Electronic Supplementary Information

Neutral and Anionic Phosphate-Diesters as Molecular Templates for the Encapsulation of Water Dimer

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Experimental Section

General considerations. Reactions involving *n*BuLi and $POCl_3$ were carried out under an argon atmosphere using standard Schlenk techniques and all remaining reactions were carried out under an open atmosphere inside a fume hood. THF was dried by Innovative Technology solvent purification system. Compounds Ar-OH[27] and **3**[32] were prepared according to literature procedures. NMR spectra were recorded on a BrukerNanoBay 300 MHz NMR spectrometer. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (^{1}H) or the deuterated solvent itself (^{13}C). ^{31}P NMR spectra were referenced to external H_3PO_4. IR spectra were recorded on a Bruker–Alpha spectrometer. Melting points were determined in Stuart melting point apparatus SMP10 and are uncorrected. Elemental analyses were performed on a Perkin Elmer-Series-II CHNS/O analyzer 2400.

Synthesis of 2·Et$_2$O. *n*BuLi (1.6 M, 7 mL, 11.2 mmol) was added dropwise to a solution of Ar-OH (4.68 g, 10 mmol, in 50 mL dry THF) at −78° C. After completion of addition the reaction mixture was allowed to reach room temperature within one hour and stirred for another 2 hrs. During this time a deep red suspension of Ar-O^-Li^+ was formed. This suspension was transferred to a solution of $POCl_3$ (1 mL, 10.5 mmol, in 5 mL THF) at −78° C in a drop by drop by cannula. Then the reaction mixture was slowly allowed to reach room temperature and an off-yellow clear solution formed. The stirring was continued for another 12 hrs followed by refluxed for 4 hrs and then the volatiles were removed under vacuum affording a yellow residue of ArO-$POCl_2$. In another Schlenk flask, ^{n}BuLi (1.6 M, 7 mL, 11.2 mmol) was added dropwise to a solution of Ar-OH (4.68 g, 10 mmol, in 50 mL dry THF) at −78° C. After completion of addition the reaction mixture was allowed to reach room temperature within one hour and stirred for another 2 hrs. During this time a deep red suspension of Ar-O^-Li^+ was formed and added to a stirred solution of Ar-O-$POCl_2$ in THF (50 mL) at −78° C. Then the reaction mixture was slowly allowed to reach room temperature and stirring was continued for overnight. During this period a deep orange-red clear solution formed, which was refluxed for 12 hrs and then the volatiles were removed under vacuum affording a yellow residue of $(Ar\text{-}O)_2POCl$. The resulting solid was dissolved in a mixture of THF/water (100mL/40mL) and refluxed for 45 hrs. The organic layer was separated and subsequently all volatiles were evaporated under vacuum affording a yellow residue. The resulting solid was extracted with DCM/water and the organic layer was separated followed by drying over Na_2SO_4, filtering and concentrating to give a yellow residue which was washed with cold diethyl ether to give pure $(Ar\text{-}O)_2PO(OH)\cdot Et_2O$. Yield: 3.39 g, 32 %. **M. P.:** 136 °C. **^{1}H NMR** (25 °C, 300 MHz, $CDCl_3$): δ = 7.01-6.94 (m, 24H, Ar–H), 6.76-6.74 (m, 16H, Ar–H), 6.64 (s, 4H, Ar–H), 6.04 (s, 4H, C*H*Ph_2), 5.02 (s, br, 1H, P–O*H*), 3.45 (q, 4H, OC*H*$_2$$CH_3$), 2.59 (sept, 2H, C*H*$(CH_3)_2$, 1.15 (t, 6H, OCH_2C*H*$_3$), 0.97 (d, 12H, CH(C*H*$_3$)$_2$ ppm. **^{13}C{^{1}H} NMR** (25 °C, 75.431 MHz, CDCl3): δ = 145.47 (Ar–C_{quart}), 145.36 (Ar–C_{quart}), 145.07 (Ar–C_{quart}), 143.29 (Ar–C_{quart}), 136.12 (Ar–C_{quart}), 136.08 (Ar–C_{quart}), 129.46 (Ar–*C*H), 127.98 (Ar–*C*H), 127.71 (Ar–*C*H), 125.94 (Ar–*C*H), 65.86 (OCH_2CH_3), 49.90 (*C*HPh_2), 33.35 (*C*H$(CH_3)_2$), 25.47 (CH(*C*H$_3$)$_2$), 15.13 (OCH_2CH_3) ppm. **^{31}P{^{1}H} NMR** (25 °C, 121.442 MHz, $CDCl_3$): δ = −11.2 ppm. **IR** (KBr pellet, cm^{-1}): $\bar{\upsilon}$ = 3425 (m, br), 3083 (w), 3059 (m), 3026 (m), 2959 (s), 2926 (m), 2869 (m), 1947 (w), 1880 (w), 1803 (w), 1754 (w), 1599 (m), 1493 (s), 1465 (s), 1445 (s), 1383 (w), 1363 (w), 1319 (w), 1260 (m), 1197 (m), 1156 (s), 1115 (s), 1078 (m), 1031 (m), 1015 (m), 977 (s) 945 (s), 893 (w), 862 (w), 828 (w), 795 (w), 761 (m), 721 (s), 698 (s), 647 (w), 634 (w), 621 (w), 605 (s), 569 (w), 524 (w). **ESI-MS:** Calcd (m/z) for $[C_{70}H_{63}O_4P + H^+]^+$: 999.4537; found: 999.4470. **Elemental analysis** calcd (%) for $C_{74}H_{73}O_5P$: C 82.81, H 6.86; found: C 82.31, H 6.60.

Synthesis of 2·(H$_2$O)$_2$. Slow evaporation of a CH_3CN/H_2O (10:1) solution of **2·Et$_2$O** at room temperature leads to almost quantitative formation of **2·(H$_2$O)$_2$**. These obtained crystals are also suitable for single crystal X-ray diffraction study. **M. P.:** 211

°C. **^{1}H NMR** (25 °C, 300 MHz, $CDCl_3$): δ = 7.02 (m, 24H, Ar–H), 6.77 (m, 16H, Ar–H), 6.64 (s, 4H, Ar–H), 6.04 (s, 4H, $CHPh_2$), 3.13 (s, 5H, P–O*H*, 2H_2O), 2.62 (sept, 2H, C*H*$(CH_3)_2$), 1.99 (s, 1H, CH_3CN), 0.98 (d, 12H, CH(CH_3)$_2$) ppm. **^{13}C{^{1}H} NMR** (25 °C, 75.431 MHz, CDCl3): δ = 145.53 (Ar–C_{quart}), 145.42 (Ar–C_{quart}), 145.09 (Ar–C_{quart}), 143.31 (Ar–C_{quart}), 136.02 (Ar–C_{quart}), 129.49 (Ar–*C*H), 128.0 (Ar–*C*H), 127.72 (Ar–*C*H), 125.98 (Ar–*C*H), 49.92 (*C*HPh_2), 33.36 (*C*H$(CH_3)_2$), 23.82 (CH(*C*H_3)$_2$) ppm. **^{31}P{^{1}H} NMR** (25 °C, 121.442 MHz, $CDCl_3$): δ = –11.3 ppm. **IR** (KBr pellet, cm^{-1}): $\bar{\upsilon}$ = 3600 (m, br), 3567 (m, br), 3417 (m, br), 3083 (w), 3059 (m), 3026 (m), 2958 (s), 2868 (w), 2372 (w), 1948 (w), 1885 (w), 1802 (w), 1758 (w) 1599 (s), 1493 (s), 1465 (s), 1445 (s), 1383 (w), 1363 (w), 1319 (s), 1258 (s), 1197 (s), 1157 (s), 1116 (s), 1078 (m), 1030 (m), 1011 (s), 972 (s), 951 (s), 894 (m), 863 (m), 828 (w), 795 (w), 761 (m), 745 (w), 722 (s), 698 (s), 648 (w), 633 (w), 621 (w), 604 (s), 585 (w), 571 (w), 553 (w), 522 (w). **Elemental analysis** calcd (%) for $C_{70}H_{67}O_6P$: C 81.21, H 6.52; found: C 82.88, H 6.65.

Synthesis of 4. Under N_2-atmosphere, to a solution of **2·Et$_2$O** (0.107 g, 0.1 mmol) in dry CH_3CN (20 mL) was added Et_3N (0.017 mL, 0.12 mmol) at room temperature and stirred for 5 hours at this temperature. The resulting reaction mixture was dried under vacuum affording a colorless compound which was re-dissolved in dry CH_3CN (5mL) and filtered through a frit. The filtrate was kept for crystallization under N_2-atmosphere affording colorless crystals of compound **4** at room temperature. **Yiel**d: 0.092 g, 76%. **M.P:** 286 °C. **^{1}H NMR** ($CDCl_3$, 25 °C): δ = 12.30 (s, br, 1H, N–*H*), 6.99–6.85 (m, 40H, Ar–*H*), 6.70 (s, 4H, Ar–*H*), 6.60 (s, 4H, C*H*Ph_2), 2.65 (sept, 2H,C*H*$(CH_3)_2$), 2.26 (m, 6H, NCH_2CH$_3$), 1.98 (s, CH_3CN), 1.01 (d, 12H, CH(CH_3)$_2$), 0.75 (t, 9H, NCH$_2$CH_3) ppm. **^{13}C{^{1}H} NMR** ($CDCl_3$, 75.431 MHz, 25 °C): 146.9 (Ar–C_{quart}), 146.8 (Ar–C_{quart}), 144.8 (Ar–C_{quart}), 143.7 (Ar–C_{quart}), 137.0 (Ar–C_{quart}), 136.9 (Ar–C_{quart}), 129.8 (Ar–*C*H), 127.7 (Ar–*C*H), 127.4 (Ar–*C*H), 125.4 (Ar–*C*H), 116.5 (CH$_3$*C*N), 49.4 (*C*HPh_2), 45.0 (N*C*H$_2$CH$_3$), 33.4 (*C*H$(CH_3)_2$), 24.1 (CH(*C*H_3)$_2$), 8.3 (NCH$_2$*C*H$_3$), 2.01 (*C*H$_3$CN) ppm. **^{31}P{^{1}H} NMR** ($CDCl_3$, 121.442 MHz, 25 °C): δ = –9.8 ppm. **IR** (KBr pellet, cm^{-1}): $\bar{\upsilon}$ = 3424 (s, br), 3082 (w), 3058 (m), 3025 (m), 2958 (s), 2868 (w), 2600 (w), 2418 (w), 1952 (w), 1804 (w), 1599 (s), 1493 (s), 1466 (s), 1445 (s), 1383 (w), 1361 (w), 1318 (w), 1291 (w), 1244 (s), 1203 (m), 1175 (w), 1159 (m), 1119 (m), 1076 (s), 1031 (m), 921 (m), 889 (s), 846 (m), 796 (w), 762 (w), 746 (w), 720 (s), 699 (s), 669 (w), 645 (w), 621 (w), 605 (m), 580 (w), 548 (w), 524 (w), 508 (w). **ESI-MS:** calcd (m/z) for $[C_{70}H_{62}O_4P]^-$: 997.4391; found: 997.4276 and calcd (m/z) for $[C_6H_{16}N]^+$ 102.1277; found: 102.1281. **Elemental analysis** calcd (%) for $C_{76}H_{78}NO_4P$: C 82.95, H 7.14, N 1.27; found: C 82.50, H 7.12, N 1.89.

Synthesis of 4·(H$_2$O)$_2$. To a solution of **2·(H$_2$O)$_2$** (0.05 g, 0.05 mmol) in CH_3CN (1 mL) was added Et_3N (0.1 mL, 0.12 mmol) at room temperature. Colorless single crystals suitable for X-ray diffraction were obtained by slow evaporation at room temperature. **Yiel**d: 0.038 g, 71%. **M.P:** 278 °C. **^{1}H NMR** ($CDCl_3$, 25 °C): δ = 12.40 (s, br, 1H, N–*H*), 6.99-6.97 (m, 24H, Ar–*H*), 6.86-6.84 (m, 16H, Ar–*H*), 6.73 (s, 4H, Ar–*H*), 6.60 (s, 4H, C*H*Ph_2), 2.65 (sept, 2H,C*H*$(CH_3)_2$), 2.24 (m, 6H, NCH_2CH$_3$), 1.82 (s, CH_3CN), 1.01 (d, 12H, CH(CH_3)$_2$), 0.78 (t, 9H, NCH$_2$CH_3) ppm. **^{13}C{^{1}H} NMR** ($CDCl_3$, 75.431 MHz, 25 °C): 146.8 (Ar–C_{quart}), 146.7 (Ar–C_{quart}), 144.6 (Ar–C_{quart}), 143.6 (Ar–C_{quart}), 136.8 (Ar–C_{quart}), 136.7 (Ar–C_{quart}), 129.7 (Ar–*C*H), 127.6 (Ar–*C*H), 127.3 (Ar–*C*H), 125.3 (Ar–*C*H), 49.3 (*C*HPh_2), 44.8 (N*C*H$_2$CH$_3$), 33.3 (*C*H$(CH_3)_2$), 24.0 (CH(*C*H_3)$_2$), 8.2 (NCH$_2$*C*H$_3$) ppm. **^{31}P{^{1}H} NMR** ($CDCl_3$, 121.442 MHz, 25 °C): δ = –10.0 ppm. **IR** (KBr pellet, cm^{-1}): $\bar{\upsilon}$ = 3417 (s, br), 3082 (w), 3058 (w), 3025 (m), 2957 (s), 2866 (w), 2608 (w), 2350 (w), 1945 (w), 1885 (w), 1807 (w), 1637 (m), 1599 (m), 1493 (s), 1466 (m), 1444 (s), 1383 (w), 1361 (w), 1320 (w), 1292 (w), 1243 (s), 1202 (m), 1158 (m), 1121 (m), 1077 (s), 1031 (m), 920 (m), 906 (m), 892 (s), 848 (m), 796 (w), 762 (m), 746 (m), 720 (s), 699 (s), 671 (w), 634 (w), 619 (w), 605 (w), 590 (w), 574 (w) 547 (w), 521 (w). **ESI-MS:** calcd (m/z) for $[C_{70}H_{62}O_4P]^-$ 997.4391; found: 997.4215 and calcd (m/z) for $[C_6H_{16}N]^+$ 102.1277; found: 102.1280. **Elemental analysis** calcd (%) for $C_{76}H_{82}NO_6P$: C 80.32, H 7.27, N 1.23; found: C 82.42, H 7.13, N 1.93.

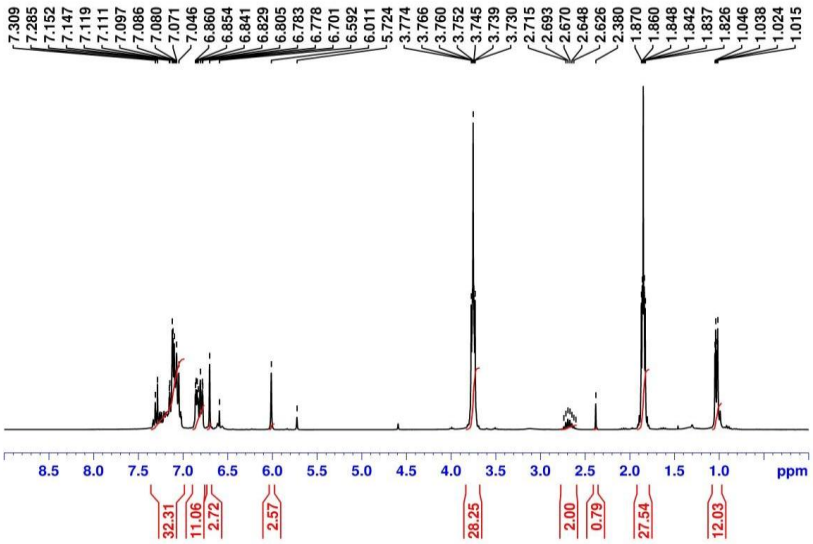


Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$ at RT.

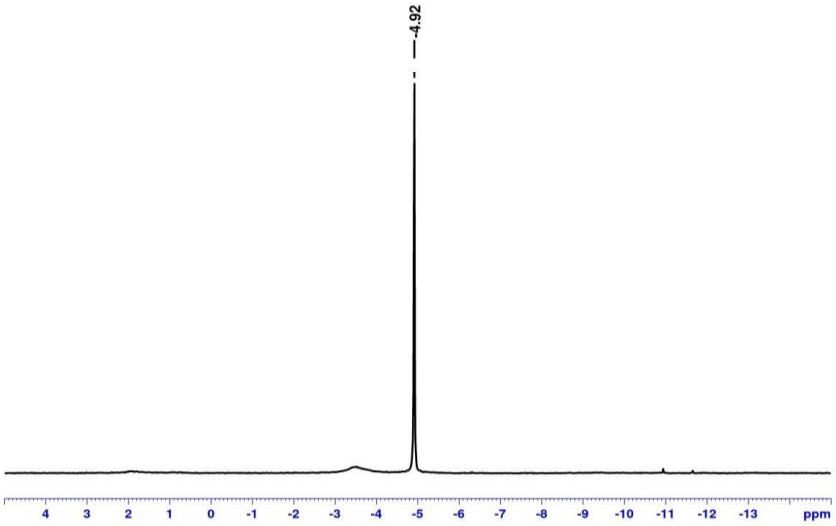


Figure S2. ^{31}P NMR spectrum of **1** in $CDCl_3$ at RT.

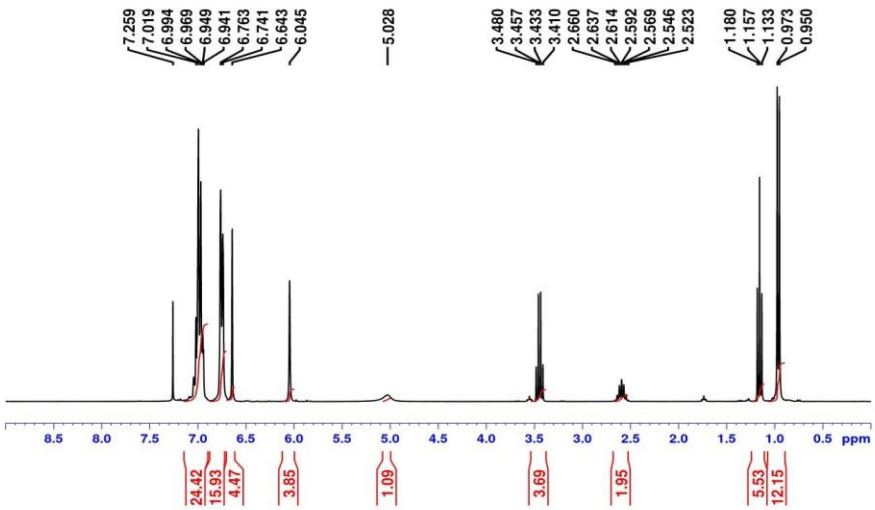


Figure S3. ^{1}H NMR spectrum of **2·Et$_2$O** in $CDCl_3$ at RT.

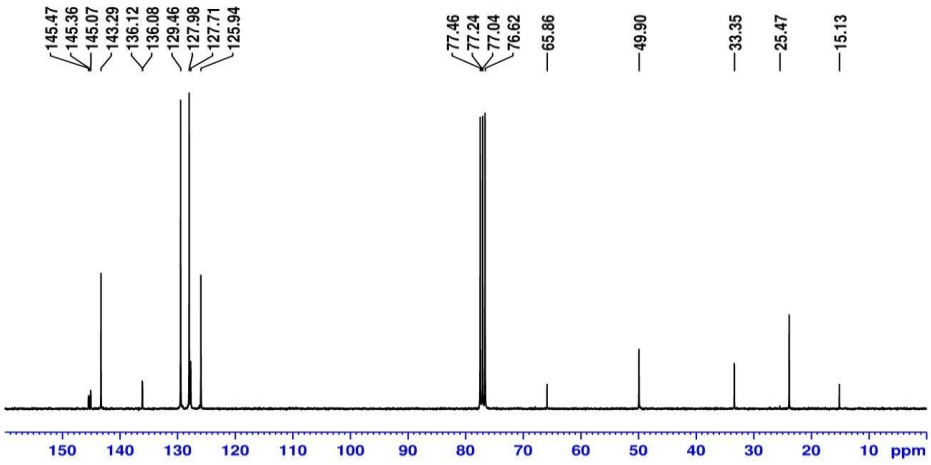


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **2·Et$_2$O** in $CDCl_3$ at RT.

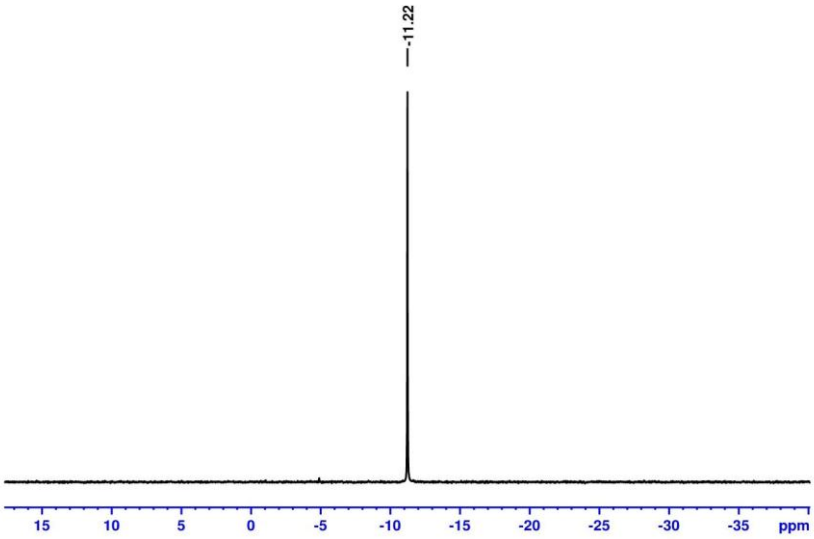


Figure S5. ^{31}P NMR spectrum of **2·Et$_2$O** in $CDCl_3$ at RT.

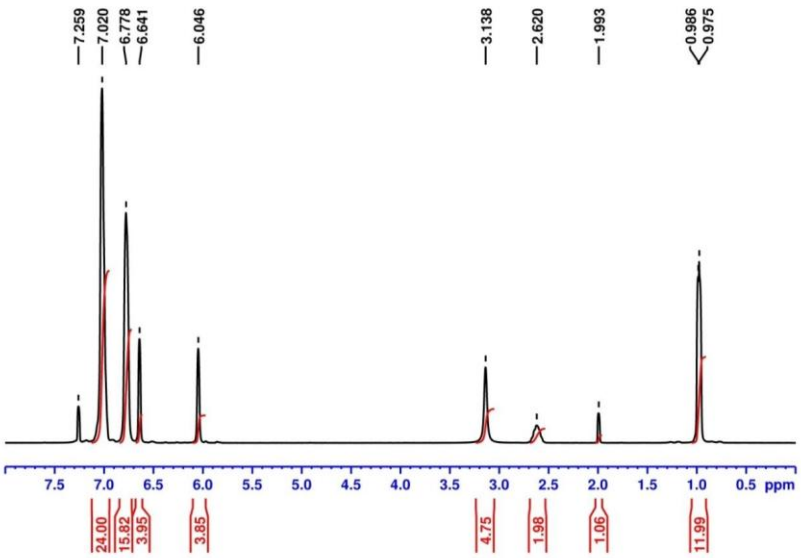


Figure S6. ^{1}H NMR spectrum of **2·(H$_2$O)$_2$** in $CDCl_3$ at RT.

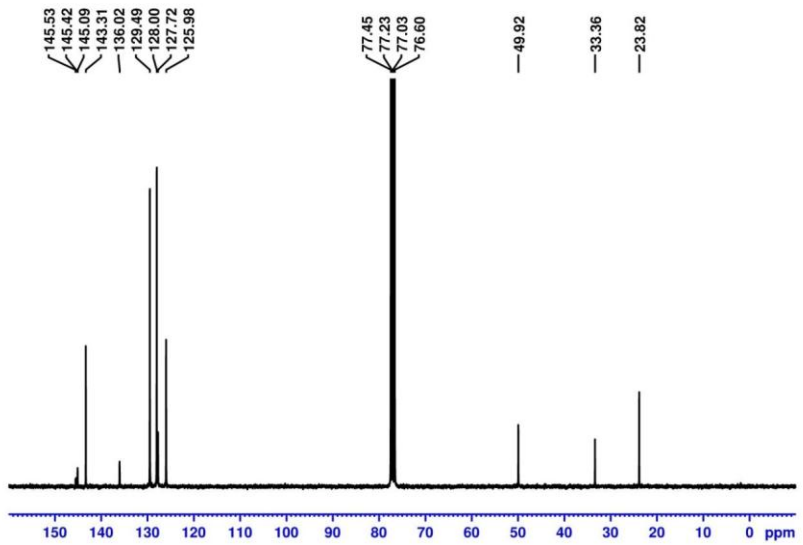


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **2·(H$_2$O)$_2$** in CDCl3 at RT.

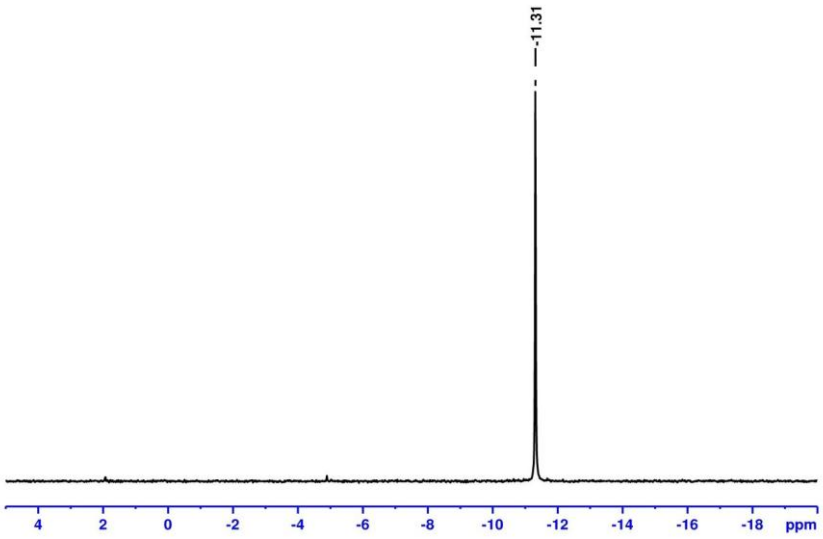


Figure S8. ^{31}P NMR spectrum of **2·(H$_2$O)$_2$** in $CDCl_3$ at RT.

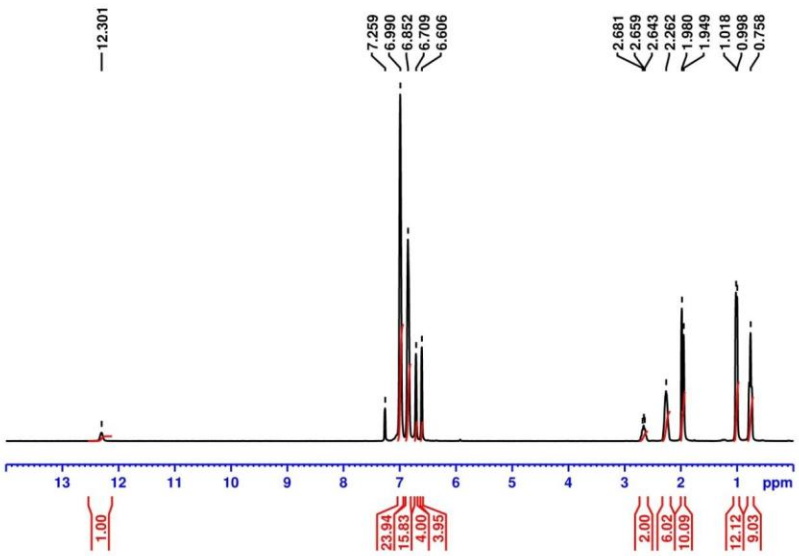


Figure S9. ^{1}H NMR spectrum of **4** in $CDCl_3$ at RT.

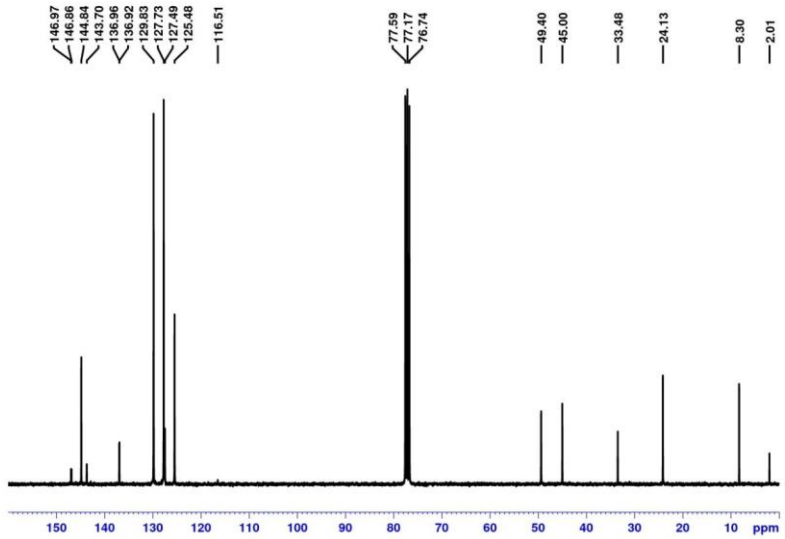


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$ at RT.

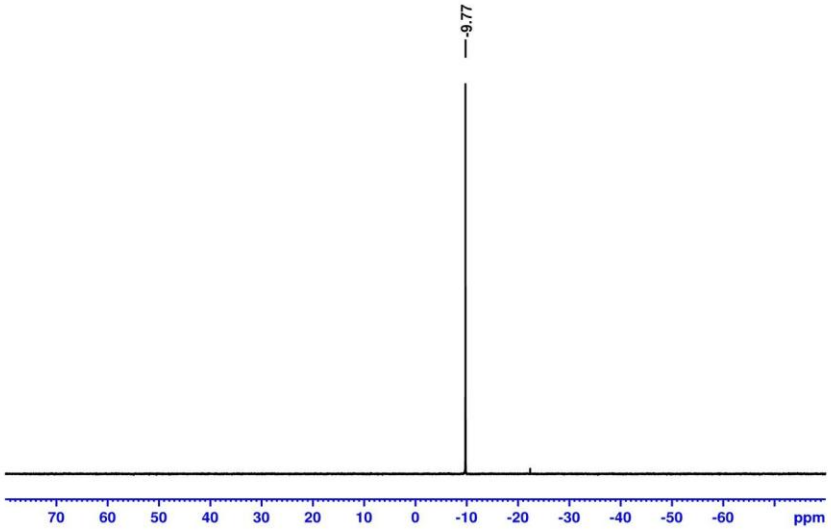


Figure S11. ^{31}P NMR spectrum of **4** in $CDCl_3$ at RT.

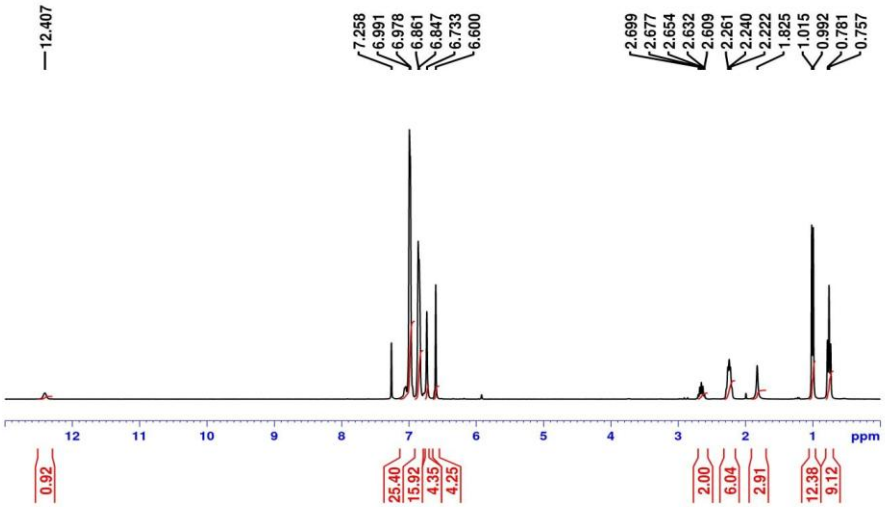


Figure S12. ^{1}H NMR spectrum of $[\mathbf{4}\cdot(H_2O)_2]_2$ in $CDCl_3$ at RT.

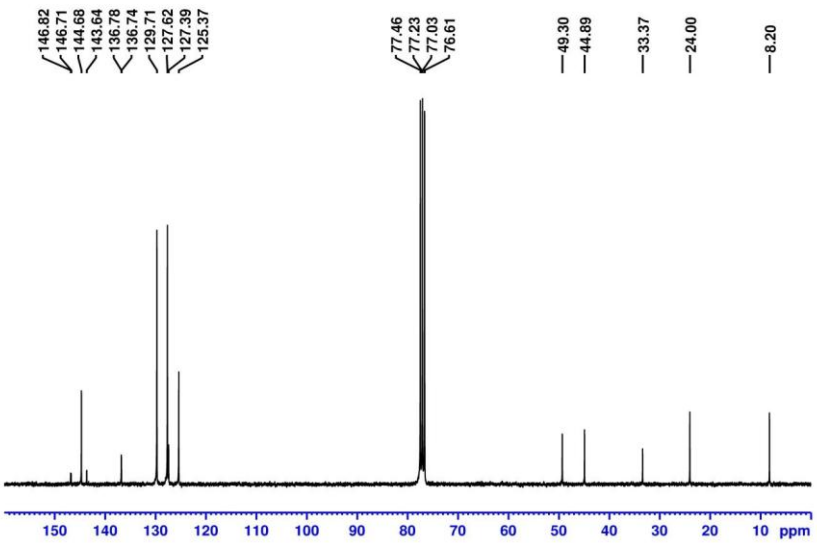


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of $[\mathbf{4}\cdot(H_2O)_2]_2$ in $CDCl_3$ at RT.

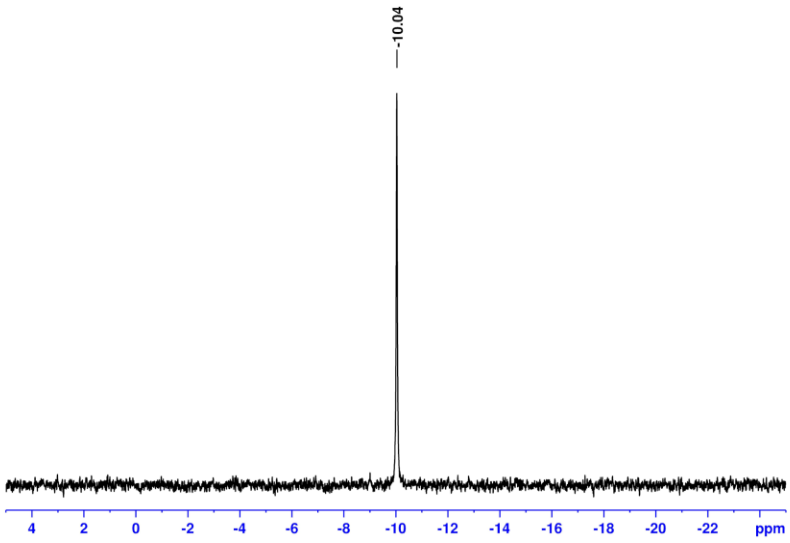


Figure S14. ^{31}P NMR spectrum of $[\mathbf{4}\cdot(H_2O)_2]_2$ in $CDCl_3$ at RT.

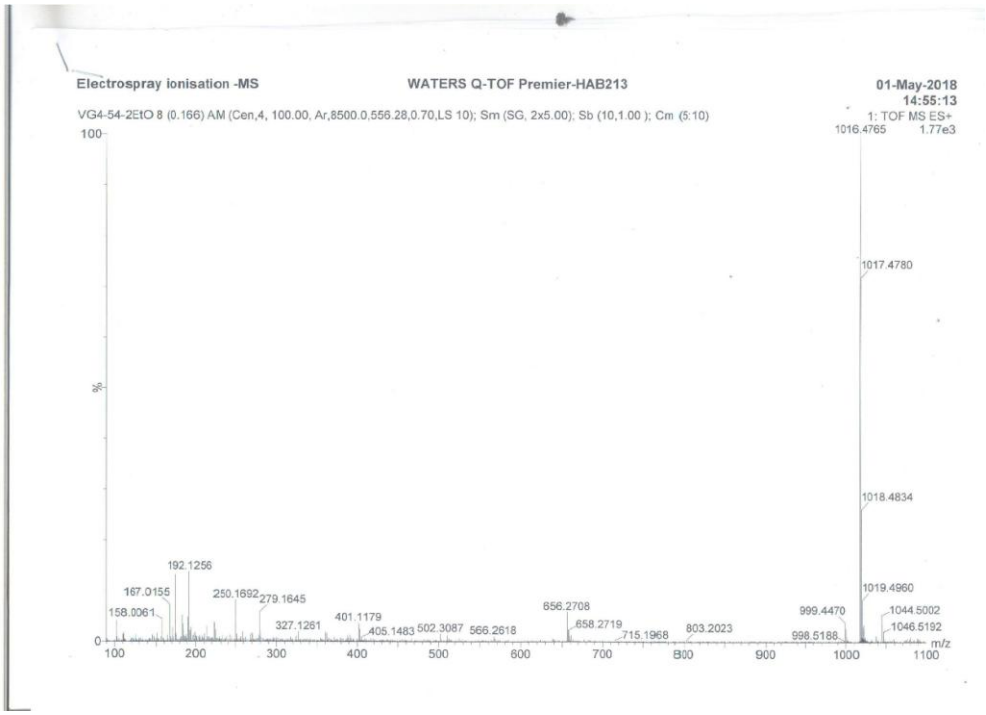


Figure S15. ESI-mass spectrum of **2·Et$_2$O** (+ve mode).

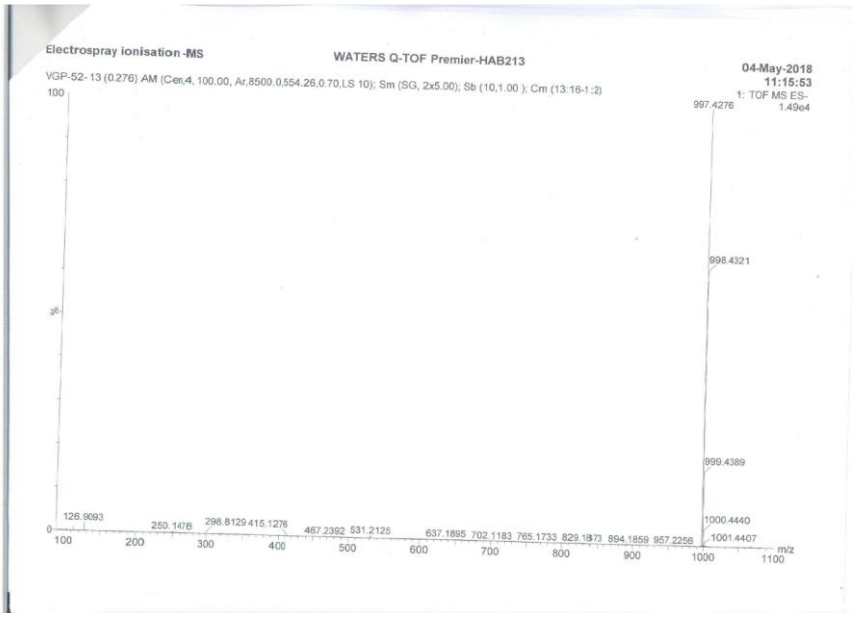


Figure S16. ESI-mass spectrum of **4** (−ve mode).

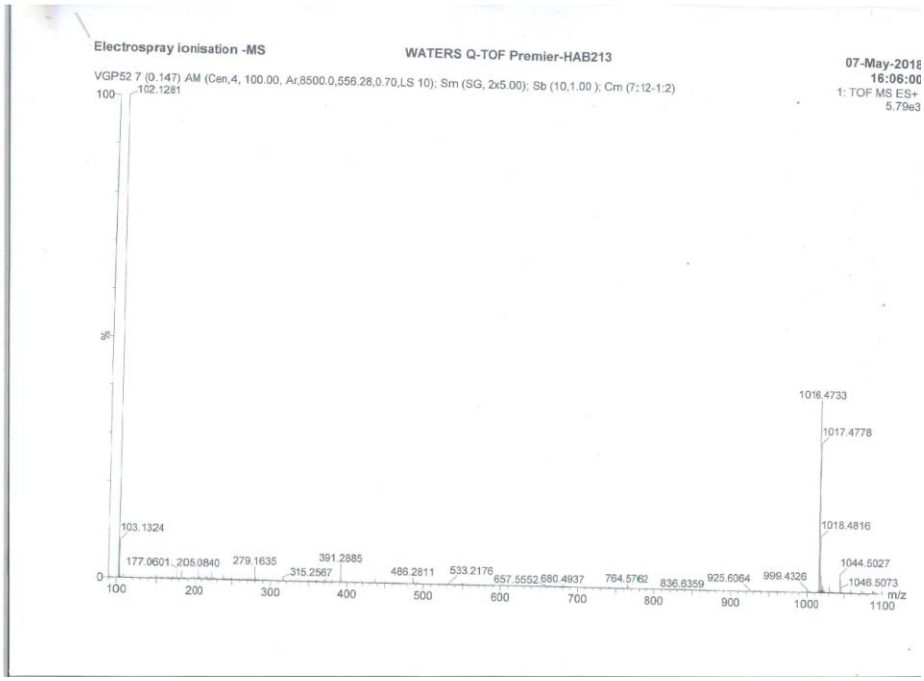


Figure S17. ESI-mass spectrum of **4** (+ve mode).

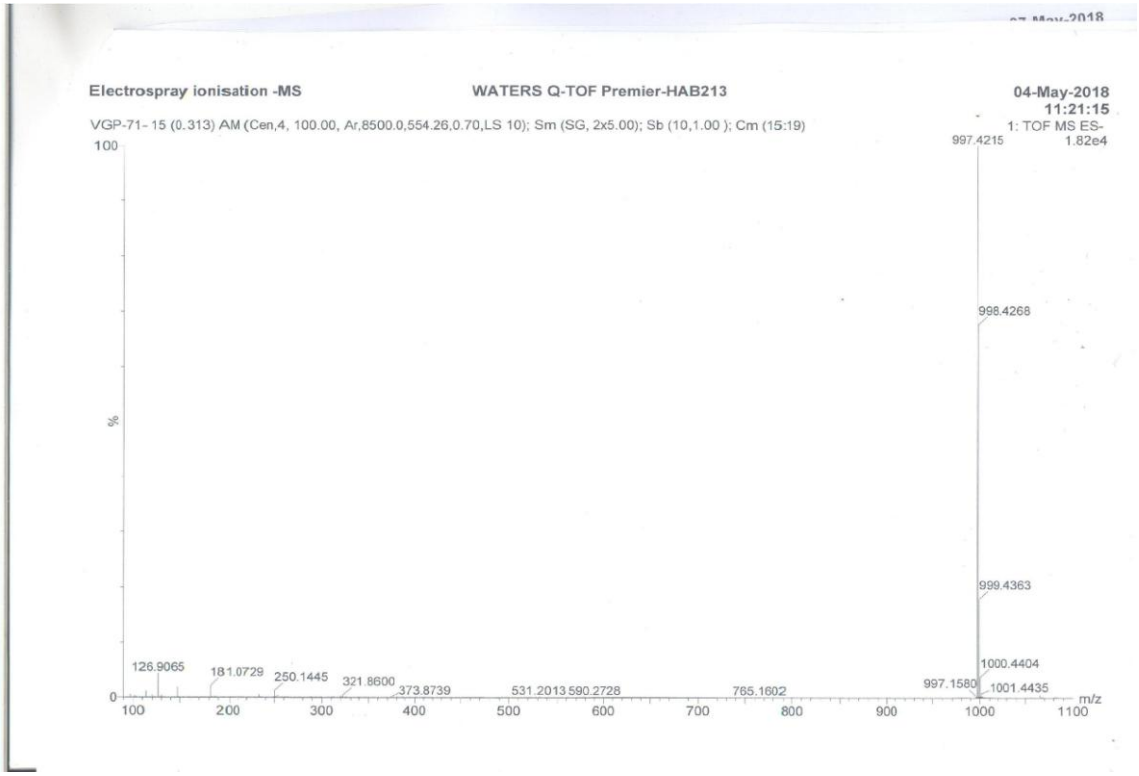


Figure S18. ESI-mass spectrum of **4·$(H_2O)_2$** (−ve mode).

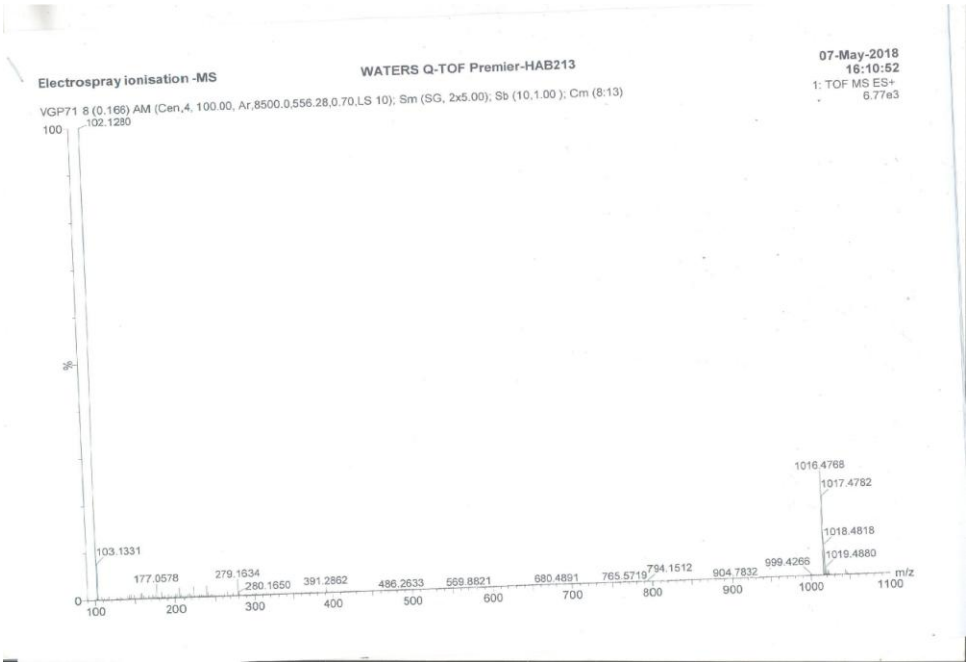
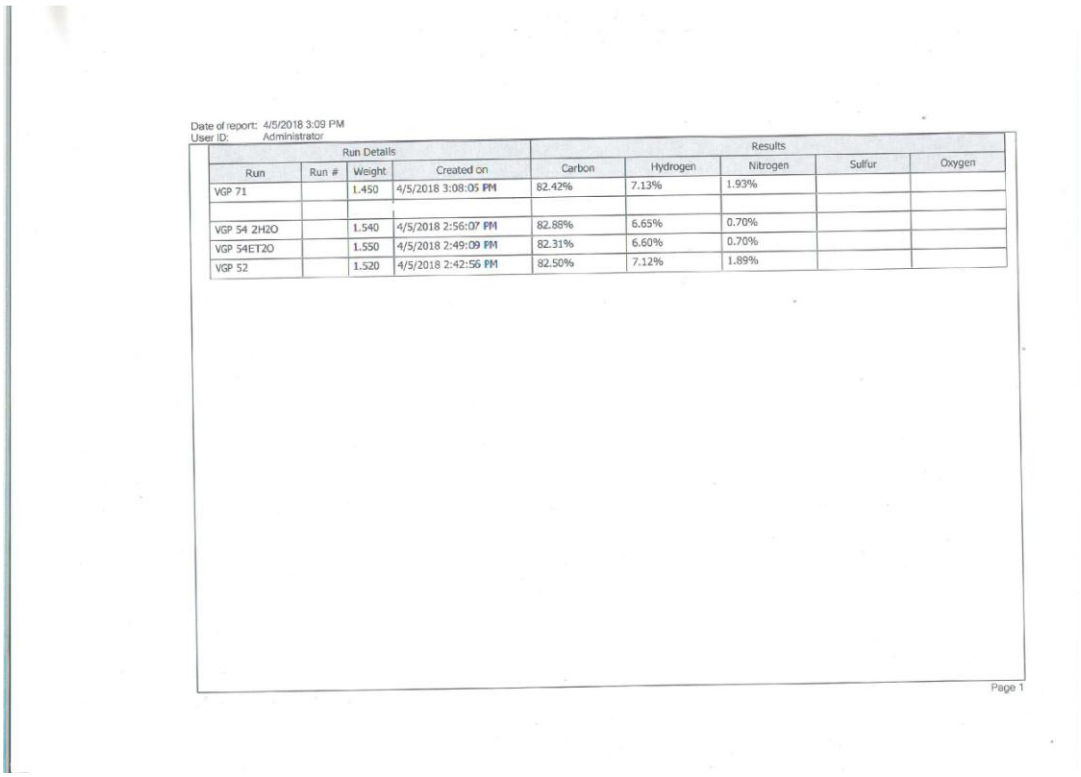


Figure S19. ESI-mass spectrum of **[4·$(H_2O)_2$]** (+ve mode).



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VGP 52		1.520	4/5/2018 2:42:56 PM	82.50%	7.12%	1.89%		

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Figure S20. CHN analysis of **2·Et$_2$O** (VGP 54ET2O), **2·(H$_2$O)$_2$** (VGP 54 2 H2O), **4** (VGP 52), and **[4·(H$_2$O)$_2$]$_2$** (VGP 71).

X-ray crystallographic studies. Single-crystal X-ray diffraction data of **2·(H$_2$O)$_2$**, **3**, **4** and **4·(H$_2$O)$_2$** were collected on a Rigaku XtaLAB X-ray Diffractometer system equipped with a CCD area detector and operated at 30 W power (50 kV, 0.6 mA) to generate Mo Kα radiation (λ = 0.71073 Å) at 120(2) K. Data were integrated using CrysAlis Pro software with a narrow frame algorithm[S1]. Data were subsequently corrected for absorption by the program SCALE3 ABSPACK scaling algorithm[S2]. The structure was solved with the SHELXT structure solution program using intrinsic phasing and refined with the SHELXL refinement package using least squares minimization with the Olex-2 software[S3,S4]. All non-hydrogen atoms were refined with anisotropic thermal parameters. All carbon bound hydrogen atoms were refined isotropically and placed in geometrically calculated positions after they were located in the Fourier difference map. They were included in the refinement process using a riding model with their U_{iso} values constrained to 1.5 times U_{eq} of their pivot atoms for methyl groups and to 1.2 times U_{eq} of their pivot atoms for all other C-H groups. All refined nitrogen or oxygen bound hydrogen atoms in the four structures were initially located. The water hydrogen atoms in **2·(H$_2$O)$_2$** were refined with DFIX restraints for the O-H and H-H distances and their U_{iso} values were constrained to 1.5 times U_{eq} of their parent oxygen atom. The orientations of the hydrogen atoms were refined without restraints. When refined completely freely, one hydrogen atom of a water molecule tended to move towards its hydrogen bond acceptor and the other, which is not engaged in strong hydrogen bonds showed signs of some sort of rotation around its pivot atom. The P-O-H hydrogen atoms in **2·(H$_2$O)$_2$** and **3** were added with HFIX 147 and their U_{iso} values were constrained to 1.5 times U_{eq} of their parent oxygen atom. The N-H hydrogen atom in **4** was found and refined freely (without any constraints or restraints). The water hydrogen atoms in **4·(H$_2$O)$_2$** were refined with DFIX restraints for the O-H and H-H distances and their U_{iso} values were constrained to 1.5 times U_{eq} of their parent oxygen atom. The orientations of the hydrogen atoms were refined without restraints. The N-H hydrogen atom in **4·(H$_2$O)$_2$** was found and refined freely (without any constraints or restraints). One ethyl substituent of the ammonium cation and one phenyl ring of the phosphate diester are disordered over two positions each. The disorder was treated using SADI/DELU/SIMU constraints and the relative occupancies were refined using free variables. Crystal and structure refinement data of all these compounds are summarized in Table S1. All crystallographic data were deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. These data can be obtained free of charge on quoting the depository numbers (CCDC 1843001 to CCDC 1843004) by FAX (+44-1223-336-033), email (deposit@ccdc.cam.ac.uk) or their web interface (at http://www.ccdc.cam.ac.uk).

Table S1 Crystal data and structure refinement for **2·$(H_2O)_2$**, **3**, **4** and **4·$(H_2O)_2$**.

Identification code	**2·$(H_2O)_2$**	**3**	**4**	**4·$(H_2O)_2$**
CCDC	1843001	1843002	1843003	1843004
Empirical formula	$C_{70}H_{67}O_6P$	$C_{24}H_{35}O_4P$	$C_{80}H_{84}N_3O_4P$	$C_{80}H_{88}N_3O_6P$
Formula weight	1035.20	418.49	1182.47	1218.50
Temperature/K	120.15	120(2)	120(2)	120(2)
Crystal system	monoclinic	triclinic	triclinic	monoclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
a/Å	10.6501(3)	8.6709(3)	12.4315(3)	16.4577(4)
b/Å	37.3357(7)	11.8216(5)	12.5478(3)	14.9850(4)
c/Å	14.6867(3)	12.5323(3)	22.9017(5)	27.7532(8)
α/°	90	71.887(3)	90.892(2)	90
β/°	97.195(2)	79.512(3)	95.969(2)	96.392(2)
γ/°	90	77.411(3)	108.698(2)	90
Volume/Å^3	5793.9(2)	1182.52(8)	3360.96(14)	6801.9(3)
Z	4	2	2	4
ρ_{calc}g/cm^3	1.187	1.175	1.168	1.190
μ, mm^1	0.100	0.142	0.093	0.096
F(000)	2200.0	452.0	1264.0	2608.0
Crystal size/mm^3	0.37 × 0.32 × 0.20	0.60 × 0.41 × 0.16	0.56 × 0.37 × 0.21	0.47 × 0.24 × 0.22
Theta range for data collection/°	5.038 to 53	5.56 to 53	5.276 to 58	4.894 to 57.67
Index ranges	-13 ≤ h ≤ 13, -46 ≤ k ≤ 46, -14 ≤ l ≤ 18	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15	-12 ≤ h ≤ 16, -16 ≤ k ≤ 16, -30 ≤ l ≤ 27	-22 ≤ h ≤ 16, -18 ≤ k ≤ 19, -36 ≤ l ≤ 37
Reflections collected	61616	17388	49656	84684
Independent reflections	11997 [R_{int} = 0.0424, R_{sigma} = 0.0349]	4872 [R_{int} = 0.0351, R_{sigma} = 0.0315]	15378 [R_{int} = 0.0409, R_{sigma} = 0.0451]	15942 [R_{int} = 0.0388, R_{sigma} = 0.0339]
Data / restraints / parameters	11997 / 6 / 711	4872 / 0 / 271	15378 / 0 / 806	15942 / 224 / 884
Goodness-of-fit on F^2	1.061	1.050	1.076	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1119	R_1 = 0.0337, wR_2 = 0.0856	R_1 = 0.0432, wR_2 = 0.1029	R_1 = 0.0580, wR_2 = 0.1527
Final R indexes [all data]	R_1 = 0.0583, wR_2 = 0.1177	R_1 = 0.0374, wR_2 = 0.0880	R_1 = 0.0581, wR_2 = 0.1095	R_1 = 0.0766, wR_2 = 0.1640
Largest diff. peak / hole / e Å^{-3}	1.34 / -0.43	0.25 / -0.43	0.37 / -0.41	0.77 / -0.56

Table S2 Selected distances (Å) and angles (°) for **2·(H$_2$O)$_2$**, **3**, **4** and **4·(H$_2$O)$_2$**.

2·(H$_2$O)$_2$	**3**	**4**	**4·(H$_2$O)$_2$**
P1–O3 1.548(11)	P1–O3 1.542(8)	P1–O3 1.490(9)	P1–O3 1.501(13)
P1–O4 1.467(11)	P1–O4 1.478(8)	P1–O4 1.477(9)	P1–O4 1.478(13)
O3–H3 0.840	O3–H3 0.840	N1–H1 0.981(17)	N1–H1N 0.98(3)
O5–H5O 1.013(17)	O3–H3…O4* 1.72	N1–H1…O3 1.629(17)	O5–H5O 0.979(10)
O5–H5P 0.975(17)	O3…O4* 2.555(11)	N1…O3 2.610(14)	O5–H5P 0.969(10)
O6–H6O 1.145(17)	O1–P1–O2 101.15(4)	O3–P1–O4 118.70(5)	O6–H6O 0.970(10)
O6–H6P 0.922(17)	O1–P1–O3 106.04(4)	N1–H1…O3 177.7(16)	O6–H6P 0.992(19)
O3…O6 2.599(2)	O1–P1–O4 115.53(5)		N1–H1N…O3 1.77(3)
O5…O4 2.808(2)	O2–P1–O3 110.23(5)		N1…O3 2.739(2)
O6…O5 2.668(3)	O2–P1–O4 108.59(5)		O3…O6 2.765(2)
H3…O6 1.76	O3–P1–O4 114.46(5)		O5…O6 2.890(5)
H5O…O4 1.816(19)	O3–H3…O4* 178.2		O4…O5 2.792(3)
H6O…O5 1.547(18)			O6…O6* 2.766(43)
O3–H3…O6 177.5			O3–P1–O4 118.20(7)
O5–H5O…O4 165(3)			N1–H1N…O(3) 168(2)
O6–H6O…O5 165(3)			O3…H6O–O6 1.837(19)
O1–P1–O2 97.25(6)			O3…H6O–O6 159(4)
O1–P1–O3 107.33(6)			O4…H5P–O5 1.88(2)
O1–P1-O4 113.70(6)			O4…H5P–O5 156(5)
O2–P1–O3 105.57(6)			O6…H5O–O5 2.14(5)
O2–P1–O4 116.01(6)			O6…H5O–O5 132(5)
O3–P1–O4 115.16(7)			O6–H6P…O6* 2.281(42)
			O6–H6P…O6* 108.88(12)

Computational Details. All geometry optimizations (for phosphodiesters and related water-dimer complexes) were performed using the GPW formalism as implemented in the QUICKSTEP module of CP2K package[S5]. We have used Perdew-Burke-Ernzerhof (PBE)[S6] exchange-correlation functional along with Goedecker-Teter-Hutter (GTH) pseudopotentials[S7-S9] and double-zeta valence polarized basis sets for all atoms. Additionally, noncovalent interactions are taken into account by Grimme's empirical DFT-D2 dispersion corrections[S10]. A supercell of 35*35*35 angstrom size is used for all calculations to avoid interaction with the periodic images. We have used a 320 Ry energy cutoff to construct the plane waves. All optimization calculations were performed with Broyden-Fletcher-Goldfarb-Shanno (BFGS)[S11-S15] minimization algorithm until a convergence of 0.0001 hartree/bohr.

Cartesian coordinates of the computed structures

PBE-D2/DZVP optimized structures are given in standard XYZ format.

$(H_2O)_2$

6

O	17.9077202523	17.9980512394	18.8046317268
H	17.9812346173	17.1741910052	19.3180343101
H	18.8293458965	18.2649149529	18.6399200665
O	17.0016014946	17.0943536146	16.1909117661
H	17.2235147866	17.4647906044	17.0734675306
H	16.2054894972	17.5801997085	15.9196807485

2-monomer

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P	18.4588676183	16.7924481814	17.1508743862
O	17.2738251230	16.4576688446	18.1713602316
O	18.0483525209	18.3111980035	16.8711257838
O	18.6431962061	15.8967767438	15.9927315215
O	19.7771741758	16.8921181686	18.0898095477
H	20.5061090575	16.4212116497	17.6419781027
C	16.5935485103	15.2190328289	18.1700978620
C	15.1510110768	12.8456052906	18.3116113603
C	16.9039535786	14.3100909078	19.1882328896
C	16.1573544932	13.1253654409	19.2443759480
H	16.3846181672	12.3965454520	20.0240265534
C	18.5060357378	13.4171019062	20.9281180879
C	14.8896364860	13.7839189936	17.3054010107
H	14.1281978434	13.5762540291	16.5519892013
C	15.5934658737	14.9905855535	17.2168700898
C	18.9615766851	19.3799238073	16.7484984430
C	19.2315580727	20.1380445780	17.8954557399
C	17.6053973120	15.7955991606	21.1120650068
C	15.2599736698	16.0354209960	16.1639227746
H	16.1893444744	16.5611362617	15.8974985029
C	20.0740997528	19.0291800475	13.1164522465

C	18.0064457290	14.6531108272	20.1863081967
H	18.8604923808	15.0261499383	19.5957496874
C	18.5878018405	19.7678540476	19.2232609933
H	18.5621934171	18.6695416924	19.2908073195
C	14.8003297209	15.3954607660	14.8576362999
C	20.5812384476	21.6249797329	16.4996189535
C	19.4800140024	19.6868408646	15.4854099897
C	14.3061947809	17.0955594113	16.6914748352
C	20.0523911719	21.2607652587	17.7457332388
H	20.2823465431	21.8560226784	18.6307024938
C	19.4261114584	20.2133752189	20.4158229708
C	19.1184335194	18.8178522932	14.2854811433
H	19.2399191715	17.7668021510	14.5965412246
C	17.6576748768	18.9723665197	13.8816317977
C	18.5659998823	16.7398614142	21.5053139583
H	19.5777837917	16.6705534038	21.1016216019
C	17.1389104477	20.2261311705	19.2806753420
C	14.3890820104	11.5348233935	18.3552566572
H	14.7018410750	11.0020938026	19.2697992683
C	20.2917121987	20.8260190036	15.3875114783
H	20.7104822964	21.0889569175	14.4147849613
C	19.7721531903	19.8703008984	12.0368780408
H	18.7994027344	20.3614019211	11.9985064181
C	16.2994325184	15.9138177735	21.6089601526
H	15.5401358355	15.2001217494	21.2849152235
C	15.7538036330	14.6840559406	14.1089844607
H	16.7713832267	14.6038765650	14.4979141369
C	18.1440347857	13.1283440699	22.2500513093
H	17.5169194542	13.8320839964	22.7981891215
C	16.9668380023	17.8593666808	13.3805330497
H	17.4644217047	16.8885045010	13.3627159356
C	19.3242348639	12.5063533897	20.2387637067
H	19.6001596120	12.7204988832	19.2039302177
C	18.9863209812	21.1543311705	21.3532252365
H	18.0059397240	21.6143456593	21.2292602385
C	20.6997408560	20.0686064607	11.0075657558
H	20.4471043362	20.7237788710	10.1728613926
C	21.4374891244	22.8691585729	16.3590260463
H	21.7581799849	22.9291723529	15.3048574336
C	15.9673491828	16.9437639432	22.4960885679
H	14.9463017460	17.0265056390	22.8710884032
C	16.9977541711	20.2085347975	13.9437184169
H	17.5189002362	21.0715720785	14.3617083752
C	16.1649997037	19.3582331838	19.7948029667
H	16.4524551746	18.3510692684	20.0986032890
C	18.2379116586	17.7734998247	22.3872898441
H	18.9921781603	18.5125074623	22.6596060297
C	19.7857794631	21.4867362036	22.4548030155
H	19.4269264275	22.2176598780	23.1807290441
C	16.9358057664	17.8737947035	22.8886903970

H	16.6725384396	18.6869125225	23.5656229317
C	18.5896440397	11.9537745610	22.8698927507
H	18.3003469479	11.7450736149	23.9007422162
C	12.8698891957	11.7587654119	18.4225382215
H	12.5940546906	12.3678279284	19.2961922462
H	12.3403057112	10.7958138485	18.4849698939
H	12.5150950413	12.2789610166	17.5190335881
C	22.6940688929	22.7895972694	17.2407366489
H	22.4160712828	22.7232427919	18.3044108981
H	23.3169906421	23.6876382267	17.1087227322
H	23.2978831902	21.9043395951	16.9929824189
C	15.6820161179	20.3322860992	13.4833439278
H	15.1788016683	21.2988721426	13.5371384063
C	15.4124623103	14.1158944078	12.8809511108
H	16.1659464869	13.5794693099	12.3024348647
C	15.6514606388	17.9773857135	12.9249956459
H	15.1253654678	17.0935714628	12.5623383114
C	15.0090923154	19.2199233086	12.9667734555
H	13.9791867812	19.3147974124	12.6214673801
C	19.4031993794	11.0537885935	22.1753856973
H	19.7514377224	10.1409289833	22.6598034003
C	13.4960751194	15.5107896320	14.3639170918
H	12.7560703565	16.0737706466	14.9334813241
C	21.9419258364	19.4274532230	11.0426914194
H	22.6621149602	19.5792028309	10.2380896603
C	14.7513319472	10.6616118655	17.1409970975
H	14.4639589333	11.1698347901	16.2068513397
H	14.2206663487	9.6977995195	17.1836763984
H	15.8329594171	10.4665472702	17.1008736053
C	13.2064102426	16.7682253585	17.4970612459
H	13.0680803195	15.7352452351	17.8205014370
C	19.7724500089	11.3355977139	20.8541524526
H	20.4092685498	10.6419559768	20.3033543884
C	20.6256739536	24.1340314969	16.6867958551
H	19.7370297723	24.2142926761	16.0434369236
H	21.2411748271	25.0365445715	16.5501256032
H	20.2861516717	24.1102901928	17.7344111873
C	16.7622867095	21.5134016313	18.8722746590
H	17.5148433471	22.1819830938	18.4503335401
C	21.0327054761	20.8810085687	22.6312879838
H	21.6503858935	21.1349924192	23.4933693853
C	12.4762420586	19.0795459510	17.4739880051
H	11.7666965887	19.8500439752	17.7787684183
C	20.6853706587	19.6153550549	20.5962274302
H	21.0259482238	18.8800375732	19.8646501058
C	21.3231302953	18.3884309460	13.1412934567
H	21.5625590523	17.7289970897	13.9780761893
C	14.8382454152	19.7763881385	19.9138937605
H	14.0861656347	19.0838360344	20.2922306016
C	22.2508763816	18.5823981767	12.1153838632

H	23.2135881583	18.0707815786	12.1496298354
C	14.4943785064	18.4295677078	16.3025034993
H	15.3579370461	18.6911655020	15.6904296816
C	14.4715940018	21.0684660109	19.5236740898
H	13.4334747083	21.3912477382	19.6106078022
C	14.1065189377	14.2414117166	12.3873480018
H	13.8394924387	13.8027010749	11.4252151200
C	12.2929751200	17.7551083822	17.8838320344
H	11.4374187358	17.4878328907	18.5058742121
C	13.5845105930	19.4153511520	16.6892365154
H	13.7524912843	20.4496911149	16.3883566409
C	21.4829685600	19.9417111354	21.6935287545
H	22.4533772705	19.4607121338	21.8239446332
C	13.1502599190	14.9355207622	13.1338665458
H	12.1319804301	15.0389483168	12.7562310905
C	15.4349247794	21.9364714924	18.9988322569
H	15.1527976998	22.9417115189	18.6821995308

2-dimer

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P	15.6151810165	17.8869071291	17.4108816234
P	19.6247406344	17.7300229344	17.9995233116
O	16.1176884509	17.3141144546	18.7687225885
O	19.0165969734	17.6451979188	16.5542100354
H	17.1392720673	17.4570909357	18.9331585548
H	18.0567587499	18.0432784613	16.5191605571
O	14.2793148998	18.7016652494	17.7365665056
O	20.8159798617	16.6505363621	18.0290956176
O	16.6510505606	18.6317753925	16.6286855735
O	18.6289909390	17.6355992493	19.1034331482
O	15.0874389065	16.7155496830	16.4481900395
O	20.4576390907	19.0858549091	18.1712660135
C	13.9651298086	19.4214405531	18.9215549847
C	20.5548774315	15.2743247626	17.7950668301
C	12.9906559352	18.8854308970	19.7843349788
C	20.7532359139	14.7782434353	16.4905501263
C	14.5487633195	20.6820558103	19.1419759003
C	20.1718889288	14.4560796009	18.8673674943
C	12.7093996746	16.7880612409	15.9659027547
C	22.8561155775	19.0696168902	17.8758027211
C	13.8186847468	16.1016942582	16.4836173139
C	21.5859499524	19.3847666070	17.3664585918
C	13.7593069876	14.7491848691	16.8594562248
C	21.4008950358	20.1253745405	16.1867175457
C	12.8976191003	18.0433532805	15.1204589530
C	23.0387171789	18.5861777509	19.3087880156
H	13.9673577107	18.2980520934	15.1468885175

H	22.0352760042	18.4136999493	19.7263487778
C	11.4652923945	16.1484248445	16.0580791527
C	23.9677152012	19.4364804656	17.1083823688
H	10.5860582824	16.6542853302	15.6550805427
H	24.9633380272	19.2059042048	17.4920730436
C	14.0795398361	21.4365918751	20.2210148068
C	19.8961859326	13.1087364429	18.5831245482
H	14.5292640603	22.4148230581	20.3931895306
H	19.5516820979	12.4816322490	19.4049680392
C	15.7658514468	21.2010935115	18.3833491081
C	20.0381402639	14.9567769790	20.2983052984
H	15.9568100673	20.5358834230	17.5304859882
H	20.1198488131	16.0549408505	20.2744718561
C	12.3890458815	17.4955340008	19.6290915483
C	21.3124855551	15.6832191085	15.3944275091
H	12.6420931350	17.1310635472	18.6195054810
H	21.0223053083	16.7131113108	15.6352737834
C	11.3267092100	14.8677638146	16.6041199648
C	23.8394667592	20.1487778879	15.9133337469
C	15.0569204238	13.9461011194	16.9147422223
C	20.0313180553	20.6361414191	15.7748427310
H	15.7719551054	14.4727381128	17.5668841894
H	19.3109109996	20.2435914711	16.5098083964
C	12.4918086258	14.1635109459	16.9413889606
C	22.5560215991	20.5198886163	15.4974881135
C	13.0903343175	20.9687029474	21.0873564261
C	20.0554927084	12.5668430157	17.3061936101
C	12.5801014942	19.6904484466	20.8600072233
C	20.4929143010	13.4195699630	16.2795661452
H	11.8041782926	19.3041272208	21.5230535597
H	20.6236727221	13.0114168546	15.2761930439
H	12.4240093837	13.1248630643	17.2615997291
H	22.4439095004	21.1848608490	14.6420589407
C	19.5241697209	20.1495388095	14.4141001985
C	18.1366966469	19.9858777521	14.2565365355
C	20.3442242879	19.8752234159	13.3090054250
C	17.5812131870	19.5943883216	13.0356496606
H	17.4832148728	20.1540750309	15.1107558154
C	19.7930162699	19.4890835876	12.0826764997
H	21.4265211412	19.9358209687	13.3945348809
C	18.4098441306	19.3585951443	11.9350479753
H	16.5009766111	19.4654478891	12.9508198733
H	20.4550443376	19.2732926453	11.2434701528
H	17.9839271068	19.0572758467	10.9772335748
C	19.9255605601	22.1658825342	15.9589475053
C	20.7929411392	22.8454646331	16.8310806488
C	18.8591565510	22.8856468814	15.3951168562
C	20.5908026942	24.1941697122	17.1406112416
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C	18.6452600190	24.2290418084	15.7162056446

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H	21.2773017947	24.6954783382	17.8247605522
H	17.7855758985	24.7499013144	15.2938813152
H	19.3384555281	25.9362757717	16.8518206284
C	23.8206523711	17.2992395407	19.5240621734
C	24.3573008545	16.5226622684	18.4913679562
C	23.9906324090	16.8635565411	20.8513097484
C	25.0663464177	15.3487919032	18.7825755743
H	24.2203877299	16.8189276614	17.4528604886
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H	23.5645365501	17.4557439995	21.6629508636
C	25.2429602673	14.9354216918	20.1033975313
H	25.4723544394	14.7610621806	17.9608233715
H	24.7985676648	15.3716888034	22.1757867677
H	25.7916549663	14.0193421898	20.3259256949
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C	24.9671174968	19.8757163908	20.4372198009
C	23.2530452116	22.0264439892	20.9538101989
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H	25.6310227774	19.0313724996	20.2486608702
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H	26.5069162821	21.0888911565	21.3417295839
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C	21.2255605942	14.3442418869	13.2135478267
C	19.7541542148	16.2410855453	13.4803691526
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H	22.0379506093	13.7198127370	13.5875527882
C	19.2299124358	16.0100827395	12.2053720233
H	19.3882821785	17.0788323046	14.0747955091
C	19.6914021748	14.9396720917	11.4353251794
H	21.0718078295	13.2749993318	11.3453843166
H	18.4557725370	16.6731306739	11.8217386277
H	19.2803604724	14.7594791981	10.4409133695
C	22.8371647587	15.6686259603	15.3377159236
C	23.5917999436	14.5139704979	15.5846638162
C	23.4998504913	16.8401362037	14.9399361043
C	24.9796250407	14.5215512801	15.4109608805
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C	24.8874860691	16.8553526713	14.7867027702
H	22.9201181797	17.7498901988	14.7723662168
C	25.6327180485	15.6922374712	15.0138939907
H	25.5538613906	13.6135370915	15.6015478464
H	25.3890558428	17.7799457597	14.4994523608
H	26.7164203935	15.7022342738	14.8922640869
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C	17.5383576045	14.9586772832	19.9999669647
C	18.3434445764	14.2964691051	22.1598220456
C	16.2316159746	14.9209843864	20.4664287248
H	15.9989100515	12.9076190039	19.2655457909
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H	19.1585326999	14.0470273160	22.8383618848
C	15.9438780526	14.5681791459	21.7923584161
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H	22.3750292805	15.3761493844	24.3109009110
H	23.3458738783	11.9493924694	21.8803704702
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C	18.1770322257	20.2825607030	21.2442889018
H	16.1816981382	19.7128207672	20.6834404857
C	19.2935721686	21.0635119718	20.9404222611
H	20.1526295891	22.4527391316	19.5155492840
H	18.1786628287	19.6376001751	22.1235556222
H	20.1696849347	21.0470512215	21.5895889933
C	15.5045176673	22.5760307912	17.7766885741
C	15.7459768672	23.7712818483	18.4717588584
C	14.9938906347	22.6498489007	16.4726233213
C	15.4791981781	25.0082463586	17.8774216365
H	16.1787315062	23.7294012149	19.4717689988
C	14.7295370090	23.8842904227	15.8730722244
H	14.7936292519	21.7248427552	15.9296926231
C	14.9703596829	25.0699829121	16.5753049664
H	15.6782341641	25.9273301006	18.4302379603
H	14.3378802669	23.9198629088	14.8554445789
H	14.7692143696	26.0356519064	16.1097658325
C	12.9930015217	16.4741893606	20.6096282493
C	13.4742139964	16.8612964347	21.9417965172
C	13.0486111138	15.1666582964	20.2690620402
C	14.1671194310	16.0115533339	22.7275475294
H	13.3190406522	17.8830685635	22.2837145925
C	13.4844548938	14.1021793175	21.2421027560
H	12.7266218067	14.8495645840	19.2779918980

C	14.5080979640	14.5956149604	22.2918078060
H	16.8291876698	13.9249589851	23.6532563474
H	12.5839256898	13.7397658143	21.7755415684
H	14.4502506971	13.9331425997	23.1713213297
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C	8.7447810579	16.2323208702	19.6975802233
H	10.6934697638	15.3571384991	19.9283286982
C	8.6867654576	18.6223227911	19.4179028124
H	10.5905301153	19.6191323430	19.3848060799
C	8.0065996366	17.4063261758	19.5171025499
H	8.2372358287	15.2697287366	19.7767664911
H	8.1308781209	19.5507187924	19.2758751041
H	6.9182829228	17.3736708459	19.4570486001
C	14.9234699202	12.5168044933	17.4363575976
C	14.2964154094	11.5173609932	16.6721612759
C	15.4828120455	12.1559895722	18.6705456572
C	14.2117999528	10.2035531952	17.1399180924
H	13.8937365034	11.7700122557	15.6910986321
C	15.4057218560	10.8395986940	19.1398945604
H	17.7258640577	15.2244140306	18.9611591422
C	14.7657039156	9.8579571703	18.3786704419
H	13.7220865119	9.4438737715	16.5291674507
H	15.8555376574	10.5854694327	20.1008515233
H	14.7074370154	8.8304035390	18.7393061583
C	15.6595043819	13.9102925514	15.5045331689
C	17.0496618344	13.8908762944	15.3346374823
C	14.8361647492	13.8281913276	14.3707450376
C	17.6059460129	13.7630188763	14.0593777088
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H	13.7527572665	13.8848223856	14.4847635289
C	16.7787880735	13.6560998681	12.9366460608
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H	17.2240091021	13.5627333947	11.9463079651
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C	13.5708967175	16.8847441777	12.9765030652
C	11.1461412389	17.4981057717	11.7336525232
H	10.6485507626	18.5314175547	13.5695009035
C	13.3264966588	16.4516113807	11.6709982894
H	14.5091082179	16.6258228247	13.4714942316
C	12.1121301753	16.7572151305	11.0442462119
H	10.1982379153	17.7420628425	11.2520366201
H	14.0873341858	15.8728944331	11.1454937531
H	11.9204708154	16.4208380134	10.0246982766
C	12.1523085038	19.3052360911	15.5228524731
C	12.4951877707	20.4933835736	14.8526805760

C	11.1427661196	19.3498544082	16.4880822798
C	11.8479284591	21.6947132943	15.1393519203
H	13.2790965937	20.4629779424	14.0925279011
C	10.4828612633	20.5534555194	16.7700799895
H	10.8707445001	18.4500980936	17.0373011511
C	10.8309052053	21.7279848508	16.1013668790
H	12.1392869777	22.6076580731	14.6193799473
H	9.6927624344	20.5635726448	17.5208215998
H	10.3205166867	22.6640904367	16.3290002188
C	9.9487217765	14.2353044183	16.6872890442
C	9.8382999226	13.1414738371	17.7555355066
C	9.5446739934	13.6825591023	15.3077063197
H	9.2459000064	15.0431803734	16.9556220552
H	10.1635990247	13.5068482560	18.7406212886
H	8.7959559958	12.7992423296	17.8377706444
H	10.4529959309	12.2652112665	17.4958846919
H	9.5924221548	14.4648951549	14.5359815968
H	10.2296092489	12.8720463614	15.0111089548
H	8.5214158925	13.2765511853	15.3345249035
C	12.6159082742	21.8117591545	22.2538910581
C	12.0265996424	23.1477499315	21.7737107371
C	13.7594527743	22.0538207078	23.2536213167
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H	11.1896716507	22.9875407210	21.0781090095
H	11.6657477531	23.7407313937	22.6281277896
H	12.7924323825	23.7398153137	21.2483129690
H	14.1698153936	21.1042385314	23.6276354979
H	14.5801311440	22.6073656674	22.7709490004
H	13.4060097356	22.6467175705	24.1112903092
C	25.0720157878	20.6072426512	15.1578013458
C	25.4336460179	22.0450928964	15.5741609885
C	24.9094187790	20.5106464329	13.6345936153
H	25.9017487029	19.9447856968	15.4611504335
H	25.5895722256	22.1136719631	16.6607458408
H	26.3489000245	22.3819053247	15.0628554419
H	24.6153738874	22.7318280183	15.3046384082
H	24.6125281225	19.4984341767	13.3212204088
H	24.1427734224	21.2145933483	13.2749737318
H	25.8536599144	20.7688891576	13.1320255015
C	19.7765453178	11.1028190040	17.0038389651
C	18.4058283918	10.9231494926	16.3259475194
C	19.8721880651	10.1983453488	18.2381711204
H	20.5502349325	10.7797234191	16.2838808941
H	18.3293224652	11.5103232419	15.4014447477
H	18.2415879643	9.8620567137	16.0813708167
H	17.5948999060	11.2467533944	16.9973324197
H	20.8237225448	10.3349860068	18.7744751735
H	19.0487540911	10.4051179404	18.9401044033
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O	10.3237137532	11.2525566512	16.8024018187
O	10.4730749484	13.2294384680	15.1785187355
C	13.5397315678	10.9954547692	15.5763168941
C	14.7092948502	11.7712197085	15.6470727031
C	13.5034077141	9.6139802029	15.8174017454
C	11.4159092122	13.5289643014	12.9623107210
C	11.1738012043	14.0461773594	14.2479912643
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C	10.9308810235	12.1610608753	12.5129596686
H	10.5034243940	11.6411787256	13.3805876440
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H	12.3033167278	13.9820748948	11.0567527088
C	14.7119073198	9.0027019203	16.1887406310
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C	12.2419627910	8.7847879739	15.6555485186
H	11.4228498247	9.4514495349	15.3562530842
C	14.7289397444	13.2417606832	15.2700751131
H	13.6941719142	13.6041925590	15.2130401645
C	12.5112592598	15.6410187552	12.4214001249
H	13.0474325152	16.2650408519	11.7056517755
C	11.1818175488	15.9329797897	15.9933605745
H	10.6834505020	15.1528698866	16.5836457873
C	12.2214078359	16.1280573147	13.6954199671
H	12.5203658074	17.1396278646	13.9739814005
C	15.8925996365	9.7381671735	16.2942824484
H	16.8205726364	9.2430947123	16.5825597447
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C	9.8146351974	12.3190350632	11.4654470270
H	8.9732473259	12.9027514777	11.8664046128
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H	10.1940197904	12.8372986649	10.5705651808
C	15.8883929837	11.1070624894	16.0161582723
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C	12.4275322811	7.7315138966	14.5498304977
H	12.6869143540	8.2044666817	13.5906987344
H	11.4994863887	7.1548003406	14.4163658168
H	13.2319661397	7.0251528289	14.8090315398
C	12.4351840742	16.3845443790	16.7577136810
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H	16.3946936458	13.0721209445	13.8662822923
H	15.3234157308	14.4758672212	13.5758235035
H	14.7892908068	12.8388920608	13.1205850349
C	10.1964641492	17.1031736790	15.8240225069
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H	9.2824312193	16.7817569073	15.3037908248
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O	12.8286480014	13.4635353062	16.3507832227
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C	9.5866260112	13.7375246886	17.4754149380
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C	15.3876334057	9.8808993490	12.7640695961
C	9.6123566301	15.1190697809	17.2359049472
C	13.3523369505	13.8000815243	9.8789889971
C	11.6477086818	11.1999126083	20.1209696451
C	13.0668972434	14.3176882004	11.1553206900
C	11.9331872751	10.6823157768	18.8446602926
C	13.4135866582	15.6183659498	11.5556721961
C	11.5864979106	9.3816569404	18.4443126459
C	12.8857463748	12.4301663618	9.4168248621
C	12.1142500316	12.5698470142	20.5831501439

H	12.4344126459	11.9102884079	10.2721003188
H	12.5656090453	13.0897261329	19.7279029540
C	14.0615600307	14.6289977526	8.9976941220
C	10.9384809610	10.3709737579	21.0022334678
H	14.2995861800	14.2520580787	8.0021924937
H	10.7004404659	10.7479003929	21.9977405060
C	16.5985688883	9.2773213005	13.1365534371
C	8.4014019503	15.7226122409	16.8633596518
H	16.6108892632	8.2044132241	13.3333023162
H	8.3890390800	16.7955463620	16.6665991099
C	14.1372691663	9.0410154198	12.5849531151
C	10.8627062640	15.9590126810	17.4150133554
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C	16.5907431133	13.5185336004	12.2290211438
C	8.4092805374	11.4814638493	17.7710095114
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H	9.4438783063	11.1380046728	17.8989742544
C	14.4606181268	15.9129680792	9.3709726480
C	10.5394430472	9.0870053998	20.6289569489
C	13.0127395141	16.2112806676	12.8933869816
C	11.9873315920	8.7887570678	17.1065887206
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C	14.1279000617	16.4004130464	10.6340412728
C	10.8721688083	8.5995795816	19.3658953906
C	17.7737048660	10.0214938492	13.2443405801
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C	14.0512405130	11.5726107693	8.8986831911
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H	13.5621736924	13.4028723500	21.9860337235
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H	12.7921174435	11.8963451492	22.5483339294
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C	14.3267894677	8.0457501638	11.4272688043
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H	18.2921649763	14.1025569838	13.4773662128
H	6.7078395301	10.8974434085	16.5227058842
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H	14.5693824749	7.6325474283	14.2028908578
H	10.4306158098	17.3673072095	15.7969385280
H	12.8505585039	7.7207677469	13.7432126049
H	12.1494315165	17.2792009611	16.2567233798
H	13.5857363669	9.0347109654	14.6960236491
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H	15.0199409565	16.5365968712	8.6729052488
H	9.9801246426	8.4633567279	21.3270055244
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H	10.5848304099	7.5874411573	19.0779997808

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C	18.8969465945	17.9509577920	15.5431455182
C	19.9114597498	18.1558563917	20.3095126703
C	16.5745414439	16.8202941968	19.0055914082
C	19.7846403137	20.9622848252	16.7015339312
C	18.9692333662	20.4918071847	15.4979585192
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C	14.5200193711	15.5278135431	18.2217461330
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C	18.8770337571	21.5211912085	14.3830443161
C	20.6566475206	20.1185121213	17.4029653764
H	20.8028234081	19.0932988010	17.0615155373

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H	18.7438026348	13.7947832954	21.9670770392
C	17.7074073856	19.4028974824	20.5012398127
C	20.7928278297	17.3278104119	19.5926901885
H	20.4234905629	16.7585307947	18.7377754539
C	19.8569233351	23.2343133634	12.9570071616
H	20.7077284694	23.8640419735	12.6930742387
C	13.3407221557	16.6941162006	20.1839453956
H	14.3003650501	16.7768299640	20.6958962598
C	21.3281958615	20.5666890963	18.5472824977
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C	17.3242672499	14.5751942527	13.8791309416
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H	18.9234173114	22.9417729170	16.6439376828
C	19.2590579627	14.3422195583	17.9886377031
H	18.1801036401	14.2858777792	18.1451398663
C	21.1435124581	15.0345452416	16.6473990597
H	21.5396386543	15.5163031462	15.7526918459
C	21.1456779872	21.8741856715	19.0032905683
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H	15.8019697397	14.5460123769	16.0991081845
C	16.8656135292	19.1643041697	21.5971879192
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C	21.7463023629	18.7627311712	21.7894068055
H	22.1109713889	19.3258430520	22.6497742627
C	12.1887492741	17.2355065660	20.7692304346
H	12.2587488911	17.7306413349	21.7391820432
C	19.0536780760	13.0905003757	14.6858905179
H	19.8754122943	12.8806234988	15.3713522926
C	13.6073916590	11.8163358733	17.7681865159
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C	22.1351608929	17.2298246036	19.9619711688
H	22.7988152791	16.5853339773	19.3854276769
C	22.0188607144	14.5276770005	17.6132484236
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H	17.8020782429	11.5164014909	21.9521578448

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H	16.0960065818	13.8209503828	12.2764708748
C	10.8808400439	16.4887154048	18.8809464438
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C	17.6015575175	12.3848144176	12.8740828712
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C	18.6617400616	12.1267840124	13.7469471299
H	19.1875685055	11.1719255539	13.7024061140
C	20.7076864307	17.0438383441	10.9181625327
H	20.3478102601	16.0307547285	11.1578327763
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H	15.8427704836	12.2288163607	15.2150925092
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H	15.5637895245	20.0227556547	23.0926964691
C	17.6871199210	21.6157629560	13.6446997145
H	16.8485546027	20.9710402406	13.9174250174
C	17.8883297915	20.7227631778	20.0606844289
H	18.5468386595	20.9146005134	19.2123155895
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H	15.9045419805	22.3647074554	22.3063272276
C	17.2480154023	21.7834581851	20.7084040165
H	17.4161946551	22.8050517389	20.3617454408
N	14.3432584028	20.7367893144	17.8913588164
H	15.0940470125	20.1731983281	17.3146097855
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H	14.0524531596	19.0222304676	19.0737789915
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4-$(H_2O)_2$

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C	20.0611946393	16.5463242391	13.9148943852
H	20.2752087116	15.5632295766	13.4917562944
C	19.8926411182	20.8479350522	16.7767076600
C	19.8559065121	14.8405658062	16.7811101999
C	14.4084639839	14.0549649253	17.7117807297

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C	20.7767719302	19.9808602382	17.4327582159
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C	19.4012636909	14.2115608760	17.9496826294
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C	17.0633573834	18.8992974471	21.7740310398
H	16.8675912008	17.8526665699	22.0118066659
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H	12.9440434714	13.4346474967	19.1691926557
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H	15.8297721162	14.3853016458	16.1252807636
C	12.2114136038	16.2443227871	18.2470965666
H	12.1974544336	16.0111270262	17.1811377017
C	11.1160071562	17.1326271988	20.2228466002
H	10.2313855751	17.5506562260	20.7053279069
C	21.3231811046	21.6955787681	19.0598428317
H	21.8733075195	22.0180230340	19.9444077253
C	22.2630024944	17.0308656870	19.8333262391
H	22.8989187154	16.4206550337	19.1925127312
C	20.4379659373	22.5709775871	18.4178373844
H	20.3001169811	23.5856561695	18.7953665804
C	12.2956261961	16.9498071197	20.9500800410
H	12.3366441532	17.2240232823	22.0056304385
C	22.1447466782	14.3974195599	17.4814116673
H	23.2166237021	14.4766573502	17.2927792475
C	13.5026218174	11.8052674572	17.8528769375
H	12.8395601184	11.0864913509	18.3369461426
C	16.8682194322	13.5578611941	13.0222471514
H	16.0105491371	13.7763797530	12.3846804178
C	17.5090850114	12.3140759168	12.9379375866
H	17.1582435503	11.5619001023	12.2301882056
C	22.7938619150	17.6688524952	20.9615799086
H	23.8519498592	17.5646579691	21.2050783875
C	20.3049950647	13.6808307171	18.8736667646
H	19.9296279258	13.2116589261	19.7837997762
C	22.6179044566	16.6957928585	12.2213737746
H	23.2521593122	17.0680101205	13.0396812214
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C	18.1435114204	20.5579996259	20.3882473586
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H	15.8266817906	19.6603563525	23.3727459656
C	14.2903525732	11.4096135464	16.7661336575
H	14.2443712861	10.3818281060	16.4035607557
C	21.6812525473	13.7650917676	18.6396936917
H	22.3877245490	13.3550846626	19.3623102516
C	17.5142175010	12.0793736868	21.1267018171
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C	11.0794758526	16.7755658545	18.8679579677
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C	17.5665298383	21.5756825442	21.1536363148
H	17.7760954649	22.6187220032	20.9092564756
C	18.7048425091	23.4374616549	12.4761228852
H	18.6106369923	24.1915753713	11.6940463356
C	17.7211542275	21.7076681871	13.8579334460
H	16.8579682411	21.1106663497	14.1601005009
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H	16.6315035195	22.8301326270	12.3682112149
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C	14.4794060417	20.0227379963	19.5564140559
H	15.5097557633	19.9379899425	19.9209506498
H	14.1273261805	19.0104280410	19.3235898184
C	15.6934052299	22.6764855096	17.0421101427
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H	16.3232326891	23.5584266001	17.2271508900
H	14.8172681984	23.0026613359	16.4660780895
C	13.5806276606	20.6973671555	20.5779963831
H	12.5409177751	20.7685352462	20.2278851115
H	13.9421887734	21.6986596136	20.8510647586
H	13.5861424144	20.0846938327	21.4895925494
C	15.3182932106	22.0574114609	18.3811505859
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H	16.2185888658	21.8154338972	18.9609632135
C	13.2234464706	20.9620136288	17.5772535413
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O	19.6412518883	17.1728525845	18.1976781863
H	20.2621238273	16.3382980122	18.2434943565
C	16.4576688877	15.3973485239	18.2438921805
C	15.0436499703	13.0062076973	18.3934510301
C	16.7840348048	14.4909661707	19.2594273375
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H	16.2918018200	12.5728769290	20.1000423192
C	18.4076664899	13.6276616389	20.9918074361
C	14.7701460807	13.9381060188	17.3836607831
H	14.0089870458	13.7212459187	16.6323849420
C	15.4607722770	15.1529698949	17.2921598141
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C	19.0481218444	20.3300251984	17.9156894540
C	17.4968666332	15.9955953698	21.1668986823
C	15.1191302463	16.1967432103	16.2409808004
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C	19.9505989450	19.0752401332	13.1873844725
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C	18.4122684106	19.9678252247	19.2496873992
H	18.4024422102	18.8708203720	19.3271980670
C	14.7018267939	15.5578889079	14.9199023840
C	20.3888961980	21.8087111978	16.4994910346
C	19.3170703933	19.8424798018	15.5142091464
C	14.1257713187	17.2290298192	16.7534294181
C	19.8536735082	21.4617238173	17.7482341000
H	20.0722012300	22.0754477032	18.6236670510
C	19.2505356861	20.4210422293	20.4393889700
C	18.9599011333	18.9445384716	14.3359843421
H	19.0386698193	17.9035834450	14.6895210222
C	17.5115868715	19.1290603119	13.8957627365
C	18.4593117704	16.9435246277	21.5453010351
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C	16.9571034328	20.4019720137	19.3134242552
C	14.3034300397	11.6824596264	18.4505473505
H	14.5742183207	11.1973140369	19.4041551388
C	20.1160142635	20.9880521357	15.3983126092
H	20.5399070072	21.2364985983	14.4238061356
C	19.7457202727	19.9608471410	12.1203571679
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C	16.1973289540	16.1104468869	21.6814430255
H	15.4351578297	15.3957180216	21.3659430865

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H	17.2271416374	13.9230935745	22.7717385077
C	16.8098976330	18.0247375685	13.3902121968
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C	19.3445941586	12.7964532479	20.3569597155
H	19.7230463592	13.0827212436	19.3741351106
C	18.7880083945	21.3172098262	21.4097146105
H	17.7938474454	21.7519759598	21.3041665375
C	20.7002582023	20.0836099647	11.1045688298
H	20.5253949219	20.7748383753	10.2789817875
C	21.2431306205	23.0534537573	16.3489566751
H	21.5575064306	23.1106780795	15.2927015021
C	15.8748332565	17.1380817104	22.5746784745
H	14.8589542772	17.2176378934	22.9642153805
C	16.8660496426	20.3726649834	13.9497023799
H	17.3923135081	21.2301409496	14.3724940447
C	16.0043265156	19.5140540286	19.8338627381
H	16.3171772970	18.5165994679	20.1447653404
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C	19.5807995908	21.6314574008	22.5217611012
H	19.2031624774	22.3258706202	23.2737012077
C	16.8462982500	18.0700983860	22.9545216654
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H	15.0618442466	21.4827074464	13.5327878724
C	15.3885349503	14.3072967981	12.9468886374
H	16.1653569082	13.7864889466	12.3850772323
C	15.4971587806	18.1546267329	12.9310082023
H	14.9638012484	17.2744390939	12.5699742455
C	14.8676345769	19.4041861967	12.9692229487
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H	12.9506124553	15.8496634639	17.9259164242
C	19.8022738201	11.6324269364	20.9786285003
H	20.5342461118	10.9992262626	20.4750638294
C	20.4358546716	24.3202477551	16.6801364211
H	19.5432253960	24.4014765895	16.0423186024
H	21.0521134591	25.2215676819	16.5386932106
H	20.1026277485	24.2986895179	17.7298236132
C	16.5505485350	21.6781292151	18.8993576629
H	17.2869660423	22.3625621713	18.4741832172
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H	21.4548479911	21.2917749003	23.5475235785
C	12.2241475286	19.1586802890	17.5029587054
H	11.4870336688	19.9078815607	17.7949998367
C	20.5278196831	19.8548981033	20.5953781121
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C	21.1273368171	18.3100256998	13.2155490530
H	21.2877853616	17.6113534309	14.0397834899
C	14.6662819624	19.8974526695	19.9453860137
H	13.9309547822	19.1882280358	20.3258942799
C	22.0803470657	18.4273895785	12.2005210347
H	22.9855140894	17.8195892914	12.2335642273
C	14.2566244804	18.5597312804	16.3278574218
H	15.1035069983	18.8395313816	15.6998767216
C	14.2683554945	21.1769713381	19.5444471628
H	13.2219055703	21.4736667805	19.6235135037
C	14.0975614646	14.4266452553	12.4135346765
H	13.8650628279	13.9987475854	11.4377391434
C	12.0984388278	17.8392164548	17.9484404302
H	11.2600970986	17.5542437938	18.5860037813
C	13.3110908314	19.5177641491	16.6982837277
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C	21.3179222750	20.1628940279	21.7031874703
H	22.3020855912	19.7054714383	21.8146181142
C	13.1118665012	15.1006170893	13.1398732608
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C	15.2123859755	22.0669263163	19.0205521269
H	14.9053768266	23.0630358257	18.6980361832
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H	22.0289793577	15.2519234127	18.5438979663
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C	22.8389026153	13.4688017326	18.1002626490
C	24.0697790850	15.6817706510	16.9097594923
H	24.5455458073	16.5420180424	16.4381311046
C	23.2620348862	15.8909071428	18.0373619282
C	21.5205558045	13.6116678831	22.9271285004
C	21.7404715919	11.2497024114	17.7143946629
C	20.3639751627	13.5988599988	22.1214704877
C	22.4096636058	14.8448378075	22.9680823778
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H	21.9818212431	17.3671986702	18.8678501502
C	23.6345487410	13.3242223251	16.9575502075
H	23.7499554502	12.3251898291	16.5337715203
C	23.8151724246	17.5613040104	19.9114651981
C	23.2083490193	11.5982785936	19.7629646196
C	18.0121448770	11.1326152144	20.6617884020
C	19.7740718759	11.4253099305	22.9679781986
H	19.0951890411	10.5731414069	22.9566135284
C	20.9115335182	11.3985307285	23.7766378643
C	19.4764468886	12.5117337692	22.1303614239
C	23.8395131949	14.5411682110	23.4092701866
C	24.2679712494	14.4141078441	16.3549900622
C	22.2475981467	12.2359737458	18.7678538800
H	21.3627302158	12.5560599615	19.3382468320
C	16.9775169174	13.0117659605	22.0583172574
C	21.7739110341	15.9610821755	23.7815771404
C	18.1984984650	12.5044926614	21.2986424889
H	18.3536681449	13.2059355992	20.4633850825
C	23.3371701886	18.3686344783	17.5654768378
C	24.4267085770	15.1267662522	24.5381694533
H	23.8405058576	15.8034399170	25.1599340460
C	24.6279801929	16.6103194815	20.5406784098
H	24.7149561369	15.6099324940	20.1154081573
C	24.6154918744	18.9317626388	17.4206021085
H	25.4070425034	18.6406195816	18.1127093243
C	21.7710881939	12.5033883859	23.7397309647
H	22.6774333971	12.4983482001	24.3479416157
C	25.1397479106	14.2239629504	15.1281951158
H	25.5304469590	15.2167613042	14.8459861780
C	23.7071636098	18.8388893402	20.4935053348

H	23.0809317325	19.5893211349	20.0071959848
C	24.5986138701	11.5853276391	19.5709990607
H	25.0264598065	12.1030180546	18.7120721233
C	21.2185218919	10.2365724862	24.7039817180
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C	22.6781306513	10.9465984498	20.8853756880
H	21.6002535030	10.9669534574	21.0551101916
C	20.7309408379	11.6834972091	16.8367900534
H	20.3310454366	12.6920265593	16.9571098289
C	21.0270006936	15.7082777074	24.9415021113
H	20.8410401558	14.6747596366	25.2386797348
C	17.0642417502	13.5853754757	23.3345928411
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H	26.2071204893	15.3422813388	25.7410207384
C	24.6132725043	13.6756112314	22.6171396293
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H	19.3174021315	11.6434408277	19.0309715315
C	15.7188641759	12.9629332287	21.4315205417
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C	25.9482302327	13.4229769358	22.9364073624
H	26.5283825221	12.7523109857	22.3025367693
C	24.4129064247	19.1618846453	21.6537776745
H	24.3222603762	20.1613902459	22.0825026987
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C	25.4370939735	10.9261740730	20.4756838377
H	26.5156434144	10.9257093484	20.3098644302
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O	17.9094756926	15.5384890949	17.0840096197
H	18.3879832390	14.9343255570	17.7034596016
H	18.4610585557	16.3750292183	17.1257384090
O	17.0908560777	19.4611595095	17.9158297912
H	16.6122260544	20.0650982978	17.2962157790
H	16.5396606415	18.6243848382	17.8742535575

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