Supplementary Information

Cation Grease/Brake Rotation in Anionic Pillar[5]arenes and Its Application for Fluorescence Switch

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1. General Methods

All reactions were performed in air atmosphere unless otherwise stated. Deuterium solvents were purchased from Aldrich. All other reagents were obtained from commercial sources and were used without further purification, unless indicated otherwise. All yields were given as isolated yields. ^{1}H NMR and ^{13}C NMR spectra were recorded on a BRUKER AVANCE III 400 MHz or BRUKER AVANCE III 600 MHz spectrometer, and the chemical shifts (δ) for ^{1}H NMR spectra, given in ppm, are referenced to the residual proton signal of the deuterated solvent. The fluorescence emission spectra were recorded on a Hitachi F-7000 Fluorescence Spectrometer.

2. Synthesis and Characterization

(1). Synthesis of WP5-M

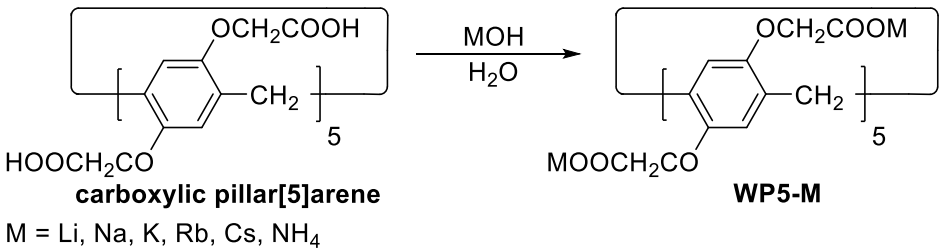
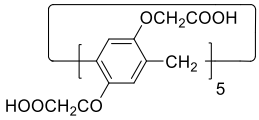


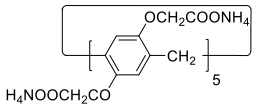
Figure S1. General synthetic routes of **WP5-M**.

General procedure for synthesis of WP5-M: To a suspension of carboxylic pillar[5]arene (50 mg, 0.042 mmol, 1.0 equiv.) in H_2O (20 ml), was added MOH (0.42 mmol, 10.0 equiv.). The reaction was stirred at room temperature until affording a clear solution. After removal of solvent and dried under vacuo, **WP5-M** was obtained quantitatively as a dark yellow solid.

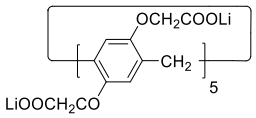


Carboxylic pillar[5]arene: The reported procedure[S1] was used to afford the title compound as a brown solid (total yield: 11%). ^{1}H NMR (400 MHz, DMSO-d_6, 298 K) δ 12.95 (br, 10H), 7.10 (s, 10H), 4.69 (d, J = 15.9 Hz, 10H), 4.41 (d,

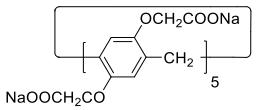
J = 15.8 Hz, 10H), 3.74 (s, 10H).



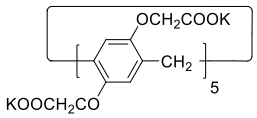
WP5-NH$_4$: The reported procedure[S2] was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.70 (s, 10H), 4.21 (s, 20H), 3.84 (s, 10H).



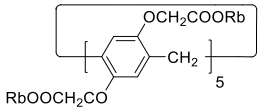
WP5-Li: The general procedure was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.80 (s, 10H), 4.47 (d, *J* = 15.9 Hz, 10H), 4.29 (d, *J* = 15.9 Hz, 10H), 3.85 (s, 10H). ^{13}C NMR (100 MHz, D_2O, 298 K) δ 177.44, 149.22, 128.68, 114.62, 67.74, 28.99.



WP5-Na: The reported procedure[S1] was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.77 (s, 10H), 4.50 (d, *J* = 16.0 Hz, 10H), 4.26 (d, *J* = 16.1 Hz, 10H), 3.83 (s, 10H).

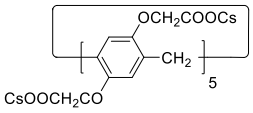


WP5-K: The general procedure was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.76 (s, 10H), 4.49 (d, *J* = 15.9 Hz, 11H), 4.26 (d, *J* = 16.1 Hz, 10H), 3.82 (s, 10H). ^{13}C NMR (100 MHz, D_2O, 298 K): δ 177.18, 149.10, 128.79, 114.47, 67.54, 28.83.



WP5-Rb: The general procedure was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.74 (s, 10H), 4.47 (d, *J* = 16.1 Hz, 10H), 4.24 (d, *J* = 16.1 Hz, 10H), 3.80 (s, 10H). ^{13}C

NMR (100 MHz, D_2O, 298 K) δ 177.15, 149.32, 128.68, 114.87, 67.69, 29.19.



WP5-Cs: The general procedure was used to quantitatively afford the title compound as a light brown solid. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 6.82 (s, 10H), 4.49 (d, J = 13.1 Hz, 10H), 4.33 (d, J = 14.7 Hz, 10H), 3.83 (s, 10H). ^{13}C NMR (100 MHz, D_2O, 298 K) δ 177.14, 149.05, 128.75, 114.43, 67.49, 28.78.

(2). NMR spectrum of synthetic compounds

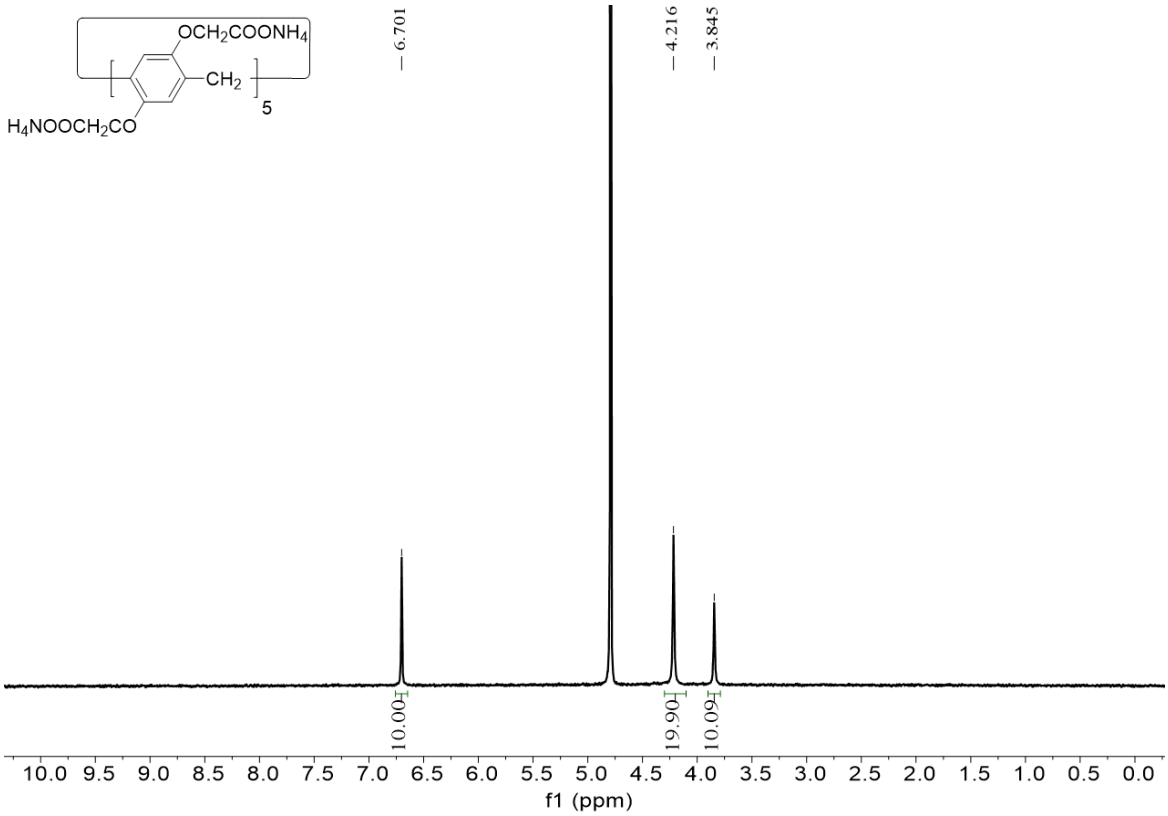


Figure S2. ^{1}H NMR spectra of **WP5-NH$_4$** in D_2O at 298 K.

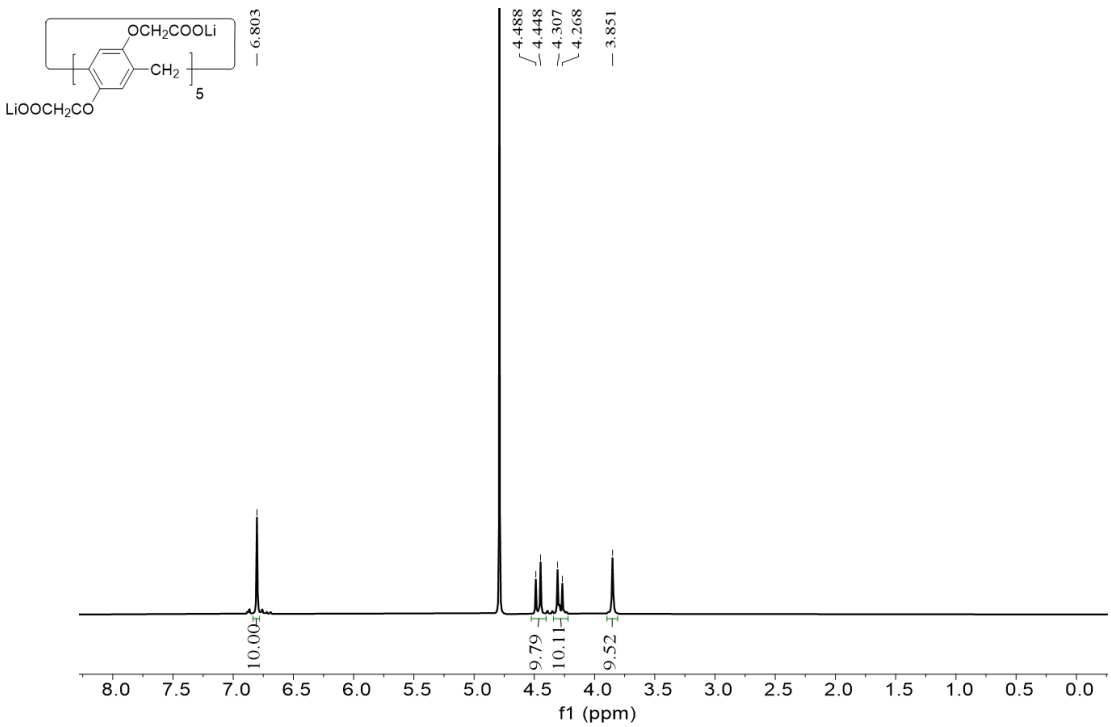


Figure S3. ^{1}H NMR spectra of **WP5-Li** in D_2O at 298 K.

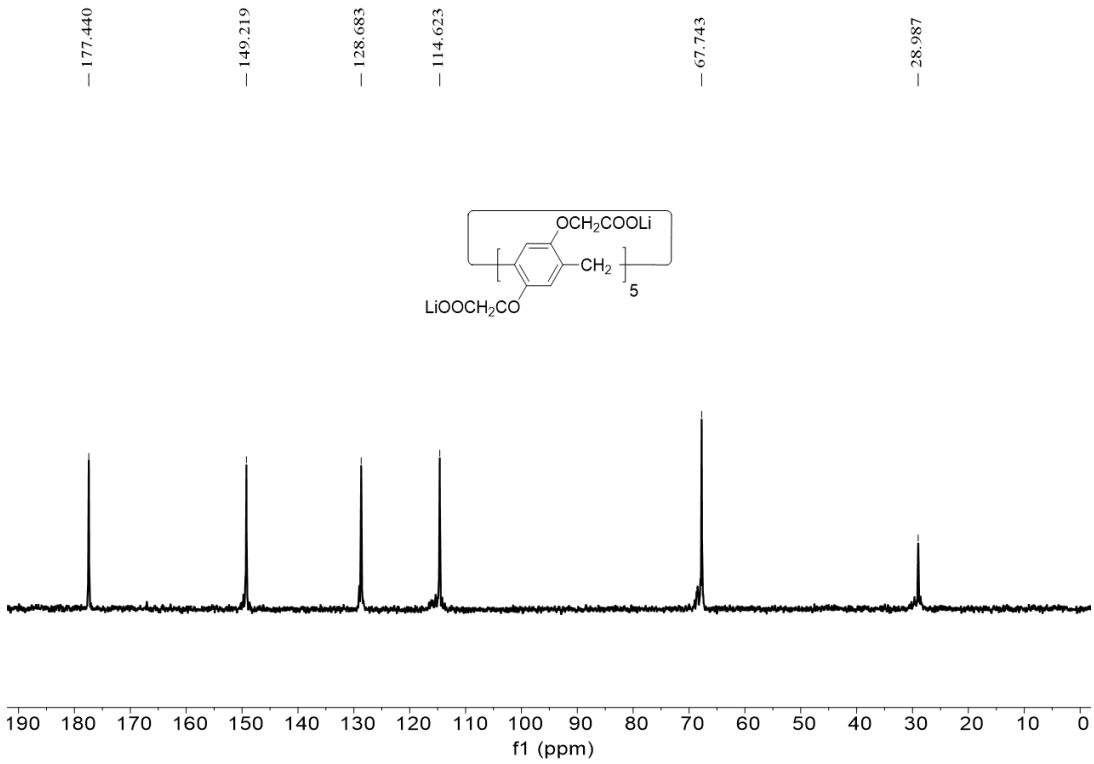


Figure S4. ^{13}C NMR spectra of **WP5-Li** in D_2O at 298 K.

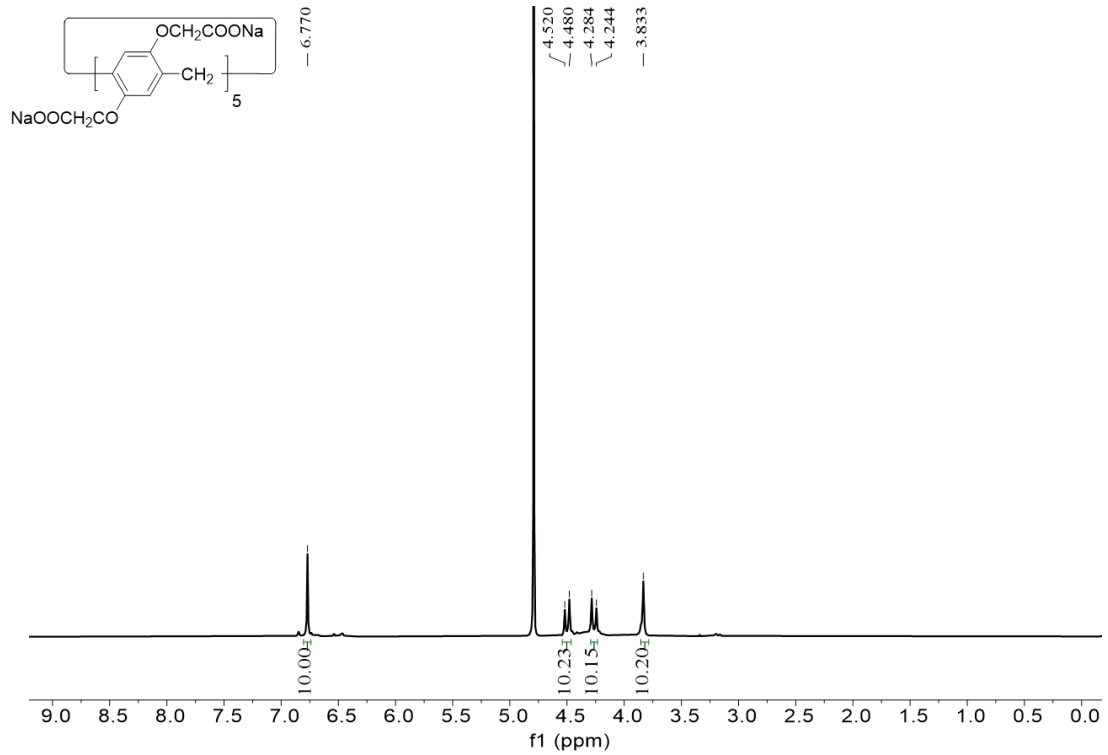


Figure S5. ^{1}H NMR spectra of **WP5-Na** in D_2O at 298 K.

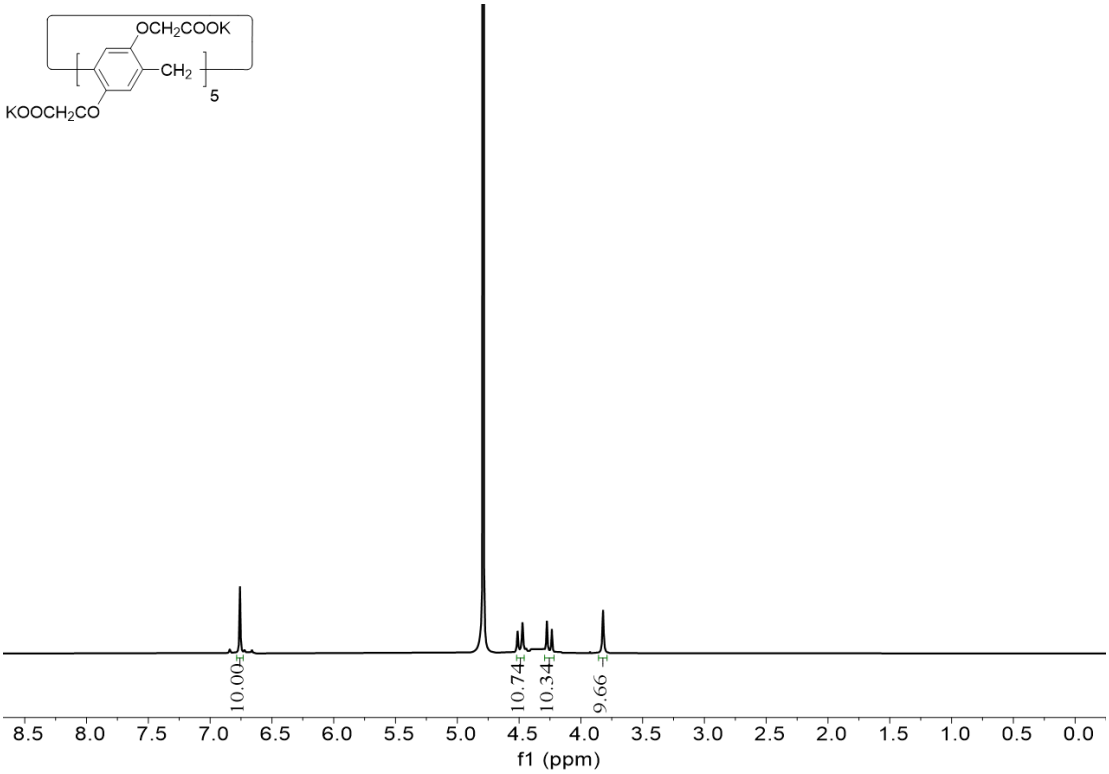


Figure S6. ^{1}H NMR spectra of **WP5-K** in D_2O at 298 K.

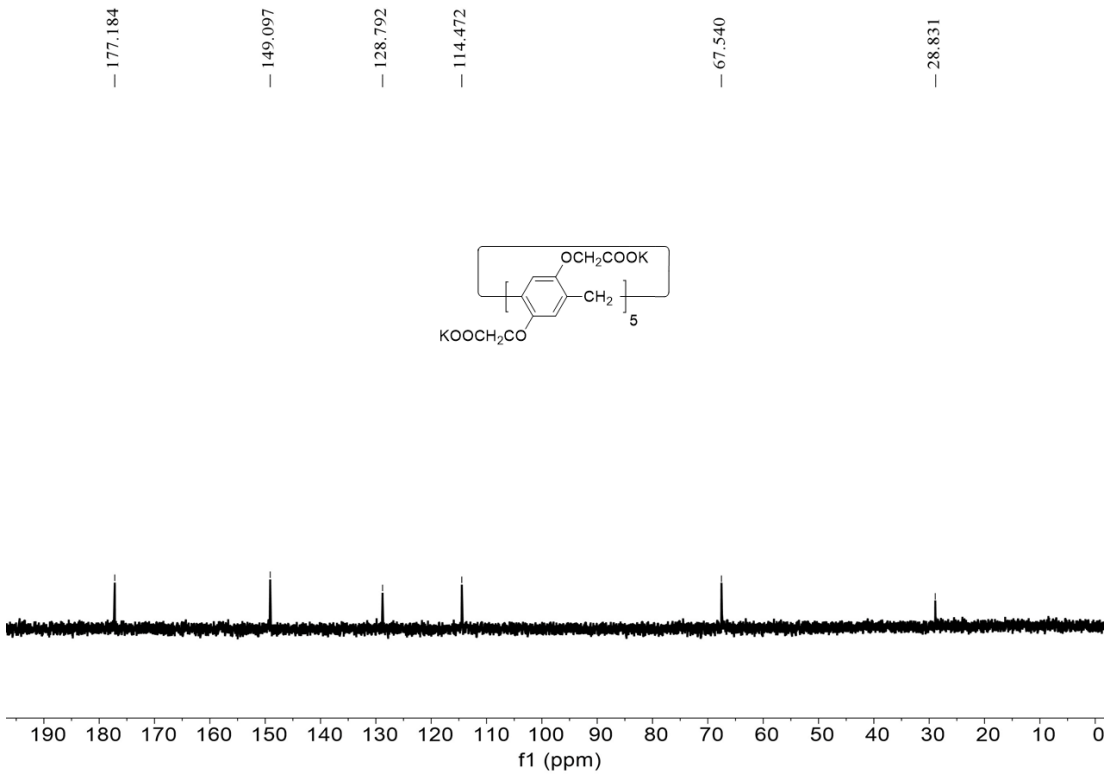


Figure S7. ^{13}C NMR spectra of **WP5-K** in D_2O at 298 K.

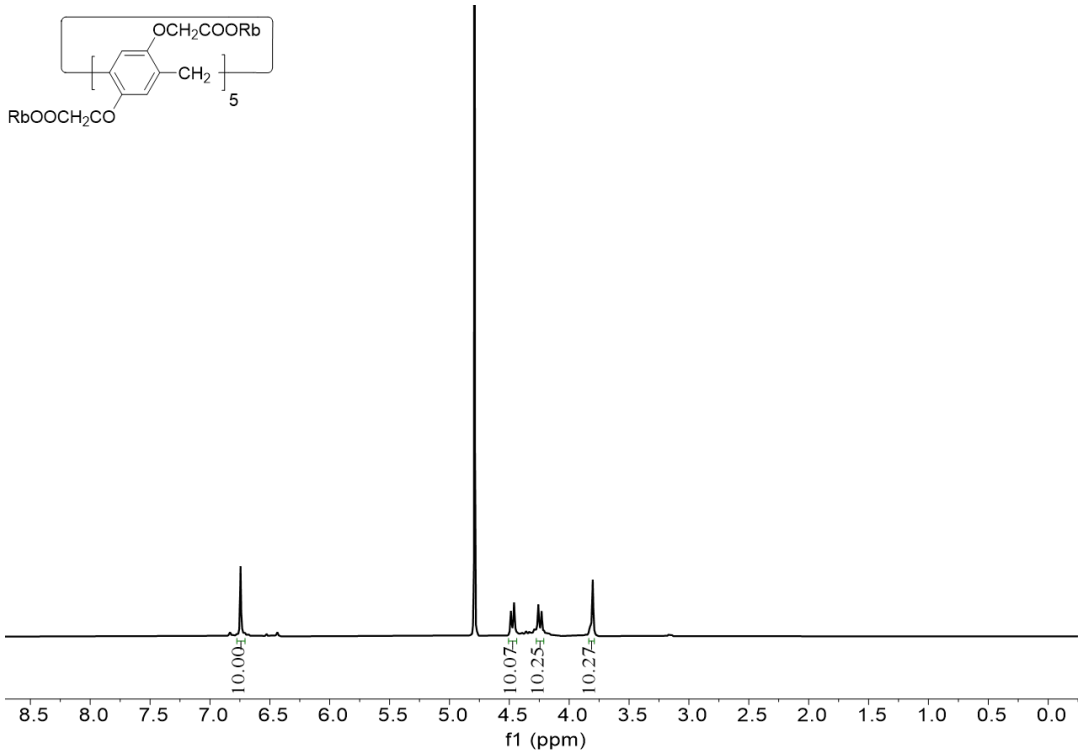


Figure S8. ^{1}H NMR spectra of **WP5-Rb** in D_2O at 298 K.

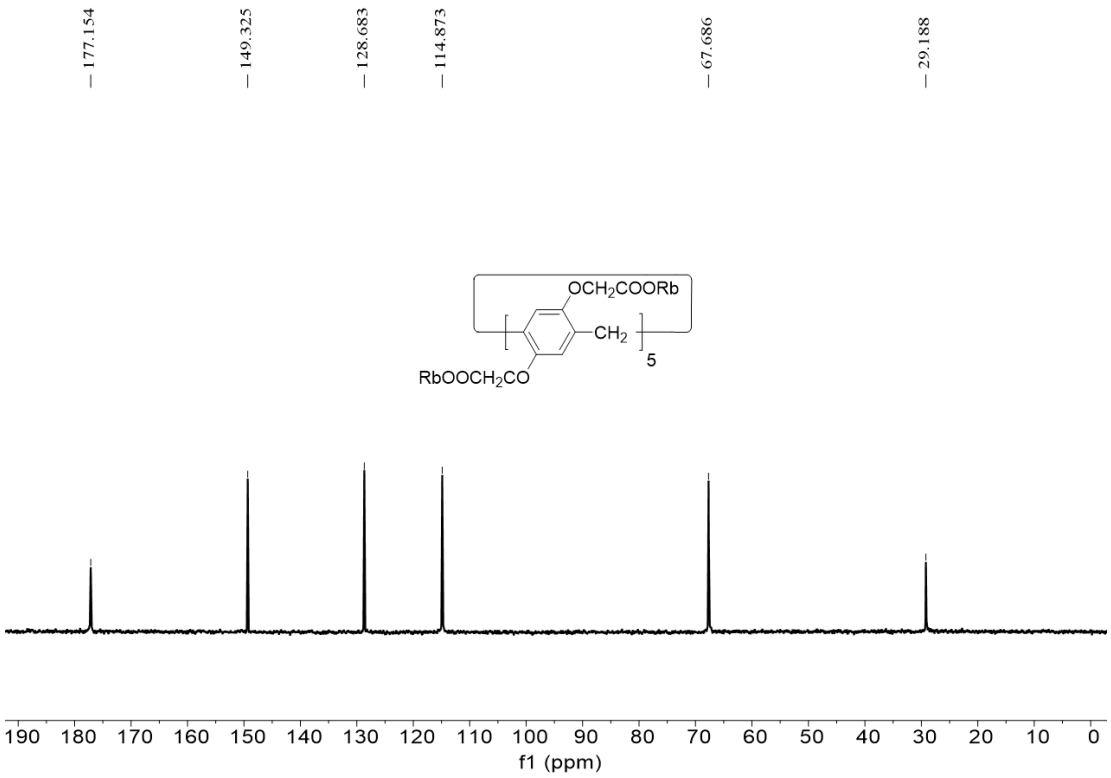


Figure S9. ^{13}C NMR spectra of **WP5-Rb** in D_2O at 298 K.

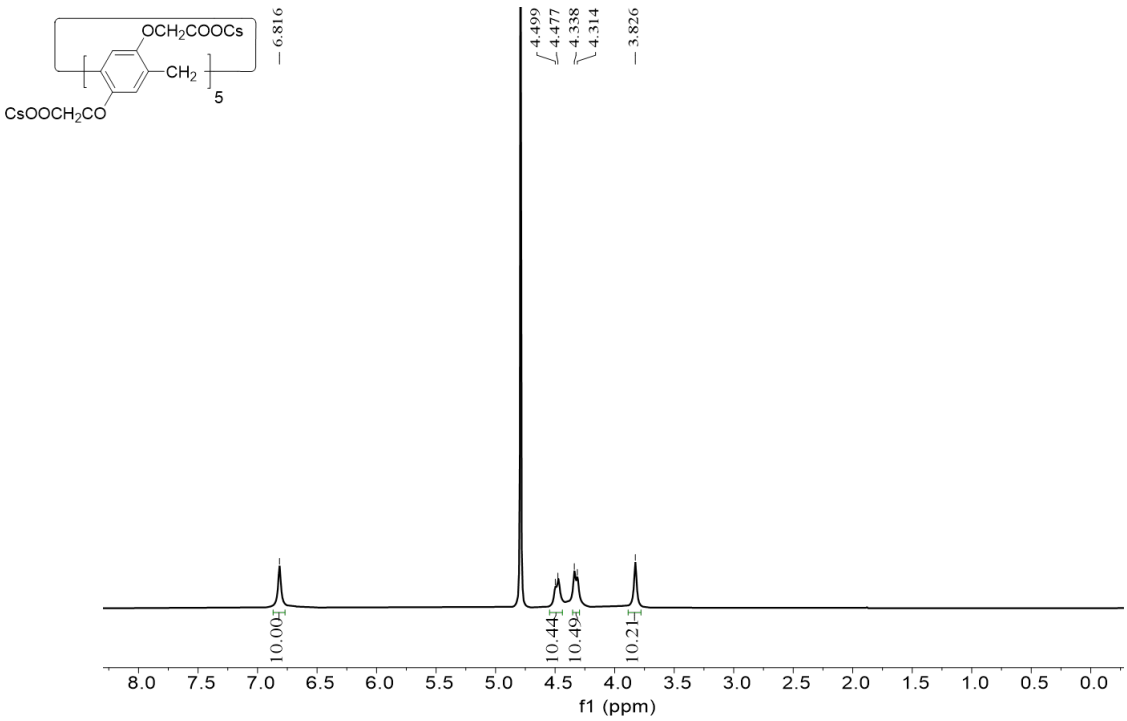


Figure S10. ^{1}H NMR spectra of **WP5-Cs** in D_2O at 298 K.

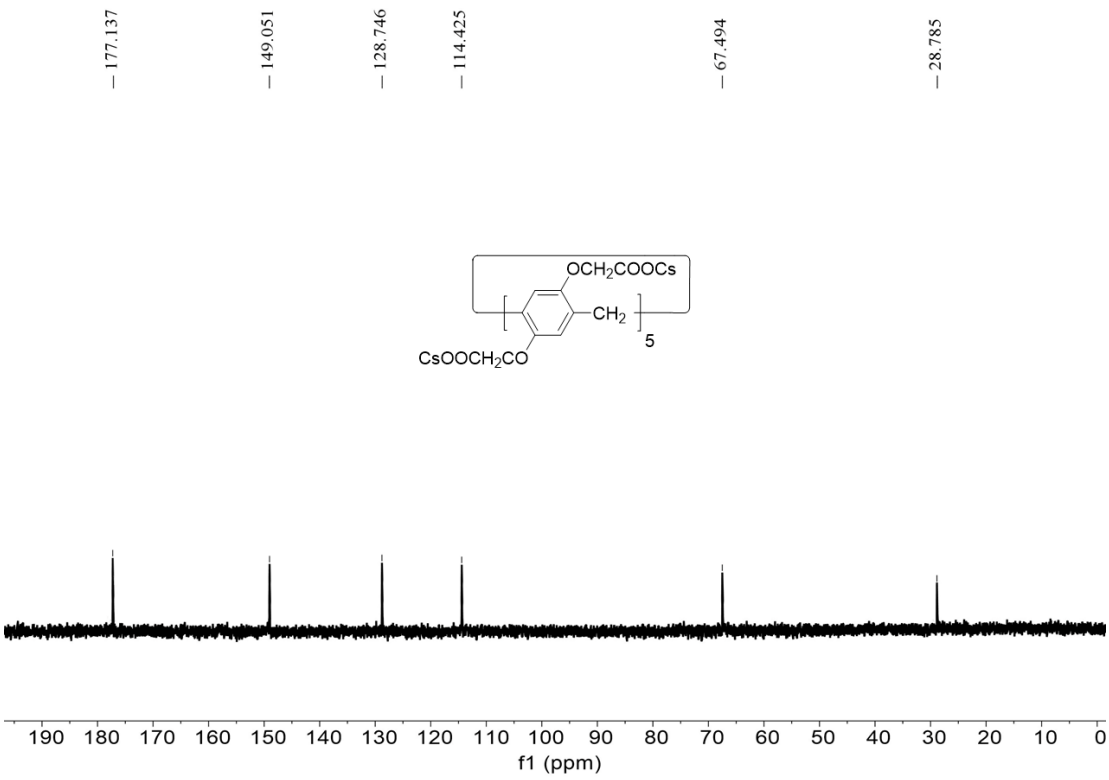


Figure S11. ^{13}C NMR spectra of **WP5-Cs** in D_2O at 298 K.

3. Dynamic NMR Studies

(1). ^{1}H NMR line shape analysis

Rotational barriers of rotors **WP5-M** were measured via variable temperature (VT) ^{1}H NMR by monitoring the broadening of diastereotopic methylene protons in the rims of **WP5-M**. Rates of exchange k_{ex} were obtained by line width analysis with the equation $k_{ex} = \pi(h - h_0)$, where h represented the width of peak at half height, h_0 represented the width of peak at slow or no exchange.[S3] The concentration of rotors were 10 mM. All VT experiments were performed three times.

(2). Kinetic parameters

By using the exchange rates (k_{ex}, s^{-1}) obtained from line width analysis of the VT ^{1}H NMR spectra, the enthalpy change ($\Delta H^{\ddagger}$) and entropy change ($\Delta S^{\ddagger}$) of the transition state were calculated from Eyring plots:

$$\ln\frac{k}{T} = -\frac{\Delta H^{\ddagger}}{R}\frac{1}{T} + \frac{\Delta S^{\ddagger}}{R} + \ln\left(\frac{k_B}{h}\right)$$

where k is the exchange rate constant, T is the absolute temperature, $\Delta H^{\ddagger}$ is the enthalpy of activation, R is the universal gas constant, k_B is the Boltzmann constant, h is the Planck's constant, and $\Delta S^{\ddagger}$ is the entropy of activation. The free energy of activation ($\Delta G^{\ddagger}$) was calculated through Gibbs equation: $\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$.

(3). VT NMR spectrum and Eyring plots of WP5-M

Since the chemical shift of deuterium oxide in NMR spectrum could shift with the increase of temperature, the chemical shifts (δ) for VT ^{1}H NMR spectra, given in ppm, are referenced to the proton signal of phenolic rings in **WP5-M**.

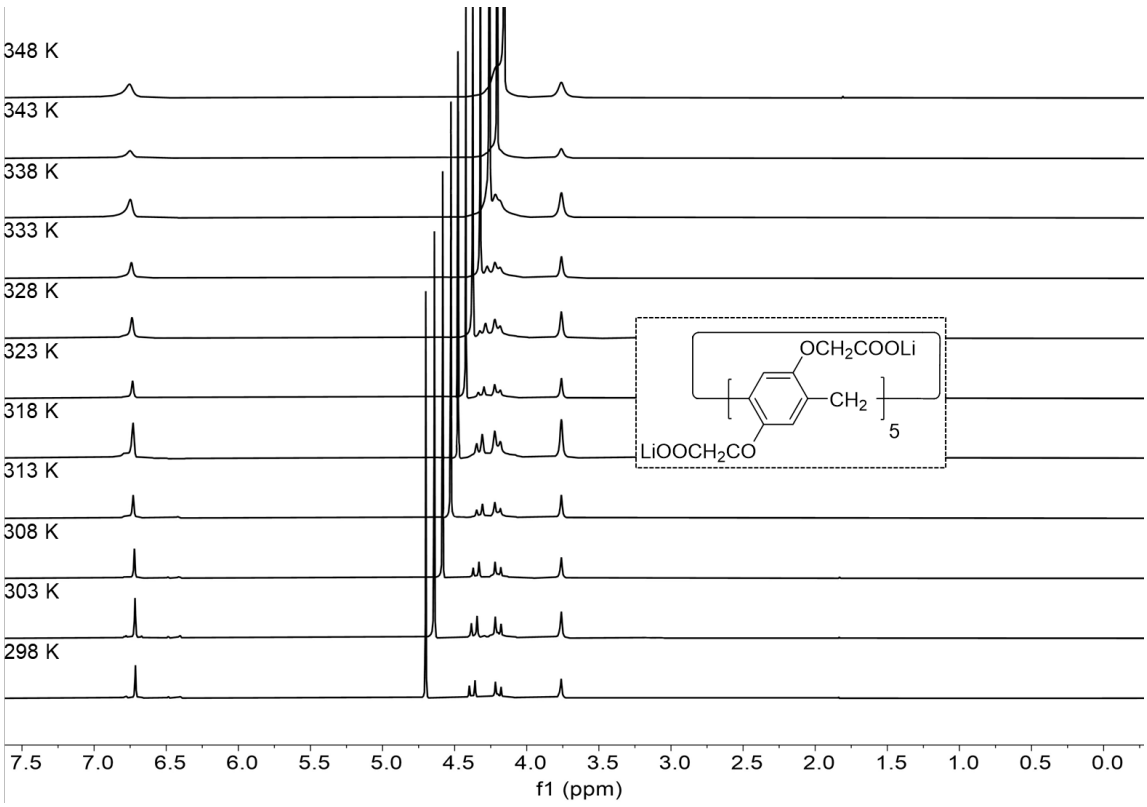


Figure S12. VT NMR spectra of **WP5-Li** in D_2O between 298 K and 348 K.

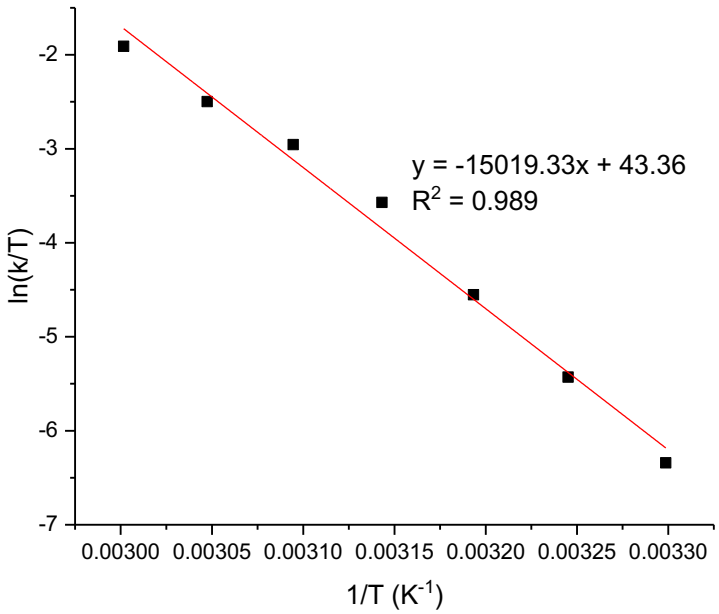


Figure S13. Eyring plot of the rates of exchange in D_2O obtained from line width analysis of methene protons on **WP5-Li**. The barrier ($\Delta G^{\ddagger}$ = 18.23 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 29.83 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = 38.92 cal·mol^{-1}·K^{-1}).

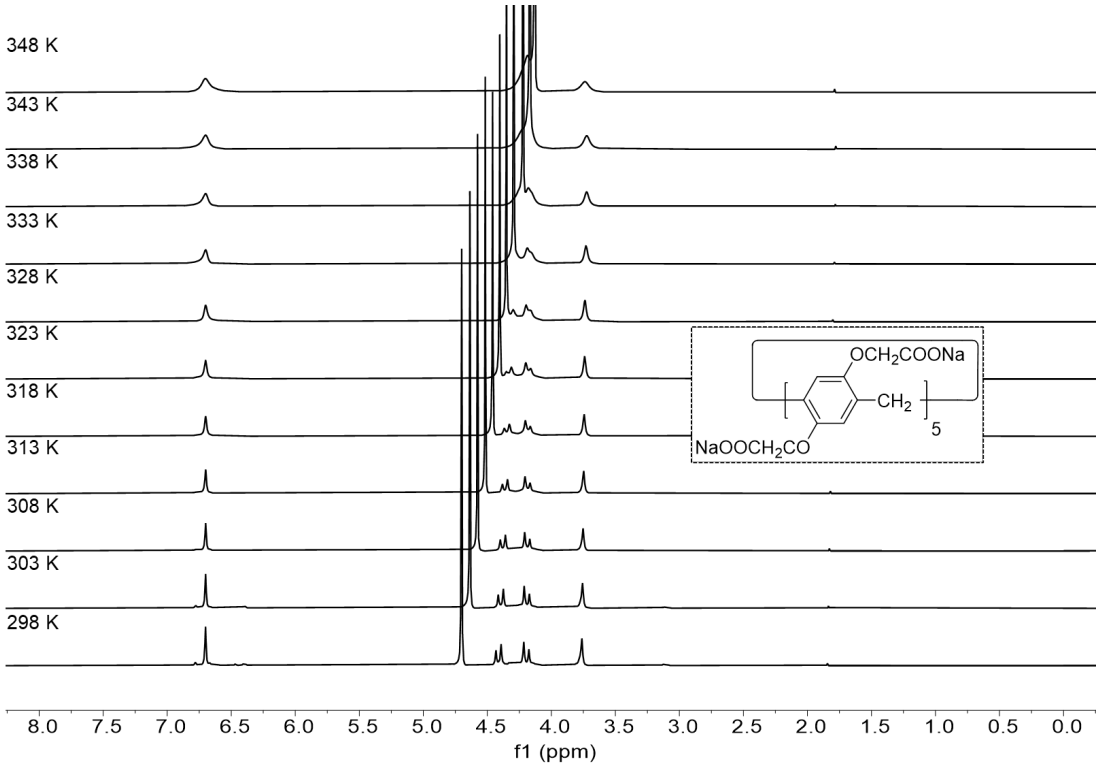


Figure S14. VT NMR spectra of **WP5-Na** in D_2O between 298 K and 348 K.

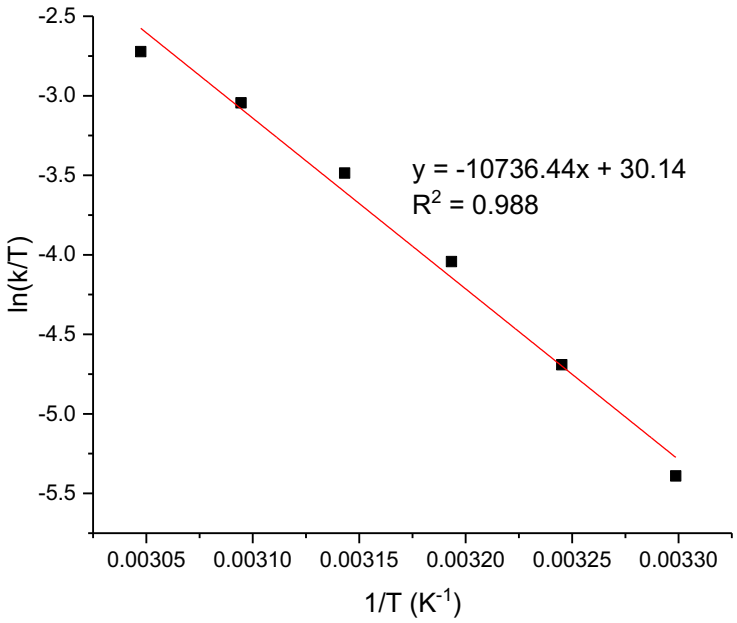


Figure S15. Eyring plot of the rates of exchange in D_2O obtained from line width analysis of methene protons on **WP5-Na**. The barrier ($\Delta G^{\ddagger}$ = 17.55 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 21.32 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = 12.67 cal·mol^{-1}·K^{-1}).

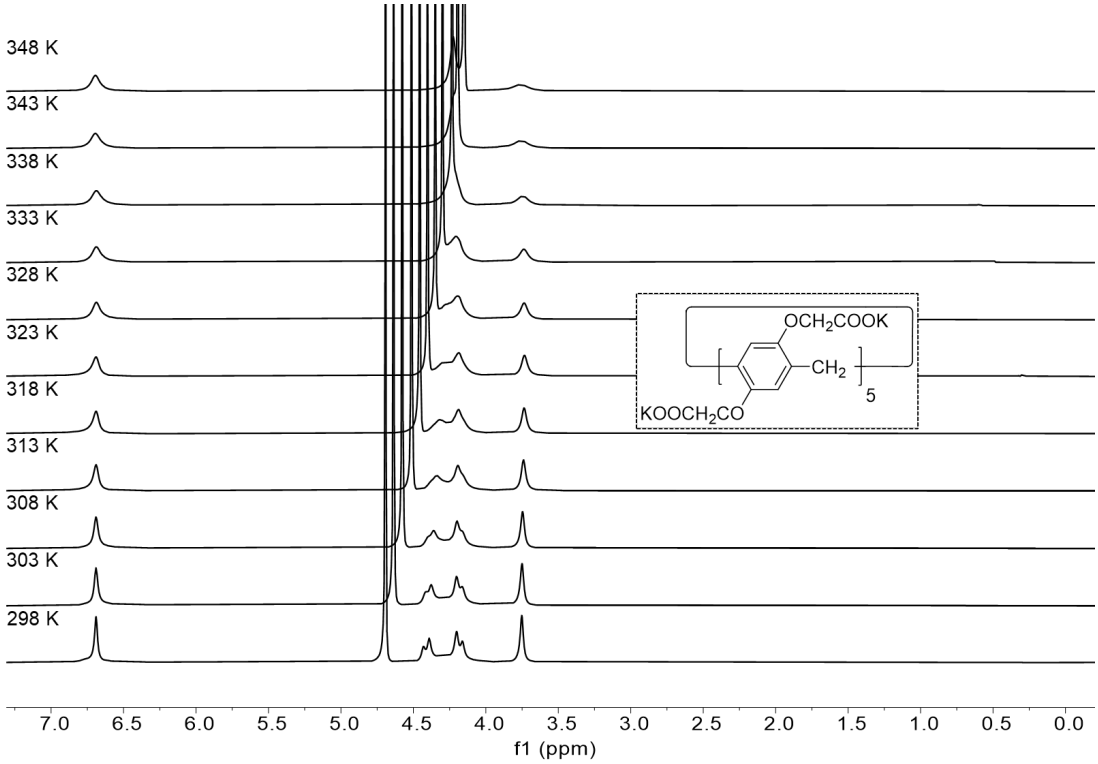


Figure S16. VT NMR spectra of **WP5-K** in D_2O between 298 K and 348 K.

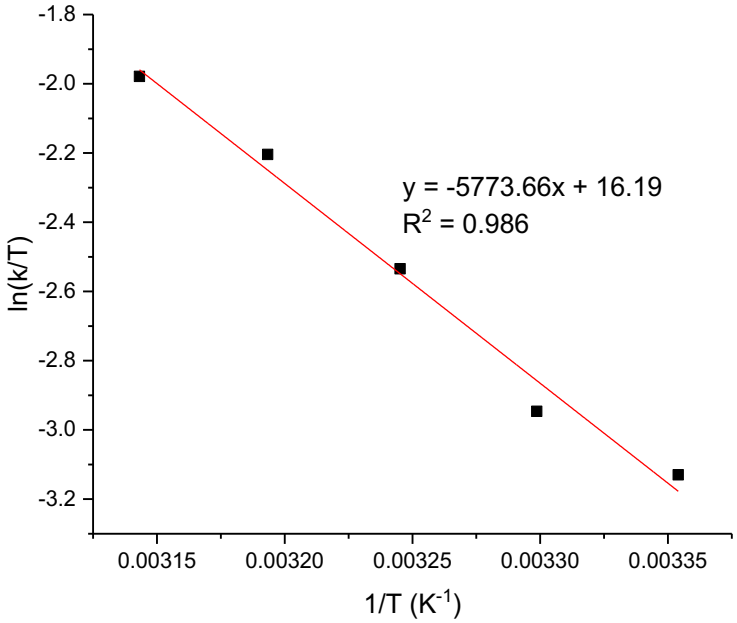


Figure S17. Eyring plot of the rates of exchange in D_2O obtained from line width analysis of methene protons on **WP5-K**. The barrier ($\Delta G^{\ddagger}$ = 15.95 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 11.47 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = -15.04 cal·mol^{-1}·K^{-1}).

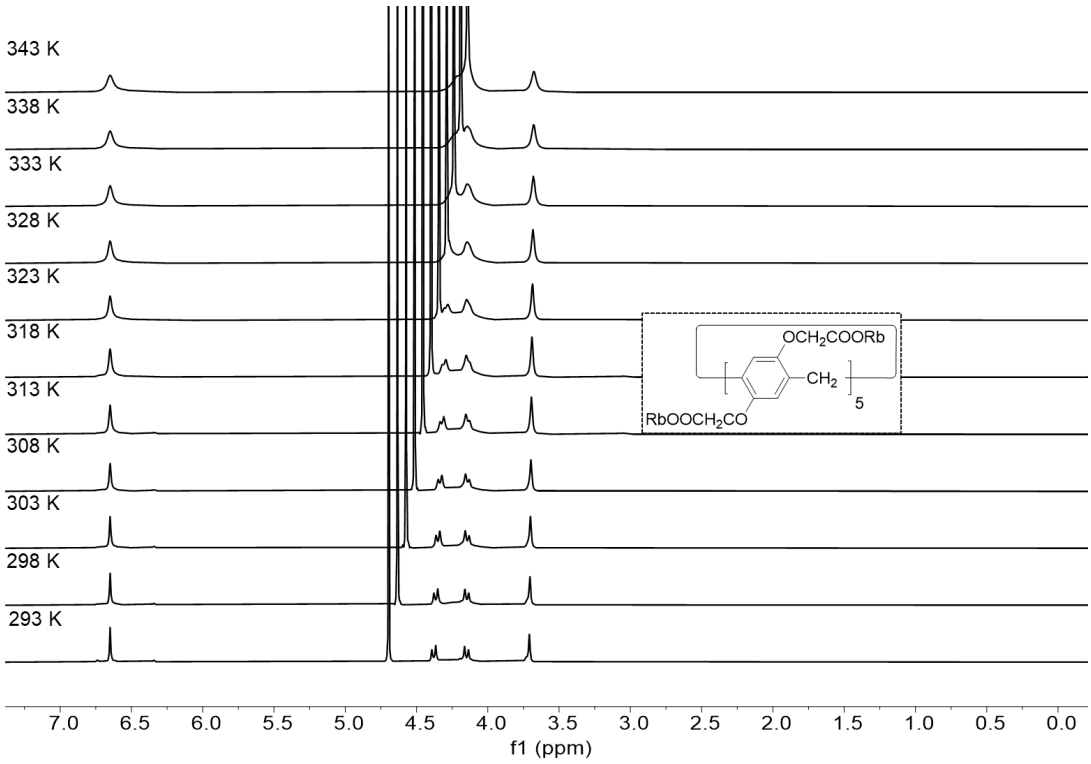


Figure S18. VT NMR spectra of **WP5-Rb** in D_2O between 293 K and 343 K.

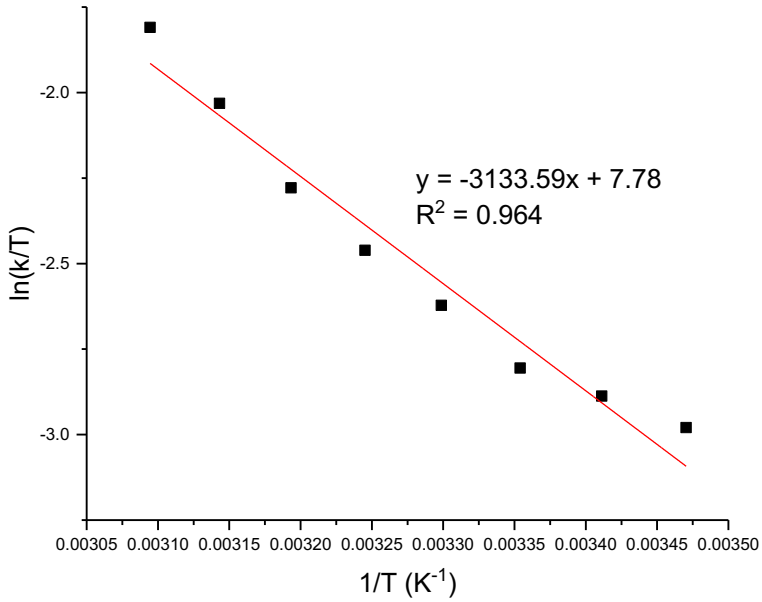


Figure S19. Eyring plot of the rates of exchange in D_2O obtained from line width analysis of methene protons on **WP5-Rb**. The barrier ($\Delta G^{\ddagger}$ = 15.68 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 6.22 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = -31.74 cal·mol^{-1}·K^{-1}).

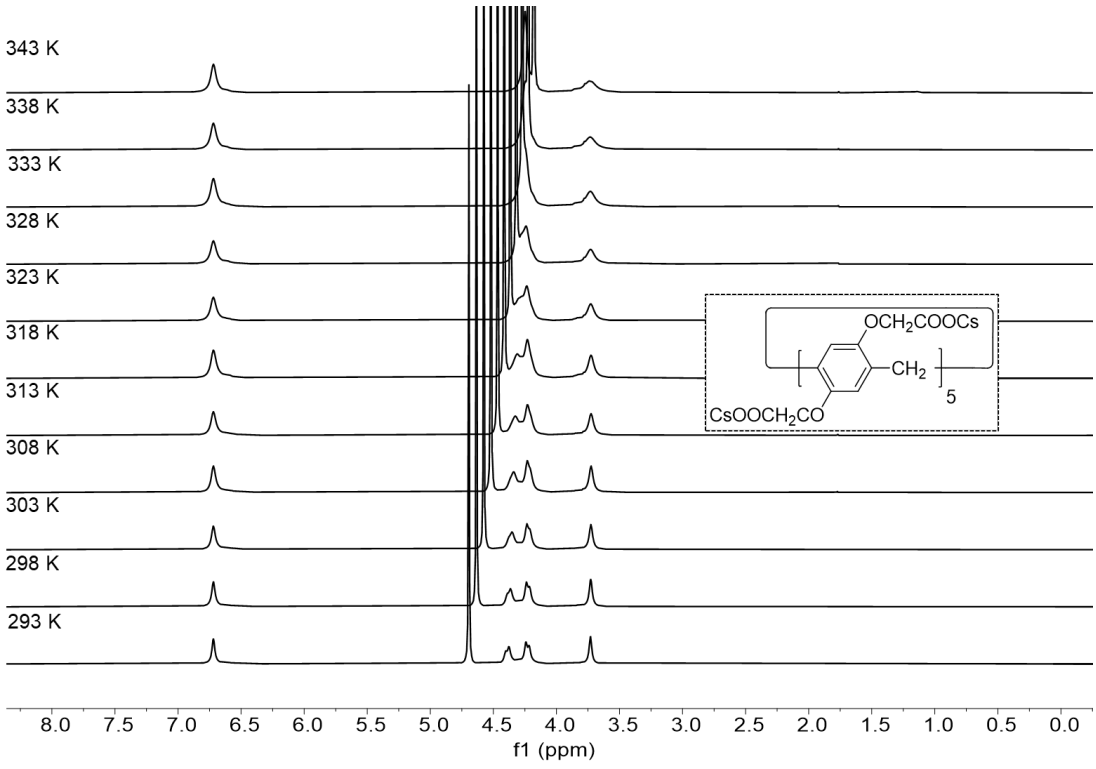


Figure S20. VT NMR spectra of **WP5-Cs** in D_2O between 293 K and 343 K.

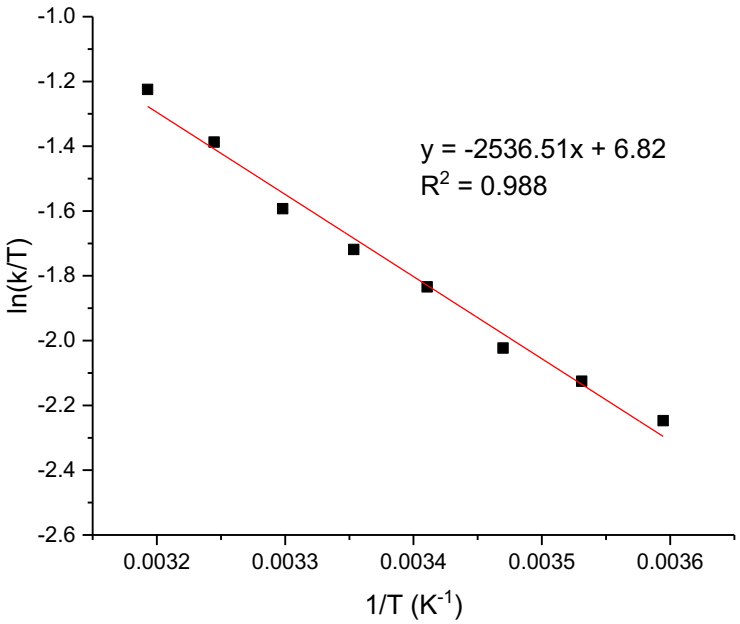


Figure S21. Eyring plot of the rates of exchange in D_2O obtained from line width analysis of methene protons on **WP5-Cs**. The barrier ($\Delta G^{\ddagger}$ = 15.06 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 5.04 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = -33.65 cal·mol^{-1}·K^{-1}).

4. Theoretical calculation

All computational calculations were carried out with Gaussian 16 software.[S4] The potential energy surface have been scanned using semi-empirical PM6 method with dispersion correction (PM6-D3). [S5,S6] The plane α was defined as original point (rotary part in horizontal position), where rotation to up and down corresponds to negative and position directions, respectively (**Figure S33a**). To give a further description of the relative position of cations in cavities of **WP5**, the angle between cation and two neighboring carbonyl oxygen atoms (θ) was also displayed (**Figure S33a**). The sampled configurations from the scanned structures were further optimized using the B3LYP-D3 functional. [S7-S10] The standard 6-31G(d) and 6-31G+(d) basis sets were used for nonmetal atoms and metal Li, Na and K, respectively.

The interaction energies are defined as:

$$E_{int} = E_{complex} - E_h - E_m$$

where E_{int} is the interactions between **WP5** and different metal, $E_{complex}$ is the total energy of the self-assembly formed by **WP5** and metal, E_h and E_m are the energy of **WP5** and different metals, respectively. The energies were calculated by the dispersion-corrected functional B3LYP-D3 with 6-31G(d) basis set for nonmetal atoms. The 6-31G+(d) basis sets were used for metal Li, Na and K, respectively.

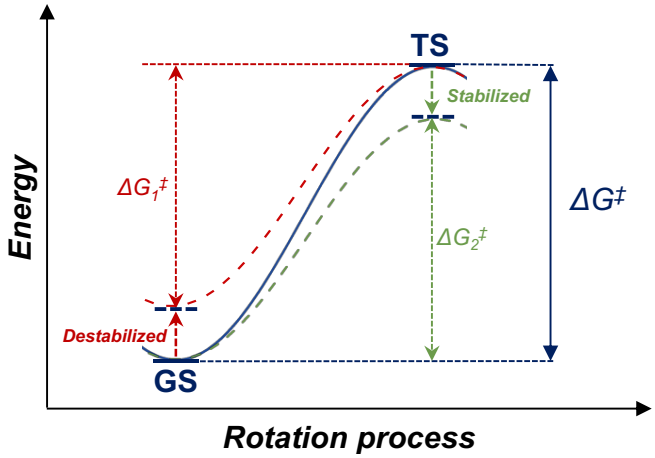


Figure S22. Relative energy between ground state (GS) and transition state (TS) of **WP5-M**. The impact of counter cations on GS or TS could change rotational barriers.

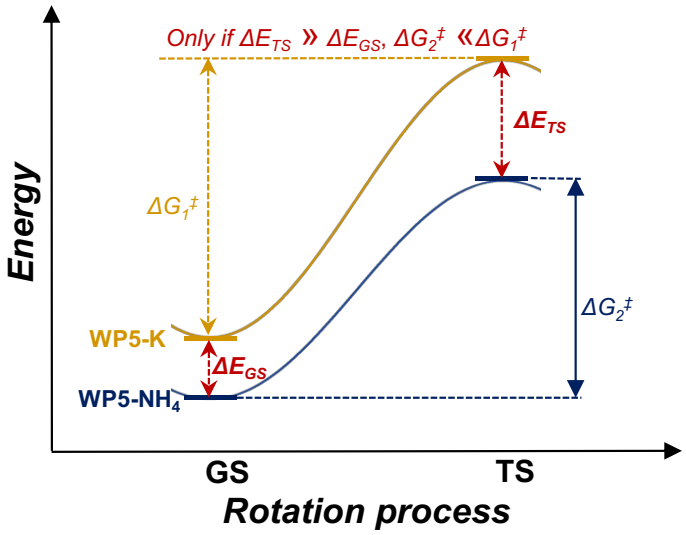


Figure S23. Relative energy between ground state (GS) and transition state (TS) of **WP5-K** and **WP5-NH4**. Only if ΔE_{TS} was much bigger than ΔE_{GS}, rotational barriers of **WP5-NH4** would much lower than that of **WP5-K** (*i.e.*, complied with experimental results), which indicated the effect of cations on transition states was much greater than that on ground states.

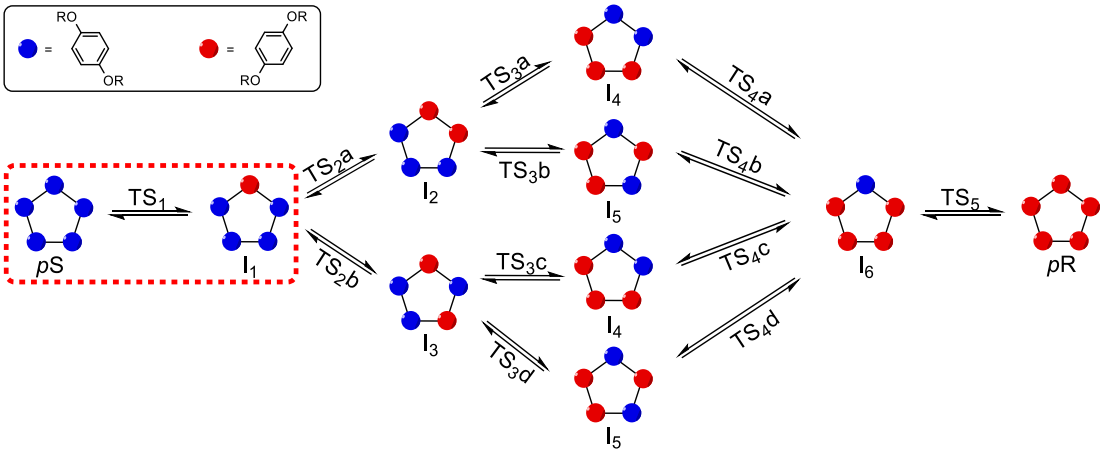


Figure S24. Pathways of transformation between *p*S and *p*R conformers of **WP5-M**.

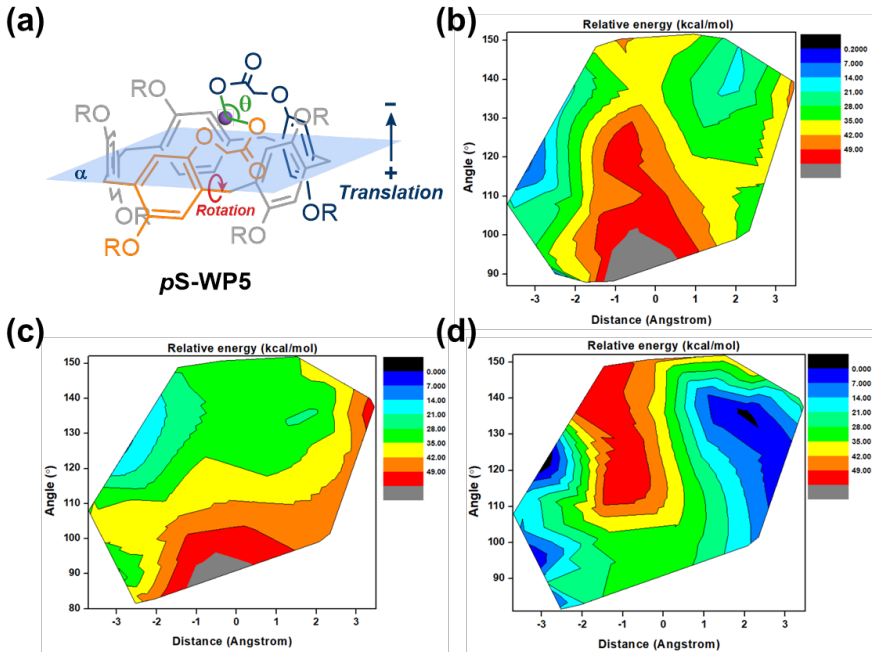


Figure S25. (a) Illustration of configuration for **WP5** when ion is located in different positions of cavity. The potential energy surface of **WP5** with Li (b), Na (c) and K (d) using semi-empirical PM6 method with dispersion correction (PM6-D3).

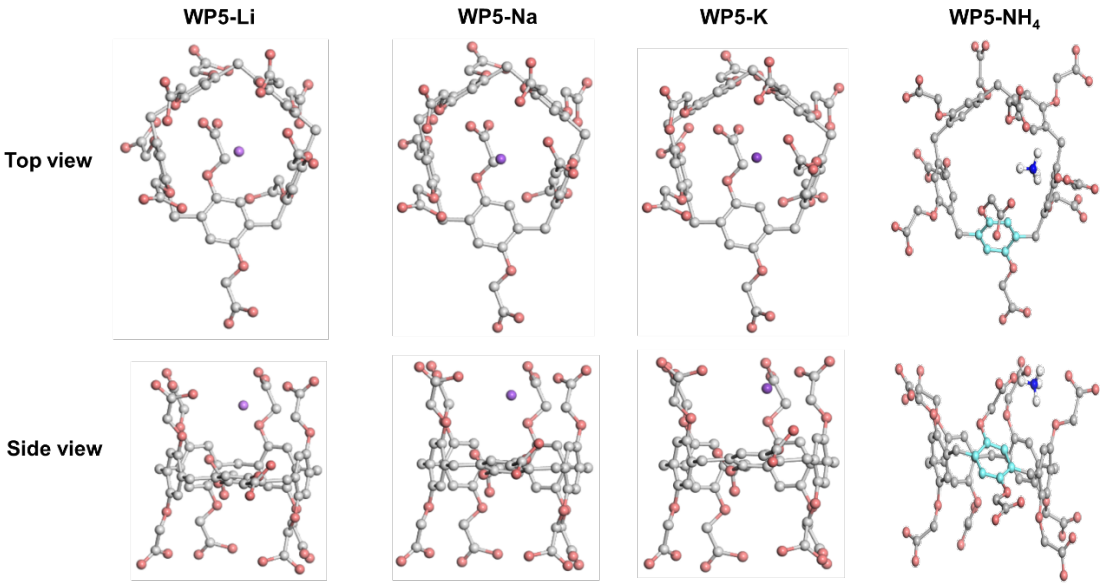


Figure S26. The sampled highest-energy configurations from the scanned structures at the PM6-D3 level for **WP5-Li**, **WP5-Na**, **WP5-K** and **WP5-NH$_4$**.

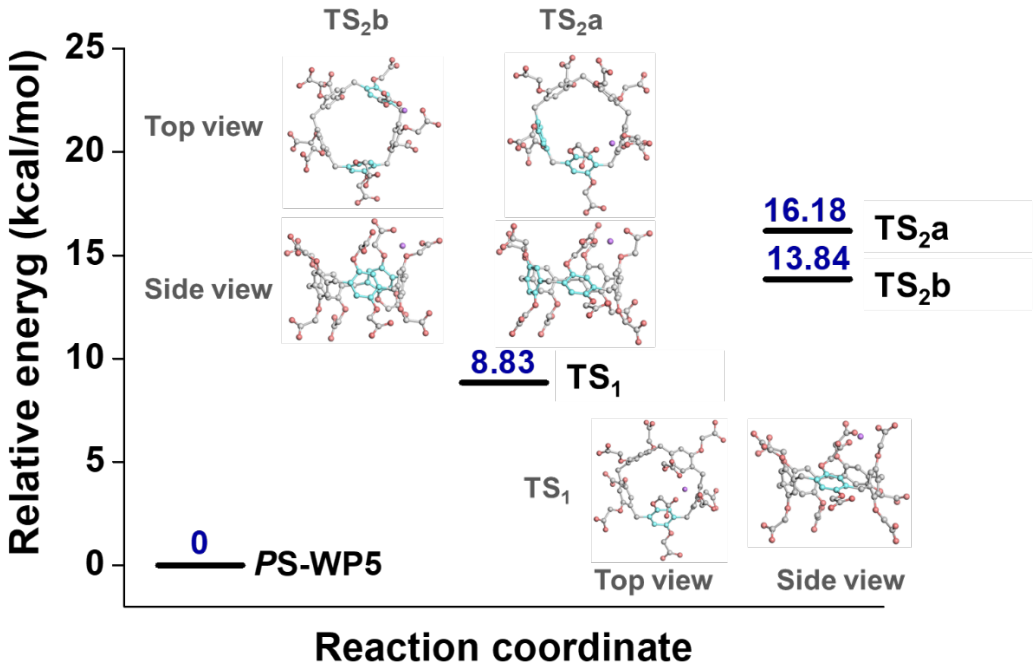


Figure S27. Relative energy diagram and optimized geometric structures of two intermediates in TS_1 and TS_2 for **WP5-Li** using B3LYP-D3 functional.

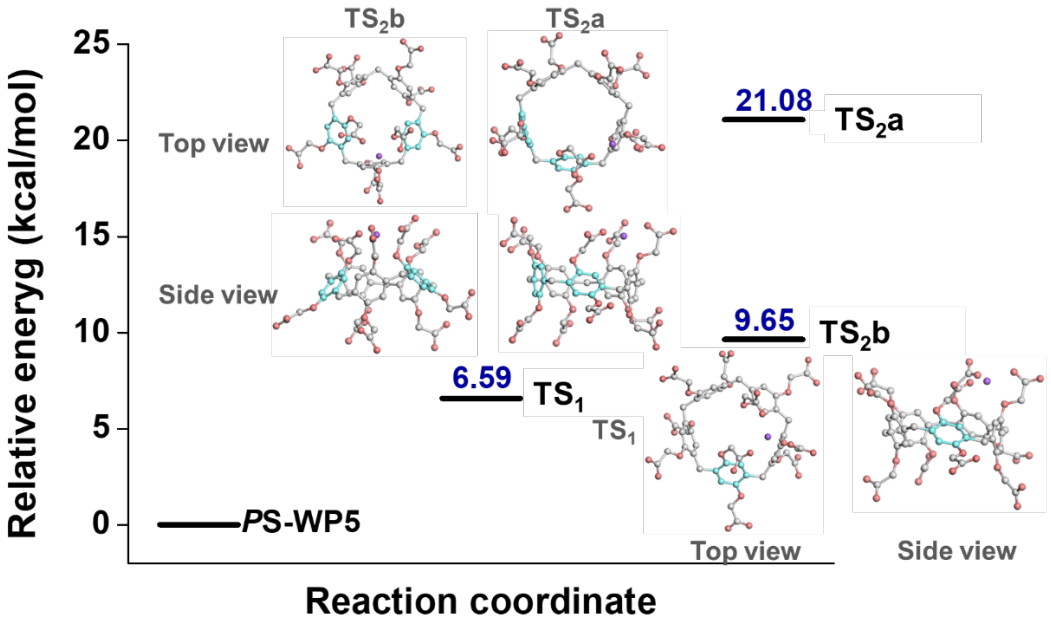


Figure S28. Relative energy diagram and optimized geometric structures of two intermediates in TS_1 and TS_2 for **WP5-Na** using B3LYP-D3 functional.

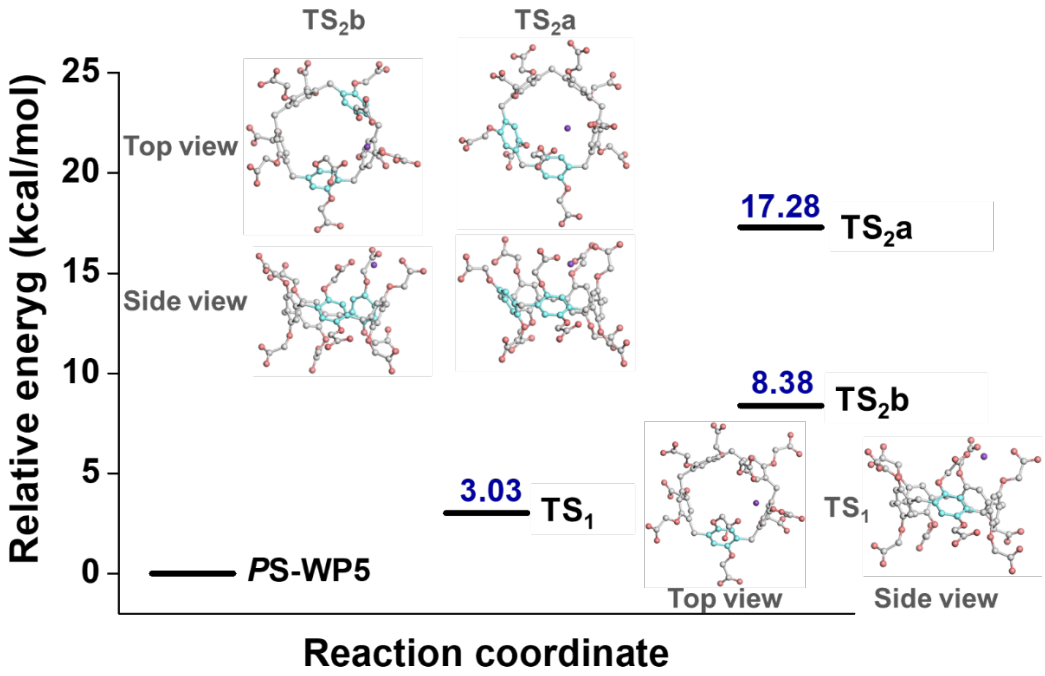


Figure S29. Relative energy diagram and optimized geometric structures of two intermediates in TS_1 and TS_2 for **WP5-K** using B3LYP-D3 functional.

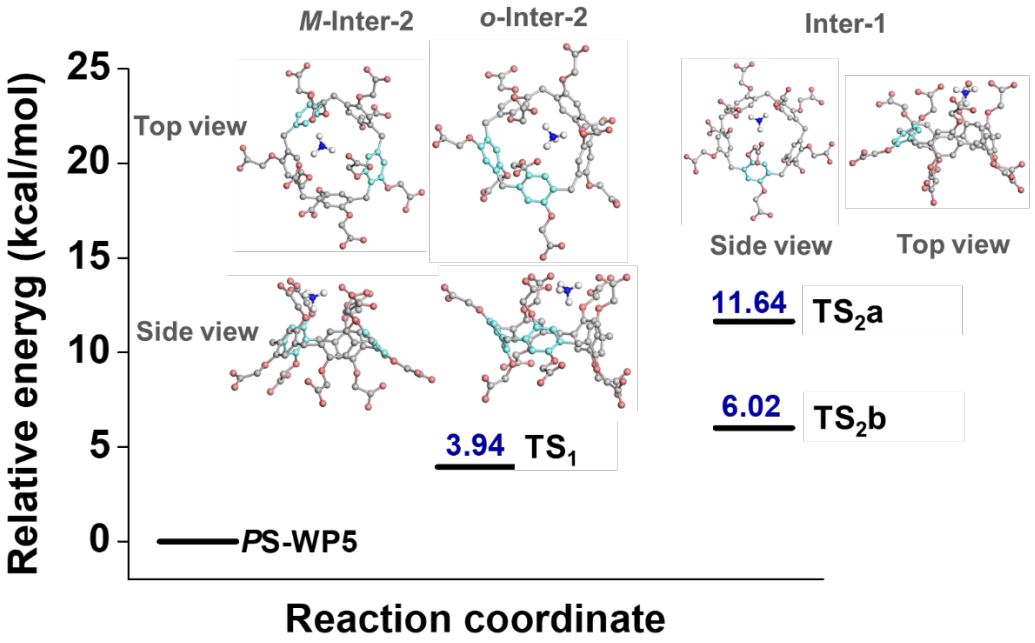


Figure S30. Relative energy diagram and optimized geometric structures of two intermediates in TS_1 and TS_2 for **WP5-NH$_4$** using B3LYP-D3 functional.

Table S1. The summery of binding energy (kcal/mol) between cations and **WP5** anion in GS and TS_1.

	Li^+	Na^+	K^+	NH_4^+
E_{GS}	−493.42	−464.44	−461.67	−513.48
E_{TS}	−535.02	−499.05	−465.84	−515.28

The binding energy in TS_1 was higher than that in GS, which indicated stronger stabilizing effect of cations on TS_1 than GS.

Table S2. Summary of calculated rotational barriers (kcal/mol) of **WP5-Li**, **WP5-Na**, **WP5-K** and **WP5-NH$_4$**.

	$\Delta G^{\ddagger}_{TS1}$	$\Delta G^{\ddagger}_{TS2a}$	$\Delta G^{\ddagger}_{TS2b}$
WP5-Li	8.83	16.18	13.84
WP5-Na	6.59	21.08	9.65
WP5-K	3.03	17.28	8.38
WP5-NH$_4$	3.94	11.64	6.02

5. Solvent effect

Since the chemical shift of deuterium oxide in NMR spectrum could shift with the increase of temperature, the chemical shifts (δ) for VT ^{1}H NMR spectra in mixed solvent, given in ppm, are referenced to the proton signal of methanol-d_4 or DMSO-d_6. **WP5-Na** was chosen as the model compound to explore the effect of ionic solvation on rotational barriers of **WP5-M** in mixed solvent (D_2O mixed with polar protic solvent methanol-d_4, or polar aprotic solvent DMSO-d_6). For further verifing our conclusion, VT studies of the remaining **WP5-M** in D_2O/methanol-d_4 were performed.

Table S3. The summery of kinetic parameters of **WP5-M** in different solvent.

Compound[a]	Solvent[b]	$\Delta H^{\ddagger}$ (kcal·mol^{-1})	$\Delta S^{\ddagger}$ (cal·mol^{-1}·K^{-1})	$\Delta G^{\ddagger}_{298K}$ (kcal·mol^{-1})
WP5-Li	D_2O	29.83	38.92	18.23
	D_2O/CD_3OD	31.09	42.99	18.28
WP5-Na	D_2O	21.32	12.67	17.55
	D_2O/CD_3OD	21.46	12.97	17.59
	D_2O/DMSO-d_6	21.39	12.87	17.55
WP5-K	D_2O	11.47	−15.04	15.95
	D_2O/CD_3OD	11.65	−14.46	15.96
WP5-Rb	D_2O	6.22	−31.74	15.68
	D_2O/CD_3OD	6.47	−31.02	15.71
WP5-Cs[c]	D_2O	5.04	−33.65	15.06
	D_2O/CD_3OD	-	-	-

(a). The concentration of rotors was 10 mM; (b). v/v of D_2O/CD_3OD = 2:1; v/v of D_2O/DMSO-d_6 = 2:1; (c). It was a failure to obtain kinetic parameters of **WP5-Cs** in mixed solvent since the limited solubility of **WP5-Cs**.

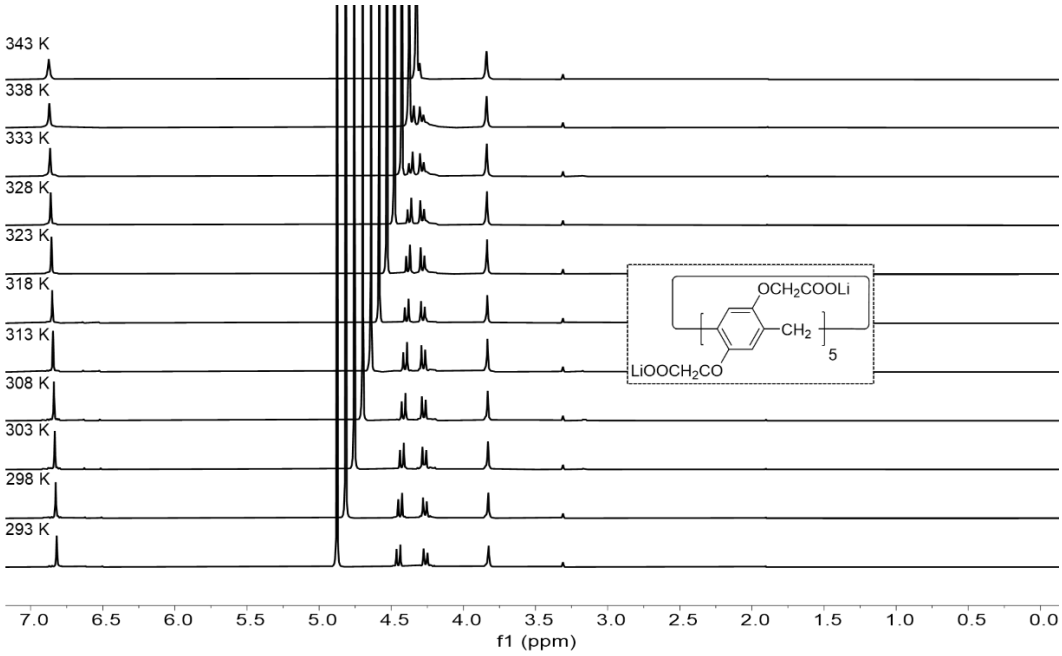


Figure S31. VT NMR spectra of **WP5-Li** in mixed solvent (v/v of D_2O/CD_3OD = 2:1) between 293 K and 343 K.

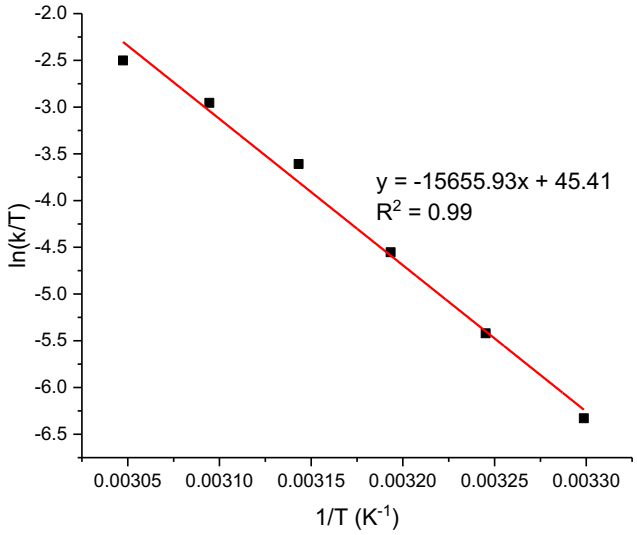


Figure S32. Eyring plot of the rates of exchange in mixed solvent obtained from line width analysis of methene protons on **WP5-Li**. The barrier ($\Delta G^{\ddagger}$ = 18.28 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 31.09 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = 42.99 cal·mol^{-1}·K^{-1}).

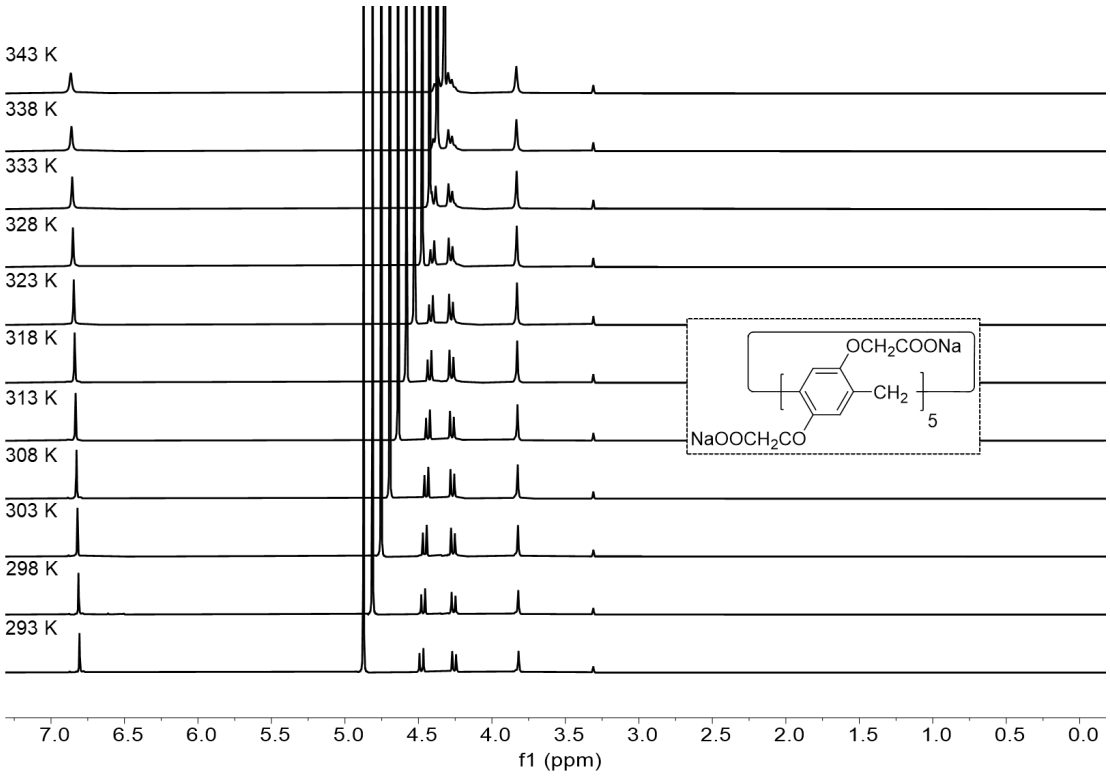


Figure S33. VT NMR spectra of **WP5-Na** in mixed solvent (v/v of D_2O/CD_3OD = 2:1) between 293 K and 343 K.

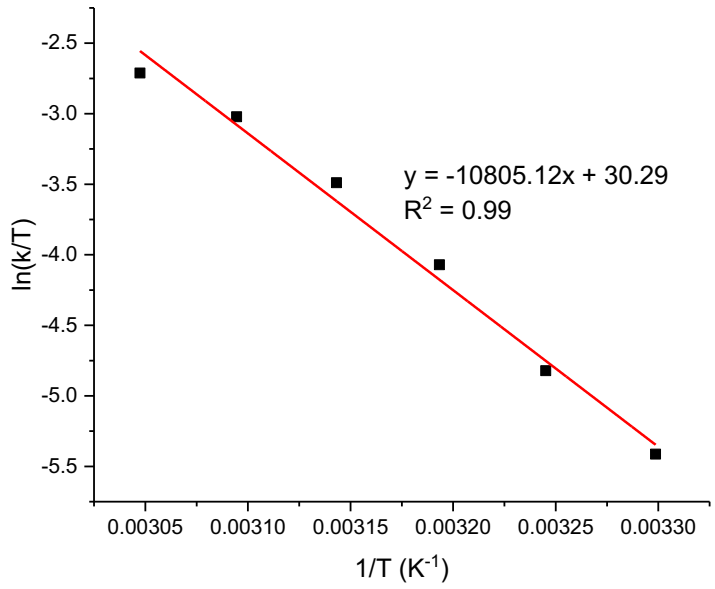


Figure S34. Eyring plot of the rates of exchange in mixed solvent obtained from line width analysis of methene protons on **WP5-Na**. The barrier ($\Delta G^{\ddagger}$ = 17.59 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 21.46 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = 12.97 cal·mol^{-1}·K^{-1}).

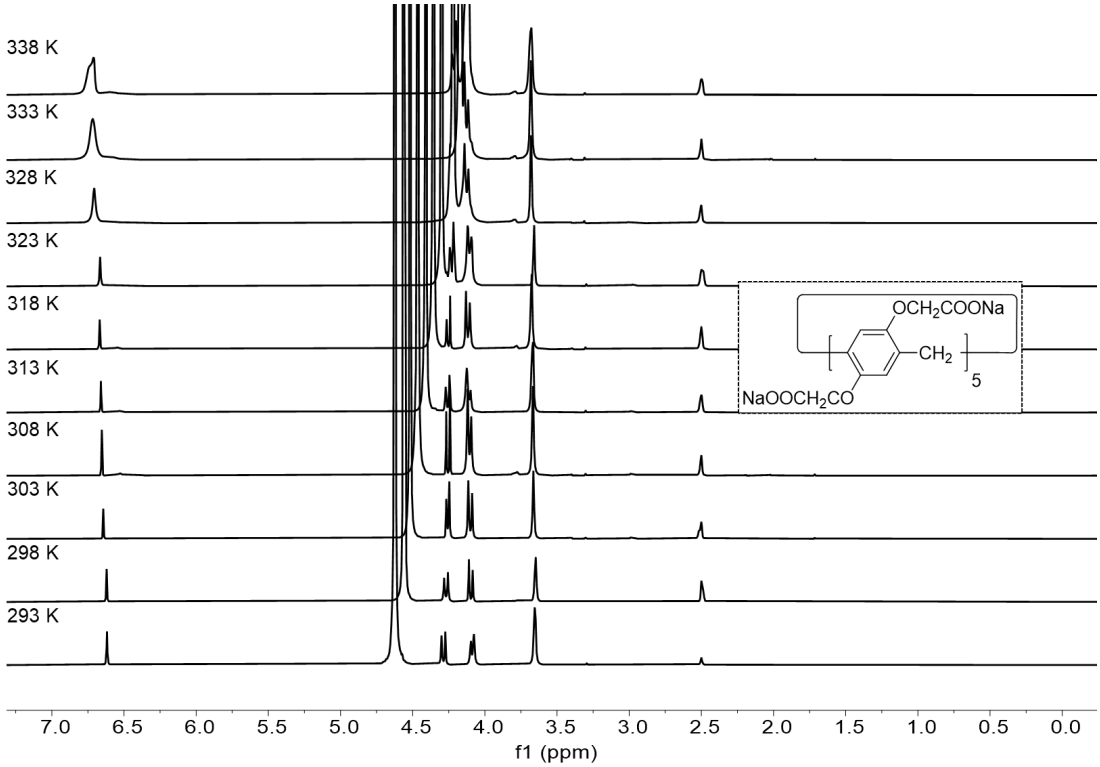


Figure S35. VT NMR spectra of **WP5-Na** in mixed solvent (v/v of D_2O/DMSO-d_6 = 2:1) between 293 K and 338 K.

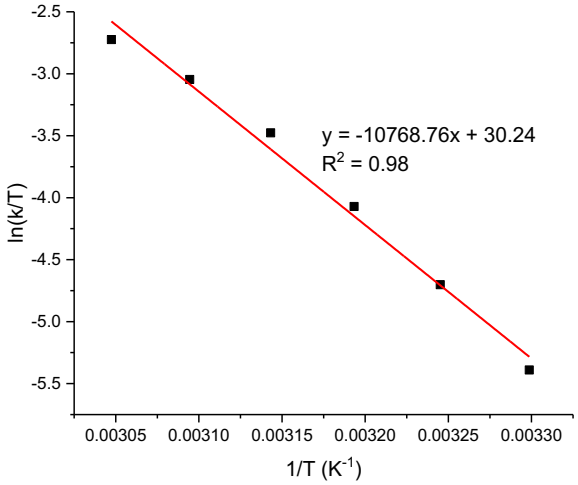


Figure S36. Eyring plot of the rates of exchange in mixed solvent obtained from line width analysis of methene protons on **WP5-Na**. The barrier ($\Delta G^{\ddagger}$ = 17.55 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 21.39 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = 12.87 cal·mol^{-1}·K^{-1}).

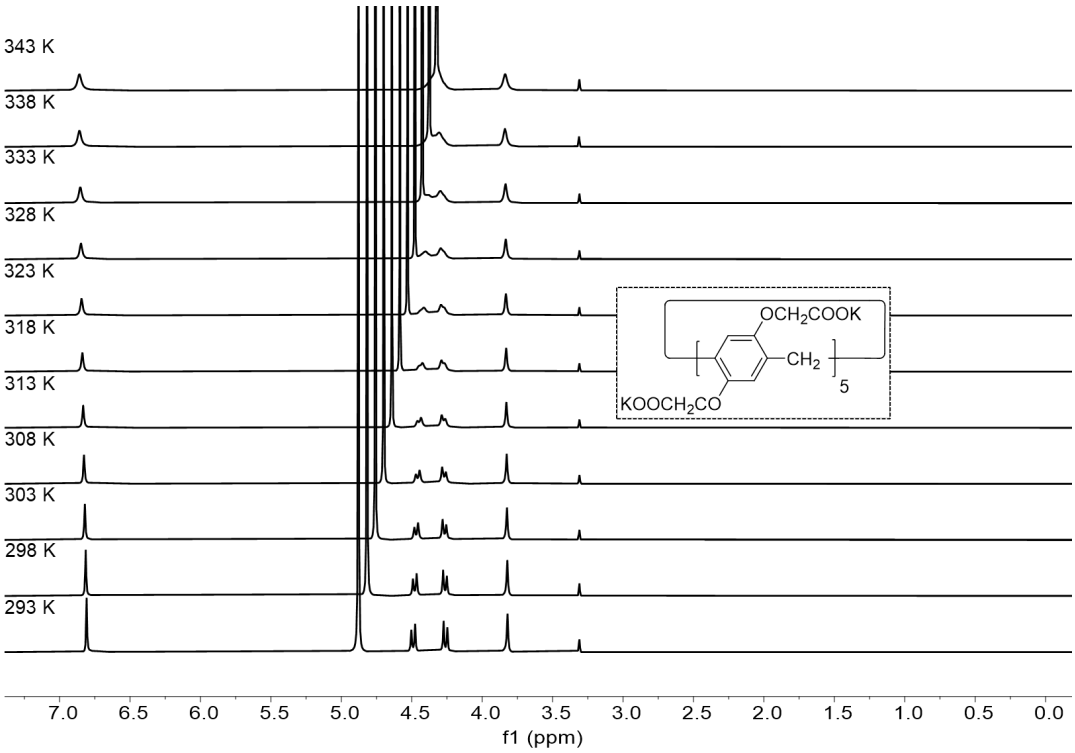


Figure S37. VT NMR spectra of **WP5-K** in mixed solvent (v/v of D_2O/CD_3OD = 2:1) between 293 K and 343 K.

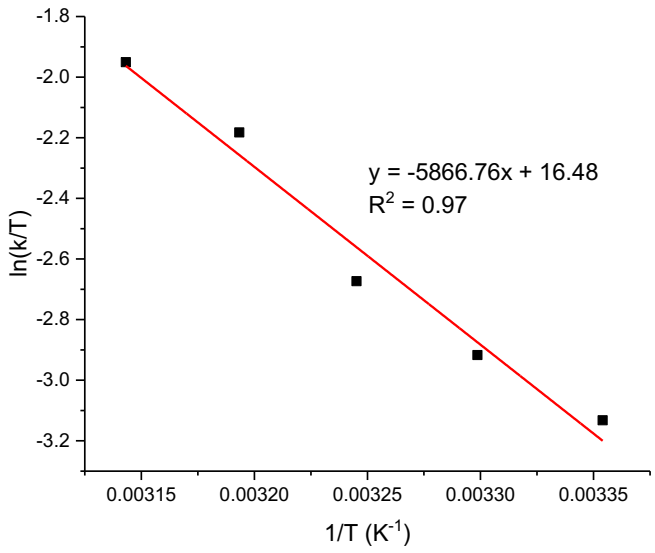


Figure S38. Eyring plot of the rates of exchange in mixed solvent obtained from line width analysis of methene protons on **WP5-K**. The barrier ($\Delta G^{\ddagger}$ = 15.96 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 11.65 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = -14.46 cal·mol^{-1}·K^{-1}).

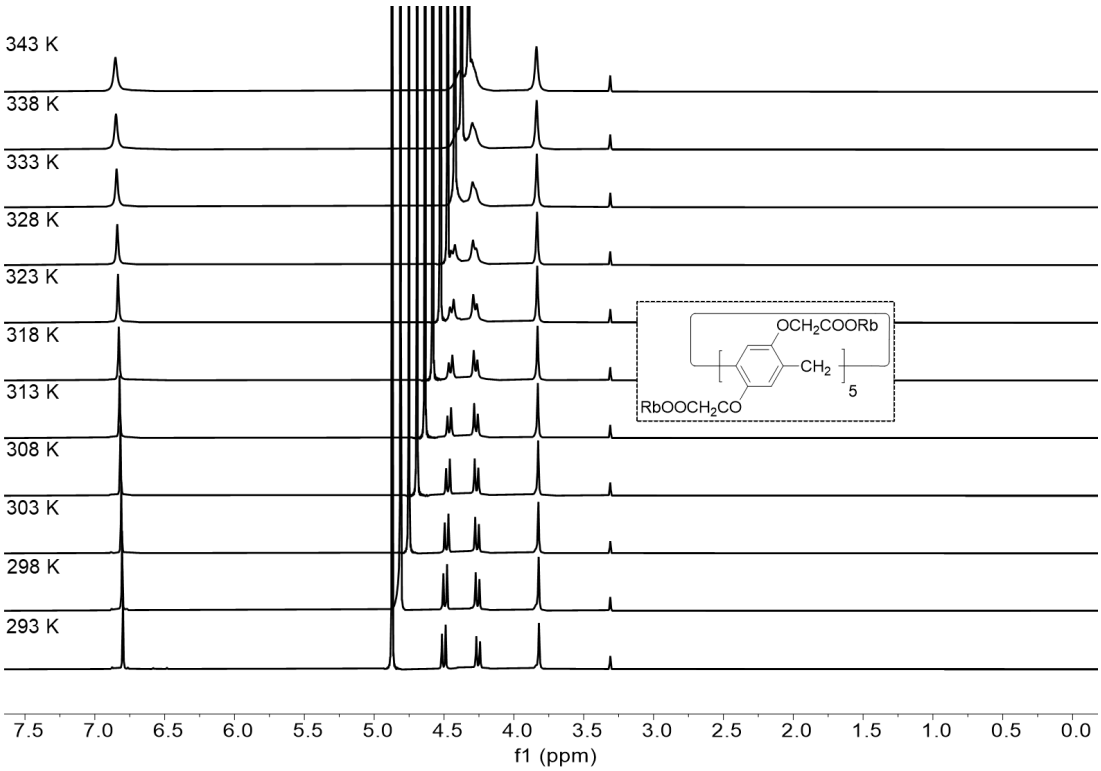


Figure S39. VT NMR spectra of **WP5-K** in mixed solvent (v/v of D_2O/CD_3OD = 2:1) between 293 K and 343 K.

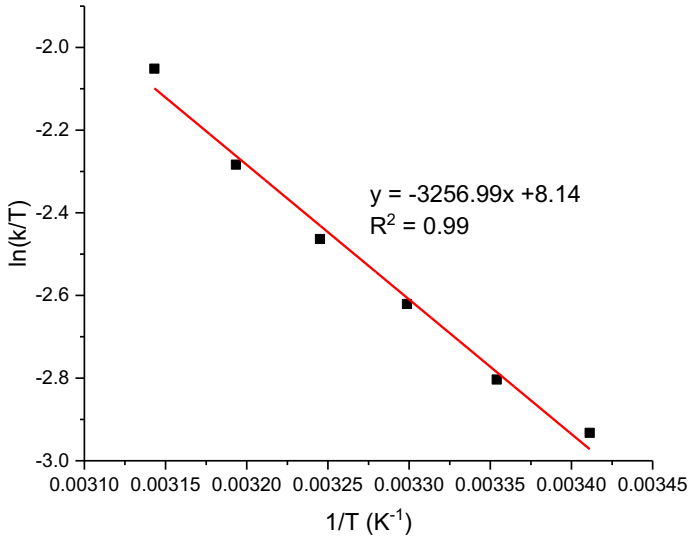


Figure S40. Eyring plot of the rates of exchange in mixed solvent obtained from line width analysis of methene protons on **WP5-Rb**. The barrier ($\Delta G^{\ddagger}$ = 15.71 kcal·mol^{-1}) was calculated from the slope ($\Delta H^{\ddagger}$ = 6.47 kcal·mol^{-1}) and y-intercept ($\Delta S^{\ddagger}$ = -31.02 cal·mol^{-1}·K^{-1}).

6. Cation switch reactions

Rate of exchange k_{ex} of **WP5-NH$_4$** at 298 K was estimated by line width analysis with the equation $k_{ex} = \frac{\sqrt{2}\pi h}{2}$, where h represented the width of peak at half height.[S3]

Li$^+$/NH$_4^+$ switching: To an aqueous solution of **WP5-Li** (10 mM, 3.0 ml, 1.0 equiv.), was added NH_4F (11.0 mg, 10.0 equiv.). After storing at 0 ℃ for 30 min, filtration of precipitate and characterization with ^{1}H NMR spectrum and fluorescence emission spectrum, LiOH (7.2 mg, 10.0 equiv.) was added. The mixture was heated to 60 ℃ and bubbled with Ar for 30 min, after which the solution was characterized with ^{1}H NMR spectrum and fluorescence emission spectrum.

Na$^+$/NH$_4^+$ switching: To an aqueous solution of **WP5-Na** (10 mM, 600 μl, 1.0 equiv.), was added 15-Crown-5 (24 μl, 20.0 equiv.) and NH_4Cl (3.2 mg, 10.0 equiv.). After characterizing with ^{1}H NMR spectrum, NaOH (2.4 mg, 10.0 equiv.) was added. The mixture was heated to 60 ℃ and bubbled with Ar for 30 min, after which the solution was characterized with ^{1}H NMR spectrum.

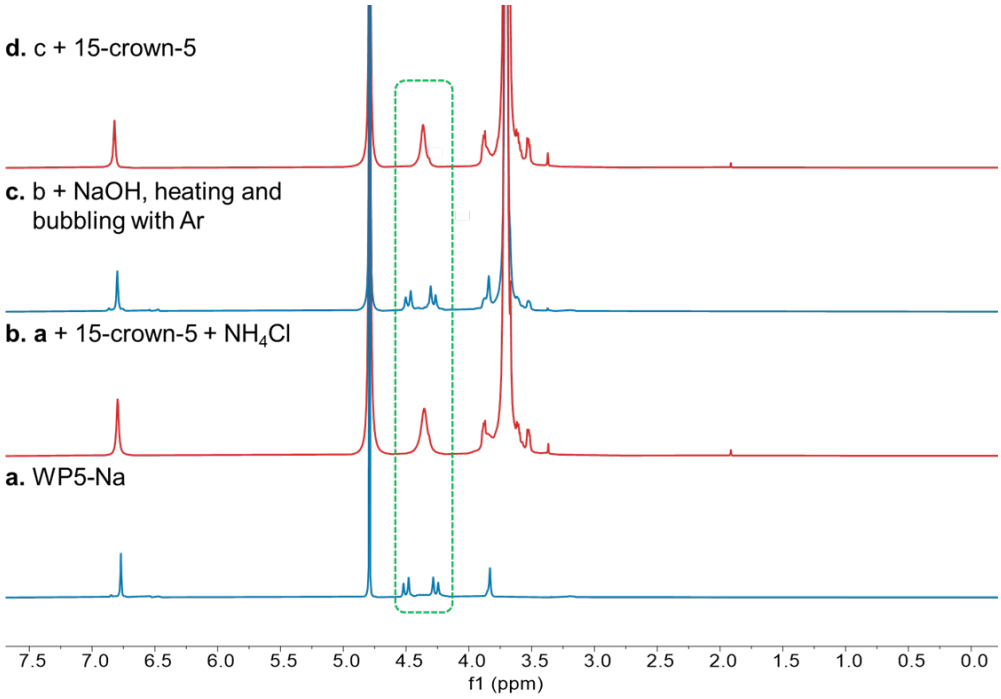


Figure S41. Stacking NMR spectra of Na$^+$/NH$_4^+$ switching: (a). **WP5-Na** (10 mM); (b). a + 15-crown-5 (20.0 equiv.) + NH_4Cl (10.0 equiv.); (c). b + NaOH (10.0 equiv.), heating and bubbling with Ar; (d). c + 15-crown-5.

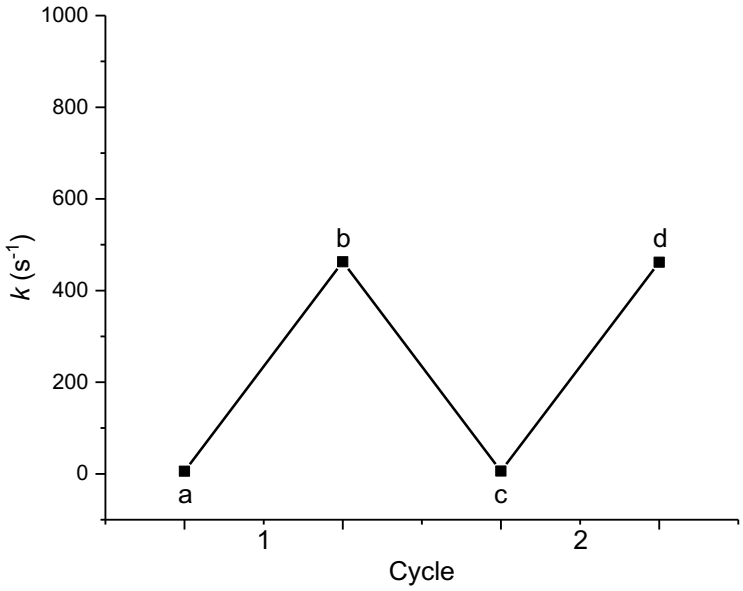


Figure S42. Switching of rate for WP5 in D_2O at 298 K with multiple cycles shown in **Figure S37**.

7. Inks writing tests.

WP5-NH_4 aqueous solution (10 mM) was employed as inks. Typically, inks were written on a filter paper and LiOH aqueous solution (10 mM) was used for revealing the preexisting images. The visible images could be erased by NH_4F aqueous solution (10 mM).

8. Reference

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Appendix: molecular coordinates

WP5-Li – configuration with highest energy extracted from potential energy surface scanning

C	1.553	2.709	-3.142
C	0.845	3.654	-2.388
C	1.347	4.082	-1.152
C	2.562	3.573	-0.675
C	3.27	2.627	-1.429
C	2.762	2.191	-2.66
C	0.561	5.109	-0.316
H	1.243	5.694	0.266
H	0.007	5.752	-0.967
C	3.532	1.139	-3.481
H	4.58	1.233	-3.29
H	3.344	1.292	-4.523
C	-0.409	4.365	0.621
C	-1.708	4.066	0.19
C	0.009	3.985	1.903
C	-2.586	3.375	1.037
C	-0.868	3.295	2.75
C	-2.164	2.985	2.315
C	3.058	-0.268	-3.073
C	3.7	-0.949	-2.03
C	1.983	-0.867	-3.743
C	3.26	-2.223	-1.649
C	1.543	-2.142	-3.362
C	2.177	-2.818	-2.311
C	1.683	-4.212	-1.882
H	2.504	-4.778	-1.494
C	-3.123	2.212	3.239
H	-2.896	2.439	4.26
C	-3.893	-0.322	3.558
C	-3.7	-1.656	3.176
C	-2.597	-2.006	2.387
C	-1.679	-1.024	1.989
C	-1.872	0.31	2.372
C	-2.982	0.662	3.151

C	-2.429	-3.549	2.272
H	-2.116	-4.033	3.173
H	-3.352	-3.975	1.94
C	-1.354	-3.738	1.185
C	-1.724	-3.783	-0.166
C	-0.006	-3.864	1.547
C	-0.744	-3.941	-1.155
C	0.974	-4.022	0.558
C	0.605	-4.054	-0.794
H	1.267	-4.72	-2.727
H	-4.132	2.497	3.027
H	-0.079	4.049	-2.756
H	-3.578	3.146	0.707
H	-4.396	-2.407	3.486
H	-1.172	1.06	2.068
H	-1.026	-3.974	-2.187
H	0.276	-3.838	2.579
H	1.498	-0.351	-4.545
H	3.75	-2.743	-0.852
H	4.197	2.238	-1.064
H	0.999	4.221	2.235
O	1.04	2.271	-4.404
O	0.445	-2.753	-4.045
O	-3.1	-3.666	-0.534
O	-5.02	0.036	4.363
O	-2.138	4.463	-1.115
O	-0.442	2.906	4.058
O	-0.547	-1.384	1.193
O	2.349	-4.149	0.927
O	4.805	-0.342	-1.354
O	3.08	4.018	0.582
C	4.508	3.963	0.555
H	4.824	2.957	0.376
H	4.875	4.597	-0.226
C	5.694	-1.359	-0.886
H	5.174	-2.006	-0.211
H	6.055	-1.927	-1.718
C	2.443	-4.769	2.212
H	1.933	-4.168	2.936

H	1.993	-5.739	2.174
C	0.969	2.671	4.05
H	1.196	1.891	3.354
H	1.478	3.567	3.76
C	-0.18	-0.28	0.361
H	-1	-0.028	-0.279
H	0.067	0.562	0.973
C	1.428	2.252	5.459
C	5.066	4.442	1.909
C	6.883	-0.706	-0.158
C	3.924	-4.905	2.61
C	1.039	-0.667	-0.497
O	8.009	-1.268	-0.161
O	4.292	-5.856	3.348
O	2.203	-0.458	-0.067
O	1.792	3.126	6.288
O	6.189	5.008	1.962
O	4.307	4.245	3.105
O	6.708	0.54	0.522
O	4.881	-3.952	2.14
O	0.849	-1.265	-1.782
O	1.442	0.87	5.825
C	0.283	3.326	-5.002
H	-0.531	3.591	-4.359
H	0.913	4.179	-5.149
C	0.414	-2.298	-5.401
H	0.297	-1.234	-5.417
H	1.329	-2.564	-5.887
C	-3.334	-4.394	-1.743
H	-2.72	-3.995	-2.524
H	-3.091	-5.425	-1.591
C	-5.377	-1.067	5.2
H	-5.627	-1.91	4.592
H	-4.551	-1.315	5.833
C	-3.11	3.533	-1.6
H	-2.675	2.557	-1.65
H	-3.95	3.517	-0.938
C	-4.816	-4.268	-2.14
C	-6.59	-0.681	6.067

C	-3.573	3.962	-3.005
C	-0.269	2.855	-6.361
C	-0.768	-2.956	-6.136
O	-0.695	-3.178	-7.373
O	0.406	3.03	-7.409
O	-4.557	4.735	-3.135
O	-6.738	-1.194	7.206
O	-5.38	-5.199	-2.771
O	-7.55	0.259	5.576
O	-5.552	-3.092	-1.791
O	-1.95	-3.314	-5.414
O	-1.548	2.22	-6.431
O	-2.885	3.48	-4.163
Li	-2.767	0.57	-2.96

WP5-Li - *pS*

C	-0.68	-4.102	1.662
C	-2.002	-3.643	1.519
C	-2.649	-3.572	0.274
C	-1.933	-4.036	-0.85
C	-0.558	-4.311	-0.727
C	0.105	-4.325	0.512
C	-4.095	-3.079	0.157
H	-4.546	-3.582	-0.705
H	-4.645	-3.379	1.053
C	1.599	-4.647	0.609
H	1.875	-5.307	-0.218
H	1.757	-5.193	1.546
C	-4.264	-1.565	-0.01
C	-4.625	-0.731	1.073
C	-4.116	-0.954	-1.265
C	-4.572	0.666	0.914
C	-4.248	0.433	-1.453
C	-4.359	1.279	-0.333
C	2.541	-3.438	0.581
C	3.365	-3.15	-0.535
C	2.661	-2.595	1.695

C	4.07	-1.933	-0.576
C	3.507	-1.474	1.709
C	4.143	-1.066	0.527
C	4.956	0.226	0.487
H	5.724	0.114	-0.284
C	-4.3	2.8	-0.471
H	-4.774	3.065	-1.425
C	-2.477	4.333	0.533
C	-1.119	4.707	0.602
C	-0.174	4.312	-0.358
C	-0.646	3.541	-1.438
C	-1.956	3.044	-1.431
C	-2.887	3.394	-0.44
C	1.278	4.793	-0.282
H	1.509	5.314	-1.222
H	1.366	5.518	0.532
C	2.339	3.714	-0.079
C	2.899	3.42	1.184
C	2.859	3.014	-1.172
C	3.713	2.281	1.332
C	3.79	1.985	-1.034
C	4.149	1.505	0.238
H	5.471	0.314	1.449
H	-4.881	3.261	0.331
H	-2.564	-3.348	2.401
H	-4.72	1.309	1.776
H	-0.778	5.336	1.417
H	-2.29	2.38	-2.221
H	4.002	1.951	2.324
H	2.5	3.281	-2.16
H	2.083	-2.834	2.584
H	4.6	-1.655	-1.482
H	0.021	-4.545	-1.616
H	-3.901	-1.589	-2.12
O	-0.095	-4.343	2.892
O	3.697	-0.722	2.857
O	2.595	4.269	2.222
O	-3.441	4.861	1.376
O	-5.024	-1.341	2.248

O	-4.236	1.017	-2.709
O	0.238	3.328	-2.478
O	4.32	1.47	-2.243
O	3.454	-4.1	-1.536
O	-2.63	-4.2	-2.033
C	-2.207	-5.22	-2.944
H	-1.613	-4.766	-3.747
H	-1.559	-5.934	-2.419
C	4.608	-4.08	-2.379
H	4.44	-3.399	-3.225
H	5.464	-3.688	-1.812
C	5.753	1.541	-2.39
H	6.174	2.13	-1.569
H	6.167	0.528	-2.329
C	-5.004	0.406	-3.756
H	-4.311	0.008	-4.507
H	-5.57	-0.441	-3.35
C	-0.293	3.076	-3.777
H	-0.643	2.035	-3.852
H	-1.147	3.735	-3.969
C	-6.029	1.339	-4.489
C	-3.355	-6.065	-3.598
C	5.061	-5.465	-2.952
C	6.203	2.162	-3.736
C	0.787	3.305	-4.861
O	5.973	-5.338	-3.834
O	7.446	2.273	-3.888
O	0.396	3.793	-5.949
O	-6.299	2.467	-4.016
O	-2.941	-6.758	-4.584
O	-4.507	-6.045	-3.104
O	4.571	-6.527	-2.504
O	5.294	2.49	-4.56
O	1.976	2.944	-4.586
O	-6.521	0.79	-5.529
C	-0.913	-4.823	3.965
H	-1.11	-3.998	4.661
H	-1.881	-5.156	3.569
C	4.235	-1.385	4.01

H	3.668	-1.015	4.872
H	4.058	-2.465	3.939
C	3.557	4.493	3.261
H	3.178	4.047	4.187
H	4.499	3.988	3.013
C	-3.161	6.111	2.009
H	-2.545	5.949	2.905
H	-2.573	6.739	1.324
C	-5.872	-0.614	3.14
H	-5.26	-0.085	3.882
H	-6.431	0.145	2.576
C	3.911	5.996	3.537
C	-4.409	6.957	2.431
C	-6.945	-1.466	3.902
C	-0.326	-6.028	4.779
C	5.756	-1.166	4.316
O	6.103	-1.661	5.438
O	0.611	-6.708	4.299
O	-7.234	-2.617	3.499
O	-4.073	7.998	3.087
O	4.502	6.158	4.654
O	-5.562	6.604	2.094
O	3.654	6.864	2.67
O	6.476	-0.563	3.485
O	-0.946	-6.217	5.876
O	-7.473	-0.822	4.866
Li	3.518	2.299	-3.974

WP5-Li - TS_1

C	0.435	-3.084	-1.063
C	1.743	-2.596	-1.166
C	2.802	-3.099	-0.403
C	2.512	-4.172	0.47
C	1.173	-4.546	0.686
C	0.099	-4	-0.047
C	4.224	-2.557	-0.583
H	4.869	-3.05	0.149
H	4.581	-2.848	-1.579

C	-1.334	-4.461	0.264
H	-1.283	-5.128	1.132
H	-1.712	-5.058	-0.578
C	4.366	-1.044	-0.449
C	4.249	-0.181	-1.556
C	4.65	-0.455	0.795
C	4.194	1.204	-1.342
C	4.738	0.937	0.982
C	4.353	1.791	-0.077
C	-2.381	-3.397	0.579
C	-2.403	-2.759	1.83
C	-3.418	-3.083	-0.316
C	-3.265	-1.671	2.037
C	-4.405	-2.124	-0.028
C	-4.255	-1.303	1.113
C	-5.122	-0.062	1.349
H	-5.4	-0.013	2.407
C	4.017	3.265	0.124
H	4.375	3.593	1.103
C	1.993	4.857	0.356
C	0.601	5.064	0.293
C	-0.294	4.12	-0.248
C	0.261	2.932	-0.752
C	1.621	2.668	-0.549
C	2.516	3.594	-0.007
C	-1.779	4.445	-0.405
H	-1.961	5.418	0.077
H	-1.997	4.589	-1.468
C	-2.783	3.419	0.122
C	-3.849	2.966	-0.686
C	-2.705	2.905	1.423
C	-4.564	1.822	-0.292
C	-3.58	1.912	1.897
C	-4.416	1.243	0.981
H	-6.035	-0.161	0.755
H	4.562	3.877	-0.611
H	1.928	-1.812	-1.892
H	3.95	1.855	-2.175
H	0.181	6.001	0.646

H	2.006	1.713	-0.869
H	-5.254	1.353	-0.986
H	-1.923	3.281	2.079
H	-3.458	-3.616	-1.261
H	-3.171	-1.081	2.945
H	0.938	-5.271	1.459
H	4.793	-1.12	1.641
O	-0.502	-2.598	-1.958
O	-5.533	-1.943	-0.814
O	-4.116	3.675	-1.842
O	2.899	5.844	0.742
O	4.166	-0.749	-2.811
O	5.182	1.521	2.151
O	-0.567	2.087	-1.425
O	-3.628	1.529	3.227
O	-1.522	-3.198	2.8
O	3.584	-4.805	1.083
C	3.389	-6.128	1.58
H	2.869	-6.096	2.549
H	2.741	-6.684	0.888
C	-2.028	-3.458	4.115
H	-1.246	-3.128	4.808
H	-2.918	-2.849	4.31
C	-3.478	2.537	4.232
H	-2.531	2.365	4.758
H	-3.416	3.524	3.76
C	5.921	0.73	3.085
H	5.233	0.288	3.817
H	6.416	-0.096	2.555
C	-0.018	0.939	-2.08
H	0.546	0.32	-1.374
H	-0.887	0.35	-2.381
C	7.063	1.482	3.851
C	4.694	-6.971	1.77
C	-2.382	-4.942	4.475
C	-4.617	2.631	5.308
C	0.846	1.218	-3.343
O	-2.671	-5.083	5.71
O	-4.309	3.423	6.259

O	0.928	2.373	-3.804
O	7.613	2.477	3.321
O	4.452	-8.122	2.267
O	5.809	-6.508	1.433
O	-2.367	-5.822	3.583
O	-5.687	1.999	5.153
O	1.395	0.165	-3.811
O	7.377	0.912	4.946
C	-0.966	-3.518	-2.946
H	-1.152	-4.502	-2.502
H	-1.93	-3.119	-3.279
C	-5.991	-3.054	-1.587
H	-5.506	-3.048	-2.573
H	-5.698	-3.988	-1.088
C	-5.413	3.574	-2.427
H	-5.435	2.747	-3.149
H	-6.151	3.342	-1.645
C	2.39	7.151	0.978
H	1.713	7.435	0.157
H	1.797	7.163	1.903
C	4.55	0.077	-3.92
H	3.795	0.859	-4.073
H	5.526	0.533	-3.709
C	-5.924	4.87	-3.148
C	3.45	8.299	1.07
C	4.615	-0.759	-5.219
C	-0.1	-3.749	-4.221
C	-7.539	-3.142	-1.811
O	-7.848	-4.052	-2.65
O	-0.549	-4.667	-4.966
O	5.577	-0.503	-6.004
O	2.971	9.354	1.609
O	-6.946	4.648	-3.879
O	4.594	8.15	0.581
O	-5.371	5.974	-2.929
O	-8.319	-2.402	-1.167
O	0.913	-3.03	-4.428
O	3.672	-1.578	-5.405
Li	1.981	-1.504	-4.341

WP5-Li – TS_2a

C	-3.244	2.388	-1.711
C	-3.928	1.169	-1.75
C	-4.474	0.572	-0.608
C	-4.447	1.351	0.579
C	-3.644	2.506	0.635
C	-2.997	3.041	-0.497
C	-5.02	-0.852	-0.655
H	-5.647	-1.032	0.221
H	-5.682	-0.961	-1.527
C	-2.124	4.296	-0.381
H	-2.588	4.986	0.335
H	-2.094	4.791	-1.357
C	-3.934	-1.943	-0.73
C	-4.163	-3.267	-0.29
C	-2.686	-1.675	-1.299
C	-3.075	-4.162	-0.222
C	-1.669	-2.63	-1.403
C	-1.802	-3.868	-0.749
C	-0.679	4.087	0.073
C	-0.364	3.915	1.429
C	0.398	4.163	-0.829
C	0.95	3.592	1.804
C	1.738	4.039	-0.419
C	2.023	3.611	0.901
C	3.441	3.252	1.359
H	3.56	3.578	2.399
C	-0.68	-4.918	-0.707
H	-1.011	-5.728	-0.047
C	1.118	-4.453	1.086
C	2.319	-3.801	1.423
C	3.224	-3.318	0.463
C	2.937	-3.609	-0.889
C	1.669	-4.102	-1.222
C	0.711	-4.466	-0.264
C	4.489	-2.559	0.879
H	4.833	-2.98	1.835

H	5.274	-2.739	0.143
C	4.335	-1.04	1.057
C	5.027	-0.107	0.249
C	3.543	-0.513	2.088
C	4.659	1.252	0.309
C	3.37	0.866	2.293
C	3.807	1.766	1.303
H	4.149	3.81	0.739
H	-0.578	-5.338	-1.719
H	-4.009	0.656	-2.706
H	-3.208	-5.128	0.254
H	2.569	-3.669	2.472
H	1.39	-4.204	-2.263
H	5.059	1.948	-0.422
H	3.05	-1.207	2.764
H	0.176	4.357	-1.875
H	1.156	3.321	2.835
H	-3.48	3.012	1.579
H	-2.51	-0.688	-1.697
O	-2.82	2.923	-2.95
O	2.806	4.339	-1.242
O	6.047	-0.583	-0.549
O	0.321	-5.103	2.015
O	-5.464	-3.615	0.042
O	-0.529	-2.416	-2.13
O	3.926	-3.346	-1.803
O	2.747	1.377	3.416
O	-1.379	4.026	2.367
O	-5.213	0.906	1.621
C	-5.577	1.775	2.704
H	-5.011	1.471	3.59
H	-5.306	2.81	2.467
C	-1.208	4.981	3.424
H	-1.607	4.508	4.329
H	-0.141	5.168	3.593
C	3.066	0.818	4.697
H	2.117	0.555	5.179
H	3.639	-0.107	4.574
C	-0.386	-1.192	-2.836

H	-0.529	-0.334	-2.171
H	0.66	-1.183	-3.159
C	3.832	-3.753	-3.167
H	2.814	-3.628	-3.553
H	4.464	-3.036	-3.702
C	-1.271	-1.034	-4.106
C	-7.107	1.792	3.046
C	-1.919	6.368	3.267
C	3.872	1.723	5.692
C	4.344	-5.184	-3.563
O	-1.799	7.094	4.308
O	3.98	1.185	6.844
O	4.721	-5.984	-2.675
O	-1.675	-2.036	-4.716
O	-7.345	2.06	4.267
O	-7.936	1.633	2.117
O	-2.515	6.645	2.199
O	4.335	2.821	5.309
O	4.336	-5.363	-4.825
O	-1.45	0.192	-4.449
C	-3.725	3.9	-3.501
H	-4.753	3.62	-3.238
H	-3.519	4.884	-3.062
C	2.593	5.246	-2.327
H	2.363	4.68	-3.239
H	1.725	5.881	-2.107
C	7.046	0.325	-1.016
H	6.768	0.699	-2.009
H	7.101	1.19	-0.341
C	0.951	-5.614	3.191
H	2.023	-5.756	2.997
H	0.86	-4.884	4.006
C	-5.772	-4.998	0.203
H	-5.201	-5.585	-0.532
H	-5.462	-5.339	1.2
C	8.502	-0.254	-1.09
C	0.425	-6.994	3.714
C	-7.273	-5.391	-0.009
C	-3.612	3.984	-5.042

C	3.773	6.228	-2.641
O	3.61	6.827	-3.755
O	-4.318	4.871	-5.589
O	-7.548	-6.537	0.48
O	0.877	-7.267	4.876
O	9.254	0.408	-1.88
O	-0.302	-7.711	2.989
O	8.829	-1.213	-0.351
O	4.696	6.391	-1.81
O	-2.846	3.145	-5.607
O	-8.034	-4.641	-0.665
Li	-2.066	1.842	-4.434

WP5-Li – TS_2b

C	3.386	-3.625	0.483
C	4.215	-2.51	0.276
C	3.995	-1.575	-0.75
C	2.943	-1.846	-1.642
C	2.003	-2.836	-1.316
C	2.175	-3.721	-0.242
C	4.886	-0.337	-0.847
H	5.734	-0.493	-0.169
H	5.32	-0.237	-1.847
C	1.128	-4.802	0.061
H	1.399	-5.296	0.996
H	1.182	-5.563	-0.733
C	4.202	0.978	-0.462
C	3.774	1.913	-1.411
C	4.007	1.32	0.887
C	3.023	3.03	-1.03
C	3.372	2.509	1.282
C	2.753	3.337	0.308
C	-0.317	-4.329	0.172
C	-0.828	-3.858	1.394
C	-1.215	-4.408	-0.908
C	-2.102	-3.269	1.43
C	-2.556	-3.986	-0.818
C	-2.98	-3.283	0.335

C	-4.355	-2.607	0.437
H	-4.82	-2.903	1.384
C	1.897	4.551	0.689
H	2.121	4.839	1.716
C	-0.507	4.502	1.637
C	-1.847	4.097	1.473
C	-2.395	3.738	0.231
C	-1.561	3.885	-0.899
C	-0.19	4.106	-0.708
C	0.38	4.362	0.549
C	-3.853	3.287	0.105
H	-4.426	3.788	0.9
H	-4.252	3.636	-0.849
C	-4.11	1.776	0.209
C	-4.716	1.038	-0.835
C	-3.819	1.074	1.388
C	-4.709	-0.37	-0.767
C	-4.043	-0.305	1.533
C	-4.347	-1.075	0.395
H	-4.979	-2.98	-0.379
H	2.2	5.388	0.043
H	5.088	-2.366	0.904
H	2.66	3.69	-1.814
H	-2.5	4.075	2.341
H	0.465	4.107	-1.571
H	-5.018	-0.948	-1.633
H	-3.41	1.628	2.229
H	-0.858	-4.847	-1.835
H	-2.44	-2.778	2.336
H	1.095	-2.931	-1.902
H	4.394	0.644	1.642
O	3.663	-4.643	1.354
O	-3.491	-4.256	-1.806
O	-5.302	1.747	-1.863
O	-0.025	5.06	2.81
O	4.169	1.782	-2.756
O	3.278	2.925	2.575
O	-2.152	3.761	-2.128
O	-3.926	-0.948	2.753

O	-0.014	-3.94	2.503
O	2.897	-1.142	-2.851
C	2.118	-1.743	-3.908
H	2.151	-2.831	-3.803
H	1.073	-1.423	-3.82
C	-0.562	-4.368	3.758
H	-0.051	-3.774	4.522
H	-1.63	-4.127	3.814
C	-4.489	-0.332	3.92
H	-3.713	-0.349	4.693
H	-4.727	0.718	3.716
C	4.106	2.394	3.613
H	3.555	2.625	4.53
H	4.174	1.302	3.549
C	-1.51	4.225	-3.316
H	-0.464	3.897	-3.359
H	-2.036	3.7	-4.119
C	5.549	2.986	3.774
C	2.648	-1.392	-5.32
C	-0.4	-5.881	4.134
C	-5.78	-0.983	4.527
C	-1.573	5.757	-3.654
O	-0.634	-6.102	5.368
O	-6.104	-0.447	5.639
O	-2.116	6.55	-2.852
O	6	3.761	2.9
O	2.093	-2.009	-6.26
O	3.585	-0.541	-5.402
O	-0.102	-6.712	3.245
O	-6.369	-1.902	3.915
O	-1.05	6.018	-4.786
O	6.113	2.588	4.844
C	4.79	-4.64	2.227
H	5.098	-3.619	2.481
H	4.424	-5.098	3.151
C	-3.22	-5.343	-2.692
H	-2.586	-5.001	-3.521
H	-2.657	-6.117	-2.151
C	-6.274	1.101	-2.686

H	-5.781	0.657	-3.56
H	-6.747	0.284	-2.123
C	-0.968	5.64	3.712
H	-1.832	6.013	3.144
H	-1.339	4.875	4.407
C	5.235	2.678	-3.138
H	4.811	3.508	-3.718
H	5.696	3.092	-2.236
C	-7.448	2.014	-3.185
C	-0.456	6.858	4.555
C	6.328	1.97	-3.978
C	6.059	-5.456	1.793
C	-4.466	-6.064	-3.309
O	-4.126	-6.912	-4.201
O	6.94	-5.497	2.712
O	7.255	2.719	-4.393
O	-1.244	7.135	5.52
O	-8.038	1.536	-4.209
O	0.578	7.476	4.213
O	-7.757	3.041	-2.536
O	-5.619	-5.818	-2.889
O	6.102	-5.994	0.661
O	6.189	0.726	-4.159
Li	4.337	0.127	-3.846

WP5-Na – configuration with highest energy extracted from potential energy surface scanning

C	1.553	2.709	-3.142
C	0.845	3.654	-2.388
C	1.347	4.082	-1.152
C	2.562	3.573	-0.675
C	3.27	2.627	-1.429
C	2.762	2.191	-2.66
C	0.561	5.109	-0.316
H	1.243	5.694	0.266
H	0.007	5.752	-0.967
C	3.532	1.139	-3.481
H	4.58	1.233	-3.29

H	3.344	1.292	-4.523
C	-0.409	4.365	0.621
C	-1.708	4.066	0.19
C	0.009	3.985	1.903
C	-2.586	3.375	1.037
C	-0.868	3.295	2.75
C	-2.164	2.985	2.315
C	3.058	-0.268	-3.073
C	3.7	-0.949	-2.03
C	1.983	-0.867	-3.743
C	3.26	-2.223	-1.649
C	1.543	-2.142	-3.362
C	2.177	-2.818	-2.311
C	1.683	-4.212	-1.882
H	2.504	-4.778	-1.494
C	-3.123	2.212	3.239
H	-2.896	2.439	4.26
C	-3.893	-0.322	3.558
C	-3.7	-1.656	3.176
C	-2.597	-2.006	2.387
C	-1.679	-1.024	1.989
C	-1.872	0.31	2.372
C	-2.982	0.662	3.151
C	-2.429	-3.549	2.272
H	-2.116	-4.033	3.173
H	-3.352	-3.975	1.94
C	-1.354	-3.738	1.185
C	-1.724	-3.783	-0.166
C	-0.006	-3.864	1.547
C	-0.744	-3.941	-1.155
C	0.974	-4.022	0.558
C	0.605	-4.054	-0.794
H	1.267	-4.72	-2.727
H	-4.132	2.497	3.027
H	-0.079	4.049	-2.756
H	-3.578	3.146	0.707
H	-4.396	-2.407	3.486
H	-1.172	1.06	2.068
H	-1.026	-3.974	-2.187

H	0.276	-3.838	2.579
H	1.498	-0.351	-4.545
H	3.75	-2.743	-0.852
H	4.197	2.238	-1.064
H	0.999	4.221	2.235
O	1.04	2.271	-4.404
O	0.445	-2.753	-4.045
O	-3.1	-3.666	-0.534
O	-5.02	0.036	4.363
O	-2.138	4.463	-1.115
O	-0.442	2.906	4.058
O	-0.547	-1.384	1.193
O	2.349	-4.149	0.927
O	4.805	-0.342	-1.354
O	3.08	4.018	0.582
C	4.508	3.963	0.555
H	4.824	2.957	0.376
H	4.875	4.597	-0.226
C	5.694	-1.359	-0.886
H	5.174	-2.006	-0.211
H	6.055	-1.927	-1.718
C	2.443	-4.769	2.212
H	1.933	-4.168	2.936
H	1.993	-5.739	2.174
C	0.969	2.671	4.05
H	1.196	1.891	3.354
H	1.478	3.567	3.76
C	-0.18	-0.28	0.361
H	-1	-0.028	-0.279
H	0.067	0.562	0.973
C	1.428	2.252	5.459
C	5.066	4.442	1.909
C	6.883	-0.706	-0.158
C	3.924	-4.905	2.61
C	1.039	-0.667	-0.497
O	8.009	-1.268	-0.161
O	4.292	-5.856	3.348
O	2.203	-0.458	-0.067
O	1.792	3.126	6.288

O	6.189	5.008	1.962
O	4.307	4.245	3.105
O	6.708	0.54	0.522
O	4.881	-3.952	2.14
O	0.849	-1.265	-1.782
O	1.442	0.87	5.825
C	0.283	3.326	-5.002
H	-0.531	3.591	-4.359
H	0.913	4.179	-5.149
C	0.414	-2.298	-5.401
H	0.297	-1.234	-5.417
H	1.329	-2.564	-5.887
C	-3.334	-4.394	-1.743
H	-2.72	-3.995	-2.524
H	-3.091	-5.425	-1.591
C	-5.377	-1.067	5.2
H	-5.627	-1.91	4.592
H	-4.551	-1.315	5.833
C	-3.11	3.533	-1.6
H	-2.675	2.557	-1.65
H	-3.95	3.517	-0.938
C	-4.816	-4.268	-2.14
C	-6.59	-0.681	6.067
C	-3.573	3.962	-3.005
C	-0.269	2.855	-6.361
C	-0.768	-2.956	-6.136
O	-0.695	-3.178	-7.373
O	0.406	3.03	-7.409
O	-4.557	4.735	-3.135
O	-6.738	-1.194	7.206
O	-5.38	-5.199	-2.771
O	-7.55	0.259	5.576
O	-5.552	-3.092	-1.791
O	-1.95	-3.314	-5.414
O	-1.548	2.22	-6.431
O	-2.885	3.48	-4.163
Na	-2.767	0.57	-2.96

WP5-Na - *pS*

C	-4.369	-2.234	-1.088
C	-3.515	-3.35	-1.087
C	-2.446	-3.502	-0.179
C	-2.311	-2.499	0.799
C	-3.025	-1.299	0.658
C	-4.052	-1.121	-0.272
C	-1.497	-4.698	-0.342
H	-1.675	-5.441	0.449
H	-1.735	-5.181	-1.296
C	-4.846	0.188	-0.363
H	-5.639	0.169	0.399
H	-5.36	0.203	-1.327
C	-0.007	-4.373	-0.37
C	0.552	-3.735	-1.487
C	0.871	-4.747	0.66
C	1.879	-3.283	-1.441
C	2.244	-4.44	0.633
C	2.744	-3.584	-0.377
C	-4.034	1.468	-0.203
C	-3.653	1.975	1.046
C	-3.647	2.218	-1.329
C	-2.751	3.04	1.145
C	-2.894	3.403	-1.224
C	-2.311	3.752	0.02
C	-1.3	4.891	0.159
H	-1.498	5.422	1.097
C	4.174	-3.033	-0.35
H	4.699	-3.501	0.487
C	4.414	-0.679	-1.357
C	4.341	0.717	-1.2
C	4.327	1.341	0.059
C	4.442	0.506	1.191
C	4.329	-0.888	1.034
C	4.287	-1.511	-0.224
C	4.265	2.866	0.187
H	4.768	3.138	1.121
H	4.822	3.316	-0.639

C	2.86	3.479	0.188
C	2.347	4.177	-0.93
C	2.045	3.416	1.329
C	0.993	4.563	-0.944
C	0.751	3.961	1.366
C	0.164	4.447	0.185
H	-1.448	5.584	-0.674
H	4.688	-3.327	-1.272
H	-3.646	-4.123	-1.837
H	2.263	-2.684	-2.263
H	4.315	1.353	-2.081
H	4.293	-1.522	1.916
H	0.565	4.986	-1.848
H	2.444	2.938	2.22
H	-3.958	1.866	-2.307
H	-2.384	3.342	2.121
H	-2.723	-0.471	1.295
H	0.469	-5.3	1.501
O	-5.505	-2.136	-1.872
O	-2.703	4.263	-2.277
O	3.219	4.46	-1.965
O	4.601	-1.293	-2.582
O	-0.252	-3.518	-2.592
O	3.141	-4.95	1.559
O	4.669	1.112	2.413
O	0.006	4.001	2.533
O	-4.233	1.441	2.219
O	-1.446	-2.571	1.873
C	-1.597	-3.667	2.779
H	-1.715	-4.61	2.241
H	-0.645	-3.719	3.315
C	-5.322	2.272	2.682
H	-4.916	3.229	3.031
H	-5.986	2.482	1.834
C	2.761	-6.132	2.266
H	2.106	-5.871	3.11
H	2.181	-6.782	1.597
C	5.382	0.384	3.418
H	4.668	-0.084	4.107

H	5.959	-0.422	2.946
C	3.935	-7.003	2.827
C	-2.732	-3.6	3.841
C	-6.168	1.64	3.816
C	6.404	1.222	4.262
O	-7.101	2.381	4.234
O	6.796	0.597	5.302
O	5.125	-6.729	2.55
O	-2.829	-4.64	4.545
O	-3.434	-2.552	3.938
O	-5.876	0.474	4.21
O	6.784	2.343	3.852
O	3.504	-7.981	3.525
C	-6.047	-3.338	-2.423
H	-5.44	-3.67	-3.276
H	-6.001	-4.135	-1.667
C	-3.608	4.215	-3.387
H	-3.191	3.568	-4.168
H	-4.56	3.774	-3.063
C	2.928	5.574	-2.814
H	2.319	5.242	-3.665
H	2.334	6.311	-2.256
C	5.361	-0.612	-3.586
H	4.676	-0.139	-4.301
H	5.952	0.187	-3.12
C	0.156	-4.111	-3.833
H	-0.131	-3.398	-4.613
H	1.248	-4.209	-3.862
C	4.174	6.343	-3.371
C	6.372	-1.504	-4.386
C	-0.462	-5.499	-4.214
C	-7.532	-3.233	-2.905
C	-3.974	5.599	-4.024
O	-4.548	5.465	-5.153
O	-8.156	-2.151	-2.809
O	-1.184	-6.108	-3.387
O	6.794	-0.929	-5.442
O	3.857	7.159	-4.298
O	6.716	-2.62	-3.932

O	5.306	6.159	-2.866
O	-3.754	6.657	-3.39
O	-7.962	-4.341	-3.366
O	-0.137	-5.869	-5.388
Na	-4.184	-0.663	3.253
C	0.594	4.608	3.693
H	1.647	4.843	3.496
H	0.57	3.868	4.502
C	-0.095	5.914	4.218
O	0.371	6.29	5.343
O	-0.984	6.468	3.529

WP5-Na - TS_1

C	0.811	-3.095	-1.003
C	2.057	-2.463	-1.036
C	3.1	-2.793	-0.167
C	2.867	-3.846	0.746
C	1.569	-4.374	0.878
C	0.506	-4	0.032
C	4.455	-2.09	-0.281
H	5.103	-2.46	0.517
H	4.916	-2.385	-1.232
C	-0.885	-4.621	0.231
H	-0.821	-5.32	1.072
H	-1.146	-5.205	-0.662
C	4.388	-0.567	-0.225
C	4.228	0.225	-1.369
C	4.491	0.113	1.004
C	3.969	1.597	-1.25
C	4.391	1.512	1.109
C	3.967	2.265	-0.019
C	-2.049	-3.677	0.517
C	-2.21	-3.095	1.784
C	-3.056	-3.43	-0.433
C	-3.19	-2.107	1.974
C	-4.153	-2.591	-0.173
C	-4.156	-1.805	1.003
C	-5.163	-0.672	1.227

H	-5.474	-0.674	2.278
C	3.49	3.711	0.09
H	3.824	4.135	1.04
C	1.307	5.045	0.46
C	-0.1	5.097	0.416
C	-0.885	4.13	-0.238
C	-0.201	3.089	-0.89
C	1.182	2.954	-0.711
C	1.965	3.896	-0.036
C	-2.401	4.282	-0.351
H	-2.688	5.192	0.197
H	-2.659	4.461	-1.4
C	-3.26	3.11	0.128
C	-4.273	2.565	-0.692
C	-3.101	2.55	1.403
C	-4.839	1.325	-0.344
C	-3.845	1.439	1.838
C	-4.608	0.715	0.902
H	-6.042	-0.864	0.604
H	3.974	4.312	-0.694
H	2.214	-1.712	-1.798
H	3.726	2.144	-2.159
H	-0.621	5.929	0.881
H	1.673	2.096	-1.142
H	-5.478	0.807	-1.052
H	-2.363	2.988	2.07
H	-2.979	-3.921	-1.398
H	-3.209	-1.546	2.904
H	1.358	-5.086	1.669
H	4.65	-0.484	1.895
O	-0.107	-2.777	-1.989
O	-5.248	-2.499	-1.017
O	-4.643	3.289	-1.81
O	2.097	6.083	0.947
O	4.318	-0.334	-2.653
O	4.687	2.207	2.255
O	-0.938	2.251	-1.669
O	-3.823	0.994	3.149
O	-1.345	-3.48	2.792

O	3.953	-4.306	1.476
C	3.893	-5.627	2.013
H	3.307	-5.631	2.943
H	3.371	-6.285	1.303
C	-1.901	-3.856	4.058
H	-1.218	-3.461	4.818
H	-2.873	-3.372	4.207
C	-3.829	1.966	4.201
H	-2.898	1.855	4.772
H	-3.834	2.976	3.775
C	5.415	1.566	3.309
H	4.707	1.184	4.053
H	5.975	0.713	2.907
C	-0.259	1.3	-2.491
H	0.382	0.65	-1.885
H	-1.058	0.67	-2.892
C	6.484	2.461	4.027
C	5.281	-6.283	2.321
C	-2.086	-5.387	4.341
C	-5.024	1.903	5.216
C	0.549	1.877	-3.695
O	-2.441	-5.616	5.545
O	-4.848	2.685	6.209
O	0.31	3.034	-4.099
O	7.038	3.386	3.387
O	5.157	-7.44	2.844
O	6.345	-5.684	2.038
O	-1.894	-6.219	3.424
O	-6.012	1.168	4.984
O	1.372	1.038	-4.19
O	6.744	2.063	5.208
C	-0.278	-3.759	-3.014
H	-0.234	-4.768	-2.586
H	-1.293	-3.605	-3.398
C	-5.533	-3.614	-1.864
H	-5.014	-3.495	-2.824
H	-5.148	-4.531	-1.398
C	-5.918	3.044	-2.399
H	-5.834	2.256	-3.159

H	-6.615	2.68	-1.629
C	1.449	7.306	1.284
H	0.717	7.559	0.502
H	0.891	7.19	2.224
C	5.646	-0.229	-3.196
H	6.008	0.798	-3.053
H	6.318	-0.898	-2.639
C	-6.601	4.293	-3.057
C	2.372	8.563	1.419
C	5.742	-0.566	-4.707
C	0.688	-3.732	-4.238
C	-7.048	-3.881	-2.162
O	-7.206	-4.764	-3.07
O	0.495	-4.694	-5.04
O	6.929	-0.527	-5.157
O	1.799	9.514	2.052
O	-7.574	3.972	-3.816
O	3.498	8.584	0.872
O	-6.213	5.45	-2.765
O	-7.939	-3.293	-1.506
O	1.523	-2.798	-4.348
O	4.684	-0.822	-5.335
Na	2.564	-0.821	-4.245

WP5-Na – TS_2a

C	-3.419	2.242	-1.558
C	-3.977	0.964	-1.668
C	-4.43	0.238	-0.56
C	-4.428	0.923	0.682
C	-3.763	2.157	0.8
C	-3.213	2.834	-0.304
C	-4.888	-1.21	-0.698
H	-5.55	-1.463	0.131
H	-5.491	-1.305	-1.614
C	-2.46	4.157	-0.125
H	-2.959	4.753	0.648
H	-2.508	4.715	-1.066
C	-3.748	-2.243	-0.758

C	-3.881	-3.544	-0.222
C	-2.547	-1.946	-1.413
C	-2.741	-4.37	-0.144
C	-1.48	-2.848	-1.494
C	-1.514	-4.041	-0.748
C	-0.989	4.042	0.275
C	-0.618	3.843	1.613
C	0.049	4.22	-0.658
C	0.727	3.6	1.935
C	1.408	4.171	-0.295
C	1.765	3.724	1
C	3.219	3.456	1.406
H	3.352	3.783	2.444
C	-0.323	-5.01	-0.684
H	-0.594	-5.824	-0.002
C	1.438	-4.386	1.095
C	2.59	-3.646	1.421
C	3.458	-3.113	0.452
C	3.191	-3.445	-0.895
C	1.961	-4.031	-1.219
C	1.032	-4.449	-0.254
C	4.668	-2.263	0.854
H	5.056	-2.661	1.804
H	5.454	-2.382	0.107
C	4.407	-0.76	1.044
C	4.999	0.224	0.218
C	3.615	-0.297	2.105
C	4.534	1.552	0.299
C	3.35	1.065	2.325
C	3.685	1.999	1.327
H	3.866	4.065	0.767
H	-0.193	-5.446	-1.685
H	-4.054	0.517	-2.659
H	-2.796	-5.306	0.404
H	2.829	-3.481	2.467
H	1.691	-4.174	-2.258
H	4.858	2.279	-0.44
H	3.201	-1.027	2.795
H	-0.223	4.442	-1.686

H	0.987	3.309	2.948
H	-3.635	2.619	1.772
H	-2.457	-0.982	-1.895
O	-3.068	2.901	-2.758
O	2.425	4.564	-1.143
O	6.023	-0.172	-0.619
O	0.69	-5.076	2.034
O	-5.144	-3.943	0.188
O	-0.378	-2.641	-2.278
O	4.159	-3.126	-1.815
O	2.733	1.526	3.474
O	-1.609	3.841	2.582
O	-5.043	0.288	1.723
C	-5.536	0.982	2.876
H	-5.289	0.341	3.727
H	-5.017	1.935	3.021
C	-1.458	4.729	3.701
H	-1.816	4.175	4.576
H	-0.398	4.953	3.863
C	3.121	0.973	4.738
H	2.204	0.643	5.241
H	3.75	0.089	4.587
C	-0.267	-1.444	-3.029
H	-0.473	-0.57	-2.4
H	0.79	-1.394	-3.313
C	4.098	-3.565	-3.171
H	3.073	-3.528	-3.558
H	4.671	-2.812	-3.72
C	-1.102	-1.366	-4.34
C	-7.078	1.27	2.914
C	-2.234	6.089	3.651
C	3.894	1.916	5.724
C	4.72	-4.959	-3.539
O	-2.147	6.735	4.747
O	4.061	1.375	6.867
O	5.151	-5.713	-2.637
O	-1.508	-2.405	-4.888
O	-7.503	1.486	4.096
O	-7.724	1.301	1.842

O	-2.838	6.422	2.605
O	4.284	3.043	5.341
O	4.732	-5.16	-4.799
O	-1.233	-0.165	-4.777
C	-4.101	3.76	-3.277
H	-5.076	3.291	-3.093
H	-4.084	4.716	-2.738
C	2.115	5.475	-2.201
H	1.878	4.913	-3.114
H	1.223	6.056	-1.931
C	6.934	0.809	-1.116
H	6.598	1.158	-2.1
H	6.944	1.678	-0.443
C	1.359	-5.54	3.209
H	2.438	-5.601	3.014
H	1.215	-4.818	4.024
C	-5.371	-5.331	0.426
H	-4.778	-5.924	-0.286
H	-5.031	-5.599	1.435
C	8.428	0.344	-1.233
C	0.937	-6.955	3.733
C	-6.851	-5.816	0.257
C	-3.973	4.032	-4.8
C	3.224	6.527	-2.545
O	2.99	7.122	-3.648
O	-4.817	4.854	-5.251
O	-7.059	-6.943	0.817
O	1.412	-7.195	4.893
O	9.1	1.054	-2.052
O	0.261	-7.722	3.01
O	8.851	-0.579	-0.498
O	4.16	6.741	-1.74
O	-3.081	3.41	-5.449
O	-7.656	-5.15	-0.435
Na	-1.877	1.824	-4.367

WP5-Na – TS_2b

C	1.061	-4.725	0.593

C	2.335	-4.176	0.37
C	2.557	-3.109	-0.522
C	1.452	-2.64	-1.25
C	0.162	-3.08	-0.911
C	-0.074	-4.101	0.016
C	3.95	-2.521	-0.722
H	4.678	-3.215	-0.278
H	4.159	-2.465	-1.795
C	-1.501	-4.575	0.339
H	-1.488	-5.072	1.311
H	-1.781	-5.342	-0.4
C	4.158	-1.122	-0.131
C	4.618	-0.055	-0.916
C	3.879	-0.83	1.216
C	4.55	1.259	-0.442
C	3.962	0.471	1.74
C	4.152	1.566	0.862
C	-2.583	-3.501	0.359
C	-2.891	-2.802	1.542
C	-3.351	-3.195	-0.78
C	-3.728	-1.676	1.476
C	-4.334	-2.188	-0.791
C	-4.435	-1.318	0.318
C	-5.293	-0.046	0.298
H	-5.869	0.009	1.229
C	3.834	3	1.259
H	3.915	3.112	2.343
C	1.798	4.584	1.391
C	0.464	4.869	1.038
C	-0.225	4.176	0.026
C	0.492	3.19	-0.676
C	1.766	2.813	-0.231
C	2.437	3.466	0.809
C	-1.653	4.548	-0.37
H	-1.934	5.447	0.2
H	-1.668	4.83	-1.426
C	-2.724	3.472	-0.169
C	-3.58	3.077	-1.22
C	-2.927	2.867	1.079

C	-4.355	1.912	-1.066
C	-3.881	1.856	1.285
C	-4.493	1.253	0.169
H	-5.996	-0.119	-0.537
H	4.586	3.677	0.826
H	3.201	-4.615	0.857
H	4.762	2.063	-1.143
H	-0.067	5.666	1.55
H	2.266	1.993	-0.726
H	-4.879	1.499	-1.923
H	-2.313	3.195	1.914
H	-3.181	-3.781	-1.679
H	-3.841	-1.038	2.347
H	-0.693	-2.601	-1.378
H	3.546	-1.643	1.855
O	0.831	-5.872	1.318
O	-5.223	-2.015	-1.843
O	-3.604	3.866	-2.354
O	2.54	5.358	2.279
O	5.092	-0.259	-2.216
O	3.771	0.765	3.065
O	-0.119	2.638	-1.761
O	-4.204	1.386	2.546
O	-2.291	-3.225	2.707
O	1.66	-1.721	-2.262
C	1.012	-1.987	-3.524
H	0.144	-2.634	-3.38
H	0.666	-1.014	-3.889
C	-3.004	-3.172	3.95
H	-2.282	-2.825	4.696
H	-3.811	-2.432	3.905
C	-4.356	2.326	3.617
H	-3.708	1.992	4.436
H	-4.006	3.315	3.304
C	4.167	-0.144	4.099
H	3.429	-0.009	4.895
H	4.094	-1.184	3.764
C	0.604	1.735	-2.598
H	1.044	0.919	-2.013

H	-0.168	1.29	-3.234
C	5.592	0.057	4.724
C	1.919	-2.602	-4.633
C	-3.632	-4.511	4.475
C	-5.799	2.522	4.202
C	1.684	2.351	-3.54
O	-3.966	-4.439	5.704
O	-5.792	3.256	5.246
O	1.765	3.589	-3.672
O	6.44	0.754	4.121
O	1.306	-3.275	-5.506
O	3.153	-2.32	-4.609
O	-3.779	-5.478	3.693
O	-6.787	2.004	3.634
O	2.369	1.457	-4.142
O	5.729	-0.572	5.823
C	1.773	-6.399	2.252
H	2.577	-5.684	2.453
H	1.221	-6.526	3.191
C	-5.488	-3.144	-2.677
H	-4.744	-3.195	-3.484
H	-5.387	-4.064	-2.085
C	-4.74	3.804	-3.214
H	-4.585	3.038	-3.984
H	-5.625	3.507	-2.632
C	1.991	6.607	2.686
H	1.558	7.118	1.813
H	1.172	6.445	3.402
C	6.513	-0.419	-2.31
H	7.004	0.345	-1.693
H	6.798	-1.404	-1.909
C	-5.115	5.15	-3.926
C	2.994	7.624	3.328
C	7.041	-0.294	-3.765
C	2.42	-7.791	1.923
C	-6.91	-3.199	-3.332
O	-7.003	-4.146	-4.183
O	3.136	-8.226	2.885
O	8.301	-0.431	-3.863

O	2.39	8.6	3.889
O	-5.925	4.977	-4.896
O	4.231	7.463	3.209
O	-4.675	6.239	-3.487
O	-7.808	-2.403	-2.974
O	2.19	-8.352	0.826
O	6.213	-0.069	-4.684
Na	3.823	-0.216	-4.093

WP5-K – configuration with highest energy extracted from potential energy surface scanning

C	1.553	2.709	-3.142
C	0.845	3.654	-2.388
C	1.347	4.082	-1.152
C	2.562	3.573	-0.675
C	3.27	2.627	-1.429
C	2.762	2.191	-2.66
C	0.561	5.109	-0.316
H	1.243	5.694	0.266
H	0.007	5.752	-0.967
C	3.532	1.139	-3.481
H	4.58	1.233	-3.29
H	3.344	1.292	-4.523
C	-0.409	4.365	0.621
C	-1.708	4.066	0.19
C	0.009	3.985	1.903
C	-2.586	3.375	1.037
C	-0.868	3.295	2.75
C	-2.164	2.985	2.315
C	3.058	-0.268	-3.073
C	3.7	-0.949	-2.03
C	1.983	-0.867	-3.743
C	3.26	-2.223	-1.649
C	1.543	-2.142	-3.362
C	2.177	-2.818	-2.311
C	1.683	-4.212	-1.882
H	2.504	-4.778	-1.494
C	-3.123	2.212	3.239

H	-2.896	2.439	4.26
C	-3.893	-0.322	3.558
C	-3.7	-1.656	3.176
C	-2.597	-2.006	2.387
C	-1.679	-1.024	1.989
C	-1.872	0.31	2.372
C	-2.982	0.662	3.151
C	-2.429	-3.549	2.272
H	-2.116	-4.033	3.173
H	-3.352	-3.975	1.94
C	-1.354	-3.738	1.185
C	-1.724	-3.783	-0.166
C	-0.006	-3.864	1.547
C	-0.744	-3.941	-1.155
C	0.974	-4.022	0.558
C	0.605	-4.054	-0.794
H	1.267	-4.72	-2.727
H	-4.132	2.497	3.027
H	-0.079	4.049	-2.756
H	-3.578	3.146	0.707
H	-4.396	-2.407	3.486
H	-1.172	1.06	2.068
H	-1.026	-3.974	-2.187
H	0.276	-3.838	2.579
H	1.498	-0.351	-4.545
H	3.75	-2.743	-0.852
H	4.197	2.238	-1.064
H	0.999	4.221	2.235
O	1.04	2.271	-4.404
O	0.445	-2.753	-4.045
O	-3.1	-3.666	-0.534
O	-5.02	0.036	4.363
O	-2.138	4.463	-1.115
O	-0.442	2.906	4.058
O	-0.547	-1.384	1.193
O	2.349	-4.149	0.927
O	4.805	-0.342	-1.354
O	3.08	4.018	0.582
C	4.508	3.963	0.555

H	4.824	2.957	0.376
H	4.875	4.597	-0.226
C	5.694	-1.359	-0.886
H	5.174	-2.006	-0.211
H	6.055	-1.927	-1.718
C	2.443	-4.769	2.212
H	1.933	-4.168	2.936
H	1.993	-5.739	2.174
C	0.969	2.671	4.05
H	1.196	1.891	3.354
H	1.478	3.567	3.76
C	-0.18	-0.28	0.361
H	-1	-0.028	-0.279
H	0.067	0.562	0.973
C	1.428	2.252	5.459
C	5.066	4.442	1.909
C	6.883	-0.706	-0.158
C	3.924	-4.905	2.61
C	1.039	-0.667	-0.497
O	8.009	-1.268	-0.161
O	4.292	-5.856	3.348
O	2.203	-0.458	-0.067
O	1.792	3.126	6.288
O	6.189	5.008	1.962
O	4.307	4.245	3.105
O	6.708	0.54	0.522
O	4.881	-3.952	2.14
O	0.849	-1.265	-1.782
O	1.442	0.87	5.825
C	0.283	3.326	-5.002
H	-0.531	3.591	-4.359
H	0.913	4.179	-5.149
C	0.414	-2.298	-5.401
H	0.297	-1.234	-5.417
H	1.329	-2.564	-5.887
C	-3.334	-4.394	-1.743
H	-2.72	-3.995	-2.524
H	-3.091	-5.425	-1.591
C	-5.377	-1.067	5.2

H	-5.627	-1.91	4.592
H	-4.551	-1.315	5.833
C	-3.11	3.533	-1.6
H	-2.675	2.557	-1.65
H	-3.95	3.517	-0.938
C	-4.816	-4.268	-2.14
C	-6.59	-0.681	6.067
C	-3.573	3.962	-3.005
C	-0.269	2.855	-6.361
C	-0.768	-2.956	-6.136
O	-0.695	-3.178	-7.373
O	0.406	3.03	-7.409
O	-4.557	4.735	-3.135
O	-6.738	-1.194	7.206
O	-5.38	-5.199	-2.771
O	-7.55	0.259	5.576
O	-5.552	-3.092	-1.791
O	-1.95	-3.314	-5.414
O	-1.548	2.22	-6.431
O	-2.885	3.48	-4.163
K	-2.853	1.322	-2.965

WP5-K – *pS*

C	-0.138	-4.21	1.858
C	-1.513	-3.903	1.808
C	-2.173	-3.573	0.609
C	-1.401	-3.602	-0.565
C	-0.015	-3.768	-0.493
C	0.659	-4.023	0.707
C	-3.671	-3.246	0.606
H	-4.132	-3.712	-0.271
H	-4.124	-3.686	1.501
C	2.181	-4.173	0.717
H	2.456	-4.834	-0.116
H	2.47	-4.678	1.642
C	-4.022	-1.761	0.585
C	-4.001	-0.998	1.766
C	-4.429	-1.117	-0.594

C	-4.109	0.399	1.678
C	-4.744	0.254	-0.634
C	-4.442	1.06	0.486
C	2.985	-2.876	0.585
C	3.111	-2.187	-0.634
C	3.693	-2.355	1.685
C	3.762	-0.949	-0.685
C	4.472	-1.185	1.598
C	4.428	-0.4	0.42
C	5.116	0.966	0.318
H	5.87	0.925	-0.477
C	-4.45	2.581	0.42
H	-5.176	2.895	-0.341
C	-2.673	4.432	0.66
C	-1.375	4.91	0.389
C	-0.509	4.283	-0.519
C	-0.995	3.148	-1.201
C	-2.229	2.593	-0.829
C	-3.087	3.208	0.095
C	0.871	4.87	-0.832
H	0.899	5.117	-1.902
H	0.977	5.802	-0.265
C	2.083	3.988	-0.537
C	2.615	3.873	0.765
C	2.745	3.301	-1.566
C	3.557	2.862	1.027
C	3.845	2.462	-1.324
C	4.16	2.112	0.003
H	5.633	1.159	1.261
H	-4.794	2.992	1.375
H	-2.098	-3.911	2.722
H	-3.928	1.003	2.563
H	-1.014	5.799	0.897
H	-2.559	1.663	-1.274
H	3.846	2.65	2.053
H	2.374	3.41	-2.581
H	3.637	-2.893	2.626
H	3.775	-0.408	-1.628
H	0.572	-3.73	-1.405

H	-4.501	-1.707	-1.503
O	0.483	-4.704	2.986
O	5.302	-0.757	2.616
O	2.167	4.765	1.719
O	-3.574	5.106	1.48
O	-3.821	-1.662	2.964
O	-5.321	0.863	-1.731
O	-0.224	2.685	-2.232
O	4.62	1.929	-2.339
O	2.628	-2.754	-1.819
O	-1.973	-3.499	-1.839
C	-2.443	-4.771	-2.33
H	-1.711	-5.545	-2.057
H	-3.392	-5.026	-1.841
C	3.659	-3.501	-2.492
H	4.474	-2.817	-2.77
H	4.077	-4.243	-1.798
C	4.889	2.757	-3.482
H	4.277	2.408	-4.322
H	4.583	3.787	-3.263
C	-6.192	0.073	-2.552
H	-5.619	-0.368	-3.378
H	-6.595	-0.756	-1.956
C	-0.632	1.517	-2.94
H	-0.399	0.632	-2.336
H	-1.717	1.536	-3.11
C	-7.419	0.83	-3.164
C	-2.641	-4.849	-3.871
C	3.191	-4.24	-3.773
C	6.383	2.818	-3.95
C	0.014	1.39	-4.348
O	4.075	-5.018	-4.248
O	6.525	3.527	-5.002
O	0.026	0.188	-4.768
O	-7.633	2.031	-2.879
O	-3.293	-5.877	-4.233
O	-2.123	-3.963	-4.593
O	2.043	-4.006	-4.225
O	7.279	2.229	-3.301

O	0.368	2.425	-4.956
O	-8.116	0.072	-3.917
C	-0.29	-5.447	3.934
H	-0.616	-4.782	4.743
H	-1.193	-5.836	3.446
C	5.709	-1.705	3.604
H	4.924	-1.816	4.365
H	5.842	-2.689	3.132
C	3.028	5.103	2.81
H	2.678	4.59	3.714
H	4.045	4.749	2.602
C	-3.405	6.518	1.616
H	-2.527	6.736	2.243
H	-3.21	6.956	0.628
C	-4.568	-1.243	4.112
H	-3.849	-1.063	4.92
H	-5.079	-0.296	3.907
C	3.161	6.632	3.13
C	-4.611	7.281	2.256
C	-5.655	-2.238	4.65
C	0.44	-6.682	4.565
C	7.053	-1.374	4.338
O	7.276	-2.175	5.304
O	1.462	-7.153	4.012
O	-5.978	-3.239	3.971
O	-4.523	8.544	2.094
O	3.679	6.842	4.276
O	-5.5	6.655	2.88
O	2.831	7.482	2.27
O	7.783	-0.441	3.932
O	-0.162	-7.126	5.597
O	-6.126	-1.866	5.775
K	-0.026	-2.31	-3.842

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C	1.362	-3.162	-0.983
C	2.516	-2.373	-1.005
C	3.478	-2.39	0.01

C	3.279	-3.313	1.06
C	2.048	-3.992	1.159
C	1.051	-3.915	0.167
C	4.715	-1.492	-0.088
H	5.375	-1.722	0.752
H	5.256	-1.75	-1.007
C	-0.27	-4.677	0.345
H	-0.158	-5.352	1.201
H	-0.448	-5.297	-0.542
C	4.407	0.005	-0.108
C	4.185	0.717	-1.296
C	4.329	0.733	1.094
C	3.727	2.04	-1.251
C	3.972	2.091	1.136
C	3.549	2.741	-0.052
C	-1.532	-3.853	0.589
C	-1.791	-3.291	1.849
C	-2.532	-3.716	-0.39
C	-2.885	-2.424	2.013
C	-3.726	-3.009	-0.159
C	-3.855	-2.236	1.018
C	-5.009	-1.249	1.224
H	-5.332	-1.295	2.271
C	2.927	4.135	-0.037
H	3.239	4.664	0.865
C	0.627	5.194	0.475
C	-0.779	5.094	0.46
C	-1.467	4.1	-0.256
C	-0.692	3.2	-1.01
C	0.702	3.207	-0.874
C	1.391	4.168	-0.124
C	-2.993	4.068	-0.307
H	-3.364	4.909	0.298
H	-3.32	4.257	-1.334
C	-3.671	2.776	0.153
C	-4.59	2.094	-0.674
C	-3.431	2.235	1.424
C	-4.967	0.782	-0.336
C	-4.005	1.024	1.85

C	-4.652	0.203	0.906
H	-5.844	-1.561	0.59
H	3.331	4.708	-0.886
H	2.691	-1.745	-1.869
H	3.487	2.526	-2.195
H	-1.374	5.82	1.006
H	1.282	2.453	-1.389
H	-5.524	0.182	-1.049
H	-2.768	2.773	2.096
H	-2.376	-4.195	-1.351
H	-2.996	-1.876	2.945
H	1.836	-4.59	2.04
H	4.56	0.205	2.013
O	0.55	-3.151	-2.109
O	-4.8	-3.04	-1.032
O	-5.059	2.763	-1.789
O	1.309	6.272	1.032
O	4.41	0.133	-2.553
O	3.955	2.851	2.273
O	-1.372	2.355	-1.834
O	-3.925	0.58	3.158
O	-0.918	-3.574	2.883
O	4.323	-3.502	1.946
C	4.399	-4.739	2.659
H	3.816	-4.672	3.587
H	3.948	-5.536	2.052
C	-1.464	-4.037	4.125
H	-0.855	-3.579	4.912
H	-2.49	-3.672	4.249
C	-4.052	1.536	4.217
H	-3.115	1.538	4.787
H	-4.184	2.541	3.798
C	4.58	2.455	3.496
H	3.922	2.841	4.281
H	4.603	1.366	3.605
C	-0.653	1.488	-2.706
H	0.093	0.911	-2.146
H	-1.406	0.777	-3.058
C	6.021	3.009	3.781

C	5.848	-5.21	3.021
C	-1.476	-5.584	4.378
C	-5.231	1.318	5.229
C	0.012	2.133	-3.964
O	-1.857	-5.877	5.559
O	-5.154	2.111	6.226
O	0.772	1.313	-4.579
O	6.692	3.502	2.846
O	5.846	-6.202	3.822
O	6.842	-4.65	2.5
O	-1.137	-6.368	3.461
O	-6.119	0.468	4.991
O	-0.268	3.306	-4.284
O	6.354	2.87	5.003
C	0.533	-4.358	-2.884
H	0.98	-5.177	-2.308
H	-0.519	-4.611	-3.062
C	-4.946	-4.185	-1.876
H	-4.434	-4.01	-2.831
H	-4.463	-5.05	-1.401
C	-6.3	2.359	-2.365
H	-6.123	1.604	-3.141
H	-6.928	1.891	-1.593
C	0.544	7.398	1.447
H	-0.225	7.616	0.69
H	0.018	7.172	2.385
C	5.738	0.394	-3.047
H	5.965	1.459	-2.902
H	6.463	-0.179	-2.453
C	-7.154	3.516	-2.989
C	1.334	8.735	1.644
C	5.955	0.063	-4.551
C	1.241	-4.326	-4.274
C	-6.419	-4.623	-2.185
O	-6.469	-5.517	-3.094
O	1.196	-5.443	-4.873
O	7.155	0.242	-4.928
O	0.661	9.596	2.306
O	-8.085	3.082	-3.744

O	2.46	8.892	1.117
O	-6.922	4.709	-2.677
O	-7.374	-4.141	-1.534
O	1.76	-3.256	-4.682
O	4.977	-0.317	-5.242
K	2.389	-0.714	-4.32

WP5-K – TS_2a

C	2.574	-2.759	-1.791
C	3.488	-1.699	-1.793
C	4.291	-1.38	-0.692
C	4.272	-2.308	0.385
C	3.278	-3.306	0.424
C	2.39	-3.542	-0.644
C	5.097	-0.084	-0.669
H	5.81	-0.112	0.157
H	5.704	-0.017	-1.585
C	1.33	-4.643	-0.567
H	1.663	-5.406	0.145
H	1.252	-5.112	-1.555
C	4.251	1.201	-0.549
C	4.755	2.376	0.064
C	2.966	1.298	-1.089
C	3.876	3.442	0.332
C	2.158	2.435	-0.984
C	2.553	3.495	-0.152
C	-0.075	-4.22	-0.144
C	-0.392	-4.037	1.211
C	-1.126	-4.103	-1.072
C	-1.657	-3.543	1.57
C	-2.443	-3.792	-0.685
C	-2.699	-3.384	0.645
C	-4.06	-2.837	1.083
H	-4.293	-3.222	2.08
C	1.659	4.682	0.237
H	2.089	5.128	1.142
C	-0.154	3.588	1.631
C	-1.478	3.149	1.77

C	-2.518	3.61	0.952
C	-2.199	4.621	0.011
C	-0.85	4.929	-0.23
C	0.196	4.382	0.531
C	-3.949	3.073	1.117
H	-4.358	3.455	2.065
H	-4.567	3.481	0.316
C	-4.094	1.553	1.117
C	-4.309	0.836	-0.077
C	-4.073	0.813	2.312
C	-4.248	-0.567	-0.056
C	-4.182	-0.59	2.347
C	-4.153	-1.309	1.132
H	-4.814	-3.221	0.388
H	1.696	5.444	-0.556
H	3.558	-1.086	-2.69
H	4.206	4.258	0.967
H	-1.7	2.406	2.532
H	-0.587	5.632	-1.014
H	-4.29	-1.122	-0.989
H	-3.987	1.36	3.246
H	-0.909	-4.3	-2.118
H	-1.849	-3.29	2.61
H	3.156	-3.918	1.31
H	2.549	0.465	-1.635
O	1.802	-2.956	-2.944
O	-3.515	-3.879	-1.553
O	-4.499	1.563	-1.229
O	0.839	3.202	2.512
O	6.103	2.404	0.369
O	0.96	2.427	-1.68
O	-3.262	5.254	-0.594
O	-4.332	-1.304	3.527
O	0.58	-4.31	2.157
O	5.247	-2.166	1.336
C	5.527	-3.214	2.273
H	5.097	-2.937	3.242
H	5.055	-4.149	1.948
C	0.253	-5.218	3.219

H	0.728	-4.813	4.12
H	-0.83	-5.225	3.39
C	-4.871	-0.609	4.653
H	-4.07	-0.072	5.18
H	-5.591	0.144	4.303
C	0.874	3.377	-2.752
H	-0.182	3.662	-2.808
H	1.451	4.274	-2.51
C	-3.125	6.113	-1.724
H	-2.122	6.056	-2.157
H	-3.817	5.724	-2.481
C	1.308	2.881	-4.164
C	7.048	-3.548	2.457
C	0.722	-6.705	3.064
C	-5.627	-1.489	5.705
C	-3.485	7.628	-1.525
O	0.494	-7.393	4.112
O	-5.96	-0.812	6.735
O	-3.445	8.279	-2.621
O	1.306	1.636	-4.388
O	7.324	-4.007	3.611
O	7.817	-3.43	1.472
O	1.247	-7.081	1.991
O	-5.87	-2.695	5.471
O	-3.786	8.065	-0.389
O	1.564	3.806	-4.984
C	2.432	-3.748	-3.962
H	3.51	-3.534	-3.967
H	2.306	-4.814	-3.725
C	-3.453	-4.846	-2.61
H	-3.122	-4.355	-3.534
H	-2.706	-5.61	-2.359
C	-5.404	1.111	-2.244
H	-4.957	1.428	-3.191
H	-5.463	0.016	-2.26
C	0.667	3.554	3.891
H	-0.397	3.529	4.157
H	1.167	2.762	4.459
C	6.682	3.648	0.768

H	6.216	4.464	0.196
H	6.473	3.833	1.829
C	-6.874	1.658	-2.203
C	1.251	4.922	4.382
C	8.223	3.788	0.53
C	1.882	-3.476	-5.389
C	-4.783	-5.618	-2.913
O	-4.699	-6.303	-3.985
O	2.364	-4.251	-6.269
O	8.732	4.741	1.209
O	1.083	5.095	5.634
O	-7.492	1.459	-3.3
O	1.81	5.691	3.566
O	-7.309	2.187	-1.155
O	-5.745	-5.554	-2.114
O	1.063	-2.534	-5.543
O	8.799	3.059	-0.311
K	0.464	-0.646	-3.611

WP5-K – TS_2b

C	1.425	-4.316	1.164
C	2.641	-3.645	0.954
C	2.918	-2.906	-0.213
C	1.941	-2.929	-1.226
C	0.665	-3.438	-0.934
C	0.357	-4.105	0.258
C	4.242	-2.159	-0.346
H	5	-2.704	0.235
H	4.563	-2.172	-1.391
C	-1.048	-4.682	0.498
H	-1.062	-5.164	1.477
H	-1.221	-5.467	-0.253
C	4.216	-0.695	0.124
C	4.611	0.356	-0.718
C	3.797	-0.336	1.418
C	4.355	1.686	-0.361
C	3.694	1.002	1.834
C	3.834	2.045	0.885

C	-2.216	-3.7	0.432
C	-2.659	-3.021	1.583
C	-2.945	-3.489	-0.752
C	-3.608	-1.993	1.454
C	-4.026	-2.591	-0.835
C	-4.285	-1.727	0.254
C	-5.285	-0.566	0.17
H	-5.903	-0.567	1.075
C	3.392	3.472	1.173
H	3.472	3.672	2.244
C	1.208	4.841	1.293
C	-0.149	4.984	0.942
C	-0.76	4.222	-0.069
C	0.056	3.318	-0.773
C	1.363	3.075	-0.33
C	1.958	3.792	0.715
C	-2.221	4.435	-0.461
H	-2.603	5.286	0.123
H	-2.27	4.729	-1.514
C	-3.16	3.239	-0.276
C	-3.927	2.727	-1.346
C	-3.323	2.628	0.974
C	-4.554	1.476	-1.196
C	-4.15	1.508	1.169
C	-4.646	0.819	0.045
H	-5.938	-0.737	-0.691
H	4.084	4.17	0.678
H	3.435	-3.734	1.688
H	4.547	2.458	-1.105
H	-0.761	5.72	1.455
H	1.953	2.314	-0.824
H	-4.996	0.991	-2.061
H	-2.781	3.04	1.821
H	-2.674	-4.072	-1.628
H	-3.841	-1.366	2.308
H	-0.12	-3.332	-1.677
H	3.516	-1.128	2.104
O	1.191	-5.181	2.198
O	-4.868	-2.528	-1.936

O	-4.014	3.493	-2.492
O	1.866	5.694	2.174
O	5.212	0.109	-1.957
O	3.368	1.371	3.11
O	-0.509	2.709	-1.853
O	-4.454	1.018	2.427
O	-2.083	-3.36	2.787
O	2.271	-2.518	-2.521
C	1.768	-3.404	-3.55
H	1.665	-4.408	-3.129
H	0.767	-3.068	-3.856
C	-2.875	-3.408	3.98
H	-2.223	-3.044	4.78
H	-3.725	-2.719	3.912
C	-4.74	1.944	3.483
H	-4.092	1.681	4.326
H	-4.48	2.962	3.174
C	3.782	0.599	4.244
H	3.017	0.786	5.002
H	3.763	-0.474	4.025
C	0.283	1.892	-2.708
H	0.841	1.146	-2.129
H	-0.449	1.345	-3.31
C	5.179	0.941	4.87
C	2.63	-3.513	-4.842
C	-3.439	-4.804	4.419
C	-6.215	1.997	4.014
C	1.25	2.618	-3.697
O	-3.866	-4.796	5.622
O	-6.32	2.736	5.05
O	1.989	1.793	-4.333
O	6.002	1.613	4.208
O	2.349	-4.53	-5.541
O	3.463	-2.606	-5.108
O	-3.454	-5.754	3.603
O	-7.124	1.377	3.417
O	1.203	3.858	-3.82
O	5.32	0.448	6.036
C	2.166	-5.493	3.191

H	2.84	-4.649	3.371
H	1.584	-5.633	4.109
C	-4.968	-3.69	-2.76
H	-4.179	-3.676	-3.525
H	-4.806	-4.586	-2.144
C	-5.113	3.288	-3.378
H	-4.845	2.544	-4.139
H	-5.968	2.886	-2.815
C	1.19	6.881	2.575
H	0.691	7.33	1.702
H	0.405	6.641	3.306
C	6.646	0.138	-1.933
H	6.978	1.013	-1.357
H	7.02	-0.757	-1.414
C	-5.634	4.574	-4.108
C	2.085	8.011	3.184
C	7.294	0.208	-3.345
C	3.023	-6.794	3.001
C	-6.337	-3.903	-3.489
O	-6.282	-4.862	-4.33
O	3.746	-7.044	4.021
O	8.567	0.199	-3.31
O	1.389	8.914	3.759
O	-6.387	4.3	-5.1
O	3.328	7.995	3.026
O	-5.349	5.711	-3.66
O	-7.334	-3.206	-3.19
O	2.925	-7.462	1.946
O	6.549	0.276	-4.353
K	3.637	-0.202	-4.046

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C	0.129	-4.327	-1.648
C	1.502	-4.017	-1.646
C	2.186	-3.626	-0.48
C	1.439	-3.593	0.71
C	0.052	-3.758	0.678
C	-0.645	-4.078	-0.493

C	3.683	-3.302	-0.514
H	4.161	-3.754	0.362
H	4.117	-3.758	-1.411
C	-2.166	-4.235	-0.471
H	-2.426	-4.843	0.405
H	-2.465	-4.798	-1.359
C	4.031	-1.817	-0.525
C	3.984	-1.075	-1.719
C	4.453	-1.15	0.636
C	4.083	0.324	-1.656
C	4.758	0.223	0.647
C	4.431	1.007	-0.481
C	-2.977	-2.937	-0.408
C	-3.105	-2.191	0.775
C	-3.687	-2.473	-1.532
C	-3.765	-0.957	0.768
C	-4.471	-1.304	-1.5
C	-4.433	-0.465	-0.361
C	-5.128	0.901	-0.322
H	-5.895	0.888	0.462
C	4.433	2.53	-0.442
H	5.155	2.858	0.316
C	2.645	4.357	-0.746
C	1.346	4.839	-0.491
C	0.486	4.245	0.445
C	0.981	3.142	1.171
C	2.215	2.578	0.817
C	3.067	3.159	-0.134
C	-0.895	4.841	0.737
H	-0.927	5.116	1.8
H	-0.997	5.757	0.144
C	-2.105	3.952	0.459
C	-2.621	3.789	-0.844
C	-2.784	3.308	1.504
C	-3.56	2.77	-1.08
C	-3.883	2.461	1.279
C	-4.179	2.06	-0.037
H	-5.631	1.056	-1.28
H	4.779	2.925	-1.401

H	2.068	-4.073	-2.571
H	3.884	0.911	-2.549
H	0.978	5.704	-1.034
H	2.552	1.667	1.298
H	-3.835	2.518	-2.101
H	-2.429	3.459	2.519
H	-3.629	-3.056	-2.446
H	-3.781	-0.373	1.685
H	-0.513	-3.671	1.601
H	4.543	-1.723	1.554
O	-0.514	-4.883	-2.735
O	-5.301	-0.927	-2.539
O	-2.158	4.642	-1.826
O	3.539	5.004	-1.595
O	3.788	-1.761	-2.901
O	5.35	0.853	1.724
O	0.21	2.72	2.223
O	-4.672	1.97	2.305
O	-2.613	-2.697	1.983
O	2.054	-3.426	1.954
C	2.445	-4.685	2.53
H	1.632	-5.411	2.383
H	3.331	-5.069	2.007
C	-3.643	-3.393	2.707
H	-4.452	-2.689	2.949
H	-4.071	-4.175	2.064
C	-4.959	2.846	3.406
H	-4.353	2.542	4.268
H	-4.66	3.868	3.143
C	6.255	0.084	2.529
H	5.711	-0.356	3.375
H	6.653	-0.745	1.931
C	0.635	1.619	3.019
H	0.359	0.685	2.515
H	1.726	1.63	3.139
C	7.487	0.865	3.101
C	2.747	-4.645	4.052
C	-3.176	-4.055	4.027
C	-6.457	2.914	3.86

C	0.053	1.652	4.46
O	-4.043	-4.832	4.528
O	-6.612	3.664	4.881
O	0.027	0.503	5.018
O	7.667	2.07	2.814
O	3.395	-5.656	4.459
O	2.302	-3.689	4.739
O	-2.042	-3.772	4.495
O	-7.343	2.294	3.228
O	-0.243	2.75	4.974
O	8.224	0.119	3.827
C	0.243	-5.679	-3.654
H	0.554	-5.06	-4.505
H	1.156	-6.038	-3.16
C	-5.708	-1.924	-3.479
H	-4.922	-2.077	-4.23
H	-5.845	-2.881	-2.956
C	-3.006	4.946	-2.937
H	-2.635	4.417	-3.823
H	-4.023	4.585	-2.738
C	3.372	6.413	-1.768
H	2.491	6.616	-2.397
H	3.183	6.878	-0.792
C	4.521	-1.361	-4.066
H	3.791	-1.176	-4.863
H	5.049	-0.42	-3.876
C	-3.152	6.466	-3.295
C	4.575	7.156	-2.435
C	5.583	-2.375	-4.614
C	-0.494	-6.948	-4.201
C	-7.047	-1.625	-4.233
O	-7.278	-2.483	-5.148
O	-1.509	-7.385	-3.61
O	5.909	-3.371	-3.929
O	4.484	8.423	-2.314
O	-3.663	6.641	-4.449
O	5.463	6.512	-3.04
O	-2.836	7.339	-2.454
O	-7.766	-0.659	-3.89

O	0.097	-7.451	-5.212
O	6.036	-2.024	-5.753
N	0.122	-2.048	3.907
H	-0.75	-2.598	4.088
H	0.224	-1.95	2.897
H	0.08	-1.081	4.335
H	0.956	-2.592	4.234

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C	-1.708	-4.153	1.56
C	-2.822	-3.326	1.802
C	-3.405	-2.519	0.808
C	-2.857	-2.618	-0.486
C	-1.671	-3.329	-0.688
C	-1.036	-4.062	0.322
C	-4.597	-1.619	1.159
H	-5.461	-1.896	0.542
H	-4.864	-1.8	2.206
C	0.28	-4.785	0.031
H	0.153	-5.353	-0.9
H	0.46	-5.508	0.831
C	-4.365	-0.122	0.999
C	-3.518	0.563	1.88
C	-5.012	0.638	0.009
C	-3.113	1.871	1.572
C	-4.761	2.008	-0.166
C	-3.678	2.601	0.521
C	1.516	-3.89	-0.118
C	1.81	-3.19	-1.3
C	2.453	-3.786	0.926
C	2.88	-2.288	-1.341
C	3.621	-3.006	0.823
C	3.791	-2.143	-0.286
C	4.949	-1.144	-0.382
H	5.477	-1.299	-1.328
C	-3.132	3.967	0.107
H	-3.573	4.208	-0.867
C	-0.865	3.196	-0.782

C	0.536	3.27	-0.769
C	1.231	4.287	-0.098
C	0.469	5.3	0.529
C	-0.924	5.135	0.637
C	-1.613	4.084	0.013
C	2.767	4.323	-0.09
H	3.108	4.923	-0.948
H	3.09	4.858	0.806
C	3.462	2.968	-0.14
C	3.679	2.21	1.032
C	3.935	2.435	-1.349
C	4.124	0.885	0.911
C	4.539	1.167	-1.442
C	4.525	0.324	-0.312
H	5.652	-1.363	0.427
H	-3.491	4.741	0.802
H	-3.243	-3.277	2.801
H	-2.308	2.321	2.149
H	1.118	2.53	-1.307
H	-1.509	5.844	1.216
H	4.176	0.249	1.79
H	3.826	3.037	-2.246
H	2.264	-4.348	1.836
H	3.027	-1.704	-2.247
H	-1.242	-3.364	-1.682
H	-5.726	0.14	-0.639
O	-1.238	-5.072	2.48
O	4.638	-3.052	1.754
O	3.367	2.818	2.222
O	-1.61	2.299	-1.485
O	-3.04	-0.103	2.994
O	-5.508	2.821	-1.001
O	1.14	6.427	0.993
O	5.155	0.707	-2.596
O	1.086	-3.426	-2.478
O	-3.438	-2.015	-1.594
C	-4.706	-2.548	-2.003
H	-4.999	-3.361	-1.329
H	-5.456	-1.752	-1.916

C	1.708	-4.47	-3.253
H	2.776	-4.236	-3.366
H	1.639	-5.418	-2.702
C	5.646	1.686	-3.517
H	4.84	1.994	-4.197
H	5.961	2.579	-2.96
C	-6.811	2.381	-1.38
H	-6.744	1.703	-2.241
H	-7.258	1.811	-0.552
C	0.355	7.507	1.486
H	-0.504	7.671	0.816
H	-0.051	7.256	2.476
C	-7.831	3.515	-1.737
C	-4.78	-3.089	-3.459
C	1.135	-4.694	-4.677
C	6.869	1.252	-4.392
C	1.069	8.896	1.592
O	1.606	-5.73	-5.236
O	7.183	2.151	-5.242
O	0.424	9.711	2.335
O	-7.545	4.719	-1.536
O	-5.882	-3.657	-3.721
O	-3.807	-2.911	-4.237
O	0.322	-3.866	-5.164
O	7.437	0.153	-4.199
O	2.105	9.13	0.929
O	-8.927	3.045	-2.19
C	-2.15	-5.578	3.46
H	-2.105	-4.957	4.363
H	-3.175	-5.512	3.07
C	4.738	-4.198	2.606
H	4.129	-4.045	3.505
H	4.336	-5.076	2.083
C	3.942	2.409	3.467
H	3.142	2.531	4.203
H	4.211	1.347	3.455
C	-1.059	1.34	-2.379
H	-0.07	1.001	-2.046
H	-1.742	0.488	-2.306

C	-3.31	0.49	4.272
H	-2.467	0.204	4.911
H	-3.305	1.584	4.19
C	5.189	3.209	3.984
C	-0.973	1.781	-3.871
C	-4.624	0.071	5.016
C	-1.931	-7.072	3.875
C	6.191	-4.581	3.049
O	6.192	-5.437	3.993
O	-1.197	-7.817	3.186
O	-5.405	-0.754	4.486
O	-0.846	0.793	-4.676
O	5.413	3.003	5.221
O	-1.016	2.991	-4.162
O	5.841	3.922	3.188
O	7.179	-4.1	2.448
O	-2.614	-7.387	4.905
O	-4.741	0.645	6.148
N	-1.204	-1.832	-3.917
H	-0.586	-2.519	-4.406
H	-0.921	-1.841	-2.937
H	-1.08	-0.836	-4.267
H	-2.201	-2.148	-3.966

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C	-0.875	-3.593	1.55
C	-2.167	-3.054	1.536
C	-3.006	-3.097	0.413
C	-2.541	-3.864	-0.686
C	-1.202	-4.299	-0.711
C	-0.333	-4.161	0.387
C	-4.348	-2.361	0.402
H	-4.955	-2.725	-0.428
H	-4.899	-2.617	1.32
C	1.1	-4.705	0.318
H	1.131	-5.489	-0.448
H	1.338	-5.169	1.281
C	-4.249	-0.825	0.311

C	-5.157	-0.043	-0.447
C	-3.29	-0.115	1.037
C	-4.879	1.322	-0.652
C	-3.132	1.272	0.974
C	-3.852	2.011	0.022
C	2.212	-3.712	-0.008
C	2.431	-3.281	-1.327
C	3.114	-3.265	0.973
C	3.338	-2.237	-1.564
C	4.166	-2.376	0.685
C	4.195	-1.735	-0.575
C	5.093	-0.537	-0.866
H	5.536	-0.639	-1.862
C	-3.608	3.493	-0.3
H	-4.137	3.716	-1.234
C	-1.41	3.487	-1.572
C	-0.02	3.681	-1.573
C	0.626	4.486	-0.629
C	-0.189	5.19	0.285
C	-1.538	4.824	0.412
C	-2.161	3.931	-0.476
C	2.15	4.59	-0.585
H	2.504	5.232	-1.406
H	2.413	5.107	0.344
C	2.916	3.271	-0.658
C	2.736	2.274	0.322
C	3.878	3.041	-1.652
C	3.439	1.066	0.217
C	4.635	1.855	-1.723
C	4.371	0.817	-0.802
H	5.922	-0.54	-0.149
H	-4.057	4.119	0.485
H	-2.53	-2.601	2.455
H	-5.458	1.88	-1.381
H	0.584	3.168	-2.318
H	-2.129	5.231	1.226
H	3.284	0.288	0.956
H	4.031	3.822	-2.39
H	2.991	-3.633	1.987

H	3.386	-1.793	-2.555
H	-0.795	-4.753	-1.608
H	-2.633	-0.64	1.715
O	-0.147	-3.523	2.738
O	5.182	-2.09	1.574
O	1.863	2.59	1.317
O	-2.056	2.794	-2.577
O	-6.288	-0.666	-0.945
O	-2.209	1.845	1.835
O	0.401	6.204	1.021
O	5.647	1.656	-2.662
O	1.691	-3.864	-2.338
O	-3.452	-4.155	-1.672
C	-3.175	-5.156	-2.66
H	-2.875	-4.657	-3.588
H	-2.342	-5.79	-2.333
C	2.362	-4.266	-3.539
H	1.675	-4.032	-4.36
H	3.27	-3.672	-3.688
C	6.073	2.788	-3.413
H	5.278	3.105	-4.105
H	6.255	3.633	-2.731
C	-2.762	2.669	2.868
H	-1.944	3.332	3.172
H	-3.567	3.293	2.468
C	-0.451	7.155	1.656
H	-1.337	7.326	1.028
H	-0.807	6.759	2.618
C	-3.296	1.961	4.148
C	-4.356	-6.143	-2.961
C	2.764	-5.775	-3.676
C	7.371	2.604	-4.266
C	0.179	8.564	1.92
O	3.248	-6.037	-4.827
O	7.684	3.679	-4.882
O	-0.581	9.301	2.632
O	-2.92	0.783	4.402
O	-4.331	-6.604	-4.148
O	-5.134	-6.46	-2.03

O	2.596	-6.556	-2.713
O	7.977	1.509	-4.29
O	1.284	8.875	1.416
O	-4.049	2.692	4.855
C	-0.251	-4.671	3.592
H	-0.995	-5.365	3.182
H	0.718	-5.19	3.599
C	5.498	-3.065	2.574
H	4.921	-2.857	3.484
H	5.202	-4.06	2.216
C	1.409	1.623	2.261
H	0.35	1.855	2.41
C	-1.852	3.235	-3.925
H	-0.823	3.59	-4.061
H	-1.974	2.338	-4.543
C	-7.319	0.152	-1.5
H	-7.384	1.09	-0.929
H	-7.069	0.417	-2.535
C	-2.812	4.333	-4.498
C	-8.765	-0.448	-1.476
C	-0.636	-4.381	5.072
C	7.01	-3.169	2.971
O	7.192	-3.989	3.931
O	-0.693	-5.433	5.781
O	-9.548	0.152	-2.286
O	-2.567	4.593	-5.722
O	-3.695	4.835	-3.765
O	7.88	-2.521	2.345
O	-0.848	-3.197	5.435
O	-9.059	-1.355	-0.663
N	-0.609	-0.724	3.93
H	-0.662	-1.598	4.498
H	-0.528	-1.023	2.958
H	-1.474	-0.138	4.042
H	0.253	-0.139	4.163
C	2.118	1.638	3.645
O	1.584	0.822	4.476
O	3.077	2.405	3.851
H	1.458	0.613	1.837

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C	0.162	-4.742	-1.153
C	1.535	-4.431	-1.197
C	2.182	-3.686	-0.193
C	1.395	-3.301	0.907
C	0.015	-3.51	0.892
C	-0.649	-4.176	-0.144
C	3.68	-3.378	-0.31
H	4.213	-3.882	0.509
H	4.042	-3.805	-1.252
C	-2.171	-4.353	-0.119
H	-2.424	-4.98	0.749
H	-2.463	-4.921	-1.006
C	4.076	-1.908	-0.287
C	3.819	-1.083	-1.388
C	4.757	-1.334	0.801
C	3.98	0.307	-1.259
C	5.101	0.027	0.843
C	4.568	0.899	-0.136
C	-3.014	-3.075	-0.03
C	-3.039	-2.297	1.132
C	-3.851	-2.684	-1.088
C	-3.756	-1.097	1.177
C	-4.649	-1.523	-1.007
C	-4.528	-0.637	0.093
C	-5.18	0.746	0.105
H	-5.685	0.923	1.056
C	4.582	2.424	0.029
H	4.989	2.646	1.02
C	2.932	4.105	-1.045
C	1.615	4.575	-1.23
C	0.553	4.08	-0.456
C	0.828	3.137	0.537
C	2.137	2.654	0.705
C	3.206	3.071	-0.125
C	-0.852	4.679	-0.642
H	-0.964	5.494	0.09

H	-0.909	5.131	-1.638
C	-2.047	3.752	-0.487
C	-2.49	2.957	-1.557
C	-2.8	3.707	0.7
C	-3.469	1.978	-1.325
C	-3.918	2.868	0.861
C	-4.174	1.881	-0.117
H	-5.941	0.766	-0.681
H	5.256	2.88	-0.704
H	2.127	-4.749	-2.049
H	3.605	0.953	-2.05
H	1.401	5.315	-1.993
H	-3.698	1.263	-2.111
H	-2.506	4.363	1.513
H	-3.876	-3.291	-1.987
H	-0.541	-3.173	1.755
H	5.014	-1.977	1.635
O	-0.448	-5.596	-2.056
O	-5.579	-1.194	-1.972
O	-1.893	3.13	-2.789
O	4.01	4.628	-1.749
O	3.335	-1.658	-2.551
O	5.931	0.567	1.811
O	2.495	1.762	1.665
O	-4.793	2.973	1.927
O	-3.671	-0.344	2.332
O	1.945	-2.673	2.016
C	2.615	-3.536	2.942
H	3.061	-4.386	2.411
H	3.43	-2.94	3.369
C	-4.767	-0.475	3.256
H	-4.967	0.533	3.633
H	-5.661	-0.817	2.722
C	-4.825	4.21	2.644
H	-4.07	4.194	3.442
H	-4.563	5.03	1.962
C	6.732	-0.333	2.575
H	6.133	-0.778	3.381
H	7.068	-1.158	1.929

C	1.536	1.114	2.492
H	0.602	0.95	1.94
H	1.967	0.128	2.694
C	8.025	0.27	3.221
C	1.776	-4.095	4.128
C	-4.528	-1.415	4.472
C	-6.2	4.602	3.282
C	1.222	1.8	3.853
O	-5.581	-1.685	5.122
O	-6.1	5.641	4.017
O	0.454	1.092	4.595
O	8.375	1.449	2.983
O	2.362	-5.018	4.768
O	0.651	-3.585	4.378
O	-3.353	-1.793	4.736
O	-7.236	3.952	3.016
O	1.719	2.91	4.126
O	8.634	-0.587	3.946
C	0.364	-6.551	-2.742
H	0.805	-6.094	-3.638
H	1.197	-6.853	-2.091
C	-6.03	-2.218	-2.865
H	-5.332	-2.309	-3.707
H	-6.035	-3.182	-2.338
C	-2.725	3.237	-3.952
H	-2.259	2.617	-4.725
H	-3.719	2.821	-3.748
C	3.828	5.887	-2.398
H	3.189	5.766	-3.285
H	3.304	6.573	-1.719
C	4.075	-1.434	-3.758
H	3.33	-1.331	-4.554
H	4.621	-0.484	-3.694
C	-2.935	4.67	-4.552
C	5.133	6.61	-2.869
C	5.092	-2.538	-4.208
C	-0.371	-7.864	-3.173
C	-7.473	-2.026	-3.44
O	-7.726	-2.861	-4.369

O	-1.517	-8.121	-2.735
O	5.322	-3.518	-3.461
O	4.883	7.765	-3.353
O	-3.483	4.636	-5.703
O	6.251	6.057	-2.761
O	-2.594	5.679	-3.891
O	-8.241	-1.168	-2.949
O	0.349	-8.588	-3.937
O	5.598	-2.29	-5.352
N	-0.772	-1.204	3.741
H	-1.743	-1.331	4.116
H	-0.851	-1.087	2.73
H	-0.301	-0.323	4.116
H	-0.184	-2.049	3.933
H	0.03	2.799	1.188
H	-2.528	-2.611	2.035