Electronic Supplementary Information

Pillar[5]arene-based supramolecular polypseudorotaxane polymer network constructed by orthogonal self-assembly

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1. General information.

All reactions were performed in atmosphere unless otherwise stated. The commercially available reagents were used as supplied without further purification. Chloroform and acetonitrile were dried according to procedures described in the literature, and other solvents were used as received without further purification unless otherwise stated. Compounds H1 and D1 were prepared according to our previously reported method.^{\$1,\$2} Column chromatography was performed with silica gel (200-300 mesh) produced by Qingdao Marine Chemical Factory, Qingdao (China). All yields were given as isolated yields. NMR spectra were recorded on a Bruker DPX 300 MHz spectrometer (or Bruker DPX 400 MHz spectrometer) with internal standard tetramethylsilane (TMS) and solvent signals as internal references at room temperature, and the chemical shifts (δ) were expressed in ppm and J values were given in Hz. Low-resolution electrospray ionization mass spectra (LR-ESI-MS) were obtained on Finnigan Mat TSQ 7000 instruments. High-resolution electrospray ionization mass spectra (HR-ESI-MS) were recorded on an Agilent 6540Q-TOF LCMS equipped with an electrospray ionization (ESI) probe operating in positive-ion mode with direct infusion. Viscosity measurements were carried out with Ubbelohde micro viscometers (Shanghai Liangjing Glass Instrument Factory, 0.40 mm inner diameter) at 298 K in CHCl₃/CH₃CN solution (v/v, 1.5/1). Dynamic light scattering (DLS) measurements were carried out on a Brookhaven BI-9000AT system (Brookhaven Instruments Corporation, USA), using a 200-mW polarized laser source ($\lambda = 532$ nm). The UV-Vis absorption spectrum was measured on a Perkin Elmer Lambda 35 UV/Vis Spectrometer. The excitation and emission spectra were recorded on a Perkin Elmer LS55 Fluorescence Spectrometer. Transmission electron microscope (TEM) investigations were carried out on a JEM-2100 instrument.

2. ESI-MS spectrum and the determination of the complex stoichiometry between H1 and D1.



Figure S1. ESI-mass spectrum of D1 in the presence of equimolar H1 in methanol solution.

From the above ESI-mass spectrum, peaks for both 1 : 1 {[**H1** + **D1**–4PF₆]⁴⁺ (m/z 447.45), [**H1** + **D1**–3PF₆]³⁺ (m/z 644.95), [**H1** + **D1**–2PF₆]²⁺ (m/z 1039.90)} and 2 : 1 {[2**H1** + **D1**–4PF₆]⁴⁺ (m/z 725.20), [2**H1** + **D1**–3PF₆]³⁺ (m/z 1015.25), [2**H1** + **D1**–2PF₆]²⁺ (m/z 1595.50)} host–guest complexes were found.



Figure S2. ¹H NMR titration spectra (300 MHz, 298 K) of 5.0 mM **D1** with various equivalents of **H1** in CDCl₃/CD₃CN (1.5/1, *v/v*) solution: (a) 0.0, (b) 0.2, (c) 0.4, (d) 0.6, (e) 0.8, (f) 1.0, (g) 2.0, (h) 4.0, (i) 6.0, (j) 10.0, (k) 30.0.

The solutions of **H1**, **D1** are both colorless, while their mixture presents yellow color with the increasing amount of **H1** in CDCl₃/CD₃CN (1.5/1, ν/ν) solution, which confirms the host-guest recognition pair in the mixed solution due to the charge transfer interaction from the π -electron rich pillar[5]arene cavity to the π -electron poor viologen aromatic rings of paraquats. As the concentration of **H1** increased, the yellow color became darker and darker, indicating the concentration dependent percentage of the complexed species of the pillararene–paraquat moieties.

(e)	(f)	(g)	(h)	(i)	(j)	(k)
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Figure S3. Naked-eye observation of the color change of the above **H1** and **D1** (5.0 mM) complex with different equivalents of **H1** in CDCl₃/CD₃CN (1.5/1, ν/ν) solution: (e) 0.8, (f) 1.0, (g) 2.0, (h) 4.0, (i) 6.0, (j) 10.0, (k) 30.0.

From the above ¹H NMR titration experiment, based on the chemical shift changes of H_a on **D1**, we can also calculate the stoichiometry of the host and guest was about 2 : 1, which was shown in Figure S4.



Figure S4. The stoichiometry of host and guest complex (based on the chemical shift changes of H_a on D1).

3. ¹H NMR spectra of H1 and H1 with D1 in different concentrations.



Figure S5. ¹H NMR spectra (300 MHz, 298 K, $CDCl_3/CD_3CN = 1.5/1$, ν/ν) of **H1** at different concentrations (mM): (a) 2.0, (b) 10.0, (c) 20.0, (d) 50.0, (e) 80.0, (f) 125.0.

In order to study the assembly behavior of **H1**, we performed the ¹H NMR experiments in CHCl₃/CH₃CN (1.5/1, v/v) solution at various concentrations of **H1** in the range of 2–125 mM. From the spectra above (Figure S5), It found that the **UPy** N–H signals showed a large downfield shift together with a little lower intensity (between 10 and 13.5 ppm), which gave direct evidence for the dimerization of **UPy** units.

Subsequently, the formation of the large supramolecular polypseudorotaxane networks was investigated by the ¹H NMR spectra of **D1** with **H1** in a 1 : 2 molar ratio at various concentrations in the range of 0.5–80 mM as shown in Figure S6.



Figure S6. ¹H NMR spectra (300 MHz, 298 K, CDCl₃/CD₃CN = 1.5/1, ν/ν) of **D1** with **H1** in 1:2 ratio at various **D1** concentrations (mM): (a) 0.5, (b) 1.0, (c) 2.5, (d) 7.5, (e) 15.0, (f) 25.0, (g) 50.0, (h) 80.0.

Moreover, on the basis of the chemical shift changes of H_a, the percentages of the complexed pillararene moieties with the paraquat units at different initial concentrations of **H1** and 0.5 equiv **D1** were estimated (Table S1)^{S3}. The value of the maximum chemical shift change $\Delta_0 = 0.2783$ ppm, was determined by extrapolation of a plot of $\Delta = \delta - \delta_u$ vs. 1/[**D1**]₀ in high initial concentration range (Figure S7). It is indicated that the percentage of complexed viologen moieties increased with increasing concentration, suggesting the [3]pseudorotaxane structure had been incorporated leading to the cross-linking.

Table S1. Calculated the association ratio of pillararene and paraquat unit at different concentration of monomers.

[H1] (mM)	7.5	15.0	25.0	50.0	80.0
Association Ratio (%) ^a	33.9%	65.3%	79.5%	90.4%	94.5%

^a The association ratio (%) was calculated from $\Delta/\Delta 0$.



Figure S7. Benesi-Hildebrand plot (298 K, $CDCl_3/CD_3CN = 1.5/1$, ν/ν) for complexation between **D1** and **H1** in 1 : 2 ratio at various **D1** concentrations. $\Delta_0 = 0.2783$ ppm.

4. UV-Vis spectroscopy & fluorescent titration experiment.

Figure S8 shows the UV-Vis absorption spectra of **D1** in CHCl₃/CH₃CN (1.5/1, v/v). It was found that the UV/vis absorption spectrum of **D1** solution showed an absorption band at 268 nm due to the π - π * transition on the aromatic rings of paraquats.



Figure S8. UV-Vis absorption spectra of D1 (1×10^{-5} M) in CHCl₃/CH₃CN (1.5/1, v/v).

Then, we made the fluorescent spectroscopy titration experiments and the results were shown in Figure S9. It was found that the emissions spectrum of the viologen derivatives at 353 nm upon excitation at 265 nm could be quenched by the host **H1**. A gradual quenching was observed upon the addition of **H1** into the solution of **D1** in CHCl₃/CH₃CN (1.5/1, ν/ν) solution.





Figure S9. Fluorescent titration of **D1** $(1 \times 10^{-5} \text{ M})$ in CHCl₃/CH₃CN $(1.5/1, \nu/\nu)$ solution with various equiv. of **H1**. (*Inset:* Titration profile of the absorption changes upon the addition of **H1**. Changes in the fluorescence intensities at 353 nm from **D1** upon the addition of **H1** were plotted.)

5. Determination of the K_a value.



To determine the association constant of our supramolecular polymer formed between H1 and D1, H2 (DMP5 host) and D3 (paraquat guest) were chosen as the model compounds. The Job Plot indicates a 1:1 binding model between H2 and D3 (Figure S10).



Figure S10. Job Plot of the complex formed between **H2** (host) and **D3** (guest) showing a 1:1 stoichiometry. (The job Plot was conducted by varying the mole fractions of the guest and host. Concentration: [Host] + [Guest] = 10 mM.)



Figure S11. Partial ¹H NMR titration spectra of 2.00 mM **D3** solution with (a) 0, (b) 0.25, (c) 0.5, (d) 1.0, (e) 1.5, (f) 2.0, (g) 3.0, (h) 4.0, (i) 5.0, (j) 7.5, (k) 10.0, (l) 15.0, (m) 25.0 equiv of **H2**. Solvent system: CHCl₃/CH₃CN (1.5/1, *v/v*).

Then, ¹H NMR titrations were performed with a constant concentration of **D3** (2.00 mM) and varying concentrations of **H2** in the range of 0.5–50.0 mM (Figure S11). However, the change in chemical shift ($\Delta\delta$) observed for H_a of **D3** is too small ($\Delta\delta < 0.4$ ppm), thus the average association constants cannot be calculated accurately.

Therefore, the association constant (K_a) between H2 and D3 was determined through fluorescence quenching titration experiments according to the reported method (Figure S12).^{S4} Fluorescence spectra were recorded at varying host concentrations (C_{host}). Changes in the ratios (I/I_0) of the fluorescence intensities at 353 nm from D3 upon addition of H2 were plotted and the association constant was calculated from Eq.1.

$$I / I_0 = \frac{1 + aK_aC_{host}}{1 + K_aC_{host}}$$
(Eq.1)

Where "a" is a constant, K_a stands for the association constant. By fitting the above spectrum data with Eq. 1, the K_a value was determined to be $(3.13 \pm 0.09) \times 10^3 \text{ M}^{-1}$ (CHCl₃/CH₃CN = 1.5/1, ν/ν) for the complex of [H2⊂ D3], which was approximated as the K_a value between H1 and D1. The reason we chose this mixed solvent system is based on the different solubility of the pillararene host and paraquat guest. Since pillararene host H2 can dissolve in CHCl₃ very well and paraquat guest D3 shows good solubility in polar solvent CH₃CN, therefore, we chose CHCl₃/CH₃CN (1.5/1, ν/ν) as the mixed solvents, in which both of the host and guest could

dissolve much better than single-solvent system.



Figure S12. (a) Fluorescent titration of **D3** $(1 \times 10^{-5} \text{ M})$ in CHCl₃/CH₃CN $(1.5/1, \nu/\nu)$ solution with various equivalence of **DMP5** host (**H2**). (b) Plot of the changes in the ratios (*I*/*I*₀) of the fluorescence intensities at 353 nm from **D3** upon addition of **DMP5** host.

6. 2D NOESY spectra of the complexation between H1 and D1.

The 2D-NOESY NMR spectrum of the solution of **H1–D1** (the concentration of **H1** and **D1** are 30.0 and 15.0 mM, respectively) showed the NOE peaks between protons H_1 and H_a , H_a' , H_2/H_3 and H_a , H_a' , H_2/H_3 and H_c , which confirmed the complexation between **H1** and **D1**.



Figure S13. 2D-NOESY analysis of **H1** with **D1** in CDCl₃/CD₃CN (1.5/1, ν/ν) solution with a mixing time of 600 ms (400 MHz, 298 K, the concentrations of host and guest are 30.0 mM and 15.0 mM, respectively)

7. DLS of the supramolecular polymers.

We also conducted the DLS measurements of **H1** with **D1** in 2:1 ratio in CHCl₃/CH₃CN solution (ν/ν , 1.5:1) to investigate the size of the aggregates. The aggregate of **H1** and **D1** at concentration of 30 mM and 50 mM in solution shows the average hydrodynamic radius (R_h) values of 322 nm and 574 nm, respectively, indicating the formation of large size supramolecular aggregates.

30 mM solution:

Sample ID Operator ID Elapsed Time Mean Diam. Rel. Var. Skew RmsError	30ml hxy 00:09 226.7 0.648 -0.15 5.940	/ 9:02 7 (nm) 8 11 01e-01				100 50 50 5.00	e-01	Diam	5000.0 eter (nm)
d	G(d)	C(d)	d	G(d)	C(d)	d	G(d)	C(d)	
1.00	0	0	12.68	0	37	160.89	0	37	
1.26	ō	ō	15.98	ō	37	202.69	ŏ	37	
1.59	0	0	20.13	0	37	255.35	62	51	
2.00	ō	ő	25.36	ō	37	321.69	100	72	
2.52	ō	0	31.95	ō	37	405.26	90	92	
3.17	59	13	40.25	ō	37	510.54	38	100	Print Window
4.00	69	28	50.71	0	37	643.17	0	100	
5.04	43	37	63.88	ő	37	810.25	ő	100	Copy For Spreadsheet
6.34	0	37	80.47	ő	37	1020.75	ő	100	
7,99	ō	37	101.38	ő	37	1285.93	ō	100	Copy to Clipboard
10.07	0	37	127.72	0	37	1619.99	ō	100	
	-								Close

50 mM solution:

Sample ID Operator ID Elapsed Time Mean Diam. Rel. Var. Skew RmsError	50ml/ hxy 00:12 390.1 0.824 0.707 4.234	1 2:03 1 (nm) 4 7 46e-01				100 50 0 5.00	e-01	Diame	5000.0 eter (nm)
d 2.61 2.21	G(d)	C(d)	d 25.56	G(d) 0	C(d) 37	d 250.50	G(d) 0	C(d) 37	
3.95 4.86	0	0	38.71 47.64	0	37 37 37	379.34 466.81	38 76	45 61	
7.36 9.06 11.15	67 53 0	26 37 37	72.14 88.77 109.24	0	37 37 37 37	706.90 869.90 1070.48	57 0 0	94 94 94	Print Window Copy For Spreadsheet
13.72 16.88 20.77	0 0	37 37 37	134.42 165.42 203.56	0 0 0	37 37 37	1317.32 1621.06 1994.85	28 0 0	100 100 100	Copy to Clipboard Close

Figure S14. Distribution of the hydrodynamic diameter of **H1** with **D1** in 2:1 ratio in $CHCl_3/CH_3CN$ solution (ν/ν , 1.5/1) at 298 K.

8. TEM micrograph of the supramolecular polymers.

Representative TEM images of the supramolecular polymers formed in chloroform/ acetonitrile (v/v, 1.5:1) solution are shown in Figure S15. In most cases, the supramolecular aggregates were observed as dark gray spherical aggregates, and all of the aggregates showed relatively large-sized structure (200 – 600 nm), indicating the formation of high-molecular-weight polymers.



Figure S15. TEM mcicrograph of the supramolecular aggregates (samples were prepared by placing one drop of the CHCl₃/CH₃CN solution of the mixtures of **H1** with 0.50 equiv. **D1** onto a carbon-coated copper grid).

9. Film forming experiments of the supramolecular polymers.

Representative film images of the supramolecular polymers with polyethylene glycol 2000 (**PEG-2000**) as the polymer matrix are shown in Figure S16. Samples were prepared by placing the CHCl₃ solution of **H1** (a) and the CHCl₃/CH₃CN solution of the mixtures of **H1** with 0.50 equiv. **D1** and **PEG-2000** (10 equiv.) (b) into a Teflon mould, respectively). For **PEG-2000**, it could not form a film individually, but was usually obtained as a waxy solid due to its strong crystallizability. However, in the presence of the above obtained supramolecular polymers (**H1** or **H1** with **D1**), translucent films could be obtained in white (**H1** with **PEG-2000**) or yellow color (**H1** and **D1** with **PEG-2000**), in which the color change also confirmed the formation of host-guest inclusion complex due to the charge transfer interaction between **H1** and **D1**. But

unfortunately, the film was so fragile that it was difficult to further investigate its mechanical property. Some other kind of conventional polymers will be examined, and especially the preparation of well-designed chemically modified polymers is underway for further exploring the complexation of conventional and supramolecular polymers.



Figure S16. Film formation experiments (Samples were prepared by placing **PEG-2000** (10 equiv.) with the CHCl₃ solution of **H1** (1 equiv.) (a), and the CHCl₃/CH₃CN solution of the mixtures of **H1** (1 equiv.) and **D1** (0.5 equiv.) (b) into a Teflon mould, respectively).

10. Optimized structure.



Using the density functional theory (DFT) method, the inclusion structure of the module compound [H2 \subset D2] was optimized. The geometry optimizations were carried out in gas phase, at the B3LYP/3-21G level by employing the Gaussian09 program.^{S5} Figure S17 shows the geometry of the optimized structure, and Table S2 shows the coordinates of [H2 \subset D2].

No.	Х	Y	Z	No.	Х	Y	Z
C1	-1.221744	3.535350	-0.870552	H83	-1.407214	0.524068	1.036275
C2	-0.963973	3.787805	0.477723	H84	0.191863	1.063908	1.591049
C3	-1.868151	3.323516	1.446211	C85	0.354854	-0.658986	3.510048
C4	-3.002007	2.608140	1.051675	C86	-1.468487	-1.691558	2.413448
C5	-3.261700	2.362533	-0.298953	C87	0.280916	-1.593947	4.531078
C6	-2.361743	2.831748	-1.267640	H88	1.106028	0.126142	3.543960
C7	-4.478097	1.555615	-0.725668	C89	-1.580383	-2.642442	3.413181
C8	0.308999	4.501368	0.907276	H90	-2.126442	-1.692188	1.553611
C9	1.411534	3.492770	1.195093	C91	-0.680703	-2.610005	4.484393
C10	-4.149593	0.070249	-0.777347	H91	0.990162	-1.529798	5.343926
C11	1.525886	2.891923	2.449622	H93	-2.275130	-3.459737	3.255701
C12	2.525633	1.954272	2.705408	C94	-0.670450	-3.689428	5.502019
C13	3.437639	1.583250	1.714387	C95	-1.796342	-4.000749	6.280319
C14	3.314077	2.173588	0.451325	C96	0.508078	-4.433844	5.680516
C15	2.313568	3.111822	0.183271	C97	-1.715503	-5.013664	7.219080
C16	-4.359269	-0.741491	0.342825	H98	-2.719436	-3.447263	6.173737
C17	-4.059273	-2.108318	0.280384	C99	0.534523	-5.439381	6.631230
C18	-3.516127	-2.677891	-0.869767	H100	1.367345	-4.225170	5.039094
C19	-3.266189	-1.852717	-1.983318	H101	-2.547807	-5.281453	7.855235
C20	-3.586694	-0.495370	-1.929454	H102	1.412160	-6.043537	6.811138
C21	-3.176170	-4.159271	-0.936950	C103	-0.524967	-6.841634	8.410526
C22	-1.759705	-4.406667	-0.438014	H104	-1.047702	-6.476003	9.297806
C23	-1.514152	-4.735450	0.895931	H105	0.526260	-7.003831	8.658437
C24	-0.202500	-4.881743	1.358905	C106	-1.169170	-8.126668	7.854806
C25	0.891943	-4.719630	0.513842	H107	-1.193714	-8.843835	8.684921
C26	0.643117	-4.436308	-0.847144	H108	-2.210499	-7.925101	7.573462
C27	-0.664967	-4.256026	-1.299652	C109	-0.403390	-8.745706	6.666528
C28	2.324985	-4.845802	1.024713	H110	0.632377	-8.944866	6.969377
C29	2.949365	-3.480614	1.310628	H111	-0.378053	-8.040175	5.824249
C30	4.504940	0.533053	2.002793	C112	-1.061307	-10.061892	6.186914
C31	3.977427	-0.877683	1.783586	H113	-1.075750	-10.780998	7.016355
C32	3.057998	-2.976020	2.610701	H114	-2.105281	-9.855619	5.915015
C33	3.535290	-1.680264	2.834385	C115	-0.332848	-10.696172	4.977896
C34	3.959013	-1.419973	0.484747	H116	-0.942781	-11.527276	4.604918

Table S2. coordinates of the optimized structure of [H2⊂D2]

C35	3.420350	-2.684766	0.257769	H117	-0.266445	-9.957960	4.166760
H36	-0.485669	3.864838	-1.591908	C118	1.076027	-11.225836	5.322823
O37	-1.538962	3.590572	2.781593	H119	1.019212	-11.971336	6.123909
H38	-3.691476	2.194004	1.776888	H120	1.531600	-11.703256	4.449319
O39	-2.664134	2.511232	-2.591441	H121	1.743697	-10.420395	5.649112
H40	-4.795430	1.893269	-1.714425	N122	-0.508058	-0.732533	2.462982
H41	-5.288797	1.720423	-0.013631	N123	-0.561671	-5.715072	7.391345
H42	0.102470	5.084151	1.807639	C124	5.079421	-1.323501	-1.689530
H43	0.643551	5.167717	0.110265	H125	5.737258	-2.131992	-1.355960
H44	0.793605	3.149261	3.205516	H126	4.302767	-1.719831	-2.348615
O45	2.583564	1.278720	3.958759	H127	5.652612	-0.561666	-2.217107
H46	3.987535	1.849084	-0.328952	C128	3.992110	-4.437022	4.277041
O47	2.125423	3.692362	-1.073216	H129	4.450177	-5.088070	3.527365
O48	-4.841213	-0.165429	1.539563	H130	4.709690	-3.670895	4.583723
H49	-4.245175	-2.746868	1.137946	H131	3.680930	-5.025662	5.143107
O50	-2.695277	-2.481999	-3.084841	C132	2.834205	2.161861	5.125375
H51	-3.379574	0.167349	-2.758685	H133	2.038938	2.904074	5.237813
H52	-3.263986	-4.491514	-1.973308	H134	2.856990	1.502003	5.993684
H53	-3.884558	-4.717655	-0.322350	H135	3.795340	2.671055	5.013355
O54	-2.603682	-4.880592	1.805401	C136	3.332439	3.942687	-1.886842
H55	-0.034572	-5.122093	2.402114	H137	4.115429	4.410494	-1.281980
O56	1.760749	-4.356290	-1.668145	H138	3.708493	3.018207	-2.334128
H57	-0.871539	-3.964612	-2.320250	H139	3.006810	4.623970	-2.672969
H58	2.920801	-5.369292	0.271639	C140	-1.912537	3.195590	-3.648155
H59	2.322654	-5.428341	1.948561	H141	-1.949890	4.282543	-3.519539
H60	4.839479	0.637797	3.037160	H142	-0.867303	2.866494	-3.673528
H61	5.354845	0.692833	1.335202	H143	-2.410610	2.916532	-4.576743
O62	2.756459	-3.808479	3.735818	C144	-2.622771	3.532189	3.765810
H63	3.575024	-1.288564	3.843197	H145	-2.941403	2.500338	3.957626
O64	4.492017	-0.623967	-0.529258	H146	-2.206407	3.963443	4.676688
H65	3.327155	-3.074809	-0.744955	H147	-3.486348	4.120036	3.437269
C66	2.625155	0.194443	-4.032301	C148	-2.632903	-1.734770	-4.346802
H67	3.604679	0.675657	-4.133155	H149	-3.620053	-1.354417	-4.629116
H68	1.978639	0.574058	-4.832160	H150	-1.922949	-0.903763	-4.279031
H69	2.759512	-0.883000	-4.192271	H151	-2.289092	-2.457732	-5.086319
C70	2.000713	0.472255	-2.647288	C152	-6.267457	-0.457805	1.820365
H71	2.673153	0.119196	-1.858468	H153	-6.442959	-1.537139	1.884059
H72	1.879948	1.552945	-2.499633	H154	-6.478600	0.013387	2.781059
C73	0.612607	-0.187586	-2.497998	H155	-6.913938	-0.034165	1.045045
H74	0.708478	-1.282098	-2.516548	C156	-3.068626	-6.284874	1.943292
H75	0.003708	0.094840	-3.369026	H157	-3.887919	-6.255718	2.662986
C76	-0.136400	0.261930	-1.222567	H158	-3.427867	-6.667968	0.984036
H77	-1.213307	0.133000	-1.366971	H159	-2.259506	-6.926442	2.307871

H78	0.036962	1.332484	-1.074028	C160	1.549899	-4.290922	-3.121058
C79	0.261336	-0.508253	0.059051	H161	0.907955	-5.109628	-3.461576
H80	1.345660	-0.539824	0.192234	H162	1.112904	-3.330267	-3.411760
H81	-0.104716	-1.539003	-0.015739	H163	2.544704	-4.394150	-3.553820
C82	-0.390592	0.201177	1.271455				



Figure S17. Side (left) and top (right) views of the optimized geometry of $[H2 \subset D2]$ (B3LYP/3-21G). Hydrogen atoms were omitted for clarity.

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