

Supporting Information

Tunable Supramolecular Ag⁺-Host Interactions in Pillar[*n*]arene[*m*]quinones and Ensuing Specific Binding to 1-Alkynes

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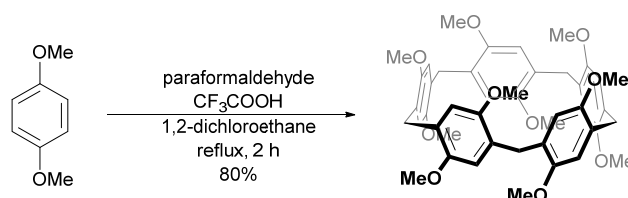
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1. Materials and General Methods

Materials: All starting materials, reagents, and solvents were purchased from commercial vendors and used as received, unless otherwise noted. Compounds **MeP5**, **EtP5**, **EtP6** and **P6Qns** were synthesized as specified per compound below. Analytical thin-layer chromatography (TLC) was performed on aluminum sheets, precoated with silica gel GF₂₅₄. Flash column chromatography was performed over silica gel (200–300 mesh).

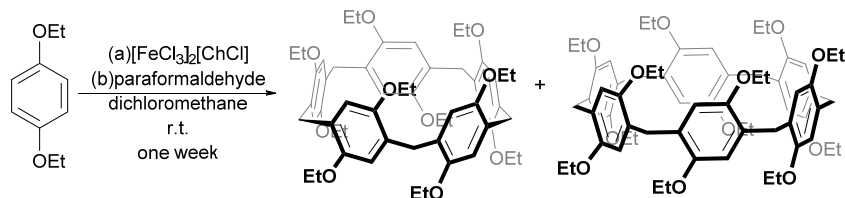
Methods: All NMR data were recorded on a Bruker Advance 400 MHz spectrometer at room temperature, unless otherwise noted. ESI-MS measurements were performed on a Q Exactive™ HF/UltiMate™ 3000 RSLCnano at 298 K.

Synthetic Procedures:



Scheme S1. Synthetic route of **MeP5**.

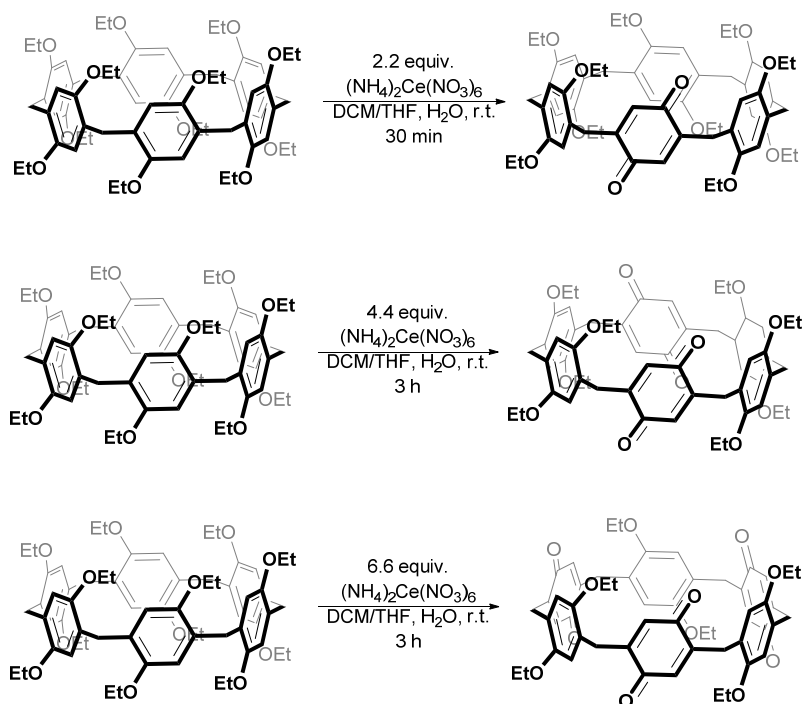
MeP5: To a solution of 1,4-dimethoxybenzene (2.77 g, 20 mmol) and paraformaldehyde (0.6 g, 20 mmol) in 1,2-dichloroethane (200 mL), trifluoroacetic acid (10 mL) was added. The reaction mixture was refluxed for 2 h. After cooling, the reaction mixture was poured into methanol. The resulting precipitate was collected by filtration. The crude product was subjected to column chromatography (*n*-hexane/EtOAc = 96:4 to 80:20, v/v) to afford **MeP5** (2.35 g, 3.13 mmol, 80%). The ¹H and ¹³C NMR data (**Figure S1**) were in accordance with literature.[1]



Scheme S2. Synthetic route of **EtP5** and **EtP6**.

EtP5 and **EtP6:** A mixture of the ferric chloride (FeCl₃) and choline chloride (ChCl) with a molar ratio of 2:1 was mixed well and heated to 120 °C with stirring until a dark brown liquid formed. To the solution of 1,4-diethoxybenzene (16.6 g, 100 mmol) in dichloromethane (1500 mL) was added paraformaldehyde (9.0 g, 300 mmol). Then this solution was added to the dark brown liquid (7.0 g, 15 mmol). The mixture was

stirred at 25 °C for one week, and quenched by addition of water. The organic phase was separated and washed with saturated aqueous NaHCO₃, H₂O and brine. The crude product was purified by column chromatography to yield **EtP5** (1.25 g, 1.4 mmol, 7%) and **EtP6** (6.20 g, 5.83 mmol, 35%) (*n*-hexane/EtOAc = 96:4 to 80:20, v/v). The ¹H and ¹³C NMR data (**Figure S2&S3**) were in accordance with literature.[2]



Scheme S3. Synthetic route towards **P6Qns**.

P6Q1 (pillar[6]arene[1]quinone): To a solution of **EtP6** (1.06 g, 1 mmol) in DCM/THF (100 mL, 9:1, v/v), an aqueous solution of (NH₄)₂[Ce(NO₃)₆] (1.33 g, 2.2 mmol) in 10 mL water was added. The resulting red-colored mixture was stirred at room temperature for 30 min, washed with water (3 × 100 mL), and concentrated under reduced pressure. The crude product was purified by column chromatography ((*n*-hexane/EtOAc = 9:1, v/v) to afford **P6Q1** product as a red solid (0.51 g, 0.50 mmol, 50%). The ¹H and ¹³C NMR data (**Figure S4**) is in accordance with literature.[3]

P6Q2 (pillar[6]arene[2]quinone): To a solution of **EtP6** (1.06 g, 1 mmol) in DCM/THF (100 mL, 8:2, v/v), an aqueous solution of (NH₄)₂[Ce(NO₃)₆] (2.66 g, 4.4 mmol) in 20 mL water was added. The resulting red-colored mixture was stirred at room temperature for 3 h, washed with water (3 × 100 mL), and concentrated under reduced pressure. The crude product was purified by column chromatography ((*n*-hexane/EtOAc = 9:1, v/v) to afford **P6Q2** product as a red solid (0.43 g, 0.45 mmol, 45%). The ¹H and ¹³C NMR data (**Figure S5**) is in accordance with literature.[3]

P6Q3 (pillar[6]arene[3]quinone): To a solution of **EtP6** (1.06 g, 1 mmol) in DCM/THF (100 mL, 7:3, v/v), an aqueous solution of (NH₄)₂[Ce(NO₃)₆] (3.99 g, 6.6 mmol) in 30 mL water was added. The resulting red-colored mixture was stirred at room temperature for 3 h, washed with water (3 × 100 mL), and concentrated under reduced pressure. The crude product was purified by column chromatography ((*n*-hexane/EtOAc = 9:1, v/v) to afford **P6Q3** product as a red solid (0.27 g, 0.30 mmol, 30%). The ¹H and ¹³C NMR data (**Figure S6**) is in accordance with literature.[3]

Note: the solvent ratios DCM/THF were optimized to balance the solubility of all the reactants, and yielded the high amount of products.

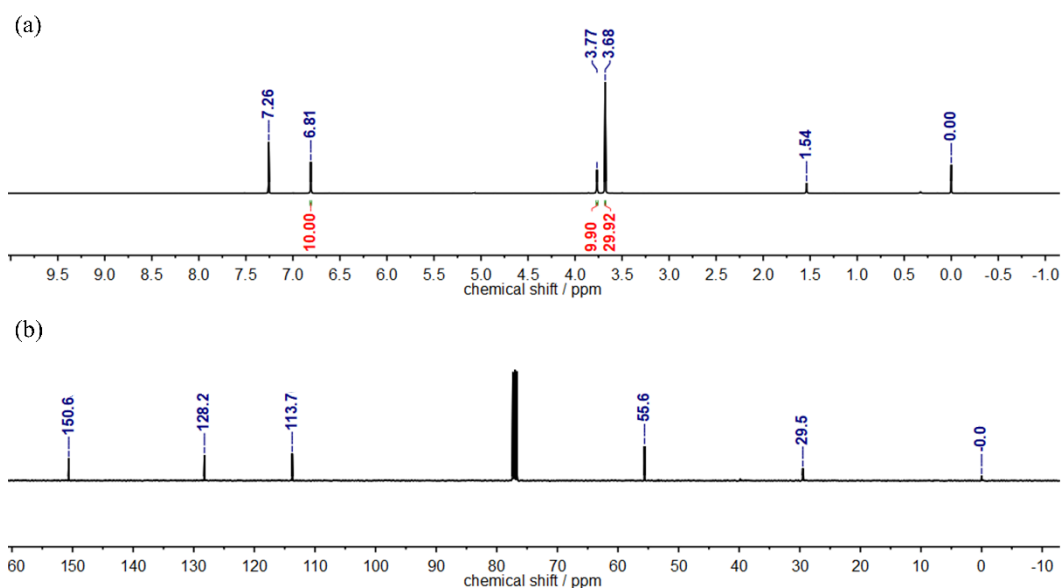


Figure S1. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of MeP5.

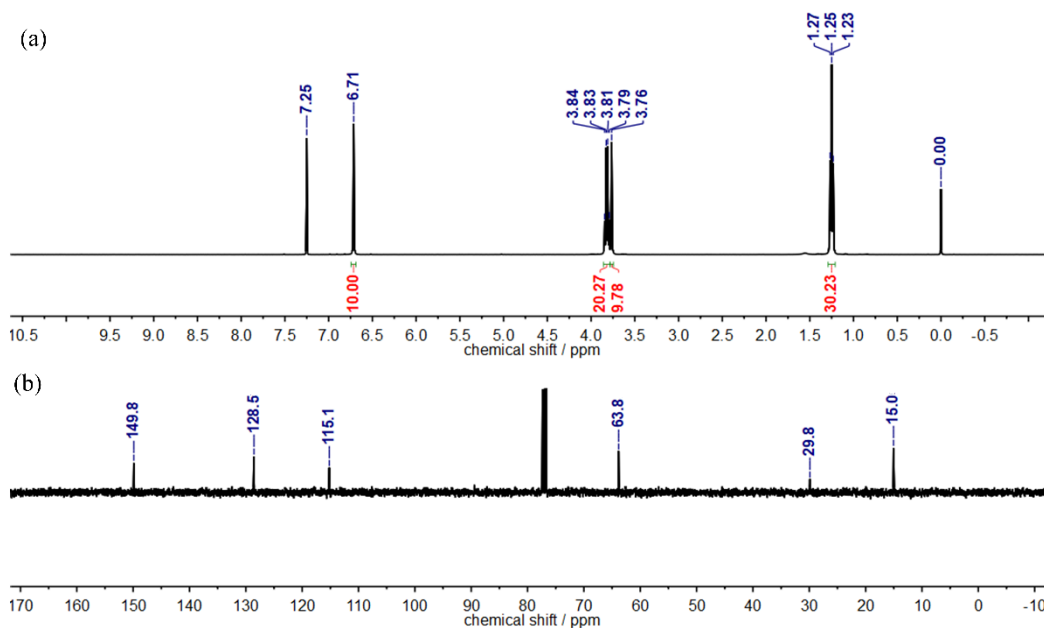


Figure S2. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of EtP5.

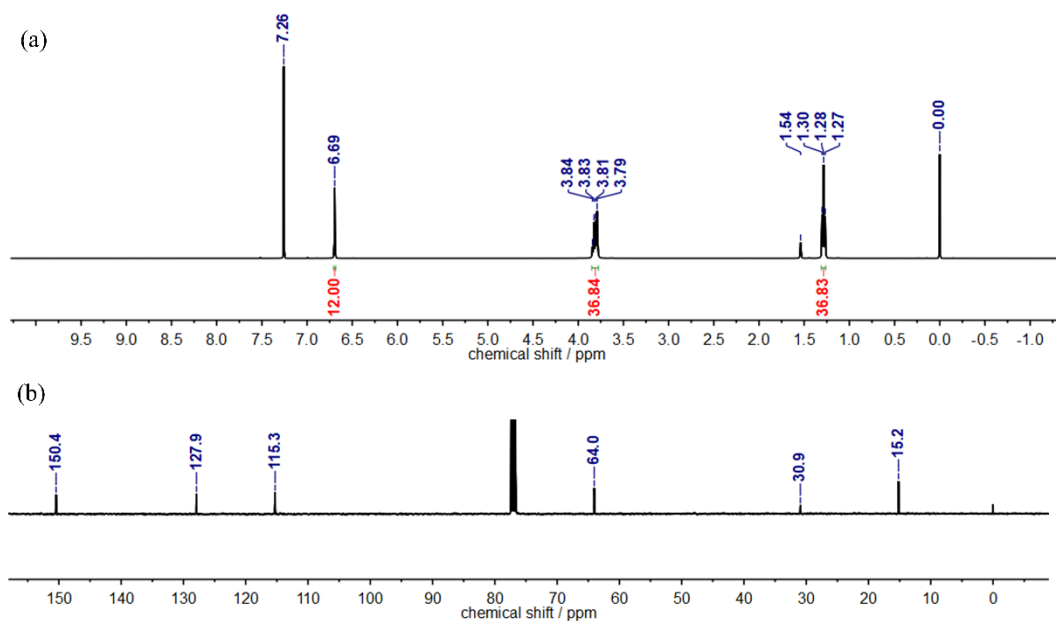


Figure S3. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of EtP6.

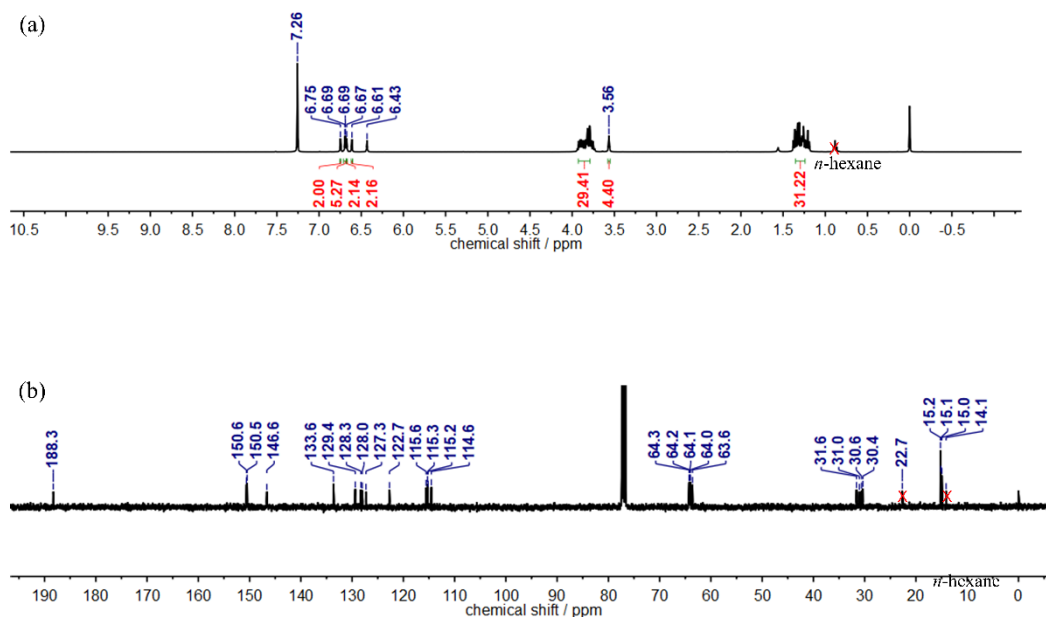


Figure S4. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of P6Q1.

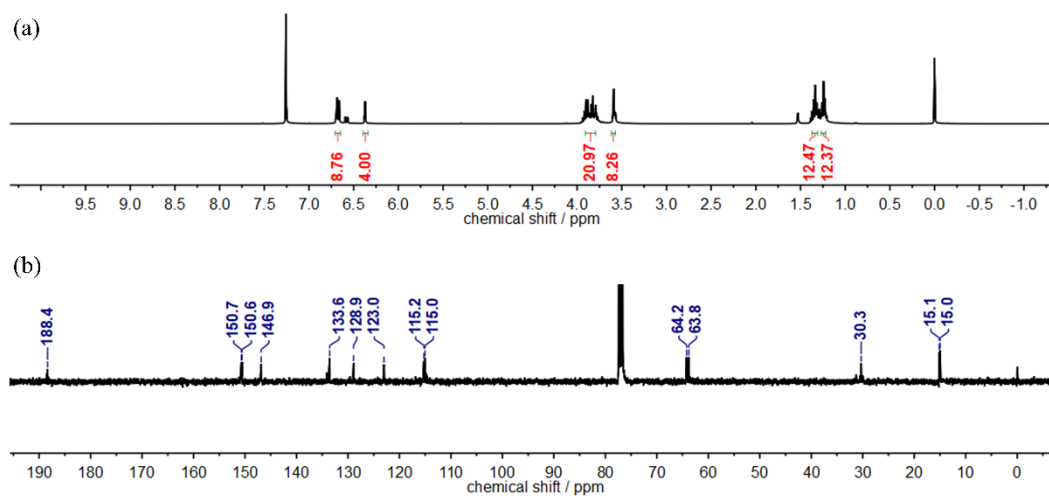


Figure S5. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of P6Q2.

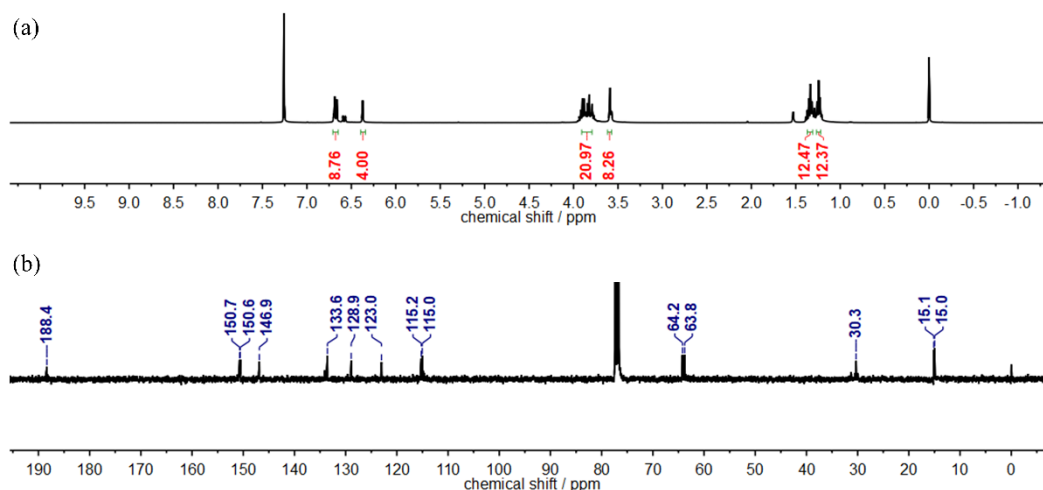


Figure S6. Partial ¹H and ¹³C NMR spectra (400 MHz, CDCl₃, room temperature) of P6Q3.

2. Stoichiometry and association constant determination for the complexation between Pillar[n]arenes and CF₃COOAg

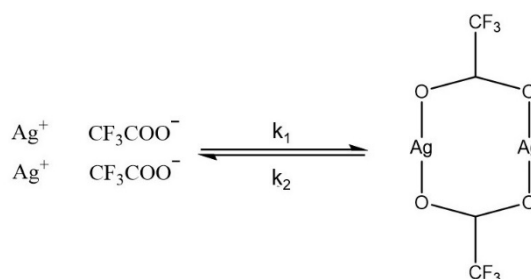


Figure S7. The possible equilibria existing in silver ion-pair recognition system.[4]

Job plots are – within limitations [5-7] – useful to determine the stoichiometry of the host-guest complexes (generally: it works well if only one type of complex is present, but is difficult to interpret if multiple different complexes are present). Here, the Job

plot and the reported crystal structures of P5s and P6s with 2 CF₃COOAg [4,8] were combined to obtain the stoichiometry.

The method of Job plot was used to determine the stoichiometry of complexation of Pillar[n]arenes and CF₃COOAg (**Figure S8-S11**). In this, we fixed the total concentration of [host + guest] at 2.0 mM, and varied the host/guest concentration to yield different ratios (host/guest) as 9:1 (pillararene : Ag⁺ = 1.8 mM : 0.2 mM), 8:2 (pillararene : Ag⁺ = 1.6 mM : 0.4 mM), 7:3 (pillararene : Ag⁺ = 1.4 mM : 0.6 mM), 6:4 (pillararene : Ag⁺ = 1.2 mM : 0.8 mM), 5:5 (pillararene : Ag⁺ = 1.0 mM : 1.0 mM), 4:6 (pillararene : Ag⁺ = 0.8 mM : 1.2 mM), 3:7 (pillararene : Ag⁺ = 0.6 mM : 1.4 mM), 2:8 (pillararene : Ag⁺ = 0.4 mM : 1.6 mM) and 1:9 (pillararene : Ag⁺ = 0.2 mM : 1.8 mM). From **Figure S8-S11** (left parts of these graphs) the highest y value in these figures are all found around X_{host} is 0.3, which indicates that **MeP5**, **EtP5**, **EtP6** and **P6Q1** each form complexes to CF₃COOAg with the ratio of 1:2 ($X_{\text{host}} = 0.33$).

To make sure that we can indeed use the Job plot as indicator of the stoichiometry of the complex, we treated the silver ion-pair as one guest (right parts of **Figure S8-S11**). In other words: the guest concentration is now half of the [Ag⁺], as only 2 Ag⁺ ions are considered to be one guest. For this, we then again systematically varied the host/guest ratios from 9:1 to 1:9, i.e., from 1.8 mM pillararene & 0.4 mM of Ag⁺ (yielding: 0.2 mM of the Ag₂²⁺ guest) to 0.2 mM pillararene & 3.6 mM of Ag⁺ (yielding: 1.8 mM of the Ag₂²⁺ guest). This yielded the right parts in **Figure S8-S11**, and these figures indicate that **MeP5**, **EtP5**, **EtP6** and **P6Q1** each complex to the silver ion pair guest Ag₂²⁺ in a ratio of 1:1.

This set of experiments thus confirms the 1:2 ratio of the pillararenes : Ag⁺.

For **P6Q2** and **P6Q3** (**Figure S12&S13**), there is no chemical shift in ¹H NMR spectra for any of the protons after adding excess CF₃COOAg.

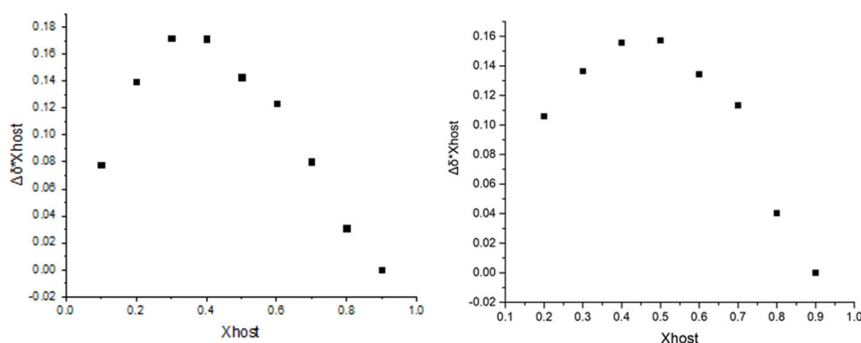


Figure S8. Job plot analysis of CF₃COOAg and **MeP5** (left) and silver ion-pair (2CF₃COOAg) and **MeP5** (right).

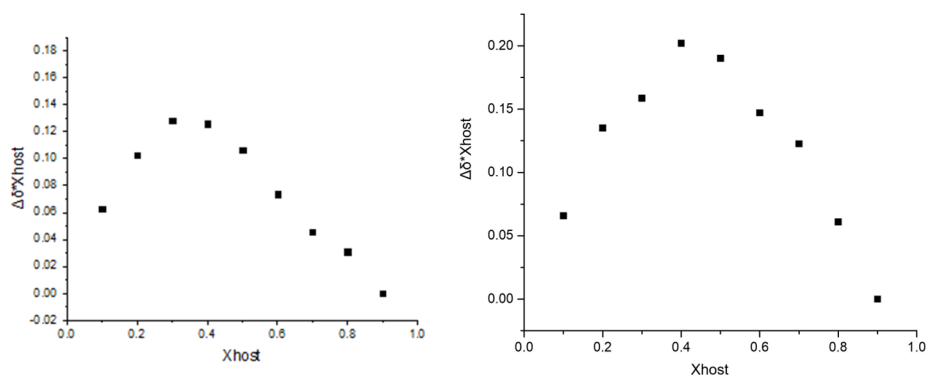


Figure S9. Job plot analysis of CF₃COOAg and **EtP5** (left) and silver ion-pair (2CF₃COOAg) and **EtP5** (right).

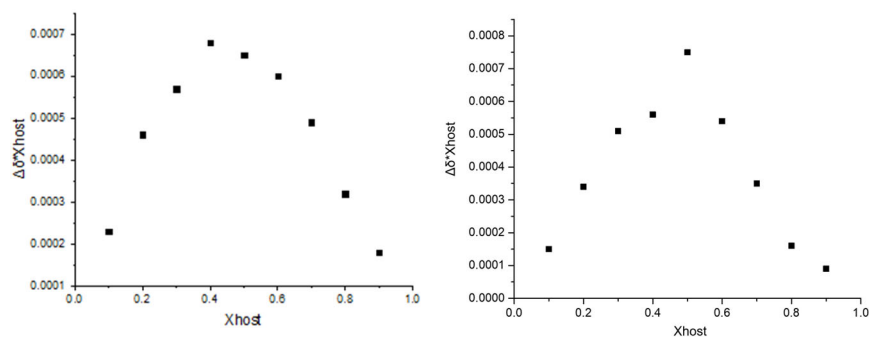


Figure S10. Job plot analysis of CF₃COOAg and **EtP6** (left) and silver ion-pair (2CF₃COOAg) and **EtP6** (right).

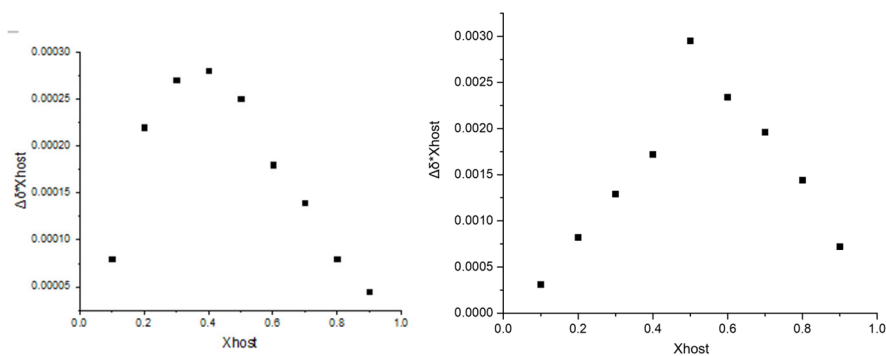


Figure S11. Job plot analysis of CF₃COOAg and **P6Q1** (left) and silver ion-pair (2CF₃COOAg) and **P6Q1** (right).

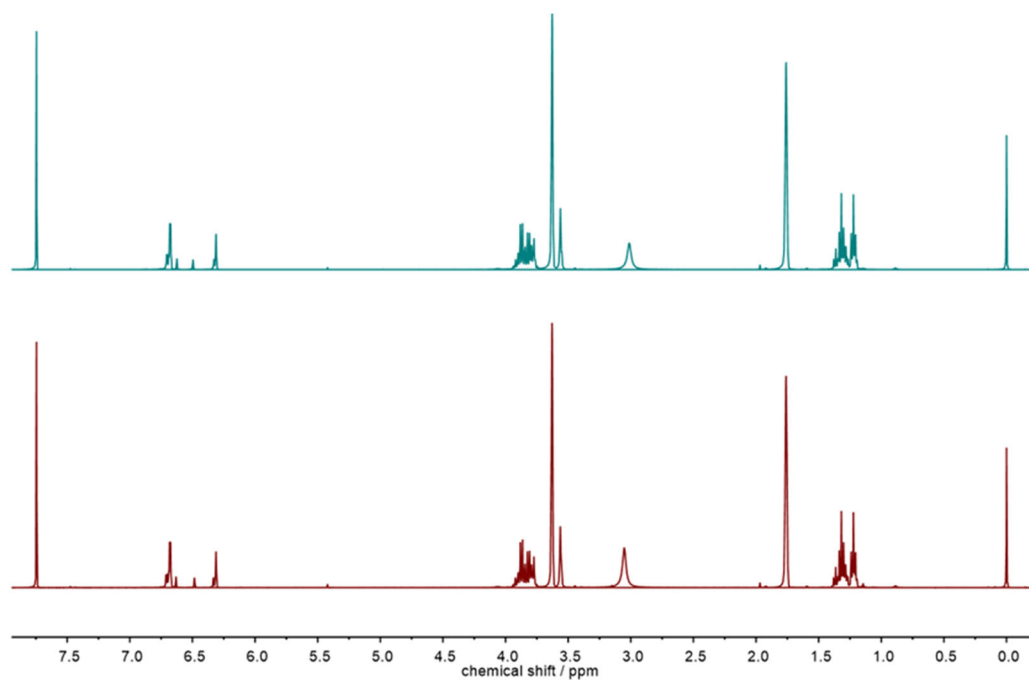


Figure S12. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **P6Q2** at a concentration of 2.00 mM (top) and 2.00 mM **P6Q2** with 10.0 mM CF₃COOAg (bottom).

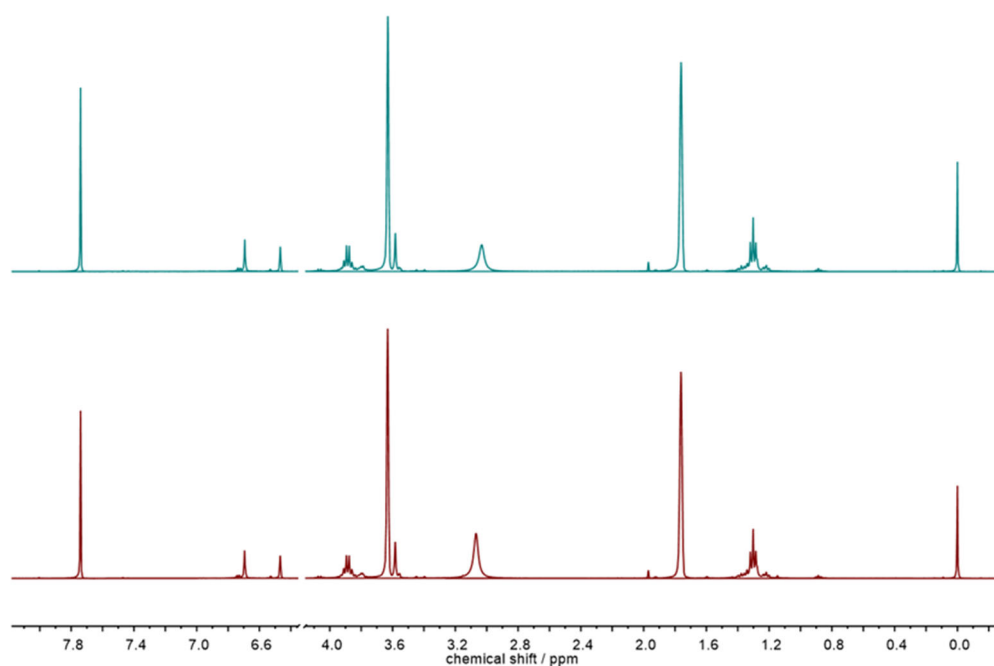


Figure S13. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **P6Q3** at a concentration of 2.00 mM (top) and 2.00 mM **P6Q3** with 10.0 mM CF₃COOAg (bottom).

An NMR titration method was used to obtain the binding constants.[9] Consider the equilibrium between the host H and a guest G that can form host-guest complex HG:



The equilibrium binding constant K for this equilibrium is defined as:

$$K = \frac{[HG]}{[H][G]} \quad (S2)$$

From S2, the equilibrium concentration of the host-guest complex [HG] can be expressed as:

$$[HG] = K [H][G] \quad (S3)$$

The mass balance for the total guest ([G]₀) and total host ([H]₀) concentration can be written as:

$$[G]_0 = [G] + [HG] = [G] K[H][G] \quad (S4)$$

$$[H]_0 = [H] + [HG] = [H] K[H][G] = [H] \times (1 + K[G]) \quad (S5)$$

The fraction of occupied host could be defined as:

$$y = \frac{[HG]}{[H]_0} = \frac{K[H][G]}{[H] \times (1 + K[G])} = \frac{K[G]}{1 + K[G]} \quad (S6)$$

Equation S6 could be used to determine the binding constant K if the fraction of occupied host is known as a function of free guest concentration at equilibrium ([G]). From S3 and S4, this free guest concentration at equilibrium is equal to:

$$[G] = [G]_0 - [HG] = [G]_0 - K[H][G] \quad (S7)$$

From S5 and S6, the free host concentration at equilibrium is equal to:

$$[H] = (1-y)[H]_0 \quad (S8)$$

S7 and S8 were combined to give:

$$[G] = [G]_0 - K(1-y)[H]_0[G] \quad (S9)$$

Rearranging S9 gives:

$$(1 + K(1 - y)[H]_0) \times [G] = [G]_0 \quad (S10)$$

From S10, the free guest concentration at equilibrium is equal to:

$$[G] = \frac{[G]_0}{1 + K(1 - y)[H]_0} \quad (S11)$$

Rearranging S6 gives:

$$y + yK[G] = K[G] \quad (S12)$$

Mixing S11 and S12 yields:

$$y + yK\left(\frac{[G]_0}{1 + K(1 - y)[H]_0}\right) = K\left(\frac{[G]_0}{1 + K(1 - y)[H]_0}\right) \quad (S13)$$

Rearranging S13 yields:

$$y(1 + K(1 - y)[H]_0) + yK[G]_0 = K[G]_0 \quad (S14)$$

Rearranging S4 gives:

$$y(1 + K[H]_0 - Ky[H]_0) + yK[G]_0 - K[G]_0 = 0 \quad (S15)$$

Rearranging S15 gives:

$$-K[H]_0y^2 + (1 + K[H]_0 + [G]_0)y - K[G]_0 = 0 \quad (S16)$$

S16 could be rewritten as:

$$K[H]_0y^2 - (1 + K[H]_0 + [G]_0)y + K[G]_0 = 0 \quad (S17)$$

Equation S17 is a quadratic equation in y, which can be solved yielding two roots:

$$y = \frac{[1 + K([H]_0 + [G]_0)] \pm \sqrt{[1 + K([H]_0 + [G]_0)]^2 - 4K^2[H]_0[G]_0}}{2K[H]_0} \quad (S18)$$

From the two roots of S18, it was found that the physically meaningful root is given by:

$$y = \frac{[1 + K([H]_0 + [G]_0)] - \sqrt{[1 + K([H]_0 + [G]_0)]^2 - 4K^2[H]_0[G]_0}}{2K[H]_0} \quad (\text{S19})$$

Equation S19 was used to fit the binding data, using Origin. So S19 was adapted to give:

$$Y = \frac{Y_0 + DY \times ((Ka \times (P + x) + 1) - \text{SQRT}(((Ka \times (P + x) + 1)^2 - 4 \times Ka \times Ka \times P \times x)))}{(2 \times Ka \times P)} \quad (\text{S20})$$

Y Measured chemical shift

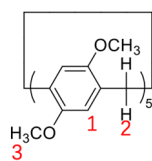
Y₀ Chemical shift of empty host solution

DY Maximal change in chemical shift: the difference in chemical shift of a fully occupied host and an empty host

Ka Binding constant

P Total host concentration

x Total guest concentration



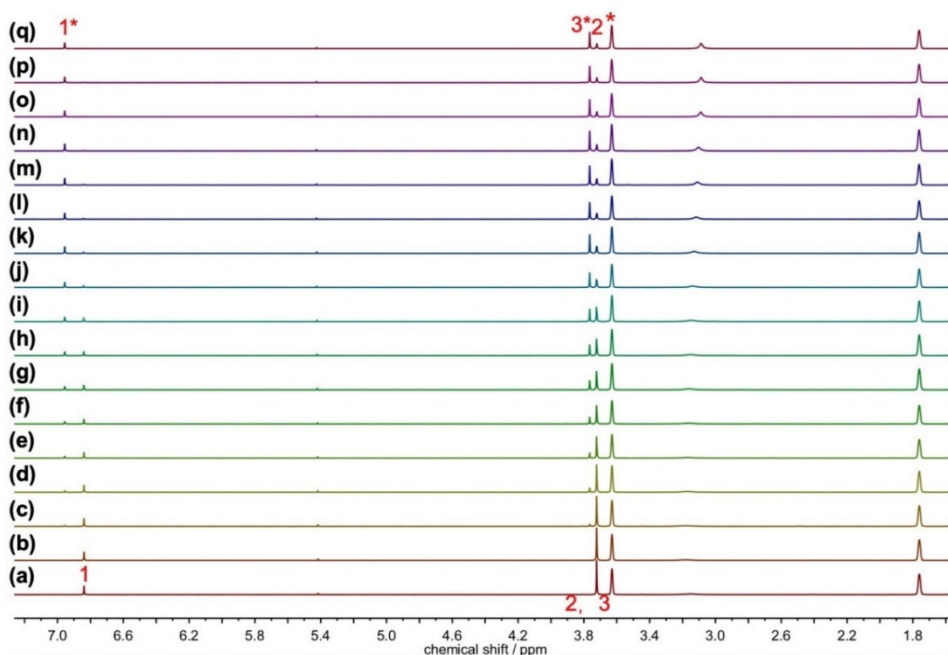


Figure S14. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **MeP5** at a concentration of 2.00 mM with different concentrations of CF₃COOAg: (a) 0 mM, (b) 0.50 mM, (c) 1.00 mM, (d) 1.50 mM, (e) 2.00 mM, (f) 2.50 mM, (g) 3.00 mM, (h) 3.50 mM, (i) 4.00 mM, (j) 6.00 mM, (k) 8.00 mM, (l) 10.00 mM, (m) 12.00 mM, (n) 14.00 mM, (o) 16.00 mM, (p) 18.00 mM and (q) 20.00 mM.

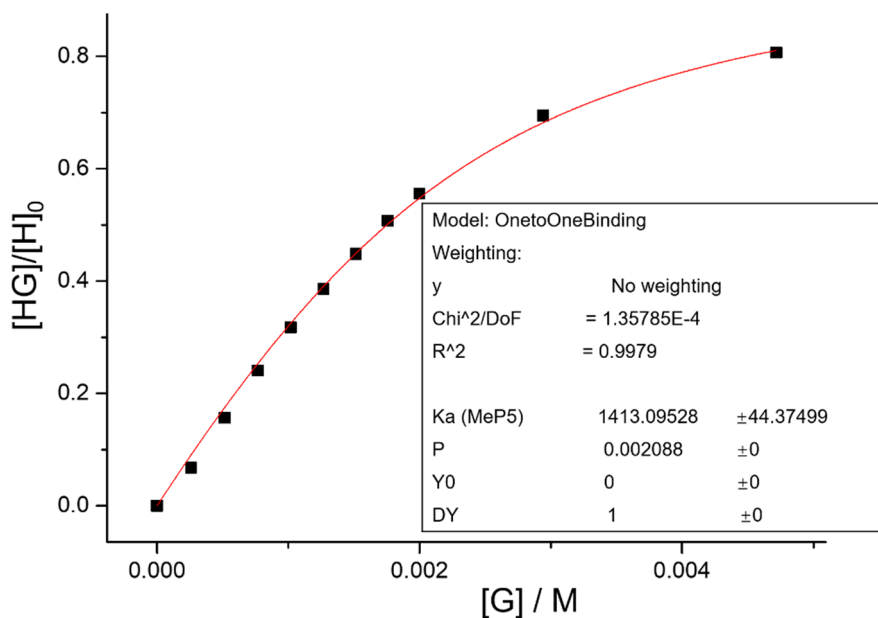


Figure S15. Data fitting for the titration of the slow exchanging [CF₃COOAg]₂ guest into a solution of **MeP5**. A binding constant of $1.41 \times 10^3 \pm 0.04 \times 10^3 \text{ M}^{-1}$ was determined for [CF₃COOAg]₂ ⊂ **MeP5**.

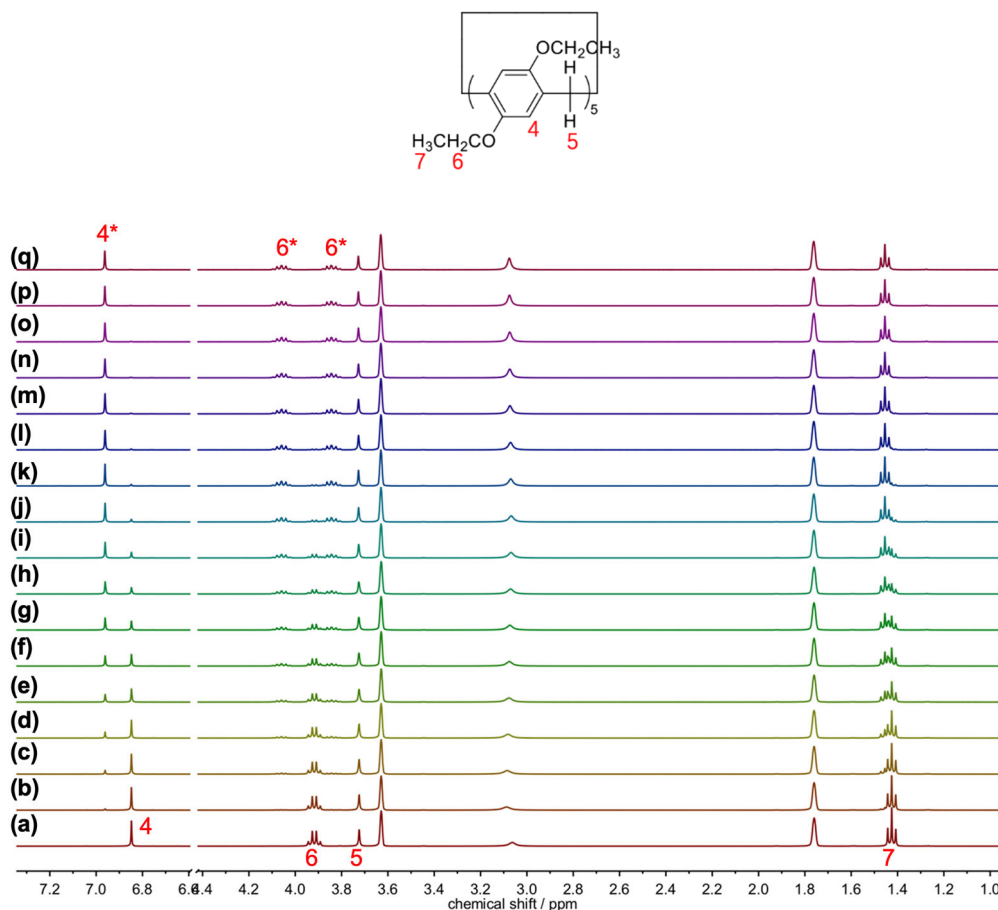


Figure S16. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **EtP5** at a concentration of 2.00 mM with different concentrations of CF₃COOAg: (a) 0 mM, (b) 0.50 mM, (c) 1.00 mM, (d) 1.50 mM, (e) 2.00 mM, (f) 2.50 mM, (g) 3.00 mM, (h) 3.50 mM, (i) 4.00 mM, (j) 6.00 mM, (k) 8.00 mM, (l) 10.00 mM, (m) 12.00 mM, (n) 14.00 mM, (o) 16.00 mM, (p) 18.00 mM and (q) 20.00 mM.

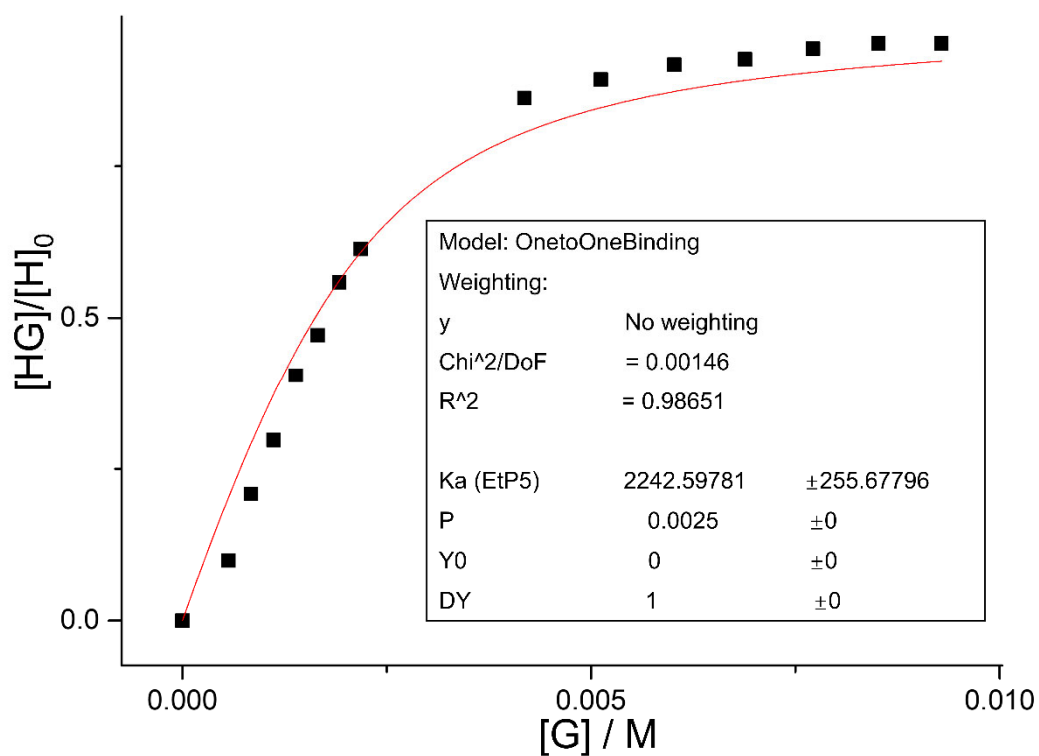


Figure S17. Data fitting for the titration of the slow exchanging [CF₃COOAg]₂ guest into a solution of **EtP5**. A binding constant of $2.24 \times 10^3 \pm 0.25 \times 10^3 \text{ M}^{-1}$ was determined for [CF₃COOAg]₂ \subset **EtP5**.

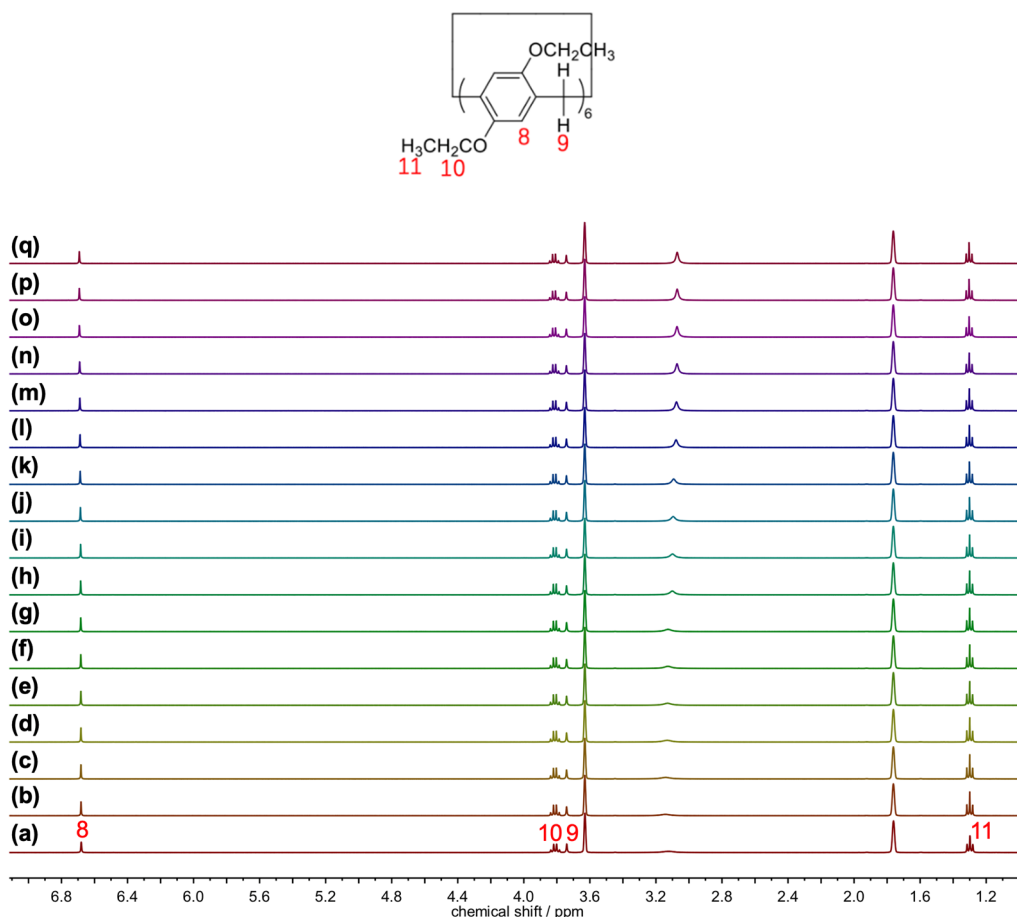


Figure S18. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **EtP6** at a concentration of 2.00 mM with different concentrations of CF₃COOAg: (a) 0 mM, (b) 0.50 mM, (c) 1.00 mM, (d) 1.50 mM, (e) 2.00 mM, (f) 2.50 mM, (g) 3.00 mM, (h) 3.50 mM, (i) 4.00 mM, (j) 6.00 mM, (k) 8.00 mM, (l) 10.00 mM, (m) 12.00 mM, (n) 14.00 mM, (o) 16.00 mM, (p) 18.00 mM and (q) 20.00 mM.

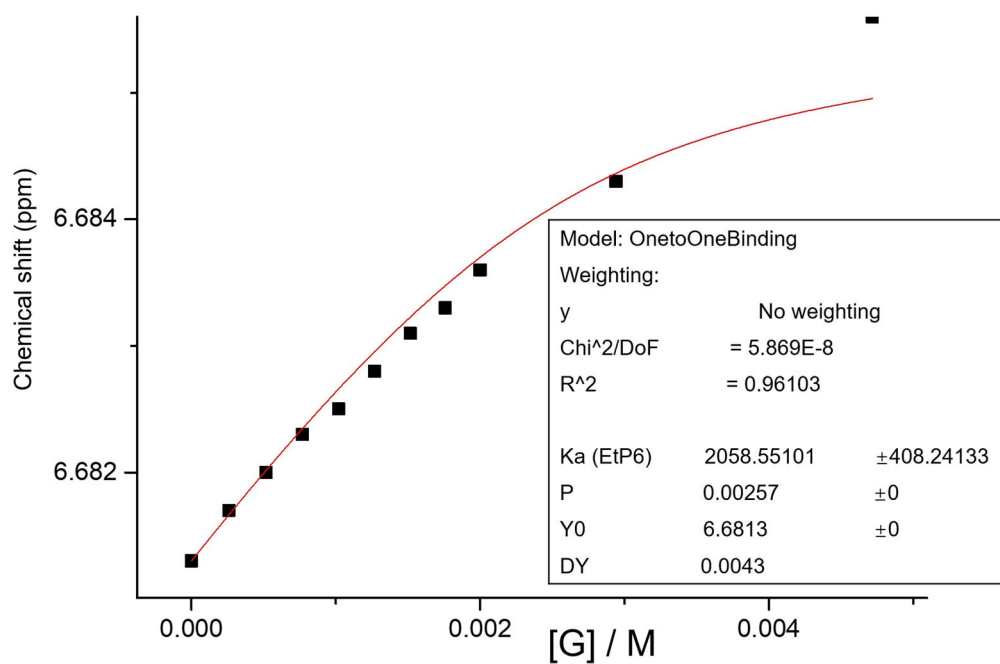


Figure S19. Data fitting for the titration of the fast exchanging $[\text{CF}_3\text{COOAg}]_2$ guest into a solution of **EtP6**. A binding constant of $2.06 \times 10^3 \pm 0.41 \times 10^3 \text{ M}^{-1}$ was determined for $[\text{CF}_3\text{COOAg}]_2 \subset \text{EtP6}$.

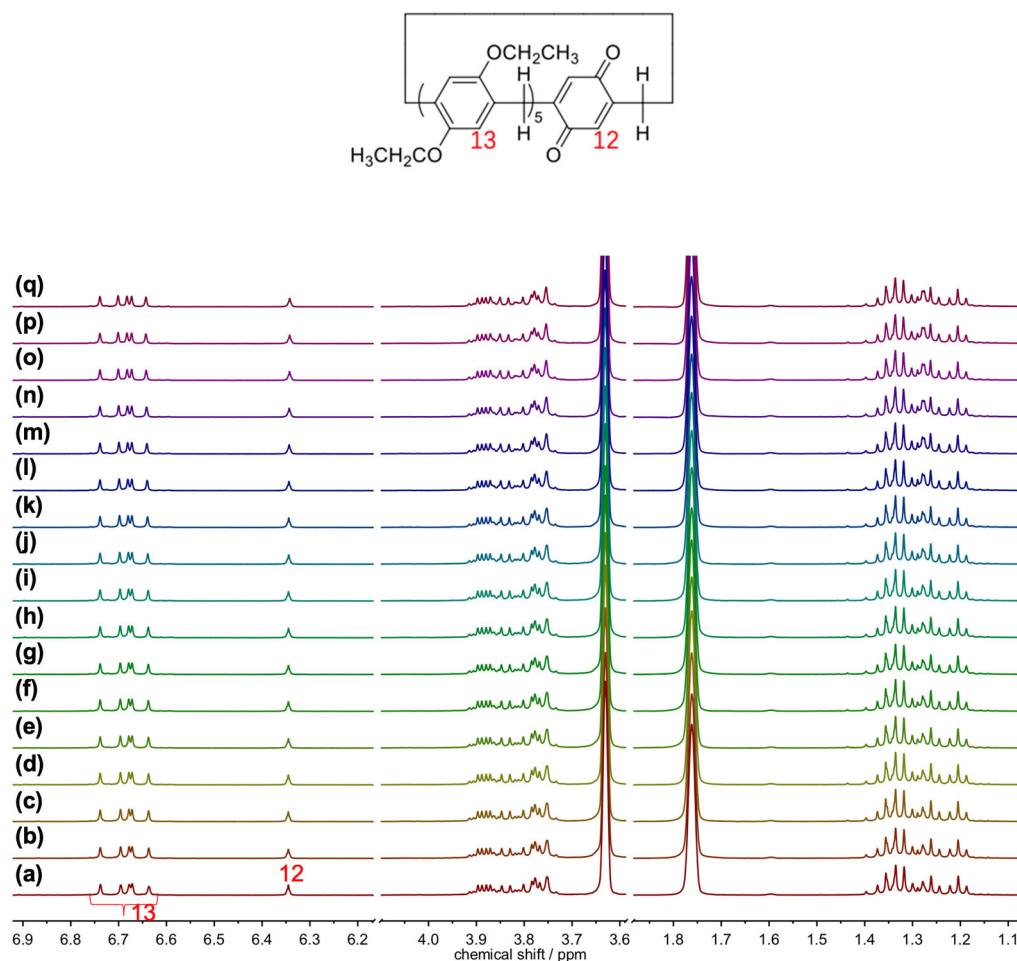


Figure S20. Partial ¹H NMR spectra (400 MHz, CDCl₃ : THF-*d*₈ = 1:2, v/v, room temperature) of **P6Q1** at a concentration of 2.00 mM with different concentrations of CF₃COOAg: (a) 0 mM, (b) 0.50 mM, (c) 1.00 mM, (d) 1.50 mM, (e) 2.00 mM, (f) 2.50 mM, (g) 3.00 mM, (h) 3.50 mM, (i) 4.00 mM, (j) 6.00 mM, (k) 8.00 mM, (l) 10.00 mM, (m) 12.00 mM, (n) 14.00 mM, (o) 16.00 mM, (p) 18.00 mM and (q) 20.00 mM.

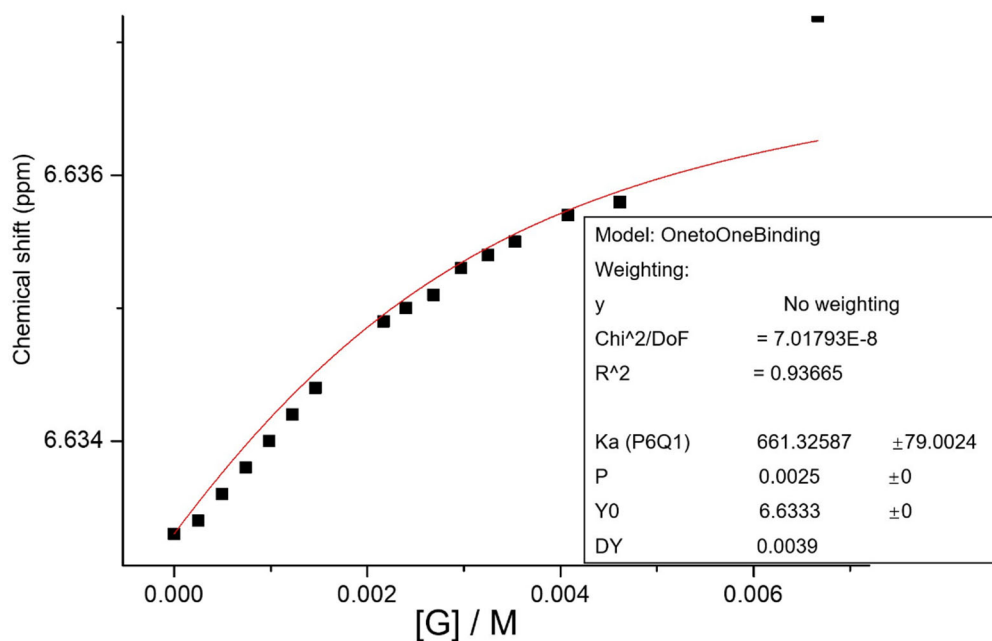


Figure S21. Data fitting for the titration of the fast exchanging $[\text{CF}_3\text{COOAg}]_2$ guest into a solution of **P6Q1**. A binding constant of $6.61 \times 10^2 \pm 0.79 \times 10^2 \text{ M}^{-1}$ was determined for $[\text{CF}_3\text{COOAg}]_2 \subset \text{P6Q1}$.

3. ESI-MS spectra of mixtures of Pillar[n]arenes and CF₃COOAg

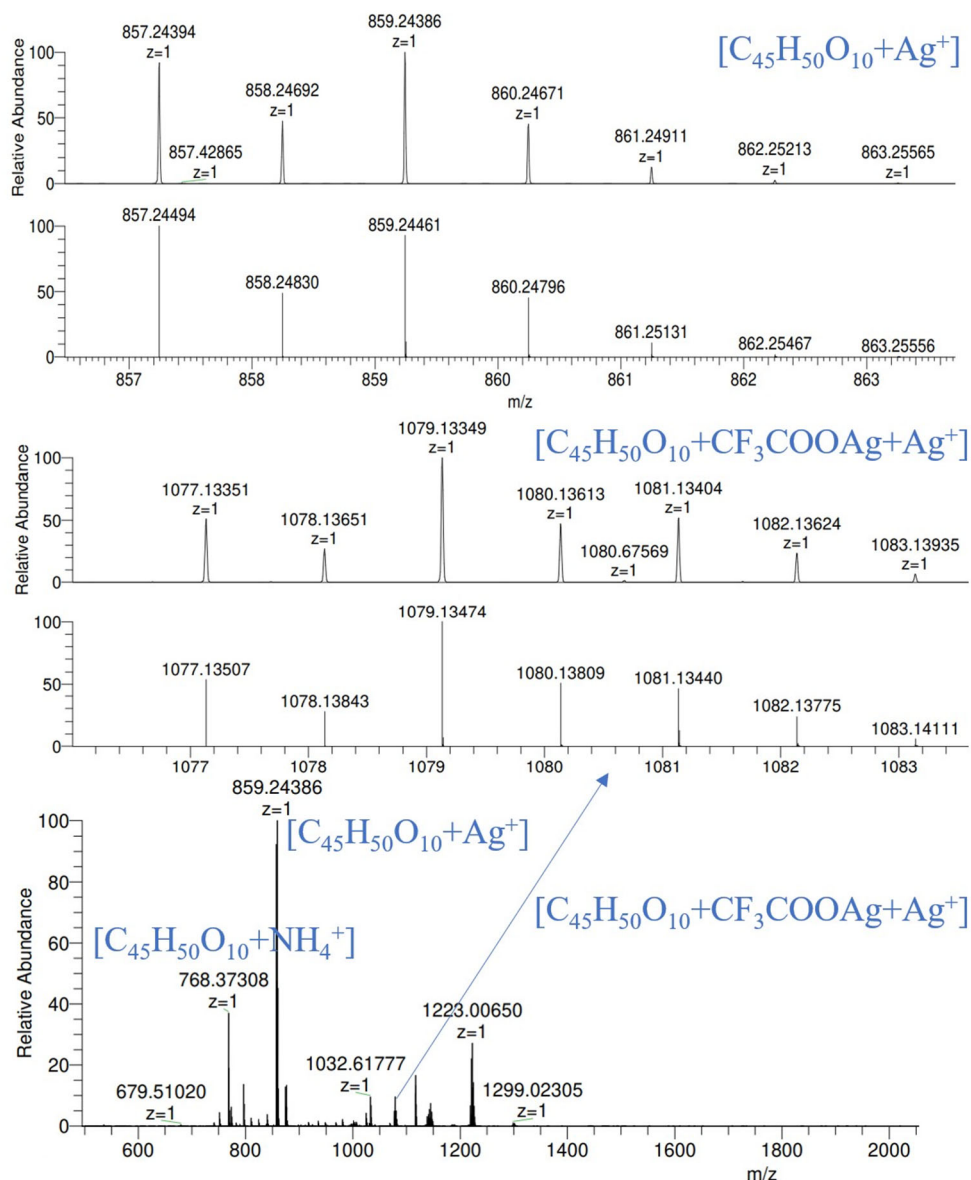


Figure S22. Electrospray ionization mass spectrum of **MeP5** and CF₃COOAg (molar ratio: 1/1). Assignment of main peaks: *m/z* 768.37 [**MeP5** + NH₄]⁺; *m/z* 859.24 [**MeP5** + Ag]⁺; 1079.13 [**MeP5** + CF₃COOAg + Ag]⁺.

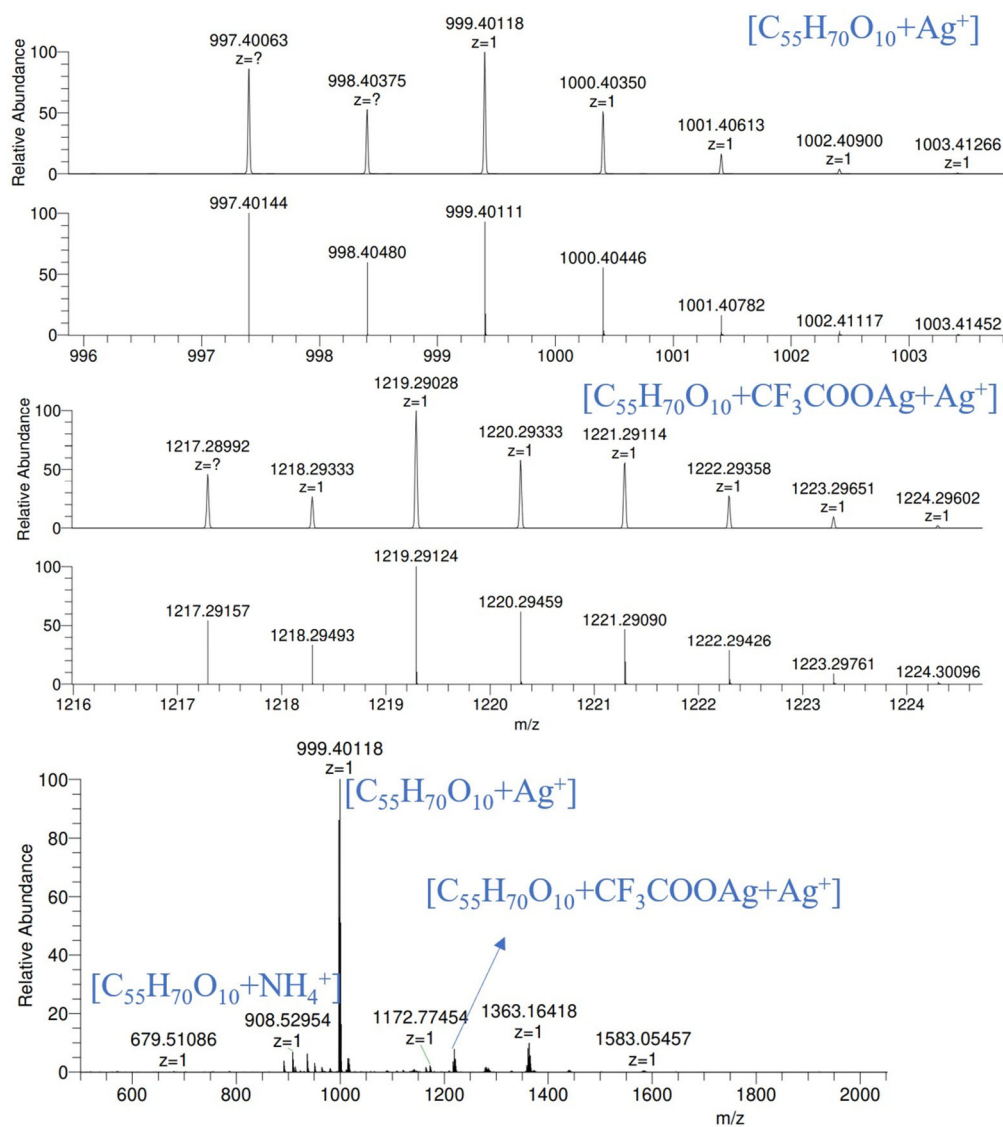


Figure S23. Electrospray ionization mass spectrum of **EtP5** and CF_3COOAg (molar ratio: 1/1). Assignment of main peaks: m/z 908.53 [**EtP5** + NH_4^+]; m/z 999.40 [**EtP5** + Ag^+]; 1219.29 [**EtP5** + $CF_3COOAg + Ag^+$].

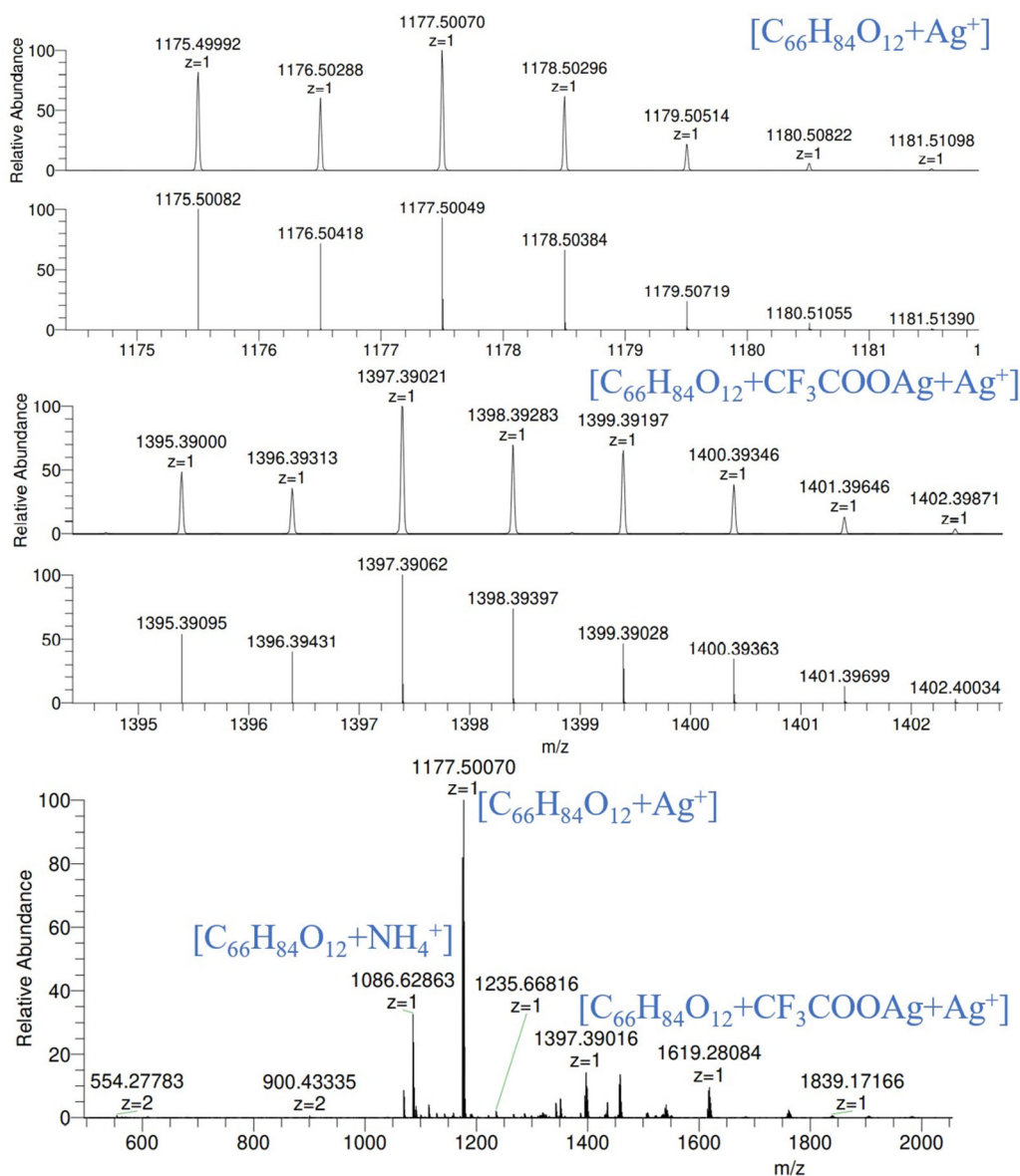


Figure S24. Electrospray ionization mass spectrum of **EtP6** and CF_3COOAg (molar ratio: 1/1). Assignment of main peaks: m/z 1086.63 [**EtP6** + NH_4^+]; m/z 1177.50 [**EtP6** + Ag]⁺; 1397.39 [**EtP6** + CF_3COOAg + Ag]⁺.

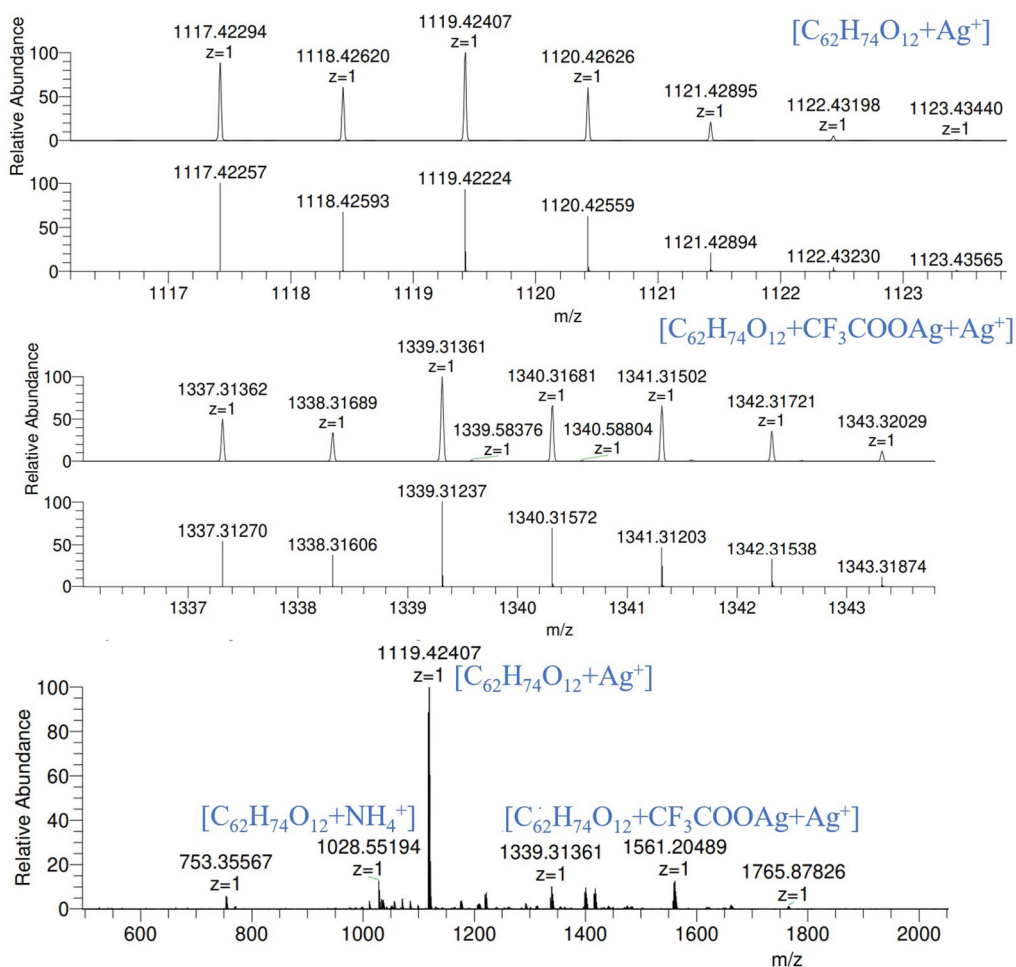


Figure S25. Electrospray ionization mass spectrum of **P6Q1** and CF_3COOAg (molar ratio: 1/1). Assignment of main peaks: m/z 1028.55 [**P6Q1** + NH_4^+]⁺; m/z 1119.42 [**P6Q1** + Ag]⁺; 1339.31 [**P6Q1** + CF_3COOAg + Ag]⁺.

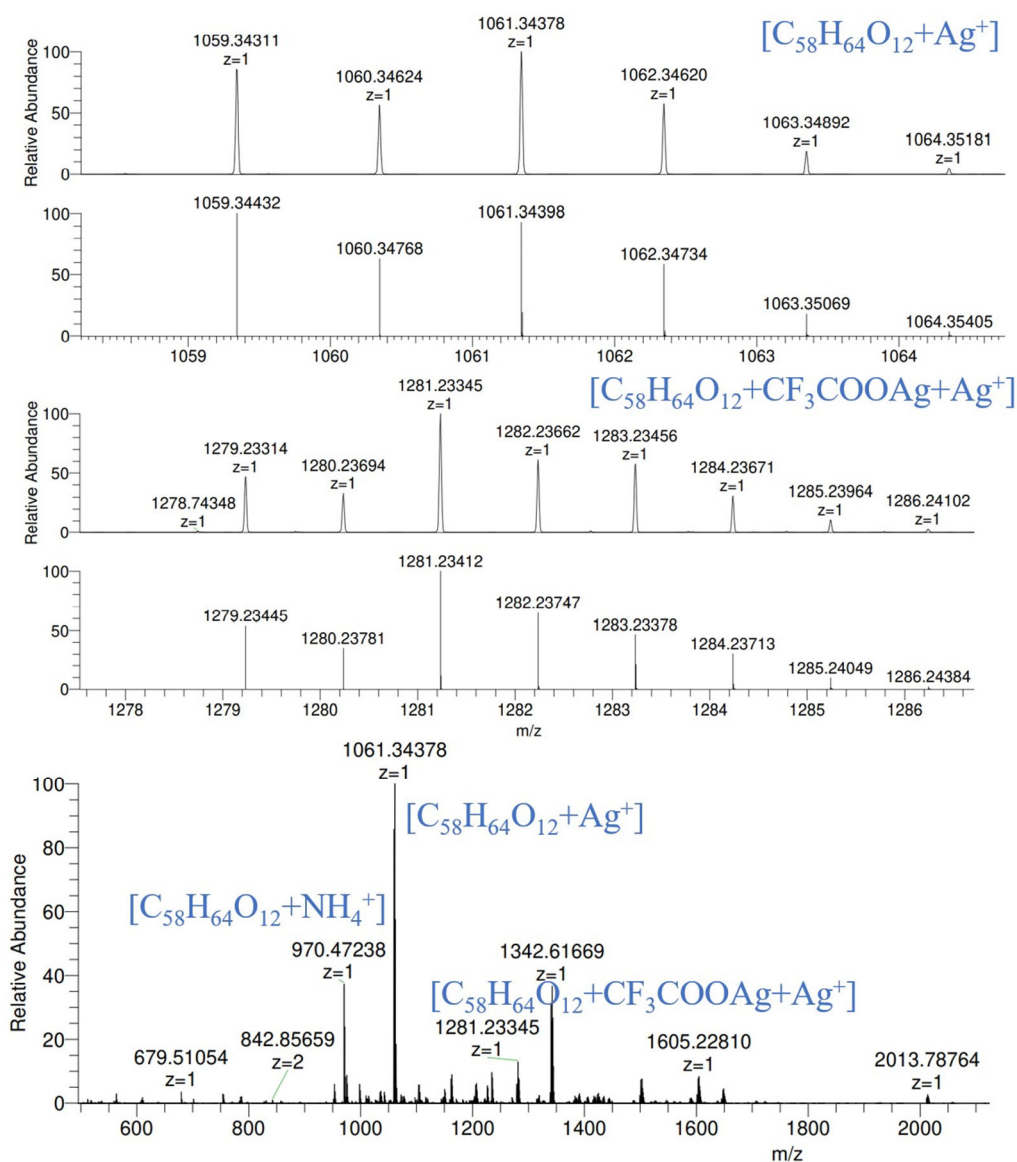


Figure S26. Electrospray ionization mass spectrum of **P6Q2** and CF_3COOAg (molar ratio: 1/1). Assignment of main peaks: m/z 970.47 [**P6Q2** + NH_4^+]; m/z 1061.34 [**P6Q2** + Ag^+]; 1281.23 [**P6Q2** + CF_3COOAg + Ag^+].

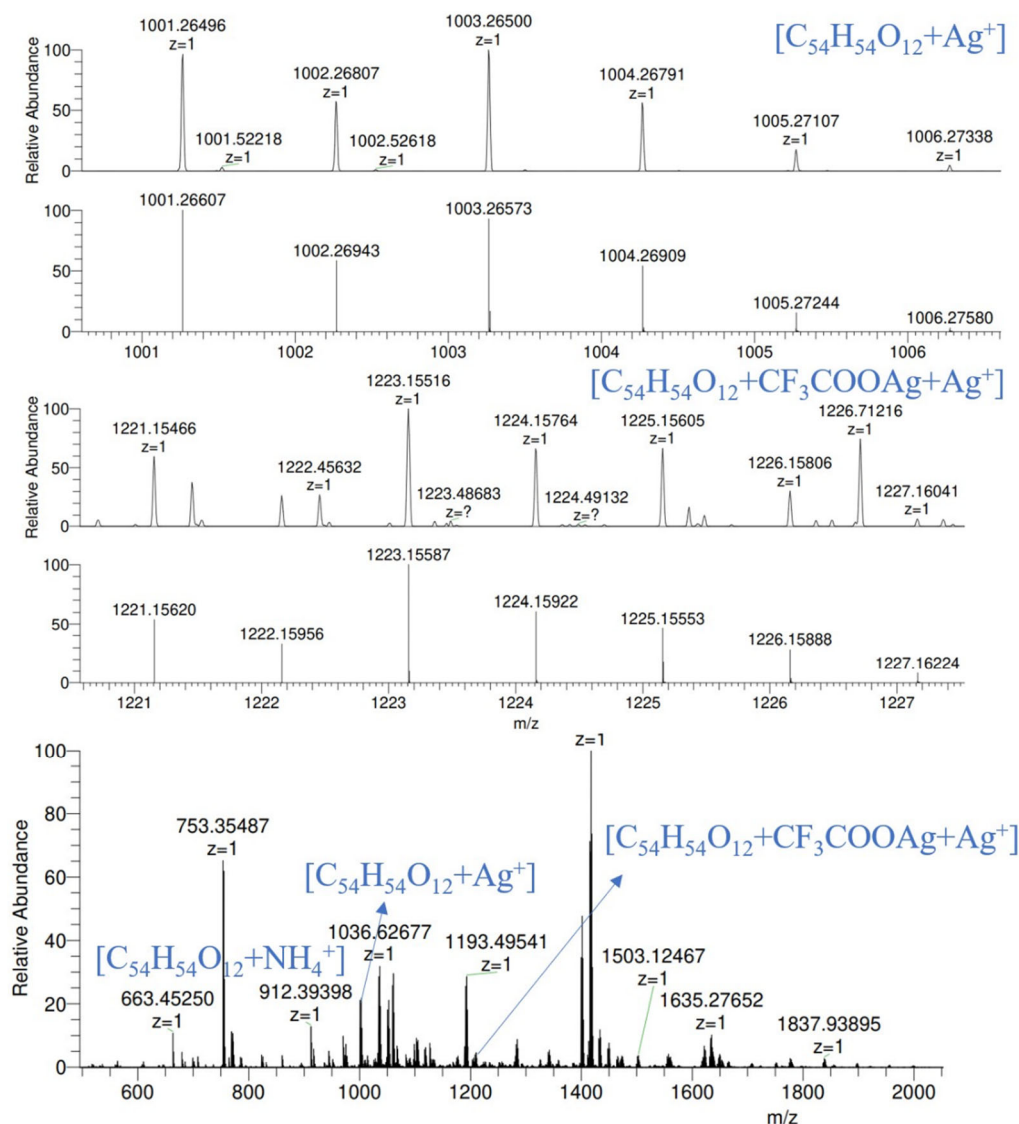


Figure S27. Electrospray ionization mass spectrum of **P6Q3** and CF₃COOAg (molar ratio: 1/1). Assignment of main peaks: m/z 912.39 [**P6Q3** + NH₄]⁺; m/z 1003.26 [**P6Q3** + Ag]⁺; 1223.15 [**P6Q3** + CF₃COOAg + Ag]⁺.

As shown in **Figure S22-S27**, peaks at m/z 1079.13, 1219.29, 1397.39, 1339.31, 1281.23 and 1223.15 were observed, corresponding to [**MeP5** + CF₃COOAg + Ag]⁺, [**EtP5** + CF₃COOAg + Ag]⁺, [**EtP6** + CF₃COOAg + Ag]⁺, [**P6Q1** + CF₃COOAg + Ag]⁺, [**P6Q2** + CF₃COOAg + Ag]⁺ and [**P6Q3** + CF₃COOAg + Ag]⁺, respectively. The results obtained from ESI-MS spectra further proved that pillararenes formed host-guest complexes with CF₃COOAg. The samples used in ESI-MS are mixtures of host and guest with the ratio of 1:1, and the concentrations of both host and guest are 1 mmol/L.



Figure S28. Histogram of NL values in ESS-MS experiments for single-host samples: [MeP5 + 1 equiv. CF₃COOAg], [EtP5 + 1 equiv. CF₃COOAg], [EtPP6 + 1 equiv. CF₃COOAg], [P6Q1 + 1 equiv. CF₃COOAg], [P6Q2 + 1 equiv. CF₃COOAg] and [P6Q3 + 1 equiv. CF₃COOAg].

4. Optimized geometry structures of Pillararenes-Ag⁺ complexes

All DFT calculations were carried out with the Gaussian 16 suite of computational programs.[10] The geometries of all stationary points were optimized using the wB97XD hybrid functional using the def2TZVP basis set.[11] All geometry optimizations were performed without symmetry constraints. Vibrational frequencies were analytically computed at the same level of theory to obtain the Gibbs free energies and to confirm whether the structures are minima.

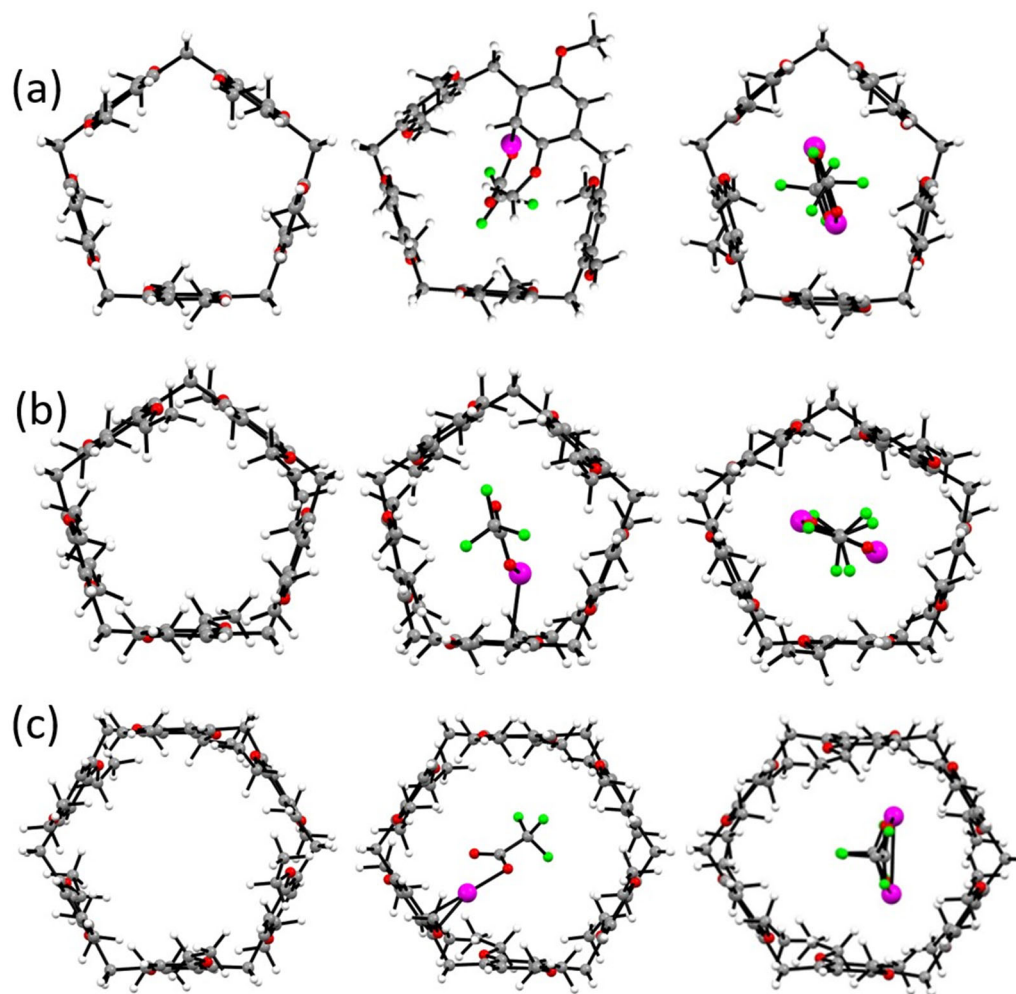
The theoretical calculations were performed using the Density Functional Theory by wB97XD/Def2TZV level of theory (in vacuum). The binding energy of CF₃COOAg with pillararenes was defined as:

$$E_{binding} = E_{(P+n*CF_3COOAg)} - E_P - n * E_{CF_3COOAg}$$

where E_(P+CF₃COOAg) refers to the free energy of stable complex of pillararenes and one or two CF₃COOAg, E_P is the free energy of pillararenes, and E_{CF₃COOAg} is the free energy of CF₃COOAg.

Host	E _{binding} with 1 CF ₃ COOAg (kcal/mol)	E _{binding} with 2 CF ₃ COOAg (kcal/mol)
MeP5	13.9	-36.3
EtP5	15.3	-42.8
EtP6	13.4	-36.5
P6Q1	20.4	-31.4
P6Q2	21.2	-27.7
P6Q3	20.3	-23.3

Table S1. Calculated binding energy of **MeP5**, **EtP5**, **EtP6**, **P6Q1**, **P6Q2** and **P6Q3** with one CF₃COOAg and two CF₃COOAg.



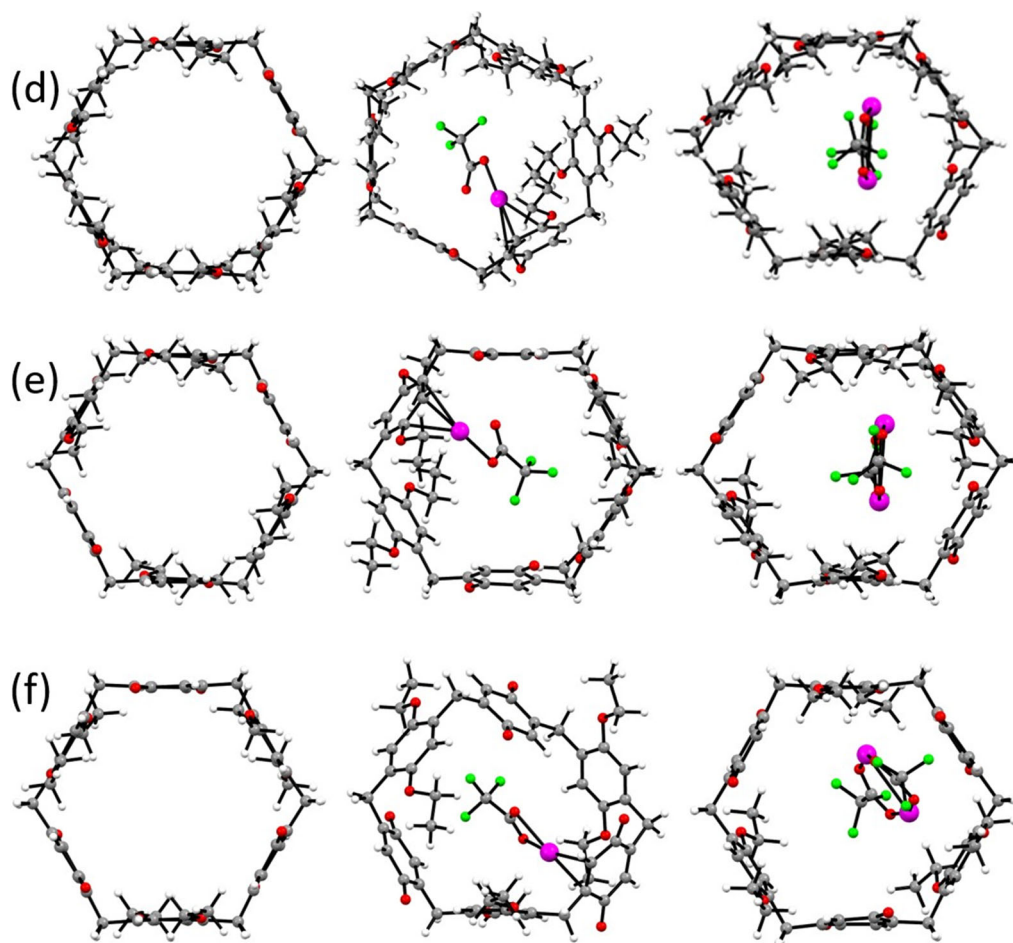
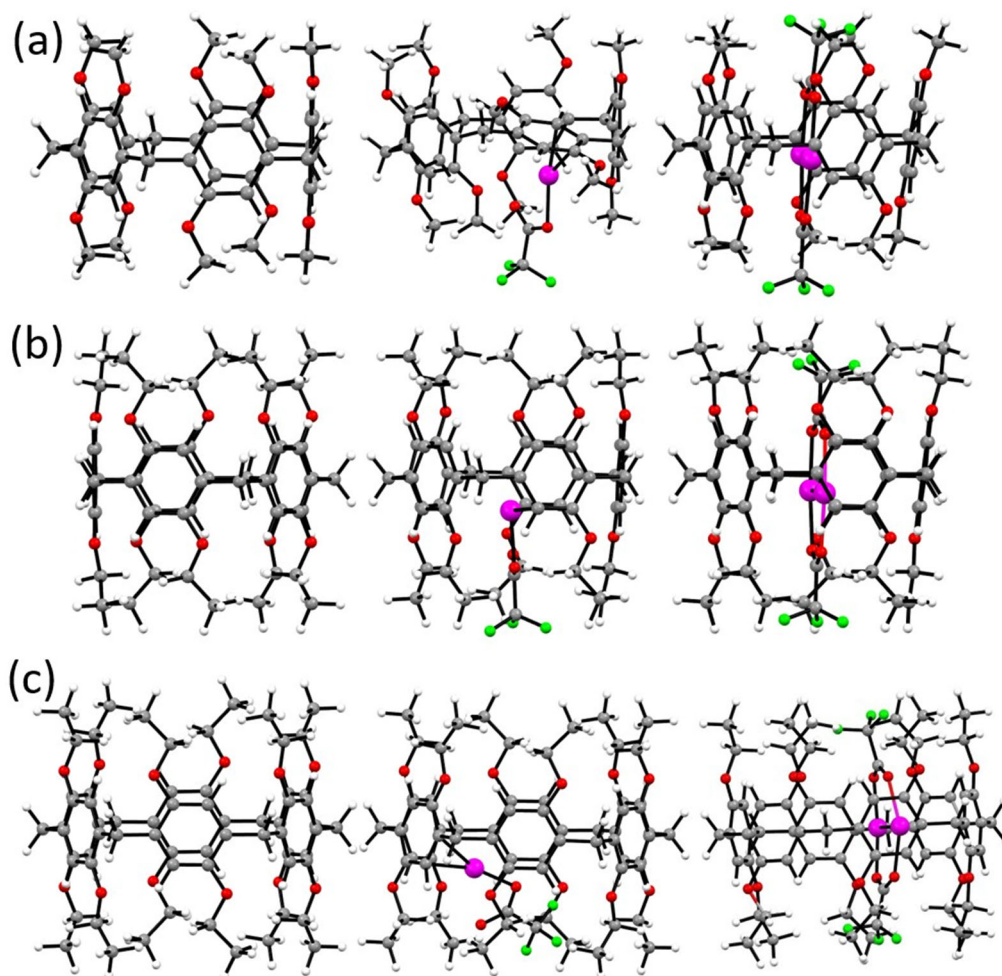


Figure S29. Top view of optimized structures of host itself, complexes with one CF₃COOAg and complexes with two CF₃COOAg in cavities of (a) **MeP5**, (b) **EtP5**, (c) **EtP6**, (d) **P6Q1**, (e) **P6Q2** and (f) **P6Q3**.



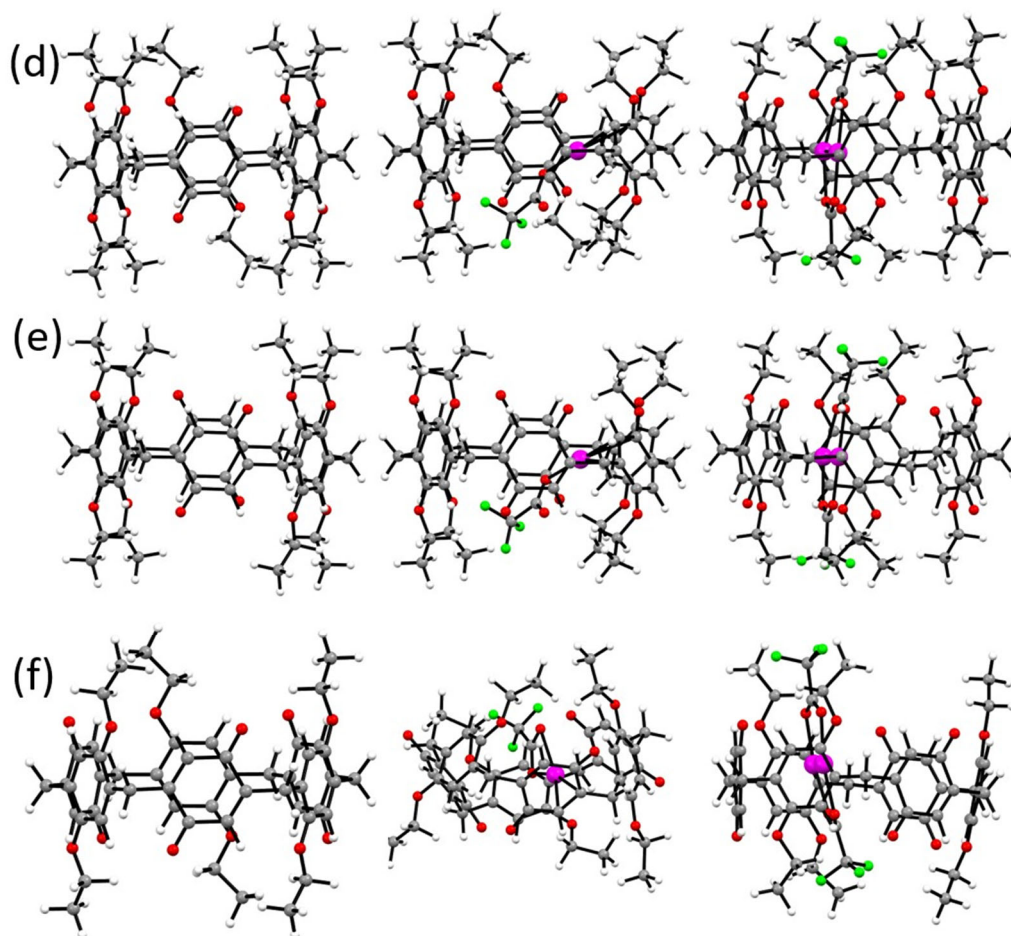


Figure S30. Side view of optimized structures of host itself, complexes with one CF₃COOAg and complexes with two CF₃COOAg in cavities of (a) **MeP5**, (b) **EtP5**, (c) **EtP6**, (d) **P6Q1**, (e) **P6Q2** and (f) **P6Q3**.

5. Selective binding of terminal alkynes by silver-loaded cavities

We did researches on the binding between 1-heptyne, 1-hexene, 3-hexene, 1-hexyne and 3-hexyne with silver-loaded cavity of **EtP6**/**P6Q1**. When silver ions were added to 1-heptyne, peaks of protons close to the alkyne group on ¹H NMR undergo a very significant chemical shift (**Figure S31** (c) & (d)). However, there is no binding between alkyne and **EtP6** (**Figure S31** (c) & (e)). When we mixed alkyne, **EtP6** and CF₃COOAg in proportion, the proton peaks on **EtP6** have little chemical shifts, partial proton peaks on the alkyne have very obvious chemical shifts (**Figure S31** (f)). This is also the case in ¹³C spectra (**Figure S32**). At the same time, we also characterized the DOSY spectra (**Figure S33** (c)) and found that the proton peaks of alkyne bound to silver ions and the proton peaks of **EtP6** have the same diffusion coefficient which means both 1-heptyne which complexed with silver was in the cavity of **EtP6**. The combination of these results shows that alkyne can bind in the cavity of **EtP6** with the exist of silver ions. The same situation is true for 1-hexyne and **P6Q1**(**Figure S33&S35**). 1-heptyne that bound to silver ions were accounted for 74% and 68% for **EtP6** and **P6Q1**, respectively (**Figure S33** (a)&(b)). Alkenes and internal alkynes can theoretically also complex with silver ions, but our experimental results show that there is no significant chemical shift in the proton peaks on NMR spectra. We also characterized the DOSY spectra (**Figure S36-38**) and found that the proton peaks of 1-hexene, 3-hexene, 3-hexyne and the proton peaks of **EtP6** have different diffusion coefficient which means either of them were loaded into the cavity of **EtP6**. Therefore, it can be concluded that only terminal alkyne could bind to silver-loaded **EtP6**.

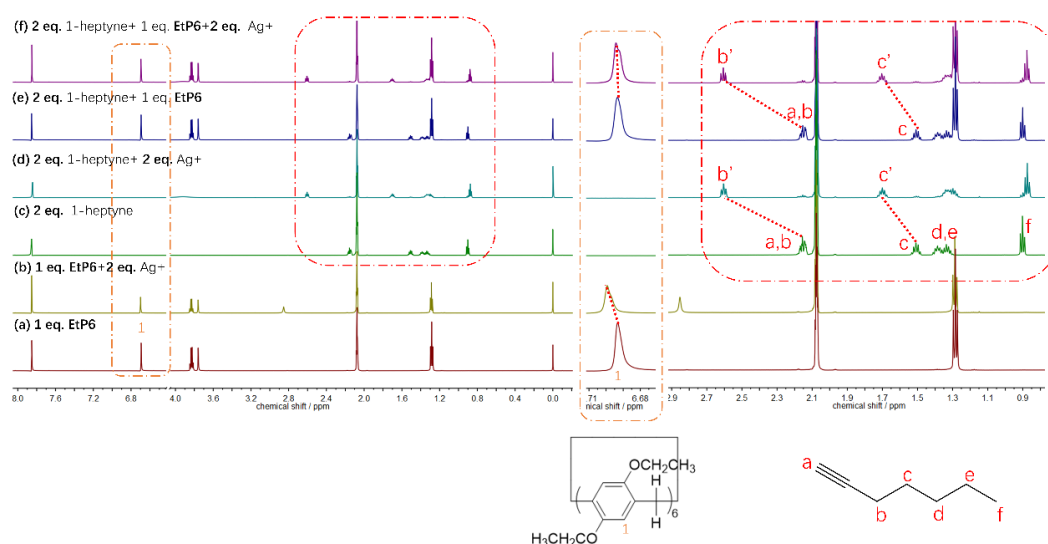


Figure S31. ¹H NMR spectra (400 MHz, CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 1 equiv. **EtP6**, (b) 1 equiv. **EtP6**+2 equiv. Ag⁺, (c) 2 equiv. 1-heptyne, (d) 2 equiv. 1-heptyne + 2 equiv. Ag⁺, (e) 2 equiv. 1-heptyne + 1 equiv. **EtP6** and (f) 2 equiv. 1-heptyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺.

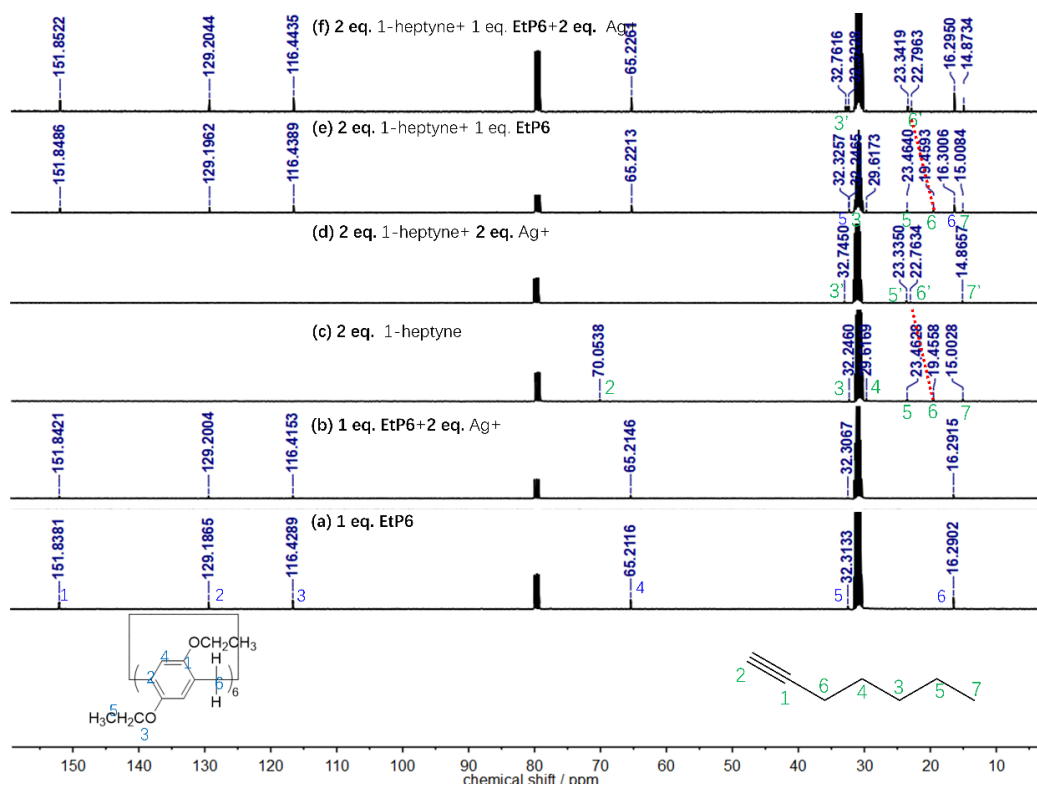
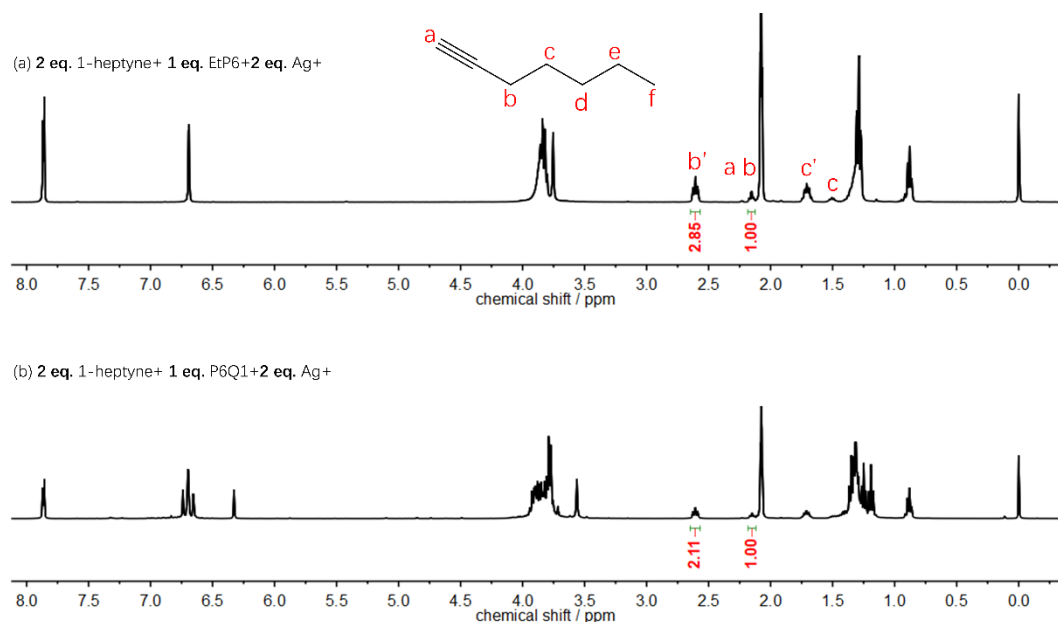


Figure S32. ¹³C NMR spectra (101 MHz, CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 1 equiv. **EtP6**, (b) 1 equiv. **EtP6**+2 equiv. Ag⁺, (c) 2 equiv. 1-heptyne, (d) 2 equiv. 1-heptyne + 2 equiv. Ag⁺, (e) 2 equiv. 1-heptyne + 1 equiv. **EtP6** and (f) 2 equiv. 1-heptyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺.



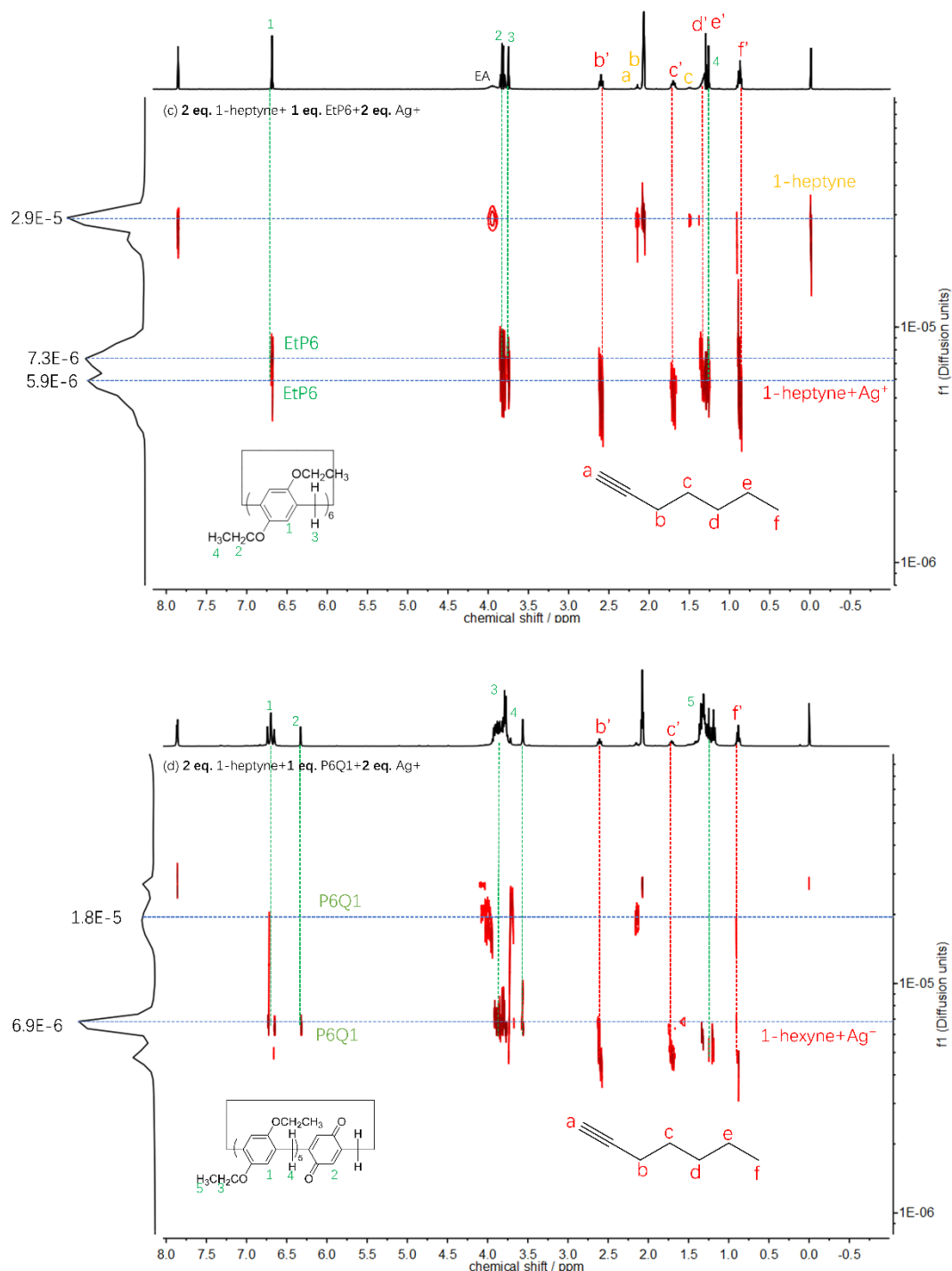


Figure S33. ¹H NMR spectra (400 MHz, CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 2 equiv. 1-heptyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺ and (b) 2 equiv. 1-heptyne + 1 equiv. **P6Q1** + 2 equiv. Ag⁺; 2D DOSY NMR spectra (CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (c) 2 equiv. 1-heptyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺ and (d) 2 equiv. 1-heptyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺.

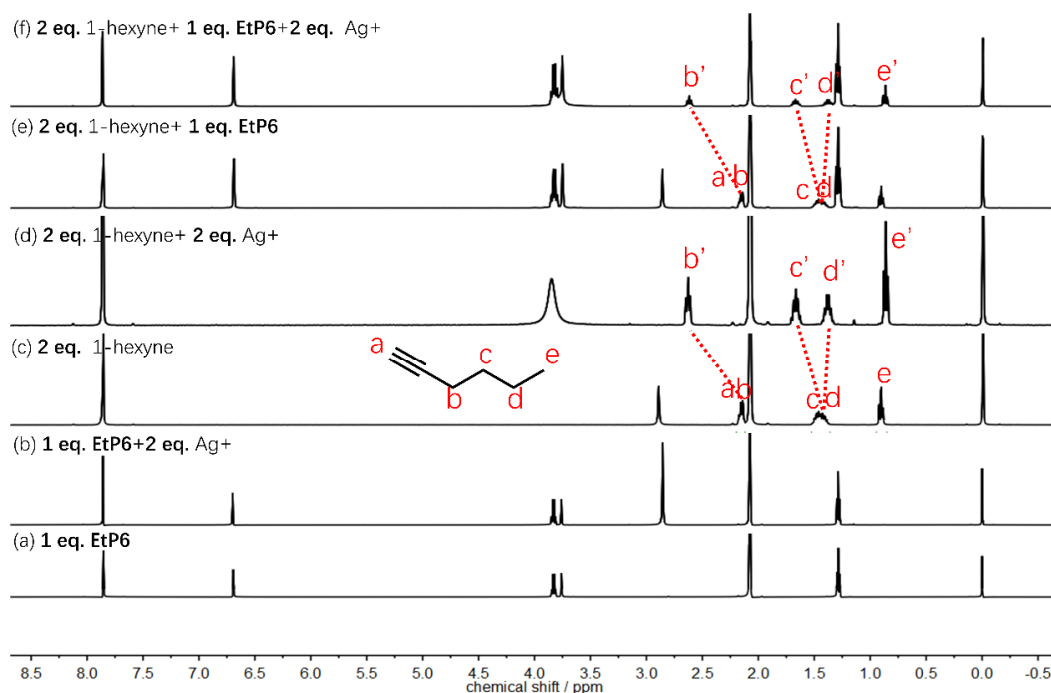
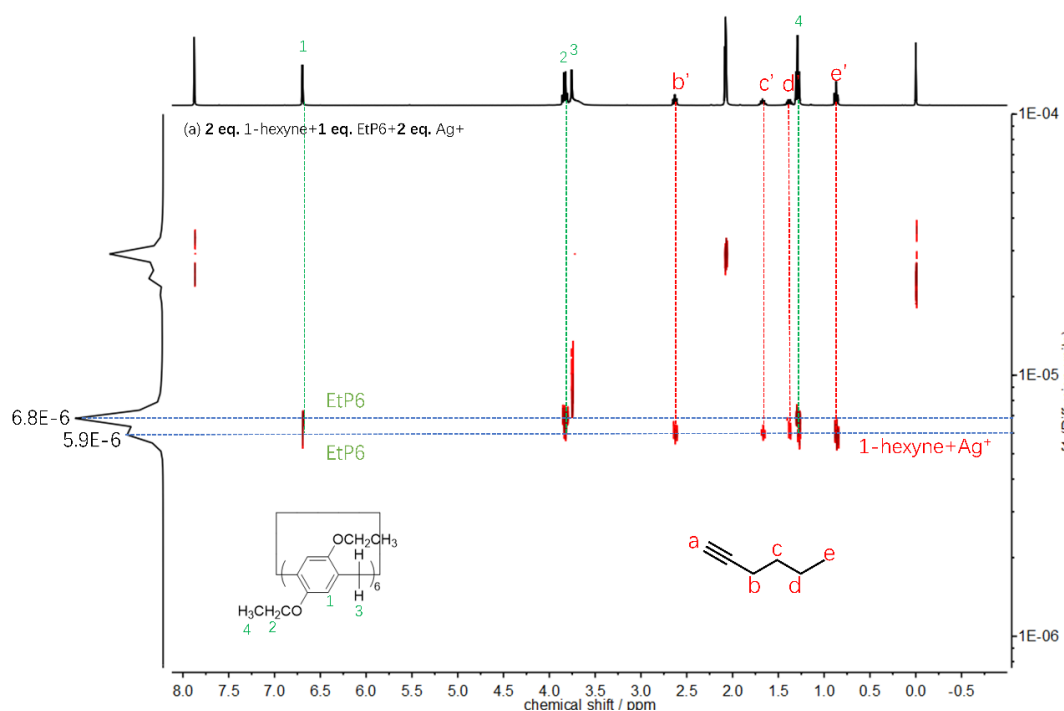


Figure S34. ¹H NMR spectra (400 MHz, CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 1 equiv. **EtP6**, (b) 1 equiv. **EtP6**+2 equiv. Ag⁺, (c) 2 equiv. 1-hexyne, (d) 2 equiv. 1-hexyne + 2 equiv. Ag⁺, (e) 2 equiv. 1-hexyne + 1 equiv. **EtP6** and (f) 2 equiv. 1-hexyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺.



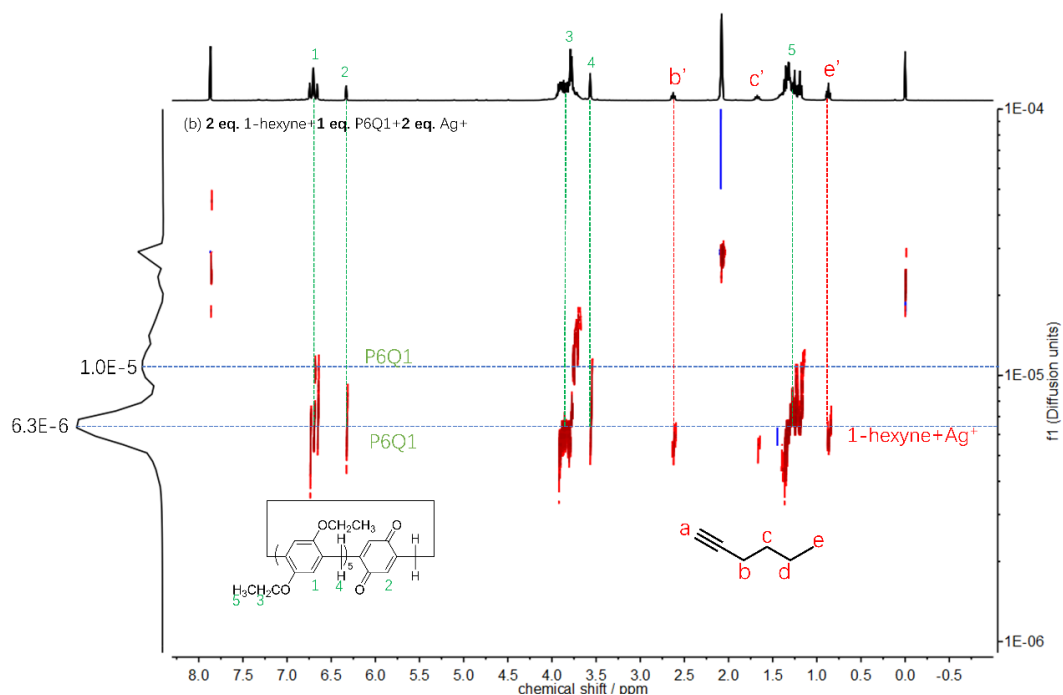
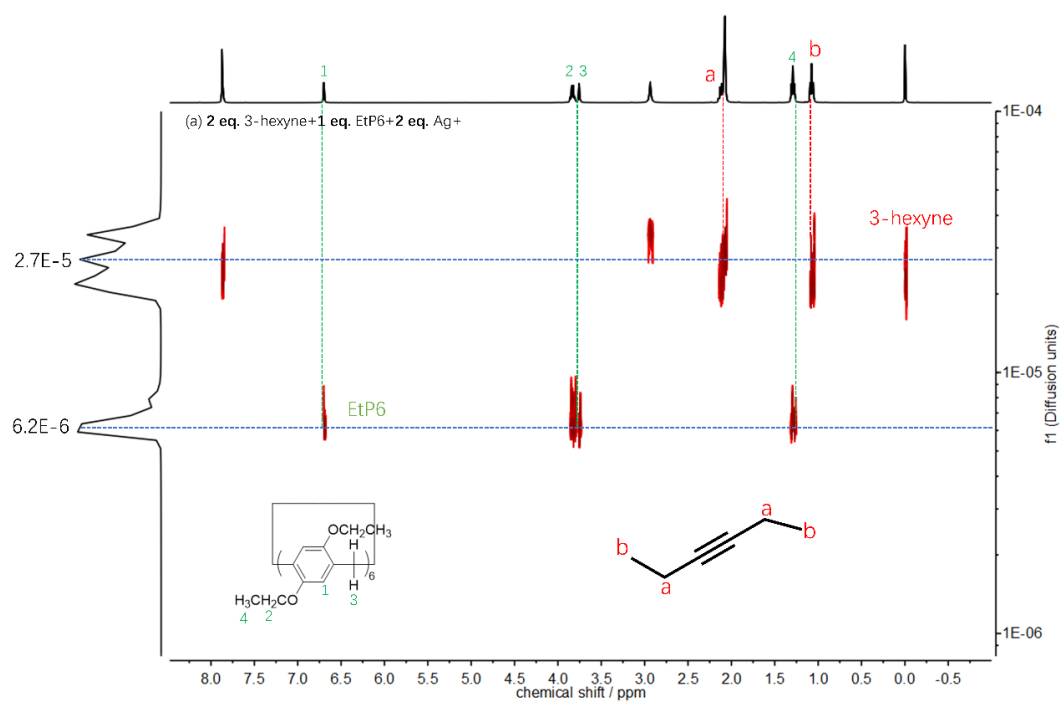
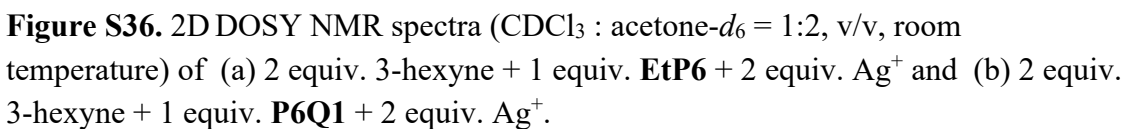


Figure S35. 2D DOSY NMR spectra (CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 2 equiv. 1-hexyne + 1 equiv. **EtP6** + 2 equiv. Ag⁺ and (b) 2 equiv. 1-hexyne + 1 equiv. **P6Q1** + 2 equiv. Ag⁺.





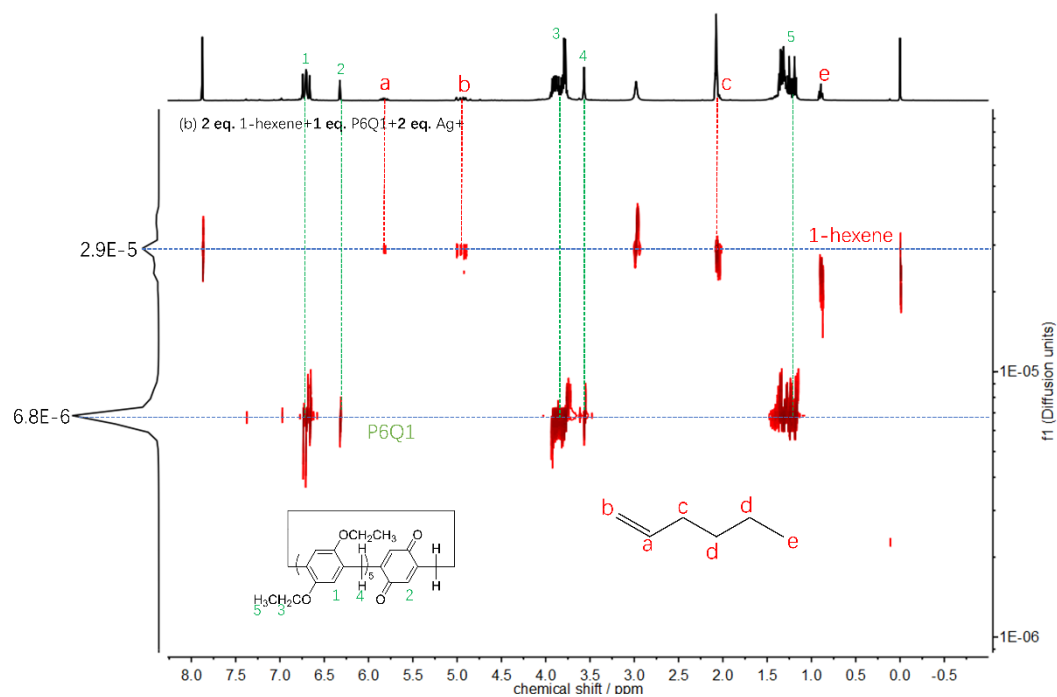
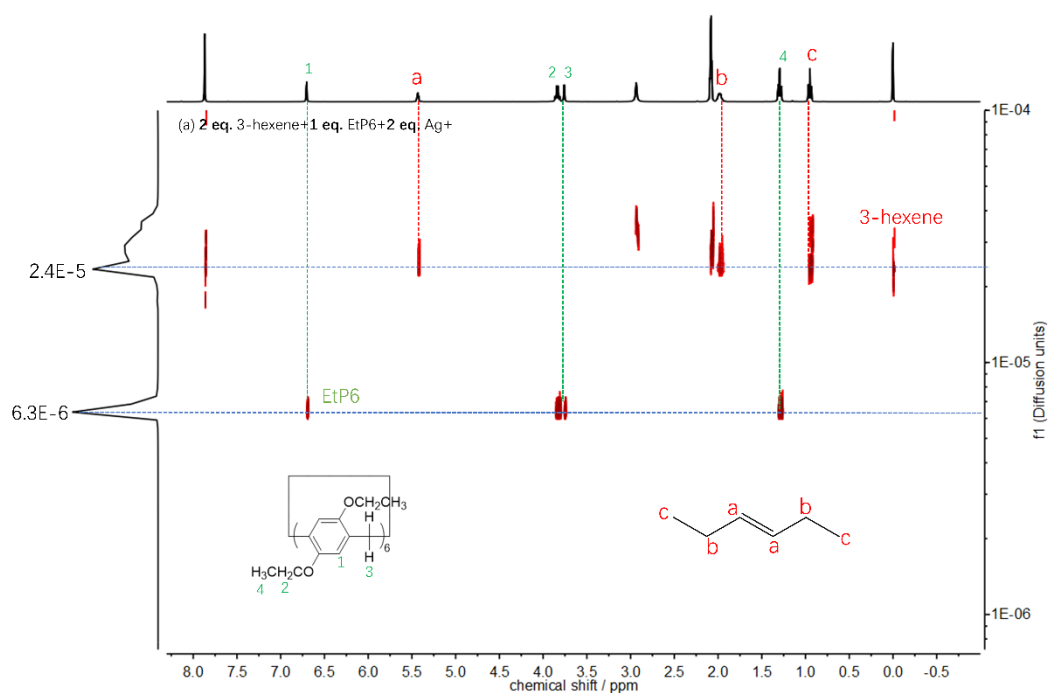


Figure S37. 2D DOSY NMR spectra (CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 2 equiv. 1-hexene + 1 equiv. **EtP6** + 2 equiv. Ag⁺ and (b) 2 equiv. 1-hexene + 1 equiv. **P6Q1** + 2 equiv. Ag⁺.



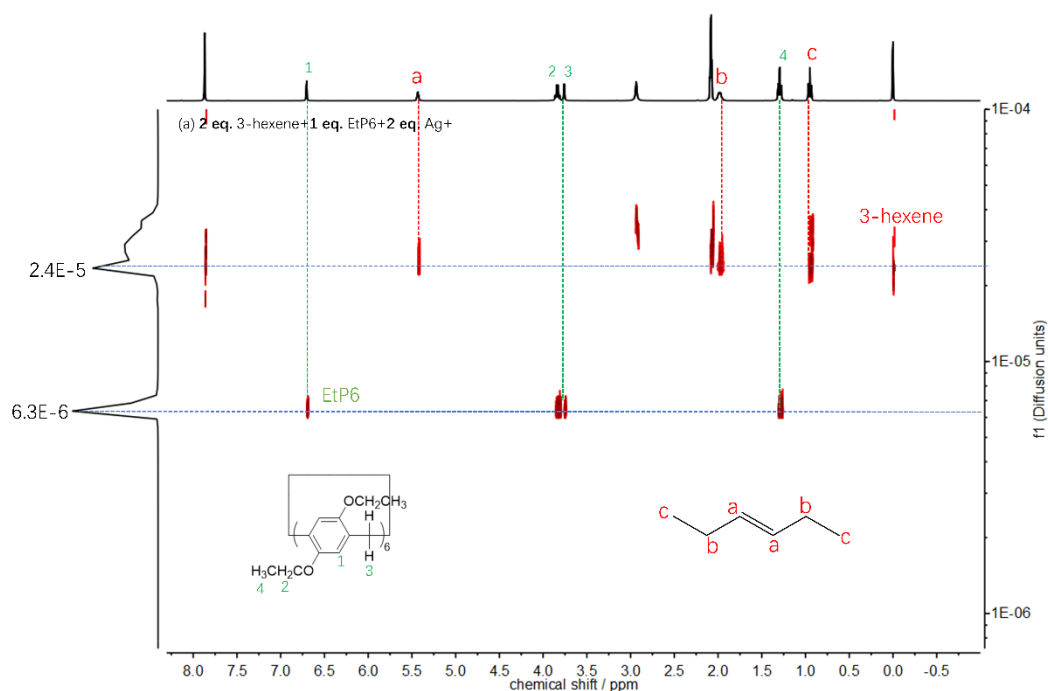


Figure S38. 2D DOSY NMR spectra (CDCl₃ : acetone-*d*₆ = 1:2, v/v, room temperature) of (a) 2 equiv. 3-hexene + 1 equiv. **EtP6** + 2 equiv. Ag⁺ and (b) 2 equiv. 3-hexene + 1 equiv. **P6Q1** + 2 equiv. Ag⁺.

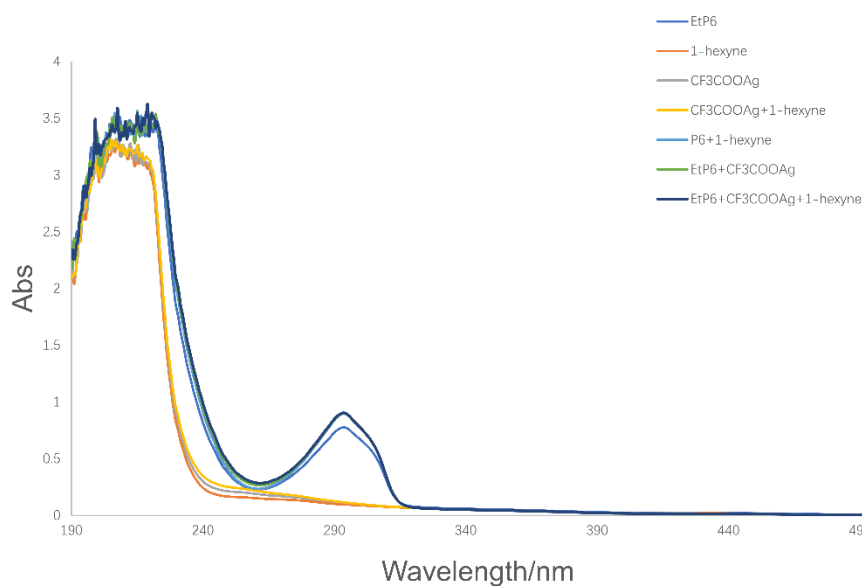


Figure S39. UV–visible spectra of **EtP6**, 1-hexyne, CF₃COOAg, CF₃COOAg+1-hexyne, **EtP6**+1-hexyne, **EtP6**+CF₃COOAg and **EtP6**+CF₃COOAg+1-hexyne.

6. Cartesian coordinates and energies of optimized structures

-----				6	1.830667000	3.888718000	0.011661000
AgOCOCF₃				6	2.340507000	3.384810000	1.206112000
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Sum of electronic and thermal Free Energies= -673.330457				1	0.795278000	5.544358000	0.882946000
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9	2.732945000	1.215418000	-0.144272000	6	-1.273752000	3.924158000	1.183649000
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6	2.207306000	0.004112000	-0.002174000	6	-2.509601000	3.278954000	-1.182748000
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-----				6	-1.275824000	3.914017000	-1.204791000
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Sum of electronic and thermal Enthalpies= -2496.255061				6	-4.241524000	0.700905000	-0.010925000
Sum of electronic and thermal Free Energies= -2496.399213				6	-4.113453000	-0.004097000	-1.205498000
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1	5.524096000	0.931922000	-0.883513000	6	-3.767389000	-2.070372000	0.011891000
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6	2.340164000	3.398213000	-1.182365000	1	-4.216553000	0.567373000	2.099734000
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1	-3.153435000	2.792158000	4.358180000	6	-2.477195000	3.035999000	3.576312000
-----				1	-2.142684000	1.991939000	3.532801000
EtP5				1	-3.557229000	3.032807000	3.767714000
Sum of electronic and zero-point Energies= -2889.246819				6	-1.752890000	3.786594000	4.669295000
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8	-2.198668000	3.675576000	2.352889000	6	-3.439858000	1.869600000	-3.581483000
8	-4.019111000	1.480361000	-2.358248000	1	-2.352191000	1.732617000	-3.536128000
8	2.817871000	3.228851000	2.352945000	1	-3.634871000	2.931475000	-3.775112000
8	0.166286000	4.278052000	-2.358303000	6	-4.043186000	1.018019000	-4.673947000
8	3.939744000	-1.678591000	2.358787000	1	-3.839532000	-0.038655000	-4.495583000
8	4.122748000	1.160812000	-2.356417000	1	-3.618872000	1.293459000	-5.640609000
8	-0.383827000	-4.262148000	2.359028000	1	-5.123642000	1.157743000	-4.717424000

6	-1.227237000	4.805066000	-0.002561000	6	4.090139000	0.428345000	-1.204333000
1	-1.397372000	5.424220000	-0.882505000	6	3.786986000	-0.996062000	3.581188000
1	-1.374819000	5.429576000	0.877654000	1	2.902886000	-0.347907000	3.535278000
6	0.193838000	4.292001000	-0.011317000	1	4.658649000	-0.358674000	3.773619000
6	0.854612000	4.035432000	1.181753000	6	3.640200000	-2.027717000	4.675146000
1	0.321777000	4.237631000	2.099864000	1	2.765914000	-2.655477000	4.498005000
6	2.139966000	3.511977000	1.201827000	1	3.521594000	-1.534558000	5.641111000
6	2.806007000	3.254336000	0.005938000	1	4.521010000	-2.668818000	4.719376000
6	2.148526000	3.519248000	-1.187124000	6	3.885899000	0.503086000	-3.579000000
1	2.674224000	3.299361000	-2.105276000	1	2.926528000	-0.027445000	-3.534315000
6	0.854344000	4.020450000	-1.207201000	1	4.669691000	-0.239965000	-3.770466000
6	2.123931000	3.297192000	3.576549000	6	3.872673000	1.545031000	-4.673009000
1	1.234947000	2.655484000	3.534288000	1	3.694208000	1.070927000	-5.639308000
1	1.786220000	4.323298000	3.766651000	1	4.827648000	2.069447000	-4.715555000
6	3.062474000	2.842976000	4.669913000	1	3.084596000	2.278393000	-4.497089000
1	3.389566000	1.817109000	4.495448000	6	3.818249000	-3.166645000	0.005318000
1	2.559001000	2.885508000	5.636893000	1	4.304057000	-3.584172000	0.886365000
1	3.944089000	3.483252000	4.709957000	1	4.319942000	-3.569010000	-0.873881000
6	4.191741000	2.652265000	-0.002884000	6	2.366707000	-3.586090000	-0.003732000
1	4.740961000	2.987052000	0.876241000	6	1.680018000	-3.763909000	1.189048000
1	4.727084000	3.004115000	-0.883896000	1	2.229068000	-3.612390000	2.107381000
6	4.143145000	1.142142000	-0.009401000	6	0.332286000	-4.095262000	1.208368000
6	4.102139000	0.436245000	1.184749000	6	-0.356781000	-4.280734000	0.012129000
1	4.128820000	1.006933000	2.102000000	6	0.332048000	-4.111286000	-1.180651000
6	4.001265000	-0.947919000	1.206743000	1	-0.221746000	-4.244146000	-2.098987000
6	3.963407000	-1.662701000	0.011775000	6	1.673808000	-3.756731000	-1.200028000
6	4.013740000	-0.957405000	-1.182337000	6	0.216240000	-3.906558000	3.582462000
1	3.968088000	-1.526810000	-2.099633000	1	0.558183000	-2.864942000	3.538302000

1	1.092374000	-4.537735000	3.775051000	1	-3.810688000	0.528985000	4.493428000
6	-0.811373000	-4.088191000	4.675035000	1	-3.764980000	-0.821166000	5.637652000
1	-1.148382000	-5.124272000	4.716981000	6	-2.842463000	-2.696739000	-3.578629000
1	-1.678746000	-3.450841000	4.498061000	1	-2.376689000	-1.704227000	-3.536107000
1	-0.380213000	-3.824514000	5.641950000	1	-3.913014000	-2.555268000	-3.770957000
6	1.687273000	-3.542176000	-3.574866000	6	-2.219870000	-3.535455000	-4.670238000
1	0.887791000	-2.791859000	-3.533576000	1	-2.685538000	-4.520501000	-4.710608000
1	1.221119000	-4.516608000	-3.765350000	1	-1.151500000	-3.666573000	-4.493457000
6	2.677413000	-3.211858000	-4.667207000	1	-2.352983000	-3.049189000	-5.637802000
1	2.173706000	-3.189403000	-5.634734000	6	0.716226000	3.847929000	-3.581411000
1	3.469766000	-3.959805000	-4.706397000	1	1.666477000	4.360935000	-3.773649000
1	3.133060000	-2.236352000	-4.492064000	1	0.921157000	2.770961000	-3.536872000
6	-1.831761000	-4.608225000	0.002682000	6	-0.278791000	4.160345000	-4.674559000
1	-2.057187000	-5.209689000	-0.877118000	1	-0.479451000	5.231210000	-4.716709000
1	-2.079866000	-5.199768000	0.883102000	1	0.115400000	3.843261000	-5.641213000
6	-2.680267000	-3.358094000	-0.007462000	1	-1.221149000	3.640087000	-4.498113000
6	-3.064301000	-2.761121000	1.185025000	-----			
1	-2.752196000	-3.237093000	2.103587000	EtP6			
6	-3.796566000	-1.582164000	1.203901000	Sum of electronic and zero-point Energies= -3467.091734			
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6	-3.656376000	-1.414099000	3.578367000	6	-5.162648000	0.132262000	0.009042000
1	-2.560014000	-1.417118000	3.535421000	6	-4.940487000	0.804746000	-1.184348000
1	-3.985748000	-2.442510000	3.770667000	6	-4.511857000	2.124955000	-1.203265000
6	-4.148320000	-0.493060000	4.670312000	6	-4.330041000	2.815193000	-0.007092000
1	-5.237870000	-0.493411000	4.711219000	6	-4.525457000	2.134428000	1.186297000

6	-4.919584000	0.803482000	1.205175000	6	-1.766246000	4.664040000	1.200932000
6	-4.602879000	-2.341944000	-0.004208000	8	-4.277311000	2.823985000	-2.352314000
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6	-3.154210000	-3.861067000	1.203214000	8	-5.119948000	0.093667000	2.354085000
6	-2.695658000	-4.404699000	0.005477000	6	-4.756058000	0.680452000	3.581737000
6	-3.168780000	-3.873951000	-1.186276000	8	-4.588944000	-2.289336000	-2.349512000
6	-4.098195000	-2.842892000	-1.202016000	6	-4.011921000	-2.662798000	-3.578924000
6	-1.727020000	-5.562896000	-0.002623000	8	-2.639389000	-4.392347000	2.350673000
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6	1.772069000	-4.678654000	-1.188314000	8	-0.309784000	-5.112248000	-2.354024000
6	0.414333000	-4.967379000	-1.205736000	6	0.302626000	-4.795151000	-3.582133000
6	-0.272810000	-5.156655000	-0.008897000	8	4.589421000	2.289299000	-2.348676000
6	0.416257000	-4.987677000	1.183763000	6	4.012672000	2.662796000	-3.578207000
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6	5.681687000	1.285575000	0.005411000	6	2.964841000	3.786828000	3.580360000
6	4.602898000	2.341913000	-0.003371000	8	0.310191000	5.112061000	-2.353959000
6	4.109155000	2.853816000	1.188241000	6	-0.302119000	4.795278000	-3.582196000
6	3.153960000	3.861008000	1.203765000	8	-2.482849000	4.485190000	2.349161000
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6	3.169030000	3.873919000	-1.185722000	8	2.482453000	-4.485193000	2.349548000
6	4.098452000	2.842863000	-1.201277000	6	1.793646000	-4.466649000	3.577963000
6	1.727018000	5.562845000	-0.002345000	6	3.954635000	-4.277657000	-0.001721000
6	-3.954638000	4.277640000	-0.002345000	6	5.162678000	-0.132285000	0.009988000
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6	4.310428000	-2.134100000	-3.579177000	1	-4.174570000	-3.730930000	-3.767708000
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6	4.755700000	-0.680614000	3.582603000	1	-4.042918000	-3.865480000	3.769724000
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1	2.328578000	-4.558003000	-2.107081000	1	-1.324533000	5.439854000	3.766161000
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1	6.314608000	1.419159000	-0.871550000	1	0.998145000	-3.712112000	3.545333000
1	6.305734000	1.436322000	0.885935000	1	1.323783000	-5.439650000	3.766397000
1	4.498477000	2.440254000	2.107892000	1	4.385328000	-4.756012000	-0.881003000
1	2.788463000	4.295567000	-2.105371000	1	4.398490000	-4.745660000	0.876619000
1	1.927120000	6.174439000	-0.881769000	1	5.116306000	-0.261963000	-2.101533000
1	1.908889000	6.182041000	0.875745000	1	4.361023000	-2.680986000	2.105073000
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1	-2.328230000	4.557862000	-2.107438000	1	5.362977000	-1.573801000	3.773473000
1	0.137070000	5.119966000	2.102633000	1	3.704643000	-0.992378000	3.546856000
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6	0.739796000	4.931525000	-4.667847000	6	-2.793560000	4.144139000	4.664055000
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1	1.570534000	4.247125000	-4.490281000	1	-2.298064000	4.125800000	5.635858000
1	0.301612000	4.698635000	-5.639446000	1	-3.585230000	4.893439000	4.692904000
6	3.909086000	-3.103655000	-4.666221000	6	-4.972544000	-0.346776000	4.668341000
1	3.927832000	-2.606855000	-5.637354000	1	-6.017036000	-0.658308000	4.700135000
1	4.594372000	-3.951259000	-4.697404000	1	-4.354585000	-1.228223000	4.491599000
1	2.900787000	-3.481173000	-4.490483000	1	-4.706320000	0.072971000	5.639523000
6	-0.739164000	-4.931228000	-4.667927000	6	-2.185846000	-4.492067000	4.664967000
1	-0.300880000	-4.698129000	-5.639431000	1	-2.439979000	-5.552069000	4.693735000
1	-1.130692000	-5.948447000	-4.699557000	1	-1.113265000	-4.398863000	4.489072000
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6	-4.655206000	-1.831439000	-4.664186000	6	2.792703000	-4.143955000	4.664482000
1	-4.478222000	-0.769252000	-4.489604000	1	3.584341000	-4.893282000	4.693530000
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1	4.705625000	-0.073180000	5.640393000	Sum of electronic and thermal Free Energies= -3308.862368			
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1	4.354330000	1.228102000	4.492433000	6	-5.012889000	1.562470000	0.249765000
6	2.184979000	4.492114000	4.665335000	6	-4.683217000	2.143296000	-0.966026000
1	1.112424000	4.398885000	4.489285000	6	-3.975589000	3.335721000	-1.029491000
1	2.415066000	4.053997000	5.637632000	6	-3.623394000	3.994328000	0.145896000
1	2.439092000	5.552121000	4.694083000	6	-3.923438000	3.399881000	1.363337000

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6	-4.008551000	-2.789490000	-0.972744000	8	-5.110377000	-0.942113000	-2.093334000
6	-4.690665000	-1.580581000	-0.961619000	6	-4.698290000	-1.444635000	-3.343425000
6	-2.905052000	-4.741238000	0.168499000	8	-3.400992000	-3.374372000	2.540927000
6	1.405219000	-4.663009000	-0.075195000	6	-3.535235000	-2.708842000	3.775616000
6	0.627956000	-4.648705000	-1.224685000	8	-1.561792000	-4.619017000	-2.265719000
6	-0.758715000	-4.633166000	-1.161878000	6	-0.964748000	-4.462715000	-3.532020000
6	-1.400141000	-4.664417000	0.074291000	8	4.898652000	1.555940000	-2.589993000
6	-0.622901000	-4.650344000	1.223779000	6	4.415080000	2.091067000	-3.803109000
6	0.763756000	-4.633409000	1.160987000	8	3.610196000	3.943595000	2.197232000
6	5.829687000	0.299497000	-0.292288000	6	3.813169000	3.247475000	3.408346000
6	5.011611000	1.567451000	-0.249034000	8	1.224965000	5.176841000	-2.338281000
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6	3.920699000	3.403732000	-1.363031000	6	2.910196000	-4.738316000	-0.169469000
6	4.591077000	2.189436000	-1.423896000	6	5.008901000	-0.966837000	-0.249820000
6	2.950180000	5.351605000	-0.091652000	6	4.572692000	-1.561873000	-1.425181000
6	-2.955573000	5.348817000	0.091573000	6	3.859198000	-2.752591000	-1.412384000
6	-1.459274000	5.272222000	-0.013049000	6	3.599277000	-3.395349000	-0.203825000
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6	0.669870000	5.219082000	-1.259990000	6	4.692137000	-1.576035000	0.961942000
6	1.453961000	5.273624000	0.013019000	8	3.405914000	-3.370600000	-2.541472000
6	0.796522000	5.256205000	1.173326000	6	3.539022000	-2.704181000	-3.775811000

8	5.110647000	-0.937283000	2.093954000	1	-3.067011000	-1.718724000	3.716729000
6	4.697741000	-1.439952000	3.343712000	1	-4.595367000	-2.563513000	4.016180000
1	-6.426080000	0.288744000	1.205021000	1	-0.355551000	-3.550636000	-3.544454000
1	-6.518567000	0.297147000	-0.550789000	1	-0.302552000	-5.309817000	-3.748224000
1	-4.998982000	1.633445000	-1.865214000	1	3.327598000	2.215121000	-3.749893000
1	-3.617926000	3.914731000	2.263458000	1	4.856188000	3.078569000	-3.982261000
1	-4.808520000	-1.069462000	2.355264000	1	3.349293000	2.256050000	3.345611000
1	-3.781441000	-3.293139000	-1.901681000	1	4.885881000	3.105692000	3.586370000
1	-3.284365000	-5.302661000	-0.685049000	1	0.359574000	-3.551542000	3.543094000
1	-3.166977000	-5.296507000	1.068828000	1	0.307834000	-5.310665000	3.747583000
1	1.142797000	-4.653099000	-2.175136000	1	3.172667000	-5.292939000	-1.070031000
1	-1.137694000	-4.656103000	2.174248000	1	3.290074000	-5.299766000	0.683817000
1	6.426707000	0.295314000	-1.203611000	1	4.811043000	-1.064383000	-2.354816000
1	6.518236000	0.303732000	0.552254000	1	3.784232000	-3.289663000	1.901355000
1	4.996606000	1.638337000	1.865955000	1	3.069727000	-1.714615000	-3.716159000
1	3.615086000	3.918284000	-2.263285000	1	4.598909000	-2.557535000	-4.016650000
1	3.205926000	5.904304000	-0.995160000	1	5.104910000	-2.445716000	3.503128000
1	3.329207000	5.903435000	0.767783000	1	3.603722000	-1.514027000	3.369951000
1	-3.335115000	5.900069000	-0.767996000	6	3.191123000	4.058160000	4.520646000
1	-3.211895000	5.901454000	0.994953000	1	2.117899000	4.171789000	4.362546000
1	-1.329607000	5.275429000	-2.118810000	1	3.346554000	3.557940000	5.477622000
1	1.324277000	5.278011000	2.118770000	1	3.642296000	5.049596000	4.572845000
1	-3.353969000	2.253429000	-3.346360000	6	-4.790240000	1.127486000	4.909030000
1	-4.891660000	3.101644000	-3.585070000	1	-5.872287000	1.002077000	4.960136000
1	-4.857544000	3.073821000	3.982819000	1	-4.336857000	0.149907000	4.737424000
1	-3.328138000	2.211942000	3.750044000	1	-4.439193000	1.507298000	5.869383000
1	-3.604234000	-1.517707000	-3.370792000	6	-2.864555000	-3.555048000	4.832381000
1	-5.104712000	-2.450794000	-3.502235000	1	-2.951134000	-3.074590000	5.807991000

1	-3.329436000	-4.539817000	4.888592000	1	-1.646334000	-4.264250000	-5.557202000
1	-1.805763000	-3.685427000	4.604129000	1	-2.676170000	-5.287744000	-4.543740000
6	2.074623000	-4.380682000	4.557949000	-----			
1	1.650637000	-4.263658000	5.556310000	P6Q2			
1	2.681434000	-5.286540000	4.543219000	Sum of electronic and zero-point Energies= -3150.401959			
1	2.723312000	-3.527230000	4.355936000	Sum of electronic and thermal Energies= -3150.333038			
6	5.195280000	-0.493922000	4.411477000	Sum of electronic and thermal Enthalpies= -3150.332094			
1	4.774577000	0.502436000	4.268552000	Sum of electronic and thermal Free Energies= -3150.513820			
1	4.900715000	-0.854350000	5.398126000	6	5.844562000	0.000345000	0.000125000
1	6.282558000	-0.417286000	4.381022000	6	5.022935000	-1.265729000	-0.013653000
6	2.868976000	-3.550511000	-4.832882000	6	4.620742000	-1.827411000	-1.216625000
1	3.334883000	-4.534756000	-4.889738000	6	3.906787000	-3.017248000	-1.255444000
1	1.810377000	-3.682131000	-4.604455000	6	3.624131000	-3.692596000	-0.070439000
1	2.954824000	-3.069434000	-5.808250000	6	3.996391000	-3.116372000	1.135622000
6	4.791175000	1.132082000	-4.908325000	6	4.669662000	-1.902965000	1.174884000
1	4.338679000	0.154072000	-4.736833000	6	5.022790000	1.266321000	0.013752000
1	4.440112000	1.511500000	-5.868828000	6	4.620428000	1.828016000	1.216667000
6	-5.197787000	-0.499233000	-4.410836000	6	3.906330000	3.017767000	1.255372000
1	-4.903812000	-0.859492000	-5.397724000	6	3.623686000	3.693024000	0.070307000
1	-6.285109000	-0.423663000	-4.379341000	6	3.996139000	3.116796000	-1.135689000
1	-4.777922000	0.497552000	-4.268432000	6	4.669563000	1.903467000	-1.174839000
6	-3.198889000	4.056133000	-4.520892000	6	2.951796000	5.046138000	0.103536000
1	-2.125627000	4.170878000	-4.363856000	6	-1.452675000	4.967467000	-0.109233000
1	-3.354751000	3.556040000	-5.477863000	6	-0.720493000	4.948231000	-1.223822000
1	-3.651180000	5.047098000	-4.572320000	6	0.753789000	4.915784000	-1.212946000
1	5.873362000	1.007718000	-4.959033000	6	1.452097000	4.967684000	0.109256000
6	-2.070104000	-4.381392000	-4.558762000	6	0.719916000	4.948719000	1.223849000
1	-2.719469000	-3.528422000	-4.356870000	6	-0.754356000	4.915968000	1.212976000

6	-5.844581000	-0.000340000	0.000195000	8	-1.379156000	-4.878972000	-2.252433000
6	-5.022798000	-1.266309000	0.013788000	8	1.379735000	-4.878885000	2.252064000
6	-4.620527000	-1.828097000	1.216682000	8	-1.379669000	4.879000000	2.252301000
6	-3.906421000	-3.017852000	1.255348000	6	-2.952382000	5.045772000	-0.103532000
6	-3.623683000	-3.693007000	0.070257000	6	-5.022963000	1.265741000	-0.013551000
6	-3.996041000	-3.116679000	-1.135730000	6	-4.620886000	1.827533000	-1.216505000
6	-4.669468000	-1.903358000	-1.174832000	6	-3.906927000	3.017376000	-1.255286000
6	-2.951787000	-5.046118000	0.103425000	6	-3.624151000	3.692602000	-0.070244000
6	2.952384000	-5.045777000	-0.103810000	6	-3.996312000	3.116271000	1.135801000
6	1.452679000	-4.967484000	-0.109466000	6	-4.669587000	1.902868000	1.175018000
6	0.720468000	-4.948395000	-1.224039000	8	-3.474786000	3.603227000	-2.407225000
6	-0.753811000	-4.915897000	-1.213128000	6	-3.624341000	2.898032000	-3.621463000
6	-1.452087000	-4.967661000	0.109093000	8	-5.041705000	1.284300000	2.330525000
6	-0.719880000	-4.948538000	1.223667000	6	-4.629703000	1.838795000	3.561798000
6	0.754394000	-4.915870000	1.212757000	1	6.487580000	-0.004929000	0.879517000
8	3.474524000	-3.602976000	-2.407395000	1	6.487733000	0.005690000	-0.879159000
6	3.623993000	-2.897660000	-3.621570000	1	4.884761000	-1.304969000	-2.125339000
8	5.041887000	-1.284506000	2.330420000	1	3.742909000	-3.643988000	2.044359000
6	4.630026000	-1.839135000	3.561677000	1	4.884372000	1.305615000	2.125428000
8	5.042020000	1.285022000	-2.330309000	1	3.742679000	3.644335000	-2.044478000
6	4.629814000	1.839283000	-3.561617000	1	3.265312000	5.613552000	-0.772342000
8	3.473913000	3.603493000	2.407261000	1	3.274081000	5.583484000	0.994617000
6	3.623539000	2.898302000	3.621489000	1	-1.184628000	4.967467000	-2.202260000
8	1.379107000	4.878842000	-2.252265000	1	1.184044000	4.968324000	2.202281000
8	-5.041801000	-1.284810000	-2.330281000	1	-6.487755000	-0.005669000	-0.879087000
6	-4.629740000	-1.839158000	-3.561597000	1	-6.487599000	0.004907000	0.879588000
8	-3.474097000	-3.603687000	2.407227000	1	-4.884535000	-1.305776000	2.125469000
6	-3.623574000	-2.898519000	3.621488000	1	-3.742494000	-3.644147000	-2.044538000

1	-3.265338000	-5.613512000	-0.772452000	1	-3.048027000	-3.185697000	5.666490000
1	-3.274032000	-5.583485000	0.994507000	1	-3.378306000	-4.688175000	4.791992000
1	3.274688000	-5.582972000	-0.994975000	6	5.062093000	-0.893088000	4.657425000
1	3.266002000	-5.613283000	0.771974000	1	6.144503000	-0.761090000	4.648344000
1	1.184573000	-4.967754000	-2.202489000	1	4.593597000	0.083786000	4.527120000
1	-1.183990000	-4.968007000	2.202111000	1	4.768964000	-1.288858000	5.630627000
1	3.173990000	-1.902348000	-3.528030000	6	2.938499000	3.693574000	4.707489000
1	4.688000000	-2.764916000	-3.851011000	1	3.048143000	3.185387000	5.666545000
1	5.085998000	-2.826123000	3.701557000	1	3.378236000	4.687912000	4.792051000
1	3.542036000	-1.969456000	3.567602000	1	1.874061000	3.800475000	4.494738000
1	3.541788000	1.969312000	-3.567389000	6	-5.061648000	0.892628000	4.657489000
1	5.085501000	2.826360000	-3.701786000	1	-4.593067000	-0.084194000	4.527109000
1	3.173741000	1.902887000	3.528035000	1	-4.768544000	1.288357000	5.630715000
1	4.687574000	2.765800000	3.850930000	1	-6.144048000	0.760533000	4.648414000
1	-3.541729000	-1.969307000	-3.567440000	6	-2.939538000	3.693477000	-4.707486000
1	-5.085544000	-2.826193000	-3.701690000	1	-3.379414000	4.687768000	-4.791899000
1	-3.173716000	-1.903130000	3.528028000	1	-1.875089000	3.800498000	-4.494861000
1	-4.687578000	-2.765950000	3.851032000	1	-3.049248000	3.185369000	-5.666575000
1	-3.274707000	5.583047000	-0.994642000	6	-5.061861000	-0.892997000	-4.657223000
1	-3.265960000	5.613210000	0.772309000	1	-4.593463000	0.083906000	-4.526782000
1	-4.884975000	1.305171000	-2.125244000	1	-4.768676000	-1.288610000	-5.630471000
1	-3.742737000	3.643807000	2.044559000	6	5.061968000	0.893138000	-4.657246000
1	-3.174325000	1.902711000	-3.528058000	1	4.768558000	1.288633000	-5.630475000
1	-4.688361000	2.765305000	-3.850846000	1	6.144417000	0.761453000	-4.648323000
1	-5.085658000	2.825768000	3.701837000	1	4.593777000	-0.083847000	-4.526673000
1	-3.541713000	1.969115000	3.567608000	6	2.939099000	-3.692983000	-4.707624000
6	-2.938503000	-3.693868000	4.707413000	1	1.874683000	-3.800088000	-4.494875000
1	-1.874090000	-3.800843000	4.494571000	1	3.048656000	-3.184721000	-5.666649000

1	3.379015000	-4.687238000	-4.792246000	6	-3.145606000	4.942263000	0.039388000
1	-6.144284000	-0.761102000	-4.648142000	6	-1.634902000	4.921289000	0.018629000
-----				6	-0.945036000	4.933802000	-1.184667000
P6Q3				6	0.442362000	4.977879000	-1.216129000
Sum of electronic and zero-point Energies= -2992.055574				6	1.157880000	5.055345000	-0.022268000
Sum of electronic and thermal Energies= -2991.992730				6	0.469659000	5.007403000	1.181060000
Sum of electronic and thermal Enthalpies= -2991.991786				6	-0.915579000	4.918328000	1.212675000
Sum of electronic and thermal Free Energies= -2992.161175				6	2.659632000	5.220908000	-0.043377000
6	3.190617000	-4.912224000	-0.047241000	6	5.854264000	0.253362000	0.046653000
6	3.798745000	-3.529195000	-0.023351000	6	4.975102000	1.470575000	0.082710000
6	4.098295000	-2.910237000	1.181317000	6	4.572557000	2.055479000	1.211664000
6	4.714473000	-1.666456000	1.215537000	6	3.745132000	3.276206000	1.228505000
6	5.080417000	-1.044241000	0.022966000	6	3.402510000	3.916070000	-0.079867000
6	4.749419000	-1.646991000	-1.181674000	6	3.771077000	3.309277000	-1.208861000
6	4.093156000	-2.870057000	-1.215883000	6	4.538424000	2.049951000	-1.225778000
6	1.689123000	-4.902516000	-0.084427000	8	5.018911000	-1.003383000	2.363549000
6	0.980098000	-4.913170000	-1.213956000	6	4.613889000	-1.560059000	3.599254000
6	-0.494194000	-4.948041000	-1.232049000	8	3.728972000	-3.502159000	-2.363979000
6	-1.215144000	-5.042759000	0.075563000	6	3.945134000	-2.847732000	-3.599277000
6	-0.508071000	-4.991618000	1.205226000	8	1.564798000	-4.813538000	2.274575000
6	0.962706000	-4.884549000	1.223528000	8	-1.100691000	-4.929865000	-2.282805000
6	-2.708799000	-5.196092000	0.037914000	8	-3.372544000	-3.850588000	2.360069000
6	-4.958536000	-1.525513000	-0.015712000	6	-3.645464000	-3.223234000	3.598192000
6	-4.568039000	-2.097195000	1.186221000	8	-1.644604000	4.852137000	2.359197000
6	-3.798544000	-3.252556000	1.215001000	6	-0.963042000	4.778453000	3.596545000
6	-3.446335000	-3.877408000	0.019684000	8	1.174459000	4.976938000	-2.362538000
6	-3.807149000	-3.286561000	-1.182290000	6	0.502958000	4.832763000	-3.599171000
6	-4.538817000	-2.106902000	-1.211111000	8	3.378975000	3.761074000	2.278766000

8	4.829930000	1.517150000	-2.276214000	1	6.501644000	0.266676000	0.922388000
8	-4.908454000	-1.472524000	-2.356211000	1	6.478862000	0.303946000	-0.844691000
6	-4.452669000	-1.982105000	-3.594589000	1	4.848766000	1.658819000	2.181005000
6	-5.852183000	-0.307277000	-0.033660000	1	3.527664000	3.726766000	-2.178220000
6	-3.759868000	3.572205000	0.079753000	1	3.534636000	-1.746872000	3.586594000
6	-4.063289000	2.933933000	1.210797000	1	5.119458000	-2.519106000	3.759609000
6	-4.706084000	1.606758000	1.231821000	1	5.019408000	-2.704745000	-3.762317000
6	-5.092755000	0.987897000	-0.074390000	1	3.473073000	-1.859413000	-3.583512000
6	-4.753099000	1.607464000	-1.205508000	1	-3.269169000	-2.194613000	3.584257000
6	-4.044580000	2.900711000	-1.226685000	1	-4.727883000	-3.183166000	3.765071000
8	-4.938995000	1.048536000	2.283676000	1	-0.261098000	3.937640000	3.584423000
8	-3.728335000	3.415845000	-2.278778000	1	-0.386266000	5.695955000	3.759606000
1	3.555894000	-5.447354000	-0.922701000	1	-0.115492000	3.928828000	-3.582791000
1	3.511335000	-5.450292000	0.844251000	1	-0.158892000	5.690168000	-3.766119000
1	3.836150000	-3.428550000	2.092937000	1	-3.360618000	-2.066521000	-3.582124000
1	5.019679000	-1.132952000	-2.093337000	1	-4.865581000	-2.983698000	-3.760117000
1	1.464222000	-4.906806000	-2.182871000	1	-6.473292000	-0.316371000	0.861480000
1	-0.990270000	-5.037043000	2.174062000	1	-6.503287000	-0.355313000	-0.905457000
1	-3.021055000	-5.767306000	0.911111000	1	-3.856213000	3.373857000	2.178708000
1	-2.976508000	-5.758710000	-0.855926000	1	-4.994856000	1.185397000	-2.173319000
1	-4.882848000	-1.613074000	2.099965000	6	1.550099000	4.745213000	-4.683822000
1	-3.499832000	-3.775266000	-2.096094000	1	2.193039000	3.877484000	-4.530534000
1	-3.482495000	5.499446000	0.912478000	1	1.068849000	4.648302000	-5.657803000
1	-3.500321000	5.454496000	-0.854444000	1	2.171288000	5.641524000	-4.693424000
1	-1.523720000	4.908404000	-2.097294000	6	3.348123000	-3.708733000	-4.686884000
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1	2.963518000	5.767093000	0.849113000	1	2.274466000	-3.830105000	-4.537384000
1	2.941731000	5.805534000	-0.917968000	1	3.508900000	-3.242731000	-5.659824000

6	-4.903646000	-1.031073000	-4.677556000	47	-1.672855000	-0.946309000	0.693985000
1	-4.583034000	-1.399699000	-5.652718000	8	1.405554000	4.174832000	1.708733000
1	-5.990415000	-0.940315000	-4.683124000	8	-0.797600000	3.768330000	-3.321459000
1	-4.472193000	-0.040778000	-4.525919000	8	3.861772000	-0.037258000	2.605675000
6	-1.997603000	4.596196000	4.681514000	8	4.276736000	2.194703000	-2.413725000
1	-2.554263000	3.670050000	4.532444000	8	0.583628000	-3.642461000	1.371894000
1	-1.509732000	4.550540000	5.655950000	8	4.955861000	-2.862900000	-1.885709000
6	4.973821000	-0.576258000	4.687027000	8	-4.426271000	-3.927371000	-0.417630000
1	4.451285000	0.369880000	4.540049000	8	0.379233000	-1.874884000	-2.122772000
1	4.689376000	-0.978122000	5.660282000	8	-3.412598000	2.950517000	1.137081000
1	6.047260000	-0.383898000	4.693315000	8	-4.000019000	0.085557000	-3.524092000
6	-2.965888000	-4.027147000	4.681040000	6	-2.572137000	4.199715000	-1.208164000
1	-1.886045000	-4.045662000	4.527992000	1	-2.784960000	4.687560000	-2.158889000
1	-3.166951000	-3.581569000	5.656059000	1	-2.993473000	4.814630000	-0.413970000
1	-3.334261000	-5.053590000	4.688041000	6	-1.076061000	4.096590000	-1.011455000
1	-2.701842000	5.428857000	4.686636000	6	-0.531016000	4.189180000	0.260621000
-----				1	-1.208752000	4.336695000	1.088594000
MeP5 with one AgOCOCF₃				6	0.835864000	4.083780000	0.476821000
Sum of electronic and zero-point Energies= -3169.668757				6	1.697166000	3.900570000	-0.603077000
Sum of electronic and thermal Energies= -3169.605909				6	1.151844000	3.792351000	-1.875170000
Sum of electronic and thermal Enthalpies= -3169.604964				1	1.834577000	3.634488000	-2.698872000
Sum of electronic and thermal Free Energies= -3169.772682				6	-0.217673000	3.877321000	-2.087528000
9	-1.913809000	0.624162000	5.236073000	6	0.563593000	4.095285000	2.835779000
9	-0.189404000	-0.681616000	5.269384000	1	-0.042811000	3.186817000	2.805231000
9	0.054342000	1.432994000	4.925042000	1	-0.081949000	4.975816000	2.919431000
8	-0.062865000	0.629875000	2.377001000	6	0.035589000	3.526035000	-4.424583000
6	-0.867302000	0.111055000	3.141569000	1	0.588419000	2.586700000	-4.314234000
6	-0.731137000	0.386678000	4.664432000	1	0.750003000	4.340943000	-4.580263000

6	3.191272000	3.811783000	-0.402534000	6	4.941231000	-3.363371000	-3.196630000
1	3.689908000	4.210273000	-1.284548000	1	4.120197000	-2.936393000	-3.783195000
1	3.474338000	4.433796000	0.446311000	1	4.859129000	-4.455262000	-3.212429000
6	3.672746000	2.401868000	-0.150327000	6	0.391600000	-4.603255000	-1.229986000
6	3.561524000	1.846507000	1.115976000	1	0.152744000	-5.497541000	-0.649915000
1	3.105638000	2.449965000	1.886648000	1	0.584175000	-4.933394000	-2.253971000
6	3.989892000	0.554459000	1.386388000	6	-0.827617000	-3.709523000	-1.222617000
6	4.585218000	-0.200598000	0.378545000	6	-2.058035000	-4.226868000	-0.826310000
6	4.691804000	0.350782000	-0.891771000	1	-2.091406000	-5.262866000	-0.518510000
1	5.133046000	-0.261898000	-1.665729000	6	-3.210360000	-3.457043000	-0.783100000
6	4.225796000	1.628709000	-1.169331000	6	-3.162554000	-2.098735000	-1.126074000
6	3.166969000	0.666935000	3.612325000	6	-1.923372000	-1.573418000	-1.528230000
1	2.158605000	0.933441000	3.286284000	1	-1.886211000	-0.576105000	-1.949854000
1	3.708762000	1.570128000	3.911953000	6	-0.770443000	-2.372279000	-1.603747000
6	5.013201000	-1.629900000	0.622208000	6	-4.531307000	-5.267535000	0.001948000
1	5.226121000	-1.776686000	1.679507000	1	-3.907809000	-5.460980000	0.880088000
1	5.919991000	-1.844173000	0.059537000	1	-4.254961000	-5.960347000	-0.798801000
6	3.901318000	-2.554466000	0.190947000	6	0.908092000	-0.690495000	-1.542193000
6	2.817836000	-2.765767000	1.030701000	1	0.989963000	-0.796437000	-0.454708000
1	2.857274000	-2.323320000	2.015643000	1	0.306229000	0.190860000	-1.781069000
6	1.692704000	-3.457049000	0.603209000	6	-4.439850000	-1.278376000	-1.152213000
6	1.643899000	-3.961429000	-0.693552000	1	-5.024387000	-1.590296000	-2.019987000
6	2.749726000	-3.797229000	-1.513738000	1	-5.032332000	-1.528359000	-0.271793000
1	2.690986000	-4.178717000	-2.523611000	6	-4.164908000	0.196330000	-1.193163000
6	3.869586000	-3.097244000	-1.091673000	6	-4.040379000	0.911038000	-0.005679000
6	0.582479000	-3.090055000	2.670510000	1	-4.308110000	0.416306000	0.919595000
1	0.768725000	-2.012604000	2.644738000	6	-3.569491000	2.218545000	0.007352000
1	1.334468000	-3.567359000	3.306299000	6	-3.215496000	2.835264000	-1.195596000

6	-3.397598000	2.140209000	-2.380291000	Sum of electronic and thermal Free Energies= -3562.720517		
1	-3.113312000	2.634494000	-3.297552000	9	-4.312378000	2.946109000 -0.938350000
6	-3.866245000	0.832630000	-2.392135000	9	-5.238238000	1.618372000 0.480990000
6	-3.736661000	2.355113000	2.372945000	9	-5.059516000	1.030352000 -1.588806000
1	-3.160298000	1.443395000	2.547786000	8	-3.196946000	-0.186942000 0.130814000
1	-4.804350000	2.120522000	2.432481000	8	-2.032485000	1.622231000 -0.479608000
6	-3.584153000	0.648297000	-4.743505000	6	-3.060279000	0.993988000 -0.288276000
1	-2.524578000	0.924215000	-4.716197000	6	-4.431342000	1.666877000 -0.587561000
1	-4.176284000	1.531389000	-5.003443000	47	-1.238950000	-1.110882000 0.614568000
8	-1.810412000	-0.674469000	2.858163000	8	2.352508000	-3.360689000 -3.252629000
6	4.836448000	1.443113000	-3.457331000	8	-1.156856000	0.753556000 -4.282783000
1	5.884549000	1.193674000	-3.260974000	8	1.407542000	-4.540111000 1.528598000
1	4.279768000	0.515276000	-3.631936000	8	-2.803575000	-3.383660000 -1.825998000
1	-3.735985000	-0.118574000	-5.499797000	8	2.314248000	-0.547824000 4.408324000
1	1.909568000	-0.562821000	-1.947813000	8	-2.889970000	-1.811225000 3.133745000
1	-0.617642000	3.457683000	-5.292826000	8	4.018926000	3.223997000 1.670149000
1	4.780352000	2.065815000	-4.348297000	8	-1.295476000	2.993909000 3.088435000
1	5.889274000	-3.072979000	-3.645116000	8	3.929419000	1.394235000 -3.119192000
1	1.219743000	4.055952000	3.702824000	8	-0.082745000	4.747704000 -1.391779000
1	-3.489883000	3.088459000	3.137159000	6	1.550499000	1.336927000 -4.566628000
1	-5.575578000	-5.421167000	0.262821000	1	0.835831000	1.801825000 -5.244847000
1	-0.408928000	-3.266494000	3.079940000	1	2.492879000	1.225267000 -5.102406000
1	3.105688000	-0.006665000	4.464906000	6	1.048148000	-0.032689000 -4.174869000
-----				6	1.941506000	-1.062046000 -3.917805000
EtP5 with one AgOCOCF₃				1	2.995522000	-0.840131000 -4.004854000
Sum of electronic and zero-point Energies= -3562.603384				6	1.505477000	-2.325933000 -3.542927000
Sum of electronic and thermal Energies= -3562.527792				6	0.142589000	-2.590790000 -3.453758000
Sum of electronic and thermal Enthalpies= -3562.526847				6	-0.754329000	-1.559228000 -3.700430000

1	-1.809019000	-1.776716000	-3.607684000	6	1.043162000	-0.881388000	4.058366000
6	-0.317825000	-0.286586000	-4.043388000	6	0.075859000	0.117880000	4.190352000
6	3.730970000	-3.089544000	-3.148132000	6	-1.238598000	-0.183734000	3.869442000
1	3.895318000	-2.279531000	-2.426573000	1	-1.975497000	0.599133000	3.977009000
1	4.129457000	-2.759335000	-4.114753000	6	-1.608752000	-1.450991000	3.417330000
6	-2.535841000	0.586157000	-4.026762000	6	3.344479000	-1.486903000	4.198416000
1	-2.680488000	0.243172000	-2.996040000	1	3.388041000	-1.755436000	3.135355000
1	-2.951938000	-0.174875000	-4.698422000	1	3.144306000	-2.402318000	4.768059000
6	-0.362358000	-3.952251000	-3.035423000	6	-3.906087000	-0.820252000	3.177773000
1	-1.303709000	-4.160466000	-3.540826000	1	-3.607443000	0.036789000	2.569036000
1	0.354360000	-4.718223000	-3.327046000	1	-4.047114000	-0.488031000	4.212235000
6	-0.562417000	-3.996309000	-1.541792000	6	0.459314000	1.506221000	4.642452000
6	0.501192000	-4.302124000	-0.706936000	1	1.254621000	1.438218000	5.384155000
1	1.442320000	-4.549628000	-1.176934000	1	-0.402378000	1.974037000	5.117029000
6	0.385315000	-4.255452000	0.676076000	6	0.927283000	2.365352000	3.490962000
6	-0.832097000	-3.901515000	1.256382000	6	2.271316000	2.417397000	3.145478000
6	-1.914481000	-3.606182000	0.417960000	1	2.965065000	1.836749000	3.736176000
1	-2.872167000	-3.406156000	0.880748000	6	2.711681000	3.171804000	2.067422000
6	-1.791608000	-3.652876000	-0.973329000	6	1.804218000	3.928332000	1.330404000
6	2.693094000	-4.769731000	0.990750000	6	0.462923000	3.881397000	1.680127000
1	3.001464000	-3.905748000	0.389563000	1	-0.230311000	4.447122000	1.075531000
1	2.675841000	-5.646818000	0.333665000	6	0.014580000	3.096745000	2.733510000
6	-0.989567000	-3.818255000	2.756485000	6	4.917184000	2.277866000	2.195802000
1	-0.343551000	-4.555939000	3.229988000	1	4.506436000	1.267860000	2.068673000
1	-2.019345000	-4.050715000	3.022496000	1	5.064970000	2.444404000	3.270316000
6	-0.632696000	-2.442584000	3.270521000	6	-2.257435000	3.676484000	2.305761000
6	0.684131000	-2.138465000	3.599382000	1	-2.176971000	3.356999000	1.261867000
1	1.419453000	-2.920581000	3.480010000	1	-2.072686000	4.756476000	2.351259000

6	2.246187000	4.720278000	0.122278000	6	-3.621177000	3.350321000	2.864243000
1	1.646741000	5.626443000	0.048173000	1	-3.700800000	3.666312000	3.905202000
1	3.288733000	5.013521000	0.233929000	1	-4.392090000	3.858199000	2.283980000
6	2.084912000	3.898237000	-1.133957000	1	-3.812941000	2.278083000	2.810202000
6	3.107428000	3.062662000	-1.560898000	6	-2.274685000	5.606963000	-1.196279000
1	4.024363000	3.062837000	-0.988418000	1	-3.284265000	5.570336000	-1.606522000
6	2.951729000	2.236647000	-2.664641000	1	-2.328330000	5.343135000	-0.139322000
6	1.752974000	2.242488000	-3.374639000	1	-1.898617000	6.627278000	-1.282171000
6	0.734015000	3.083250000	-2.950689000	6	-3.211057000	1.917726000	-4.247668000
1	-0.197372000	3.060752000	-3.497715000	1	-3.041377000	2.269707000	-5.265916000
6	0.885271000	3.905388000	-1.842233000	1	-4.284291000	1.823287000	-4.083564000
6	5.117893000	1.281792000	-2.374899000	1	-2.823602000	2.660107000	-3.550065000
1	4.888577000	0.960624000	-1.350572000	6	4.643731000	-0.861613000	4.647752000
1	5.622352000	2.253804000	-2.312656000	1	4.854271000	0.042937000	4.076702000
6	-1.383258000	4.640897000	-1.939240000	1	4.597857000	-0.599630000	5.704979000
1	-1.742183000	3.614941000	-1.819587000	1	5.465978000	-1.563114000	4.499929000
1	-1.361038000	4.888896000	-3.007389000	6	3.644430000	-4.991227000	2.142317000
6	-4.069108000	-2.993110000	-1.309543000	1	3.673774000	-4.116046000	2.792659000
1	-4.513987000	-3.832022000	-0.761924000	1	3.336562000	-5.852399000	2.735676000
1	-3.946731000	-2.147194000	-0.629385000	1	4.651104000	-5.173227000	1.763918000
6	-5.165552000	-1.429946000	2.616313000	6	4.421845000	-4.356012000	-2.699277000
1	-5.457494000	-2.316218000	3.181141000	1	4.043437000	-4.678638000	-1.727865000
1	-5.977359000	-0.703354000	2.660976000	1	4.256273000	-5.159875000	-3.416949000
1	-5.011766000	-1.698961000	1.571003000	1	5.495839000	-4.185810000	-2.611504000
6	-4.930197000	-2.590302000	-2.481349000	6	6.006218000	0.273171000	-3.065611000
1	-5.045467000	-3.413778000	-3.186958000	1	6.941957000	0.158934000	-2.516341000
1	-5.917079000	-2.290918000	-2.127220000	1	5.515929000	-0.699882000	-3.119079000
1	-4.485937000	-1.740322000	-3.001174000	1	6.237647000	0.597428000	-4.080568000

6	6.228292000	2.419799000	1.458111000	6	-1.426454000	-4.831390000	1.542456000
1	6.090717000	2.234520000	0.391741000	6	-0.045520000	-4.964184000	1.582180000
1	6.632155000	3.424772000	1.583030000	6	5.797972000	-0.780258000	0.732307000
1	6.955680000	1.703619000	1.843658000	6	5.123799000	0.562256000	0.627450000
-----				6	4.628595000	1.189048000	1.760503000
EtP6 with one AgOCOCF₃				6	3.963493000	2.408247000	1.700807000
Sum of electronic and zero-point Energies= -4140.452649				6	3.793533000	3.048890000	0.471240000
Sum of electronic and thermal Energies= -4140.362407				6	4.283859000	2.411489000	-0.686217000
Sum of electronic and thermal Enthalpies= -4140.361463				6	4.948489000	1.175835000	-0.614793000
Sum of electronic and thermal Free Energies= -4140.587229				6	3.232890000	4.451171000	0.393904000
6	-6.028177000	0.618176000	0.265736000	6	-2.526464000	5.269953000	0.168521000
6	-5.073312000	1.787339000	0.254701000	6	-1.047041000	4.982422000	0.247225000
6	-4.602957000	2.294400000	-0.947121000	6	-0.324716000	4.714093000	-0.904461000
6	-3.749672000	3.388068000	-0.989292000	6	1.041652000	4.477876000	-0.862362000
6	-3.384939000	4.028545000	0.191968000	6	1.726499000	4.559130000	0.349031000
6	-3.834582000	3.506908000	1.397297000	6	0.997052000	4.792815000	1.507931000
6	-4.651427000	2.385588000	1.439955000	6	-0.377624000	4.979222000	1.470106000
6	-5.344314000	-0.727474000	0.271477000	8	-3.252026000	3.906338000	-2.149087000
6	-5.044521000	-1.356416000	1.471716000	6	-3.449826000	3.177421000	-3.342664000
6	-4.453263000	-2.611482000	1.502791000	8	-5.103429000	1.826617000	2.601162000
6	-4.177505000	-3.280482000	0.312561000	6	-4.571087000	2.283766000	3.821238000
6	-4.452167000	-2.639864000	-0.886855000	8	-5.298516000	-0.703616000	-2.073862000
6	-5.014195000	-1.371013000	-0.919121000	6	-4.876774000	-1.265010000	-3.298238000
6	-3.619686000	-4.683217000	0.319896000	8	-4.139910000	-3.268232000	2.659519000
6	0.678949000	-5.055047000	0.396470000	6	-4.292648000	-2.588041000	3.882122000
6	-0.002688000	-4.947720000	-0.807494000	8	-2.092494000	-4.678209000	-2.004110000
6	-1.381065000	-4.784139000	-0.847963000	6	-1.389149000	-4.620428000	-3.226184000
6	-2.111963000	-4.756578000	0.338424000	8	5.477762000	0.553956000	-1.688476000

6	5.092408000	0.966904000	-2.992249000	1	0.578049000	-5.003343000	-1.717386000
8	3.483976000	3.059399000	2.789607000	1	-2.010383000	-4.788491000	2.451020000
6	3.583403000	2.434763000	4.054310000	1	6.520680000	-0.888628000	-0.074720000
8	1.786638000	4.171687000	-1.968634000	1	6.339032000	-0.833910000	1.675586000
6	1.104021000	3.945902000	-3.192964000	1	4.763880000	0.678603000	2.703800000
8	-1.137785000	5.196587000	2.580246000	1	4.274312000	2.972591000	-1.612556000
6	-0.570014000	4.951458000	3.846205000	1	3.643867000	4.931896000	-0.494174000
8	0.670939000	-5.049881000	2.743732000	1	3.591089000	5.005650000	1.261330000
6	-0.006113000	-4.877463000	3.965716000	1	-2.723023000	5.821098000	-0.750721000
6	2.165893000	-5.315078000	0.413191000	1	-2.810409000	5.908795000	1.003648000
6	4.799868000	-1.911603000	0.657874000	1	-0.867716000	4.686864000	-1.837885000
6	4.371133000	-2.387974000	-0.573984000	1	1.537015000	4.832363000	2.443540000
6	3.472651000	-3.442024000	-0.668688000	1	-3.094650000	2.150460000	-3.209292000
6	3.029107000	-4.079235000	0.491245000	1	-4.518030000	3.139315000	-3.587736000
6	3.428549000	-3.576194000	1.720440000	1	-4.854685000	3.329615000	3.993680000
6	4.281767000	-2.484928000	1.814291000	1	-3.475363000	2.235537000	3.790095000
8	3.009993000	-3.929430000	-1.848306000	1	-3.801221000	-1.463207000	-3.261783000
6	3.333887000	-3.237475000	-3.040808000	1	-5.391831000	-2.217267000	-3.473761000
8	4.676646000	-1.933201000	3.002551000	1	-3.720813000	-1.651933000	3.861133000
6	4.044430000	-2.366426000	4.185298000	1	-5.346299000	-2.331378000	4.047289000
1	-6.667117000	0.688041000	1.145397000	1	-0.645164000	-3.819586000	-3.187285000
1	-6.669083000	0.686834000	-0.613033000	1	-0.861248000	-5.565798000	-3.401423000
1	-4.919796000	1.799378000	-1.853680000	1	3.999274000	0.985366000	-3.055862000
1	-3.526963000	4.006975000	2.305273000	1	5.478731000	1.971716000	-3.195306000
1	-5.291175000	-0.832845000	2.384876000	1	3.066779000	1.468329000	4.029509000
1	-4.208540000	-3.164034000	-1.799956000	1	4.635531000	2.249648000	4.299181000
1	-3.986280000	-5.204373000	-0.564227000	1	0.309391000	3.208980000	-3.035119000
1	-4.001677000	-5.210805000	1.193780000	1	0.646358000	4.880778000	-3.534568000

1	0.230307000	5.672275000	4.053439000	6	-5.112942000	1.401346000	4.921799000
1	-0.129578000	3.947120000	3.861064000	1	-6.202054000	1.446386000	4.949035000
1	-0.517020000	-3.906723000	3.973862000	1	-4.814468000	0.364146000	4.762112000
1	-0.768138000	-5.655833000	4.093084000	1	-4.728180000	1.727819000	5.889174000
1	2.428107000	-5.866938000	-0.489126000	6	-3.792198000	-3.495167000	4.982178000
1	2.401481000	-5.951276000	1.266546000	1	-3.898218000	-3.004701000	5.951000000
1	4.762248000	-1.913803000	-1.462847000	1	-4.360486000	-4.425647000	5.000795000
1	3.050564000	-4.066855000	2.606300000	1	-2.739380000	-3.737177000	4.830035000
1	3.054845000	-2.182650000	-2.951050000	6	1.015130000	-4.952991000	5.076858000
1	4.414825000	-3.299510000	-3.220469000	1	0.526639000	-4.829589000	6.044551000
1	4.281836000	-3.418832000	4.381075000	1	1.523942000	-5.917422000	5.066085000
1	2.956361000	-2.285268000	4.074432000	1	1.763434000	-4.167045000	4.965063000
8	1.779429000	-0.143672000	-3.319768000	6	4.533814000	-1.494857000	5.318282000
6	0.681350000	0.009550000	-2.799779000	1	4.277824000	-0.449325000	5.137359000
47	2.180519000	1.486563000	-0.940812000	1	4.071707000	-1.804983000	6.256523000
8	0.379386000	0.653581000	-1.759932000	1	5.616378000	-1.571715000	5.423622000
6	-0.557205000	-0.625970000	-3.492138000	6	2.571728000	-3.882987000	-4.172348000
9	-1.307442000	0.332419000	-4.067011000	1	2.834242000	-4.937407000	-4.269221000
9	-0.218757000	-1.487240000	-4.452593000	1	1.498247000	-3.800972000	-4.002408000
9	-1.332699000	-1.277204000	-2.623888000	1	2.803096000	-3.375003000	-5.109162000
6	2.954766000	3.353844000	5.073642000	6	5.649425000	-0.031349000	-3.975987000
1	1.904309000	3.526372000	4.838545000	1	5.232203000	-1.021059000	-3.789045000
1	3.017706000	2.906853000	6.066496000	1	5.378596000	0.264900000	-4.989788000
1	3.468917000	4.315187000	5.093845000	6	-5.196403000	-0.279039000	-4.396638000
6	-1.667441000	5.069812000	4.877642000	1	-4.894978000	-0.687470000	-5.362241000
1	-2.111563000	6.065239000	4.853588000	1	-6.265608000	-0.066017000	-4.427198000
1	-2.452450000	4.336582000	4.687435000	1	-4.658862000	0.656527000	-4.238772000
1	-1.264012000	4.894463000	5.876007000	6	-2.683202000	3.866893000	-4.445800000

1	-1.616224000	3.881421000	-4.221469000	6	-2.654535000	4.320510000	-0.272708000
1	-2.825881000	3.332664000	-5.386027000	6	-3.198513000	4.021896000	0.968347000
1	-3.026462000	4.894239000	-4.573201000	6	-4.194056000	3.065815000	1.110983000
6	2.103822000	3.432501000	-4.200067000	6	-1.629846000	5.419893000	-0.414594000
1	2.485076000	2.455344000	-3.900522000	6	2.542005000	4.309972000	-0.298033000
1	1.620092000	3.314855000	-5.170437000	6	1.837951000	4.557628000	0.873844000
1	2.936711000	4.128510000	-4.310223000	6	0.486042000	4.871563000	0.857110000
6	-2.388707000	-4.353776000	-4.325652000	6	-0.190439000	4.967902000	-0.358470000
1	-2.889926000	-3.399866000	-4.158892000	6	0.503960000	4.688480000	-1.524633000
1	-1.878669000	-4.307956000	-5.288645000	6	1.851844000	4.354996000	-1.506249000
1	-3.141302000	-5.142252000	-4.365578000	6	5.674409000	-1.542679000	0.082636000
1	6.736201000	-0.086560000	-3.905691000	6	4.577004000	-2.550159000	0.306655000
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P6Q1 with one AgOCOCF₃				6	3.297037000	-4.485245000	-0.422294000
Sum of electronic and zero-point Energies= -3982.098896				6	2.479187000	-4.416487000	0.696435000
Sum of electronic and thermal Energies= -3982.015577				6	2.699419000	-3.373013000	1.627902000
Sum of electronic and thermal Enthalpies= -3982.014633				6	3.762844000	-2.471783000	1.451095000
Sum of electronic and thermal Free Energies= -3982.225438				6	1.458339000	-5.495225000	0.973798000
6	-5.823387000	1.415300000	0.105338000	6	-4.280198000	-4.105953000	1.092230000
6	-5.365142000	-0.003269000	0.342330000	6	-2.802262000	-4.366367000	1.095508000
6	-5.118721000	-0.449537000	1.632127000	6	-2.030827000	-4.218071000	2.174443000
6	-4.722625000	-1.755176000	1.881572000	6	-0.589800000	-4.505361000	2.169635000
6	-4.615308000	-2.657027000	0.826858000	6	0.019571000	-5.060418000	0.923645000
6	-4.836709000	-2.208729000	-0.467460000	6	-0.735637000	-5.165671000	-0.169171000
6	-5.185843000	-0.888386000	-0.720674000	6	-2.176336000	-4.830047000	-0.182972000
6	-4.690213000	2.406042000	-0.010615000	8	-4.445957000	-2.237150000	3.129076000
6	-4.127841000	2.684738000	-1.247695000	6	-4.439900000	-1.332771000	4.211859000
6	-3.108225000	3.616329000	-1.386329000	8	-5.389753000	-0.389521000	-1.967767000

6	-5.128013000	-1.216194000	-3.084337000	1	-4.506846000	2.142585000	-2.102612000
8	-4.757851000	2.739488000	2.313177000	1	-2.821664000	4.566053000	1.822836000
6	-4.198124000	3.278694000	3.487089000	1	-1.798038000	6.150030000	0.377220000
8	-2.520934000	3.918784000	-2.578037000	1	-1.790842000	5.926837000	-1.366117000
6	-2.921424000	3.207555000	-3.729524000	1	2.383714000	4.514727000	1.807014000
8	-0.244353000	5.133407000	1.978533000	1	-0.041181000	4.747320000	-2.455954000
8	4.098366000	-1.542588000	2.360203000	1	6.412504000	-1.631344000	0.882916000
6	3.158883000	-1.158506000	3.350276000	1	6.179794000	-1.798546000	-0.850910000
8	3.103649000	-5.468766000	-1.347624000	1	4.926947000	-3.629159000	-1.494533000
6	2.344741000	-5.052143000	-2.487572000	1	2.158780000	-3.410836000	2.565360000
8	0.088150000	-4.307959000	3.160794000	1	1.658480000	-5.900861000	1.967419000
8	-2.833976000	-4.984382000	-1.186161000	1	1.608135000	-6.290340000	0.246836000
8	2.572554000	4.091179000	-2.635812000	1	-4.688240000	-4.398621000	2.058850000
6	4.025857000	4.040692000	-0.241977000	1	-4.739294000	-4.722315000	0.320607000
6	5.205665000	-0.108440000	0.024185000	1	-2.442930000	-3.875048000	3.115281000
6	5.669858000	0.821419000	0.942072000	1	-0.343494000	-5.537560000	-1.107908000
6	5.277419000	2.152981000	0.895162000	1	-3.760559000	-0.499870000	3.994551000
6	4.406668000	2.583285000	-0.105785000	1	-5.443334000	-0.915929000	4.359831000
6	3.929217000	1.647685000	-1.011891000	1	-5.869044000	-2.023139000	-3.131497000
6	4.312079000	0.315486000	-0.956557000	1	-4.138085000	-1.670525000	-2.991370000
8	5.699964000	3.089917000	1.793182000	1	-3.129030000	3.036980000	3.532446000
6	6.619404000	2.709507000	2.791577000	1	-4.292992000	4.371275000	3.488920000
8	3.871642000	-0.630436000	-1.829908000	1	-2.806352000	2.132556000	-3.561348000
6	2.966652000	-0.233246000	-2.846550000	1	-3.978615000	3.405811000	-3.944150000
1	-6.412246000	1.450518000	-0.810080000	1	2.186478000	-0.978706000	2.872614000
1	-6.473459000	1.712043000	0.928182000	1	3.030345000	-1.963381000	4.080858000
1	-5.241632000	0.260655000	2.437303000	1	1.485011000	-4.457792000	-2.157841000
1	-4.729238000	-2.920463000	-1.274379000	1	2.967826000	-4.408716000	-3.117501000

1	4.449905000	4.594815000	0.592444000	6	2.568239000	-1.466144000	-3.617938000
1	4.489926000	4.428699000	-1.151069000	1	2.069696000	-2.181543000	-2.964143000
1	6.340638000	0.475421000	1.715906000	1	1.871308000	-1.197254000	-4.412720000
1	3.256789000	1.994187000	-1.781574000	1	3.440718000	-1.943974000	-4.066648000
1	6.193150000	1.912337000	3.412998000	6	6.922958000	3.928283000	3.630771000
1	7.534753000	2.320155000	2.329801000	1	7.353058000	4.719754000	3.016569000
1	3.453018000	0.498245000	-3.501961000	1	6.013995000	4.309033000	4.097814000
1	2.087304000	0.235630000	-2.396892000	1	7.635383000	3.672669000	4.416399000
9	-1.662323000	-1.197647000	-3.787540000	6	3.669603000	0.102126000	4.004020000
9	-0.453392000	0.500848000	-3.257621000	1	3.769545000	0.897538000	3.264919000
9	-2.235668000	0.045614000	-2.123643000	1	2.972428000	0.424680000	4.778180000
8	0.214252000	-0.692436000	-0.884663000	6	-4.931374000	2.684302000	4.667004000
8	-0.330278000	-2.587477000	-1.950705000	1	-4.529753000	3.085409000	5.598731000
6	-0.359704000	-1.379133000	-1.777205000	1	-5.994575000	2.921141000	4.617649000
6	-1.192040000	-0.501591000	-2.753335000	1	-4.820510000	1.599091000	4.682379000
47	1.399634000	-1.979941000	0.321059000	6	-3.988218000	-2.082881000	5.442649000
6	1.901960000	-6.280365000	-3.241279000	1	-2.977895000	-2.472235000	5.309367000
1	1.269458000	-6.911886000	-2.615179000	1	-3.988192000	-1.416145000	6.306165000
1	1.328766000	-5.985387000	-4.120863000	1	-4.657540000	-2.917975000	5.651770000
1	2.761506000	-6.868454000	-3.564516000	1	4.642173000	-0.071961000	4.466123000
6	-5.192765000	-0.349717000	-4.319176000	6	0.377576000	5.024809000	3.237342000
1	-6.172624000	0.119882000	-4.414075000	1	0.787192000	4.015786000	3.367490000
1	-4.433473000	0.432103000	-4.270498000	1	1.209063000	5.736125000	3.311541000
1	-5.007187000	-0.953484000	-5.208275000	6	1.874062000	3.883267000	-3.845255000
6	-2.049685000	3.658784000	-4.877128000	1	1.360018000	4.801743000	-4.151492000
1	-2.338725000	3.139675000	-5.791972000	1	1.114671000	3.105872000	-3.700473000
1	-2.149562000	4.732603000	-5.040516000	6	2.877625000	3.468643000	-4.894840000
1	-1.003052000	3.432837000	-4.670456000	1	3.390946000	2.553788000	-4.596649000

1	2.370953000	3.288198000	-5.843944000	6	-0.250886000	5.059486000	0.973227000
1	3.625113000	4.248588000	-5.042512000	6	-1.018147000	5.164740000	-0.305633000
6	-0.664586000	5.316670000	4.291853000	6	-0.360377000	5.053259000	-1.460310000
1	-1.484719000	4.600352000	4.227726000	6	1.097906000	4.865536000	-1.535062000
1	-0.222295000	5.248088000	5.286722000	6	5.851283000	-0.440687000	-0.251227000
1	-1.071762000	6.319887000	4.161854000	6	4.935772000	-1.611048000	-0.003437000
-----				6	4.770547000	-2.612704000	-0.935266000
P6Q2 with one AgOCOCF₃				6	3.912591000	-3.693643000	-0.731429000
Sum of electronic and zero-point Energies= -3823.752236				6	3.183099000	-3.792060000	0.443647000
Sum of electronic and thermal Energies= -3823.674025				6	3.316079000	-2.764941000	1.408586000
Sum of electronic and thermal Enthalpies= -3823.673081				6	4.214893000	-1.704794000	1.202440000
Sum of electronic and thermal Free Energies= -3823.875602				6	2.347343000	-5.015991000	0.734601000
6	-5.951990000	0.767873000	0.342773000	6	-3.519671000	-4.460229000	1.100824000
6	-5.259811000	-0.561938000	0.519683000	6	-2.020704000	-4.500415000	1.041121000
6	-4.895564000	-0.996052000	1.785565000	6	-1.235237000	-4.265247000	2.094218000
6	-4.286592000	-2.227198000	1.979269000	6	0.230490000	-4.347537000	2.029108000
6	-4.080281000	-3.072994000	0.893102000	6	0.860593000	-4.789977000	0.748772000
6	-4.418097000	-2.631377000	-0.378020000	6	0.084703000	-4.977425000	-0.317838000
6	-4.980972000	-1.377374000	-0.576790000	6	-1.387369000	-4.841477000	-0.271802000
6	-5.001056000	1.933155000	0.215291000	8	-3.887172000	-2.690417000	3.199857000
6	-4.539388000	2.324733000	-1.032082000	6	-3.980796000	-1.824389000	4.310409000
6	-3.689094000	3.412076000	-1.179491000	8	-5.307146000	-0.883768000	-1.799956000
6	-3.321102000	4.156892000	-0.061440000	6	-4.945197000	-1.621000000	-2.950947000
6	-3.759375000	3.750906000	1.190766000	8	-5.027900000	2.193284000	2.547428000
6	-4.577338000	2.640181000	1.339828000	6	-4.569226000	2.829434000	3.720014000
6	-2.496462000	5.412901000	-0.218411000	8	-3.195087000	3.830974000	-2.376010000
6	1.882279000	4.872076000	-0.259296000	6	-3.463653000	3.058418000	-3.529792000
6	1.219236000	4.934826000	0.895676000	8	-0.807661000	5.116848000	2.049202000

8	4.484639000	-0.775308000	2.133548000	1	6.634253000	-0.429873000	0.510029000
6	3.604639000	-0.611865000	3.233950000	1	6.339985000	-0.593270000	-1.215337000
8	3.802322000	-4.665479000	-1.681709000	1	5.305323000	-2.553534000	-1.875124000
6	2.941681000	-4.322577000	-2.772860000	1	2.856472000	-2.920477000	2.376357000
8	0.913962000	-4.075796000	2.998631000	1	2.644500000	-5.407046000	1.709357000
8	-2.055745000	-5.058045000	-1.256297000	1	2.579702000	-5.765445000	-0.018810000
8	1.651228000	4.733512000	-2.607248000	1	-3.839299000	-4.834639000	2.072507000
6	3.382257000	4.833373000	-0.351010000	1	-3.914131000	-5.119218000	0.328604000
6	5.163285000	0.903741000	-0.246562000	1	-1.653564000	-4.004040000	3.058404000
6	5.478116000	1.851740000	0.715037000	1	0.487657000	-5.273790000	-1.278719000
6	4.884515000	3.107172000	0.724732000	1	-3.455096000	-0.886915000	4.093761000
6	3.973305000	3.443420000	-0.275132000	1	-5.031098000	-1.580664000	4.510003000
6	3.647842000	2.492119000	-1.230494000	1	-5.539503000	-2.540857000	-3.005583000
6	4.216257000	1.225990000	-1.217289000	1	-3.889803000	-1.901746000	-2.899590000
8	5.144701000	4.054369000	1.670880000	1	-3.473524000	2.824203000	3.744884000
6	6.165166000	3.811469000	2.615494000	1	-4.898784000	3.874984000	3.735458000
8	3.917814000	0.260377000	-2.123351000	1	-3.185388000	2.016404000	-3.348843000
6	2.891825000	0.526209000	-3.069236000	1	-4.536018000	3.089419000	-3.757007000
1	-6.574975000	0.727768000	-0.549610000	1	2.571078000	-0.570216000	2.865694000
1	-6.607075000	0.935106000	1.197409000	1	3.685719000	-1.468323000	3.910512000
1	-5.099647000	-0.336967000	2.617237000	1	2.028785000	-3.856458000	-2.385136000
1	-4.230353000	-3.295486000	-1.210413000	1	3.443821000	-3.586938000	-3.409407000
1	-4.857114000	1.746894000	-1.888467000	1	3.795850000	5.439570000	0.451301000
1	-3.440317000	4.327761000	2.047212000	1	3.677776000	5.282296000	-1.300862000
1	-2.686755000	6.063558000	0.635060000	1	6.192991000	1.579416000	1.478612000
1	-2.810077000	5.934220000	-1.122645000	1	2.953634000	2.773799000	-2.008350000
1	1.735907000	4.931190000	1.849038000	1	5.919423000	2.928442000	3.216953000
1	-0.878020000	5.102051000	-2.410006000	1	7.111101000	3.612357000	2.098132000

1	3.214401000	1.324211000	-3.746751000	1	5.341900000	5.225012000	4.013649000
1	1.991517000	0.860406000	-2.547110000	1	7.063226000	4.881085000	4.241874000
9	-1.530741000	-0.960009000	-3.656964000	6	3.971703000	0.675320000	3.930081000
9	-0.640370000	0.896899000	-3.036508000	1	3.857882000	1.519260000	3.249158000
9	-2.270199000	0.047726000	-1.900798000	1	3.319987000	0.828700000	4.790727000
8	0.365335000	-0.285995000	-0.804341000	6	-5.135421000	2.077562000	4.901961000
8	0.026912000	-2.212438000	-1.895498000	1	-4.811252000	2.544575000	5.832904000
6	-0.159004000	-1.022848000	-1.687400000	1	-6.225511000	2.079813000	4.873761000
6	-1.163470000	-0.253374000	-2.588310000	1	-4.792398000	1.041739000	4.898273000
47	1.764285000	-1.480110000	0.269891000	6	-3.361079000	-2.522030000	5.498098000
6	2.628294000	-5.578766000	-3.545232000	1	-2.307902000	-2.738299000	5.313366000
1	2.115359000	-6.305261000	-2.912737000	1	-3.430979000	-1.886003000	6.381673000
1	1.979768000	-5.339901000	-4.388766000	1	-3.877160000	-3.459827000	5.706316000
1	3.541242000	-6.038614000	-3.924929000	1	5.004234000	0.641888000	4.280197000
6	-5.197166000	-0.743571000	-4.153615000	-----			
1	-6.244812000	-0.444406000	-4.204159000	P6Q3 with one AgOCOCF₃			
1	-4.579395000	0.154179000	-4.102192000	Sum of electronic and zero-point Energies= -3665.409885			
1	-4.943597000	-1.282114000	-5.067453000	Sum of electronic and thermal Energies= -3665.338006			
6	-2.653882000	3.630568000	-4.668377000	Sum of electronic and thermal Enthalpies= -3665.337062			
1	-2.851530000	3.069239000	-5.582625000	Sum of electronic and thermal Free Energies= -3665.524423			
1	-2.913606000	4.675692000	-4.842137000	6	0.216617000	4.756059000	-0.996218000
1	-1.587384000	3.565151000	-4.450271000	6	1.564966000	4.229609000	-0.605187000
6	2.616917000	-0.749393000	-3.824427000	6	2.255716000	3.362487000	-1.435455000
1	2.262163000	-1.525065000	-3.146038000	6	3.508819000	2.870910000	-1.085287000
1	1.841244000	-0.576645000	-4.571477000	6	4.076699000	3.241330000	0.133875000
1	3.515511000	-1.103420000	-4.332529000	6	3.382372000	4.105764000	0.969477000
6	6.282157000	5.033076000	3.495731000	6	2.144094000	4.611105000	0.607416000
1	6.536222000	5.911756000	2.902387000	6	-0.938941000	4.228736000	-0.195923000

6	-0.857450000	3.351535000	0.803442000	6	3.700301000	1.579888000	-3.096278000
6	-2.034779000	2.923419000	1.582818000	8	1.425636000	5.473768000	1.366631000
6	-3.382724000	3.400452000	1.144753000	6	1.794871000	5.663961000	2.718974000
6	-3.461113000	4.285863000	0.152659000	8	-2.395266000	5.555071000	-1.495709000
6	-2.278900000	4.762469000	-0.584337000	8	-1.906756000	2.240965000	2.576839000
6	-4.584355000	2.835274000	1.843141000	8	-5.808171000	2.401688000	-0.598613000
6	-5.399801000	-1.127457000	0.357950000	6	-6.139766000	2.290076000	-1.970799000
6	-5.755113000	-0.007631000	-0.378850000	8	1.511794000	-3.340109000	-2.863295000
6	-5.498823000	1.272572000	0.089207000	6	2.437208000	-2.473000000	-3.501387000
6	-4.889171000	1.446585000	1.331813000	8	1.908198000	-4.288925000	2.541746000
6	-4.528042000	0.327894000	2.064461000	6	0.797742000	-4.836406000	3.232683000
6	-4.769065000	-0.953244000	1.588003000	8	5.878324000	-1.997842000	-0.587848000
6	-0.496889000	-4.907550000	-1.727706000	8	4.204845000	1.557799000	2.913044000
6	0.651611000	-4.337672000	-0.922157000	8	-4.427307000	-2.082164000	2.267538000
6	0.742156000	-4.574851000	0.440450000	6	-3.451494000	-1.979450000	3.288145000
6	1.809332000	-4.110754000	1.198985000	6	-5.670465000	-2.514146000	-0.177623000
6	2.858015000	-3.447752000	0.564981000	6	-1.829156000	-4.290082000	-1.406866000
6	2.768126000	-3.199745000	-0.805695000	6	-2.378208000	-3.309976000	-2.125590000
6	1.659772000	-3.599054000	-1.546509000	6	-3.711992000	-2.744659000	-1.821682000
6	4.081599000	-3.021778000	1.347332000	6	-4.403246000	-3.206964000	-0.579409000
6	5.409677000	2.670648000	0.563079000	6	-3.867819000	-4.208021000	0.117652000
6	5.246022000	1.204668000	0.815245000	6	-2.589283000	-4.836680000	-0.240396000
6	5.721957000	0.263534000	-0.001824000	8	-4.239001000	-1.960161000	-2.578340000
6	5.391111000	-1.158267000	0.135687000	8	-2.162628000	-5.773102000	0.407016000
6	4.389995000	-1.556291000	1.194392000	1	0.198902000	5.845831000	-0.910725000
6	3.935255000	-0.604656000	2.050458000	1	0.021937000	4.543529000	-2.048936000
6	4.430894000	0.799893000	2.000572000	1	1.793785000	3.065775000	-2.366376000
8	4.242445000	2.038287000	-1.865937000	1	3.828501000	4.369452000	1.917812000

1	0.084512000	2.923525000	1.122747000	1	-6.325658000	-2.434967000	-1.045509000
1	-4.412604000	4.675743000	-0.185311000	1	-6.174138000	-3.116548000	0.579307000
1	-5.437449000	3.491870000	1.673525000	1	-1.884349000	-2.895055000	-2.996090000
1	-4.388723000	2.786081000	2.914061000	1	-4.342865000	-4.594020000	1.010699000
1	-6.213476000	-0.158518000	-1.345534000	8	0.146559000	0.195418000	0.198794000
1	-4.026482000	0.479265000	3.009560000	6	0.209387000	0.251919000	-1.041548000
1	-0.290522000	-4.770359000	-2.786039000	47	2.293150000	-0.616122000	0.330321000
1	-0.557287000	-5.978640000	-1.527084000	8	1.201635000	-0.030133000	-1.737879000
1	-0.044512000	-5.154099000	0.900357000	6	-1.049045000	0.713193000	-1.819111000
1	3.610920000	-2.740884000	-1.304220000	9	-1.359118000	-0.169754000	-2.772269000
1	4.946616000	-3.589002000	1.000891000	9	-2.113010000	0.863146000	-1.040325000
1	3.923409000	-3.244303000	2.399799000	9	-0.812304000	1.888489000	-2.422801000
1	6.162847000	2.820210000	-0.210953000	6	1.095196000	-4.778159000	4.711145000
1	5.738700000	3.170880000	1.473738000	1	1.239563000	-3.747192000	5.036303000
1	6.332087000	0.517405000	-0.858724000	1	0.261270000	-5.203246000	5.271062000
1	3.355892000	-0.864255000	2.930588000	1	1.994587000	-5.347341000	4.947943000
1	2.714622000	1.140353000	-2.926528000	6	0.699739000	6.461064000	3.386086000
1	3.596748000	2.425084000	-3.786020000	1	0.569460000	7.424368000	2.892205000
1	2.751684000	6.196308000	2.774855000	1	-0.245058000	5.918484000	3.344508000
1	1.919335000	4.690272000	3.206032000	1	0.953023000	6.638645000	4.432091000
1	-5.394243000	1.669282000	-2.478835000	6	-3.007582000	-3.377805000	3.650135000
1	-7.116481000	1.804398000	-2.079732000	1	-2.268988000	-3.335275000	4.452536000
1	2.541905000	-1.559056000	-2.911507000	1	-3.852359000	-3.976567000	3.992917000
1	3.413862000	-2.965769000	-3.573462000	1	-2.559007000	-3.878145000	2.790530000
1	-0.103433000	-4.261313000	2.994930000	6	1.889678000	-2.147145000	-4.868900000
1	0.631264000	-5.869748000	2.910859000	1	0.941603000	-1.616983000	-4.777778000
1	-2.606798000	-1.381449000	2.929935000	1	2.592650000	-1.507698000	-5.404502000
1	-3.874844000	-1.474115000	4.163606000	6	4.652106000	0.546486000	-3.650047000

1	4.735593000	-0.305724000	-2.972831000	47	-1.475835000	-0.176842000	-0.192159000
1	4.285026000	0.183363000	-4.610734000	8	2.164538000	4.173906000	-1.952628000
1	5.647057000	0.967875000	-3.799629000	8	-1.017074000	0.209429000	-4.067471000
6	-6.169011000	3.681724000	-2.556939000	8	4.816269000	1.597571000	1.789403000
1	-5.186759000	4.151451000	-2.494323000	8	3.688183000	-0.882850000	-2.997275000
1	-6.459947000	3.634532000	-3.607193000	8	0.688728000	0.035940000	4.457206000
1	-6.889821000	4.307096000	-2.028476000	8	3.321124000	-3.568103000	1.234465000
1	1.735008000	-3.054015000	-5.454556000	8	-3.979111000	1.197324000	3.163120000
-----				8	-1.816342000	-3.673460000	1.776740000
MeP5 with two AgOCOCF₃				8	-2.993223000	3.857927000	-0.936503000
Sum of electronic and zero-point Energies= -3843.072873				8	-4.759884000	-1.328219000	-1.487915000
Sum of electronic and thermal Energies= -3843.001856				6	-2.312506000	2.558285000	-3.302500000
Sum of electronic and thermal Enthalpies= -3843.000912				1	-2.607129000	2.151213000	-4.270616000
Sum of electronic and thermal Free Energies= -3843.183185				1	-2.514326000	3.628455000	-3.318823000
9	-0.111426000	4.380197000	0.872660000	6	-0.825332000	2.351278000	-3.120519000
9	-0.535997000	3.544452000	2.815697000	6	-0.030251000	3.347689000	-2.572326000
9	1.498551000	3.751206000	2.154214000	1	-0.520388000	4.244730000	-2.220167000
9	-1.527192000	-4.226518000	-2.783822000	6	1.351319000	3.214335000	-2.480470000
9	-0.087574000	-5.058583000	-1.413321000	6	1.969265000	2.062727000	-2.960572000
9	0.574806000	-4.083906000	-3.222038000	6	1.171047000	1.046752000	-3.470949000
8	1.254327000	1.464116000	0.898280000	1	1.667272000	0.159373000	-3.834862000
8	0.919325000	-2.387006000	-1.115787000	6	-0.207682000	1.174346000	-3.547278000
8	-1.305863000	-2.084996000	-1.294865000	6	1.653131000	5.478701000	-1.819445000
6	0.173326000	2.032625000	1.103719000	1	0.884602000	5.538804000	-1.045936000
6	0.267834000	3.443860000	1.749873000	1	1.240135000	5.839648000	-2.766872000
6	-0.234828000	-2.684102000	-1.465541000	6	-0.420594000	-0.976150000	-4.528328000
6	-0.329006000	-4.031875000	-2.239317000	1	0.198740000	-1.441457000	-3.756950000
47	1.443086000	-0.494377000	-0.083661000	1	0.200239000	-0.795717000	-5.412025000

6	3.472783000	1.902602000	-2.942454000	6	2.658955000	-4.735748000	0.810139000
1	3.786843000	1.408558000	-3.861536000	1	1.743793000	-4.493903000	0.266210000
1	3.939801000	2.885150000	-2.911783000	1	2.423635000	-5.391993000	1.654175000
6	3.924786000	1.097536000	-1.751137000	6	-0.637430000	-2.355610000	3.936343000
6	4.241625000	1.731666000	-0.560586000	1	-0.680955000	-1.978328000	4.958324000
1	4.192182000	2.811004000	-0.541895000	1	-0.748282000	-3.438863000	3.980417000
6	4.538470000	1.015132000	0.592663000	6	-1.798865000	-1.777411000	3.165119000
6	4.514232000	-0.376784000	0.563836000	6	-2.340125000	-0.550447000	3.522547000
6	4.230599000	-1.017770000	-0.640468000	1	-1.872480000	-0.018727000	4.337794000
1	4.225037000	-2.098435000	-0.643841000	6	-3.430727000	-0.009697000	2.855211000
6	3.951440000	-0.299156000	-1.797615000	6	-4.018143000	-0.714000000	1.805922000
6	4.858040000	3.003182000	1.847617000	6	-3.476362000	-1.942761000	1.444661000
1	3.894918000	3.442195000	1.578661000	1	-3.932887000	-2.467124000	0.617994000
1	5.637418000	3.405421000	1.192201000	6	-2.375254000	-2.475925000	2.104277000
6	4.669264000	-1.195019000	1.822796000	6	-3.365982000	1.965225000	4.169118000
1	5.241396000	-0.635504000	2.560306000	1	-2.321109000	2.174218000	3.927227000
1	5.209028000	-2.113721000	1.599231000	1	-3.421886000	1.468718000	5.143452000
6	3.305846000	-1.524637000	2.385724000	6	-2.498522000	-4.486981000	0.850402000
6	2.651356000	-0.606087000	3.195741000	1	-2.567277000	-4.008469000	-0.130079000
1	3.166280000	0.316947000	3.419688000	1	-3.505663000	-4.729349000	1.204557000
6	1.370895000	-0.843539000	3.672576000	6	-5.151548000	-0.120603000	0.999951000
6	0.721860000	-2.038132000	3.360056000	1	-5.814971000	-0.914681000	0.661494000
6	1.369728000	-2.949466000	2.537579000	1	-5.727253000	0.566180000	1.617552000
1	0.846883000	-3.861790000	2.288698000	6	-4.572897000	0.617321000	-0.183235000
6	2.646611000	-2.705515000	2.043860000	6	-4.163090000	1.936083000	-0.047063000
6	1.321560000	1.244855000	4.799395000	1	-4.354670000	2.421440000	0.898141000
1	1.608972000	1.814015000	3.911555000	6	-3.452480000	2.584263000	-1.048285000
1	2.210783000	1.070407000	5.414044000	6	-3.149448000	1.908497000	-2.229001000

6	-3.604478000	0.604398000	-2.386609000	Sum of electronic and thermal Free Energies= -4236.143694			
1	-3.362351000	0.096909000	-3.307661000	9	4.263834000	0.505087000	-0.958404000
6	-4.310893000	-0.047414000	-1.383146000	9	4.197839000	1.540619000	0.929962000
6	-3.232492000	4.537407000	0.272372000	9	4.447186000	-0.590288000	0.885016000
1	-2.795859000	4.002782000	1.119915000	9	-5.210988000	0.574830000	-0.913148000
1	-4.304677000	4.679875000	0.443585000	9	-5.172030000	-0.949181000	0.604429000
6	-4.408505000	-2.062202000	-2.638469000	9	-4.845318000	-1.475860000	-1.459975000
1	-3.323134000	-2.134124000	-2.741972000	8	1.872225000	-0.916844000	0.349697000
1	-4.841902000	-1.620550000	-3.541524000	8	-2.449743000	-1.405587000	-0.118449000
8	-0.992107000	1.675481000	0.869267000	8	-2.658103000	0.819905000	-0.386963000
6	3.692020000	-2.292029000	-3.067560000	6	2.267944000	0.255198000	0.286981000
1	4.678201000	-2.697917000	-2.820942000	6	3.814232000	0.427016000	0.300504000
1	2.937241000	-2.724667000	-2.406290000	6	-3.065772000	-0.348660000	-0.329356000
1	-4.821881000	-3.058910000	-2.498334000	6	-4.598019000	-0.543429000	-0.535168000
1	-1.916496000	-5.401271000	0.761886000	47	-0.246405000	-1.510388000	0.184313000
1	-1.234109000	-1.649812000	-4.789530000	47	-0.538420000	1.401991000	-0.083140000
1	3.452243000	-2.541966000	-4.098879000	8	3.311621000	-1.764068000	-3.298786000
1	3.348078000	-5.249625000	0.143086000	8	-1.681317000	0.444044000	-3.998988000
1	2.493678000	6.106924000	-1.530815000	8	2.920902000	-4.185355000	1.276781000
1	-2.752839000	5.508738000	0.176113000	8	-1.348236000	-4.172852000	-2.197111000
1	-3.918454000	2.901550000	4.216162000	8	1.979537000	-0.154496000	4.221822000
1	0.595901000	1.817825000	5.372804000	8	-2.176068000	-3.431064000	2.714086000
1	5.093961000	3.256774000	2.879036000	8	1.670724000	4.450743000	2.113772000
-----				8	-2.868401000	1.538856000	3.205063000
EtP5 with two AgOCOCF₃				8	2.502544000	3.302548000	-2.721440000
Sum of electronic and zero-point Energies= -4236.016655				8	-2.644456000	4.257065000	-1.022504000
Sum of electronic and thermal Energies= -4235.931715				6	0.476610000	2.179921000	-4.245884000
Sum of electronic and thermal Enthalpies= -4235.930771				1	-0.348236000	2.289045000	-4.950213000

1	1.381827000	2.536205000	-4.735752000	1	4.561674000	-4.650322000	0.117994000
6	0.648568000	0.714266000	-3.915737000	6	0.393670000	-4.466787000	2.414625000
6	1.910007000	0.166306000	-3.734484000	1	1.274218000	-4.896071000	2.889219000
1	2.759455000	0.832692000	-3.789140000	1	-0.452997000	-5.121324000	2.615615000
6	2.089310000	-1.192257000	-3.495801000	6	0.128178000	-3.097932000	2.999570000
6	0.985646000	-2.040299000	-3.456208000	6	1.185897000	-2.281022000	3.377013000
6	-0.281194000	-1.486996000	-3.598806000	1	2.185718000	-2.669130000	3.247936000
1	-1.125884000	-2.158418000	-3.555191000	6	0.973261000	-1.000106000	3.866650000
6	-0.459340000	-0.129251000	-3.820126000	6	-0.327136000	-0.522198000	4.024417000
6	4.460730000	-1.089136000	-3.769503000	6	-1.384446000	-1.334547000	3.639754000
1	4.586034000	-0.135749000	-3.250310000	1	-2.384877000	-0.945278000	3.760054000
1	4.348180000	-0.877624000	-4.839393000	6	-1.172412000	-2.605738000	3.117604000
6	-2.819748000	-0.388315000	-3.974662000	6	3.311525000	-0.610203000	4.109381000
1	-2.870189000	-0.922007000	-3.019346000	1	3.505013000	-0.944910000	3.086281000
1	-2.748171000	-1.142176000	-4.768111000	1	3.469976000	-1.464886000	4.778307000
6	1.141752000	-3.533100000	-3.269136000	6	-3.499176000	-2.934115000	2.718618000
1	0.407766000	-4.046022000	-3.889817000	1	-3.531660000	-1.974764000	2.197112000
1	2.134028000	-3.834830000	-3.599558000	1	-3.833651000	-2.777301000	3.751215000
6	0.955661000	-3.926505000	-1.826179000	6	-0.584483000	0.841791000	4.619978000
6	2.043442000	-3.967445000	-0.969128000	1	0.185033000	1.055856000	5.361069000
1	3.017564000	-3.761919000	-1.388927000	1	-1.544860000	0.820512000	5.134765000
6	1.888936000	-4.185463000	0.394419000	6	-0.596433000	1.954707000	3.600702000
6	0.613455000	-4.370897000	0.923782000	6	0.552115000	2.687396000	3.341846000
6	-0.479366000	-4.371523000	0.057865000	1	1.448965000	2.417075000	3.880199000
1	-1.459935000	-4.525569000	0.485704000	6	0.563857000	3.720519000	2.413108000
6	-0.320462000	-4.165778000	-1.309219000	6	-0.603078000	4.047330000	1.725508000
6	4.213706000	-3.866446000	0.801362000	6	-1.757370000	3.312027000	1.981923000
1	4.180125000	-2.922220000	0.252550000	1	-2.649370000	3.567646000	1.427794000

6	-1.764681000	2.275069000	2.907942000	6	-4.374425000	-3.940803000	2.013243000
6	2.908278000	4.049011000	2.662451000	1	-4.321698000	-4.913586000	2.503462000
1	3.065253000	2.985891000	2.464658000	1	-5.410778000	-3.601804000	2.020204000
1	2.903147000	4.198885000	3.748855000	1	-4.059375000	-4.052527000	0.974983000
6	-4.105118000	1.889901000	2.617147000	6	-3.601142000	-4.255754000	-2.898827000
1	-4.049480000	1.759832000	1.530999000	1	-3.372853000	-5.029792000	-3.632204000
1	-4.328019000	2.944069000	2.819719000	1	-4.632868000	-4.380020000	-2.568247000
6	-0.601559000	5.115167000	0.655133000	1	-3.514609000	-3.281699000	-3.382274000
1	-1.565130000	5.621617000	0.644257000	6	-5.163402000	0.998048000	3.221071000
1	0.168811000	5.852629000	0.871962000	1	-5.247518000	1.173378000	4.294016000
6	-0.334279000	4.481700000	-0.689395000	1	-6.129921000	1.196955000	2.756781000
6	0.969284000	4.271901000	-1.118306000	1	-4.917601000	-0.051568000	3.058760000
1	1.766972000	4.632676000	-0.485870000	6	-4.986035000	3.975174000	-0.898601000
6	1.244358000	3.554686000	-2.274551000	1	-5.857065000	3.538719000	-1.388579000
6	0.197303000	3.030720000	-3.031568000	1	-4.917164000	3.558116000	0.107208000
6	-1.109201000	3.273953000	-2.624890000	1	-5.132451000	5.053027000	-0.820661000
1	-1.908176000	2.859863000	-3.222097000	6	-4.038528000	0.479216000	-4.172104000
6	-1.386697000	3.995392000	-1.468491000	1	-3.990571000	0.997098000	-5.130552000
6	3.594609000	3.726051000	-1.931926000	1	-4.939390000	-0.134710000	-4.150937000
1	3.534173000	3.257685000	-0.944389000	1	-4.113827000	1.221678000	-3.377934000
1	3.559104000	4.813787000	-1.796346000	6	4.226462000	0.534018000	4.474029000
6	-3.739235000	3.655130000	-1.686687000	1	4.080253000	1.372848000	3.792764000
1	-3.584765000	2.574501000	-1.730128000	1	4.034955000	0.873772000	5.492462000
1	-3.813888000	4.043359000	-2.709360000	1	5.267068000	0.214855000	4.403479000
8	1.642418000	1.320501000	0.172554000	6	5.127672000	-3.753800000	1.997714000
6	-2.668849000	-4.343154000	-1.714763000	1	4.786377000	-2.960152000	2.663887000
1	-2.760000000	-5.317718000	-1.220779000	1	5.153991000	-4.689720000	2.556754000
1	-2.896592000	-3.559405000	-0.986885000	1	6.140628000	-3.514638000	1.671380000

6	5.652747000	-1.978604000	-3.507858000	6	-0.444528000	4.502884000	-1.281977000
1	5.756089000	-2.167933000	-2.438441000	6	0.940939000	4.432024000	-1.317157000
1	5.543576000	-2.934319000	-4.021624000	6	1.671803000	4.601394000	-0.139789000
1	6.564753000	-1.495880000	-3.861680000	6	0.984264000	4.703654000	1.060009000
6	4.863659000	3.327777000	-2.646048000	6	-0.404514000	4.721574000	1.104387000
1	5.731296000	3.618556000	-2.052248000	6	3.171756000	4.762250000	-0.180398000
1	4.897061000	2.248597000	-2.794287000	6	5.631897000	1.227156000	-0.061843000
1	4.928484000	3.815982000	-3.619033000	6	5.155049000	1.800202000	1.108613000
6	3.993501000	4.873627000	2.013348000	6	4.317364000	2.904840000	1.083111000
1	4.010753000	4.700285000	0.936546000	6	3.975756000	3.488325000	-0.135164000
1	3.833136000	5.937269000	2.192542000	6	4.437165000	2.904041000	-1.305113000
1	4.966287000	4.595136000	2.420851000	6	5.244025000	1.774913000	-1.281018000
-----				6	3.151854000	-4.772657000	0.180381000
EtP6 with two AgOCOCF₃				6	1.652494000	-4.606606000	0.138938000
Sum of electronic and zero-point Energies= -4813.851519				6	0.965147000	-4.707371000	-1.061092000
Sum of electronic and thermal Energies= -4813.752279				6	-0.423655000	-4.720791000	-1.106131000
Sum of electronic and thermal Enthalpies= -4813.751334				6	-1.149461000	-4.682501000	0.082641000
Sum of electronic and thermal Free Energies= -4813.997205				6	-0.464072000	-4.500515000	1.280062000
6	-2.623461000	4.898085000	-0.090942000	6	0.921635000	-4.434191000	1.315874000
6	-3.404746000	3.611263000	-0.082158000	6	-2.643789000	-4.889035000	0.088157000
6	-3.713279000	2.993186000	1.125105000	6	-5.770048000	0.011028000	-0.001975000
6	-4.454831000	1.821078000	1.167679000	6	-4.933540000	-1.242483000	0.015955000
6	-4.928106000	1.260897000	-0.019607000	6	-4.605417000	-1.846294000	1.220731000
6	-4.597069000	1.863389000	-1.224250000				
6	-3.829543000	3.019832000	-1.270894000				
6	-1.129864000	4.686388000	-0.084786000				

6	-3.842905000	-3.006039000	1.267646000	6	5.087732000	1.460220000	-3.637847000
6	-3.420324000	-3.599357000	0.079051000	6	6.489982000	-0.012115000	0.001069000
6	-3.725953000	-2.980104000	-1.128297000	6	3.960643000	-3.501736000	0.135781000
6	-4.462430000	-1.804840000	-1.171144000	6	4.424142000	-2.919646000	1.305997000
8	-4.766989000	1.175913000	2.323491000	6	5.235744000	-1.793903000	1.282393000
6	-4.228533000	1.677263000	3.531485000	6	5.626418000	-1.247608000	0.063470000
8	-3.473195000	3.642754000	-2.425548000	6	5.147432000	-1.818324000	-1.107258000
6	-3.586543000	2.919529000	-3.635230000	6	4.304941000	-2.919309000	-1.082248000
8	-1.120971000	4.834670000	2.256666000	8	5.705501000	-1.183524000	2.410501000
6	-0.479802000	4.504496000	3.473559000	6	5.079278000	-1.478336000	3.639069000
8	1.650856000	4.253697000	-2.462138000	8	3.793011000	-3.500527000	-2.204788000
6	0.938233000	3.950016000	-3.645689000	6	3.986156000	-2.850075000	-3.441364000
8	3.807826000	3.488645000	2.205401000	1	-2.889480000	5.473373000	-0.976416000
6	3.997930000	2.837739000	3.442201000	1	-2.902360000	5.484507000	0.783064000
8	1.631545000	-4.257605000	2.461101000	1	-3.350715000	3.461332000	2.028852000
6	0.919207000	-3.951526000	3.644238000	1	-4.950608000	1.397806000	-2.132727000
8	-1.139856000	-4.832217000	-2.258721000	1	-1.030463000	4.447948000	-2.188213000
6	-0.497294000	-4.503398000	-3.475254000	1	1.566383000	4.795889000	1.966120000
8	-3.489582000	-3.630358000	2.422497000	1	3.465444000	5.390323000	0.661070000
6	-3.600924000	-2.906677000	3.632095000	1	3.433737000	5.298811000	-1.092601000
8	-4.771578000	-1.158416000	-2.327092000	1	5.448682000	1.343361000	2.042764000
6	-4.234490000	-1.661806000	-3.534812000	1	4.145156000	3.358352000	-2.241590000
8	5.711611000	1.162333000	-2.408828000	1	3.411409000	-5.310302000	1.092646000

1	3.443783000	-5.401661000	-0.661010000	1	-3.111919000	-1.935213000	3.512092000
1	1.547332000	-4.802023000	-1.966917000	1	-4.656550000	-2.737792000	3.875206000
1	-1.050225000	-4.443302000	2.186013000	1	-4.626273000	-2.668004000	-3.725673000
1	-2.912218000	-5.463425000	0.973495000	1	-3.145252000	-1.735517000	-3.449927000
1	-2.924343000	-5.474414000	-0.786010000	1	4.004701000	1.319626000	-3.539995000
1	-6.412019000	0.019215000	0.878409000	1	5.265658000	2.505304000	-3.916888000
1	-6.411757000	0.005637000	-0.882570000	1	7.129981000	0.036558000	0.880602000
1	-4.957187000	-1.379145000	2.129082000	1	7.130274000	-0.063586000	-0.878097000
1	-3.365002000	-3.449744000	-2.031915000	1	4.130025000	-3.372948000	2.242308000
1	-3.138989000	1.746770000	3.447082000	1	5.443353000	-1.362555000	-2.041204000
1	-4.616558000	2.684955000	3.722130000	1	3.996964000	-1.333009000	3.540259000
1	-4.642653000	2.754930000	-3.879169000	1	5.252358000	-2.524115000	3.918550000
1	-3.101577000	1.946071000	-3.514939000	1	5.052282000	-2.842382000	-3.699575000
1	-0.004957000	3.523071000	3.372803000	1	3.649810000	-1.809096000	-3.369627000
1	0.294363000	5.244245000	3.707529000	9	-0.925956000	0.950926000	-4.824522000
1	0.266467000	3.104246000	-3.463593000	9	-0.820411000	-1.195452000	-4.769975000
1	0.329436000	4.812406000	-3.944144000	9	0.921725000	-0.021158000	-4.274284000
1	3.656132000	1.798483000	3.370992000	8	-0.945982000	-1.072790000	2.176562000
1	5.064062000	2.824559000	3.700156000	8	-0.865470000	-1.181748000	-2.118355000
1	0.249706000	-3.104135000	3.461361000	8	-0.940419000	1.074746000	-2.173232000
1	0.308083000	-4.812236000	3.942791000	6	-0.797960000	0.064074000	2.652417000
1	-0.019708000	-3.523378000	-3.373848000	6	-0.795498000	-0.062586000	-2.648842000
1	0.274889000	-5.245204000	-3.709235000	6	-0.412310000	-0.083828000	-4.157651000

47	-1.165212000	-1.570836000	0.036132000	6	5.657587000	0.536221000	-4.688182000
47	-1.160881000	1.574018000	-0.033079000	1	5.195413000	0.741157000	-5.654946000
8	-0.863611000	1.183413000	2.121811000	1	6.734714000	0.677487000	-4.781469000
6	-0.416495000	0.083745000	4.161699000	1	5.468118000	-0.506314000	-4.429687000
9	-0.936826000	-0.947857000	4.828334000	6	3.192353000	-3.591037000	-4.490664000
9	0.917020000	0.013496000	4.279930000	1	2.128148000	-3.560174000	-4.256736000
9	-0.818956000	1.197853000	4.773161000	1	3.342199000	-3.128016000	-5.466958000
6	-1.545323000	-4.479143000	-4.561245000	1	3.508098000	-4.633391000	-4.549030000
1	-2.300319000	-3.722620000	-4.346335000	6	5.652304000	-0.556555000	4.689625000
1	-1.082529000	-4.236278000	-5.518483000	1	6.728725000	-0.702508000	4.783837000
1	-2.035965000	-5.449331000	-4.647366000	1	5.467611000	0.486729000	4.430683000
6	-4.622581000	-0.723480000	-4.651302000	1	5.188440000	-0.759202000	5.656061000
1	-5.707167000	-0.643520000	-4.731756000	6	1.921531000	-3.618358000	4.722257000
1	-4.212397000	0.271630000	-4.479349000	1	2.509014000	-2.745272000	4.439435000
1	-4.229690000	-1.095016000	-5.598450000	1	1.400960000	-3.393095000	5.653939000
6	-2.910221000	3.717747000	-4.722549000	6	-1.528315000	4.483585000	4.559148000
1	-3.368297000	4.702210000	-4.823192000	1	-1.066573000	4.239730000	5.516640000
1	-1.850774000	3.844304000	-4.499132000				
1	-2.997234000	3.193721000	-5.675118000	1	-2.016264000	5.455176000	4.644760000
6	1.940170000	3.614765000	-4.723441000	1	-2.285314000	3.729074000	4.344210000
1	1.419435000	3.391299000	-5.655464000	6	-4.620747000	0.740436000	4.647791000
1	2.619902000	4.450260000	-4.895921000	1	-4.214177000	-0.256208000	4.476126000
1	2.525311000	2.740045000	-4.440791000	1	-4.226980000	1.110544000	5.595136000

1	-5.705666000	0.664526000	4.727660000	6	-2.084811000	-4.172803000	0.659236000
6	-2.928638000	-3.707542000	4.719964000	6	-1.452524000	-3.885101000	1.867790000
1	-1.869475000	-3.838089000	4.497509000	6	-0.084897000	-4.068253000	2.028160000
1	-3.014501000	-3.183238000	5.672483000	6	0.669047000	-4.597179000	0.977940000
1	-3.390554000	-4.690259000	4.820137000	6	0.050755000	-4.806690000	-0.245085000
6	3.208406000	3.583437000	4.491378000	6	-1.307064000	-4.574536000	-0.425539000
1	2.144051000	3.558935000	4.257363000	6	2.107320000	-5.003238000	1.187773000
1	3.355433000	3.119616000	5.467721000	6	5.135366000	-1.991661000	0.609414000
1	3.530278000	4.623914000	4.549679000	6	4.619205000	-2.695206000	-0.468685000
1	2.599037000	-4.455510000	4.895452000	6	3.615009000	-3.637564000	-0.303706000
-----				6	3.127685000	-3.914920000	0.971627000
P6Q1 with two AgOCOCF₃				6	3.633771000	-3.200745000	2.048109000
Sum of electronic and zero-point Energies= -4655.496526				6	4.619240000	-2.238297000	1.878708000
Sum of electronic and thermal Energies= -4655.402736				6	3.737691000	4.221942000	-0.737130000
Sum of electronic and thermal Enthalpies= -4655.401792				6	2.231853000	4.312799000	-0.766094000
Sum of electronic and thermal Free Energies= -4655.638469				6	1.525905000	4.652238000	0.378633000
6	-3.589361000	-4.121032000	0.560609000	6	0.159123000	4.899217000	0.341401000
6	-4.128113000	-2.745867000	0.267208000	6	-0.507897000	4.866063000	-0.881925000
6	-4.177285000	-2.285812000	-1.045362000	6	0.178338000	4.445555000	-2.015409000
6	-4.715240000	-1.043548000	-1.351433000	6	1.530990000	4.136424000	-1.961054000
6	-5.273598000	-0.268928000	-0.334750000	6	-1.934005000	5.351582000	-0.980972000
6	-5.188287000	-0.708070000	0.977181000	6	-5.938328000	1.044723000	-0.664284000
6	-4.592809000	-1.921619000	1.293305000	6	-4.920433000	2.134494000	-0.803197000

6	-4.440460000	2.541746000	-1.978550000	6	6.186208000	-0.932799000	0.385908000
6	-3.414837000	3.589782000	-2.095576000	6	4.307186000	2.858371000	-0.442107000
6	-2.933790000	4.246411000	-0.839519000	6	4.664961000	2.006927000	-1.476929000
6	-3.391713000	3.818309000	0.339224000	6	5.263034000	0.779089000	-1.229091000
6	-4.406739000	2.758066000	0.455835000	6	5.544291000	0.398031000	0.080407000
8	-4.749151000	-0.525291000	-2.604892000	6	5.166090000	1.240094000	1.116329000
6	-4.016889000	-1.180969000	-3.626260000	6	4.533541000	2.449311000	0.870004000
8	-4.443799000	-2.379794000	2.561377000	8	5.621560000	-0.094317000	-2.214263000
6	-4.600563000	-1.462929000	3.631492000	6	5.134277000	0.131337000	-3.518958000
8	-1.954432000	-4.768035000	-1.606126000	8	4.126921000	3.300773000	1.855693000
6	-1.178429000	-4.791975000	-2.790084000	6	4.197768000	2.860531000	3.193474000
8	0.571924000	-3.804012000	3.186187000	1	-4.010620000	-4.476481000	1.499387000
6	-0.147704000	-3.178562000	4.232950000	1	-3.914429000	-4.798270000	-0.227642000
8	3.073610000	-4.346172000	-1.335508000	1	-3.791687000	-2.935516000	-1.818739000
6	3.445902000	-3.997534000	-2.651372000	1	-5.584685000	-0.068635000	1.752554000
8	2.245214000	3.712173000	-3.034041000	1	-2.073098000	-3.554833000	2.689084000
6	1.540003000	3.362046000	-4.212331000	1	0.658347000	-5.179140000	-1.057523000
8	-0.579308000	5.239750000	1.429600000	1	2.326718000	-5.829785000	0.511314000
6	-0.035476000	4.987986000	2.713028000	1	2.214526000	-5.378146000	2.205739000
8	-2.976247000	3.912371000	-3.179290000	1	5.018982000	-2.470584000	-1.446870000
8	-4.833636000	2.423803000	1.540553000	1	3.232388000	-3.418669000	3.027851000
8	5.143589000	-1.507800000	2.905984000	1	4.119806000	4.551178000	-1.703152000
6	4.495103000	-1.543738000	4.156665000	1	4.102513000	4.923237000	0.013567000

1	2.079969000	4.748341000	1.301729000	1	4.540864000	-2.552375000	4.583823000
1	-0.368329000	4.395198000	-2.946671000	1	6.827515000	-1.231501000	-0.441901000
1	-2.074538000	5.828567000	-1.949965000	1	6.808224000	-0.836435000	1.274575000
1	-2.112558000	6.089596000	-0.200989000	1	4.461926000	2.333698000	-2.487219000
1	-6.494034000	0.953530000	-1.596659000	1	5.371590000	0.912524000	2.125302000
1	-6.634007000	1.302519000	0.133558000	1	4.043511000	0.232857000	-3.489627000
1	-4.779479000	2.105794000	-2.909477000	1	5.547360000	1.061819000	-3.925665000
1	-3.047702000	4.252703000	1.269731000	1	5.243996000	2.707409000	3.485233000
1	-3.025269000	-1.451432000	-3.251370000	1	3.677069000	1.900765000	3.296103000
1	-4.532520000	-2.105135000	-3.912893000	9	-1.431307000	0.085014000	4.815859000
1	-5.659586000	-1.209708000	3.753270000	9	-2.497597000	1.884777000	4.303370000
1	-4.052011000	-0.543880000	3.406702000	9	-0.338966000	1.896673000	4.426678000
1	-0.495560000	-3.936667000	-2.785905000	8	-0.395156000	0.887032000	-2.291195000
1	-0.585337000	-5.712622000	-2.833331000	8	-1.051471000	1.808062000	1.814229000
1	-0.639447000	-2.276358000	3.854975000	8	-1.556255000	-0.351258000	2.235393000
1	-0.922468000	-3.858260000	4.608078000	6	-0.463527000	-0.321313000	-2.581252000
1	3.254101000	-2.931653000	-2.819459000	6	-1.324268000	0.827649000	2.532723000
1	4.518169000	-4.174870000	-2.798249000	6	-1.396724000	1.173376000	4.048313000
1	0.726803000	2.674698000	-3.961272000	47	-0.743855000	1.652682000	-0.310995000
1	1.104476000	4.259867000	-4.665908000	47	-1.525868000	-1.326296000	0.219258000
1	0.350988000	3.964721000	2.744017000	8	-0.830362000	-1.295210000	-1.909920000
1	0.791280000	5.680316000	2.910554000	6	0.037824000	-0.656308000	-4.016154000
1	3.437735000	-1.283198000	4.028402000	9	-0.234887000	0.314511000	-4.884126000

9	1.368486000	-0.823175000	-3.990324000	1	6.626379000	-1.141047000	-4.407569000
9	-0.500353000	-1.781387000	-4.487580000	1	5.119584000	-1.969619000	-3.990170000
6	-1.138584000	5.168460000	3.726491000	1	5.177905000	-0.899530000	-5.397819000
1	-1.942033000	4.454213000	3.546433000	6	2.518035000	2.709958000	-5.159330000
1	-0.750491000	4.995708000	4.730972000	1	2.924463000	1.799153000	-4.719159000
1	-1.545969000	6.179204000	3.680531000	1	2.012223000	2.444170000	-6.088201000
6	-4.056964000	-2.116315000	4.878346000	6	-2.120974000	-4.716752000	-3.966268000
1	-4.585851000	-3.045753000	5.092310000	1	-1.554803000	-4.752878000	-4.897716000
1	-2.995217000	-2.333664000	4.757815000	1	-2.824670000	-5.549773000	-3.953884000
1	-4.172778000	-1.444653000	5.729566000	1	-2.682583000	-3.782380000	-3.945975000
6	0.829245000	-2.834385000	5.330493000	6	-3.902460000	-0.238381000	-4.799816000
1	0.300990000	-2.366689000	6.162091000	1	-3.357973000	0.664342000	-4.519196000
1	1.333872000	-3.729161000	5.697128000	1	-3.360643000	-0.724945000	-5.611702000
1	1.581485000	-2.134586000	4.965936000	1	-4.888926000	0.048373000	-5.166198000
6	5.184651000	-0.555964000	5.068118000	1	3.342826000	3.384695000	-5.392584000
1	4.708417000	-0.558054000	6.049590000	6	2.636460000	-4.838433000	-3.609018000
1	6.236054000	-0.816569000	5.192231000	1	1.572510000	-4.631346000	-3.496001000
1	5.125947000	0.453223000	4.658299000	1	2.921902000	-4.609445000	-4.636638000
6	3.552166000	3.910308000	4.066443000	1	2.807517000	-5.900613000	-3.430098000
1	2.500959000	4.033168000	3.804271000	-----			
1	3.611375000	3.612359000	5.114150000	P6Q2 with two AgOCOCF₃			
1	4.055581000	4.870723000	3.950402000	Sum of electronic and zero-point Energies= -4497.148406			
6	5.540891000	-1.041778000	-4.378985000	Sum of electronic and thermal Energies= -4497.060727			

Sum of electronic and thermal Enthalpies= -4497.059783				6	-3.664415000	-3.238740000	-0.127833000
Sum of electronic and thermal Free Energies= -4497.283987				6	-3.009448000	-3.645453000	1.025351000
6	4.514259000	3.032708000	-0.152991000	6	-1.791037000	-4.311758000	0.970050000
6	4.581594000	1.536835000	-0.314780000	6	-1.243740000	-4.632415000	-0.272214000
6	4.355520000	0.962403000	-1.562961000	6	-1.856637000	-4.155280000	-1.425331000
6	4.475388000	-0.407552000	-1.755976000	6	-3.040095000	-3.432208000	-1.361614000
6	4.880055000	-1.216449000	-0.693818000	6	-0.046911000	-5.549686000	-0.359418000
6	5.070742000	-0.650325000	0.556988000	6	5.079098000	-2.696903000	-0.905033000
6	4.899047000	0.711287000	0.765736000	6	3.772296000	-3.425387000	-0.825575000
6	3.122701000	3.563937000	0.087718000	6	3.067774000	-3.784472000	-1.899113000
6	2.594128000	3.581216000	1.375964000	6	1.773484000	-4.477995000	-1.802711000
6	1.384372000	4.206061000	1.648415000	6	1.250539000	-4.806689000	-0.438904000
6	0.721911000	4.891721000	0.629318000	6	1.940717000	-4.420314000	0.636771000
6	1.201574000	4.797859000	-0.667992000	6	3.236528000	-3.726840000	0.538321000
6	2.374145000	4.110308000	-0.955841000	8	4.233312000	-1.026576000	-2.937869000
6	-0.459797000	5.774975000	0.954370000	6	3.684394000	-0.265197000	-4.000619000
6	-4.373227000	3.784745000	0.653829000	8	5.039023000	1.312246000	1.973015000
6	-3.802030000	4.319084000	-0.426556000	6	5.074076000	0.497044000	3.132804000
6	-2.480170000	4.965150000	-0.390963000	8	2.882808000	3.978711000	-2.207737000
6	-1.776687000	5.060179000	0.925432000	6	2.014437000	4.184467000	-3.310305000
6	-2.344974000	4.524859000	2.005893000	8	0.813517000	4.235029000	2.878435000
6	-3.656180000	3.853686000	1.965051000	6	1.360030000	3.405070000	3.890949000
6	-5.059047000	-2.668138000	-0.053409000	8	-1.982207000	5.418431000	-1.400794000

8	-3.669605000	-2.928720000	-2.453320000	1	0.645571000	5.294502000	-1.451135000
6	-2.982632000	-2.949229000	-3.693313000	1	-0.490844000	6.589190000	0.230877000
8	-1.109549000	-4.737526000	2.064360000	1	-0.317107000	6.201904000	1.946234000
6	-1.464297000	-4.202098000	3.327167000	1	-4.285079000	4.283326000	-1.394699000
8	1.153604000	-4.778160000	-2.800678000	1	-1.866740000	4.569548000	2.976716000
8	3.861500000	-3.435808000	1.535805000	1	-5.587370000	-2.928502000	-0.969975000
8	-4.145264000	3.393306000	2.975338000	1	-5.578830000	-3.151499000	0.773426000
6	-5.690061000	3.068716000	0.622142000	1	-3.492730000	-3.453568000	1.973114000
6	-5.137010000	-1.174860000	0.131448000	1	-1.395903000	-4.387784000	-2.375153000
6	-5.191220000	-0.335393000	-0.970791000	1	-0.148265000	-6.172223000	-1.247506000
6	-5.332980000	1.037552000	-0.824499000	1	-0.030086000	-6.194309000	0.517364000
6	-5.478776000	1.582793000	0.448971000	1	5.528189000	-2.873648000	-1.881419000
6	-5.395010000	0.748092000	1.554059000	1	5.750148000	-3.079859000	-0.136846000
6	-5.196870000	-0.617141000	1.407588000	1	3.417706000	-3.574370000	-2.901741000
8	-5.360045000	1.909152000	-1.869412000	1	1.583799000	-4.620956000	1.639575000
6	-4.996525000	1.431706000	-3.150441000	1	2.843013000	0.327657000	-3.630638000
8	-5.075844000	-1.478254000	2.455757000	1	4.441296000	0.427883000	-4.386208000
6	-4.987024000	-0.947415000	3.762455000	1	6.021537000	-0.051614000	3.173489000
1	5.144108000	3.327199000	0.684937000	1	4.257743000	-0.229518000	3.091444000
1	4.917159000	3.497677000	-1.051165000	1	1.084880000	3.630570000	-3.147137000
1	4.096477000	1.622696000	-2.379047000	1	1.772060000	5.248597000	-3.403611000
1	5.341704000	-1.304342000	1.372847000	1	1.515963000	2.396931000	3.495079000
1	3.176421000	3.124479000	2.164311000	1	2.332165000	3.801928000	4.206915000

1	-1.979364000	-2.534019000	-3.561583000	8	0.869805000	0.890769000	-2.087964000
1	-2.884294000	-3.981997000	-4.046823000	6	-0.299730000	0.301308000	-4.062198000
1	-1.511255000	-3.110867000	3.255158000	9	-0.336768000	-0.804030000	-4.804018000
1	-2.450748000	-4.575051000	3.626467000	9	-1.536034000	0.817509000	-4.031675000
1	-6.288937000	3.455486000	-0.200918000	9	0.488734000	1.177325000	-4.682320000
1	-6.219950000	3.249463000	1.556646000	6	-0.409363000	-4.624989000	4.319302000
1	-5.120735000	-0.787677000	-1.950128000	1	0.565251000	-4.234410000	4.027532000
1	-5.476703000	1.198087000	2.533082000	1	-0.650958000	-4.232016000	5.307501000
1	-4.051327000	0.884021000	-3.081374000	1	-0.350703000	-5.712288000	4.382481000
1	-5.761182000	0.740334000	-3.523499000	6	4.923812000	1.399994000	4.332205000
1	-5.933548000	-0.468361000	4.038188000	1	5.723297000	2.141014000	4.363670000
1	-4.201244000	-0.185028000	3.802536000	1	3.964289000	1.916806000	4.297907000
9	1.845900000	0.049589000	4.697033000	1	4.959329000	0.808836000	5.247773000
9	2.114597000	-2.054883000	4.330501000	6	0.390669000	3.382221000	5.047560000
9	0.133375000	-1.252401000	4.655703000	1	0.789330000	2.759652000	5.849211000
8	-0.251195000	-1.067623000	-2.149431000	1	0.225852000	4.387147000	5.438208000
8	0.507304000	-1.699140000	1.996796000	1	-0.569066000	2.967092000	4.737051000
8	1.712248000	0.207034000	2.086235000	6	-4.671685000	-2.087505000	4.701688000
6	0.170900000	0.009861000	-2.607548000	1	-3.711399000	-2.538516000	4.447436000
6	1.164707000	-0.800553000	2.554289000	1	-4.617706000	-1.721728000	5.727761000
6	1.318133000	-1.011517000	4.088292000	1	-5.442857000	-2.856743000	4.647856000
47	0.022113000	-1.684713000	-0.104186000	6	-4.854069000	2.619939000	-4.070938000
47	1.747255000	0.904021000	-0.034385000	1	-5.786540000	3.183216000	-4.123030000

1	-4.061598000	3.284335000	-3.724172000	6	-3.974490000	2.986965000	0.519863000
1	-4.598750000	2.280268000	-5.075545000	6	-4.167270000	2.604781000	-0.812172000
6	-3.779351000	-2.125095000	-4.675555000	6	-3.364528000	3.155497000	-1.801322000
1	-3.851590000	-1.091356000	-4.336264000	6	-2.391023000	4.096044000	-1.495831000
1	-3.286221000	-2.130599000	-5.648195000	6	0.153060000	5.192386000	0.277746000
6	2.723666000	3.690813000	-4.547791000	6	1.037281000	5.255123000	-0.717348000
1	2.091209000	3.841248000	-5.423225000	6	2.447763000	4.861443000	-0.552837000
1	3.660587000	4.228387000	-4.698237000	6	2.922409000	4.497645000	0.818835000
1	2.938996000	2.625197000	-4.462562000	6	2.026311000	4.381682000	1.800274000
6	3.230141000	-1.223944000	-5.074118000	6	0.591926000	4.662719000	1.604976000
1	2.459942000	-1.895086000	-4.691758000	6	4.394089000	4.266642000	1.004456000
1	2.810200000	-0.666722000	-5.912185000	6	5.633427000	0.157909000	0.715340000
1	4.065325000	-1.822445000	-5.439774000	6	5.362784000	0.727219000	1.950524000
1	-4.786763000	-2.526301000	-4.793543000	6	4.909102000	2.034878000	2.054247000
-----				6	4.776376000	2.809606000	0.903468000
P6Q3 with two AgOCOCF₃				6	5.011348000	2.230070000	-0.334608000
Sum of electronic and zero-point Energies= -4338.792638				6	5.411185000	0.904855000	-0.440680000
Sum of electronic and thermal Energies= -4338.710817				6	2.118611000	-5.457673000	-0.136879000
Sum of electronic and thermal Enthalpies= -4338.709873				6	0.725958000	-4.960802000	-0.439693000
Sum of electronic and thermal Free Energies= -4338.924367				6	0.363393000	-4.629946000	-1.735889000
6	-1.273297000	5.641344000	0.145025000	6	-0.928492000	-4.224295000	-2.044141000
6	-2.239789000	4.528089000	-0.178102000	6	-1.901624000	-4.216420000	-1.044303000
6	-3.016046000	3.952144000	0.818714000	6	-1.528108000	-4.498235000	0.269646000

6	-0.216298000	-4.844887000	0.586551000	8	5.634289000	0.274260000	-1.623156000
6	-3.349947000	-3.970036000	-1.396440000	6	5.249049000	0.923569000	-2.822089000
6	-5.247629000	1.610085000	-1.165676000	6	6.182766000	-1.245697000	0.618963000
6	-4.729718000	0.202055000	-1.151717000	6	3.092752000	-4.342725000	0.108646000
6	-4.749135000	-0.578084000	-0.068003000	6	3.353168000	-3.846099000	1.318423000
6	-4.243394000	-1.962916000	-0.080109000	6	4.359490000	-2.790424000	1.545805000
6	-3.743862000	-2.522352000	-1.374563000	6	5.118931000	-2.272804000	0.365785000
6	-3.673231000	-1.725592000	-2.441637000	6	4.827101000	-2.741377000	-0.848117000
6	-4.130017000	-0.324850000	-2.418615000	6	3.802671000	-3.772987000	-1.079262000
8	-4.779591000	2.404971000	1.440350000	8	4.583921000	-2.383316000	2.665798000
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8	-0.203832000	4.499874000	2.506668000	1	-2.861658000	4.280280000	1.836518000
8	3.204061000	4.857299000	-1.501056000	1	-3.513926000	2.821779000	-2.817973000
8	4.594607000	2.635976000	3.234053000	1	0.755923000	5.605321000	-1.702111000
6	4.662519000	1.873408000	4.423859000	1	2.320108000	4.085417000	2.800488000
8	0.212658000	-5.110944000	1.842002000	1	4.686964000	4.647135000	1.981336000
6	-0.704370000	-4.981404000	2.922213000	1	4.932039000	4.825124000	0.239398000
8	-1.323359000	-3.847219000	-3.283376000	1	5.507329000	0.116439000	2.829976000
6	-0.319149000	-3.517921000	-4.235091000	1	4.879876000	2.845012000	-1.214440000
8	-4.244969000	-2.634535000	0.929740000	1	2.087062000	-6.097654000	0.742779000
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1	1.122190000	-4.691382000	-2.502989000	1	5.343966000	-2.384036000	-1.729846000
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1	-1.496947000	-5.730694000	2.816912000	9	-1.908734000	-1.960786000	4.833174000
1	0.428936000	-2.876908000	-3.760708000	9	-2.580618000	0.083588000	4.904237000
1	0.176293000	-4.431657000	-4.580086000	6	-0.987913000	-2.803807000	-5.384218000
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1	5.885513000	1.799113000	-2.992253000	1	-0.247229000	-2.560221000	-6.146657000
1	6.688371000	-1.489443000	1.553133000	1	-1.756769000	-3.430782000	-5.837617000
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1	2.851755000	-4.219260000	2.203779000	1	-0.413968000	5.717631000	-4.520738000

1	0.628285000	4.430807000	-3.883275000	1	-5.257216000	0.720914000	3.396595000
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6	5.388243000	-0.069414000	-3.950912000	1	-6.506638000	1.981822000	3.373676000
1	5.117247000	0.404453000	-4.895114000	6	4.166475000	2.740297000	5.556349000
1	6.415787000	-0.427394000	-4.026813000	1	3.131318000	3.039932000	5.388144000
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6	0.065658000	-5.186638000	4.203242000	1	4.777714000	3.638378000	5.651238000
1	0.838236000	-4.424608000	4.311488000	1	0.536336000	-6.170327000	4.224382000
1	-0.611742000	-5.106886000	5.053980000	-----			
6	-5.463416000	1.769178000	3.610808000				

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