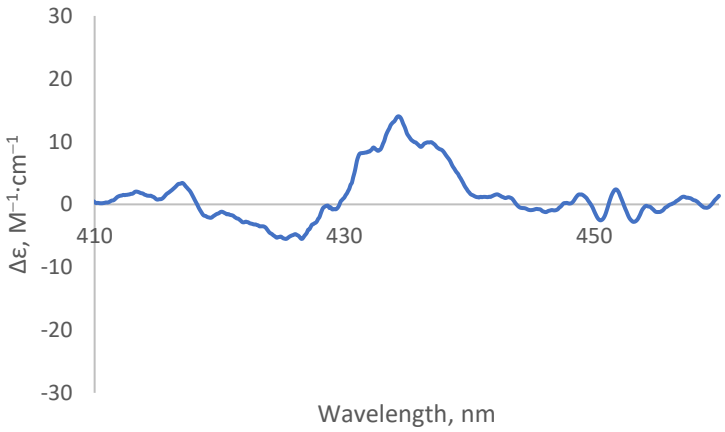


Figure S16. Experimental CD spectrum generated by mixing **P5** ($2.2 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($4.3 \cdot 10^{-3}$ M), 91% conversion to complex.

Spectroscopic data of system **1a** + **P6**

Table S6. Absorptions (AU) of **P6** (2.0×10^{-6} M) derived from the UV-Vis titration of **P6** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 417.8 nm	AU 429.2 nm	$C_{\mathbf{1a}}$, M
1	1.257	0.092	0.00
2	1.164	0.194	$4.96\cdot10^{-5}$
3	1.082	0.283	$9.90\cdot10^{-5}$
4	1.002	0.366	$1.48\cdot10^{-4}$
5	0.936	0.436	$1.97\cdot10^{-4}$
6	0.881	0.496	$2.46\cdot10^{-4}$
7	0.828	0.551	$2.94\cdot10^{-4}$
8	0.752	0.628	$3.91\cdot10^{-4}$
9	0.685	0.696	$4.86\cdot10^{-4}$
10	0.629	0.754	$5.80\cdot10^{-4}$
11	0.585	0.797	$6.74\cdot10^{-4}$
12	0.533	0.848	$8.13\cdot10^{-4}$
13	0.503	0.878	$9.04\cdot10^{-4}$
14	0.479	0.900	$9.95\cdot10^{-4}$
15	0.456	0.926	$1.08\cdot10^{-3}$
16	0.431	0.952	$1.22\cdot10^{-3}$
17	0.404	0.980	$1.39\cdot10^{-3}$
18	0.380	1.005	$1.56\cdot10^{-3}$
19	0.356	1.028	$1.78\cdot10^{-3}$

20	0.335	1.051	$2.02 \cdot 10^{-3}$
21	0.319	1.069	$2.26 \cdot 10^{-3}$
22	0.296	1.094	$2.65 \cdot 10^{-3}$
23	0.269	1.125	$3.38 \cdot 10^{-3}$
24	0.252	1.145	$4.05 \cdot 10^{-3}$
25	0.241	1.162	$4.67 \cdot 10^{-3}$
26	0.233	1.175	$5.25 \cdot 10^{-3}$

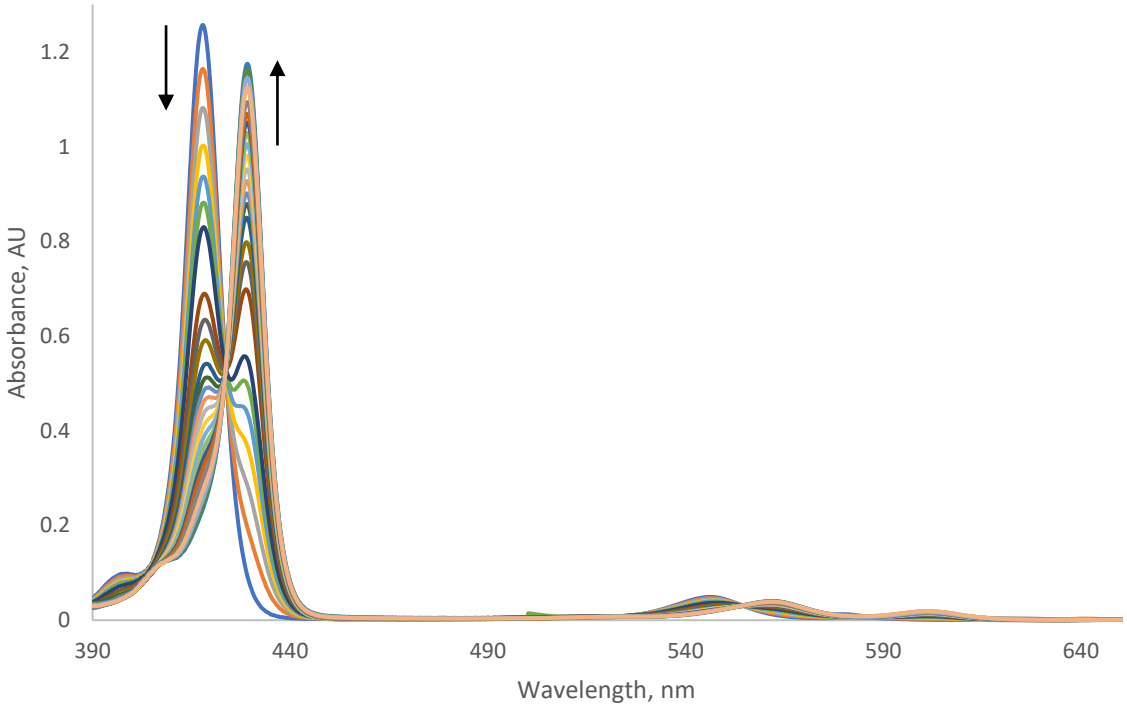


Figure S17. Changes in UV-Vis spectrum of **P6** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$5.25 \cdot 10^{-3}$ M).

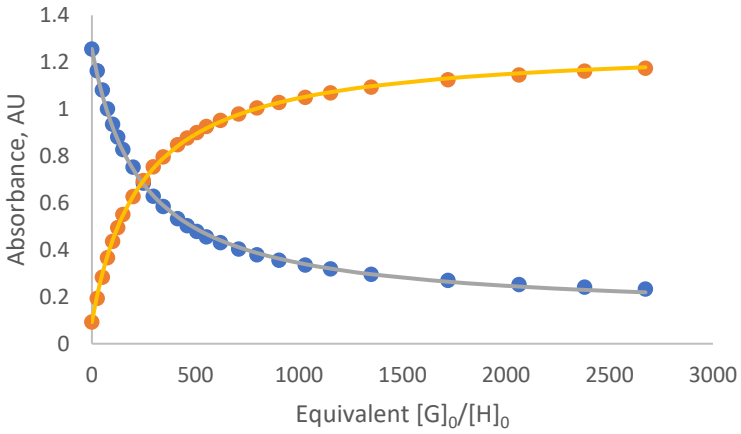


Figure S18. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P6** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P6** host. Blue points – absorption at 417.8 nm, orange points – absorption at 429.2 nm.

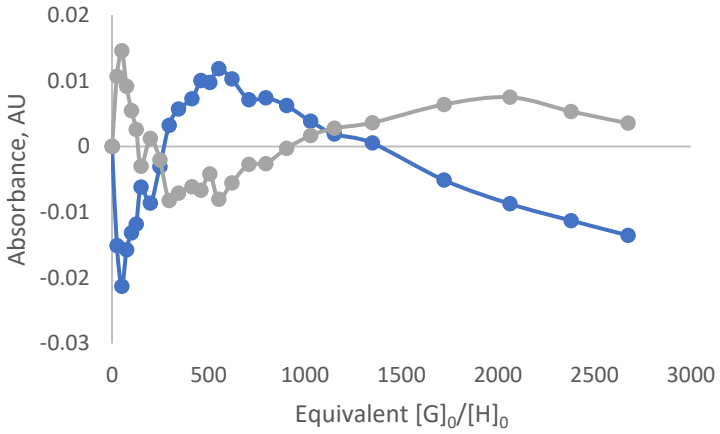


Figure S19. Residual analysis of UV-Vis titration between **P6** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P6** host. Blue points – absorption at 417.8 nm, grey points – absorption at 429.2 nm.

K_a (**1a** + **P6**) = (2.13 ± 0.02) × 10^3 M^{-1}

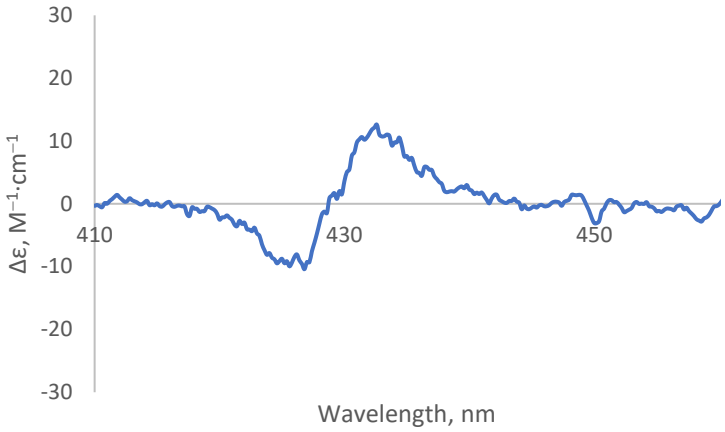


Figure S20. Experimental CD spectrum generated by mixing **P6** ($2.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($5.3 \cdot 10^{-3}$ M), 92% conversion to complex.

Spectroscopic data of system **1a** + **P7**

Table S7. Absorptions (AU) of **P7** (2.1×10^{-6} M) derived from the UV-Vis titration of **P7** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 420.6 nm	AU 432.0 nm	C_{1a}, M
1	0.914	0.112	0.00
2	0.829	0.197	$9.26 \cdot 10^{-5}$
3	0.757	0.270	$1.85 \cdot 10^{-4}$
4	0.693	0.333	$2.77 \cdot 10^{-4}$
5	0.643	0.384	$3.68 \cdot 10^{-4}$
6	0.596	0.428	$4.59 \cdot 10^{-4}$
7	0.554	0.469	$5.49 \cdot 10^{-4}$
8	0.491	0.532	$7.29 \cdot 10^{-4}$
9	0.443	0.578	$9.07 \cdot 10^{-4}$
10	0.407	0.614	$1.08 \cdot 10^{-3}$

11	0.378	0.641	$1.26 \cdot 10^{-3}$
12	0.352	0.667	$1.43 \cdot 10^{-3}$
13	0.316	0.702	$1.77 \cdot 10^{-3}$
14	0.289	0.729	$2.11 \cdot 10^{-3}$
15	0.268	0.750	$2.44 \cdot 10^{-3}$
16	0.234	0.780	$3.08 \cdot 10^{-3}$
17	0.217	0.798	$3.70 \cdot 10^{-3}$
18	0.205	0.812	$4.30 \cdot 10^{-3}$
19	0.196	0.823	$4.87 \cdot 10^{-3}$
20	0.183	0.836	$5.97 \cdot 10^{-3}$
21	0.175	0.846	$7.01 \cdot 10^{-3}$
22	0.170	0.852	$7.98 \cdot 10^{-3}$
23	0.165	0.860	$8.89 \cdot 10^{-3}$
24	0.160	0.863	$9.75 \cdot 10^{-3}$
25	0.160	0.870	$1.06 \cdot 10^{-2}$
26	0.157	0.872	$1.13 \cdot 10^{-2}$
27	0.157	0.875	$1.20 \cdot 10^{-2}$

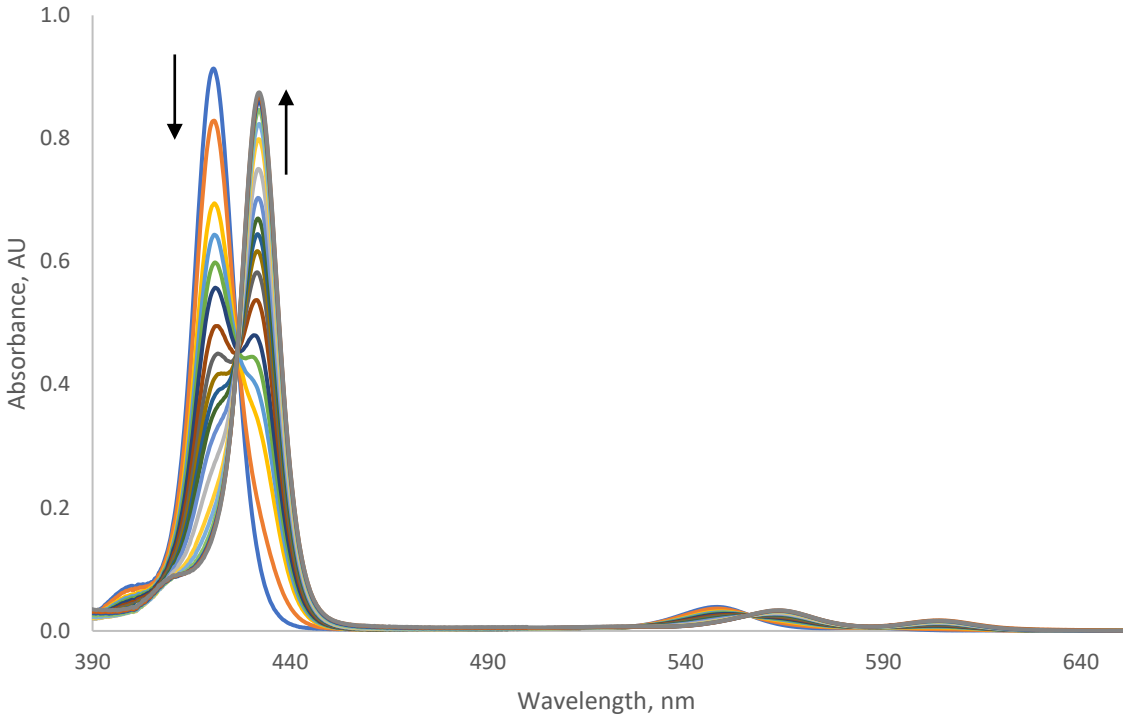


Figure S21. Changes in UV-Vis spectrum of **P7** (2.1×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$1.2\cdot10^{-2}$ M).

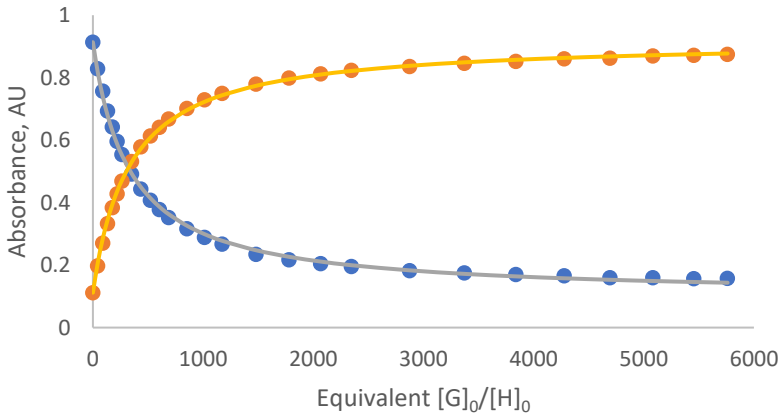


Figure S22. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P7** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P7** host. Blue points – absorption at 420.6 nm, orange points – absorption at 432.2 nm.

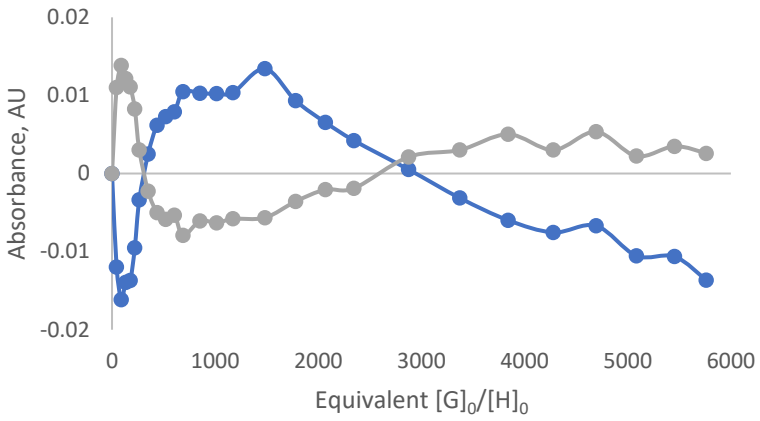


Figure S23. Residual analysis of UV-Vis titration between **P7** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P7** host. Blue points – absorption at 420.6 nm, grey points – absorption at 432.2 nm.

K_a (**1a** + **P7**) = (1.42 ± 0.02) × 10^3 M^{-1}

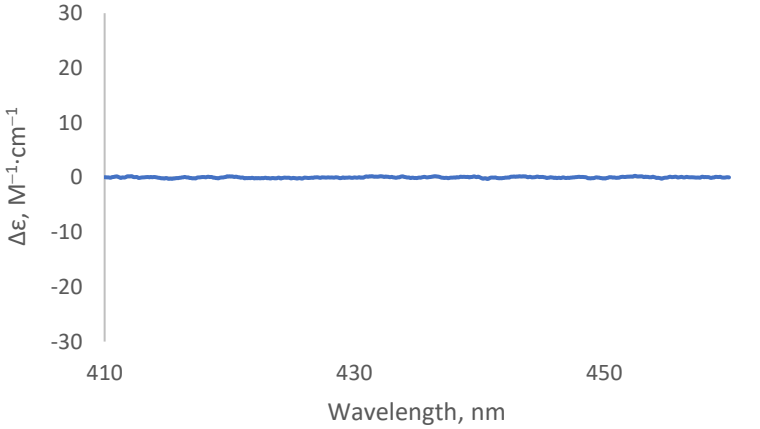


Figure S24. Experimental CD spectrum generated by mixing **P7** ($1.9 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($2.4 \cdot 10^{-2}$ M), 99% conversion to complex.

Spectroscopic data of system **1a** + **P8**

Table S8. Absorptions (AU) of **P8** (2.1×10^{-6} M) derived from the UV-Vis titration of **P8** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 412.6 nm	AU 425.0 nm	C_{1a}, M
1	0.960	0.054	0.00
2	0.944	0.070	$2.62\cdot10^{-6}$
3	0.921	0.099	$5.22\cdot10^{-6}$
4	0.898	0.127	$7.83\cdot10^{-6}$
5	0.874	0.153	$1.04\cdot10^{-5}$
6	0.832	0.203	$1.56\cdot10^{-5}$
7	0.791	0.248	$2.07\cdot10^{-5}$
8	0.755	0.290	$2.59\cdot10^{-5}$
9	0.722	0.327	$3.10\cdot10^{-5}$
10	0.689	0.365	$3.61\cdot10^{-5}$
11	0.661	0.395	$4.11\cdot10^{-5}$
12	0.614	0.447	$5.11\cdot10^{-5}$
13	0.571	0.496	$6.11\cdot10^{-5}$
14	0.534	0.537	$7.09\cdot10^{-5}$
15	0.491	0.583	$8.56\cdot10^{-5}$
16	0.453	0.626	$1.00\cdot10^{-4}$
17	0.413	0.669	$1.19\cdot10^{-4}$
18	0.379	0.708	$1.37\cdot10^{-4}$
19	0.353	0.736	$1.56\cdot10^{-4}$

20	0.333	0.757	$1.74 \cdot 10^{-4}$
21	0.298	0.794	$2.09 \cdot 10^{-4}$
22	0.264	0.832	$2.59 \cdot 10^{-4}$
23	0.234	0.864	$3.29 \cdot 10^{-4}$
24	0.215	0.885	$3.95 \cdot 10^{-4}$
25	0.200	0.899	$4.56 \cdot 10^{-4}$
26	0.189	0.912	$5.14 \cdot 10^{-4}$
27	0.182	0.919	$5.67 \cdot 10^{-4}$

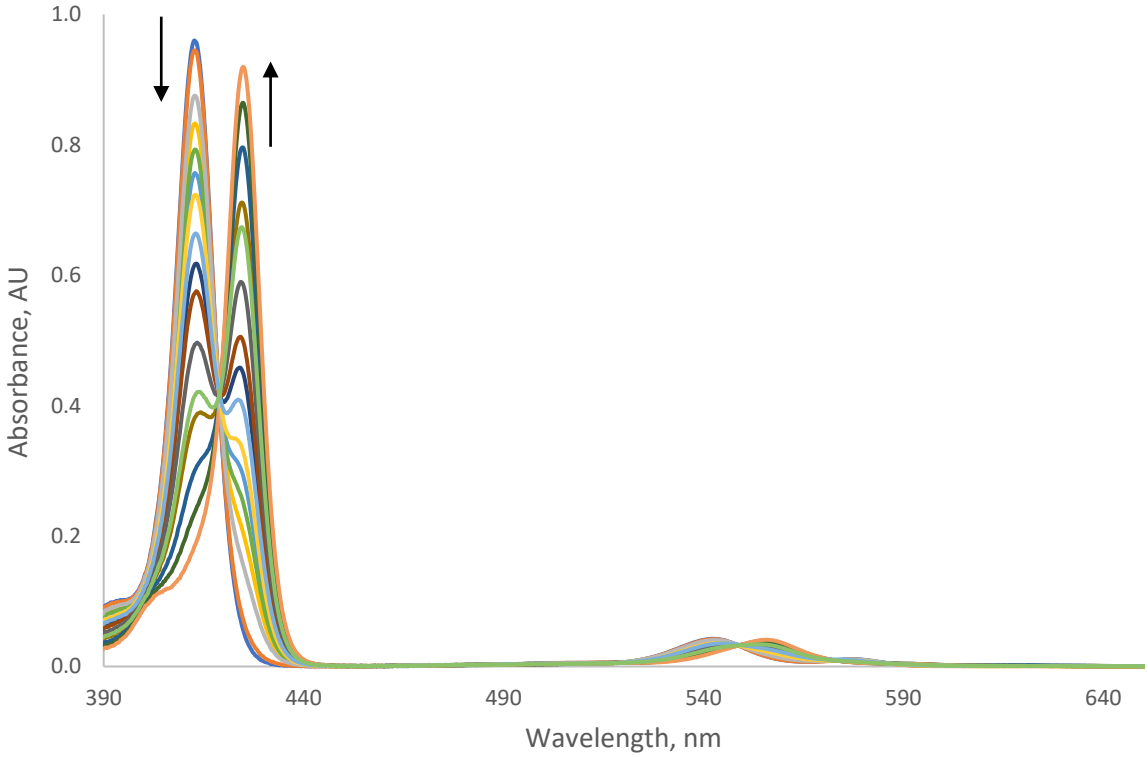


Figure S25. Changes in UV-Vis spectrum of **P8** (2.1×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$5.67 \cdot 10^{-4}$ M).

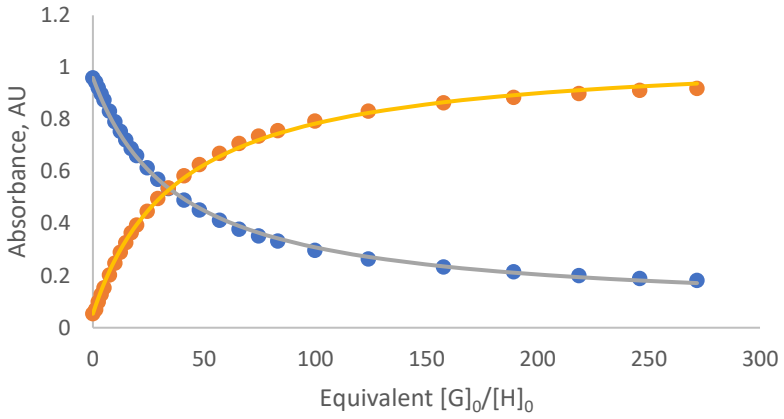


Figure S26. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P8** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P8** host. Blue points – absorption at 412.6 nm, orange points – absorption at 425.0 nm.

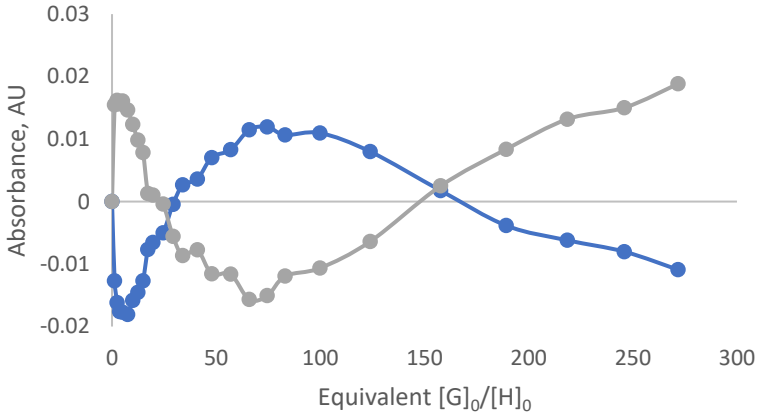


Figure S27. Residual analysis of UV-Vis titration between **P8** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P8** host. Blue points – absorption at 412.6 nm, grey points – absorption at 425.0 nm.

K_a (**1a** + **P8**) = (1.27 ± 0.02) × 10^4 M^{-1}

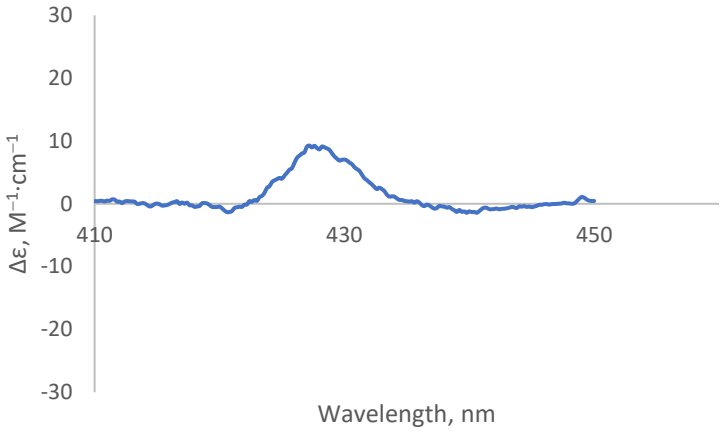


Figure S28. Experimental CD spectrum generated by mixing **P8** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1a** ($1.0 \cdot 10^{-3}$ M), 93% conversion to complex

Spectroscopic data of system **1a** + **P9**

Table S9. Absorptions (AU) of **P9** (2.0×10^{-6} M) derived from the UV-Vis titration of **P9** with **1a** in CH_2Cl_2 and concentrations of **1a** at 293 K.

Sample no	AU 456.8 nm	AU 470.0 nm	C_{1a}, M
1	0.391	0.248	0.00
2	0.350	0.291	$1.07 \cdot 10^{-6}$
3	0.326	0.312	$2.14 \cdot 10^{-6}$
4	0.317	0.322	$3.22 \cdot 10^{-6}$
5	0.308	0.331	$4.29 \cdot 10^{-6}$
6	0.295	0.342	$6.43 \cdot 10^{-6}$
7	0.285	0.353	$8.57 \cdot 10^{-6}$
8	0.280	0.358	$1.07 \cdot 10^{-5}$
9	0.271	0.365	$1.60 \cdot 10^{-5}$
10	0.261	0.374	$2.67 \cdot 10^{-5}$

11	0.255	0.377	$3.72 \cdot 10^{-5}$
12	0.250	0.379	$5.82 \cdot 10^{-5}$
13	0.246	0.379	$8.94 \cdot 10^{-5}$
14	0.243	0.379	$1.30 \cdot 10^{-4}$

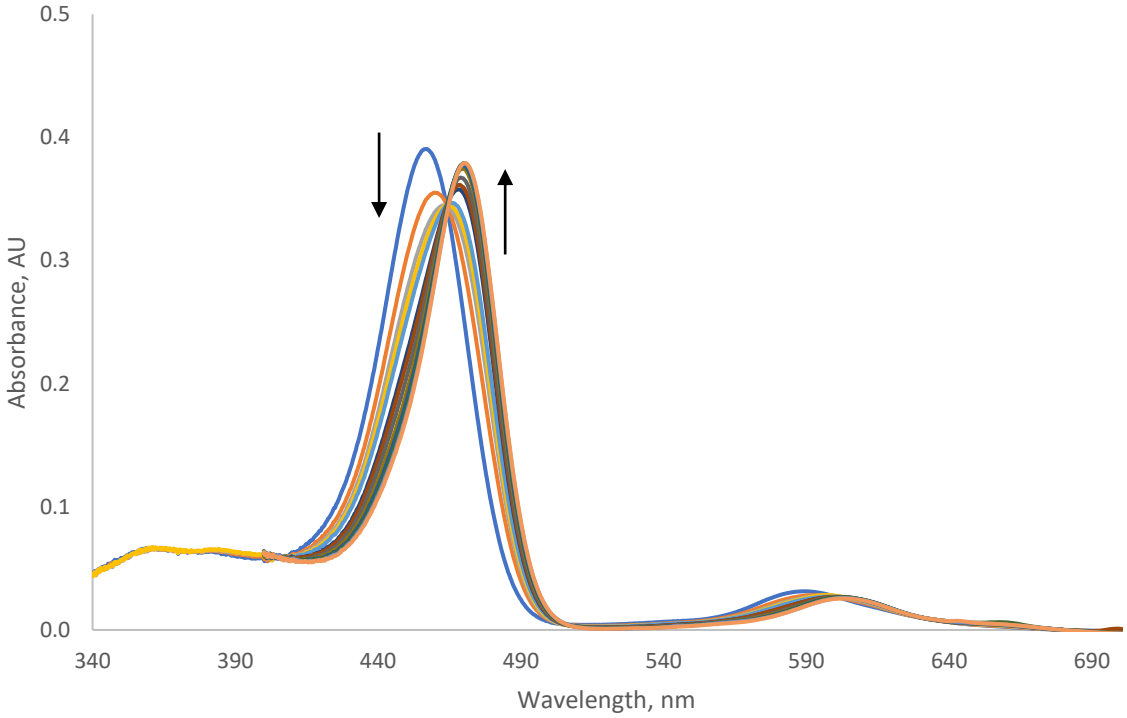


Figure S29. Changes in UV-Vis spectrum of **P9** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1a** (0–$1.30 \cdot 10^{-4}$ M).

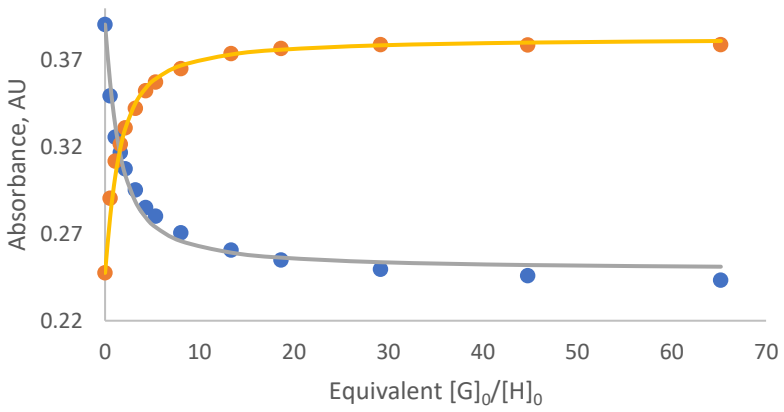


Figure S30. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P9** and **1a** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P9** host. Blue points – absorption at 456.8 nm, orange points – absorption at 470.0 nm.

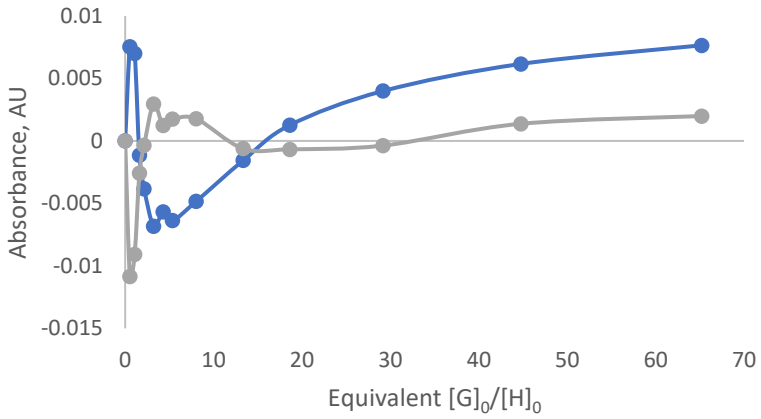


Figure S31. Residual analysis of UV-Vis titration between **P9** and **1a** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1a** guest and **P9** host. Blue points – absorption at 456.8 nm, grey points – absorption at 470.0 nm.

K_a (**1a** + **P9**) = (5.2 ± 0.2) × 10^5 M^{-1}

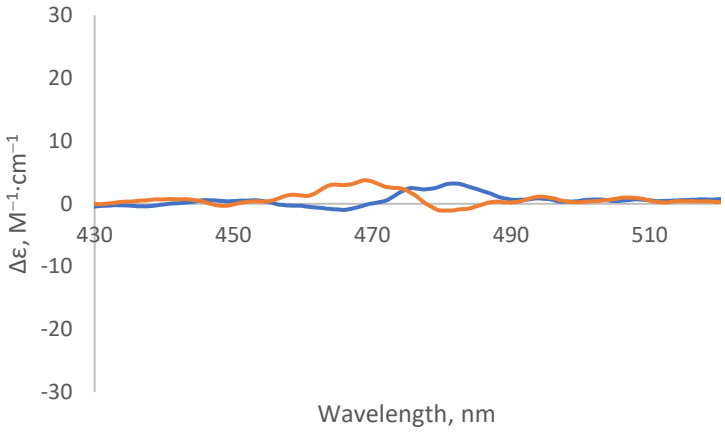


Figure S32. Experimental CD spectra generated by mixing host and guest. Blue line: **P9** ($4.0\cdot10^{-6}$ M, CH_2Cl_2, 293 K) and (*R*,*R*)-**1a** ($1.3\cdot10^{-4}$ M); orange line: **P9** ($4.0\cdot10^{-6}$ M, CH_2Cl_2, 293 K) and (*S*,*S*)-**1a** ($1.3\cdot10^{-4}$ M), >99% conversion to complex in both cases. Since the CD signal for complex (*R*,*R*)-**1a**·**P9** is small, complex (*S*,*S*)-**1a**·**P9** CD signal was measured for comparison.

Spectroscopic data of system **1b** + **P2**

Table S10. Absorptions (AU) of **P2** (2.0×10^{-6} M) derived from the UV-Vis titration of **P2** with **1b** in CH_2Cl_2 and concentrations of **1b** at 293 K.

Sample no	AU 422.6 nm	AU 432.0 nm	C_{1b}, M
1	1.020	0.177	0.00
2	0.967	0.233	$2.24\cdot10^{-5}$
3	0.868	0.342	$4.47\cdot10^{-5}$
4	0.804	0.408	$6.69\cdot10^{-5}$
5	0.748	0.469	$8.91\cdot10^{-5}$
6	0.705	0.514	$1.11\cdot10^{-4}$
7	0.669	0.552	$1.33\cdot10^{-4}$
8	0.633	0.591	$1.55\cdot10^{-4}$
9	0.603	0.618	$1.76\cdot10^{-4}$

10	0.570	0.655	$1.98 \cdot 10^{-4}$
11	0.557	0.665	$2.20 \cdot 10^{-4}$
12	0.533	0.692	$2.41 \cdot 10^{-4}$
13	0.518	0.707	$2.62 \cdot 10^{-4}$
14	0.503	0.723	$2.83 \cdot 10^{-4}$
15	0.492	0.734	$3.04 \cdot 10^{-4}$
16	0.479	0.746	$3.25 \cdot 10^{-4}$
17	0.470	0.756	$3.46 \cdot 10^{-4}$
18	0.461	0.766	$3.67 \cdot 10^{-4}$
19	0.451	0.776	$3.88 \cdot 10^{-4}$
20	0.443	0.784	$4.09 \cdot 10^{-4}$
21	0.435	0.793	$4.29 \cdot 10^{-4}$
22	0.421	0.806	$4.70 \cdot 10^{-4}$
23	0.409	0.818	$5.10 \cdot 10^{-4}$
24	0.395	0.837	$5.50 \cdot 10^{-4}$
25	0.388	0.840	$5.90 \cdot 10^{-4}$
26	0.379	0.852	$6.29 \cdot 10^{-4}$
27	0.371	0.859	$6.68 \cdot 10^{-4}$
28	0.363	0.868	$7.07 \cdot 10^{-4}$
29	0.357	0.874	$7.45 \cdot 10^{-4}$
30	0.351	0.880	$7.83 \cdot 10^{-4}$
31	0.345	0.887	$8.21 \cdot 10^{-4}$

32	0.338	0.892	$8.58 \cdot 10^{-4}$

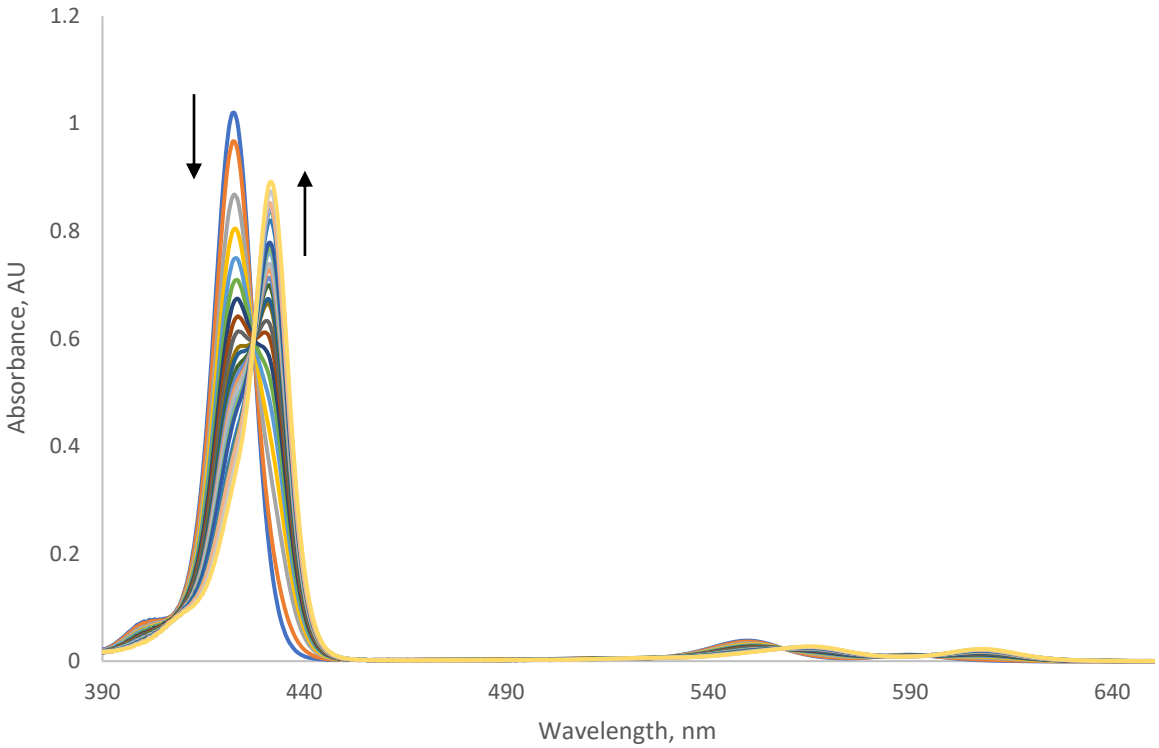


Figure S33. Changes in UV-Vis spectrum of **P2** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1b** (0–$8.58 \cdot 10^{-4}$ M).

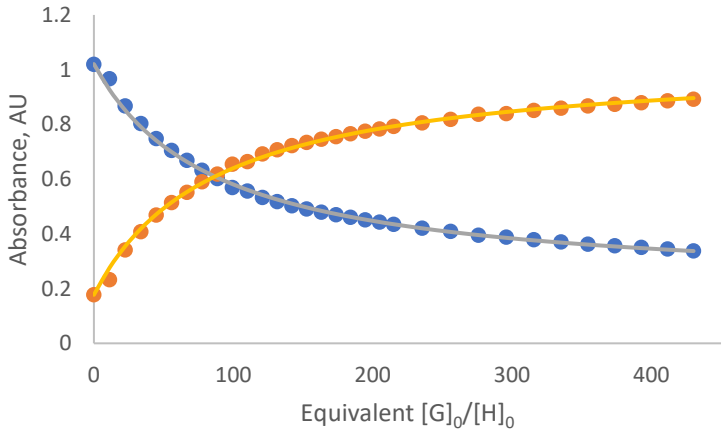


Figure S34. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P2** and **1b** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P2** host. Blue points – absorption at 422.6 nm, orange points – absorption at 432.0 nm.

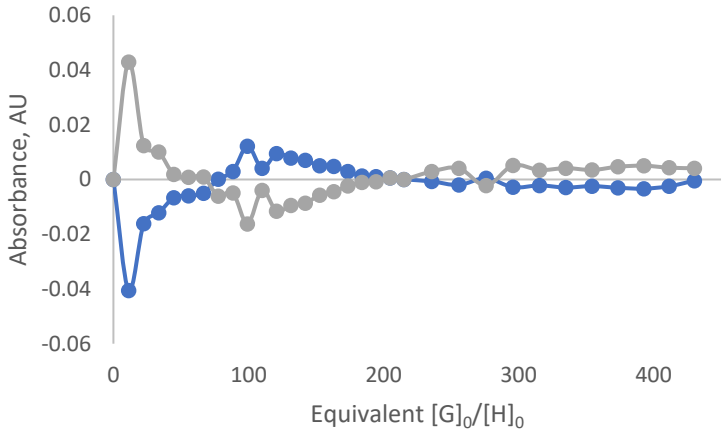


Figure S35. Residual analysis of UV-Vis titration between **P2** and **1b** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P2** host. Blue points – absorption at 422.6 nm, grey points – absorption at 432.0 nm.

K_a (**1b** + **P2**) = (5.8 ± 0.3) × 10^3 M^{-1}

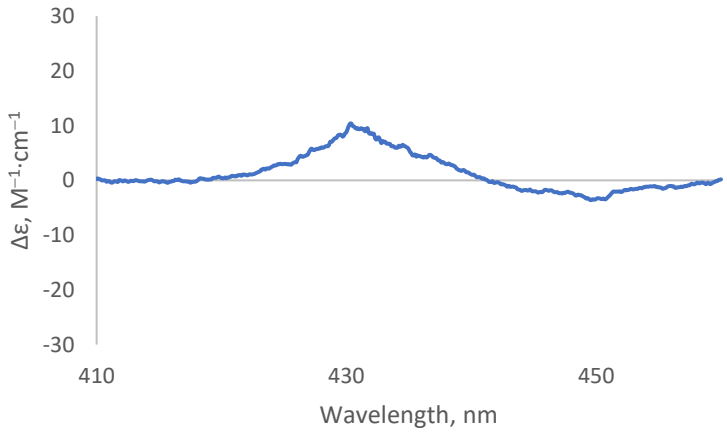


Figure S36. Experimental CD spectrum generated by mixing **P2** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1b** ($3.6 \cdot 10^{-3}$ M), 97% conversion to complex.

Spectroscopic data of system **1b** + **P5**

Table S11. Absorptions (AU) of **P5** (2.1×10^{-6} M) derived from the UV-Vis titration of **P5** with **1b** in CH_2Cl_2 and concentrations of **1b** at 293 K.

Sample no	AU 418.0 nm	AU 428.6 nm	$C_{\mathbf{1b}}$, M
1	1.281	0.108	0.00
2	1.109	0.299	$2.10\cdot10^{-5}$
3	0.974	0.444	$4.18\cdot10^{-5}$
4	0.869	0.559	$6.26\cdot10^{-5}$
5	0.788	0.641	$8.33\cdot10^{-5}$
6	0.752	0.678	$9.36\cdot10^{-5}$
7	0.711	0.726	$1.04\cdot10^{-4}$
8	0.690	0.743	$1.14\cdot10^{-4}$
9	0.655	0.781	$1.24\cdot10^{-4}$
10	0.634	0.802	$1.35\cdot10^{-4}$
11	0.612	0.824	$1.45\cdot10^{-4}$
12	0.582	0.858	$1.55\cdot10^{-4}$
13	0.572	0.864	$1.65\cdot10^{-4}$
14	0.542	0.895	$1.85\cdot10^{-4}$
15	0.509	0.934	$2.05\cdot10^{-4}$
16	0.493	0.947	$2.25\cdot10^{-4}$
17	0.465	0.979	$2.45\cdot10^{-4}$
18	0.455	0.984	$2.65\cdot10^{-4}$
19	0.436	1.008	$2.85\cdot10^{-4}$

20	0.418	1.022	$3.24 \cdot 10^{-4}$
21	0.397	1.042	$3.63 \cdot 10^{-4}$
22	0.374	1.067	$4.01 \cdot 10^{-4}$
23	0.346	1.096	$4.39 \cdot 10^{-4}$
24	0.327	1.112	$5.15 \cdot 10^{-4}$
25	0.327	1.112	$5.89 \cdot 10^{-4}$

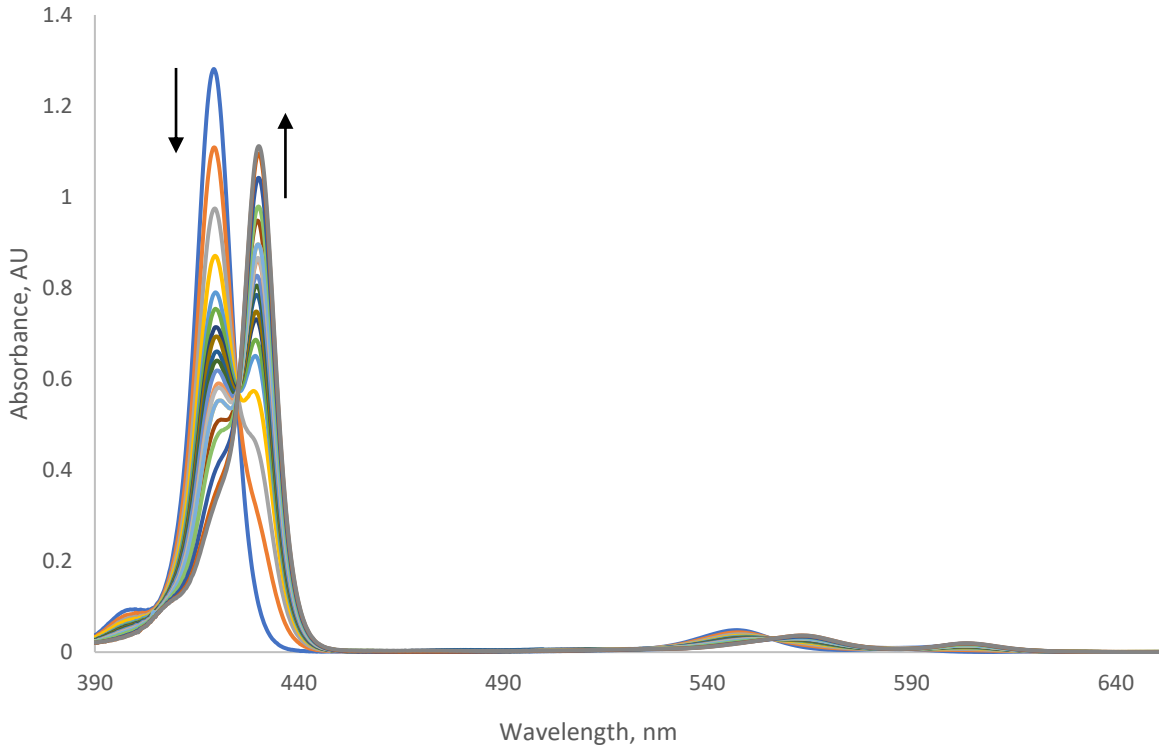


Figure S37. Changes in UV-Vis spectrum of **P5** (2.1×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1b** (0–$5.89 \cdot 10^{-4}$ M).

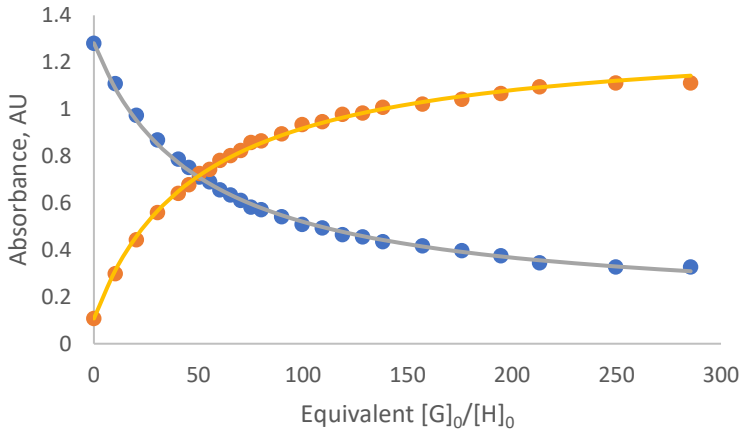


Figure S38. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P5** and **1b** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P5** host. Blue points – absorption at 419.0 nm, orange points – absorption at 428.6 nm.

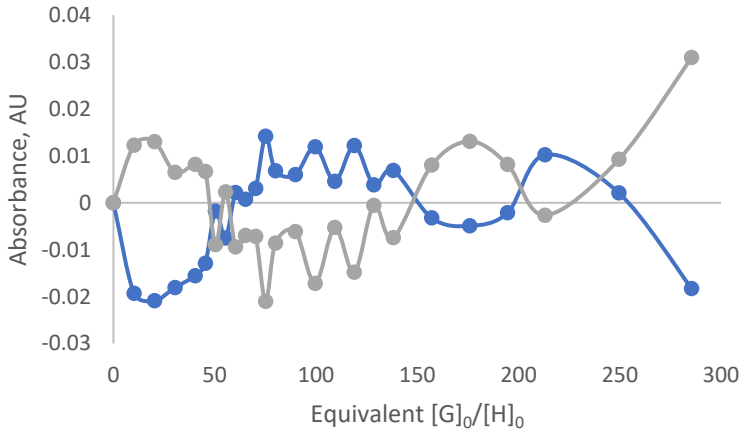


Figure S39. Residual analysis of UV-Vis titration between **P5** and **1b** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P5** host. Blue points – absorption at 419.0 nm, grey points – absorption at 428.6 nm.

K_a (**1b** + **P5**) = (9.8 ± 0.1) × 10^3 M^{-1}

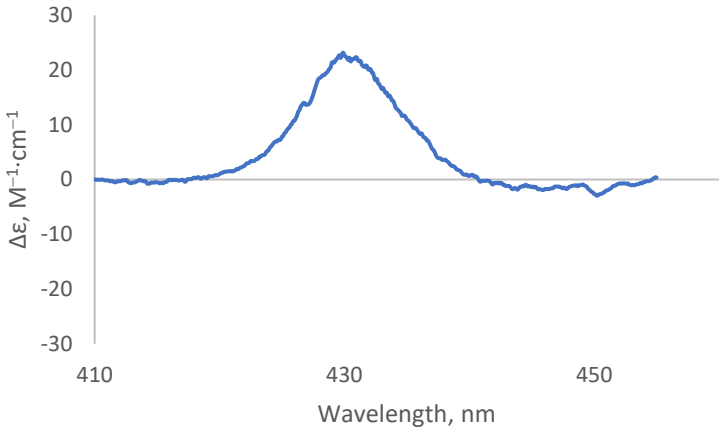


Figure S40. Experimental CD spectrum generated by mixing **P5** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1b** ($3.7 \cdot 10^{-3}$ M), 98% conversion to complex.

Spectroscopic data of system **1b** + **P6**

Table S12. Absorptions (AU) of **P6** (2.0×10^{-6} M) derived from the UV-Vis titration of **P6** with **1b** in CH_2Cl_2 and concentrations of **1b** at 293 K.

Sample no	AU 418.2 nm	AU 429.0 nm	$C_{\mathbf{1b}}$, M
1	1.269	0.104	0.00
2	1.088	0.301	$1.40 \cdot 10^{-5}$
3	0.956	0.440	$2.80 \cdot 10^{-5}$
4	0.858	0.545	$4.19 \cdot 10^{-5}$
5	0.784	0.623	$5.58 \cdot 10^{-5}$
6	0.733	0.676	$6.68 \cdot 10^{-5}$
7	0.689	0.723	$7.78 \cdot 10^{-5}$
8	0.651	0.762	$8.87 \cdot 10^{-5}$
9	0.620	0.794	$9.96 \cdot 10^{-5}$
10	0.590	0.823	$1.10 \cdot 10^{-4}$

11	0.563	0.852	$1.21 \cdot 10^{-4}$
12	0.539	0.876	$1.32 \cdot 10^{-4}$
13	0.519	0.898	$1.43 \cdot 10^{-4}$
14	0.500	0.916	$1.54 \cdot 10^{-4}$
15	0.482	0.935	$1.64 \cdot 10^{-4}$
16	0.467	0.952	$1.75 \cdot 10^{-4}$
17	0.450	0.967	$1.88 \cdot 10^{-4}$
18	0.434	0.984	$2.01 \cdot 10^{-4}$
19	0.420	0.998	$2.14 \cdot 10^{-4}$
20	0.406	1.010	$2.27 \cdot 10^{-4}$
21	0.384	1.032	$2.53 \cdot 10^{-4}$
22	0.367	1.048	$2.79 \cdot 10^{-4}$
23	0.337	1.078	$3.30 \cdot 10^{-4}$
24	0.299	1.118	$4.28 \cdot 10^{-4}$
25	0.254	1.162	$6.38 \cdot 10^{-4}$
26	0.230	1.187	$8.32 \cdot 10^{-4}$

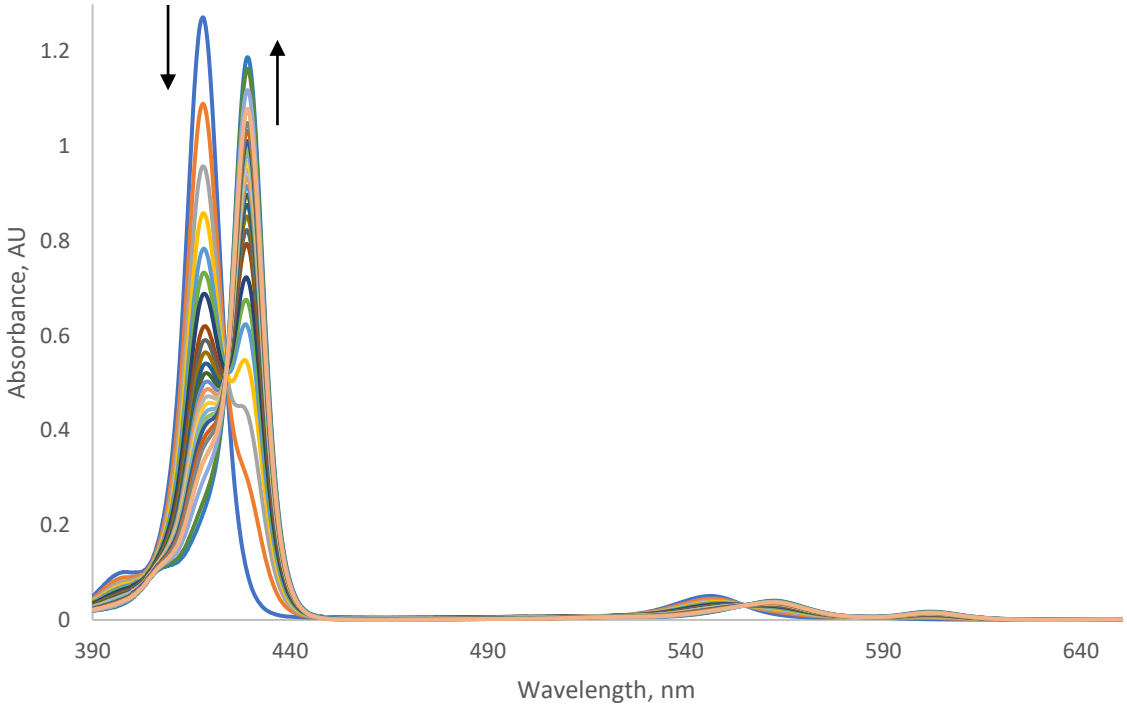


Figure S41. Changes in UV-Vis spectrum of **P6** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1b** (0–$8.32\cdot10^{-4}$ M).

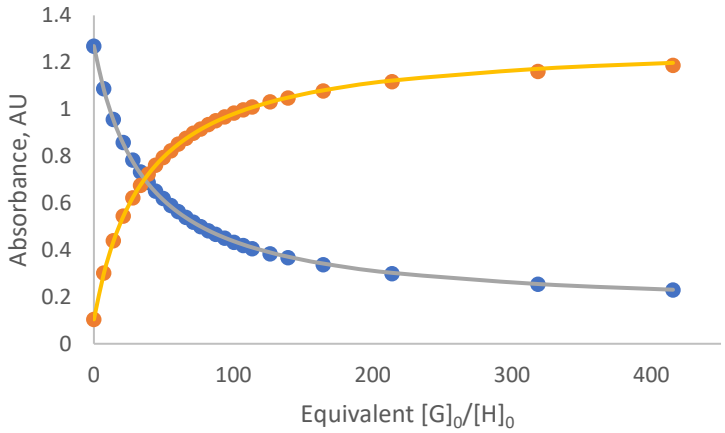


Figure S42. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P6** and **1b** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P6** host. Blue points – absorption at 418.2 nm, orange points – absorption at 429.0 nm.

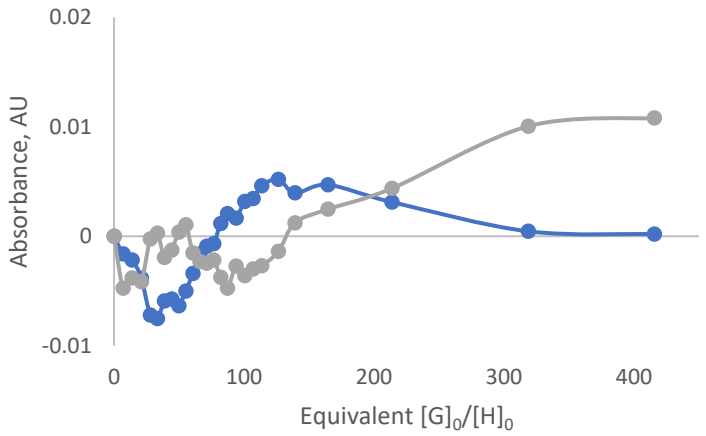


Figure S43. Residual analysis of UV-Vis titration between **P6** and **1b** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P6** host. Blue points – absorption at 418.2 nm, grey points – absorption at 429.0 nm.

K_a (**1b** + **P6**) = (1.413 ± 0.007) × 10^4 M^{-1}

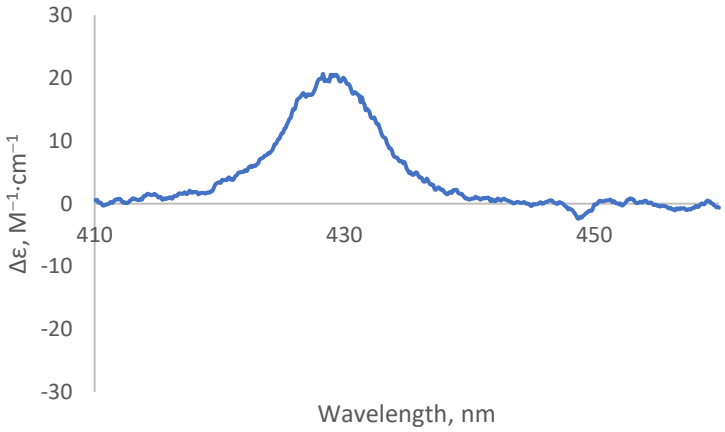


Figure S44. Experimental CD spectrum generated by mixing **P6** ($1.9 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1b** ($1.7 \cdot 10^{-2}$ M), >99% conversion to complex.

Spectroscopic data of system **1b** + **P7**

Table S13. Absorptions (AU) of **P7** (2.2×10^{-6} M) derived from the UV-Vis titration of **P7** with **1b** in CH_2Cl_2 and concentrations of **1b** at 293 K.

Sample no	AU 420.6 nm	AU 432.0 nm	$C_{\mathbf{1b}}$, M
1	0.918	0.114	0.00
2	0.789	0.244	$1.13\cdot10^{-5}$
3	0.686	0.347	$2.25\cdot10^{-5}$
4	0.616	0.416	$3.37\cdot10^{-5}$
5	0.550	0.482	$4.49\cdot10^{-5}$
6	0.498	0.534	$5.61\cdot10^{-5}$
7	0.468	0.560	$6.73\cdot10^{-5}$
8	0.408	0.619	$8.95\cdot10^{-5}$
9	0.366	0.662	$1.12\cdot10^{-4}$
10	0.335	0.692	$1.34\cdot10^{-4}$
11	0.307	0.719	$1.55\cdot10^{-4}$
12	0.293	0.731	$1.77\cdot10^{-4}$
13	0.264	0.759	$2.21\cdot10^{-4}$
14	0.240	0.783	$2.66\cdot10^{-4}$
15	0.227	0.795	$3.06\cdot10^{-4}$
16	0.202	0.821	$3.90\cdot10^{-4}$
17	0.191	0.830	$4.72\cdot10^{-4}$
18	0.180	0.841	$5.53\cdot10^{-4}$
19	0.173	0.847	$6.32\cdot10^{-4}$

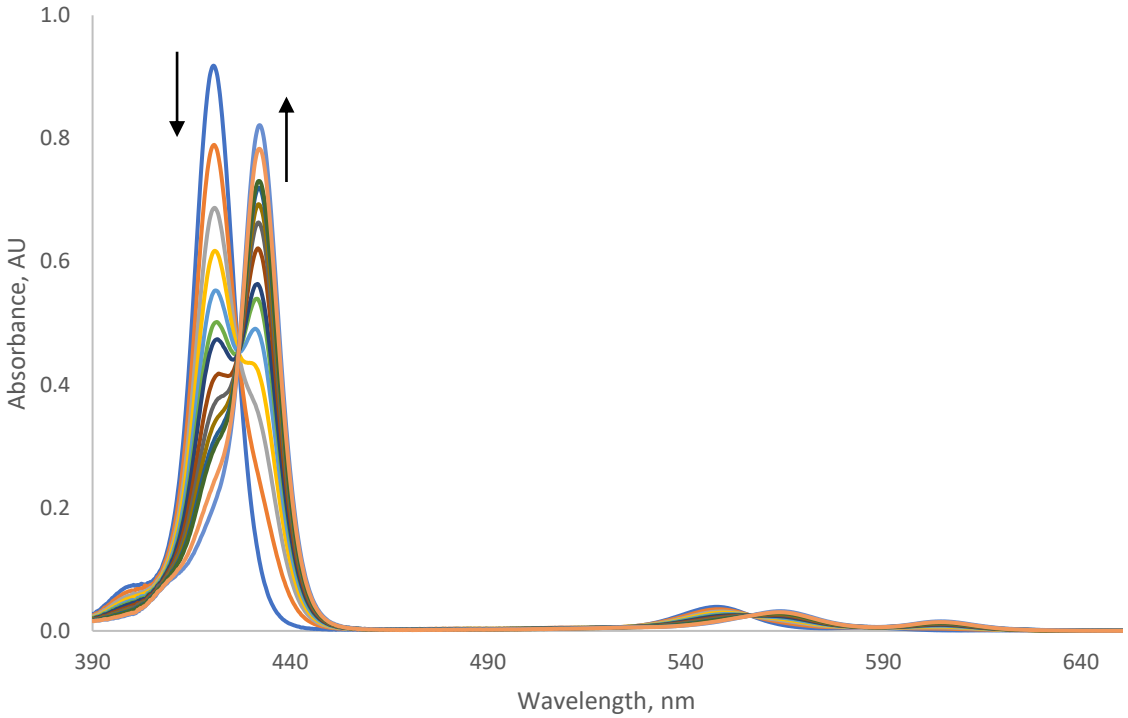


Figure S45. Changes in UV-Vis spectrum of **P7** (2.2×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1b** ($0–6.32\cdot10^{-4}$ M).

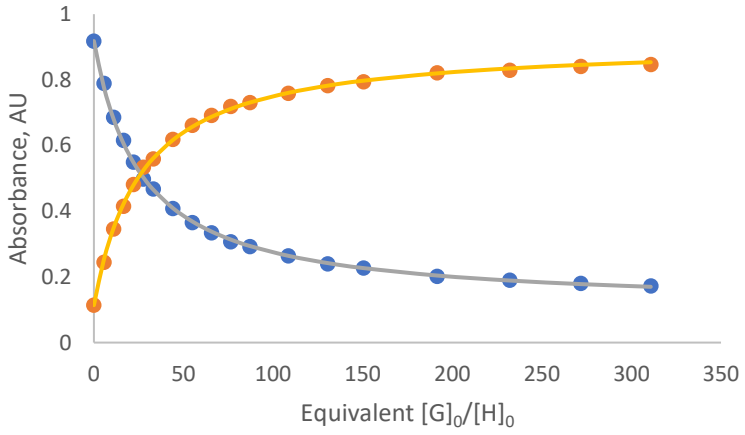


Figure S46. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P7** and **1b** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P7** host. Blue points – absorption at 420.6 nm, orange points – absorption at 432.0 nm.

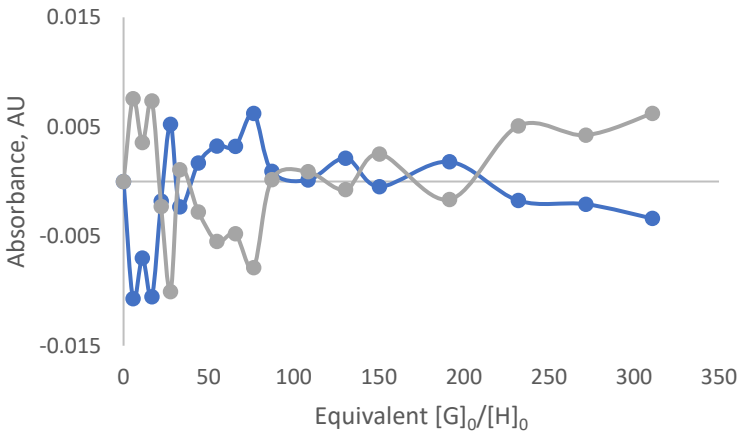


Figure S47. Residual analysis of UV-Vis titration between **P7** and **1b** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1b** guest and **P7** host. Blue points – absorption at 420.6 nm, grey points – absorption at 432.0 nm.

K_a (**1b** + **P7**) = (1.91 ± 0.02) × 10^4 M^{-1}

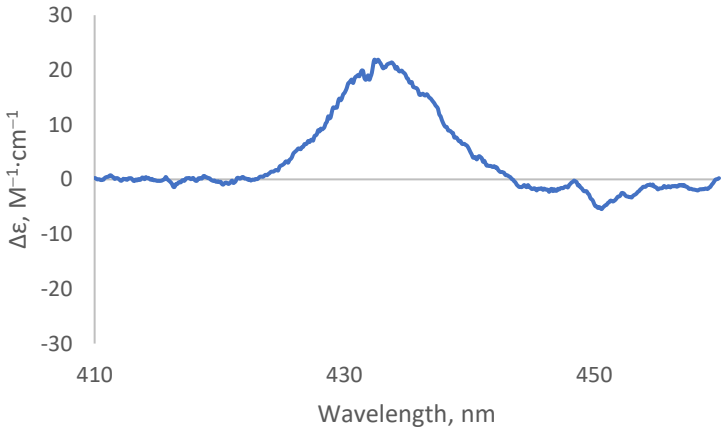


Figure S48. Experimental CD spectrum generated by mixing **P7** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1b** ($4.1 \cdot 10^{-3}$ M), 99% conversion to complex.

Spectroscopic data of system **1c** + **P1**

Table S14. Absorptions (AU) of **P1** (2.1×10^{-6} M) derived from the UV-Vis titration of **P1** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 423.0 nm	AU 433.0 nm	C_{1c}, M
1	1.103	0.182	0.00
2	1.059	0.231	$7.45\cdot10^{-6}$
3	1.013	0.285	$1.49\cdot10^{-5}$
4	0.969	0.333	$2.23\cdot10^{-5}$
5	0.930	0.376	$2.97\cdot10^{-5}$
6	0.865	0.447	$4.44\cdot10^{-5}$
7	0.810	0.510	$5.91\cdot10^{-5}$
8	0.762	0.563	$7.37\cdot10^{-5}$
9	0.722	0.608	$8.82\cdot10^{-5}$
10	0.686	0.646	$1.03\cdot10^{-4}$
11	0.656	0.681	$1.17\cdot10^{-4}$
12	0.628	0.711	$1.31\cdot10^{-4}$
13	0.604	0.739	$1.46\cdot10^{-4}$
14	0.582	0.763	$1.60\cdot10^{-4}$
15	0.563	0.784	$1.74\cdot10^{-4}$
16	0.531	0.818	$2.02\cdot10^{-4}$
17	0.504	0.848	$2.30\cdot10^{-4}$
18	0.471	0.885	$2.71\cdot10^{-4}$
19	0.437	0.921	$3.25\cdot10^{-4}$

20	0.410	0.952	$3.78 \cdot 10^{-4}$
21	0.373	0.991	$4.82 \cdot 10^{-4}$
22	0.337	1.028	$6.30 \cdot 10^{-4}$
23	0.302	1.065	$8.40 \cdot 10^{-4}$
24	0.281	1.089	$1.03 \cdot 10^{-3}$
25	0.267	1.101	$1.21 \cdot 10^{-3}$
26	0.257	1.112	$1.38 \cdot 10^{-3}$

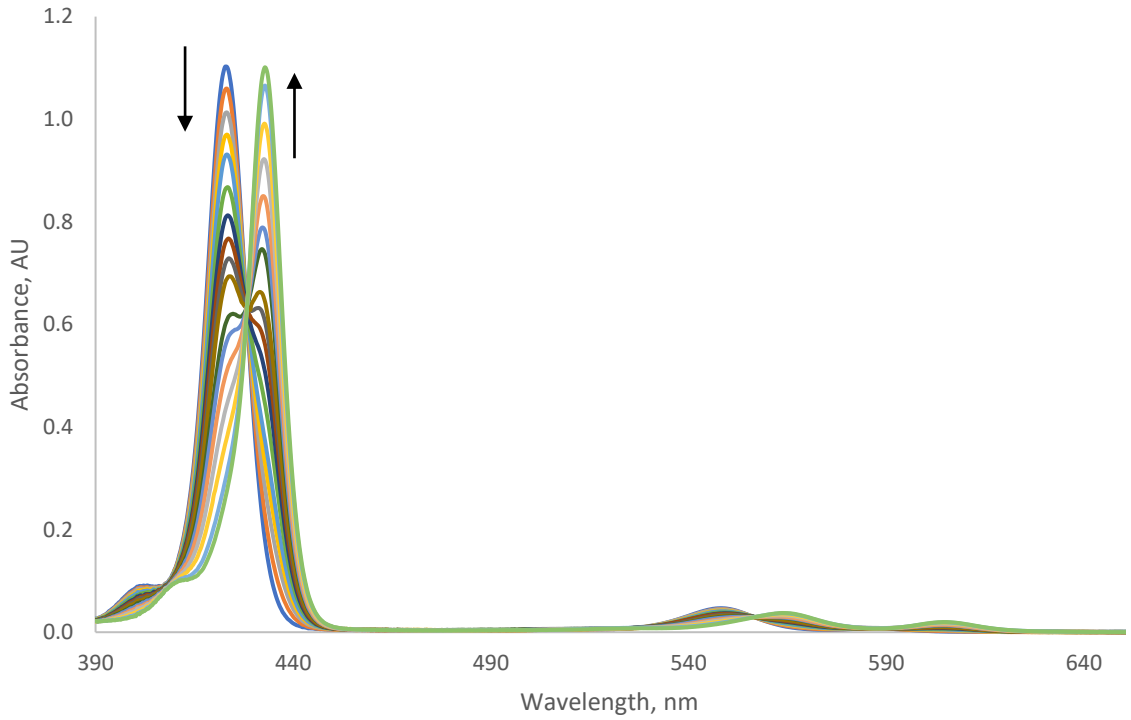


Figure S49. Changes in UV-Vis spectrum of **P1** (2.1×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$1.38 \cdot 10^{-3}$ M).

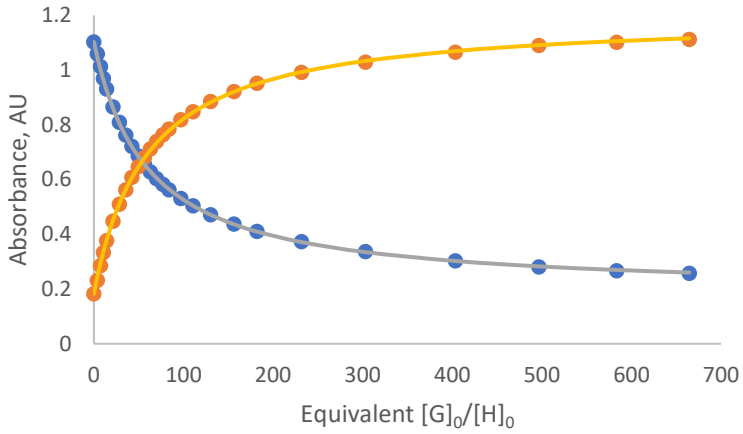


Figure S50. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P1** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P1** host. Blue points – absorption at 423.0 nm, orange points – absorption at 433.0 nm.

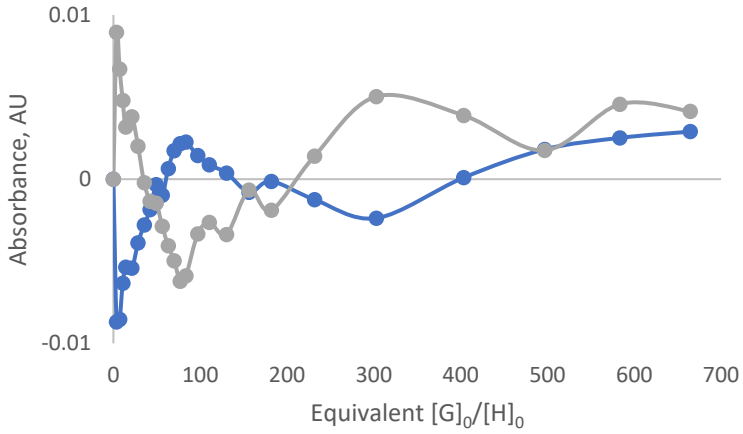


Figure S51. Residual analysis of UV-Vis titration between **P1** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P1** host. Blue points – absorption at 423.0 nm, grey points – absorption at 433.0 nm.

K_a (**1c** + **P1**) = (8.2 ± 0.5) × 10^3 M^{-1}

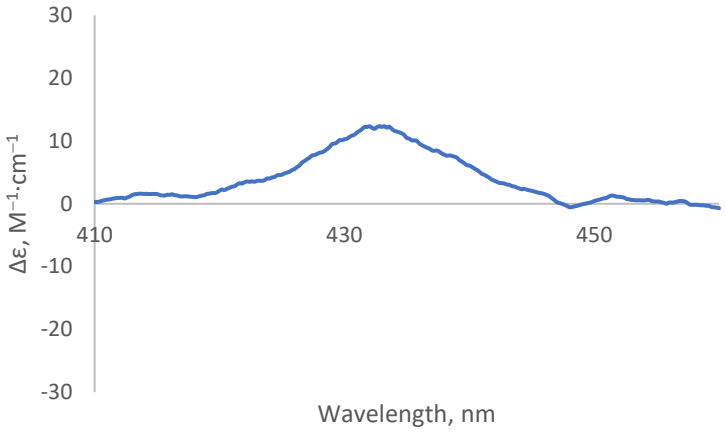


Figure S52. Experimental CD spectrum generated by mixing **P1** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($1.4 \cdot 10^{-4}$ M), 92% conversion to complex.

Spectroscopic data of system **1c** + **P2**

Table S15. Absorptions (AU) of **P2** (2.0×10^{-6} M) derived from the UV-Vis titration of **P2** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 422.4 nm	AU 431.8 nm	C_{1c}, M
1	1.137	0.201	0.00
2	0.994	0.356	$2.30 \cdot 10^{-5}$
3	0.886	0.475	$4.58 \cdot 10^{-5}$
4	0.803	0.564	$6.86 \cdot 10^{-5}$
5	0.726	0.644	$9.58 \cdot 10^{-5}$
6	0.688	0.686	$1.14 \cdot 10^{-4}$
7	0.654	0.722	$1.32 \cdot 10^{-4}$
8	0.622	0.755	$1.50 \cdot 10^{-4}$
9	0.595	0.781	$1.67 \cdot 10^{-4}$
10	0.571	0.807	$1.85 \cdot 10^{-4}$

11	0.552	0.828	$2.03 \cdot 10^{-4}$
12	0.534	0.847	$2.21E \cdot 10^{-4}$
13	0.517	0.865	$2.38 \cdot 10^{-4}$
14	0.502	0.879	$2.56 \cdot 10^{-4}$
15	0.488	0.893	$2.73 \cdot 10^{-4}$
16	0.475	0.908	$2.90 \cdot 10^{-4}$
17	0.464	0.919	$3.08 \cdot 10^{-4}$
18	0.441	0.940	$3.51 \cdot 10^{-4}$
19	0.420	0.963	$3.93 \cdot 10^{-4}$
20	0.404	0.979	$4.35 \cdot 10^{-4}$
21	0.379	1.005	$5.19 \cdot 10^{-4}$
22	0.357	1.029	$6.01 \cdot 10^{-4}$
23	0.328	1.059	$7.79 \cdot 10^{-4}$

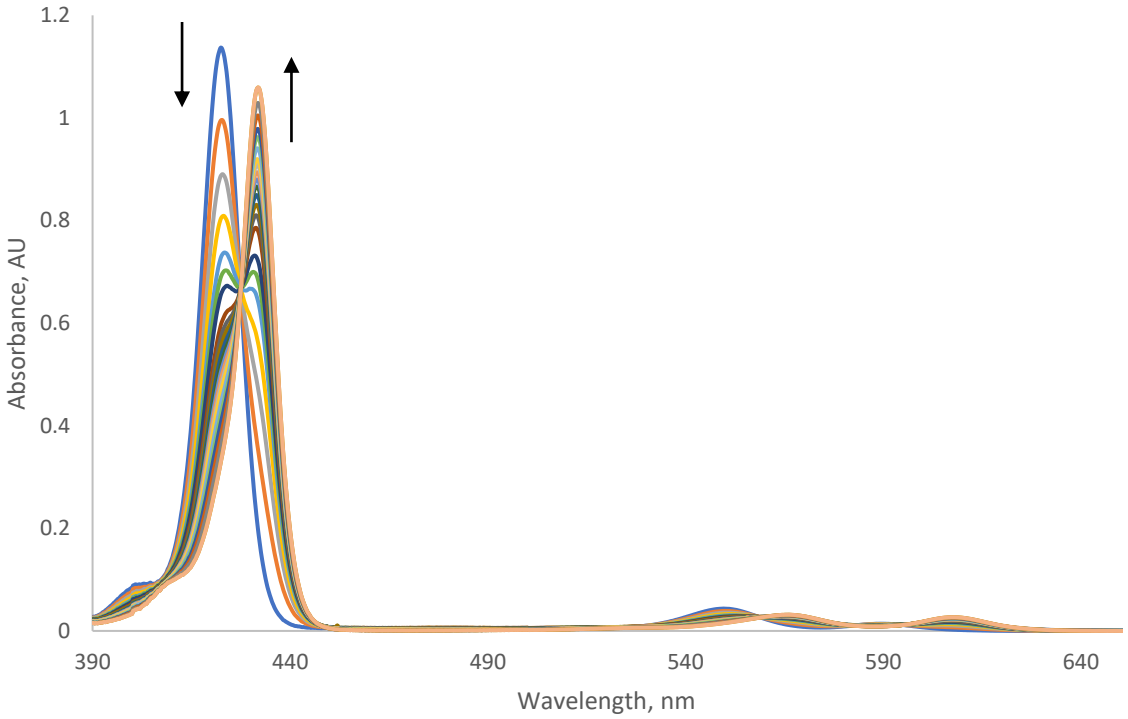


Figure S53. Changes in UV-Vis spectrum of **P2** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$7.79\cdot10^{-4}$ M).

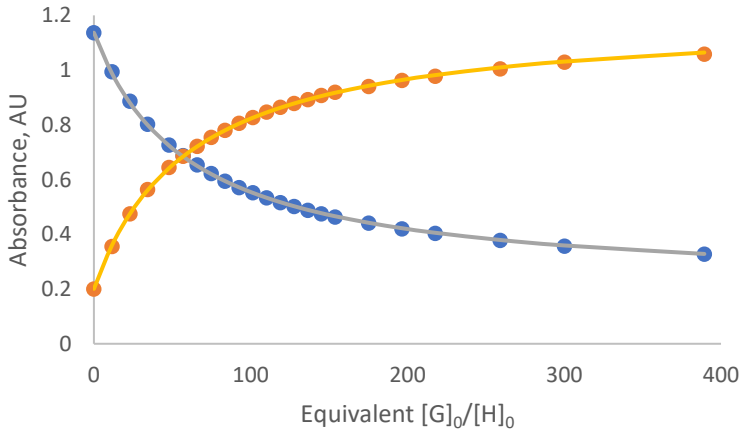


Figure S54. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P2** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P2** host. Blue points – absorption at 422.4 nm, orange points – absorption at 431.8 nm.

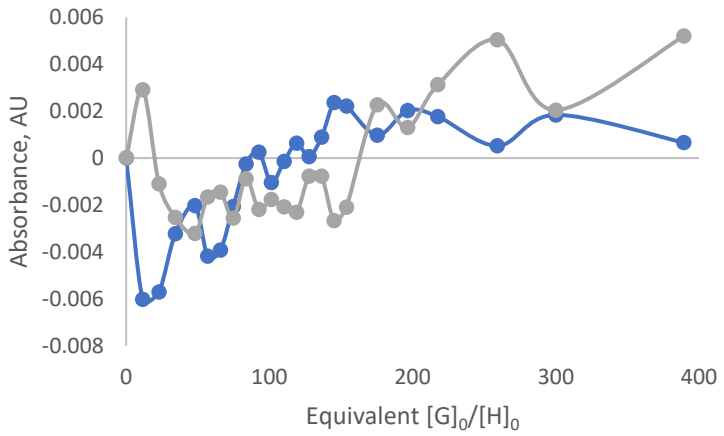


Figure S55. Residual analysis of UV-Vis titration between **P2** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P2** host. Blue points – absorption at 422.4 nm, grey points – absorption at 431.8 nm.

K_a (**1c** + **P2**) = (8.35 ± 0.03) × 10^3 M^{-1}

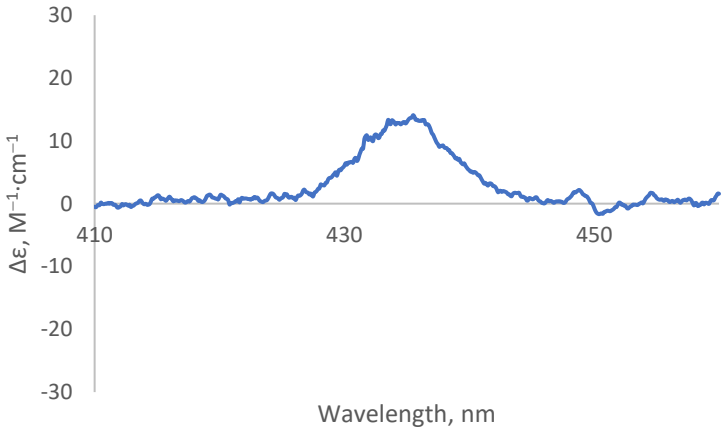


Figure S56. Experimental CD spectrum generated by mixing **P2** ($2.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($7.8 \cdot 10^{-4}$ M), 87% conversion to complex.

Spectroscopic data of system **1c** + **P4**

Table S16. Absorptions (AU) of **P4** (2.0×10^{-6} M) derived from the UV-Vis titration of **P4** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 417.8 nm	AU 428.8 nm	C_{1c}, M
1	1.182	0.085	0.00
2	1.047	0.238	$1.45\cdot10^{-5}$
3	0.937	0.359	$2.90\cdot10^{-5}$
4	0.870	0.428	$4.05\cdot10^{-5}$
5	0.818	0.485	$5.19\cdot10^{-5}$
6	0.763	0.544	$6.62\cdot10^{-5}$
7	0.716	0.595	$8.04\cdot10^{-5}$
8	0.676	0.639	$9.45\cdot10^{-5}$
9	0.642	0.676	$1.09\cdot10^{-4}$
10	0.612	0.706	$1.23\cdot10^{-4}$
11	0.587	0.733	$1.37\cdot10^{-4}$
12	0.565	0.760	$1.50\cdot10^{-4}$
13	0.544	0.778	$1.64\cdot10^{-4}$
14	0.526	0.799	$1.78\cdot10^{-4}$
15	0.509	0.814	$1.92\cdot10^{-4}$
16	0.495	0.828	$2.05\cdot10^{-4}$
17	0.483	0.839	$2.19\cdot10^{-4}$
18	0.472	0.851	$2.32\cdot10^{-4}$
19	0.462	0.862	$2.46\cdot10^{-4}$

20	0.444	0.880	$2.72 \cdot 10^{-4}$
21	0.427	0.899	$2.99 \cdot 10^{-4}$
22	0.414	0.912	$3.25 \cdot 10^{-4}$
23	0.393	0.932	$3.77 \cdot 10^{-4}$
24	0.376	0.952	$4.28 \cdot 10^{-4}$
25	0.357	0.973	$5.02 \cdot 10^{-4}$
26	0.336	0.997	$6.10 \cdot 10^{-4}$
27	0.321	1.012	$7.14 \cdot 10^{-4}$
28	0.299	1.034	$9.32 \cdot 10^{-4}$

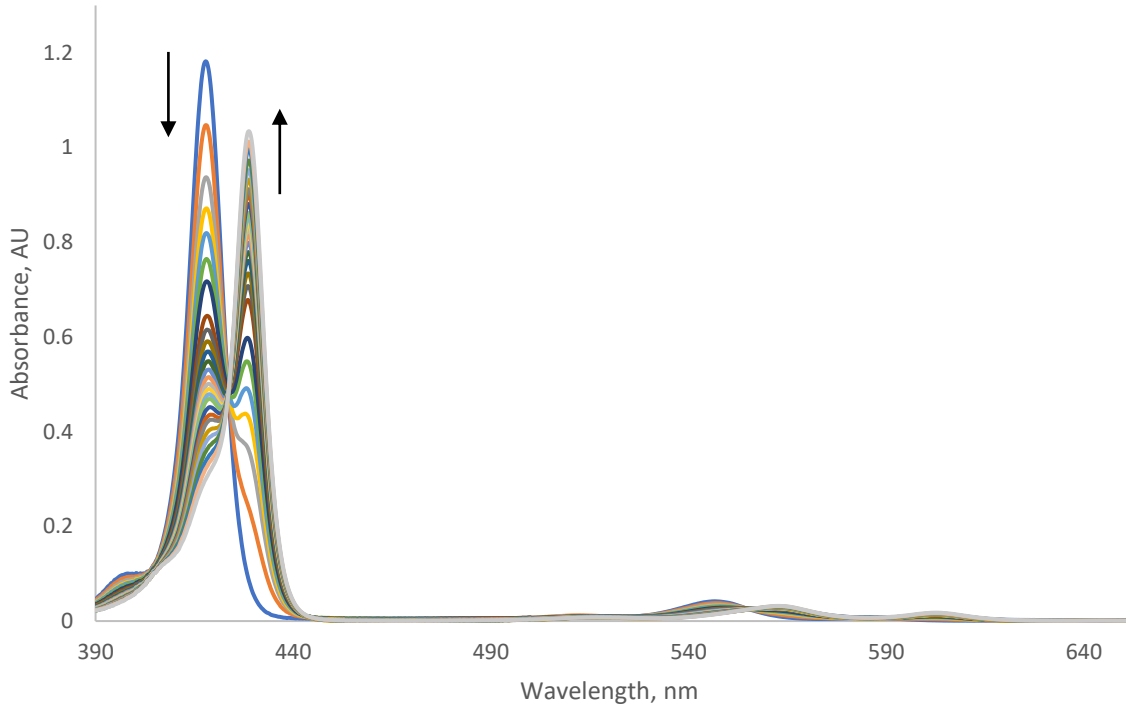


Figure S57. Changes in UV-Vis spectrum of **P4** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$9.32 \cdot 10^{-4}$ M).

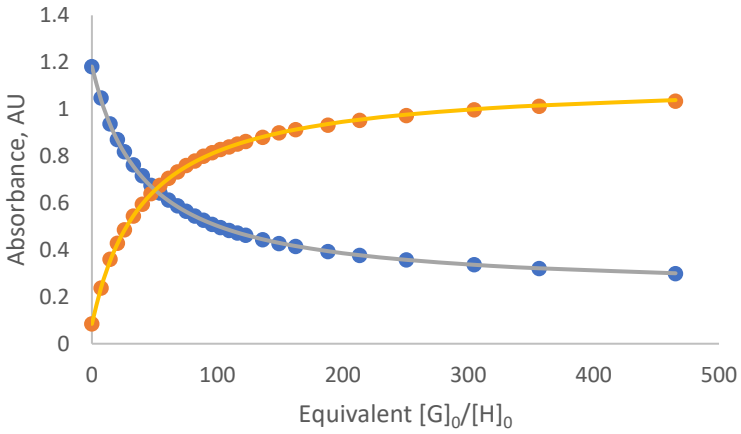


Figure S58. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P4** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P4** host. Blue points – absorption at 417.8 nm, orange points – absorption at 428.8 nm.

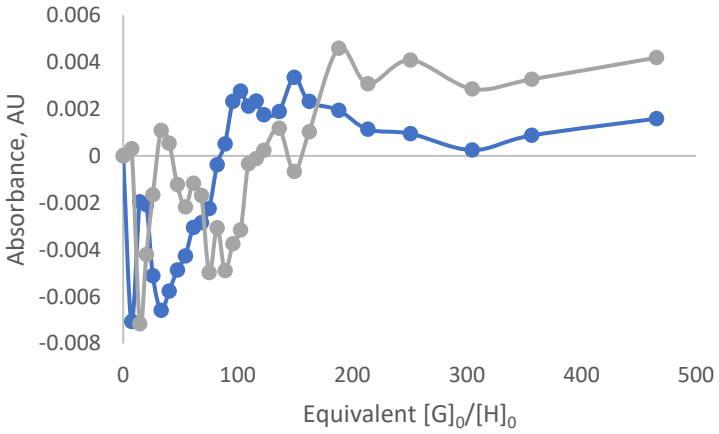


Figure S59. Residual analysis of UV-Vis titration between **P4** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P4** host. Blue points – absorption at 417.8 nm, grey points – absorption at 428.8 nm.

K_a (**1c** + **P4**) = (1.221 ± 0.005) × 10^4 M^{-1}

Spectroscopic data of system **1c** + **P5**

Table S17. Absorptions (AU) of **P5** (2.0×10^{-6} M) derived from the UV-Vis titration of **P5** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 419.4nm	AU 430.4 nm	C_{1c}, M
1	1.268	0.110	0.00
2	1.086	0.311	$1.37\cdot10^{-5}$
3	0.981	0.423	$2.73\cdot10^{-5}$
4	0.882	0.531	$4.09\cdot10^{-5}$
5	0.811	0.606	$5.44\cdot10^{-5}$
6	0.751	0.670	$6.78\cdot10^{-5}$
7	0.696	0.728	$8.12\cdot10^{-5}$
8	0.665	0.761	$9.19\cdot10^{-5}$
9	0.639	0.787	$1.03\cdot10^{-4}$
10	0.611	0.817	$1.13\cdot10^{-4}$
11	0.587	0.843	$1.24\cdot10^{-4}$
12	0.564	0.870	$1.34\cdot10^{-4}$
13	0.544	0.887	$1.45\cdot10^{-4}$
14	0.524	0.910	$1.55\cdot10^{-4}$
15	0.507	0.928	$1.65\cdot10^{-4}$
16	0.491	0.944	$1.76\cdot10^{-4}$
17	0.476	0.959	$1.86\cdot10^{-4}$
18	0.461	0.975	$1.96\cdot10^{-4}$
19	0.449	0.986	$2.07\cdot10^{-4}$

20	0.437	1.002	$2.17 \cdot 10^{-4}$
21	0.413	1.024	$2.42 \cdot 10^{-4}$
22	0.390	1.049	$2.67 \cdot 10^{-4}$
23	0.368	1.071	$2.92 \cdot 10^{-4}$
24	0.352	1.089	$3.17 \cdot 10^{-4}$
25	0.338	1.102	$3.41 \cdot 10^{-4}$
26	0.326	1.116	$3.65 \cdot 10^{-4}$
27	0.306	1.137	$4.13 \cdot 10^{-4}$
28	0.275	1.174	$5.17 \cdot 10^{-4}$
29	0.255	1.197	$6.18 \cdot 10^{-4}$

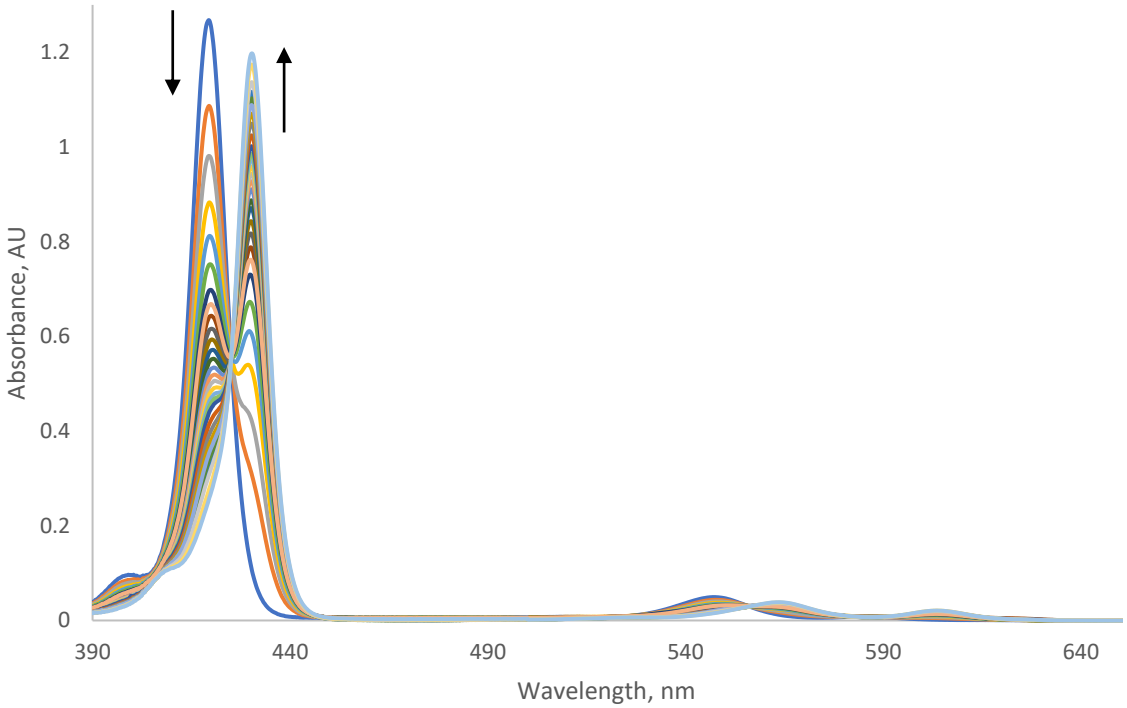


Figure S60. Changes in UV-Vis spectrum of **P5** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$6.18 \cdot 10^{-4}$ M).

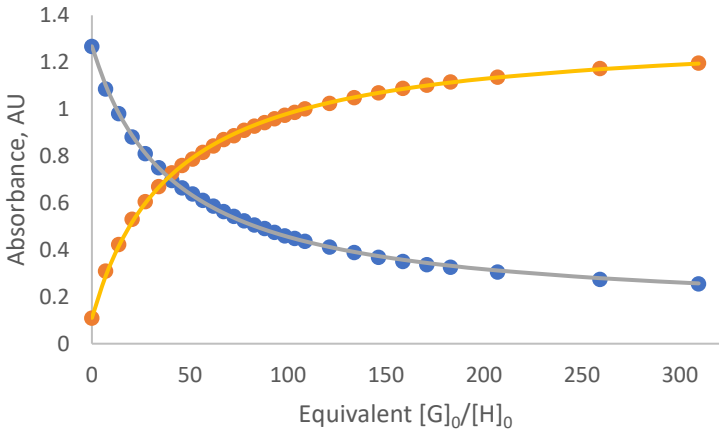


Figure S61. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P5** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P5** host. Blue points – absorption at 419.4 nm, orange points – absorption at 430.4 nm.

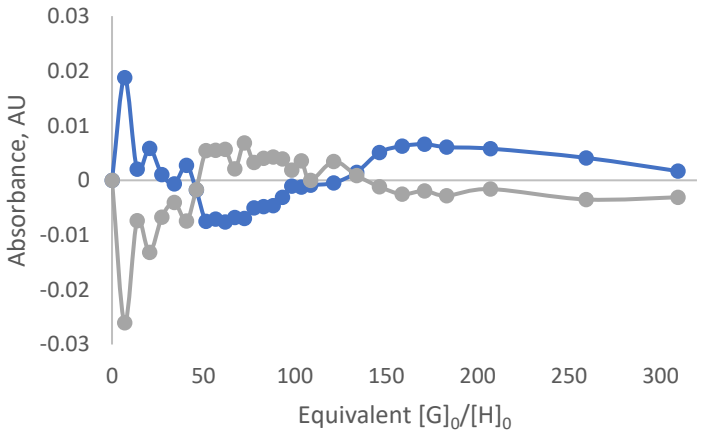


Figure S62. Residual analysis of UV-Vis titration between **P5** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P5** host. Blue points – absorption at 419.4 nm, grey points – absorption at 430.4 nm.

K_a (**1c** + **P5**) = (1.24 ± 0.01) × 10^4 M^{-1}

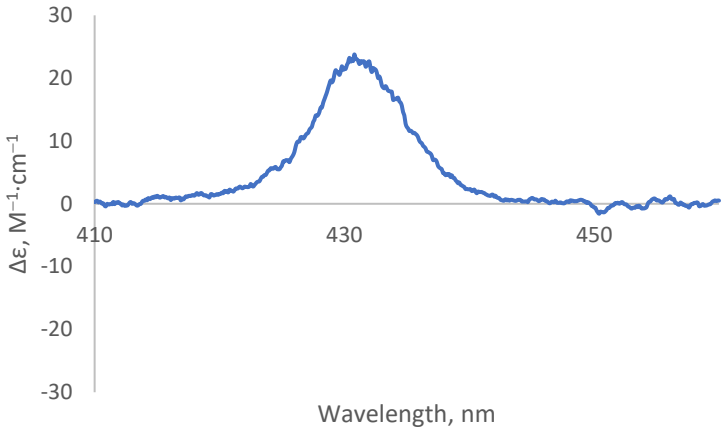


Figure S63. Experimental CD spectrum generated by mixing **P5** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($6.2 \cdot 10^{-4}$ M), 88% conversion to complex.

Spectroscopic data of system **1c** + **P6**

Table S18. Absorptions (AU) of **P6** (2.0×10^{-6} M) derived from the UV-Vis titration of **P6** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	Abs 417.8 nm	Abs 429.4 nm	C_{1c}, M
1	1.228	0.086	0.00
2	1.094	0.233	$7.20 \cdot 10^{-6}$
3	0.969	0.365	$1.44 \cdot 10^{-5}$
4	0.883	0.458	$2.15 \cdot 10^{-5}$
5	0.817	0.528	$2.86 \cdot 10^{-5}$
6	0.756	0.591	$3.56 \cdot 10^{-5}$
7	0.705	0.646	$4.27 \cdot 10^{-5}$
8	0.663	0.689	$4.97 \cdot 10^{-5}$
9	0.626	0.725	$5.66 \cdot 10^{-5}$
10	0.593	0.760	$6.36 \cdot 10^{-5}$

11	0.559	0.791	$7.04 \cdot 10^{-5}$
12	0.539	0.815	$7.73 \cdot 10^{-5}$
13	0.513	0.842	$8.41 \cdot 10^{-5}$
14	0.491	0.866	$9.09 \cdot 10^{-5}$
15	0.472	0.883	$9.77 \cdot 10^{-5}$
16	0.455	0.900	$1.04 \cdot 10^{-4}$
17	0.439	0.916	$1.11 \cdot 10^{-4}$
18	0.414	0.940	$1.24 \cdot 10^{-4}$
19	0.390	0.965	$1.38 \cdot 10^{-4}$
20	0.371	0.982	$1.51 \cdot 10^{-4}$
21	0.354	0.999	$1.64 \cdot 10^{-4}$
22	0.329	1.029	$1.89 \cdot 10^{-4}$
23	0.308	1.047	$2.14 \cdot 10^{-4}$
24	0.285	1.071	$2.51 \cdot 10^{-4}$
25	0.260	1.098	$3.05 \cdot 10^{-4}$
26	0.230	1.126	$4.06 \cdot 10^{-4}$

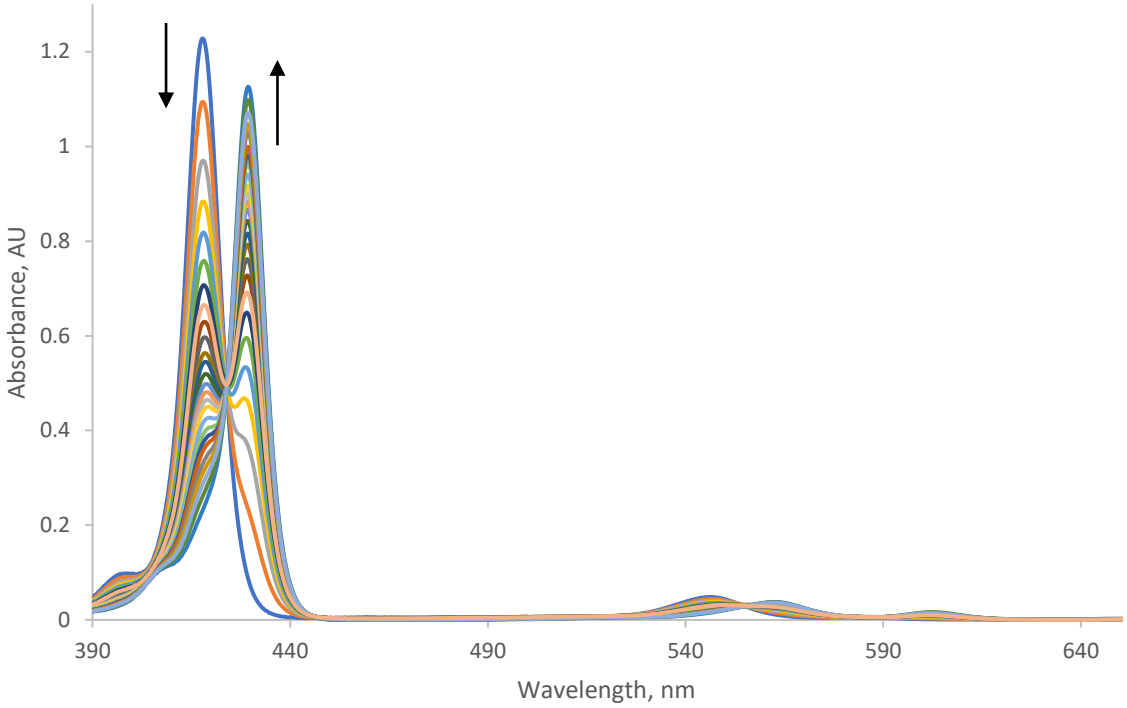


Figure S64. Changes in UV-Vis spectrum of **P6** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$4.06\cdot10^{-4}$ M).

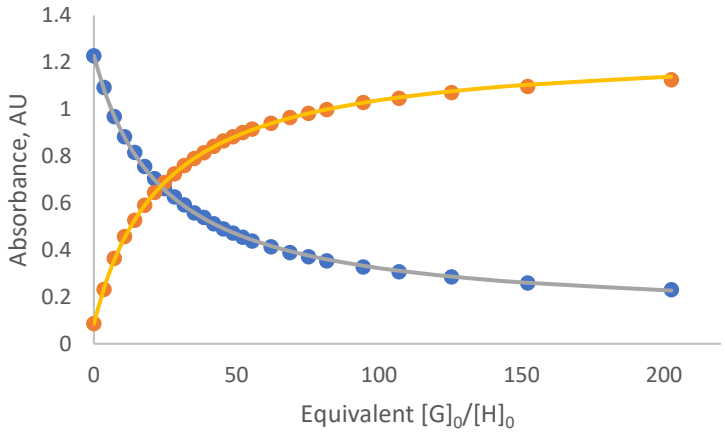


Figure S65. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P6** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P6** host. Blue points – absorption at 417.8 nm, orange points – absorption at 429.4 nm.

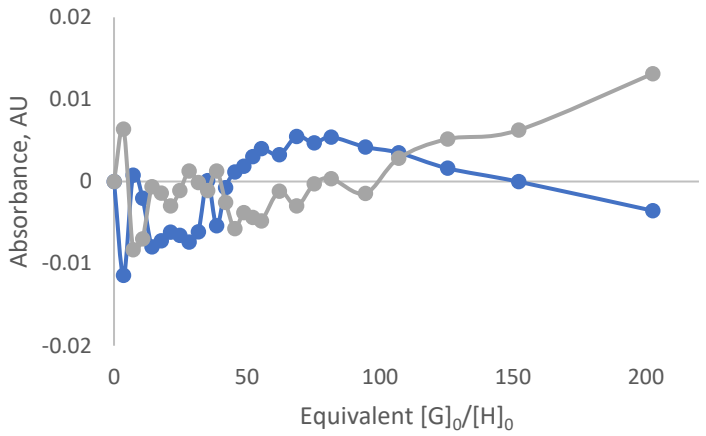


Figure S66. Residual analysis of UV-Vis titration between **P6** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P6** host. Blue points – absorption at 417.8 nm, grey points – absorption at 429.4 nm.

K_a (**1c** + **P6**) = (2.16 ± 0.01) × 10^4 M^{-1}

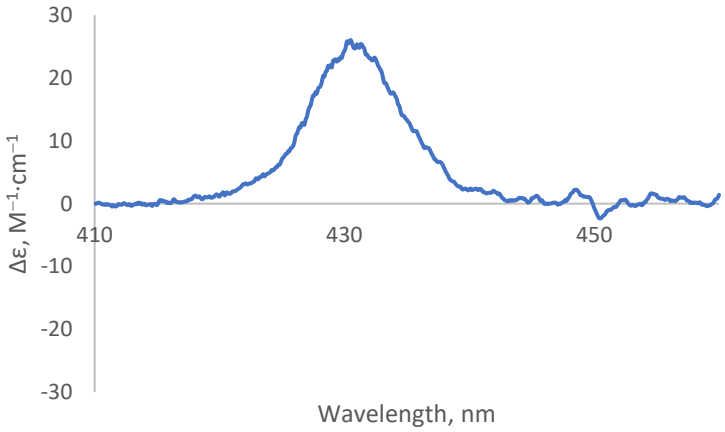


Figure S67. Experimental CD spectrum generated by mixing **P6** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($1.8 \cdot 10^{-2}$ M), >99% conversion to complex.

Spectroscopic data of system **1c** + **P7**

Table S19. Absorptions (AU) of **P7** (2.0×10^{-6} M) derived from the UV-Vis titration of **P7** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 420.6 nm	AU 432.6 nm	C_{1c}, M
1	0.850	0.094	0.00
2	0.689	0.255	$1.13\cdot10^{-5}$
3	0.579	0.367	$2.26\cdot10^{-5}$
4	0.503	0.441	$3.38\cdot10^{-5}$
5	0.446	0.497	$4.50\cdot10^{-5}$
6	0.402	0.543	$5.62\cdot10^{-5}$
7	0.339	0.605	$7.85\cdot10^{-5}$
8	0.320	0.621	$8.96\cdot10^{-5}$
9	0.284	0.657	$1.12\cdot10^{-4}$
10	0.260	0.681	$1.34\cdot10^{-4}$
11	0.240	0.701	$1.56\cdot10^{-4}$
12	0.223	0.718	$1.77\cdot10^{-4}$
13	0.205	0.732	$2.21\cdot10^{-4}$
14	0.189	0.748	$2.64\cdot10^{-4}$
15	0.177	0.761	$3.06\cdot10^{-4}$
16	0.163	0.772	$3.90\cdot10^{-4}$
17	0.152	0.783	$4.73\cdot10^{-4}$
18	0.143	0.783	$5.53\cdot10^{-4}$
19	0.138	0.797	$6.33\cdot10^{-4}$

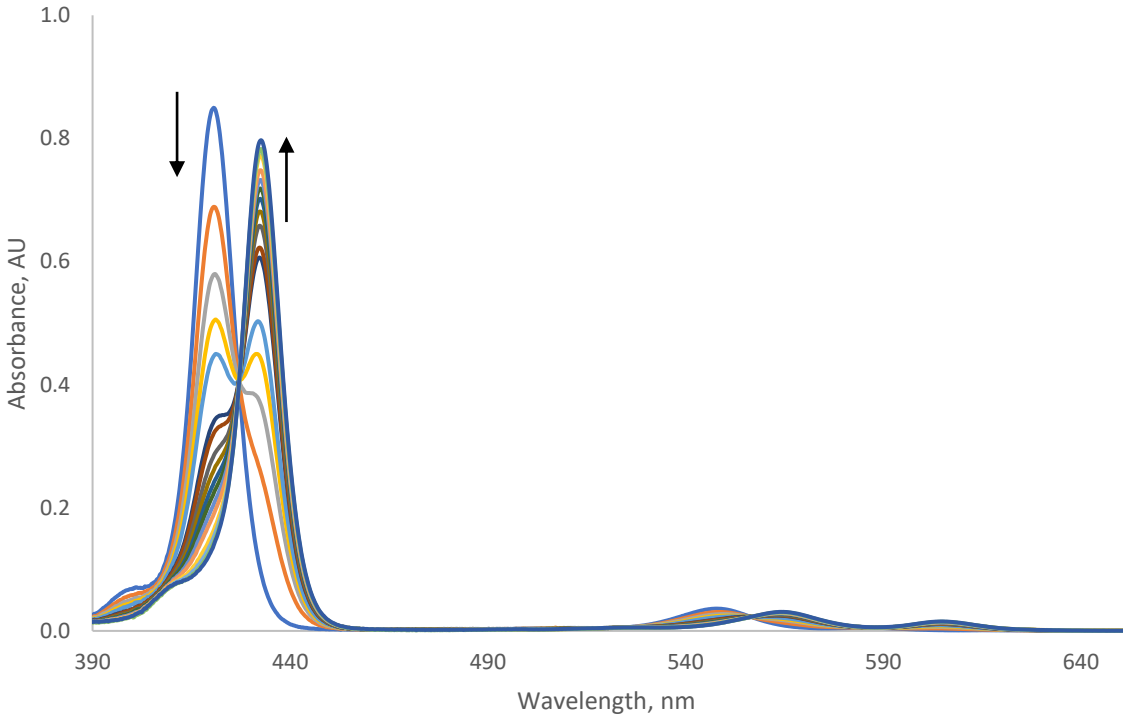


Figure S68. Changes in UV-Vis spectrum of **P7** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** ($0–6.63\cdot10^{-4}$ M).

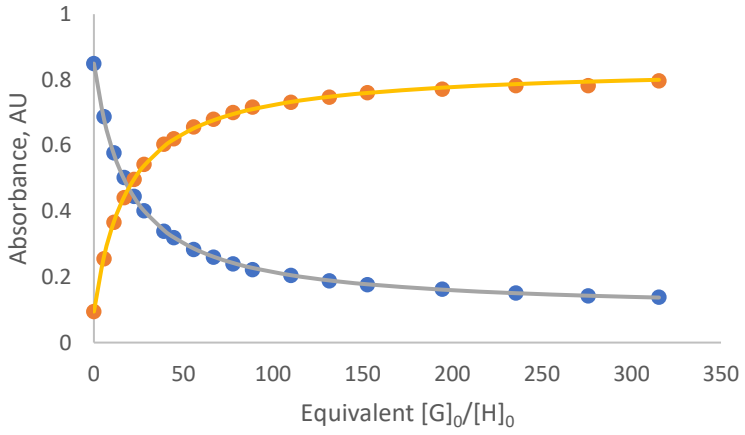


Figure S69. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P7** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P7** host. Blue points – absorption at 420.6 nm, orange points – absorption at 432.6 nm.

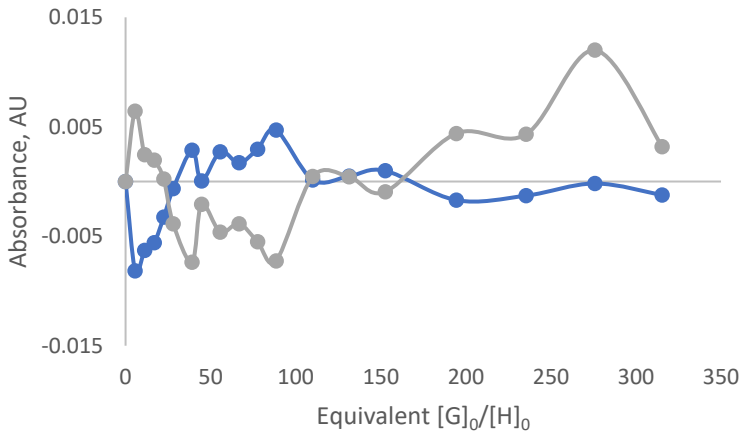


Figure S70. Residual analysis of UV-Vis titration between **P7** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P7** host. Blue points – absorption at 420.6 nm, grey points – absorption at 432.6 nm.

K_a (**1c** + **P7**) = (2.66 ± 0.03) × 10^4 M^{-1}

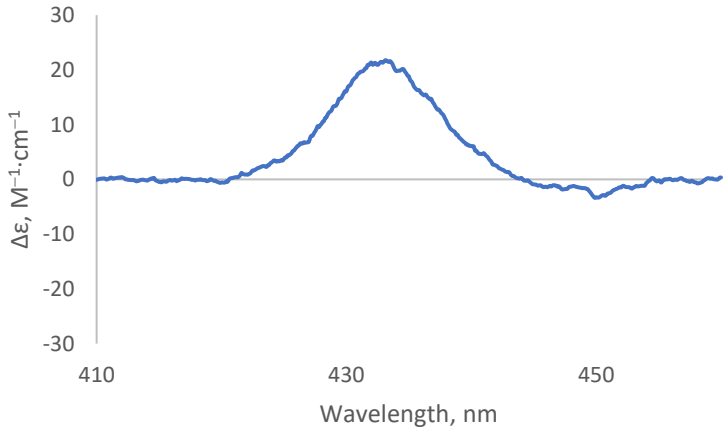


Figure S71. Experimental CD spectrum generated by mixing **P7** ($2.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($6.0 \cdot 10^{-3}$ M), 95% conversion to complex.

Spectroscopic data of system **1c** + **P8**

Table S20. Absorptions (AU) of **P8** (2.0×10^{-6} M) derived from the UV-Vis titration of **P8** with **1c** in CH_2Cl_2 and concentrations of **1c** at 293 K.

Sample no	AU 412.8 nm	AU 425.0 nm	C_{1c}, M
1	0.960	0.022	0.00
2	0.931	0.051	$6.15\cdot10^{-7}$
3	0.892	0.079	$1.23\cdot10^{-6}$
4	0.849	0.145	$1.84\cdot10^{-6}$
5	0.796	0.200	$2.45\cdot10^{-6}$
6	0.750	0.252	$3.06\cdot10^{-6}$
7	0.707	0.300	$3.67\cdot10^{-6}$
8	0.660	0.352	$4.28\cdot10^{-6}$
9	0.633	0.384	$4.88\cdot10^{-6}$
10	0.605	0.414	$5.49\cdot10^{-6}$
11	0.580	0.441	$6.09\cdot10^{-6}$
12	0.557	0.468	$6.69\cdot10^{-6}$
13	0.536	0.492	$7.29\cdot10^{-6}$
14	0.518	0.512	$7.89\cdot10^{-6}$
15	0.500	0.532	$8.48\cdot10^{-6}$
16	0.469	0.567	$9.67\cdot10^{-6}$
17	0.450	0.587	$1.09\cdot10^{-5}$
18	0.422	0.619	$1.20\cdot10^{-5}$
19	0.388	0.659	$1.44\cdot10^{-5}$

20	0.358	0.691	$1.67 \cdot 10^{-5}$
21	0.325	0.728	$2.01 \cdot 10^{-5}$
22	0.297	0.760	$2.35 \cdot 10^{-5}$
23	0.271	0.791	$2.80 \cdot 10^{-5}$
24	0.252	0.812	$3.23 \cdot 10^{-5}$
25	0.224	0.845	$4.09 \cdot 10^{-5}$
26	0.201	0.873	$5.31 \cdot 10^{-5}$
27	0.180	0.899	$7.03 \cdot 10^{-5}$
28	0.165	0.918	$8.62 \cdot 10^{-5}$
29	0.156	0.931	$1.01 \cdot 10^{-4}$

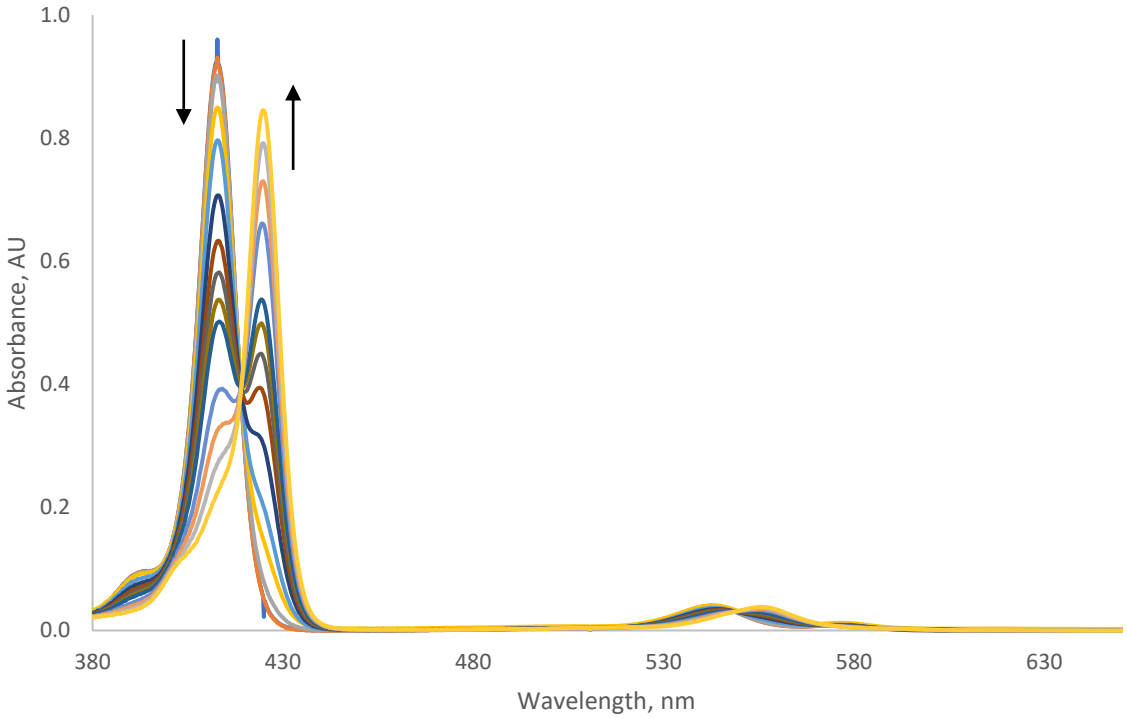


Figure S72. Changes in UV-Vis spectrum of **P8** (2.0×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1c** (0–$1.01 \cdot 10^{-4}$ M).

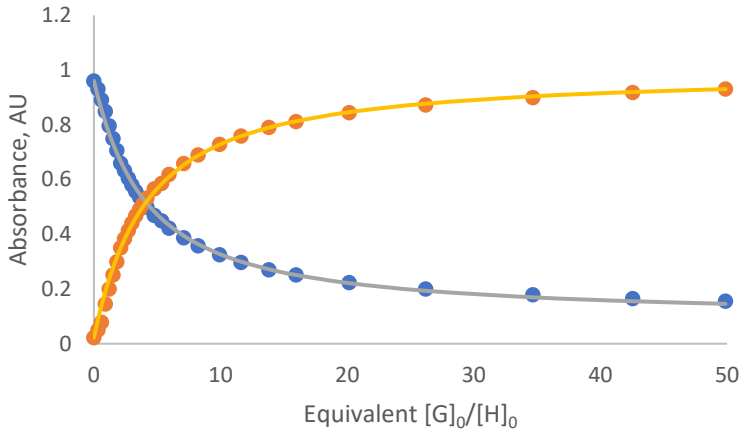


Figure S73. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P8** and **1c** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P8** host. Blue points – absorption at 412.8 nm, orange points – absorption at 425.0 nm.

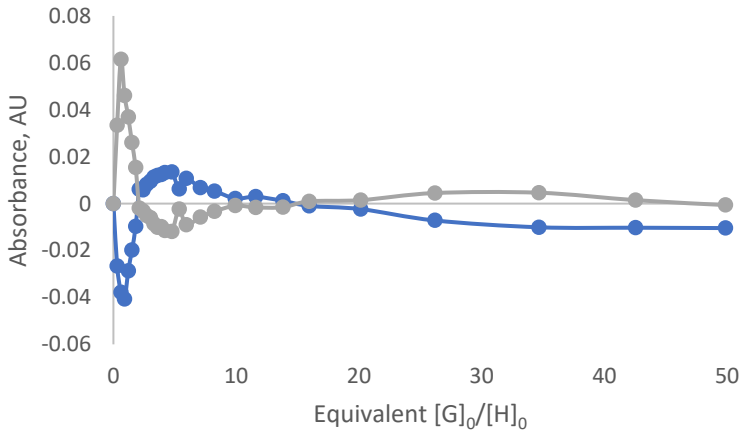


Figure S74. Residual analysis of UV-Vis titration between **P8** and **1c** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1c** guest and **P8** host. Blue points – absorption at 412.8 nm, grey points – absorption at 425.0 nm.

K_a (**1c** + **P8**) = (1.41 ± 0.04) × 10^5 M^{-1}

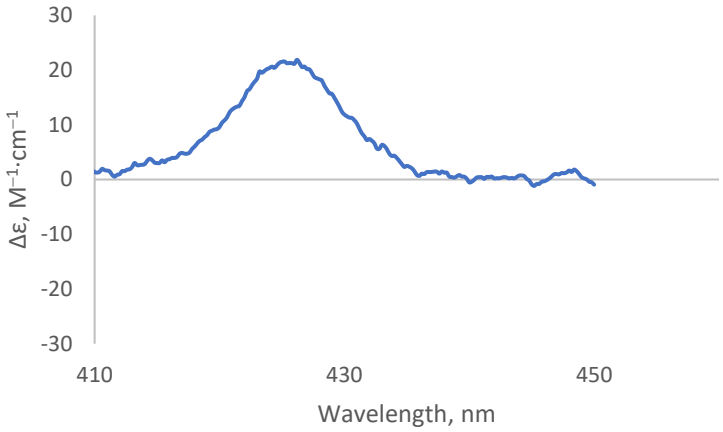


Figure S75. Experimental CD spectrum generated by mixing **P8** ($2.1 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1c** ($1.4 \cdot 10^{-4}$ M), 92% conversion to complex.

Spectroscopic data of system **1d** + **P8**

Table S21. Absorptions (AU) of **P8** (2.3×10^{-6} M) derived from the UV-Vis titration of **P8** with **1d** in CH_2Cl_2 and concentrations of **1d** at 293 K.

Sample no	AU 412.8 nm	AU 425.0 nm	$C_{\mathbf{1d}}$, M
1	1.047	0.072	0.00
2	1.027	0.088	$1.96 \cdot 10^{-5}$
3	1.016	0.104	$3.92 \cdot 10^{-5}$
4	0.999	0.118	$7.83 \cdot 10^{-5}$
5	0.979	0.132	$1.17 \cdot 10^{-4}$
6	0.960	0.148	$1.56 \cdot 10^{-4}$
7	0.939	0.166	$1.94 \cdot 10^{-4}$
8	0.922	0.182	$2.33 \cdot 10^{-4}$
9	0.899	0.201	$3.09 \cdot 10^{-4}$
10	0.875	0.223	$3.84 \cdot 10^{-4}$

11	0.843	0.249	$4.96 \cdot 10^{-4}$
12	0.811	0.275	$6.06 \cdot 10^{-4}$
13	0.778	0.305	$7.51 \cdot 10^{-4}$
14	0.747	0.330	$8.93 \cdot 10^{-4}$
15	0.718	0.358	$1.03 \cdot 10^{-3}$
16	0.684	0.390	$1.17 \cdot 10^{-3}$
17	0.659	0.413	$1.30 \cdot 10^{-3}$
18	0.635	0.437	$1.44 \cdot 10^{-3}$
19	0.602	0.467	$1.69 \cdot 10^{-3}$
20	0.574	0.494	$1.94 \cdot 10^{-3}$
21	0.533	0.536	$2.30 \cdot 10^{-3}$
22	0.500	0.570	$2.64 \cdot 10^{-3}$
23	0.459	0.616	$3.12 \cdot 10^{-3}$
24	0.426	0.653	$3.57 \cdot 10^{-3}$
25	0.394	0.694	$3.99 \cdot 10^{-3}$
26	0.374	0.723	$4.39 \cdot 10^{-3}$
27	0.354	0.750	$4.76 \cdot 10^{-3}$
28	0.346	0.772	$4.90 \cdot 10^{-3}$
29	0.330	0.790	$5.19 \cdot 10^{-3}$
30	0.319	0.810	$5.94 \cdot 10^{-3}$
31	0.302	0.830	$7.04 \cdot 10^{-3}$

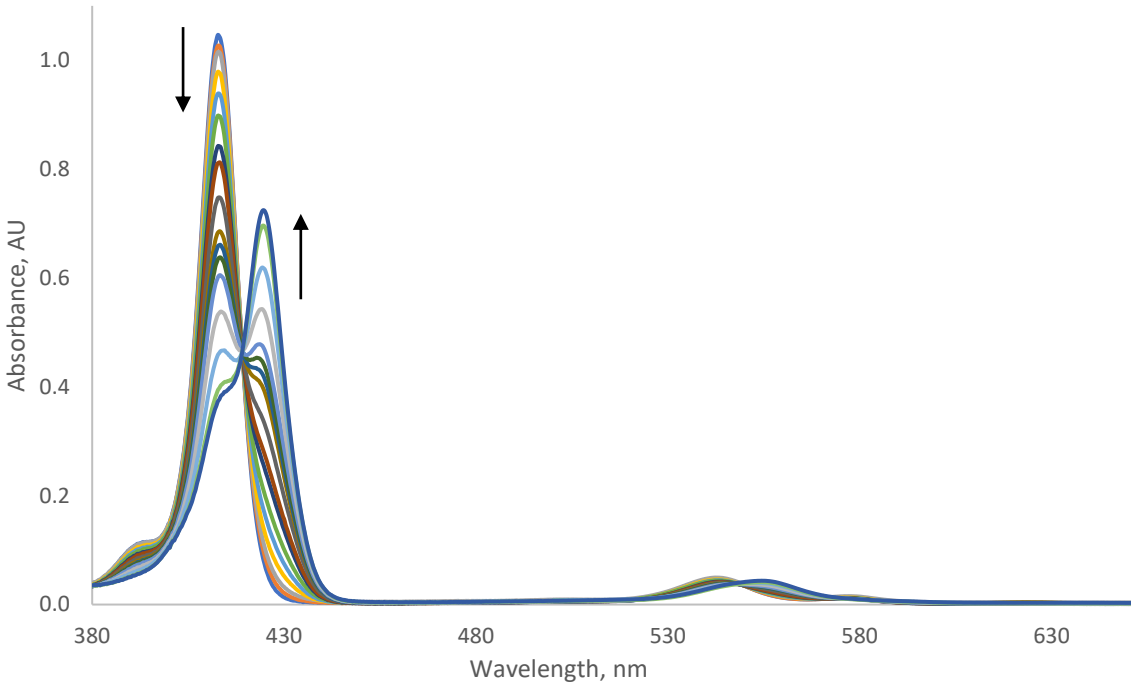


Figure S76. Changes in UV-Vis spectrum of **P8** (2.3×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1d** (0–$7.04\cdot10^{-3}$ M).

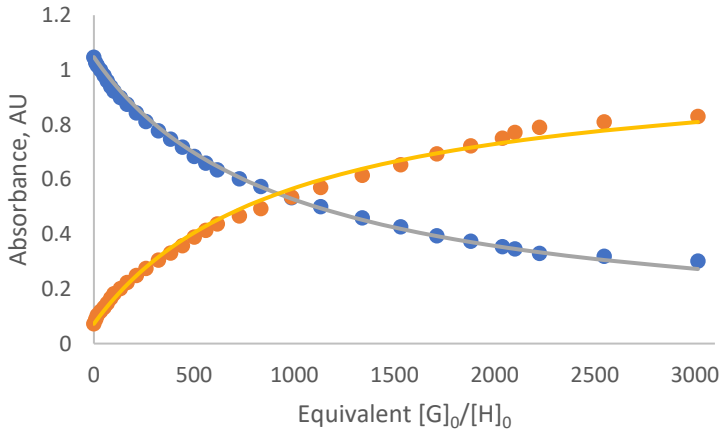


Figure S77. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P8** and **1d** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1d** guest and **P8** host. Blue points – absorption at 412.8 nm, orange points – absorption at 425.0 nm.

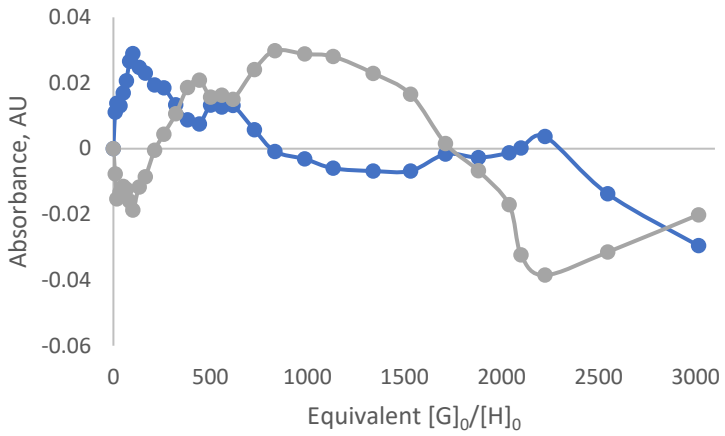


Figure S78. Residual analysis of UV-Vis titration between **P8** and **1d** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1d** guest and **P8** host. Blue points – absorption at 412.8 nm, grey points – absorption at 425.0 nm.

K_a (**1d** + **P8**) = (4.5 ± 0.1) × 10^2 M^{-1}

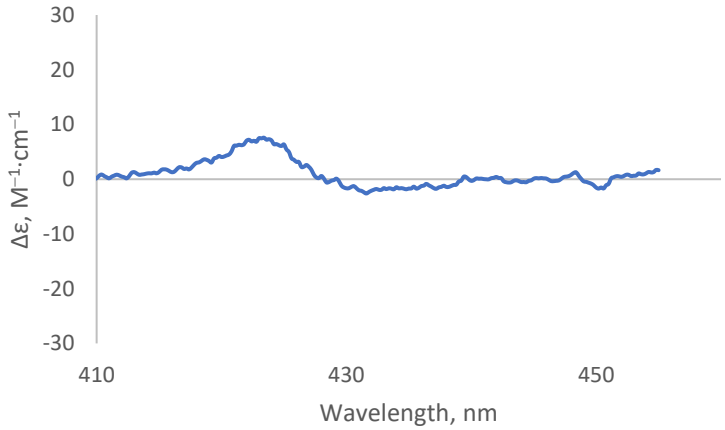


Figure S79. Experimental CD spectrum generated by mixing **P8** ($2.3 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1d** ($1.8 \cdot 10^{-2}$ M), 90% conversion to complex.

Spectroscopic data of system **1d** + **P9**

Table S22. Absorptions (AU) of **P9** (1.9×10^{-6} M) derived from the UV-Vis titration of **P9** with **1d** in CH_2Cl_2 and concentrations of **1d** at 293 K.

Sample no	AU 455.8 nm	AU 472.4 nm	C_{1d}, M
1	0.368	0.187	0.00
2	0.326	0.210	$2.59\cdot10^{-5}$
3	0.297	0.227	$5.18\cdot10^{-5}$
4	0.276	0.240	$7.75\cdot10^{-5}$
5	0.261	0.250	$1.03\cdot10^{-4}$
6	0.248	0.260	$1.29\cdot10^{-4}$
7	0.240	0.267	$1.55\cdot10^{-4}$
8	0.228	0.277	$2.06\cdot10^{-4}$
9	0.221	0.285	$2.56\cdot10^{-4}$
10	0.212	0.293	$3.57\cdot10^{-4}$
11	0.206	0.299	$5.07\cdot10^{-4}$
12	0.201	0.305	$7.03\cdot10^{-4}$
13	0.198	0.309	$8.95\cdot10^{-4}$
14	0.196	0.310	$1.08\cdot10^{-3}$
15	0.196	0.312	$1.27\cdot10^{-3}$

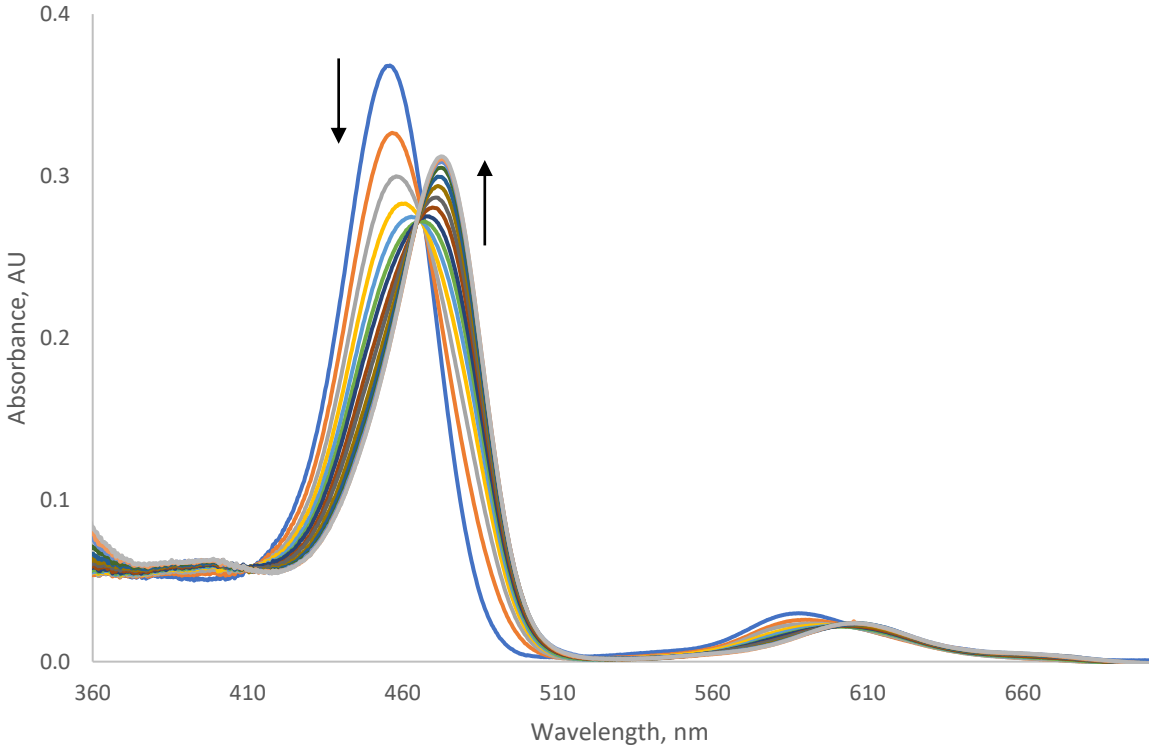


Figure S80. Changes in UV-Vis spectrum of **P9** (1.9×10^{-6} M, CH_2Cl_2, 293 K) caused by portion-wise addition of guest **1d** (0–$1.27\cdot10^{-3}$ M).

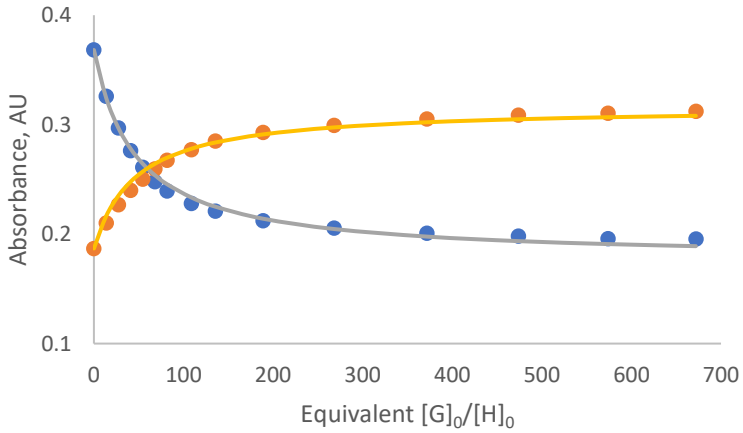


Figure S81. UV-Vis experimental (points) and 1:1 fitted (line) titration curves of **P9** and **1d** in CH_2Cl_2. $[G]_0/[H]_0$ defines the ratio of **1d** guest and **P9** host. Blue points – absorption at 455.8nm, orange points – absorption at 472.4 nm.

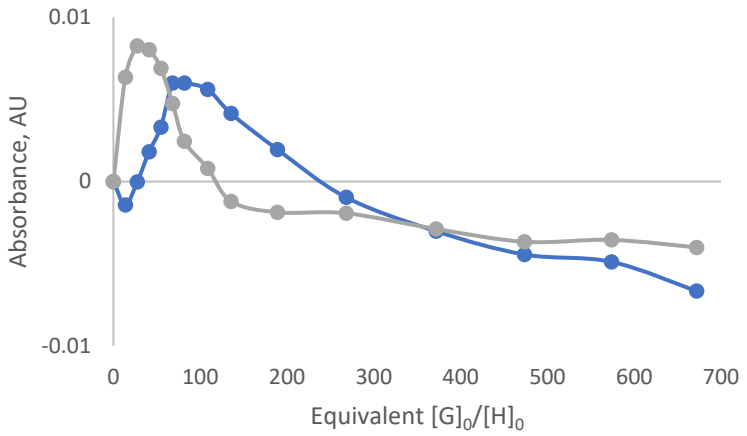


Figure S82. Residual analysis of UV-Vis titration between **P9** and **1d** in CH_2Cl_2 using 1:1 model. $[G]_0/[H]_0$ defines the ratio of **1d** guest and **P9** host. Blue points – absorption at 455.8 nm, grey points – absorption at 472.4 nm.

K_a (**1d** + **P9**) = (1.16 ± 0.07) × 10^4 M^{-1}

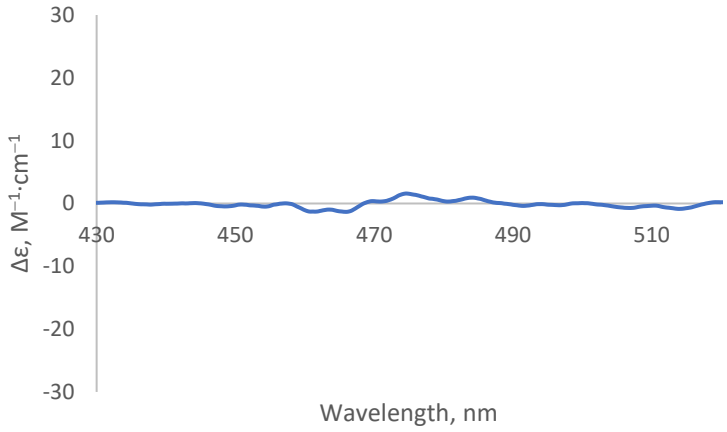


Figure S83. Experimental CD spectrum generated by mixing **P9** ($4.0 \cdot 10^{-6}$ M, CH_2Cl_2, 293 K) and **1d** ($1.3 \cdot 10^{-3}$ M), 96% conversion to complex.

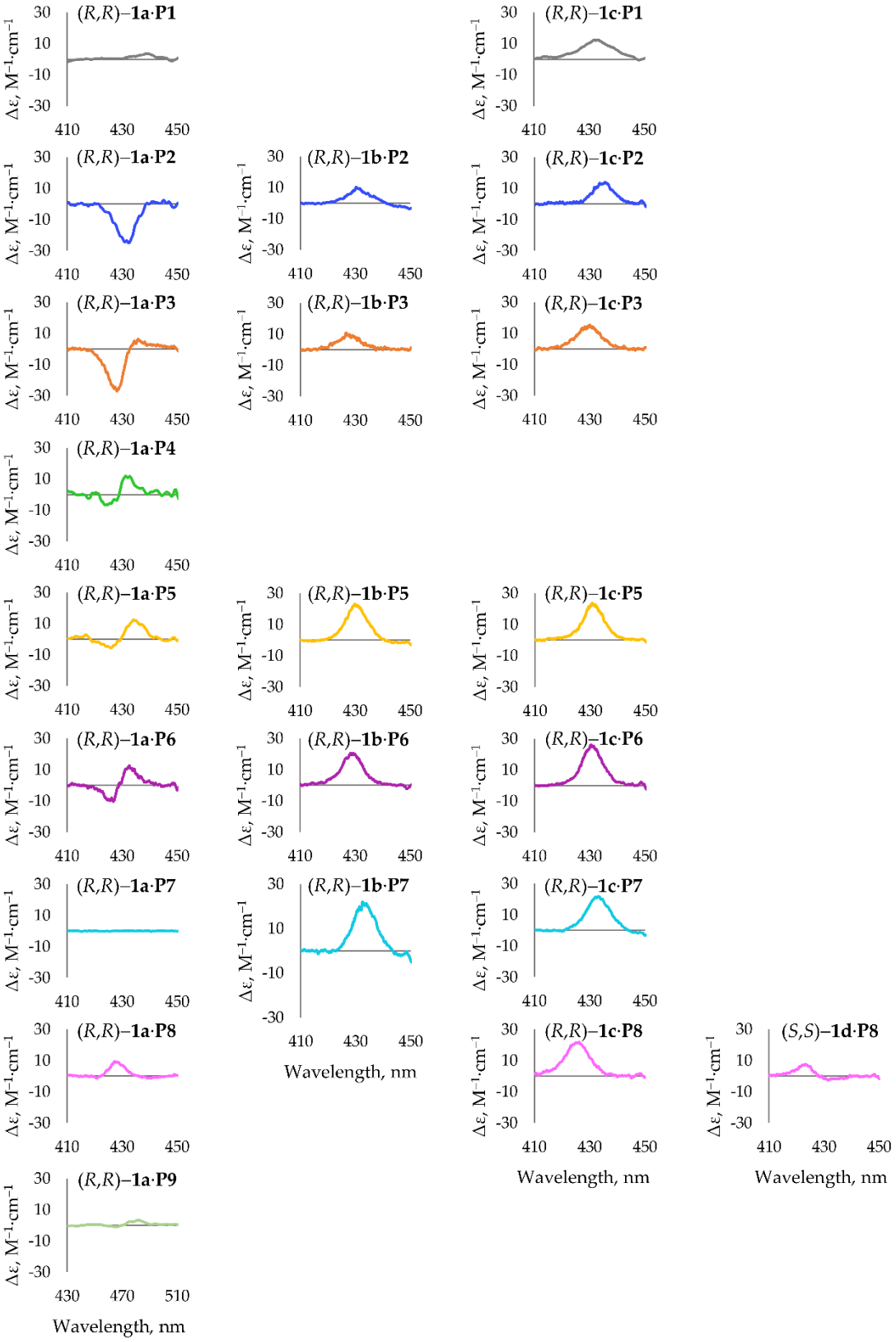


Figure S84. Overview of experimental CD spectra obtained for the complexes of thioureas **1a-d** with zinc porphyrins **P1-P9** (CH_2Cl_2, 293 K).

2. UV-Vis and CD spectra of compound 1a

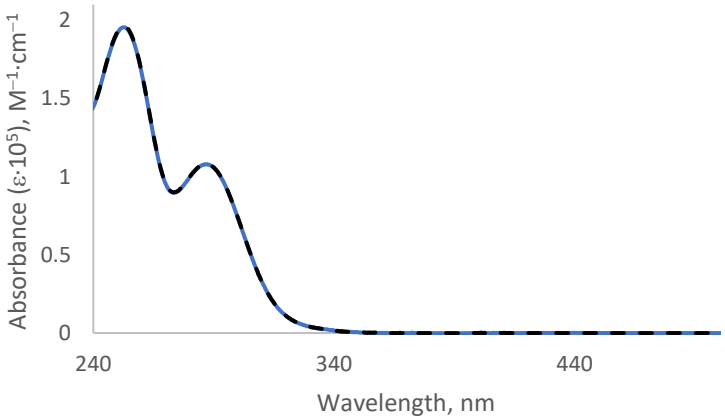


Figure S85. Experimental UV-Vis spectra of (*R*,*R*)-**1a** ($5.25 \cdot 10^{-5}$ M, CH_2Cl_2, 293 K, blue solid line) and (*S*,*S*)-**1a** ($5.24 \cdot 10^{-5}$ M, CH_2Cl_2, 293 K, black dotted line). The solvent cutoff is at 239 nm.

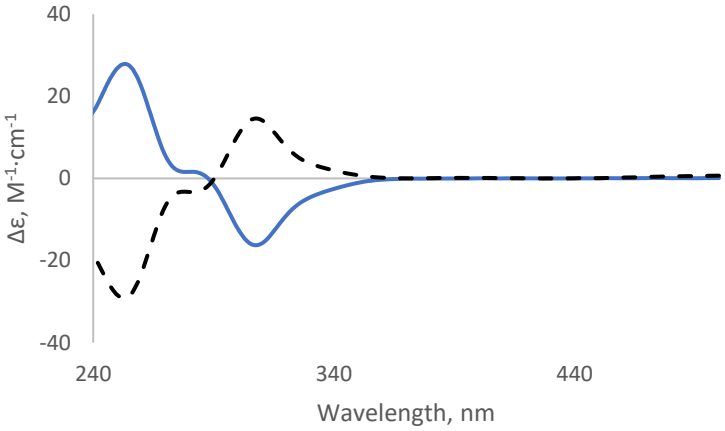


Figure S86. Experimental CD spectra of (*R*,*R*)-**1a** ($5.25 \cdot 10^{-5}$ M, CH_2Cl_2, 293 K, blue solid line) and (*S*,*S*)-**1a** ($5.24 \cdot 10^{-5}$ M, CH_2Cl_2, 293 K, black dotted line). The solvent cutoff is at 239 nm.

3. NSD distortion analysis for the porphyrin core in 1b·P5 complex

The porphyrin core was extracted from X-ray data (CCDC 2081478). All atoms were deleted except 24 atoms of the porphyrin core. The porphyrin core was subjected to NSD analysis with on-line tool [2–4].

Table S23. Summary of the NSD (in Å)

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.20	0.00	0.00	0.01	0.00	0.02	0.20	-0.01
ext.	0.20	0.00	0.00	0.01	0.00	0.02	0.20	-0.01
			0.01	0.00	0.00	-0.01	-0.02	-0.01
total	0.20	0.00	0.00	0.01	0.00	0.02	0.20	-0.01
			0.01	0.00	0.00	-0.01	-0.02	-0.01
			-0.01	0.01	0.00	0.00	0.02	0.00
			0.00	0.00	0.00	0.00	-0.01	0.00
			0.00	0.00	-0.01	0.00	0.01	-0.01
			0.01	-0.01	0.00	0.00	0.00	
					0.00	0.01		
					0.01	0.00		
					0.01	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.20	0.00	0.01	0.01	0.02	0.02	0.20	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.45	0.00	0.35	-0.24	0.02	0.03	0.14	0.00
ext.	0.46	0.00	0.35	-0.24	0.02	0.03	0.14	0.00
			-0.06	0.00	0.02	-0.06	0.09	0.00
total	0.46	0.00	0.35	-0.24	0.02	0.03	0.14	0.00
			-0.06	0.00	0.02	-0.06	0.09	0.00
			0.00	0.00	-0.01	0.01	0.00	
						0.01	-0.01	
						0.00	0.01	
comp.	0.46	0.00	0.35	0.24	0.03	0.07	0.17	0.00

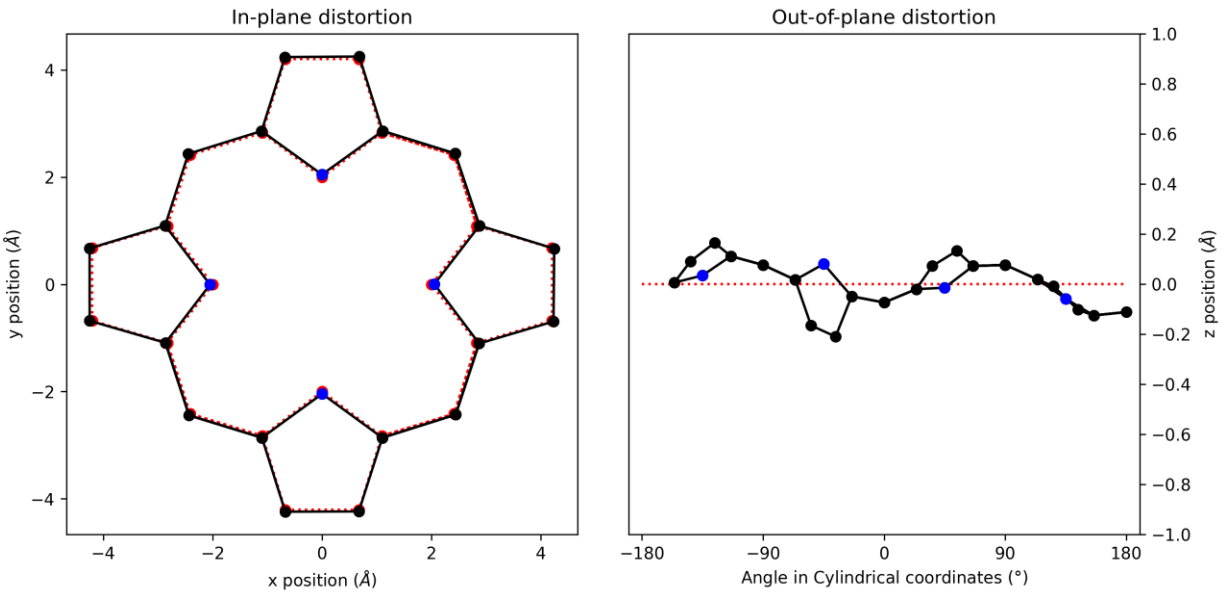


Figure S87. (a) in-plane and **(b)** out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

Table S24. Summary of structural parameters

Bond Distances, Bond Angles, Atom Displacements	**Mean Value (standard error)**	**Units**
$N–C_a$	1.373(6)	(Å)
$C_a–C_b$	1.444(6)	(Å)
$C_a–C_m$	1.405(9)	(Å)
$C_b–C_b$	1.355(5)	(Å)
$\angle C_aC_bC_b$	107.1(3)	(°)
$\angle NC_aC_b$	109.6(4)	(°)
$\angle NC_aC_m$	125.6(4)	(°)
$\angle C_aNC_a$	106.7(4)	(°)
$\angle C_mC_aC_b$	124.8(3)	(°)
$\angle C_aC_mC_a$	125.4(4)	(°)
Δ24	0.0786	(Å)
ΔN	0.05(3)	(Å)
ΔC_a	0.05(5)	(Å)
ΔC_b	0.12(5)	(Å)
ΔC_m	0.08(2)	(Å)
∠ pyrrole tilt	4.7(14)	(°)
N···N dist (adj)	2.897(4)	(Å)

Bond Distances, Bond Angles, Atom Displacements	Mean Value (standard error)	Units
N···N dist (opp)	4.097(5)	(Å)

Table S25. Porphyrin structure tests

test	value
Probable correct structure (Σ residual total values = 0):	True
Solution symmetry guess (ip > 0.2, oop > 0.5):	D4h
Crystal phase symmetry guess (ip > 0.03, oop > 0.1):	C1
Exact centrosymmetry (Σ|ungerade| > 0.01):	False
Approx. centrosymmetry (Σ|ungerade| > 0.1):	False
B_{2g} tests:	
B_{1g} tests:	
A_{1g} tests:	Expanded porphyrin core (Zn-like)
A_{2g} tests:	
B_{2u} tests:	
B_{1u} tests:	
A_{2u} tests:	
CCDC most similar in plane (leastsq):	NANZAG
CCDC most similar out of plane (leastsq):	NEFTUN
CCDC most similar in plane (leastsum):	HALXEX
CCDC most similar out of plane (leastsum):	NEFTUN
PDB most similar in plane (leastsq):	1SHR_HEM_A_142
PDB most similar out of plane (leastsq):	4YBN_HEM_B_301
PDB most similar in plane (leastsum):	2LDO_HEM_A_154
PDB most similar out of plane (leastsum):	1MPW_HEM_A_417
mode energy calc:	15.4 kJ/mol

4. Determination of dimerization constants for 1a and 1c by ^{1}H NMR spectroscopy

Dimerization constants were determined by tracking changes in the chemical shifts of diagnostic NH protons in **1a** and **1c** upon dilution [5, 6]. To determine the dimerization constants, the experimental data were fitted using numpy (1.18.5) and scipy (1.4.1) libraries of Python 3. Fitting of the experimental data points was performed with the simplest dimerization model [5, 6], which does not take into account the conformational changes [7, 8] and continuous aggregation [9].

Equilibrium constant for a dimerization process is defined as follows:

$$2\mathrm{M} \rightleftharpoons \mathrm{D}, \qquad K_{dim} = \frac{[\mathrm{D}]}{[\mathrm{M}]^2} \tag{1},$$

where the sum of monomer $[\mathrm{M}]$ and dimer $[\mathrm{D}]$ concentrations gives the initial concentration, $[\mathrm{M}]_0$

$$[\mathrm{M}]_0 = [\mathrm{M}] + 2[\mathrm{D}] \tag{2}$$

The observed chemical shift, δ_{obs}, is defined as follows:

$$\delta_{obs} = \delta_M + (\delta_D - \delta_M)\chi_D \tag{3}$$

$$\delta_{obs} = \delta_M + (\delta_D - \delta_M)(1 - \frac{[\mathrm{M}]}{[\mathrm{M}]_0}) \tag{4}$$

where δ_M and δ_D are the chemical shifts of monomer and dimer, respectively, and χ_D is the mole fraction of dimer. From the equations (1–4), the following equation (5) was derived and used for fitting the experimental data:

$$K_{dim} = \frac{(\delta_D - \delta_M)(\delta_{obs} - \delta_M)}{2\,(\delta_D - \delta_{obs})^2\,[\mathrm{M}]_0} \tag{5}$$

It was found for both **1a** and **1c** that chemical shifts values remain virtually constant in the concentrations range 10^{-4}–10^{-2} M used for UV-Vis titrations (Figures S86-88 below). This result confirms the dominance of monomeric species in the diluted solutions. The chemical shifts showed a significant change only at concentrations higher than 10^{-2} M.

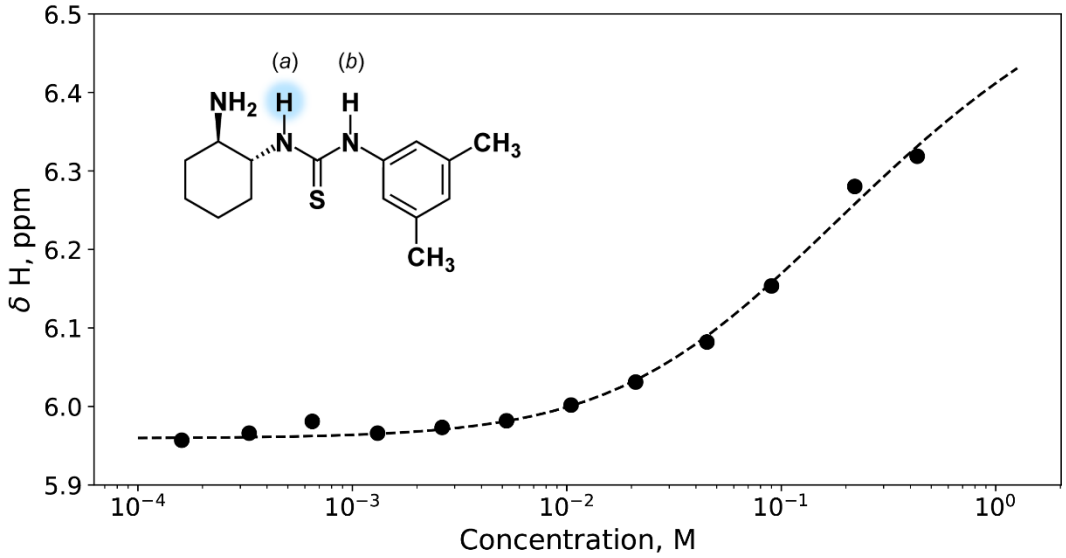


Figure S88. Concentration dependence of the chemical shift of NH(*a*) proton for thiourea **1c** (293 K, $CDCl_3$).

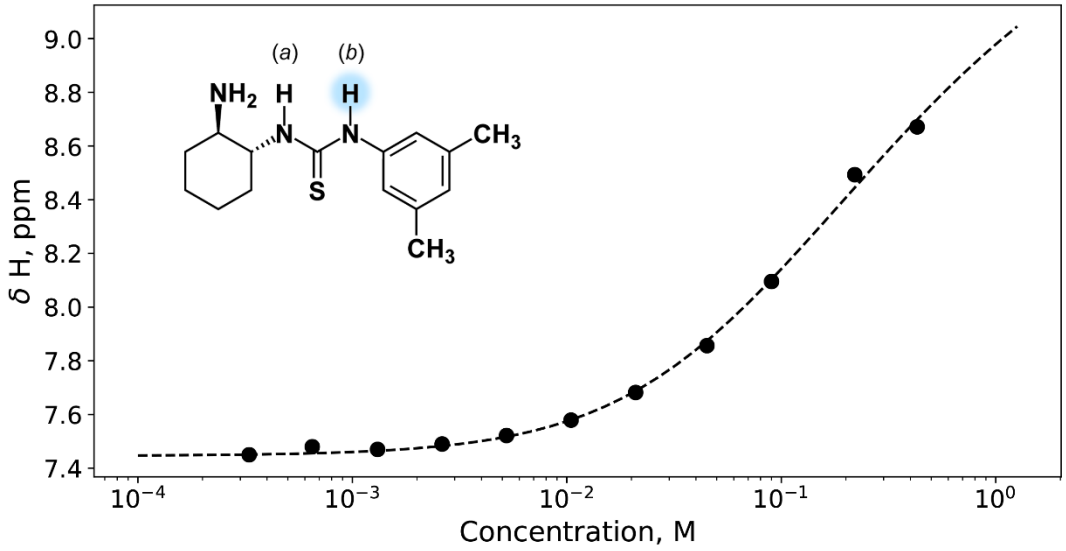


Figure S89. Concentration dependence of the chemical shift of NH(*b*) proton for thiourea **1c** (293 K, $CDCl_3$).

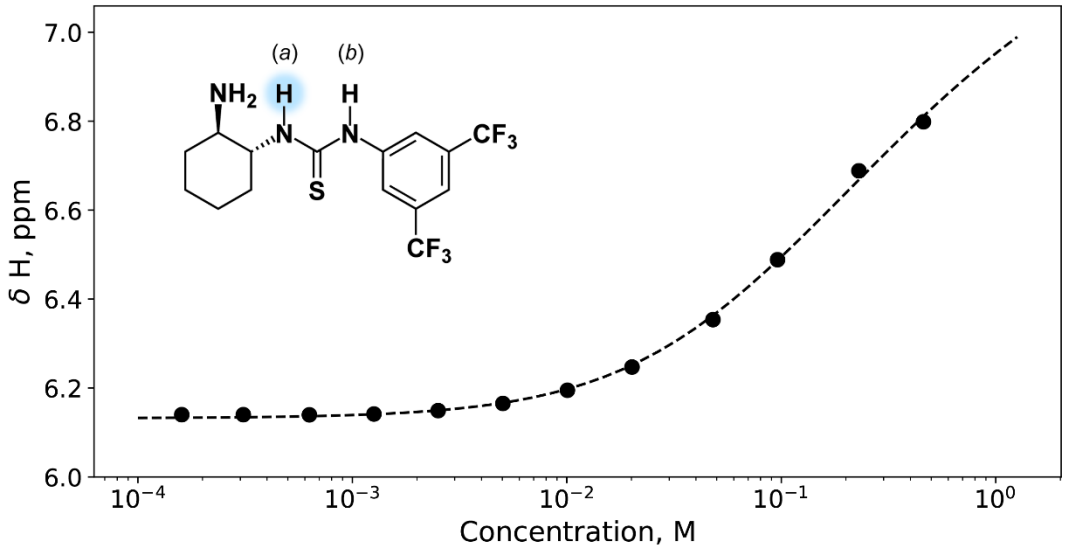


Figure S90. Concentration dependence of the chemical shift of NH(*a*) proton for thiourea **1a** (293 K, $CDCl_3$).

Table S26. Sample data and fitting results for compound **1c**

$[M]_0$, M	δ_{obs}, ppm	
	NH(*a*)	**NH(*b*)**
0.43	6.3187	8.6713
0.22	6.2802	8.4932
0.090	6.1535	8.0953
0.045	6.0821	7.8564
0.0209	6.0311	7.682
0.0105	6.0018	7.579
0.00523	5.9818	7.5217
0.00262	5.9733	7.49
0.00131	5.966	7.47
0.00065	5.981	7.48
0.00033	5.966	7.45
0.00016	5.957	–
δ_D, ppm	6.62 ± 0.04	9.72 ± 0.10
δ_M, ppm	5.959 ± 0.006	7.45 ± 0.02
K_{dim}, M^{-1}	**3.4 ± 0.6**	**3.2 ± 0.4**
R^2	0.995	0.998
χ^2	1.20×10^{-4}	4.23×10^{-4}

Table S27. Sample data and fitting results for compound **1a**

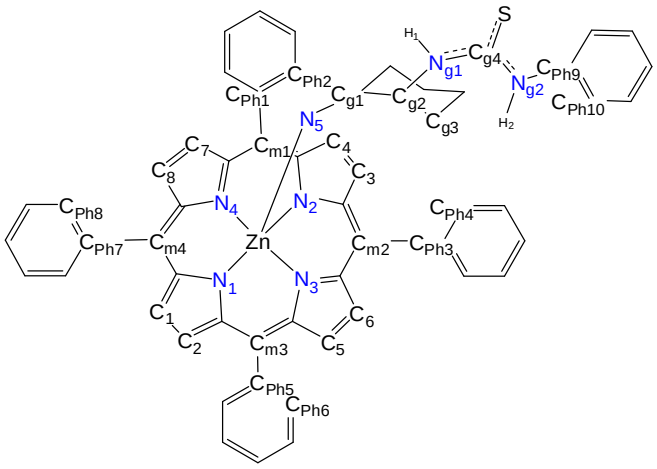
$[M]_0$, M	δ_{obs}, ppm
	NH(*a*)
0.46	6.7986
0.23	6.6884
0.096	6.4885
0.048	6.3538
0.0201	6.2472
0.0101	6.195
0.00503	6.1653
0.00251	6.1492
0.00126	6.1416
0.00063	6.1398
0.00031	6.1401
0.00016	6.1401
δ_D, ppm	7.37 ± 0.04
δ_M, ppm	6.132 ± 0.004
K_{dim}, M^{-1}	**2.9 ± 0.2**
R^2	0.999
χ^2	1.09×10^{-4}

5. Computational studies

Table S28. Electronic energies, zero point energies, enthalpies, entropies, relative energies and Boltzmann distribution of conformer of complex **1a**·**P6** (two most abundant conformers are highlighted in blue).

	Complex 1a·P6					
Conformer	**1**	**2**	**3**	**4**	**5**	**6**
$E_{electr.def2\text{-}SV(P)}$. Hartree	-6780.62524395849	-6780.62656054079	-6780.62335277556	-6780.62142767010	-6780.62802170832	-6780.61881009232
$E_{electr.def2\text{-}TZVP}$. Hartree	-6786.26514959499	-6786.26488763996	-6786.26400398201	-6786.26110608537	-6786.26614867179	-6786.25935256310
ZPE. Hartree	0.9147005	0.9149808	0.9137806	0.9139507	0.9147805	0.9134594
H. kJ/mol/K	2584.3	2587.08	2579.83	2582.15	2584.13	2583.95
S. kJ/mol	1.72756	1.74105	1.7054	1.71126	1.70668	1.74421
Relative energy						
def2-SV(P). kJ/mol	4.66	0.00	11.69	17.34	3.35	16.29
def2-TZVP. kJ/mol	0.51	0.00	5.59	13.79	3.88	10.47
Boltzmann. %	**37.9**	**46.6**	4.9	0.2	9.7	0.7

Table S29. Selected structural parameters for the six conformers of complexes **1a**·**P6** and **1a**·**P3** (two most abundant conformers are highlighted in blue).



	Complex 1a·P6						Complex 1a·P3					
Conformer	**1**	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**	**6**
Abundance	37.9	46.6	4.9	0.2	9.7	0.7	10.7	7.4	48.6	4.1	24.5	4.7
Zn-N5. Å	2.158	2.155	2.135	2.151	2.156	2.137	2.198	2.191	2.129	2.150	2.139	2.142
Averaged Zn-N5. Å*	**2.155**						**2.145**					
N1-Zn-N5	90.34	90.86	93.96	91.7	89.09	91.51	89.9	89.9	93.22	92.99	88.74	93.33
N3-Zn-N5	108.51	106.27	113.78	113.34	105.25	109.69	105.02	105.02	114.88	115.06	102.18	114.85
N2-ZN-N5-Cg1	-28.48	-28.19	5.19	-19.95	-20.88	-10.57	25.1	25.1	-19.81	-16.78	49.5	-12.88
Porphyrin												
C1-C2-C3-C4	8.98	9.95	-0.41	4.67	9.84	3.38	6.14	6.14	6.24	5.01	9.49	5.23
C5-C6-C7-C8	-8.05	-9.42	1.97	-3.11	-9.41	-3.5	-5.57	-5.57	-5.16	-3.68	-9.71	-5.55
N1-Zn-N2	158.33	159.72	158.88	159.48	160.71	159.89	160.61	160.61	158.45	157.68	158.93	157.24
N3-Zn-N4	161.98	160.36	163.02	161.54	159.96	163.16	164.66	164.66	160.84	160.09	159.73	160.56
Aryl in host												
C7-C_{m1}-C_{Ph1}-C_{Ph2}	65.9	113.25	109.01	-114.05	66.61	-100.31	70.5	70.5	109.98	67.22	60.53	66.43
C3-C_{m2}-C_{Ph3}-C_{Ph4}	119.01	118.71	120.89	123.42	115.82	119.02	117.2	117.2	124.78	124.67	73.35	122.55
C5-C_{m3}-C_{Ph5}-C_{Ph6}	63.38	65.69	60.24	59.12	117.04	115.09	66.35	66.35	57.73	61.14	117.71	116.86
C1-C_{m4}--C_{Ph7}-C_{Ph8}	116.04	65.79	115.42	70.57	64.56	112.83	112.41	112.41	115.99	67.84	65.94	115.13
Guest conf.												
Cg3-Cg2-Ng1-H1	-73.86	-76.97	82.37	90.77	-86.57	89.29	-24.68	-24.68	-0.95	-20.59	-1.51	-14.37
H1-Ng1-Cg4-S	169.66	169.87	-169.33	-169.77	169.82	-168.97	-89.67	-89.67	83.97	92.48	-86.87	92.54
S-Cg4-Ng2-H2	18.99	20.1	-27.3	164.55	17.3	168.32	170.62	170.62	-170.28	-171.13	170.23	-170.83
H2-Ng2-C_{Ph9}-C_{Ph10}	24.87	26.11	-16	-10.88	24.35	-5.8	16.75	16.75	-23.51	166.55	14.95	167.41

* Boltzmann-averaged distance

Table S30. Topological analysis (QTAIM) of the electron density of main conformers in complexes **1a**·**P6** and **1a**·**P3**.

weak dispersion – $\rho(r)$ <0.005 a.u., positive Laplacian [10],

strong noncovalent interactions – 0.005 < $\rho(r)$ < 0.05 a.u., positive Laplacian [10],

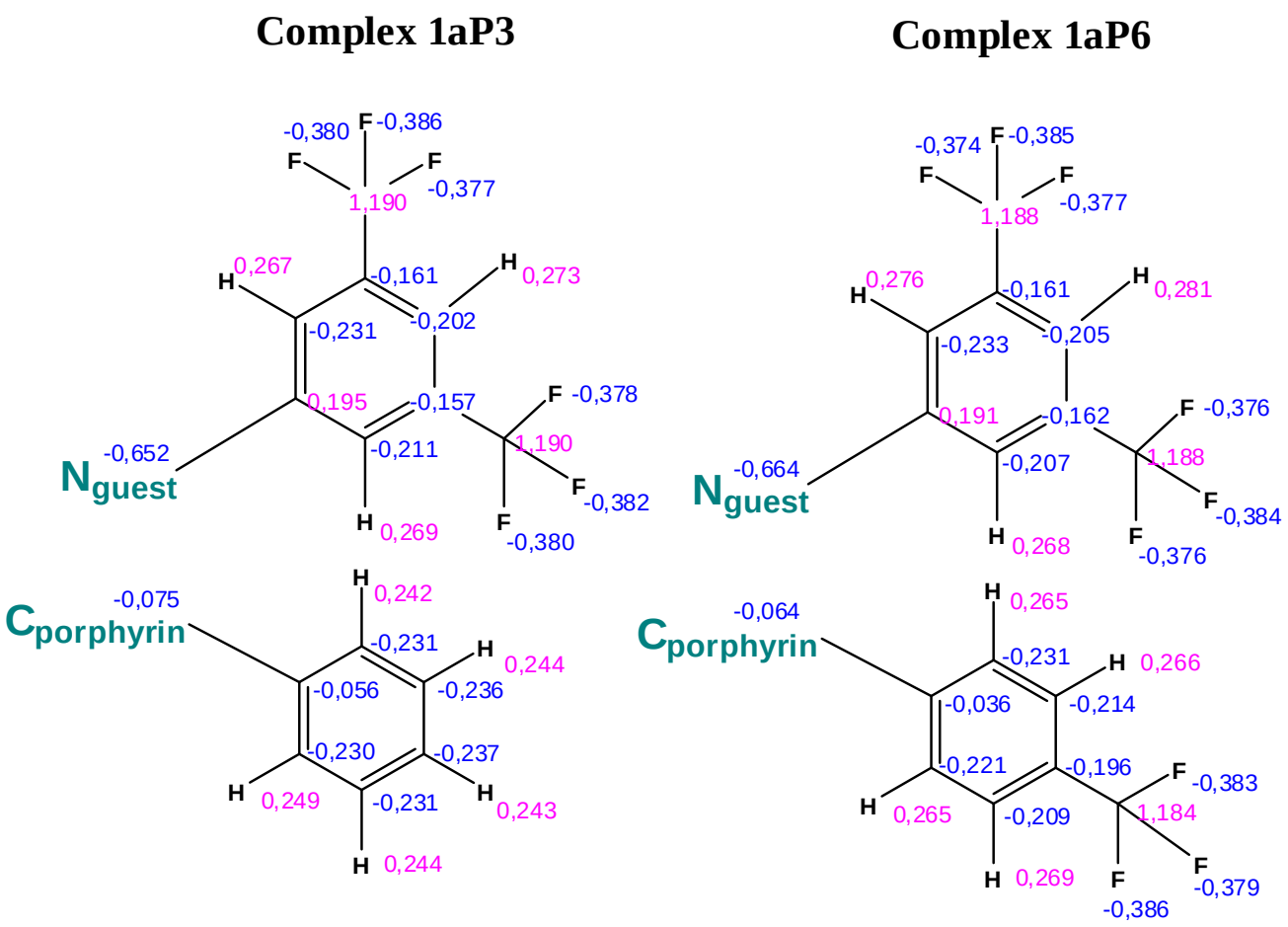
σ/π interactions – 0.007 <$\rho(r)$ < 0.010 a.u., positive Laplacian [11],

π–π stacking – $\rho(r)$ < 0.0125 a.u., positive Laplacian, the presence of a C···C bond path between the C atoms belonging to different rings [12],

covalent bond – $\rho(r)$ > 0.100 a.u., negative Laplacian [13].

Atoms	Electron Delocalization Index.	Electron Density ($\rho(r)$), a.u.	Laplacian of Rho
Complex 1a·P6			
BCP (bond critical point)			
C_{69} H_{58}	0.015	0.008	0.029
C_{61} H_{33}	0.023	0.010	0.031
H_{50} H_{65}	0.011	0.005	0.021
C_{77} H_{33}	0.03	0.011	0.042
C_{73} H_{66}	0.89	0.009	0.029
S_{55} H_{70}	0.037	0.007	0.019
C_{75} F_{124}	0.018	0.005	0.021
C_{75} F_{125}	0.012	0.004	0.016
H_{48} H_{100}	0.015	0.006	0.021
F_{116} F_{125}	0.016	0.005	0.027
F_{126} F_{130}	0.001	0.000	0.005
H_{50} F_{128}	0.011	0.003	0.016
Complex 1a·P3			
H_{14} C_{118}	0.027	0.011	0.045
F_{75} H_{14}	0.010	0.003	0.018
C_{63} C_{112}	0.030	0.008	0.022
F_{73} C_{114}	0.018	0.004	0.017
F_{75} C_{116}	0.016	0.004	0.015
F_{72} H_{113}	0.019	0.006	0.029
H_{111} F_{72}	0.013	0.005	0.024
Complex 1a·P6			
RCP (ring critical point)			
C_{15} C_{17} H_{33} H_{77} C_{68} C_{26}	0.010	0.048	
H_{33} C_{61} C_{64} C_{113} F_{124} C_{75} C_{77} F_{125}	0.003	0.011	
C_{37} C_{38} H_{48} H_{100} C_{99} F_{128} H_{50}	0.001	0.006	
C_{17} C_{21} C_{19} C_{22} C_{90} C_{99} F_{128} C_{112} C_{62} C_{60} C_{59} C_{61} H_{33}	0.001	0.001	
N_4 C_{15} C_{26} C_{68} C_{69} H_{58} N_{57} C_{54} N_{53}	0.003	0.011	
C_{36} C_{37} H_{50} H_{65} C_{60} H_{56} N_{53}	0.005	0.020	

N_{57} $H5_8$ C_{69} C_{71} C_{73} H_{66} C_{61} C_{59}	0.004	0.016	
C_{17} C_{21} H_{56} C_{60} C_{59} C_{61} H_{33}	0.006	0.017	
H_{33} C_{61} H_{66} C_{73} C_{75} C_{77}	0.004	0.012	
C_{73} C_{74} F_{116} F_{125} C_{75}	0.003	0.016	
C_{54} S_{55} H_{70} C_{69} H_{58} N_{57}	0.005	0.020	
C_{61} C_{64} C_{113} F_{125} C_{75} C_{73} H_{66}	0.004	0.015	
C_{75} F_{124} C_{113} F_{125}	0.004	0.016	
H_{50} H_{65} C_{60} C_{62} C_{112} F_{128}	0.003	0.013	
C_{95} C_{96} F_{130} F_{126} C_{112} F_{128} C_{99} C_{97}	0.000	0.004	
CCP (cage critical point)			
N_4 C_{17} C_{19} C_{20} C_{21} C_{22} C_{23} H_{33} C_{36} C_{37} C_{38} H_{48} H_{50} H_{52} N_{53} H_{56} C_{59} C_{60} C_{61} C_{62} H_{65} C_{90} C_{99} H_{100} C_{112} F_{128}	0.001	0.003	
N_4 C_{15} C_{17} C_{21} C_{26} H_{33} N_{53} C_{54} H_{56} N_{57} H_{58} C_{59} C_{60} C_{61} H_{66} C_{68} C_{69} C_{71} C_{73} C_{75} C_{77}	0.003	0.010	
H_{33} C_{61} C_{64} H_{66} C_{73} C_{75} C_{77} C_{113} F_{124} F_{125}	0.003	0.010	
Complex 1a·P3			
RCP			
C_{13} H_{14} C_{118} C_{109} C_{27} C_{25}	0.011	0.051	
C_{59} C_{60} C_{62} C_{63} C_{64} C_{61} C_{110} H_{111} C_{112}	0.004	0.011	
C_{13} H_{14} F_{75} C_{68} C_{62} C_{60} H_{65}	0.003	0.017	
C_{13} C_{25} C_{27} C_{109} C_{110} C_{112} C_{63} C_{62} C_{60} H_{65}	0.003	0.009	
C_{63} C_{64} C_{69} F_{72} H_{113} C_{112}	0.004	0.016	
C_{63} C_{64} C_{69} F_{72} H_{111} C_{110} C_{112}	0.004	0.019	
CCP			
C_{68} F_{73} C_{114} C_{116} F_{75}	0.003	0.012	
C_{62} C_{63} C_{112} C_{114} F_{73} C_{68}	0.003	0.012	
F_{72} H_{111} C_{110} C_{112} H_{113}	0.004	0.022	
H_{14} F_{75} C_{116} C_{118}	0.002	0.010	



.

Figure S91. NBO partial atomic charges of main conformers in complexes **1a**·**P3** and **1a**·**P6**.

Table S31. NBO partial atomic charges of main conformers in complexes **1a**·**P6** and **1a**·**P3**.

No	Atom	Natural Charge		No	Atom	Natural Charge
1	Zn	1.16739		1	Zn	1.14926
2	N	-0.65638		2	N	-0.65663
3	N	-0.65835		3	N	-0.66114
4	N	-0.66374		4	N	-0.65117
5	N	-0.66657		5	N	-0.66347
6	C	-0.25865		6	C	-0.25195
7	C	-0.06327		7	C	-0.05896
8	C	-0.25874		8	C	-0.25673
9	C	0.19927		9	C	0.20022

10	C	0.19741		10	C	0.19899
11	C	-0.25767		11	C	-0.25329
12	H	0.26248		12	H	0.25396
13	C	-0.25931		13	C	-0.26361
14	H	0.26185		14	H	0.2549
15	C	0.19855		15	C	0.18744
16	C	0.19292		16	C	0.19234
17	C	-0.26601		17	C	-0.2548
18	C	-0.25574		18	C	-0.25741
19	C	0.18431		19	C	0.19294
20	C	0.19437		20	C	0.19213
21	C	-0.26707		21	C	-0.25857
22	C	-0.0716		22	C	-0.06764
23	C	-0.25845		23	C	-0.25451
24	C	0.20146		24	C	0.19649
25	C	0.19779		25	C	0.19876
26	C	-0.06449		26	C	-0.06537
27	C	-0.0641		27	C	-0.07494
28	H	0.26333		28	H	0.25441
29	H	0.26331		29	H	0.25518
30	H	0.26324		30	H	0.25528
31	H	0.26225		31	H	0.2537
32	H	0.26205		32	H	0.25494
33	H	0.25643		33	H	0.25419
34	N	-0.96082		34	N	-0.95574
35	C	-0.03631		35	C	-0.02581
36	C	-0.03644		36	C	-0.04206
37	C	-0.45722		37	C	-0.44842
38	C	-0.45002		38	C	-0.43936
39	C	-0.45936		39	C	-0.45345
40	C	-0.44741		40	C	-0.44018
41	H	0.42878		41	H	0.42016
42	H	0.42272		42	H	0.42228
43	H	0.23141		43	H	0.22582
44	H	0.24517		44	H	0.24114
45	H	0.24517		45	H	0.2254

46	H	0.24095		46	H	0.23928
47	H	0.22709		47	H	0.21925
48	H	0.22315		48	H	0.22337
49	H	0.24472		49	H	0.23908
50	H	0.24131		50	H	0.24204
51	H	0.2353		51	H	0.22609
52	H	0.24988		52	H	0.25523
53	N	-0.66542		53	N	-0.65699
54	C	0.37006		54	C	0.37518
55	S	-0.32718		55	S	-0.31285
56	H	0.44829		56	H	0.44364
57	N	-0.66437		57	N	-0.65233
58	H	0.45986		58	H	0.45572
59	C	0.19133		59	C	0.19473
60	C	-0.23267		60	C	-0.21086
61	C	-0.20703		61	C	-0.23141
62	C	-0.16112		62	C	-0.1566
63	C	-0.20474		63	C	-0.20219
64	C	-0.16238		64	C	-0.16128
65	H	0.2764		65	H	0.2688
66	H	0.268		66	H	0.26683
67	H	0.28068		67	H	0.27288
68	C	-0.03633		68	C	1.19027
69	C	-0.23101		69	C	1.18989
70	H	0.26519		70	F	-0.38005
71	C	-0.21439		71	F	-0.37711
72	H	0.26584		72	F	-0.38581
73	C	-0.19571		73	F	-0.37816
74	C	1.18382		74	F	-0.37952
75	C	-0.20945		75	F	-0.38201
76	H	0.26868		76	C	-0.05941
77	C	-0.22127		77	C	-0.22326
78	H	0.26524		78	H	0.24863
79	C	-0.0414		79	C	-0.2334
80	C	-0.21811		80	H	0.24437
81	H	0.26167		81	C	-0.23821

82	C	-0.20728		82	H	0.24307
83	H	0.26352		83	C	-0.23357
84	C	-0.19122		84	H	0.24431
85	C	1.18308		85	C	-0.22588
86	C	-0.20917		86	H	0.24756
87	H	0.26543		87	C	-0.05983
88	C	-0.21715		88	C	-0.22551
89	H	0.26258		89	H	0.24842
90	C	-0.04211		90	C	-0.2331
91	C	-0.21794		91	H	0.2441
92	H	0.26256		92	C	-0.24033
93	C	-0.2096		93	H	0.24273
94	H	0.26565		94	C	-0.23368
95	C	-0.19144		95	H	0.24337
96	C	1.1833		96	C	-0.22534
97	C	-0.20265		97	H	0.24611
98	H	0.26295		98	C	-0.05818
99	C	-0.21385		99	C	-0.22534
100	H	0.25434		100	H	0.24348
101	C	-0.04026		101	C	-0.23373
102	C	-0.21594		102	H	0.24437
103	H	0.2573		103	C	-0.23625
104	C	-0.20706		104	H	0.24345
105	H	0.26336		105	C	-0.23293
106	C	-0.19092		106	H	0.24479
107	C	1.18313		107	C	-0.22363
108	C	-0.20854		108	H	0.24963
109	H	0.2657		109	C	-0.05614
110	C	-0.21796		110	C	-0.23099
111	H	0.26289		111	H	0.2424
112	C	1.18844		112	C	-0.23565
113	C	1.18808		113	H	0.24448
114	F	-0.37853		114	C	-0.23715
115	F	-0.38288		115	H	0.24313
116	F	-0.38568		116	C	-0.2307
117	F	-0.38195		117	H	0.2443

118	F	-0.38399		118	C	-0.22958
119	F	-0.38345		119	H	0.24923
120	F	-0.38172				
121	F	-0.38397				
122	F	-0.38366				
123	F	-0.37589				
124	F	-0.38441				
125	F	-0.37564				
126	F	-0.37435				
127	F	-0.37731				
128	F	-0.38524				
129	F	-0.38176				
130	F	-0.38369				
131	F	-0.38389				

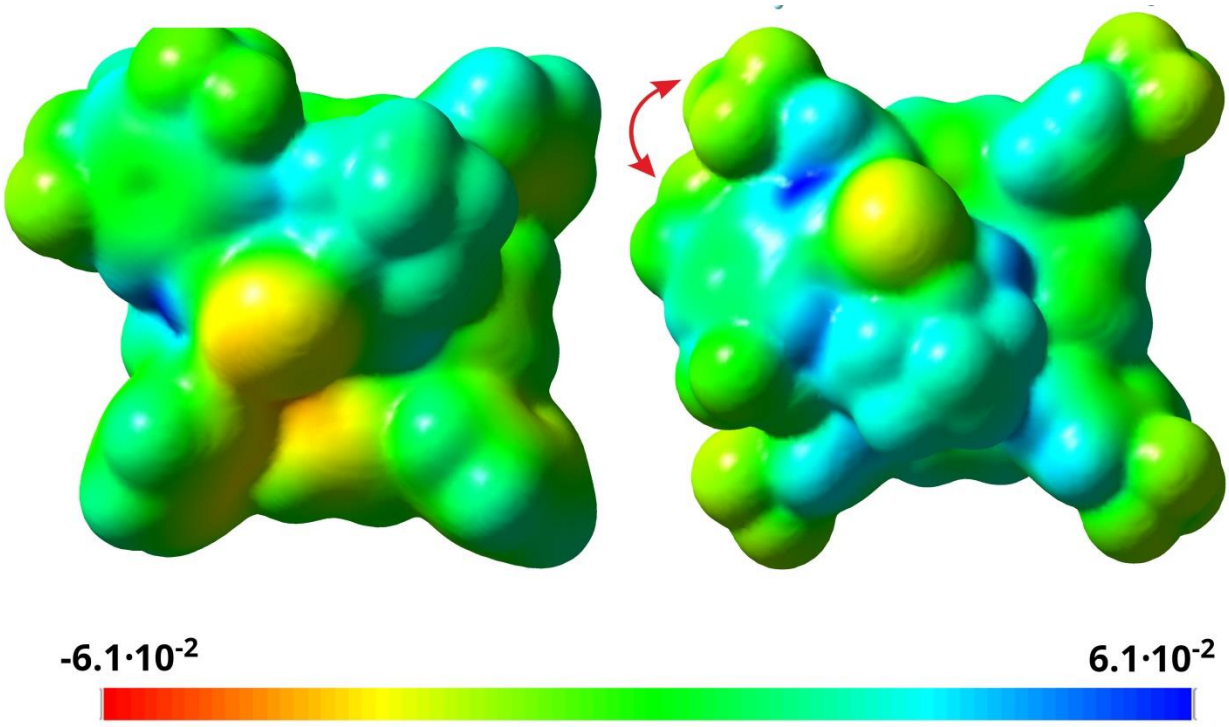


Figure S92. Molecular electrostatic surface potential for the dominant conformers of complexes **1a**·**P3** (left) and **1a**·**P6** (right) calculated based on the NBO partial charges, mapped over the electron density isosurface at 0.002 au.

Table S32. Perturbation theory energy analysis of the main conformers of complexes **1a**·**P6** and **1a**·**P3**

Complex 1a·P6

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
91. BD (2) C 68 - C 77	/***. BD*(1) C 17 - H 33	0.51
88. BD (1) C 64 - C 113	/616. RY*(1) H 33	0.3
323. LP (1) F 124	/616. RY*(1) H 33	0.09
323. LP (1) F 124	/***. BD*(1) C 17 - H 33	0.17
324. LP (2) F 124	/616. RY*(1) H 33	0.08
324. LP (2) F 124	/***. BD*(1) C 17 - H 33	0.36
92. BD (1) C 69 - H 70	/771. RY*(1) H 58	0.07
92. BD (1) C 69 - H 70	/***. BD*(1) N 57 - H 58	0.12
93. BD (1) C 69 - C 71	/771. RY*(1) H 58	0.14
94. BD (2) C 69 - C 71	/771. RY*(1) H 58	0.17
94. BD (2) C 69 - C 71	/***. BD*(1) N 57 - H 58	1.02
73. BD (1) N 57 - H 58	/852. RY*(3) C 69	0.07
73. BD (1) N 57 - H 58	/***. BD*(2) C 69 - C 71	0.14
71. BD (1) C 54 - S 55	/859. RY*(1) H 70	0.41
289. LP (1) S 55	/***. BD*(1) C 69 - H 70	0.24
290. LP (2) S 55	/***. BD*(1) C 69 - H 70	0.32
291. LP (3) S 55	/***. BD*(1) C 69 - H 70	1.35
161. BD (1) C 113 - F 124	/896. RY*(3) C 75	0.06
323. LP (1) F 124	/616. RY*(1) H 33	0.09
323. LP (1) F 124	/***. BD*(1) C 17 - H 33	0.17
324. LP (2) F 124	/616. RY*(1) H 33	0.08
324. LP (2) F 124	/***. BD*(1) C 17 - H 33	0.36
325. LP (3) F 124	/896. RY*(3) C 75	0.08
325. LP (3) F 124	/***. BD*(2) C 73 - C 75	0.21
326. LP (1) F 125	/***. BD*(1) C 74 - F 115	0.06
326. LP (1) F 125	/***. BD*(1) C 74 - F 116	0.05
328. LP (3) F 125	/896. RY*(3) C 75	0.06
138. BD (2) C 97 - C 99	/***. BD*(1) C 112 - F 128	0.2
335. LP (1) F 128	/***. RY*(3) C 97	0.07
335. LP (1) F 128	/***. RY*(3) C 99	0.11
336. LP (2) F 128	/***. BD*(2) C 97 - C 99	0.14
300. LP (2) F 116	/833. RY*(1) H 66	0.06
300. LP (2) F 116	/***. BD*(1) C 61 - H 66	0.08
Total bonds		**7.58**
89. BD (1) C 68 - C 69	/833. RY*(1) H 66	0.05
90. BD (1) C 68 - C 77	/833. RY*(1) H 66	0.06
93. BD (1) C 69 - C 71	/833. RY*(1) H 66	0.25

94. BD (2) C 69 - C 71	/833. RY*(1) H 66	0.12
94. BD (2) C 69 - C 71	/***. BD*(1) C 61 - H 66	0.31
96. BD (1) C 71 - C 73	/833. RY*(1) H 66	0.6
97. BD (1) C 73 - C 74	/833. RY*(1) H 66	0.3
98. BD (1) C 73 - C 75	/833. RY*(1) H 66	0.42
99. BD (2) C 73 - C 75	/833. RY*(1) H 66	0.41
99. BD (2) C 73 - C 75	/***. BD*(1) C 61 - H 66	0.88
104. BD (1) C 75 - C 77	/833. RY*(1) H 66	0.19
Total rings		**1.90**
164. CR (2)Zn 1	/***. BD*(1) N 34 - C 35	0,07
165. CR (3)Zn 1	/***. BD*(1) N 34 - C 35	0,43
165. CR (3)Zn 1	/***. BD*(1) N 34 - H 41	0,2
165. CR (3)Zn 1	/***. BD*(1) N 34 - H 42	0,11
171. CR (9)Zn 1	/***. BD*(1) N 34 - C 35	0,19
171. CR (9)Zn 1	/***. BD*(1) N 34 - H 41	0,05
265. LP (1)Zn 1	/620. RY*(1) N 34	0,06
266. LP (2)Zn 1	/***. BD*(1) N 34 - H 41	0,05
266. LP (2)Zn 1	/***. BD*(1) N 34 - H 42	0,15
269. LP (5)Zn 1	/***. BD*(1) N 34 - C 35	0,21
269. LP (5)Zn 1	/***. BD*(1) N 34 - H 41	0,09
270. LP*(6)Zn 1	/620. RY*(1) N 34	0,5
270. LP*(6)Zn 1	/621. RY*(2) N 34	0,05
270. LP*(6)Zn 1	/622. RY*(3) N 34	0,05
270. LP*(6)Zn 1	/627. RY*(8) N 34	0,07
270. LP*(6)Zn 1	/***. BD*(1) N 34 - C 35	0,7
270. LP*(6)Zn 1	/***. BD*(1) N 34 - H 41	0,88
270. LP*(6)Zn 1	/***. BD*(1) N 34 - H 42	0,65
271. LP*(7)Zn 1	/621. RY*(2) N 34	0,06
271. LP*(7)Zn 1	/622. RY*(3) N 34	0,17
271. LP*(7)Zn 1	/***. BD*(1) N 34 - C 35	0,66
272. LP*(8)Zn 1	/621. RY*(2) N 34	0,2
272. LP*(8)Zn 1	/622. RY*(3) N 34	0,06
272. LP*(8)Zn 1	/***. BD*(1) N 34 - C 35	0,25
272. LP*(8)Zn 1	/***. BD*(1) N 34 - H 42	0,1
273. LP*(9)Zn 1	/623. RY*(4) N 34	0,09
273. LP*(9)Zn 1	/***. BD*(1) N 34 - C 35	0,57
273. LP*(9)Zn 1	/***. BD*(1) N 34 - H 41	1,01
273. LP*(9)Zn 1	/***. BD*(1) N 34 - H 42	0,86
49. BD (1) N 34 - C 35	/270. LP*(6)Zn 1	1,11
49. BD (1) N 34 - C 35	/271. LP*(7)Zn 1	0,08
49. BD (1) N 34 - C 35	/273. LP*(9)Zn 1	6,24
49. BD (1) N 34 - C 35	/347. RY*(1)Zn 1	0,13
49. BD (1) N 34 - C 35	/353. RY*(7)Zn 1	0,13
49. BD (1) N 34 - C 35	/354. RY*(8)Zn 1	0,28
49. BD (1) N 34 - C 35	/356. RY*(10)Zn 1	0,19
50. BD (1) N 34 - H 41	/270. LP*(6)Zn 1	2,61
50. BD (1) N 34 - H 41	/272. LP*(8)Zn 1	0,19
50. BD (1) N 34 - H 41	/273. LP*(9)Zn 1	8,49

50. BD (1) N 34 - H 41	/347. RY*(1)Zn 1	0,41
50. BD (1) N 34 - H 41	/353. RY*(7)Zn 1	0,43
50. BD (1) N 34 - H 41	/355. RY*(9)Zn 1	0,06
50. BD (1) N 34 - H 41	/357. RY*(11)Zn 1	0,06
51. BD (1) N 34 - H 42	/270. LP*(6)Zn 1	2,64
51. BD (1) N 34 - H 42	/271. LP*(7)Zn 1	0,13
51. BD (1) N 34 - H 42	/272. LP*(8)Zn 1	0,52
51. BD (1) N 34 - H 42	/273. LP*(9)Zn 1	8,6
51. BD (1) N 34 - H 42	/347. RY*(1)Zn 1	0,37
51. BD (1) N 34 - H 42	/353. RY*(7)Zn 1	0,36
51. BD (1) N 34 - H 42	/356. RY*(10)Zn 1	0,08
196. CR (1) N 34	/270. LP*(6)Zn 1	1,38
196. CR (1) N 34	/271. LP*(7)Zn 1	0,1
196. CR (1) N 34	/273. LP*(9)Zn 1	4,96
196. CR (1) N 34	/347. RY*(1)Zn 1	0,1
196. CR (1) N 34	/353. RY*(7)Zn 1	0,08
286. LP (1) N 34	/270. LP*(6)Zn 1	45,61
286. LP (1) N 34	/271. LP*(7)Zn 1	1,44
286. LP (1) N 34	/272. LP*(8)Zn 1	0,15
286. LP (1) N 34	/273. LP*(9)Zn 1	41,32
286. LP (1) N 34	/347. RY*(1)Zn 1	0,12
286. LP (1) N 34	/352. RY*(6)Zn 1	1,26
286. LP (1) N 34	/353. RY*(7)Zn 1	0,31
286. LP (1) N 34	/356. RY*(10)Zn 1	0,3
286. LP (1) N 34	/357. RY*(11)Zn 1	0,12
286. LP (1) N 34	/359. RY*(13)Zn 1	0,08
286. LP (1) N 34	/364. RY*(18)Zn 1	0,1
Total Zn-N_{quest}		**139,08**

Complex 1a·P3

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
271. LP (1) F 72	/***. RY*(1) H 113	0.06
271. LP (1) F 72	/***. BD*(1) C 110 - H 111	0.11
271. LP (1) F 72	/***. BD*(1) C 112 - H 113	0.17
272. LP (2) F 72	/***. RY*(2) C 110	0.08
272. LP (2) F 72	/***. BD*(1) C 109 - C 110	0.07
272. LP (2) F 72	/***. BD*(1) C 110 - H 111	0.17
272. LP (2) F 72	/***. BD*(1) C 112 - H 113	0.1
272. LP (2) F 72	/***. BD*(1) C 112 - C 114	0.07
273. LP (3) F 72	/***. RY*(1) H 113	0.05
273. LP (3) F 72	/***. BD*(1) C 112 - H 113	0.2
276. LP (3) F 73	/***. RY*(3) C 114	0.07
276. LP (3) F 73	/***. BD*(2) C 112 - C 114	0.13
280. LP (1) F 75	/411. RY*(1) H 14	0.1
280. LP (1) F 75	/***. BD*(1) C 13 - H 14	0.2

281. LP (2) F 75	/***. BD*(1) C 13 - H 14	0.28
282. LP (3) F 75	/***. RY*(3) C 116	0.07
282. LP (3) F 75	/***. BD*(2) C 116 - C 118	0.07
26. BD (1) C 13 - H 14	/***. BD*(2) C 116 - C 118	0.6
27. BD (1) C 13 - C 25	/***. BD*(1) C 13 - H 14	1.31
26. BD (1) C 13 - H 14	/720. RY*(1) C 60	0.13
26. BD (1) C 13 - H 14	/722. RY*(3) C 60	0.29
26. BD (1) C 13 - H 14	/765. RY*(1) H 65	0.18
26. BD (1) C 13 - H 14	/***. BD*(2) C 60 - C 62	0.28
26. BD (1) C 13 - H 14	/***. BD*(1) C 60 - H 65	0.13
78. BD (1) C 60 - C 62	/411. RY*(1) H 14	0.05
79. BD (2) C 60 - C 62	/411. RY*(1) H 14	0.09
79. BD (2) C 60 - C 62	/***. BD*(1) C 13 - H 14	0.09
80. BD (1) C 60 - H 65	/411. RY*(1) H 14	0.23
80. BD (1) C 60 - H 65	/***. BD*(1) C 13 - H 14	0.09
280. LP (1) F 75	/411. RY*(1) H 14	0.1
280. LP (1) F 75	/***. BD*(1) C 13 - H 14	0.2
281. LP (2) F 75	/***. BD*(1) C 13 - H 14	0.28
Total bonds		**2.90**
140. BD (1) C 110 - H 111	/***. BD*(2) C 59 - C 61	0.06
75. BD (1) C 59 - C 60	/***. RY*(3) C 109	0.09
76. BD (1) C 59 - C 61	/***. RY*(1) C 110	0.08
76. BD (1) C 59 - C 61	/***. RY*(3) C 110	0.08
77. BD (2) C 59 - C 61	/***. BD*(2) C 109 - C 110	0.11
77. BD (2) C 59 - C 61	/***. BD*(1) C 110 - H 111	0.07
140. BD (1) C 110 - H 111	/731. RY*(3) C 61	0.07
140. BD (1) C 110 - H 111	/***. BD*(2) C 59 - C 61	0.06
76. BD (1) C 59 - C 61	/***. RY*(1) C 110	0.08
81. BD (1) C 61 - C 64	/***. RY*(1) C 110	0.17
81. BD (1) C 61 - C 64	/***. RY*(3) C 110	0.12
81. BD (1) C 61 - C 64	/***. RY*(1) H 111	0.11
137. BD (1) C 109 - C 110	/722. RY*(3) C 60	0.06
137. BD (1) C 109 - C 110	/***. BD*(2) C 60 - C 62	0.14
78. BD (1) C 60 - C 62	/***. RY*(3) C 110	0.06
141. BD (1) C 110 - C 112	/740. RY*(3) C 62	0.11
143. BD (1) C 112 - C 114	/740. RY*(3) C 62	0.06
144. BD (2) C 112 - C 114	/***. BD*(2) C 60 - C 62	0.14
83. BD (1) C 62 - C 63	/***. RY*(2) C 110	0.06
83. BD (1) C 62 - C 63	/***. RY*(3) C 110	0.06
83. BD (1) C 62 - C 63	/***. RY*(3) C 112	0.29
84. BD (1) C 62 - C 68	/***. RY*(3) C 114	0.09
140. BD (1) C 110 - H 111	/***. BD*(2) C 63 - C 64	0.07
141. BD (1) C 110 - C 112	/749. RY*(3) C 63	0.2
141. BD (1) C 110 - C 112	/751. RY*(5) C 63	0.06
142. BD (1) C 112 - H 113	/747. RY*(1) C 63	0.05
142. BD (1) C 112 - H 113	/749. RY*(3) C 63	0.17
142. BD (1) C 112 - H 113	/***. BD*(2) C 63 - C 64	0.09

144. BD (2) C 112 - C 114	/749. RY*(3) C 63	0.1
144. BD (2) C 112 - C 114	/***. BD*(2) C 63 - C 64	0.69
83. BD (1) C 62 - C 63	/***. RY*(2) C 110	0.06
83. BD (1) C 62 - C 63	/***. RY*(3) C 110	0.06
83. BD (1) C 62 - C 63	/***. RY*(3) C 112	0.29
85. BD (1) C 63 - C 64	/***. RY*(2) C 110	0.12
85. BD (1) C 63 - C 64	/***. RY*(3) C 110	0.09
85. BD (1) C 63 - C 64	/***. RY*(2) C 112	0.07
85. BD (1) C 63 - C 64	/***. RY*(3) C 112	0.12
86. BD (2) C 63 - C 64	/***. RY*(2) C 110	0.08
86. BD (2) C 63 - C 64	/***. RY*(3) C 110	0.08
86. BD (2) C 63 - C 64	/***. RY*(3) C 112	0.2
86. BD (2) C 63 - C 64	/***. BD*(2) C 109 - C 110	0.31
86. BD (2) C 63 - C 64	***. BD*(2) C 112 - C 114	0.66
87. BD (1) C 63 - H 67	/***. RY*(1) C 112	0.06
87. BD (1) C 63 - H 67	/***. RY*(3) C 112	0.18
87. BD (1) C 63 - H 67	/***. BD*(2) C 112 - C 114	0.06
140. BD (1) C 110 - H 111	/758. RY*(3) C 64	0.15
140. BD (1) C 110 - H 111	/***. BD*(2) C 63 - C 64	0.07
141. BD (1) C 110 - C 112	/757. RY*(2) C 64	0.07
141. BD (1) C 110 - C 112	/758. RY*(3) C 64	0.12
142. BD (1) C 112 - H 113	/***. BD*(2) C 63 - C 64	0.09
144. BD (2) C 112 - C 114	/***. BD*(2) C 63 - C 64	0.69
81. BD (1) C 61 - C 64	/***. RY*(1) C 110	0.17
81. BD (1) C 61 - C 64	/***. RY*(3) C 110	0.12
81. BD (1) C 61 - C 64	/***. RY*(1) H 111	0.11
88. BD (1) C 64 - C 69	/***. RY*(2) C 110	0.06
88. BD (1) C 64 - C 69	/***. RY*(1) H 111	0.09
Total rings		**7.78**
152. CR (2)Zn 1	/***. BD*(1) N 34 - C 35	0,06
152. CR (2)Zn 1	/***. BD*(1) N 34 - H 42	0,06
153. CR (3)Zn 1	/***. BD*(1) N 34 - C 35	0,36
153. CR (3)Zn 1	/***. BD*(1) N 34 - H 41	0,09
153. CR (3)Zn 1	/***. BD*(1) N 34 - H 42	0,31
159. CR (9)Zn 1	/***. BD*(1) N 34 - C 35	0,15
159. CR (9)Zn 1	/***. BD*(1) N 34 - H 42	0,08
237. LP (1)Zn 1	/556. RY*(1) N 34	0,07
238. LP (2)Zn 1	/***. BD*(1) N 34 - H 42	0,06
239. LP (3)Zn 1	/***. BD*(1) N 34 - H 41	0,11
241. LP (5)Zn 1	/***. BD*(1) N 34 - C 35	0,08
241. LP (5)Zn 1	/***. BD*(1) N 34 - H 42	0,12
242. LP*(6)Zn 1	/556. RY*(1) N 34	0,7
242. LP*(6)Zn 1	/561. RY*(6) N 34	0,07
242. LP*(6)Zn 1	/***. BD*(1) N 34 - C 35	0,67
242. LP*(6)Zn 1	/***. BD*(1) N 34 - H 41	0,45
242. LP*(6)Zn 1	/***. BD*(1) N 34 - H 42	0,73
243. LP*(7)Zn 1	/557. RY*(2) N 34	0,2
243. LP*(7)Zn 1	/558. RY*(3) N 34	0,09

243. LP*(7)Zn 1	/***. BD*(1) N 34 - C 35	0,37
243. LP*(7)Zn 1	/***. BD*(1) N 34 - H 41	0,31
243. LP*(7)Zn 1	/***. BD*(1) N 34 - H 42	0,19
244. LP*(8)Zn 1	/557. RY*(2) N 34	0,09
244. LP*(8)Zn 1	/558. RY*(3) N 34	0,19
244. LP*(8)Zn 1	/***. BD*(1) N 34 - C 35	0,59
245. LP*(9)Zn 1	/557. RY*(2) N 34	0,08
245. LP*(9)Zn 1	/564. RY*(9) N 34	0,05
245. LP*(9)Zn 1	/***. BD*(1) N 34 - C 35	0,35
245. LP*(9)Zn 1	/***. BD*(1) N 34 - H 41	0,61
245. LP*(9)Zn 1	/***. BD*(1) N 34 - H 42	0,93
49. BD (1) N 34 - C 35	/242. LP*(6)Zn 1	1,33
49. BD (1) N 34 - C 35	/244. LP*(8)Zn 1	0,11
49. BD (1) N 34 - C 35	/245. LP*(9)Zn 1	7,32
49. BD (1) N 34 - C 35	/286. RY*(4)Zn 1	0,07
49. BD (1) N 34 - C 35	/289. RY*(7)Zn 1	0,09
49. BD (1) N 34 - C 35	/291. RY*(9)Zn 1	0,09
49. BD (1) N 34 - C 35	/292. RY*(10)Zn 1	0,21
49. BD (1) N 34 - C 35	/293. RY*(11)Zn 1	0,07
50. BD (1) N 34 - H 41	/242. LP*(6)Zn 1	2,9
50. BD (1) N 34 - H 41	/243. LP*(7)Zn 1	0,92
50. BD (1) N 34 - H 41	/245. LP*(9)Zn 1	9,81
50. BD (1) N 34 - H 41	/283. RY*(1)Zn 1	0,11
50. BD (1) N 34 - H 41	/284. RY*(2)Zn 1	0,21
50. BD (1) N 34 - H 41	/289. RY*(7)Zn 1	0,39
50. BD (1) N 34 - H 41	/292. RY*(10)Zn 1	0,07
50. BD (1) N 34 - H 41	/294. RY*(12)Zn 1	0,06
50. BD (1) N 34 - H 41	/297. RY*(15)Zn 1	0,09
51. BD (1) N 34 - H 42	/242. LP*(6)Zn 1	1,87
51. BD (1) N 34 - H 42	/244. LP*(8)Zn 1	0,26
51. BD (1) N 34 - H 42	/245. LP*(9)Zn 1	8,09
51. BD (1) N 34 - H 42	/283. RY*(1)Zn 1	0,12
51. BD (1) N 34 - H 42	/284. RY*(2)Zn 1	0,15
51. BD (1) N 34 - H 42	/289. RY*(7)Zn 1	0,34
51. BD (1) N 34 - H 42	/290. RY*(8)Zn 1	0,2
51. BD (1) N 34 - H 42	/292. RY*(10)Zn 1	0,16
184. CR (1) N 34	/242. LP*(6)Zn 1	1,26
184. CR (1) N 34	/245. LP*(9)Zn 1	5,45
184. CR (1) N 34	/284. RY*(2)Zn 1	0,06
184. CR (1) N 34	/287. RY*(5)Zn 1	0,07
184. CR (1) N 34	/289. RY*(7)Zn 1	0,08
258. LP (1) N 34	/242. LP*(6)Zn 1	44,54
258. LP (1) N 34	/244. LP*(8)Zn 1	0,45
258. LP (1) N 34	/245. LP*(9)Zn 1	46,26
258. LP (1) N 34	/287. RY*(5)Zn 1	0,79
258. LP (1) N 34	/288. RY*(6)Zn 1	0,18
258. LP (1) N 34	/289. RY*(7)Zn 1	0,22
258. LP (1) N 34	/292. RY*(10)Zn 1	0,66

258. LP (1) N 34	/293. RY*(11)Zn 1	0,05
258. LP (1) N 34	/296. RY*(14)Zn 1	0,1
258. LP (1) N 34	/297. RY*(15)Zn 1	0,15
258. LP (1) N 34	/300. RY*(18)Zn 1	0,06
49. BD (1) N 34 - C 35	/292. RY*(10)Zn 1	0,21
49. BD (1) N 34 - C 35	/293. RY*(11)Zn 1	0,07
50. BD (1) N 34 - H 41	/242. LP*(6)Zn 1	2,9
50. BD (1) N 34 - H 41	/243. LP*(7)Zn 1	0,92
50. BD (1) N 34 - H 41	/245. LP*(9)Zn 1	9,81
50. BD (1) N 34 - H 41	/283. RY*(1)Zn 1	0,11
50. BD (1) N 34 - H 41	/284. RY*(2)Zn 1	0,21
50. BD (1) N 34 - H 41	/289. RY*(7)Zn 1	0,39
50. BD (1) N 34 - H 41	/292. RY*(10)Zn 1	0,07
50. BD (1) N 34 - H 41	/294. RY*(12)Zn 1	0,06
50. BD (1) N 34 - H 41	/297. RY*(15)Zn 1	0,09
51. BD (1) N 34 - H 42	/242. LP*(6)Zn 1	1,87
51. BD (1) N 34 - H 42	/244. LP*(8)Zn 1	0,26
51. BD (1) N 34 - H 42	/245. LP*(9)Zn 1	8,09
51. BD (1) N 34 - H 42	/283. RY*(1)Zn 1	0,12
51. BD (1) N 34 - H 42	/284. RY*(2)Zn 1	0,15
51. BD (1) N 34 - H 42	/289. RY*(7)Zn 1	0,34
51. BD (1) N 34 - H 42	/290. RY*(8)Zn 1	0,2
51. BD (1) N 34 - H 42	/292. RY*(10)Zn 1	0,16
184. CR (1) N 34	/242. LP*(6)Zn 1	1,26
184. CR (1) N 34	/245. LP*(9)Zn 1	5,45
184. CR (1) N 34	/284. RY*(2)Zn 1	0,06
184. CR (1) N 34	/287. RY*(5)Zn 1	0,07
184. CR (1) N 34	/289. RY*(7)Zn 1	0,08
258. LP (1) N 34	/242. LP*(6)Zn 1	44,54
258. LP (1) N 34	/244. LP*(8)Zn 1	0,45
258. LP (1) N 34	/245. LP*(9)Zn 1	46,26
258. LP (1) N 34	/287. RY*(5)Zn 1	0,79
258. LP (1) N 34	/288. RY*(6)Zn 1	0,18
258. LP (1) N 34	/289. RY*(7)Zn 1	0,22
258. LP (1) N 34	/292. RY*(10)Zn 1	0,66
258. LP (1) N 34	/293. RY*(11)Zn 1	0,05
258. LP (1) N 34	/296. RY*(14)Zn 1	0,1
258. LP (1) N 34	/297. RY*(15)Zn 1	0,15
258. LP (1) N 34	/300. RY*(18)Zn 1	0,06
Total Zn-N_{guest}		**143,64**

6. Cartesian coordinates

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Complex 1a·P6 Conformer 1

Zn	1.7020786	0.2299911	-0.5566790
N	1.5772213	2.3130663	-0.7842127
N	3.8011509	0.3978941	-0.6763781
N	-0.2915683	0.1093835	-1.2208351
N	1.9089164	-1.8118581	-0.9796766
C	2.0900449	4.5731005	-0.7702050
C	3.9879914	2.8813096	-0.5816543
C	5.9059545	1.2494095	-0.2052080
C	2.6154865	3.2147724	-0.7169669
C	4.5170829	1.5630581	-0.5181112
C	0.7212564	4.4652170	-0.8180428
H	-0.0124968	5.2778371	-0.8852408
C	6.0052099	-0.1205965	-0.1744132
H	6.8946540	-0.7202039	0.0536015
C	-1.2088197	1.1390039	-1.1647685
C	3.0686220	-2.5467950	-0.8546244
C	-2.5510689	0.6038780	-1.3388742
C	2.7844712	-3.9559814	-1.0799843
C	-1.0018877	-1.0554725	-1.4247020
C	0.8991426	-2.7042944	-1.2684714
C	-2.4234869	-0.7567605	-1.4988627
C	-0.4632173	-2.3686542	-1.4651327
C	1.4381015	-4.0529835	-1.3416315
C	0.4131436	3.0406823	-0.8251387
C	4.6818174	-0.6437820	-0.4856893
C	-0.8993625	2.5048619	-0.9216039
C	4.3557803	-2.0225916	-0.5658302
H	-3.2285061	-1.4878947	-1.6369410
H	0.8664279	-4.9543532	-1.5934106
H	3.5258590	-4.7641517	-1.0758366
H	2.6897611	5.4913225	-0.7873471
H	6.6984656	1.9805844	-0.0057205
H	-3.4856777	1.1719020	-1.3377396
N	1.6968216	0.4511450	1.5883054
C	1.2110296	-0.6269381	2.4765100
C	-0.1428371	-1.1320897	1.9467985
C	-0.6744722	-2.3198346	2.7736553
C	0.3558029	-3.4613103	2.8076886
C	2.2222297	-1.7831453	2.5213091
C	1.7065425	-2.9682468	3.3496661
H	1.1406916	1.3058622	1.8175111
H	2.6764839	0.6828724	1.8265302
H	2.4302235	-2.1101905	1.4794292
H	3.1841507	-1.4040916	2.9361813
H	1.0639864	-0.2324041	3.5080643
H	2.4542385	-3.7929047	3.3377901
H	1.5891679	-2.6592235	4.4149953
H	0.5057449	-3.8469242	1.7707055
H	-0.0323662	-4.3077644	3.4163656
H	-1.6271748	-2.6751035	2.3196718
H	-0.9088014	-1.9700566	3.8062345
H	0.0604871	-1.5066721	0.9220966
N	-1.1869153	-0.1110637	1.7503966
C	-1.5270627	1.0082991	2.4395855
S	-0.5249689	1.9619008	3.4142258
H	-1.8373482	-0.3734091	0.9960596
N	-2.8328802	1.4566061	2.2460680
H	-2.9475352	2.4529096	2.4569985
C	-3.9153645	0.8106578	1.6308302
C	-4.1145172	-0.5816913	1.7420053
C	-4.8295680	1.5750522	0.8730996
C	-5.1346008	-1.2055313	1.0105036
C	-6.0091867	-0.4602104	0.2062258
C	-5.8583372	0.9376430	0.1685496
H	-3.4667483	-1.1842325	2.3933150
H	-4.7080254	2.6662219	0.7987083
H	-6.7990960	-0.9562906	-0.3739894
C	-2.0319184	3.4435400	-0.6729796
C	-2.0921337	4.1218075	0.5709577
H	-1.2873834	3.9590275	1.3077896
C	-3.1757852	4.9496871	0.8850535
H	-3.2187733	5.4591675	1.8613089
C	-4.2271073	5.1143862	-0.0400598
C	-5.4301972	5.9270246	0.3741684
C	-4.1674383	4.4761956	-1.2893522
H	-4.9870711	4.6067814	-2.0102708
C	-3.0720257	3.6570237	-1.6044892
H	-3.0240115	3.1695356	-2.5904715
C	4.9679512	4.0019921	-0.4525481
C	4.9274250	4.8818238	0.6540786
H	4.1441145	4.7480240	1.4173958
C	5.8795292	5.8987480	0.7963714
H	5.8464497	6.5703751	1.6691620
C	6.8912506	6.0550469	-0.1711228
C	7.9356218	7.1277993	0.0340267
C	6.9347776	5.2000801	-1.2848125
H	7.7197103	5.3316385	-2.0445092
C	5.9788439	4.1828988	-1.4222183
H	6.0126370	3.5099618	-2.2939078
C	-1.4299574	-3.4817085	-1.7048844
C	-2.1173933	-3.5814792	-2.9339868
H	-1.9009102	-2.8511506	-3.7299348
C	-3.0693407	-4.5893769	-3.1449113
H	-3.6018915	-4.6581793	-4.1054579
C	-3.3453951	-5.5144741	-2.1243175
C	-4.3900583	-6.5907827	-2.3039806
C	-2.6568068	-5.4376081	-0.8992343
H	-2.8840685	-6.1559430	-0.0960154
C	-1.7066903	-4.4305502	-0.6952857
H	-1.1844304	-4.3538195	0.2716120
C	5.4470288	-3.0115254	-0.3151605
C	5.3683799	-3.8866819	0.7939369
H	4.4971948	-3.8191576	1.4656994
C	6.3786475	-4.8236812	1.0422405
H	6.3075686	-5.4995689	1.9092710
C	7.4902907	-4.9031808	0.1805197
C	8.5744263	-5.9135806	0.4800318
C	7.5831790	-4.0407635	-0.9249646
H	8.4477172	-4.1120463	-1.6018308
C	6.5682103	-3.1029106	-1.1686325
H	6.6338830	-2.4346330	-2.0419586
C	-5.2677864	-2.7085404	1.1304615
C	-6.7219084	1.7658814	-0.7581135
F	-6.3153761	6.1028513	-0.6314010
F	-5.0680487	7.1555385	0.8254117
F	-6.0893807	5.3142673	1.3973083
F	8.7876647	7.2293909	-1.0145537
F	8.6831405	6.8747733	1.1411092
F	7.3659530	8.3468804	0.2173406
F	9.4802802	-6.0150595	-0.5220945
F	8.0504569	-7.1501876	0.6840613
F	9.2564402	-5.5864514	1.6094672
F	-7.9020917	1.1662176	-1.0295401
F	-6.0864346	1.9586201	-1.9533650
F	-6.9811644	2.9923380	-0.2504169
F	-6.1221654	-3.2237858	0.2229986
F	-5.6975882	-3.0743869	2.3622194
F	-4.0562517	-3.3115763	0.9451253
F	-4.9656723	-6.5559880	-3.5296654
F	-5.3821045	-6.4656778	-1.3835884
F	-3.8572051	-7.8296608	-2.1381308

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Complex 1a·P6 Conformer 2

Zn	1.7342593	0.2439185	-0.5356646
N	-0.2447469	0.1628146	-1.2216276
N	1.6389269	2.3377641	-0.6918250
N	1.9571313	-1.7722147	-1.0805918
N	3.8343254	0.4067864	-0.5750661
C	-2.4777705	0.7014510	-1.5065338
C	-0.8323230	2.5570790	-0.8869599
C	0.7994097	4.4968892	-0.6709941
C	-1.1470984	1.2058244	-1.1987018
C	0.4812142	3.0754376	-0.7278533
C	-2.3551067	-0.6526855	-1.7191095
H	-3.1488649	-1.3542294	-2.0013956
C	2.1685363	4.5929600	-0.6116350
H	2.7753267	5.5065649	-0.5968363
C	0.9253817	-2.6551090	-1.3104763
C	4.5745058	1.5622976	-0.4656901
C	1.4090029	-4.0228287	-1.1935957
C	5.9796790	1.2299140	-0.2635018
C	3.0856199	-2.5302619	-0.8430481
C	4.7125440	-0.6454487	-0.4499033
C	2.7492932	-3.9450140	-0.8981192
C	4.3732873	-2.0196917	-0.5374601
C	6.0645135	-0.1413744	-0.2541206
C	-0.9534272	-0.9834322	-1.5162078
C	2.6835714	3.2300393	-0.5982264
C	-0.4272450	-2.3009161	-1.5503226
C	4.0555768	2.8846791	-0.4955520
H	3.4429044	-4.7751353	-0.7193095
H	6.9655520	-0.7567040	-0.1411367
H	6.7966143	1.9502396	-0.1368662
H	-3.3989698	1.2864179	-1.5761182
H	0.0725337	5.3169722	-0.7196352
H	0.8008506	-4.9281509	-1.3067704
N	1.6241560	0.3664350	1.6094004
C	1.1031480	-0.7338143	2.4492818
C	-0.2504687	-1.2095602	1.8895711
C	-0.8084656	-2.3855015	2.7166253
C	0.1888338	-3.5553359	2.7295412
C	2.0931197	-1.9093124	2.4719240
C	1.5552273	-3.1052636	3.2708171
H	1.0643872	1.2169393	1.8447710
H	2.5945167	0.5855916	1.8926692
H	2.3032907	-2.2170505	1.4248886
H	3.0597764	-1.5565474	2.9002946
H	0.9449413	-0.3707345	3.4906283
H	2.2850003	-3.9439156	3.2285115
H	1.4525582	-2.8215360	4.3447861
H	0.3139540	-3.9326615	1.6867493
H	-0.2172648	-4.3972346	3.3327006
H	-1.7795851	-2.7135248	2.2822664
H	-1.0182525	-2.0306341	3.7528833
H	-0.0351590	-1.5862575	0.8677245
N	-1.2761125	-0.1749915	1.6721442
C	-1.6243806	0.9366153	2.3686804
S	-0.6499782	1.8391782	3.4161066
H	-1.8935908	-0.4075112	0.8813558
N	-2.9077572	1.4181090	2.1179807
H	-3.0106923	2.4158278	2.3287523
C	-3.9742747	0.8010873	1.4470693
C	-4.8161778	1.5843813	0.6310728
C	-4.2378143	-0.5810568	1.5806305
C	-5.8371572	0.9758856	-0.1121962
C	-6.0617276	-0.4078750	-0.0373381
C	-5.2659365	-1.1714180	0.8353912
H	-4.6460062	2.6675545	0.5432071
H	-3.6444316	-1.1905949	2.2754568
H	-6.8529305	-0.8812905	-0.6353218
C	-1.3837896	-3.4207732	-1.7957611
C	-1.2660939	-4.2334182	-2.9442906
H	-0.4692680	-4.0184382	-3.6739294
C	-2.1498091	-5.3013466	-3.1621702
H	-2.0536146	-5.9272706	-4.0620806
C	-3.1639054	-5.5707795	-2.2278108
C	-4.1421399	-6.7035757	-2.4324351
C	-3.2942785	-4.7700795	-1.0775031
H	-4.0841316	-4.9839304	-0.3439691
C	-2.4121988	-3.7039703	-0.8684133
H	-2.5129698	-3.0794295	0.0321977
C	-1.9608749	3.5029681	-0.6461752
C	-2.9545806	3.7803747	-1.6107605
H	-2.8686744	3.3451107	-2.6181584
C	-4.0527695	4.5973411	-1.3010542
H	-4.8376131	4.7766157	-2.0498915
C	-4.1627338	5.1684623	-0.0223674
C	-5.3939769	5.9424038	0.3827807
C	-3.1522022	4.9479467	0.9353186
H	-3.2301988	5.4100346	1.9326352
C	-2.0635550	4.1247956	0.6240847
H	-1.2898845	3.9195762	1.3834193
C	5.4554602	-3.0137474	-0.2666643
C	5.9221117	-3.8819629	-1.2769527
H	5.4970171	-3.8033421	-2.2903277
C	6.9153872	-4.8346729	-1.0039618
H	7.2734349	-5.5064271	-1.7986190
C	7.4589536	-4.9288107	0.2881485
C	8.5027646	-5.9683970	0.6261700
C	7.0132425	-4.0608621	1.3038070
H	7.4412217	-4.1363808	2.3162271
C	6.0208124	-3.1130171	1.0261180
H	5.6611302	-2.4389870	1.8203049
C	5.0484393	3.9969461	-0.3898336
C	6.0038147	4.1983180	-1.4099048
H	5.9844853	3.5483870	-2.2994080
C	6.9733161	5.2056070	-1.2990790
H	7.7163715	5.3521706	-2.0972204
C	6.9973669	6.0306227	-0.1627349
C	8.0544659	7.0964252	0.0082239
C	6.0392082	5.8555140	0.8544918
H	6.0592725	6.5043155	1.7448790
C	5.0740034	4.8474455	0.7392722
H	4.3327271	4.6981412	1.5408640
C	-6.6083664	1.8272978	-1.0991776
C	-5.5879931	-2.6351211	1.0420094
F	8.8801576	7.1828048	-1.0624560
F	8.8272620	6.8470243	1.0984699
F	7.4985116	8.3214831	0.1952110
F	8.9015635	-6.6738746	-0.4588101
F	8.0274760	-6.8591517	1.5365513
F	9.6078385	-5.4012240	1.1759522
F	-6.1518892	6.3028894	-0.6766973
F	-5.0735960	7.0699560	1.0671436
F	-6.1779817	5.1947872	1.2090273
F	-5.9842624	-3.2295504	-0.1086087
F	-6.5804405	-2.8012941	1.9459255
F	-4.5089100	-3.3306503	1.5093159
F	-3.8380838	-7.4606494	-3.5137735
F	-5.4067266	-6.2370929	-2.6043345
F	-4.1728844	-7.5266010	-1.3518369
F	-7.7519217	1.2353866	-1.5065483
F	-5.8545576	2.0585831	-2.2170325
F	-6.9223246	3.0383180	-0.5853384

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Complex 1a·P6 Conformer 3

Zn	-1.6760564	0.1741755	-0.6062376
N	-2.7753398	1.9509102	-0.4820700
N	0.0286334	1.2863088	-1.0801683
N	-3.5214506	-0.8623039	-0.8914900
N	-0.6894848	-1.5315132	-1.3351900
C	-3.2900177	4.1648569	-0.0238126
C	-0.8841906	3.5519048	-0.5756493
C	1.4662103	3.0757521	-1.3920206
C	-2.2427851	3.2134647	-0.3676918
C	0.1370836	2.6567039	-0.9784801
C	-4.4607307	3.4504567	0.0503062
H	-5.4660249	3.8355096	0.2583962
C	2.1537238	1.9332765	-1.7323087
H	3.1846146	1.8625450	-2.0935139
C	-4.7475362	-0.3745827	-0.4924403
C	0.6496872	-1.6320488	-1.6461885
C	-5.6848135	-1.4763695	-0.3148318
C	0.9631200	-3.0032827	-2.0243893
C	-3.6426808	-2.2298761	-0.9680715
C	-1.2375519	-2.7880119	-1.5004329
C	-4.9977453	-2.6297375	-0.6073485
C	-2.5972257	-3.1374402	-1.2916497
C	-0.2076477	-3.7171111	-1.9399974
C	-4.1212800	2.0582171	-0.2200262
C	1.2473334	0.8151099	-1.5209258
C	-5.0500751	0.9841327	-0.2090554
C	1.5786649	-0.5562706	-1.7058180
H	-5.3705719	-3.6596903	-0.5562514
H	-0.3645488	-4.7713432	-2.1979054
H	1.9403550	-3.3661927	-2.3635738
H	-3.1494719	5.2415489	0.1305465
H	1.8173152	4.1138619	-1.4457768
H	-6.7255579	-1.3846288	0.0188277
N	-1.8675046	-0.2635111	1.4750740
C	-1.1904654	-1.5140317	1.8844976
C	0.1542275	-1.1906266	2.5654904
C	0.9179390	-2.4924918	2.8725191
C	0.0710453	-3.4381749	3.7429725
C	-2.0462160	-2.4197245	2.7827870
C	-1.2995126	-3.7235798	3.1061111
H	-2.8904737	-0.3463823	1.5901401
H	-1.5459910	0.5499048	2.0498449
H	-2.2995994	-1.8747980	3.7237769
H	-3.0059386	-2.6408138	2.2604046
H	-0.9614987	-2.0857980	0.9564168
H	-1.9132945	-4.3657119	3.7752442
H	-1.1535359	-4.2967634	2.1605007
H	-0.0788824	-2.9693518	4.7439034
H	0.6260473	-4.3862602	3.9176785
H	1.8785739	-2.2552531	3.3812237
H	1.1777647	-2.9942704	1.9089814
H	-0.0594893	-0.6532001	3.5174572
N	0.9892224	-0.2827629	1.7790279
C	1.1264219	1.0570367	1.9837975
S	0.0299622	2.0317676	2.8163261
H	1.4816163	-0.6856482	0.9691096
N	2.2726009	1.6261983	1.4483569
H	2.1704298	2.6177702	1.2124752
C	3.5378137	1.0615597	1.2337061
C	4.4537396	1.7618057	0.4119016
C	3.9615896	-0.1391639	1.8393075
C	5.7205691	1.2331709	0.1501129
C	6.1276985	0.0088833	0.7113593
C	5.2390696	-0.6520603	1.5672269
H	4.1628075	2.7246102	-0.0294743
H	3.3007409	-0.6817044	2.5265567
H	7.1052527	-0.4258395	0.4649927
C	-6.4576797	1.3065385	0.1758976
C	-7.5187485	1.1294063	-0.7385039
H	-7.2986364	0.7468985	-1.7481858
C	-8.8382680	1.4462282	-0.3806818
H	-9.6567657	1.3135319	-1.1043652
C	-9.1145743	1.9431857	0.9037347
C	-10.5192372	2.3056997	1.3267224
C	-8.0688168	2.1159556	1.8307703
H	-8.2889916	2.4966650	2.8410729
C	-6.7545104	1.8014958	1.4675086
H	-5.9356590	1.9353385	2.1927974
C	-0.4877574	4.9810839	-0.3813704
C	-0.8841663	5.9791226	-1.2958248
H	-1.4960075	5.6968615	-2.1677416
C	-0.5018535	7.3164884	-1.1073126
H	-0.8114573	8.0896910	-1.8264805
C	0.2831983	7.6690724	0.0032304
C	0.7098704	9.0999095	0.2399994
C	0.6835011	6.6820498	0.9253456
H	1.2881447	6.9645867	1.8020328
C	0.3004105	5.3485122	0.7335390
H	0.5777776	4.5731870	1.4684467
C	-2.9663822	-4.5770034	-1.4317282
C	-2.3797577	-5.5654909	-0.6066032
H	-1.6408849	-5.2601610	0.1518163
C	-2.7319541	-6.9139519	-0.7369655
H	-2.2735780	-7.6732359	-0.0834063
C	-3.6835379	-7.3009373	-1.7002906
C	-4.0455632	-8.7628240	-1.8208595
C	-4.2755423	-6.3332594	-2.5287755
H	-5.0135099	-6.6381060	-3.2859996
C	-3.9167901	-4.9843310	-2.3944999
H	-4.3727218	-4.2261175	-3.0508967
C	3.0005345	-0.9103740	-1.9997977
C	3.7000850	-1.7799234	-1.1308955
H	3.1964351	-2.1798394	-0.2372003
C	5.0323786	-2.1290032	-1.3757009
H	5.5608755	-2.8025141	-0.6841470
C	5.7054872	-1.5937068	-2.4876596
C	7.1564256	-1.9565658	-2.6942603
C	5.0258588	-0.7384000	-3.3700868
H	5.5495063	-0.3288238	-4.2464818
C	3.6818030	-0.4141203	-3.1347361
H	3.1421676	0.2274107	-3.8490258
C	6.6804955	1.9671549	-0.7624963
C	5.5922509	-1.9887265	2.1775645
F	0.2484484	9.9440927	-0.7135889
F	2.0644589	9.2121585	0.2630118
F	0.2605342	9.5555171	1.4381196
F	-4.9800429	-8.9867642	-2.7746286
F	-4.5336177	-9.2473745	-0.6490372
F	-2.9574749	-9.5155963	-2.1308403
F	-11.4312241	2.0846132	0.3507036
F	-10.6042655	3.6168985	1.6742941
F	-10.9033914	1.5880114	2.4151607
F	7.7010851	-1.3456668	-3.7695825
F	7.3120603	-3.2960333	-2.8598802
F	7.9091078	-1.6159471	-1.6078321
F	7.0081900	1.2113390	-1.8424793
F	7.8362058	2.2631635	-0.1216003
F	6.8252829	-2.4110849	1.8266025
F	4.7063971	-2.9526492	1.7704303
F	5.5264186	-1.9596140	3.5302835
F	6.1587575	3.1280553	-1.2298326

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Complex 1a·P6 Conformer 4

Zn	-1.3805462	0.3200872	-0.6977626
N	-1.4696678	2.3964678	-0.9344873
N	0.6260930	0.3504190	-1.2535963
N	-3.5088172	0.2772662	-0.8854050
N	-1.4087462	-1.7462534	-1.1248809
C	-0.8142142	4.6166248	-0.8255973
C	0.9674026	2.8219277	-1.1364376
C	2.8036430	1.1084260	-1.4914801
C	-0.3813886	3.2332063	-0.9769153
C	1.4136800	1.4851949	-1.2940652
C	-2.1766333	4.5867809	-0.6524058
H	-2.8508803	5.4370010	-0.4939995
C	2.8385215	-0.2608396	-1.5660197
H	3.7362738	-0.8773184	-1.6725141
C	-4.3195215	1.3585975	-0.6158180
C	-0.2992595	-2.5381115	-1.3331943
C	-5.6923417	0.9124496	-0.4236048
C	-0.7150239	-3.9117952	-1.5766382
C	-4.3135843	-0.8382087	-0.8680781
C	-2.5146461	-2.5712663	-1.2192690
C	-5.6873446	-0.4540711	-0.5696452
C	-3.8670248	-2.1757635	-1.0525204
C	-2.0880509	-3.9288473	-1.5142181
C	-2.5765465	3.1868273	-0.7222696
C	1.4671371	-0.7308376	-1.4109597
C	-3.9024933	2.7139111	-0.5439070
C	1.0544508	-2.0944800	-1.3857743
H	-6.5392344	-1.1374450	-0.4743129
H	-2.7525514	-4.7815493	-1.6970431
H	-0.0494049	-4.7472715	-1.8245170
H	-0.1595968	5.4961903	-0.8481082
H	3.6564788	1.7949456	-1.5254732
H	-6.5513829	1.5603358	-0.2116028
N	-1.6790857	0.4850752	1.4262248
C	-2.2892937	-0.7749854	1.9141226
C	-1.2518414	-1.6479227	2.6463789
C	-1.8488890	-3.0497308	2.8607400
C	-3.1609790	-2.9587521	3.6664714
C	-3.5462893	-0.6017219	2.7748423
C	-4.1751398	-1.9802226	3.0429085
H	-2.3605598	1.2597713	1.4824649
H	-0.8609165	0.7549184	2.0152454
H	-3.2842104	-0.0895852	3.7314908
H	-4.2723440	0.0461670	2.2302588
H	-2.6059388	-1.3488778	1.0202883
H	-5.0647840	-1.8801427	3.7029285
H	-4.5456571	-2.3902768	2.0748120
H	-2.9173003	-2.6208950	4.7010791
H	-3.6133633	-3.9708492	3.7645276
H	-1.1096744	-3.6925348	3.3876503
H	-2.0379670	-3.5143204	1.8620490
H	-1.0289133	-1.1839055	3.6326451
N	0.0310785	-1.7105168	1.9482496
C	1.1309588	-0.9555674	2.2811255
S	1.0718407	0.3448719	3.3568128
H	0.0220236	-2.1674457	1.0244391
N	2.2820764	-1.4214909	1.6767811
H	2.2002939	-2.3548811	1.2534763
C	3.5222149	-0.8194326	1.4152650
C	3.7967420	0.5546927	1.5905171
C	4.5125757	-1.6512978	0.8469199
C	5.0265776	1.0711447	1.1666467
C	6.0058828	0.2560867	0.5729095
C	5.7305493	-1.1094337	0.4152111
H	3.0341737	1.2118452	2.0252424
H	4.3147425	-2.7234075	0.6905887
H	6.9628927	0.6792660	0.2358646
C	-4.9523883	3.7345495	-0.2302696
C	-5.5194546	3.8032465	1.0627260
H	-5.1817330	3.0934389	1.8354786
C	-6.4905658	4.7646144	1.3699791
H	-6.9175577	4.8179586	2.3840376
C	-6.9138307	5.6752574	0.3828844
C	-7.9825077	6.6870276	0.7320657
C	-6.3622960	5.6161317	-0.9082279
H	-6.6962959	6.3266616	-1.6793817
C	-5.3881454	4.6518051	-1.2098248
H	-4.9545744	4.6031110	-2.2215354
C	2.0150760	3.8879230	-1.0816515
C	2.2551395	4.5709859	0.1318515
H	1.6595182	4.3110976	1.0211466
C	3.2579664	5.5421671	0.2178827
H	3.4572187	6.0483849	1.1752734
C	4.0422304	5.8408494	-0.9108534
C	5.1689036	6.8346769	-0.7634091
C	3.8054245	5.1818400	-2.1278049
H	4.4177744	5.4242768	-3.0092443
C	2.7930037	4.2148732	-2.2120668
H	2.6037588	3.6952481	-3.1650355
C	-4.8985384	-3.2531539	-1.0237202
C	-5.9639000	-3.2686766	-1.9509498
H	-6.0106139	-2.4891440	-2.7282466
C	-6.9525809	-4.2619974	-1.8962910
H	-7.7768961	-4.2652760	-2.6252446
C	-6.8888011	-5.2606819	-0.9105159
C	-7.9440687	-6.3376503	-0.8133461
C	-5.8252128	-5.2702084	0.0121484
H	-5.7754385	-6.0540435	0.7849931
C	-4.8415233	-4.2769963	-0.0478020
H	-4.0125311	-4.2808143	0.6775798
C	2.1033113	-3.1538901	-1.3397739
C	2.0876904	-4.1031530	-0.2822763
H	1.2492680	-4.1009827	0.4353094
C	3.1075297	-5.0502302	-0.1358924
H	3.0833187	-5.7655044	0.7016013
C	4.1762427	-5.0728112	-1.0511091
C	5.2748995	-6.0926145	-0.8599103
C	4.1885806	-4.1741051	-2.1294436
H	5.0170589	-4.2017316	-2.8514842
C	3.1582023	-3.2349604	-2.2764589
H	3.1674194	-2.5518324	-3.1394111
C	5.2899750	2.5596938	1.2366155
C	6.6959373	-1.9878821	-0.3459144
F	6.5341521	2.8285888	1.6975709
F	4.4058677	3.2111244	2.0269525
F	7.9718733	-1.5535139	-0.2507752
F	6.3781161	-1.9979115	-1.6774417
F	6.6609469	-3.2751247	0.0726499
F	6.2868936	-5.9317763	-1.7410872
F	4.7959899	-7.3565256	-1.0125044
F	5.7955907	-6.0215721	0.3915512
F	5.8005281	7.0833312	-1.9365043
F	6.1038543	6.3825486	0.1135238
F	4.7228187	8.0236750	-0.2804846
F	-8.1422358	7.6234878	-0.2325972
F	-7.6885696	7.3363280	1.8887603
F	-9.1879539	6.0869100	0.9162659
F	5.2057725	3.1113293	-0.0095973
F	-8.9116388	-6.1981773	-1.7500606
F	-8.5488168	-6.3248149	0.4039083
F	-7.4018964	-7.5739762	-0.9664558

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Complex 1a·P6 Conformer 5

Zn	1.7370101	-0.1539830	-0.5974307
N	-0.1079203	0.5815777	-1.2680288
N	2.4587808	1.8221807	-0.6217830
N	1.1597164	-2.0593958	-1.2585039
N	3.7346039	-0.8088700	-0.6365767
C	-1.9703475	1.9519528	-1.3962273
C	0.2486394	2.9623642	-0.6387949
C	2.4790683	4.0915572	-0.1538402
C	-0.5469853	1.8797729	-1.1041550
C	1.6580690	2.9285580	-0.4658990
C	-2.3803558	0.6771260	-1.7151721
H	-3.3953359	0.3492262	-1.9664529
C	3.7827335	3.6589536	-0.1263905
H	4.6805035	4.2534002	0.0813826
C	-0.1274721	-2.4565286	-1.5511761
C	4.8679272	-0.0340186	-0.5176648
C	-0.1881918	-3.9072758	-1.6372227
C	6.0496334	-0.8863624	-0.5364628
C	1.9205696	-3.2063256	-1.1616716
C	4.1490045	-2.1184982	-0.7019084
C	1.0795801	-4.3735457	-1.3790892
C	3.3088918	-3.2495247	-0.8747872
C	5.6024791	-2.1818200	-0.6337277
C	-1.2065644	-0.1769564	-1.6172957
C	3.7552857	2.2293535	-0.4087291
C	-1.2373446	-1.5922919	-1.7308436
C	4.8939330	1.3802644	-0.3933537
H	1.4137600	-5.4172192	-1.3487147
H	6.2041256	-3.0966695	-0.6956753
H	7.0891707	-0.5392196	-0.5053964
H	-2.5962270	2.8484380	-1.3606354
H	2.1098997	5.1127216	-0.0001211
H	-1.0816023	-4.4950050	-1.8803429
N	1.6387764	-0.0550693	1.5553072
C	0.8107710	-1.0028487	2.3302952
C	-0.6295695	-0.9740204	1.7821063
C	-1.5281533	-1.9654681	2.5459594
C	-0.9505605	-3.3888618	2.4593109
C	1.3785021	-2.4265343	2.2376071
C	0.4938922	-3.4367268	2.9829265
H	1.3528153	0.9075504	1.8281122
H	2.6285662	-0.1423059	1.8421445
H	1.4639490	-2.7116330	1.1673913
H	2.4128179	-2.4305355	2.6530897
H	0.7818193	-0.6927174	3.3983457
H	0.9131554	-4.4610296	2.8698505
H	0.4992357	-3.2050485	4.0739771
H	-0.9540262	-3.7199640	1.3926749
H	-1.5970695	-4.0991660	3.0207219
H	-2.5532987	-1.9330732	2.1131872
H	-1.6093259	-1.6358139	3.6075223
H	-0.5580806	-1.3191097	0.7298519
N	-1.2515267	0.3567468	1.6696427
C	-1.2871081	1.4005537	2.5387595
S	-0.1692657	1.7376585	3.7627145
H	-1.8266238	0.4579477	0.8219544
N	-2.3073440	2.3261004	2.3389935
H	-2.0976600	3.2333533	2.7675770
C	-3.4354074	2.2732275	1.5059654
C	-4.1414623	1.0727798	1.2597133
C	-3.8769951	3.4683021	0.8996124
C	-5.2059664	1.0670314	0.3509297
C	-5.6171259	2.2439771	-0.2967399
C	-4.9517104	3.4428102	0.0011440
H	-3.8574717	0.1431871	1.7699189
H	-3.3503035	4.4137452	1.0955777
H	-6.4454078	2.2268159	-1.0199352
C	-2.5723837	-2.2227037	-1.9694236
C	-3.1885807	-2.9754109	-0.9445938
H	-2.6600833	-3.1099634	0.0121714
C	-4.4580875	-3.5340513	-1.1264176
H	-4.9367408	-4.1000925	-0.3125304
C	-5.1379086	-3.3420065	-2.3418584
C	-6.5555899	-3.8445139	-2.4683760
C	-4.5327197	-2.6115126	-3.3781198
H	-5.0660296	-2.4699761	-4.3304826
C	-3.2569546	-2.0592486	-3.1924578
H	-2.7811325	-1.4836203	-4.0026312
C	-0.4497102	4.2099272	-0.2059694
C	-0.3520331	4.5985230	1.1537292
H	0.2423415	3.9815573	1.8487134
C	-1.0282467	5.7278422	1.6280716
H	-0.9535288	6.0108025	2.6905733
C	-1.8223028	6.4919999	0.7492995
C	-2.6275897	7.6368558	1.3152750
C	-1.9096847	6.1350138	-0.6060368
H	-2.5304012	6.7311460	-1.2899380
C	-1.2221738	5.0061169	-1.0785550
H	-1.2857459	4.7369613	-2.1443479
C	3.9530058	-4.5887963	-0.7243931
C	4.0640085	-5.4911798	-1.8035361
H	3.6687981	-5.2011069	-2.7902128
C	4.6839681	-6.7391955	-1.6344789
H	4.7730865	-7.4341220	-2.4831923
C	5.2015542	-7.1002917	-0.3792739
C	5.8804113	-8.4319491	-0.1580861
C	5.0984098	-6.2104198	0.7070863
H	5.5011512	-6.4977678	1.6915071
C	4.4808744	-4.9671202	0.5325978
H	4.3951940	-4.2672210	1.3797143
C	6.2271732	2.0300736	-0.2173743
C	7.0311096	1.7511846	0.9128165
H	6.6578764	1.0527031	1.6789332
C	8.2843174	2.3552691	1.0676972
H	8.9020173	2.1337046	1.9527784
C	8.7567094	3.2532522	0.0912817
C	10.1099615	3.8951433	0.2884717
C	7.9686117	3.5449706	-1.0343956
H	8.3422860	4.2425751	-1.7990880
C	6.7138288	2.9367384	-1.1846399
H	6.0980515	3.1555440	-2.0717728
C	-5.9047459	-0.2259289	-0.0110508
C	-5.2870440	4.6951569	-0.7784929
F	5.8751648	-9.2081181	-1.2670491
F	5.2710606	-9.1323239	0.8347750
F	7.1760936	-8.2686533	0.2190908
F	-7.2463791	-0.1227299	0.1091617
F	-5.4983282	-1.2681684	0.7541392
F	-5.6450296	-0.5450489	-1.3096841
F	-6.5759517	4.7153028	-1.1836182
F	-4.5134458	4.7658702	-1.9038960
F	-5.0536713	5.8221445	-0.0688415
F	-6.9863651	-3.8611927	-3.7526649
F	-7.4143286	-3.0569156	-1.7647468
F	-6.6876295	-5.1023954	-1.9735906
F	10.4768582	4.6628665	-0.7649621
F	11.0772579	2.9584686	0.4686550
F	10.1231140	4.6863390	1.3932181
F	-3.2092719	8.3905080	0.3560033
F	-1.8597762	8.4560560	2.0776335
F	-3.6198250	7.1697609	2.1263157

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Complex 1a·P6 Conformer 6

Zn	-1.5646770	0.3566969	-0.6490454
N	-1.5998444	2.4435412	-0.7987911
N	0.4452531	0.3564355	-1.1768989
N	-3.6743515	0.3758837	-0.8478928
N	-1.6196793	-1.6987169	-1.1068767
C	-0.8829879	4.6410909	-0.6298615
C	0.8507947	2.8000657	-0.8981927
C	2.6349056	1.0806559	-1.4142759
C	-0.4865909	3.2461748	-0.7629697
C	1.2596954	1.4708389	-1.1565790
C	-2.2570410	4.6570724	-0.5989424
H	-2.9160540	5.5316530	-0.5379048
C	2.6351369	-0.2827272	-1.5740943
H	3.5113443	-0.9191405	-1.7374587
C	-4.4850504	1.4859264	-0.7484048
C	-0.5200001	-2.5210444	-1.2221853
C	-5.8814355	1.0719079	-0.6931785
C	-0.9497602	-3.9126232	-1.2443328
C	-4.5003069	-0.7241889	-0.8535648
C	-2.7325306	-2.5151290	-1.0624399
C	-5.8912775	-0.2995090	-0.7710485
C	-4.0767935	-2.0770044	-0.9379598
C	-2.3198075	-3.9081560	-1.1301034
C	-2.6939890	3.2680102	-0.6866420
C	1.2588339	-0.7323177	-1.4012422
C	-4.0454659	2.8350804	-0.6699956
C	0.8313428	-2.0911241	-1.3564848
H	-6.7655918	-0.9613518	-0.7828202
H	-2.9867164	-4.7778800	-1.1096003
H	-0.2989200	-4.7863084	-1.3677972
H	-0.1957718	5.4954361	-0.5935488
H	3.4970656	1.7573975	-1.4322097
H	-6.7456117	1.7411299	-0.6070420
N	-1.7504017	0.4496122	1.4774890
C	-2.1171300	-0.8658360	2.0521650
C	-0.8955609	-1.5034720	2.7389572
C	-1.2362239	-2.9353770	3.1938082
C	-2.4565119	-2.9377392	4.1318102
C	-3.3167690	-0.8269840	3.0089864
C	-3.6685875	-2.2481312	3.4817661
H	-2.5143411	1.1327857	1.6032224
H	-0.9003287	0.8396783	1.9423614
H	-3.0769329	-0.1747928	3.8826478
H	-4.1847980	-0.3679241	2.4808967
H	-2.4027528	-1.5304599	1.2069324
H	-4.5269522	-2.2193405	4.1887474
H	-3.9976983	-2.8487199	2.6014441
H	-2.1895241	-2.4046712	5.0747907
H	-2.7114234	-3.9817637	4.4192656
H	-0.3486813	-3.3794140	3.6960260
H	-1.4518993	-3.5571270	2.2907400
H	-0.6331074	-0.8849510	3.6269435
N	0.2951251	-1.5047953	1.8933350
C	1.3893023	-0.6874154	2.0519453
S	1.3225257	0.7868381	2.8718648
H	0.2574671	-2.1030983	1.0558872
N	2.5265378	-1.2507954	1.5063879
H	2.4111285	-2.2299010	1.2153739
C	3.8054389	-0.7573700	1.2082212
C	4.1934031	0.5956275	1.3166993
C	4.7292994	-1.6962190	0.6955337
C	5.4691412	0.9834933	0.8863111
C	6.3895173	0.0579500	0.3664116
C	6.0037331	-1.2868272	0.2789872
H	3.4831786	1.3355693	1.7067197
H	4.4409809	-2.7550419	0.5863439
H	7.3861979	0.3800524	0.0359940
C	-5.1034278	3.8851852	-0.5560124
C	-5.2425848	4.6496987	0.6249222
H	-4.5500844	4.4733700	1.4638458
C	-6.2547857	5.6100750	0.7408657
H	-6.3631406	6.1927204	1.6698007
C	-7.1468565	5.8220710	-0.3277801
C	-8.2385115	6.8539954	-0.1688480
C	-7.0134559	5.0794918	-1.5123812
H	-7.7067377	5.2543872	-2.3487582
C	-5.9969094	4.1197425	-1.6234994
H	-5.8893419	3.5359610	-2.5517592
C	1.9276642	3.8260053	-0.7243400
C	2.3116755	4.2062783	0.5802810
H	1.8182348	3.7316245	1.4440062
C	3.3211979	5.1560155	0.7746802
H	3.6326612	5.4328723	1.7934464
C	3.9684390	5.7278666	-0.3358457
C	5.1130444	6.6824520	-0.0933116
C	3.5898246	5.3634695	-1.6377001
H	4.1007114	5.8129524	-2.5023961
C	2.5702938	4.4182085	-1.8292088
H	2.2697397	4.1260069	-2.8481733
C	-5.1315267	-3.1334254	-0.8776854
C	-5.9100656	-3.3058557	0.2905951
H	-5.7490625	-2.6304949	1.1458465
C	-6.8679313	-4.3232156	0.3715247
H	-7.4582240	-4.4578233	1.2920776
C	-7.0674416	-5.1873756	-0.7221549
C	-8.0970576	-6.2858044	-0.6004229
C	-6.3183547	-5.0160858	-1.8978830
H	-6.4865911	-5.6841991	-2.7559523
C	-5.3603161	-3.9943251	-1.9731328
H	-4.7730038	-3.8573194	-2.8952852
C	1.8850104	-3.1483375	-1.3603278
C	1.9980642	-4.0482745	-0.2682772
H	1.2540681	-4.0160325	0.5465604
C	3.0263267	-4.9961007	-0.2085663
H	3.1018519	-5.6791816	0.6526629
C	3.9741222	-5.0645184	-1.2456110
C	5.1047511	-6.0587023	-1.1253538
C	3.8613890	-4.2072600	-2.3513321
H	4.5966430	-4.2715712	-3.1667336
C	2.8234005	-3.2672052	-2.4095568
H	2.7320896	-2.6086696	-3.2875866
C	5.8123121	2.4567035	0.8686016
C	6.9441628	-2.3325097	-0.2783545
F	-8.1342028	-7.0828724	-1.6944840
F	-9.3442200	-5.7767478	-0.4238905
F	-7.8424073	-7.0783977	0.4741172
F	5.9146897	-6.0562097	-2.2063904
F	4.6286134	-7.3232316	-0.9708125
F	5.8671823	-5.7926324	-0.0337255
F	-7.7210596	8.0955695	0.0214218
F	-9.0143153	6.5832198	0.9137137
F	6.1213656	6.0701799	0.5837449
F	4.7283333	7.7458212	0.6602820
F	-9.0538625	6.9144046	-1.2488016
F	5.6361672	7.1693904	-1.2441809
F	7.1450818	2.6753630	0.9329247
F	5.2315871	3.1248151	1.8916486
F	5.3714371	3.0267550	-0.2913980
F	8.1345562	-1.8119143	-0.6521961
F	6.4047565	-2.9343864	-1.3782811
F	7.1847220	-3.3098653	0.6259079

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