

Supporting Information

Self-assembling study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach

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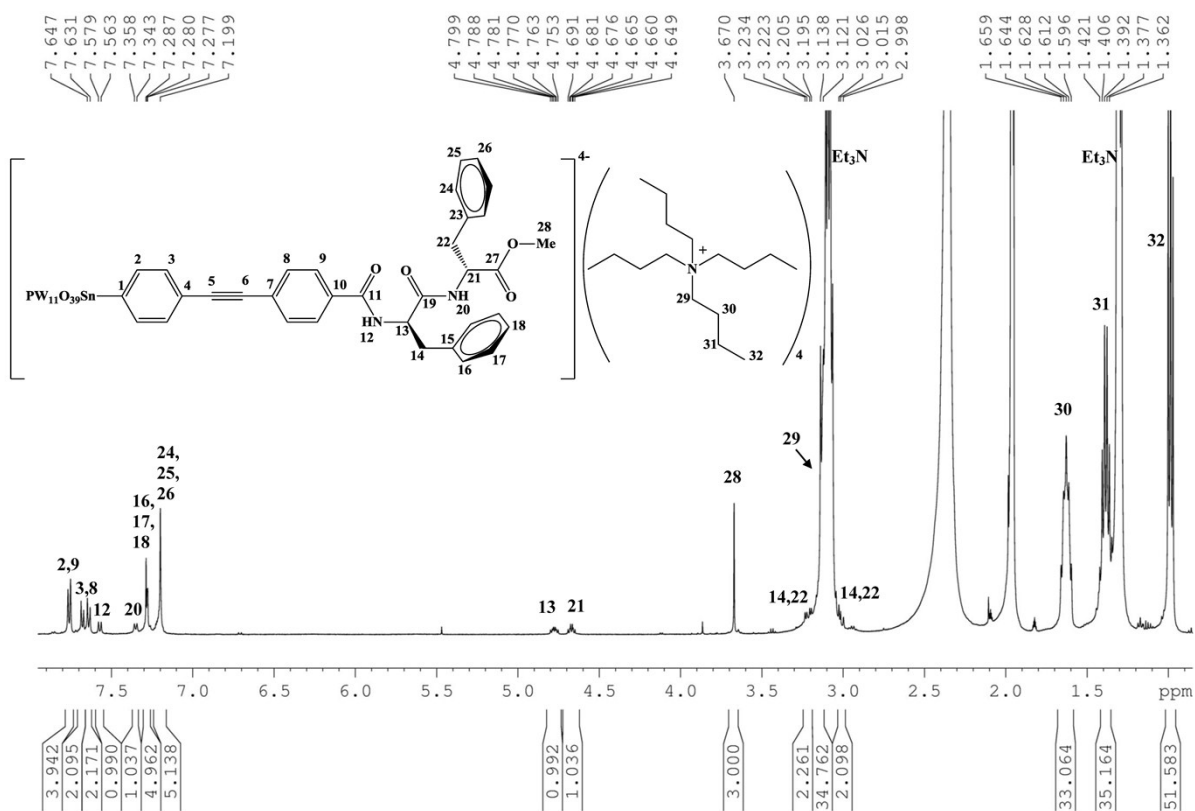


Fig. S1 1H NMR spectrum of **POM-FF** (500 MHz, CD_3CN).

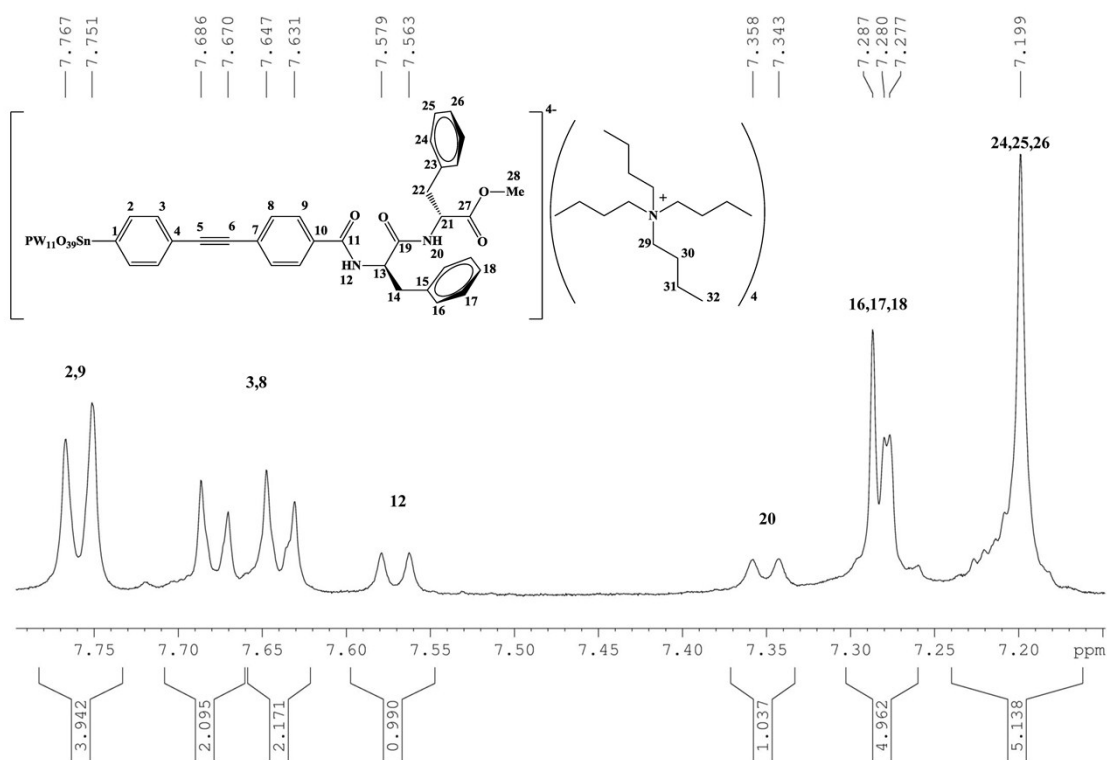
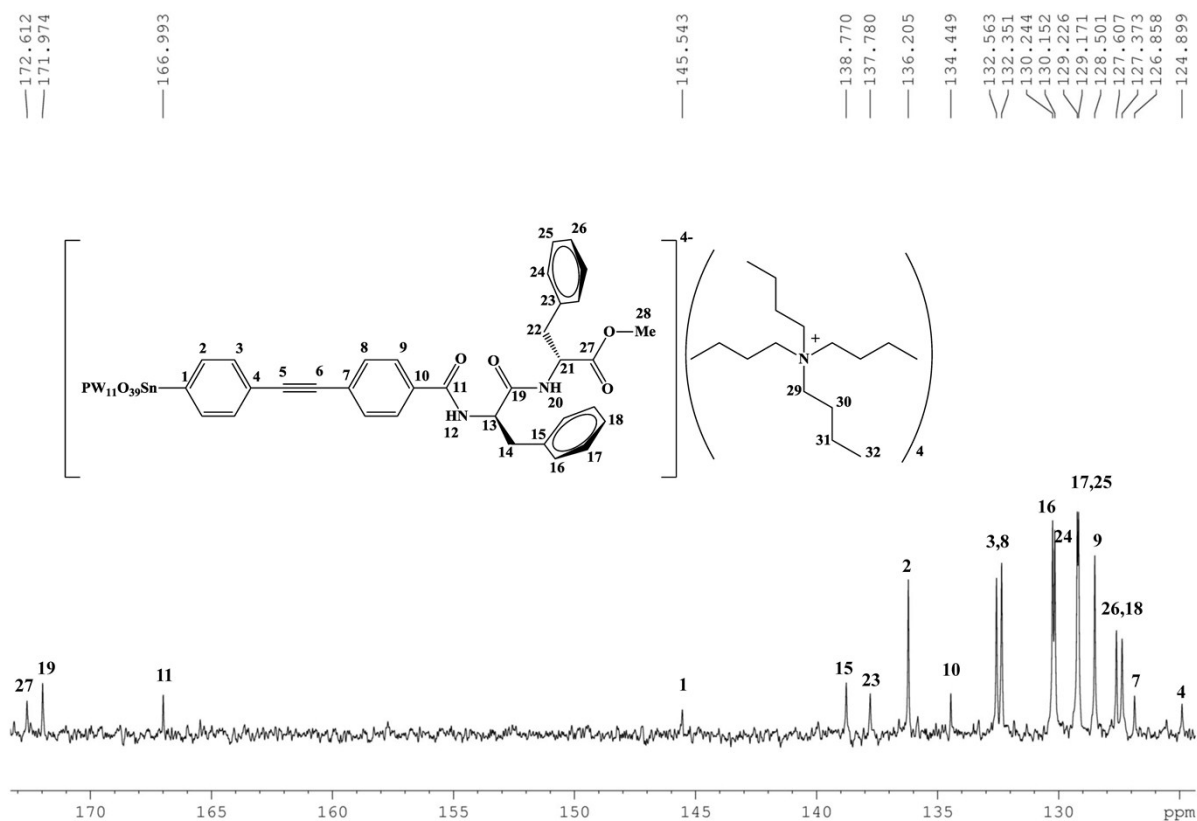
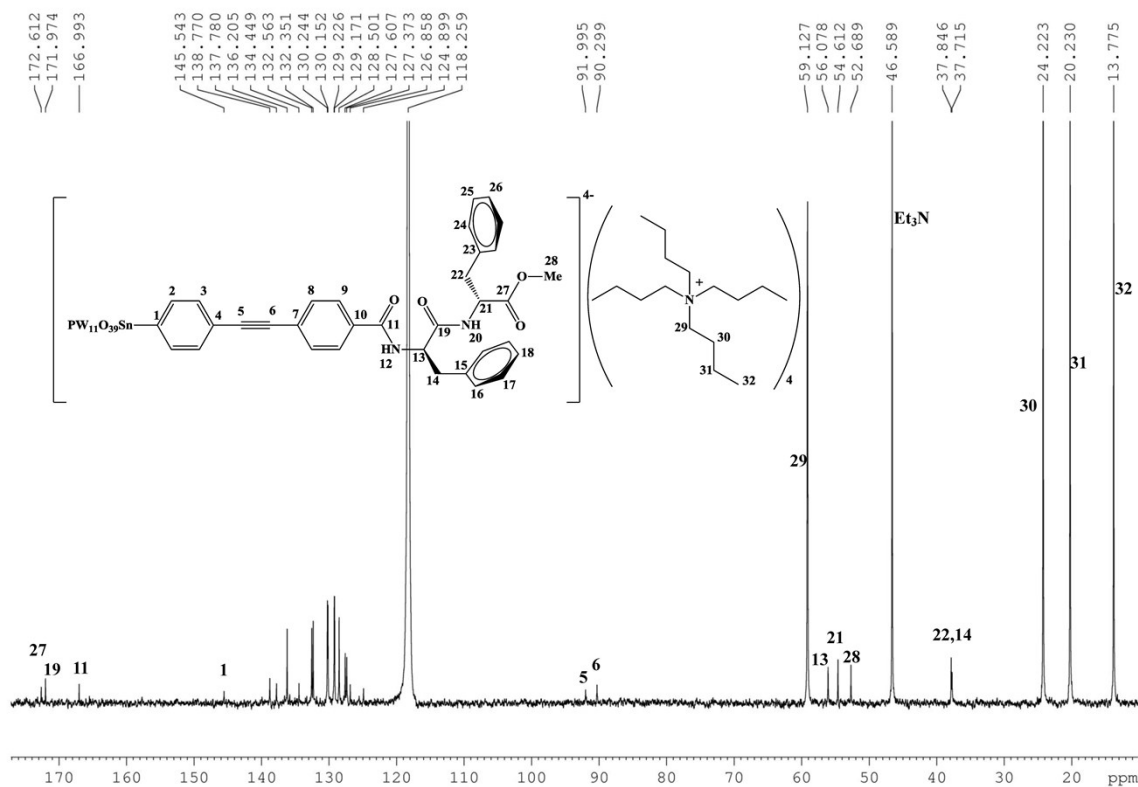


Fig. S2 1H NMR spectrum of **POM-FF** (500 MHz, CD_3CN).



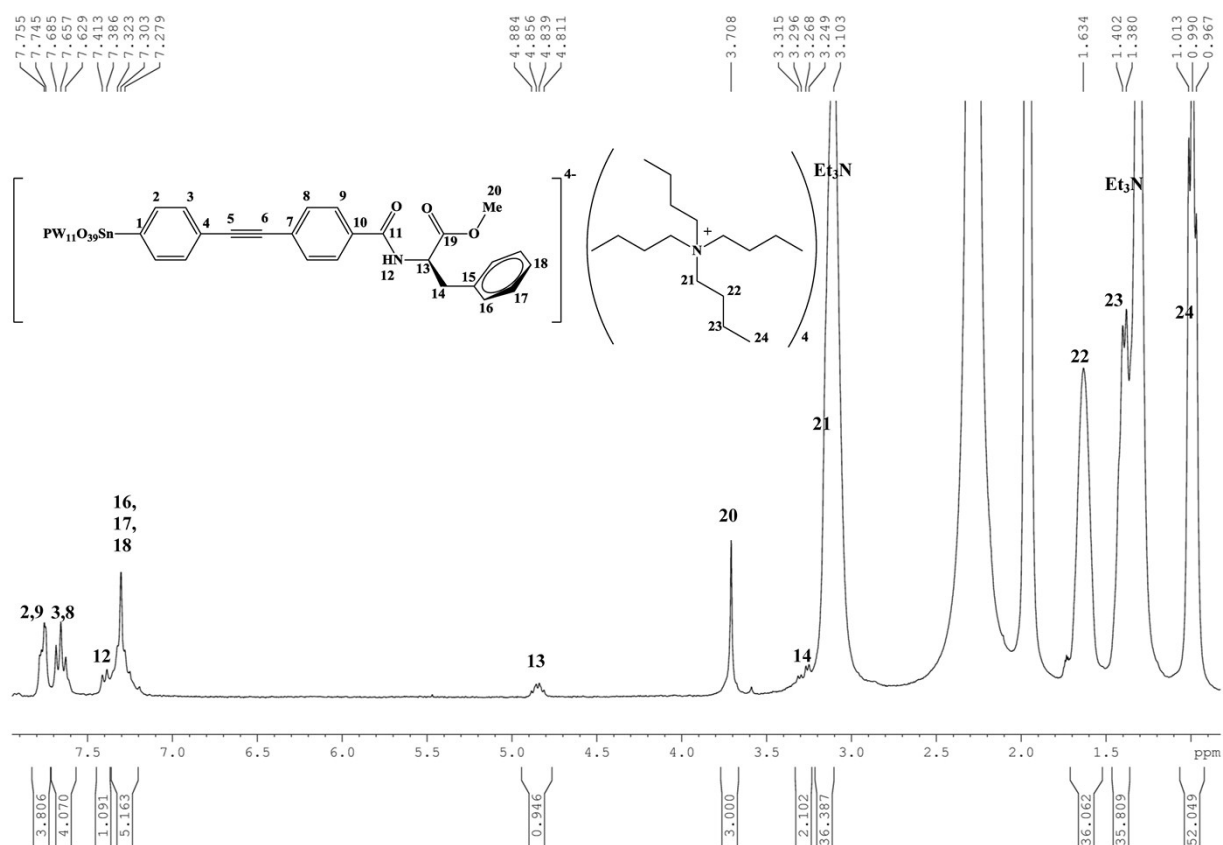


Fig. S5 ¹H NMR spectrum of **POM-F** (300 MHz, CD₃CN).

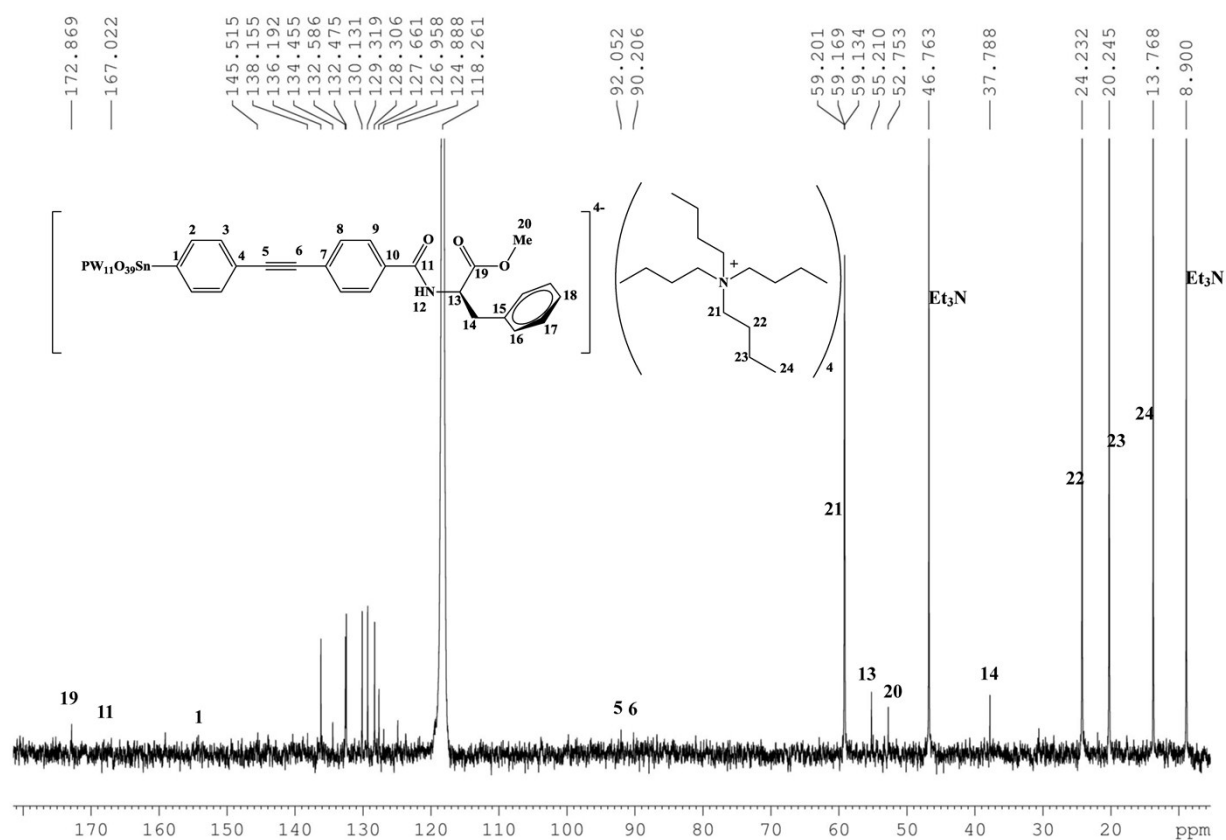


Fig. S6 ¹³C NMR spectrum of **POM-F** (75 MHz, CD₃CN).

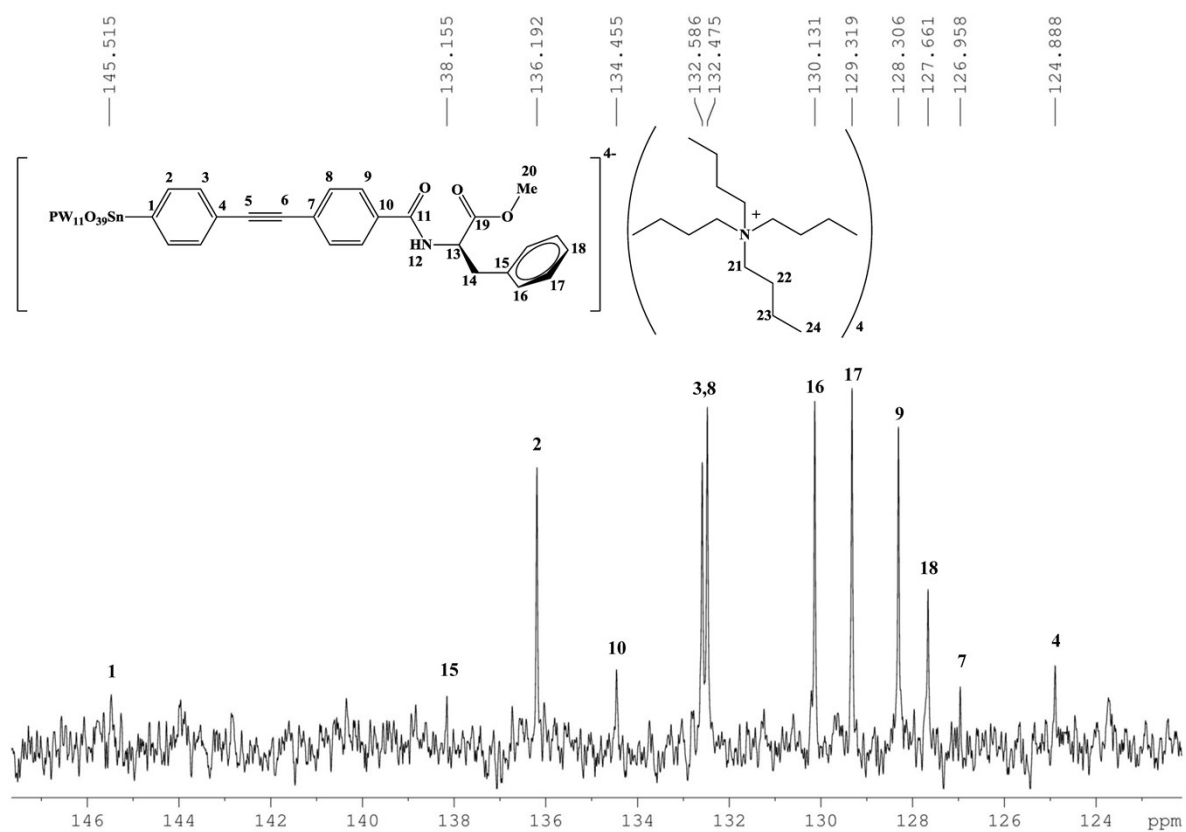


Fig. S7 ^{13}C NMR spectrum of POM-F (75 MHz, CD_3CN).

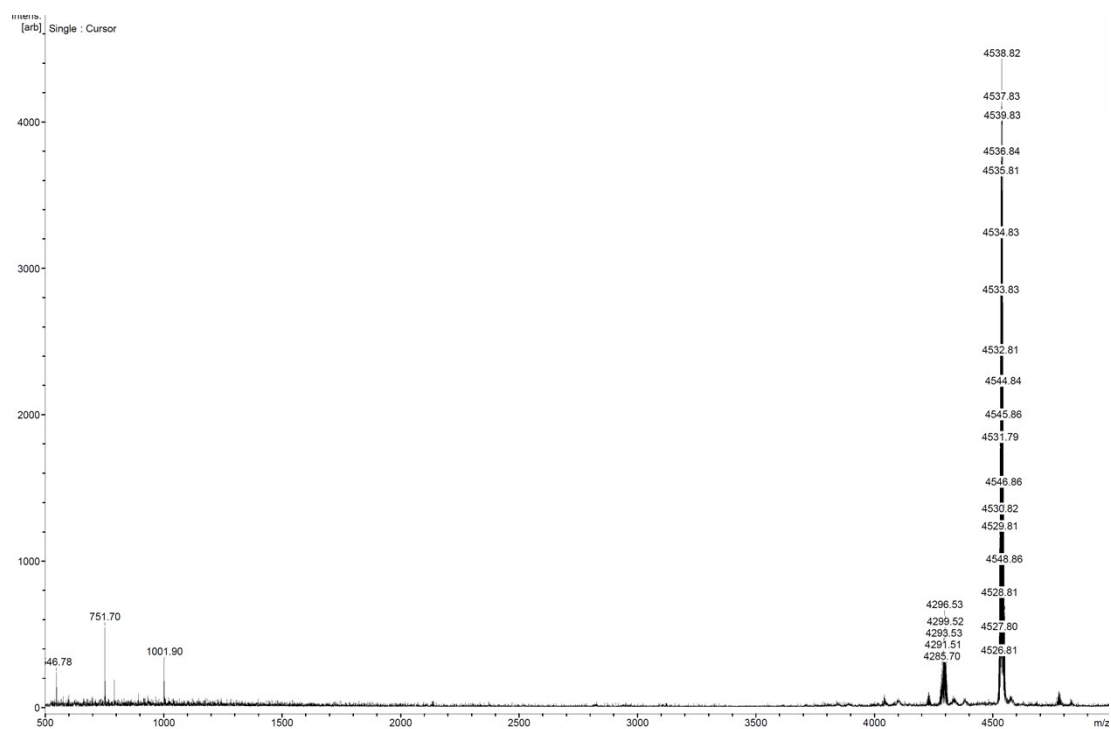


Fig. S8 MALDI-TOF mass spectra of POM-FF.

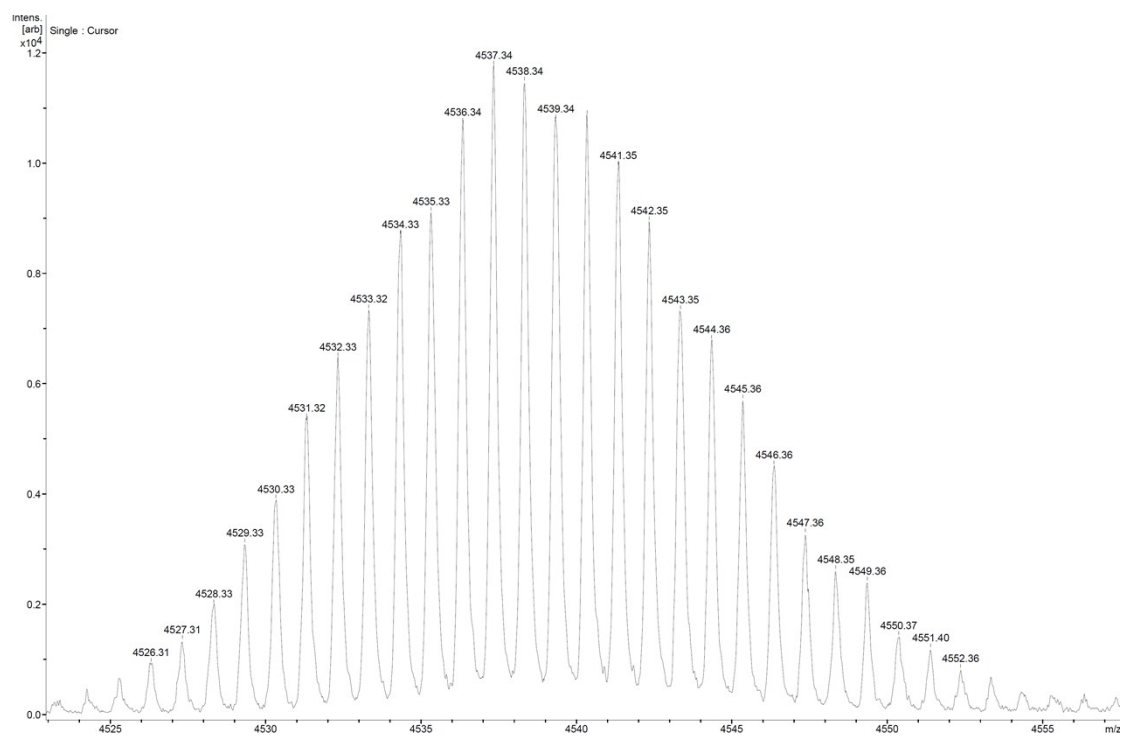


Fig. S9 MALDI-TOF mass spectra of **POM-FF**.

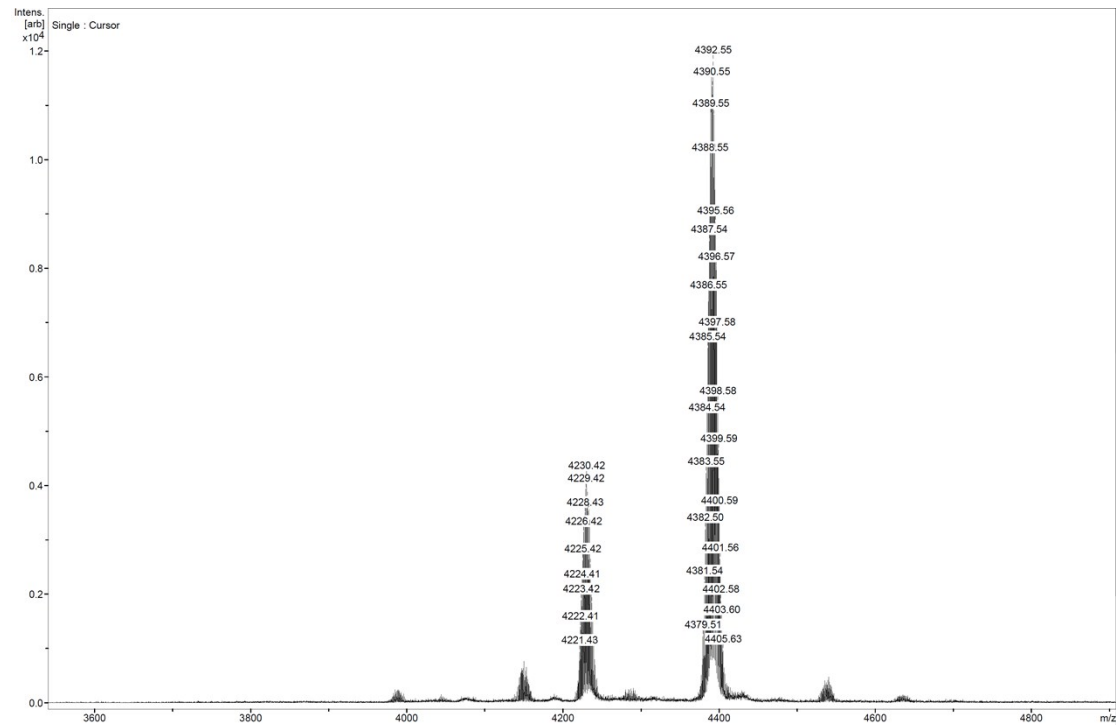


Fig. S10 MALDI-TOF mass spectra of **POM-F**.

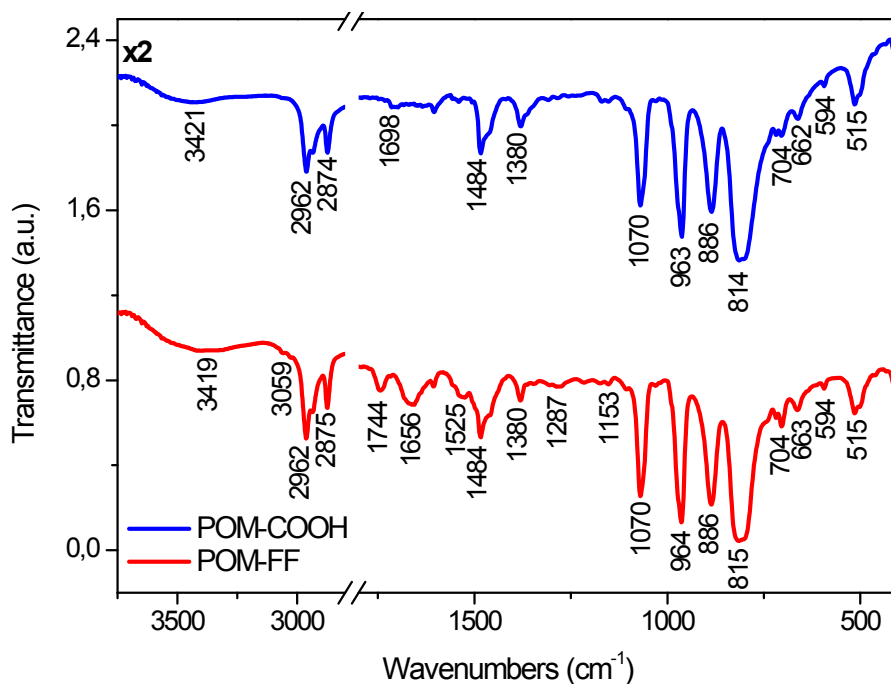


Fig. S11 FT-IR spectra of **POM-COOH** and **POM-FF**.

Table S1 FT-IR bands (cm^{-1}) of **POM-COOH** and **POM-FF**. For comparison the FT-IR bands of $[\text{PW}_{11}\text{O}_{39}]^{7-}$ and $[\text{PW}_{12}\text{O}_{40}]^{3-}$ are also given.⁷⁻¹³

POM-COOH	POM-FF	$[\text{PW}_{11}\text{O}_{39}]^{7-}$	$[\text{PW}_{12}\text{O}_{40}]^{3-}$	Assignment
3421				$\nu(\text{O-H})$ acid
	3419			$\nu(\text{N-H})$ <i>sec</i> -amide
	3059, 3026			$\nu(-\text{CH})$ arom. FF
2962, 2935, 2874	2962, 2935, 2875			$\nu(-\text{CH}_2, -\text{CH}_3)$ aliph. TBA
	1744			$\nu(\text{C=O})$ ester
1698				$\nu(\text{C=O})$ acid
	1656			$\nu(\text{C=O})$ <i>sec</i> -amide (amide I)
	1525			$\delta(\text{N-H})$ <i>sec</i> -amide (amide II)
1484	1484			$\delta(-\text{CH}_2, -\text{CH}_3)$ TBA
1380	1380			$\delta(-\text{CH}_3)$ TBA
	1287			$\nu(-\text{C}(\text{O})-\text{O})$ ester, (amide III)
	1174, 1153			$\nu(\text{C-N})$ aliph.
1070	1070	1085, 1040	1080	$\nu_{\text{as}}(\text{P-O}_a)$
963	964	950	987, 976	$\nu_{\text{as}}(\text{W-O}_d)$
886	886	900, 860	895	$\nu_{\text{as}}(\text{W-O}_b-\text{W})$
814, 704, 662	815, 704, 663	810, 725	810	$\nu_{\text{as}}(\text{W-O}_c-\text{W})$
594	594	590	598, 525, 480	$\delta(\text{O}_a-\text{P}-\text{O}_a)$
515	515	510		$\delta(\text{W-O}_{b,c}-\text{W})$

FT-IR spectroscopy discussion

Comments:

1) A single band at 886 cm^{-1} assigned to $\nu_{\text{as}}(\text{W}-\text{O}_{\text{b}}-\text{W})$ appears in both **POM-COOH** and **POM-FF**, whereas a split band ($900, 860\text{ cm}^{-1}$) is observed in lacunary $[\text{PW}_{11}\text{O}_{39}]^{7-}$ and a single band (895 cm^{-1}) in Keggin $[\text{PW}_{12}\text{O}_{40}]^{3-}$. This result indicates that some O_{b} oxygens (i.e. oxygens that link corner-sharing WO_6 octahedra) possibly interact with Sn^{4+} cations leading also to restoration of the pseudo-tetrahedral symmetry of the Keggin structure.

2) A broad single band with high intensity at $\sim 815\text{ cm}^{-1}$ and possibly the two small bands at 704 and 663 cm^{-1} are attributed to $\nu_{\text{as}}(\text{W}-\text{O}_{\text{c}}-\text{W})$ in both **POM-COOH** and **POM-FF**, whereas a split band ($810, 725\text{ cm}^{-1}$) is present in lacunary $[\text{PW}_{11}\text{O}_{39}]^{7-}$ and a single band (810 cm^{-1}) in Keggin $[\text{PW}_{12}\text{O}_{40}]^{3-}$ anions. Thus, it seems possible that the O_{c} oxygens (i.e. oxygens that link edge-sharing WO_6 octahedra) also participate in the coordination of $\text{PW}_{11}\text{O}_{39}^{7-}$ anion to Sn^{4+} cation.

3) For the **POM-COOH** a broad band at 3421 cm^{-1} attributed to $\nu(\text{O}-\text{H})$ of acid, three peaks at $2962, 2935,$ and 2874 cm^{-1} attributed to $\nu(-\text{CH}_2, -\text{CH}_3)$ of TBA cation, a peak at 1698 cm^{-1} attributed to $\nu(\text{C}=\text{O})$ of acid, a band at 1484 cm^{-1} attributed to bending (δ) of $-\text{CH}_2$ and $-\text{CH}_3$ of TBA cation, and a band at 1380 cm^{-1} assigned to $\delta(-\text{CH}_3)$ of TBA cation.^[7,8] The aromatic groups and the triple $\text{C}\equiv\text{C}$ bond could not be clearly observed.

4) For the **POM-FF** a broad band at 3419 cm^{-1} attributed to $\nu(\text{N}-\text{H})$ of *sec*-amides, two small peaks at 3059 and 3026 cm^{-1} attributed to $\nu(-\text{CH})$ aromatic of FF, three peaks at $2962, 2935,$ and 2874 cm^{-1} attributed to $\nu(-\text{CH}_2, -\text{CH}_3)$ of TBA cation, one peak at 1744 cm^{-1} assigned to $\nu(\text{C}=\text{O})$ of ester, a peak at 1656 cm^{-1} attributed to $\nu(\text{C}=\text{O})$ of *sec*-amide (amide I), a peak at 1525 cm^{-1} assigned to $\delta(\text{N}-\text{H})$ of *sec*-amide (amide II), a peak at 1484 cm^{-1} attributed to bending (δ) of $-\text{CH}_2$ and $-\text{CH}_3$ of TBA cation, a peak at 1380 cm^{-1} assigned to $\delta(-\text{CH}_3)$ of TBA cation, a peak at 1287 cm^{-1} attributed mainly to $\nu(-\text{C}(\text{O})-\text{O})$ of ester and possibly to amide III band, and two peaks at 1174 and 1153 cm^{-1} attributed to $\nu(\text{C}-\text{N})$ aliphatic.^{[2],[7,8]}

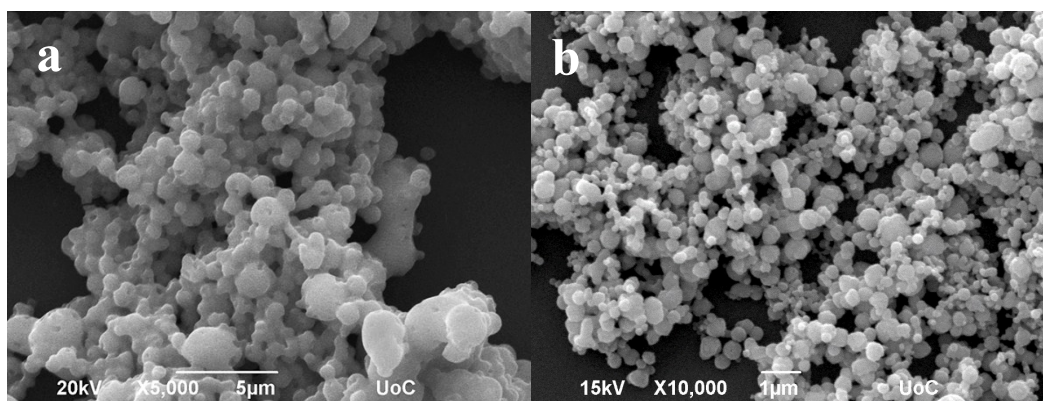


Fig. S12 POM-FF in 1mM solutions of a) DCM-Toluene 1:1, b) DCM-Heptane 1:1

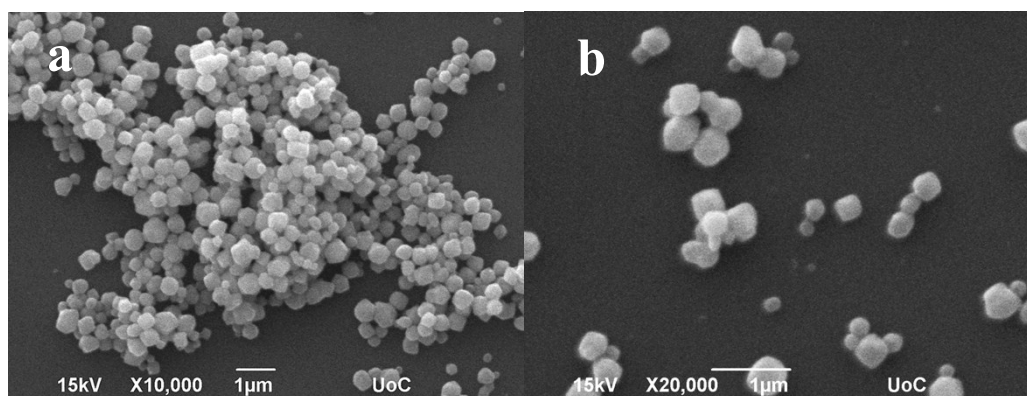


Fig. S13 POM-FF in 1mM solution of DCM-EtOH 1:1.

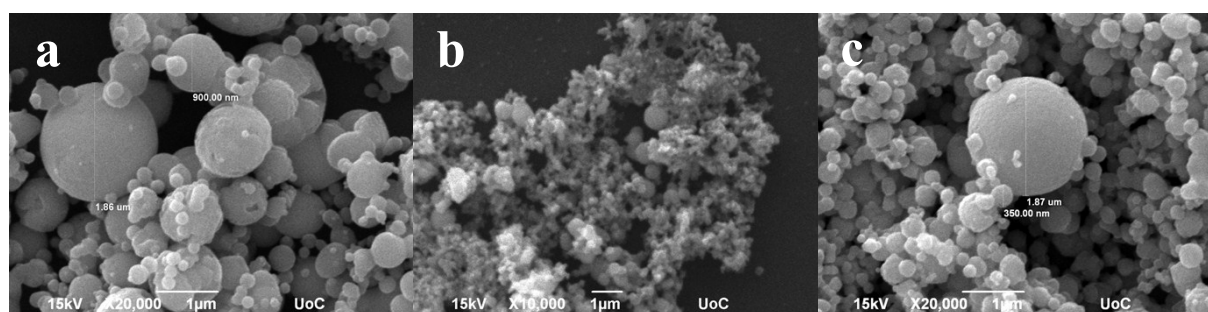


Fig. S14 POM-FF in 1mM solutions of a) DCM-Heptane 1:1, b) DCM-Heptane 1:4, c) DCM-Heptane 1:8.

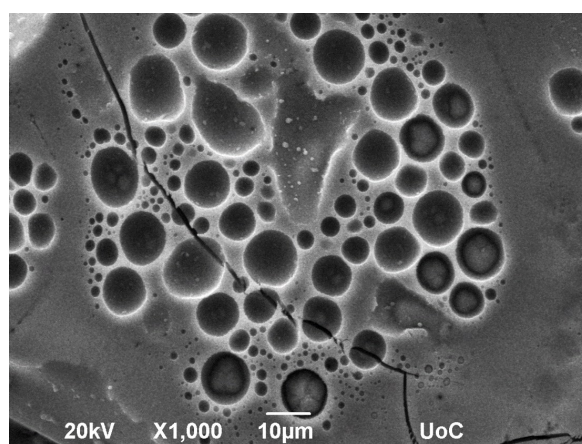


Fig. S15 POM-FF in 1mM solution of MeCN.

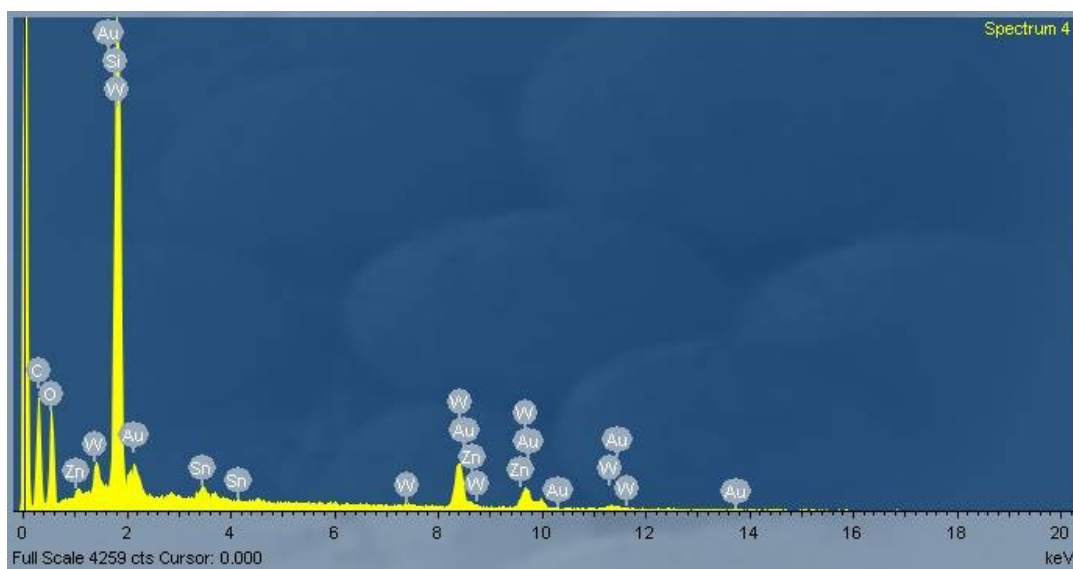


Fig. S16 EDS spectra analysis of compound **POM-FF**. Structure composition of **POM-FF** was verified by conducting SEM/EDS analysis on the structure. The tungsten peak is indicative for defining our compound.

Table S2 Elemental analysis of **POM-FF**.

Element	Weight %
W	39.90
C	28.85
O	20.97
Sn	1.85
Au	3.83
Si	1.62
Zn	2.98
Total	100

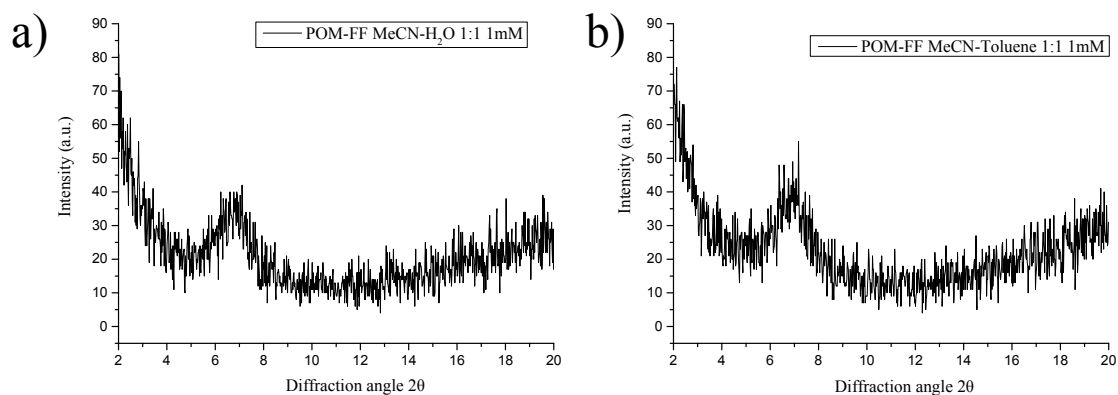


Fig. S17 XRD pattern of **POM-FF** in a) MeCN-H₂O 1:1 1mM, b) MeCN-Toluene 1:1 1mM.

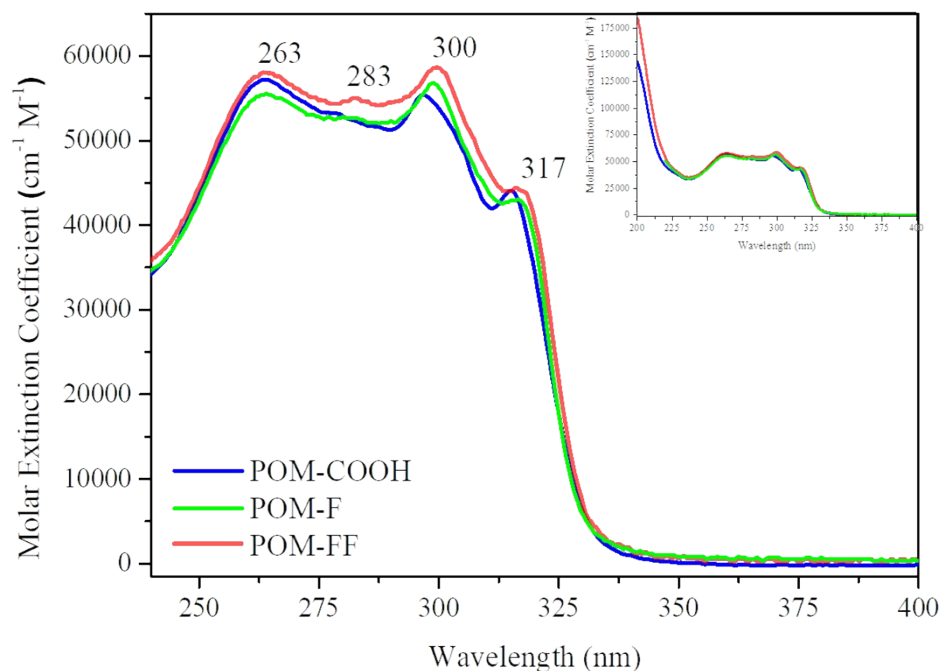


Fig. S18 UV-Vis absorption spectra of **POM-COOH**, **POM-F** and **POM-FF** in MeCN.

Table S3 UV-Vis bands (nm) of **POM-COOH**, **POM-F** and **POM-FF**. For comparison the UV-Vis bands of $[\text{PW}_{11}\text{O}_{39}]^{7-}$ and $[\text{PW}_{12}\text{O}_{40}]^{3-}$ are also given.¹⁻⁵

POM-COOH	POM-F	POM-FF	$[\text{PW}_{11}\text{O}_{39}]^{7-}$	$[\text{PW}_{12}\text{O}_{40}]^{3-}$	Assignment
~200	~200	~200	199	200	$\text{O}_d \rightarrow \text{W(VI)}$
265, 276 (sh)	264, 280 (sh)	263, 283 (sh)	252	263	$\text{O}_{b,c} \rightarrow \text{W(VI)}$
297, 315	299, 317	300, 317, 319 (sh)			$\text{O} \rightarrow \text{Sn(IV)}$ or $\pi \rightarrow \pi^*$

UV-Vis absorption spectroscopy discussion

Comments:

1) A band at ~200 nm attributed to $\text{O}_d \rightarrow \text{W(VI)}$ charge transfer (CT) is essentially unchanged in functionalized POMs in relation to both the lacunary $[\text{PW}_{11}\text{O}_{39}]^{7-}$ and Keggin $[\text{PW}_{12}\text{O}_{40}]^{3-}$ anions.^[1-5] This indicates that the terminal O_d oxygens of the POM ligand are not affected neither by the coordination of Sn^{4+} cations nor by the subsequent attachment of F or FF.

2) The contribution of F and FF groups to the band at 263 nm is rather negligible, due to the relatively low molar extinction coefficient of the initial molecules, e.g. for phenylalanine, F, $\lambda_{\text{abs}} = 257 \text{ nm}$, $\epsilon = 195 \text{ cm}^{-1} \text{ M}^{-1}$.^[6]

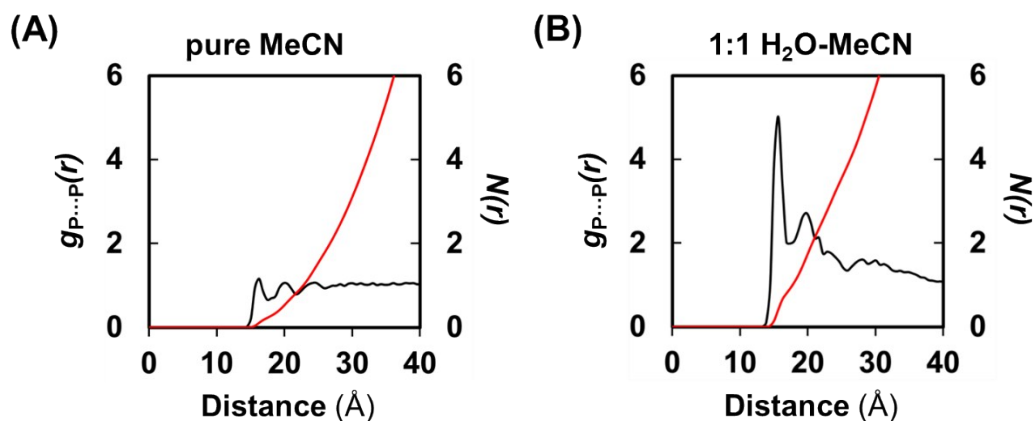


Fig. S19 POM...POM radial distribution function (RDF) between P centres, averaged over the last 10 ns of MD simulation in pure MeCN (A) and in the 1:1 solvent mixture of water and acetonitrile (B). In both cases, the black solid curve represent the RDF itself, $g(r)$, while red ones represent the coordination numbers, $N(r)$, which is obtained by integration of the RDFs. This later gives information about the number of species placed, in average, at a given distance from a reference. Values taken every 2 ps.

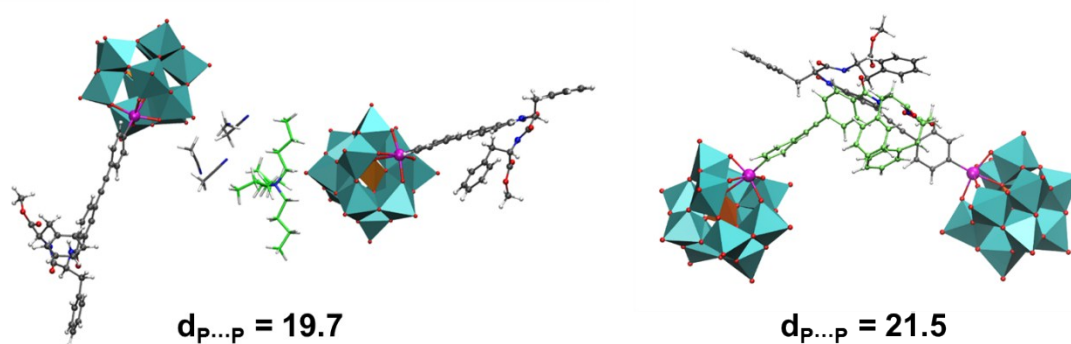


Fig. S20 Snapshots of the simulation in the solvent mixture showing a TBA- and MeCN-mediated interaction between two POM moieties (left, $t = 36788$ ps), and a direct interaction through the organic chains (right, $t = 7616$ ps). Both structures can be included in the array of configurations leading to the second broad peak in the P...P RDF (Fig. S18B). Color code: W (cyan), P (orange), Sn (magenta), C (grey), H (white), O (red) and N (blue). TBA counter cation on the left is represented in green sticks, and C atoms belonging to one of the arms on the right are colored in lime for clarity. Distances in Å.

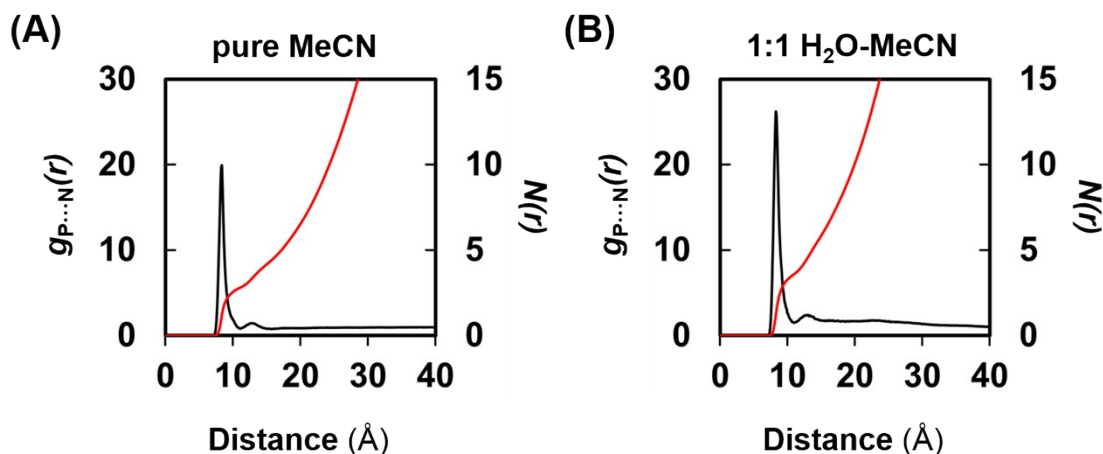


Fig. S21 POM...TBA⁺ radial distribution function (RDF) between P and N centres of each species, respectively, averaged over the last 10 ns of MD simulation in pure MeCN (A) and in the 1:1 solvent mixture of water and acetonitrile (B). In both cases, the black solid curve represent the RDF itself, $g(r)$, while red ones represent the coordination numbers, $N(r)$, which is obtained by integration of the RDFs. This later gives information about the number of species placed, in average, at a given distance from a reference. Values taken every 2 ps.

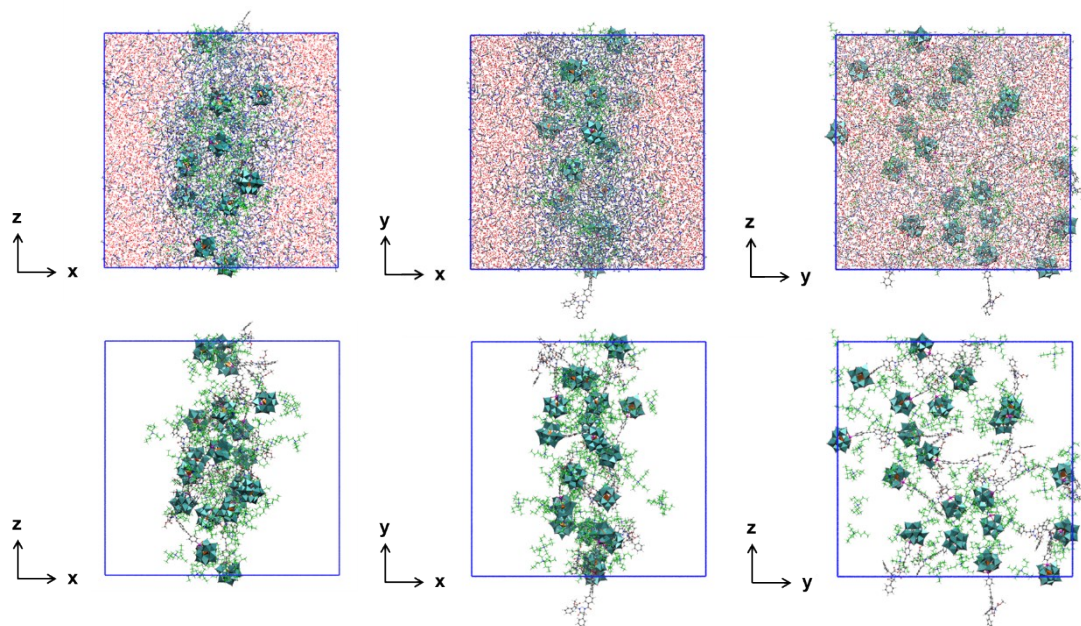


Fig. S22 Snapshots of the simulation box in H₂O-MeCN mixture at the last step of the simulation. Different views from different axis (y, z and x from left to right) are shown including and omitting the solvent molecules (top and bottom, respectively). TBA⁺ carbons are coloured in green.

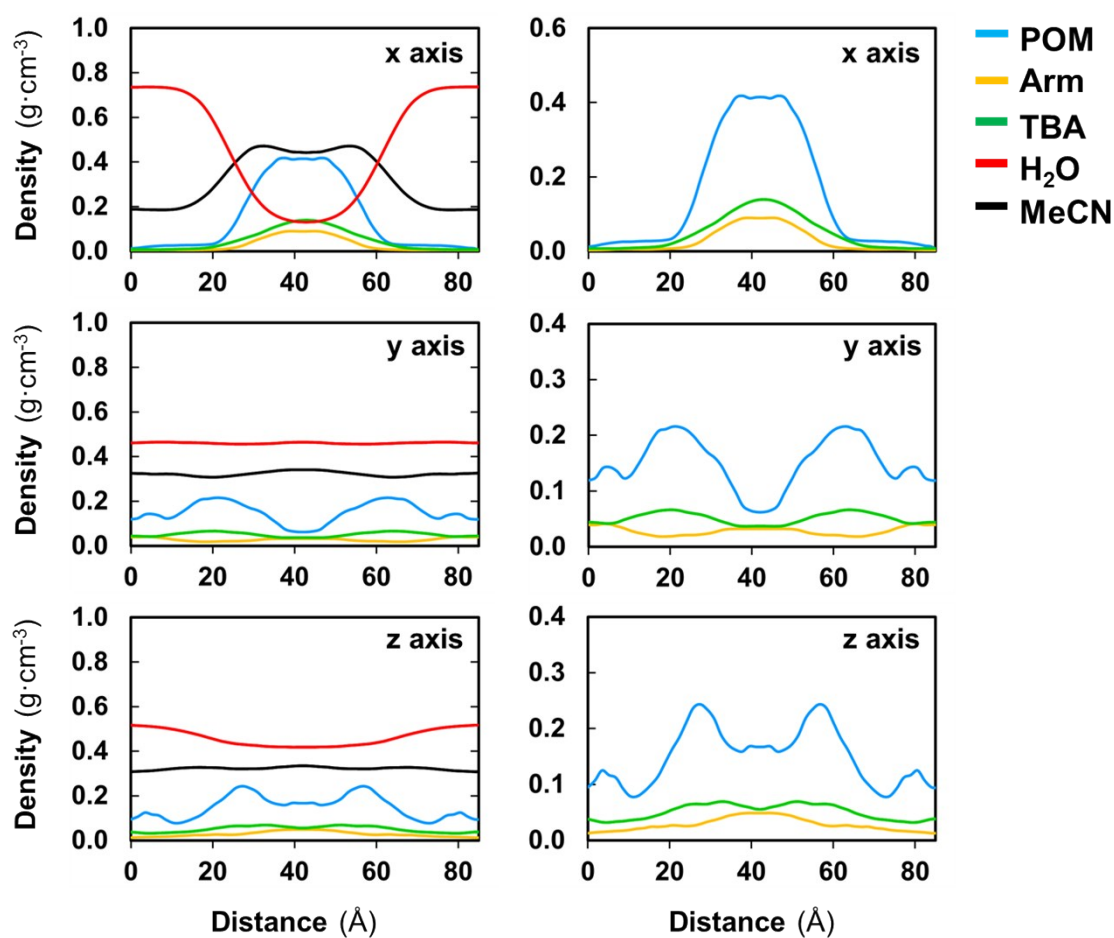


Fig. S23 Density curves of the different species/fragments in the simulation of **POM-FF** salt in H₂O-MeCN mixture along the simulation box in x, y and z directions of the space (left), averaged over the last 10 ns. Graphs on the right represent the same curves but omitting the density of the solvent.

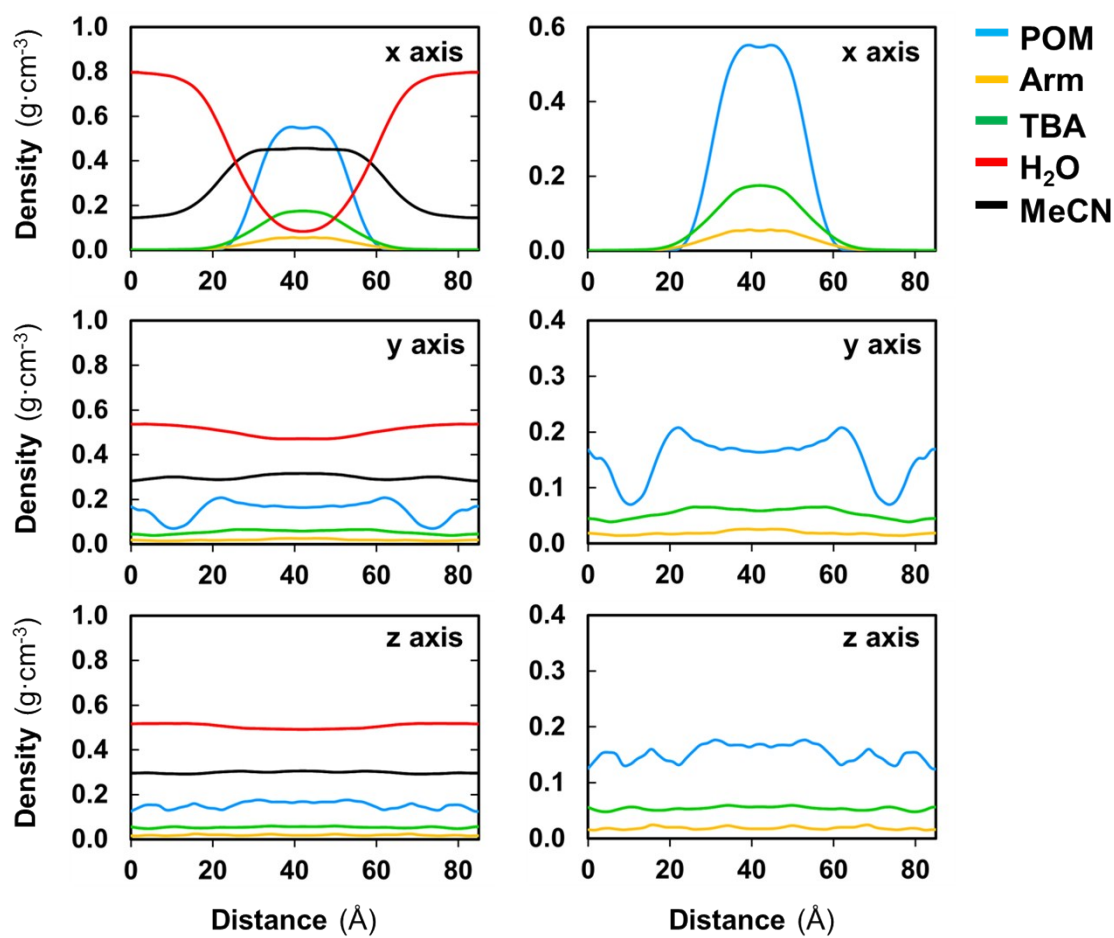


Fig. S24 Density curves of the different species/fragments in the simulation of **POM-COOH** salt in H₂O-MeCN mixture along the simulation box in x, y and z directions of the space (left), averaged over the last 10 ns. Graphs on the right represent the same curves but omitting the density of the solvent.

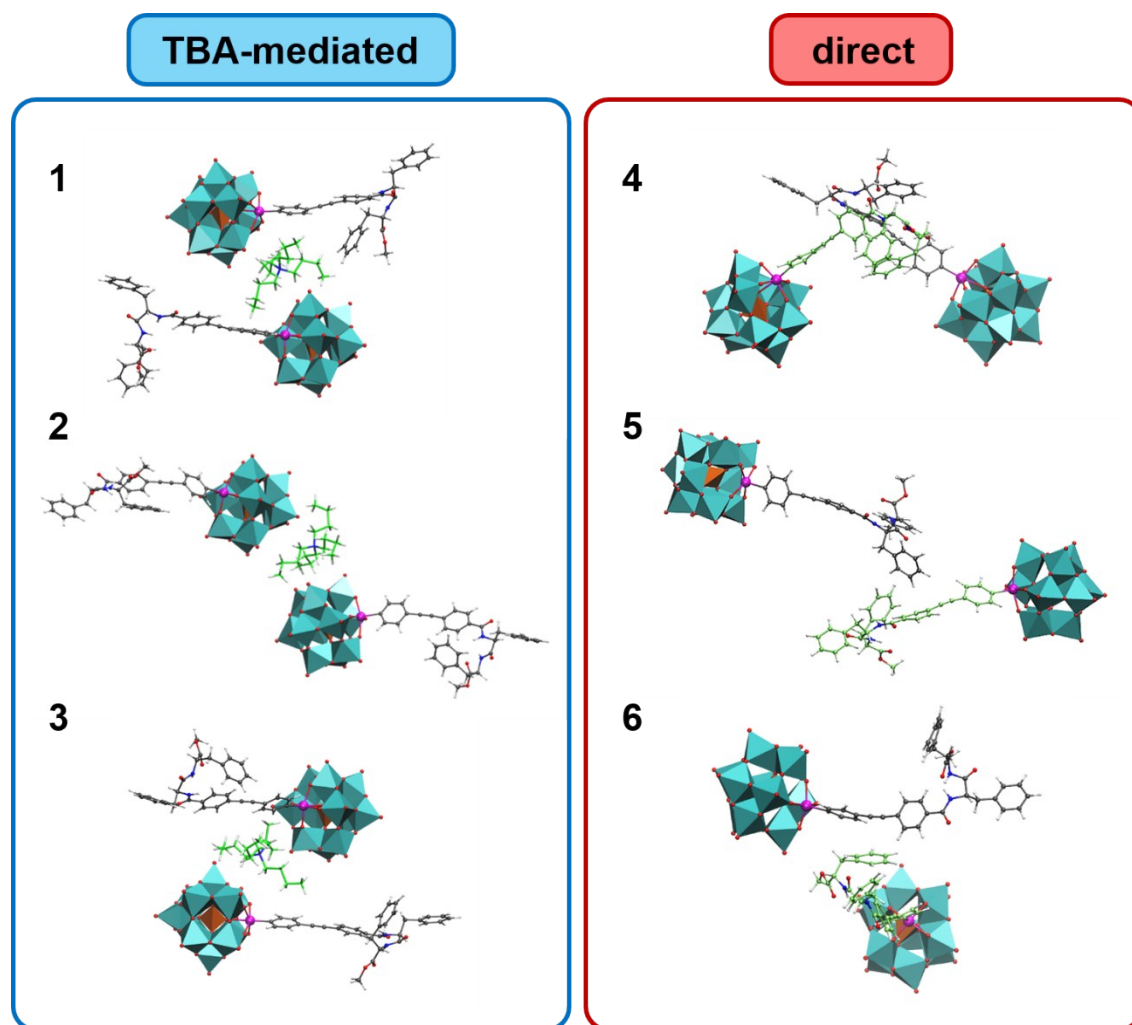


Fig. S25 Representation of the six dimers studied at QM level, labelled according to Table 1. Color code: W (cyan), P (orange), Sn (magenta), C (grey), H (white), O (red) and N (blue). TBA counter cation is represented in green sticks and the C atoms of one of the **POM-FF** monomers involved in direct contacts are coloured in lime for the sack of clarity.

Cartesian coordinates (Å) and electronic energies (a.u.) with IEF-PCM continuous solvent model of the dimeric structures taken directly from snapshots of the MD simulations:

1: $\Delta E = -12188.35226$ a.u.

P	39.17000000	33.85000000	50.81000000
W	37.29000000	33.65000000	47.65000000
W	37.16000000	31.02000000	52.15000000
W	41.17000000	33.91000000	53.93000000
W	37.45000000	36.96000000	49.66000000
W	37.28000000	34.06000000	54.00000000
W	41.04000000	30.90000000	52.07000000
W	40.91000000	33.53000000	47.57000000
W	39.00000000	30.76000000	48.77000000
W	42.85000000	33.67000000	50.79000000
W	39.26000000	37.09000000	52.75000000
W	35.44000000	33.93000000	50.97000000
O	39.23000000	35.55000000	50.74000000
O	39.10000000	33.22000000	49.32000000

O	37.75000000	33.42000000	51.63000000
O	40.49000000	33.31000000	51.64000000
O	42.25000000	33.23000000	48.98000000
O	36.09000000	35.69000000	50.43000000
O	40.38000000	30.49000000	50.22000000
O	37.98000000	35.82000000	53.60000000
O	35.91000000	33.61000000	49.10000000
O	40.56000000	35.82000000	53.61000000
O	37.78000000	30.63000000	50.36000000
O	42.42000000	35.49000000	50.36000000
O	39.10000000	30.69000000	52.48000000
O	40.99000000	35.37000000	48.10000000
O	39.19000000	33.70000000	54.40000000
O	37.38000000	35.57000000	48.19000000
O	37.87000000	37.70000000	51.47000000
O	40.31000000	31.58000000	47.58000000
O	35.68000000	34.30000000	52.88000000
O	42.65000000	31.76000000	51.42000000
O	40.50000000	37.75000000	51.46000000
O	35.58000000	31.93000000	51.44000000
O	42.73000000	34.00000000	52.73000000
O	37.65000000	31.71000000	47.74000000
O	39.05000000	33.81000000	46.84000000
O	41.41000000	31.95000000	53.71000000
O	39.11000000	37.59000000	48.99000000
O	36.75000000	32.16000000	53.74000000
O	36.33000000	33.86000000	46.24000000
O	36.47000000	29.54000000	52.60000000
O	41.91000000	34.02000000	55.49000000
O	36.34000000	38.18000000	49.04000000
O	36.50000000	34.31000000	55.56000000
O	41.63000000	29.35000000	52.55000000
O	41.89000000	33.42000000	46.16000000
O	38.80000000	29.18000000	48.02000000
O	44.61000000	33.69000000	50.52000000
O	39.23000000	38.41000000	53.94000000
O	33.69000000	34.07000000	50.76000000
Sn	40.95000000	36.83000000	49.63000000
C	42.26000000	38.29000000	48.82000000
C	41.69000000	39.52000000	48.43000000
C	43.65000000	38.06000000	48.73000000
C	42.46000000	40.53000000	47.94000000
H	40.64000000	39.68000000	48.65000000
C	44.39000000	39.12000000	48.24000000
H	44.08000000	37.14000000	49.11000000
C	43.82000000	40.32000000	47.87000000
H	41.95000000	41.47000000	47.83000000
H	45.47000000	39.11000000	48.24000000
C	44.73000000	41.35000000	47.61000000
C	45.58000000	42.19000000	47.39000000
C	46.60000000	43.16000000	47.05000000
C	47.93000000	42.69000000	47.11000000
C	46.30000000	44.46000000	46.68000000
C	48.91000000	43.48000000	46.60000000
H	48.08000000	41.64000000	47.33000000
C	47.39000000	45.34000000	46.43000000
H	45.28000000	44.80000000	46.78000000
C	48.68000000	44.84000000	46.25000000
H	49.89000000	43.06000000	46.41000000
H	47.15000000	46.34000000	46.12000000
C	49.79000000	45.65000000	45.91000000
O	49.55000000	46.80000000	45.63000000

N	51.01000000	45.18000000	45.82000000
C	52.16000000	46.02000000	45.73000000
H	51.23000000	44.20000000	45.91000000
C	52.86000000	45.41000000	44.61000000
O	53.96000000	44.92000000	44.86000000
N	51.99000000	44.68000000	43.98000000
H	51.00000000	44.86000000	44.01000000
C	52.38000000	43.63000000	43.09000000
C	51.24000000	43.61000000	42.13000000
O	50.29000000	44.24000000	42.51000000
C	50.33000000	43.47000000	40.00000000
H	49.66000000	42.67000000	40.31000000
H	49.79000000	44.41000000	40.12000000
H	50.54000000	43.33000000	38.94000000
O	51.42000000	43.33000000	40.88000000
H	53.27000000	43.86000000	42.51000000
H	51.88000000	47.05000000	45.48000000
C	52.99000000	46.07000000	47.01000000
H	52.26000000	46.42000000	47.75000000
H	53.33000000	45.05000000	47.22000000
C	52.39000000	42.27000000	43.79000000
H	53.41000000	42.16000000	44.16000000
H	51.76000000	42.14000000	44.67000000
C	54.18000000	46.97000000	46.94000000
C	55.37000000	46.39000000	47.35000000
C	54.06000000	48.34000000	46.70000000
C	56.45000000	47.26000000	47.53000000
H	55.48000000	45.35000000	47.59000000
C	55.18000000	49.19000000	46.92000000
H	53.10000000	48.78000000	46.47000000
C	56.38000000	48.61000000	47.37000000
H	57.38000000	46.93000000	47.96000000
H	55.10000000	50.25000000	46.76000000
H	57.20000000	49.24000000	47.67000000
C	52.09000000	41.12000000	42.83000000
C	50.82000000	40.61000000	42.80000000
C	53.14000000	40.57000000	42.00000000
C	50.46000000	39.64000000	41.81000000
H	50.12000000	40.93000000	43.56000000
C	52.77000000	39.63000000	41.01000000
H	54.15000000	40.92000000	42.07000000
C	51.43000000	39.13000000	40.89000000
H	49.48000000	39.20000000	41.70000000
H	53.53000000	39.32000000	40.31000000
H	51.23000000	38.38000000	40.13000000
P	38.18000000	38.42000000	36.14000000
W	39.45000000	37.66000000	32.76000000
W	36.89000000	41.67000000	34.87000000
W	36.65000000	39.09000000	39.40000000
W	41.79000000	37.54000000	35.88000000
W	39.00000000	41.61000000	37.76000000
W	34.56000000	39.12000000	36.60000000
W	37.25000000	35.30000000	34.34000000
W	36.01000000	38.35000000	33.12000000
W	35.83000000	36.04000000	37.78000000
W	40.42000000	38.27000000	39.09000000
W	40.41000000	40.90000000	34.57000000
O	39.46000000	37.63000000	36.87000000
O	37.87000000	37.71000000	34.69000000
O	38.46000000	40.03000000	35.92000000
O	36.87000000	38.24000000	37.07000000
O	36.10000000	35.41000000	35.95000000

O	41.53000000	39.47000000	35.34000000
O	34.81000000	38.60000000	34.70000000
O	40.05000000	40.21000000	38.59000000
O	40.03000000	39.49000000	33.23000000
O	38.50000000	38.52000000	39.68000000
O	36.39000000	40.27000000	33.52000000
O	37.57000000	35.31000000	38.06000000
O	35.45000000	40.78000000	35.94000000
O	38.66000000	34.84000000	35.60000000
O	37.57000000	40.78000000	38.81000000
O	40.89000000	37.37000000	34.11000000
O	41.88000000	38.09000000	37.82000000
O	35.97000000	36.43000000	33.28000000
O	40.27000000	41.88000000	36.27000000
O	34.33000000	37.30000000	37.18000000
O	40.37000000	36.37000000	39.01000000
O	38.73000000	41.96000000	34.14000000
O	36.00000000	37.26000000	39.35000000
O	37.66000000	38.18000000	32.08000000
O	38.60000000	35.85000000	33.01000000
O	34.96000000	39.47000000	38.48000000
O	41.35000000	35.80000000	36.50000000
O	37.61000000	42.45000000	36.55000000
O	40.31000000	37.42000000	31.26000000
O	36.08000000	43.12000000	34.28000000
O	36.23000000	39.42000000	41.11000000
O	43.49000000	37.33000000	35.45000000
O	39.52000000	43.00000000	38.70000000
O	32.92000000	39.62000000	36.68000000
O	36.83000000	33.80000000	33.66000000
O	34.91000000	38.54000000	31.80000000
O	34.92000000	34.79000000	38.51000000
O	41.32000000	38.60000000	40.54000000
O	41.62000000	41.88000000	33.83000000
Sn	39.56000000	35.31000000	37.42000000
C	40.04000000	33.32000000	38.07000000
C	41.17000000	32.71000000	37.61000000
C	39.06000000	32.68000000	38.81000000
C	41.50000000	31.41000000	38.05000000
H	41.96000000	33.33000000	37.20000000
C	39.34000000	31.34000000	39.16000000
H	38.13000000	33.14000000	39.10000000
C	40.51000000	30.70000000	38.78000000
H	42.49000000	31.00000000	37.96000000
H	38.65000000	30.84000000	39.82000000
C	40.94000000	29.41000000	39.18000000
C	41.34000000	28.28000000	39.63000000
C	41.80000000	27.00000000	40.09000000
C	40.87000000	26.02000000	40.42000000
C	43.16000000	26.78000000	40.26000000
C	41.26000000	24.76000000	40.91000000
H	39.84000000	26.14000000	40.14000000
C	43.56000000	25.51000000	40.72000000
H	43.94000000	27.50000000	40.06000000
C	42.62000000	24.51000000	41.02000000
H	40.51000000	23.98000000	40.86000000
H	44.62000000	25.31000000	40.83000000
C	43.14000000	23.22000000	41.52000000
O	44.34000000	23.12000000	41.43000000
N	42.27000000	22.27000000	41.94000000
C	42.65000000	21.11000000	42.67000000
H	41.27000000	22.35000000	41.79000000

C	41.50000000	20.18000000	42.33000000
O	40.71000000	19.92000000	43.21000000
N	41.15000000	20.51000000	41.11000000
H	41.85000000	20.98000000	40.57000000
C	40.14000000	19.90000000	40.34000000
C	40.94000000	19.62000000	39.13000000
O	42.06000000	20.08000000	39.08000000
C	41.07000000	18.73000000	37.05000000
H	41.33000000	19.63000000	36.50000000
H	41.94000000	18.18000000	37.41000000
H	40.56000000	18.02000000	36.40000000
O	40.28000000	19.11000000	38.12000000
H	39.81000000	18.99000000	40.84000000
H	43.55000000	20.64000000	42.29000000
C	42.74000000	21.39000000	44.20000000
H	43.46000000	22.18000000	44.41000000
H	41.77000000	21.72000000	44.56000000
C	39.00000000	20.95000000	40.05000000
H	38.54000000	21.06000000	41.03000000
H	39.29000000	21.92000000	39.65000000
C	43.32000000	20.25000000	45.00000000
C	44.74000000	20.10000000	44.87000000
C	42.56000000	19.37000000	45.78000000
C	45.37000000	19.02000000	45.54000000
H	45.38000000	20.86000000	44.45000000
C	43.22000000	18.25000000	46.38000000
H	41.50000000	19.53000000	45.94000000
C	44.60000000	18.09000000	46.24000000
H	46.44000000	18.97000000	45.57000000
H	42.76000000	17.48000000	46.98000000
H	45.11000000	17.23000000	46.65000000
C	37.81000000	20.48000000	39.15000000
C	37.17000000	21.33000000	38.26000000
C	37.37000000	19.16000000	39.34000000
C	36.13000000	20.76000000	37.41000000
H	37.39000000	22.37000000	38.07000000
C	36.36000000	18.63000000	38.57000000
H	37.88000000	18.49000000	40.01000000
C	35.79000000	19.37000000	37.56000000
H	35.62000000	21.37000000	36.68000000
H	36.10000000	17.58000000	38.65000000
H	34.99000000	18.90000000	37.00000000
C	39.16000000	38.80000000	43.25000000
H	40.01000000	38.91000000	42.57000000
H	38.33000000	38.94000000	42.57000000
C	39.29000000	40.02000000	44.18000000
H	38.37000000	40.19000000	44.73000000
H	40.10000000	39.89000000	44.90000000
C	39.72000000	41.18000000	43.38000000
H	39.65000000	42.01000000	44.08000000
H	40.77000000	41.00000000	43.11000000
C	39.03000000	41.62000000	42.12000000
H	39.26000000	40.95000000	41.29000000
H	39.31000000	42.64000000	41.87000000
H	37.97000000	41.58000000	42.34000000
C	37.98000000	37.44000000	45.07000000
H	38.10000000	38.27000000	45.77000000
H	38.04000000	36.53000000	45.66000000
C	36.55000000	37.63000000	44.49000000
H	36.22000000	36.72000000	43.99000000
H	36.50000000	38.45000000	43.77000000
C	35.50000000	37.84000000	45.62000000

H	34.54000000	37.47000000	45.27000000
H	35.74000000	37.17000000	46.45000000
C	35.33000000	39.29000000	46.02000000
H	36.22000000	39.60000000	46.58000000
H	34.49000000	39.43000000	46.70000000
H	35.36000000	39.86000000	45.09000000
C	40.31000000	37.36000000	44.84000000
H	40.38000000	37.89000000	45.79000000
H	40.34000000	36.31000000	45.14000000
C	41.63000000	37.62000000	44.13000000
H	41.76000000	38.68000000	43.90000000
H	41.70000000	37.04000000	43.21000000
C	42.72000000	37.18000000	45.12000000
H	42.38000000	37.18000000	46.15000000
H	42.88000000	36.12000000	44.94000000
C	44.05000000	37.87000000	44.88000000
H	44.12000000	37.98000000	43.80000000
H	44.95000000	37.37000000	45.26000000
H	44.09000000	38.85000000	45.35000000
C	38.92000000	36.58000000	42.90000000
H	39.72000000	36.69000000	42.18000000
H	38.00000000	36.85000000	42.39000000
C	38.80000000	35.09000000	43.22000000
H	39.71000000	34.62000000	43.62000000
H	37.94000000	35.04000000	43.87000000
C	38.52000000	34.32000000	41.93000000
H	39.24000000	34.57000000	41.15000000
H	38.71000000	33.29000000	42.21000000
C	37.11000000	34.44000000	41.52000000
H	36.52000000	34.11000000	42.37000000
H	36.80000000	33.80000000	40.68000000
H	36.94000000	35.44000000	41.14000000
N	39.08000000	37.56000000	44.01000000

2: $\Delta E = -12188.39638$ a.u.

P	30.910000	7.730000	26.020000
W	29.530000	4.870000	24.080000
W	29.750000	6.210000	29.160000
W	32.480000	10.480000	27.910000
W	28.490000	8.530000	23.310000
W	28.800000	9.540000	28.420000
W	33.460000	7.160000	28.690000
W	32.910000	5.710000	23.580000
W	31.940000	4.220000	26.680000
W	34.420000	8.630000	25.590000
W	29.890000	11.240000	25.150000
W	27.380000	6.810000	26.600000
O	30.500000	8.790000	24.810000
O	31.200000	6.230000	25.350000
O	29.670000	7.630000	27.110000
O	32.260000	8.260000	26.810000
O	34.150000	6.910000	24.610000
O	27.460000	7.760000	24.860000
O	33.090000	5.450000	27.760000
O	28.940000	10.620000	26.790000
O	28.210000	5.390000	25.440000
O	31.350000	11.360000	26.550000
O	30.650000	4.840000	28.060000
O	33.490000	9.350000	24.110000
O	31.630000	6.650000	29.370000
O	32.330000	7.330000	22.680000
O	30.670000	10.180000	28.710000

O	28.980000	6.620000	23.190000
O	28.510000	10.410000	24.040000
O	33.100000	4.380000	25.080000
O	27.350000	8.460000	27.730000
O	34.780000	7.700000	27.350000
O	31.050000	11.100000	23.640000
O	28.020000	5.970000	28.290000
O	34.070000	10.190000	26.840000
O	30.520000	3.740000	25.400000
O	31.260000	4.700000	23.180000
O	33.220000	9.040000	29.080000
O	29.940000	8.990000	22.140000
O	29.100000	8.050000	29.680000
O	28.490000	3.640000	23.230000
O	29.420000	5.260000	30.620000
O	32.950000	11.900000	28.840000
O	27.100000	8.600000	22.160000
O	27.830000	10.560000	29.420000
O	34.490000	6.650000	29.970000
O	34.010000	5.080000	22.380000
O	32.310000	2.600000	27.270000
O	36.110000	8.990000	25.270000
O	29.460000	12.980000	24.910000
O	25.750000	6.160000	26.580000
Sn	31.830000	9.340000	22.850000
C	32.670000	10.050000	21.020000
C	33.690000	9.330000	20.550000
C	32.180000	11.160000	20.300000
C	34.310000	9.510000	19.300000
H	33.960000	8.510000	21.200000
C	32.840000	11.440000	19.040000
H	31.370000	11.780000	20.650000
C	33.900000	10.630000	18.540000
H	35.060000	8.820000	18.940000
H	32.540000	12.350000	18.540000
C	34.470000	10.800000	17.230000
C	35.040000	10.940000	16.120000
C	35.820000	10.990000	14.940000
C	36.870000	10.100000	14.710000
C	35.440000	11.880000	13.890000
C	37.530000	10.120000	13.520000
H	37.170000	9.420000	15.490000
C	36.150000	11.870000	12.640000
H	34.630000	12.550000	14.120000
C	37.230000	11.000000	12.450000
H	38.290000	9.350000	13.430000
H	35.990000	12.570000	11.830000
C	37.960000	10.980000	11.240000
O	37.620000	11.660000	10.310000
N	38.950000	10.120000	11.070000
C	39.750000	10.020000	9.860000
H	39.310000	9.690000	11.910000
C	40.230000	8.690000	10.100000
O	41.440000	8.390000	10.080000
N	39.460000	7.960000	10.890000
H	38.480000	8.190000	10.970000
C	39.660000	6.460000	11.010000
C	38.360000	6.090000	11.570000
O	37.710000	7.000000	12.040000
C	37.060000	4.390000	12.470000
H	37.000000	3.310000	12.560000
H	37.280000	4.850000	13.430000

H	36.110000	4.740000	12.060000
O	38.100000	4.800000	11.640000
H	39.900000	5.970000	10.070000
H	39.070000	10.190000	9.030000
C	40.910000	11.030000	9.770000
H	40.540000	12.050000	9.910000
H	41.600000	10.870000	10.600000
C	40.720000	6.180000	12.080000
H	40.600000	5.120000	12.310000
H	41.750000	6.230000	11.710000
C	41.610000	11.020000	8.410000
C	42.970000	11.090000	8.330000
C	40.860000	11.020000	7.250000
C	43.630000	11.060000	7.100000
H	43.520000	11.200000	9.260000
C	41.470000	10.880000	6.030000
H	39.790000	11.090000	7.370000
C	42.870000	11.000000	5.930000
H	44.680000	11.300000	6.990000
H	40.920000	10.920000	5.090000
H	43.330000	11.140000	4.960000
C	40.650000	6.990000	13.350000
C	39.870000	6.520000	14.450000
C	41.350000	8.260000	13.520000
C	39.720000	7.270000	15.630000
H	39.360000	5.570000	14.490000
C	41.230000	9.010000	14.710000
H	41.900000	8.580000	12.650000
C	40.390000	8.520000	15.740000
H	39.140000	6.900000	16.460000
H	41.550000	10.030000	14.860000
H	40.240000	9.140000	16.610000
P	28.380000	18.370000	35.640000
W	30.950000	15.780000	35.010000
W	26.650000	17.450000	32.530000
W	25.730000	20.830000	36.340000
W	31.920000	19.440000	35.560000
W	27.640000	20.850000	33.010000
W	24.780000	17.490000	35.810000
W	29.270000	15.760000	38.130000
W	27.550000	14.820000	35.130000
W	26.500000	18.370000	38.780000
W	29.460000	21.880000	36.290000
W	30.090000	18.380000	32.340000
O	29.570000	19.300000	36.300000
O	28.850000	16.810000	35.900000
O	28.270000	18.690000	34.050000
O	26.940000	18.640000	36.380000
O	27.630000	16.710000	38.720000
O	31.320000	19.100000	33.640000
O	25.880000	15.850000	35.640000
O	28.730000	21.720000	34.380000
O	30.620000	16.790000	33.350000
O	27.510000	21.630000	36.610000
O	27.190000	15.810000	33.480000
O	28.150000	19.170000	39.180000
O	25.300000	17.530000	33.890000
O	30.110000	17.390000	38.650000
O	26.250000	20.960000	34.390000
O	31.910000	17.420000	35.450000
O	31.250000	21.320000	35.620000
O	28.170000	14.550000	36.980000

O	29.180000	20.080000	32.060000
O	25.060000	17.470000	37.730000
O	29.860000	21.430000	38.090000
O	28.420000	17.570000	31.630000
O	25.610000	20.020000	38.130000
O	29.420000	14.560000	34.650000
O	30.710000	15.260000	36.880000
O	24.470000	19.430000	35.880000
O	31.930000	19.510000	37.460000
O	26.580000	19.370000	32.130000
O	32.310000	14.760000	34.550000
O	25.670000	16.840000	31.160000
O	24.590000	22.180000	36.550000
O	33.670000	19.710000	35.270000
O	27.170000	22.180000	32.040000
O	23.200000	16.810000	35.630000
O	29.540000	14.680000	39.510000
O	26.870000	13.220000	34.780000
O	25.820000	18.200000	40.400000
O	29.760000	23.570000	36.350000
O	31.060000	18.320000	30.880000
Sn	30.150000	19.440000	38.630000
C	30.990000	19.690000	40.560000
C	32.180000	19.030000	40.750000
C	30.500000	20.540000	41.500000
C	32.780000	19.120000	41.980000
H	32.560000	18.260000	40.090000
C	31.120000	20.710000	42.750000
H	29.590000	21.050000	41.210000
C	32.310000	19.980000	43.000000
H	33.630000	18.520000	42.260000
H	30.710000	21.310000	43.550000
C	32.720000	19.890000	44.360000
C	33.040000	19.830000	45.550000
C	33.350000	19.690000	46.930000
C	34.460000	18.940000	47.390000
C	32.480000	20.150000	47.910000
C	34.710000	18.630000	48.730000
H	35.180000	18.510000	46.710000
C	32.770000	19.930000	49.290000
H	31.590000	20.680000	47.610000
C	33.860000	19.190000	49.700000
H	35.520000	17.960000	48.950000
H	32.180000	20.470000	50.010000
C	34.190000	19.150000	51.050000
O	33.490000	19.640000	51.890000
N	35.290000	18.510000	51.330000
C	35.880000	18.230000	52.620000
H	35.820000	18.170000	50.540000
C	37.320000	18.600000	52.250000
O	38.290000	18.220000	52.840000
N	37.400000	18.930000	50.950000
H	36.650000	19.510000	50.600000
C	38.680000	18.990000	50.250000
C	38.370000	20.080000	49.350000
O	37.210000	20.360000	49.140000
C	39.420000	21.860000	48.080000
H	38.900000	22.670000	48.590000
H	40.450000	22.200000	47.900000
H	38.980000	21.550000	47.130000
O	39.430000	20.730000	48.910000
H	39.490000	19.200000	50.950000

H	35.590000	18.850000	53.470000
C	35.700000	16.760000	52.880000
H	34.620000	16.590000	52.870000
H	36.030000	16.310000	51.950000
C	38.930000	17.700000	49.450000
H	39.220000	16.920000	50.160000
H	37.980000	17.360000	49.020000
C	36.370000	16.290000	54.140000
C	37.540000	15.540000	54.090000
C	35.820000	16.680000	55.340000
C	38.340000	15.290000	55.230000
H	38.030000	15.310000	53.160000
C	36.560000	16.400000	56.490000
H	34.890000	17.210000	55.430000
C	37.830000	15.790000	56.410000
H	39.190000	14.630000	55.200000
H	36.210000	16.690000	57.470000
H	38.480000	15.560000	57.250000
C	40.070000	17.810000	48.480000
C	41.420000	17.760000	48.950000
C	39.830000	17.840000	47.050000
C	42.440000	17.910000	48.000000
H	41.620000	17.740000	50.010000
C	40.910000	17.870000	46.130000
H	38.820000	17.890000	46.670000
C	42.190000	18.010000	46.600000
H	43.460000	18.090000	48.300000
H	40.670000	17.860000	45.080000
H	43.090000	18.100000	46.010000
C	29.920000	15.390000	27.520000
H	30.490000	14.460000	27.530000
H	29.620000	15.420000	26.470000
C	30.960000	16.510000	27.770000
H	30.510000	17.490000	27.640000
H	31.430000	16.440000	28.750000
C	32.040000	16.420000	26.660000
H	31.600000	16.260000	25.670000
H	32.650000	17.320000	26.620000
C	32.920000	15.240000	27.000000
H	33.800000	15.310000	26.360000
H	32.460000	14.300000	26.690000
H	33.180000	15.120000	28.050000
C	28.240000	16.740000	28.570000
H	28.860000	17.420000	29.150000
H	27.330000	16.670000	29.170000
C	27.890000	17.530000	27.210000
H	26.960000	17.060000	26.870000
H	28.600000	17.440000	26.390000
C	27.520000	19.040000	27.570000
H	28.410000	19.670000	27.560000
H	26.840000	19.380000	26.780000
C	26.700000	19.270000	28.830000
H	27.360000	19.150000	29.690000
H	25.910000	18.530000	28.910000
H	26.250000	20.260000	28.910000
C	29.230000	14.940000	29.780000
H	29.980000	15.620000	30.200000
H	28.440000	15.040000	30.520000
C	29.830000	13.570000	29.930000
H	30.840000	13.570000	29.520000
H	29.210000	12.800000	29.460000
C	29.990000	13.320000	31.460000

H	30.460000	14.170000	31.960000
H	29.070000	12.960000	31.910000
C	31.040000	12.200000	31.690000
H	31.970000	12.770000	31.730000
H	30.980000	11.560000	30.810000
H	30.850000	11.740000	32.660000
C	27.730000	14.420000	28.010000
H	28.090000	13.480000	27.600000
H	27.190000	14.750000	27.120000
C	26.600000	13.970000	28.920000
H	26.950000	13.380000	29.770000
H	26.090000	14.860000	29.280000
C	25.600000	13.180000	28.110000
H	24.970000	13.820000	27.490000
H	26.100000	12.370000	27.570000
C	24.580000	12.670000	29.100000
H	23.850000	13.420000	29.420000
H	25.060000	12.170000	29.940000
H	24.120000	11.860000	28.540000
N	28.800000	15.360000	28.430000

3: $\Delta E = -12188.39651$ a.u.

P	54.210000	53.190000	27.910000
W	56.350000	50.360000	26.930000
W	57.100000	55.470000	27.680000
W	51.970000	56.020000	28.690000
W	54.360000	50.180000	30.220000
W	55.230000	55.410000	30.680000
W	53.800000	56.120000	25.690000
W	53.440000	50.900000	25.030000
W	56.100000	53.140000	24.740000
W	51.140000	53.830000	25.940000
W	52.200000	52.930000	31.010000
W	57.320000	52.660000	29.860000
O	53.370000	52.120000	28.890000
O	54.770000	52.250000	26.660000
O	55.460000	53.880000	28.690000
O	53.180000	54.330000	27.340000
O	52.200000	52.440000	25.080000
O	56.010000	51.360000	30.470000
O	54.930000	54.790000	24.770000
O	53.810000	54.130000	31.350000
O	57.370000	51.480000	28.280000
O	51.590000	54.550000	29.970000
O	57.060000	54.240000	26.130000
O	50.760000	52.470000	27.190000
O	55.530000	56.280000	26.740000
O	52.230000	50.330000	26.440000
O	53.630000	56.190000	29.780000
O	55.390000	49.750000	28.520000
O	53.170000	51.310000	31.340000
O	54.780000	51.980000	23.990000
O	56.730000	54.110000	31.060000
O	52.150000	55.370000	25.090000
O	50.910000	51.910000	30.060000
O	58.070000	54.240000	28.830000
O	50.750000	55.210000	27.330000
O	56.970000	51.550000	25.460000
O	54.980000	49.760000	25.630000
O	52.740000	56.920000	27.110000
O	52.680000	49.640000	29.550000
O	56.580000	56.200000	29.410000
O	57.480000	49.060000	26.710000

O	58.370000	56.660000	27.120000
O	51.010000	57.350000	29.230000
O	54.740000	48.830000	31.250000
O	55.400000	56.520000	32.020000
O	53.920000	57.490000	24.590000
O	52.760000	49.940000	23.680000
O	57.040000	53.420000	23.320000
O	49.650000	54.040000	25.010000
O	51.330000	53.230000	32.520000
O	58.680000	52.120000	30.740000
Sn	51.400000	50.840000	28.310000
C	49.690000	49.610000	28.030000
C	49.020000	49.210000	29.160000
C	49.340000	49.230000	26.750000
C	47.990000	48.340000	29.060000
H	49.430000	49.610000	30.080000
C	48.170000	48.420000	26.560000
H	49.780000	49.680000	25.870000
C	47.590000	47.940000	27.760000
H	47.400000	48.100000	29.930000
H	47.860000	48.170000	25.550000
C	46.500000	47.060000	27.590000
C	45.550000	46.330000	27.320000
C	44.410000	45.470000	27.020000
C	43.610000	45.600000	25.870000
C	44.190000	44.440000	27.940000
C	42.640000	44.590000	25.640000
H	43.870000	46.320000	25.110000
C	43.140000	43.580000	27.750000
H	44.830000	44.290000	28.790000
C	42.410000	43.590000	26.570000
H	41.980000	44.750000	24.800000
H	43.050000	42.770000	28.460000
C	41.390000	42.650000	26.400000
O	41.020000	41.950000	27.350000
N	40.580000	42.640000	25.340000
C	39.370000	41.810000	25.210000
H	40.610000	43.400000	24.670000
C	39.420000	41.540000	23.740000
O	38.400000	41.630000	23.050000
N	40.570000	42.010000	23.340000
H	41.350000	41.700000	23.890000
C	40.910000	42.310000	21.950000
C	42.260000	41.700000	21.940000
O	42.640000	41.190000	22.930000
C	44.170000	41.180000	20.670000
H	44.210000	40.090000	20.710000
H	44.600000	41.560000	19.750000
H	44.810000	41.530000	21.470000
O	42.890000	41.810000	20.730000
H	40.260000	41.740000	21.290000
H	39.370000	40.910000	25.830000
C	38.140000	42.690000	25.560000
H	38.220000	43.350000	26.420000
H	37.850000	43.360000	24.750000
C	40.860000	43.730000	21.490000
H	41.500000	44.410000	22.050000
H	41.250000	43.770000	20.470000
C	37.020000	41.790000	25.810000
C	37.050000	41.030000	27.000000
C	35.930000	41.720000	25.020000
C	35.940000	40.270000	27.430000

H	37.870000	41.100000	27.700000
C	34.850000	40.900000	25.420000
H	36.000000	42.200000	24.060000
C	34.810000	40.180000	26.650000
H	36.020000	39.660000	28.320000
H	34.010000	40.830000	24.740000
H	33.950000	39.610000	26.970000
C	39.440000	44.240000	21.570000
C	39.050000	44.820000	22.780000
C	38.590000	44.260000	20.460000
C	37.730000	45.290000	22.930000
H	39.730000	44.860000	23.620000
C	37.260000	44.660000	20.630000
H	38.880000	43.780000	19.530000
C	36.840000	45.160000	21.860000
H	37.410000	45.590000	23.910000
H	36.620000	44.840000	19.780000
H	35.770000	45.340000	21.910000
P	39.640000	54.700000	31.950000
W	39.890000	51.950000	29.610000
W	38.700000	52.360000	34.670000
W	39.520000	57.510000	34.380000
W	37.580000	54.930000	28.840000
W	36.600000	55.170000	33.980000
W	41.640000	54.790000	35.010000
W	42.680000	54.080000	29.930000
W	41.870000	51.870000	32.580000
W	42.460000	57.010000	32.380000
W	37.420000	57.620000	31.150000
W	36.750000	52.450000	31.690000
O	39.030000	55.640000	30.720000
O	40.620000	53.620000	31.270000
O	38.400000	53.980000	32.750000
O	40.470000	55.640000	32.990000
O	43.070000	55.500000	31.210000
O	36.680000	53.650000	30.130000
O	42.250000	53.250000	33.910000
O	36.480000	56.430000	32.490000
O	38.250000	51.690000	30.660000
O	38.540000	58.040000	32.750000
O	40.220000	51.650000	33.670000
O	41.600000	57.510000	30.780000
O	40.090000	53.600000	35.330000
O	41.710000	55.400000	29.040000
O	37.880000	56.400000	34.780000
O	38.790000	53.330000	28.700000
O	36.740000	56.510000	29.650000
O	43.130000	52.730000	31.340000
O	35.810000	53.720000	32.920000
O	42.870000	56.000000	34.100000
O	38.740000	58.200000	29.900000
O	37.410000	51.680000	33.390000
O	41.220000	58.050000	33.550000
O	41.010000	51.010000	31.000000
O	41.610000	52.640000	29.020000
O	40.610000	56.390000	35.600000
O	38.930000	56.040000	28.090000
O	37.190000	53.630000	35.090000
O	39.820000	50.690000	28.490000
O	38.450000	51.120000	35.870000
O	39.280000	58.880000	35.450000
O	36.590000	54.800000	27.370000

O	35.170000	55.610000	34.920000
O	42.610000	54.430000	36.460000
O	44.030000	54.030000	28.870000
O	42.770000	50.510000	33.200000
O	43.770000	58.160000	32.430000
O	36.300000	58.990000	31.020000
O	35.430000	51.410000	31.340000
Sn	40.370000	57.030000	29.220000
C	41.260000	58.230000	27.670000
C	42.620000	58.560000	27.790000
C	40.420000	58.780000	26.630000
C	43.130000	59.400000	26.890000
H	43.130000	58.170000	28.650000
C	40.970000	59.690000	25.690000
H	39.390000	58.460000	26.660000
C	42.390000	59.900000	25.790000
H	44.170000	59.660000	27.050000
H	40.370000	60.100000	24.890000
C	43.030000	60.860000	24.950000
C	43.700000	61.640000	24.280000
C	44.540000	62.530000	23.610000
C	44.010000	63.240000	22.540000
C	45.930000	62.610000	23.920000
C	44.840000	64.130000	21.860000
H	42.950000	63.280000	22.330000
C	46.800000	63.430000	23.130000
H	46.440000	62.080000	24.710000
C	46.260000	64.150000	22.060000
H	44.440000	64.910000	21.230000
H	47.850000	63.530000	23.330000
C	47.050000	65.150000	21.440000
O	48.190000	65.340000	21.740000
N	46.460000	65.730000	20.400000
C	46.950000	66.770000	19.520000
H	45.560000	65.380000	20.110000
C	45.660000	67.470000	19.210000
O	45.420000	67.940000	18.110000
N	44.800000	67.280000	20.180000
H	45.250000	66.950000	21.030000
C	43.700000	68.120000	20.440000
C	43.530000	68.100000	21.940000
O	44.120000	67.140000	22.400000
C	43.440000	69.200000	23.860000
H	42.880000	68.300000	24.140000
H	44.480000	68.950000	24.090000
H	43.120000	70.110000	24.350000
O	43.240000	69.300000	22.500000
H	43.950000	69.130000	20.120000
H	47.520000	67.460000	20.140000
C	47.600000	66.110000	18.270000
H	48.440000	65.580000	18.710000
H	46.870000	65.420000	17.830000
C	42.400000	67.670000	19.770000
H	41.640000	68.410000	20.010000
H	42.540000	67.620000	18.680000
C	48.140000	67.160000	17.280000
C	49.030000	68.220000	17.600000
C	47.610000	67.110000	15.970000
C	49.400000	69.100000	16.620000
H	49.490000	68.380000	18.570000
C	48.070000	67.970000	14.980000
H	46.950000	66.340000	15.610000

C	48.960000	69.040000	15.280000
H	49.970000	69.980000	16.900000
H	47.590000	67.950000	14.020000
H	49.150000	69.750000	14.480000
C	41.860000	66.330000	20.230000
C	42.000000	65.140000	19.530000
C	41.260000	66.250000	21.500000
C	41.500000	63.970000	20.070000
H	42.580000	65.090000	18.620000
C	40.810000	65.050000	22.120000
H	41.160000	67.150000	22.080000
C	40.910000	63.920000	21.330000
H	41.510000	63.040000	19.520000
H	40.310000	65.070000	23.080000
H	40.560000	62.960000	21.680000
C	48.970000	55.630000	32.370000
H	49.290000	55.350000	33.370000
H	49.780000	55.170000	31.800000
C	49.260000	57.130000	32.440000
H	49.170000	57.410000	31.390000
H	48.440000	57.640000	32.940000
C	50.640000	57.430000	32.970000
H	51.360000	56.740000	32.540000
H	50.920000	58.440000	32.680000
C	50.780000	57.250000	34.480000
H	51.759318	57.553545	34.786097
H	50.630564	56.220864	34.731887
C	47.050000	55.830000	30.810000
H	46.890000	56.890000	30.970000
H	46.090000	55.360000	30.620000
C	47.870000	55.720000	29.490000
H	47.580000	54.800000	28.970000
H	48.930000	55.890000	29.650000
C	47.390000	56.830000	28.590000
H	47.640000	57.800000	29.000000
H	47.950000	56.810000	27.660000
C	45.890000	56.810000	28.330000
H	45.270000	57.140000	29.170000
H	45.460000	55.840000	28.060000
H	45.730000	57.330000	27.390000
C	46.710000	55.340000	33.080000
H	46.780000	56.400000	33.320000
H	45.660000	55.210000	32.820000
C	46.960000	54.370000	34.330000
H	47.860000	53.760000	34.240000
H	46.090000	53.740000	34.500000
C	47.250000	55.280000	35.510000
H	47.340000	54.690000	36.430000
H	48.220000	55.750000	35.320000
C	46.180000	56.380000	35.800000
H	45.230000	55.910000	36.070000
H	46.050000	57.060000	34.960000
H	46.610000	56.880000	36.670000
C	47.840000	53.680000	31.590000
H	48.400000	53.170000	32.370000
H	48.500000	53.740000	30.730000
C	46.560000	52.870000	31.140000
H	45.730000	52.930000	31.840000
H	46.290000	53.210000	30.140000
C	46.960000	51.360000	30.960000
H	47.580000	51.300000	30.060000
H	47.480000	50.950000	31.830000

C	45.700000	50.600000	30.760000
H	45.150000	50.650000	31.700000
H	45.950000	49.550000	30.620000
H	45.100000	51.100000	30.000000
N	47.610000	55.090000	31.980000
H	50.048211	57.849471	34.980019

4: $\Delta E = -11502.29761$ a.u.

P	41.590000	26.880000	32.440000
W	44.670000	28.080000	34.040000
W	43.600000	25.220000	29.780000
W	38.530000	25.550000	30.980000
W	41.890000	30.570000	33.100000
W	41.060000	27.560000	28.850000
W	41.090000	23.270000	31.950000
W	42.390000	26.240000	36.030000
W	44.380000	24.590000	33.500000
W	39.220000	24.940000	34.430000
W	38.910000	29.340000	31.560000
W	44.040000	28.770000	30.320000
O	40.790000	28.280000	32.870000
O	42.790000	26.520000	33.560000
O	42.290000	27.070000	30.950000
O	40.530000	25.660000	32.450000
O	40.810000	25.110000	35.570000
O	43.010000	30.030000	31.510000
O	42.830000	23.470000	32.830000
O	39.980000	28.790000	29.890000
O	44.830000	28.420000	32.060000
O	38.260000	27.500000	31.260000
O	44.480000	24.790000	31.500000
O	38.860000	26.780000	34.750000
O	42.280000	23.970000	30.540000
O	41.120000	27.660000	36.010000
O	39.680000	26.300000	29.490000
O	43.440000	29.570000	33.910000
O	40.220000	30.780000	32.080000
O	43.610000	24.790000	35.300000
O	42.660000	28.700000	28.940000
O	40.010000	23.350000	33.520000
O	38.470000	29.390000	33.400000
O	44.480000	26.960000	29.550000
O	38.060000	25.000000	32.830000
O	45.420000	26.210000	33.920000
O	43.980000	27.400000	35.740000
O	39.420000	23.780000	31.030000
O	40.880000	30.370000	34.680000
O	42.360000	26.120000	28.530000
O	46.160000	28.770000	34.720000
O	44.550000	24.260000	28.650000
O	37.070000	25.210000	30.080000
O	42.360000	32.220000	33.450000
O	40.500000	27.790000	27.170000
O	41.140000	21.490000	31.530000
O	42.500000	25.840000	37.730000
O	45.660000	23.420000	33.740000
O	38.170000	24.080000	35.550000
O	37.560000	30.210000	30.970000
O	45.130000	29.900000	29.580000
Sn	39.640000	28.700000	34.990000
C	38.380000	29.330000	36.630000
C	38.670000	29.070000	37.920000

C	37.070000	29.970000	36.390000
C	37.850000	29.500000	38.980000
H	39.630000	28.590000	38.020000
C	36.150000	30.160000	37.360000
H	36.900000	30.280000	35.370000
C	36.500000	29.910000	38.710000
H	38.120000	29.370000	40.010000
H	35.170000	30.540000	37.130000
C	35.490000	30.160000	39.710000
C	34.740000	30.440000	40.530000
C	33.760000	30.710000	41.470000
C	33.070000	29.610000	42.020000
C	33.380000	32.020000	41.830000
C	32.120000	29.840000	43.010000
H	33.220000	28.620000	41.630000
C	32.380000	32.250000	42.740000
H	33.860000	32.920000	41.480000
C	31.820000	31.180000	43.410000
H	31.670000	29.020000	43.540000
H	32.120000	33.290000	42.870000
C	30.720000	31.420000	44.290000
O	30.500000	32.600000	44.560000
N	29.950000	30.450000	44.760000
C	28.790000	30.720000	45.560000
H	30.100000	29.490000	44.480000
C	28.660000	29.350000	46.200000
O	27.590000	28.740000	46.180000
N	29.790000	28.680000	46.260000
H	30.650000	29.200000	46.220000
C	30.000000	27.350000	46.790000
C	31.520000	27.400000	46.940000
O	32.130000	28.280000	46.310000
C	33.430000	26.540000	47.870000
H	33.770000	25.600000	48.300000
H	33.920000	26.640000	46.900000
H	33.660000	27.310000	48.600000
O	32.080000	26.510000	47.650000
H	29.480000	27.110000	47.720000
H	28.990000	31.400000	46.390000
C	27.580000	31.110000	44.730000
H	26.780000	31.280000	45.450000
H	27.710000	32.090000	44.280000
C	29.660000	26.370000	45.680000
H	30.020000	25.430000	46.090000
H	28.570000	26.400000	45.620000
C	26.960000	30.170000	43.650000
C	27.560000	30.070000	42.430000
C	25.870000	29.290000	43.790000
C	27.310000	29.240000	41.350000
H	28.350000	30.780000	42.250000
C	25.620000	28.350000	42.760000
H	25.200000	29.280000	44.640000
C	26.320000	28.300000	41.540000
H	27.910000	29.280000	40.450000
H	24.860000	27.610000	42.930000
H	25.920000	27.730000	40.710000
C	30.380000	26.480000	44.330000
C	29.720000	27.220000	43.360000
C	31.520000	25.730000	44.070000
C	30.340000	27.180000	42.090000
H	28.770000	27.660000	43.600000
C	32.090000	25.660000	42.800000

H	31.980000	25.150000	44.860000
C	31.490000	26.430000	41.790000
H	29.840000	27.680000	41.270000
H	33.010000	25.110000	42.670000
H	31.930000	26.540000	40.810000
P	41.110000	16.110000	51.050000
W	37.900000	17.120000	52.460000
W	40.710000	12.730000	52.470000
W	44.240000	15.080000	49.360000
W	41.090000	19.130000	53.180000
W	43.720000	14.510000	53.170000
W	41.280000	13.260000	48.700000
W	38.420000	17.630000	48.960000
W	37.960000	14.360000	50.290000
W	41.700000	16.600000	47.400000
W	44.150000	18.120000	51.760000
W	40.680000	15.560000	54.710000
O	41.710000	17.640000	51.270000
O	39.500000	16.240000	50.770000
O	41.410000	15.180000	52.370000
O	41.790000	15.480000	49.650000
O	39.780000	16.850000	47.740000
O	41.100000	17.430000	54.290000
O	39.380000	13.510000	49.200000
O	44.180000	16.390000	52.820000
O	39.000000	16.140000	53.890000
O	44.510000	16.760000	50.340000
O	39.010000	13.340000	51.640000
O	42.060000	18.260000	48.230000
O	41.270000	12.610000	50.570000
O	39.660000	18.990000	49.360000
O	44.240000	14.410000	51.280000
O	39.240000	18.490000	52.880000
O	43.050000	19.010000	53.150000
O	37.440000	15.840000	49.160000
O	42.590000	14.980000	54.750000
O	41.270000	14.600000	47.280000
O	43.560000	19.420000	50.570000
O	40.300000	13.680000	54.160000
O	43.590000	15.970000	47.750000
O	37.200000	15.410000	51.720000
O	37.470000	17.910000	50.760000
O	43.260000	13.440000	48.670000
O	41.100000	20.310000	51.660000
O	42.620000	12.900000	52.960000
O	36.590000	17.680000	53.450000
O	40.440000	11.020000	52.900000
O	45.870000	14.600000	48.840000
O	40.730000	20.330000	54.420000
O	45.100000	13.850000	54.030000
O	41.120000	11.740000	47.810000
O	37.330000	18.450000	47.830000
O	36.600000	13.250000	50.020000
O	41.770000	16.970000	45.680000
O	45.750000	18.760000	52.050000
O	40.300000	15.540000	56.460000
Sn	41.610000	19.560000	49.810000
C	41.580000	21.410000	48.740000
C	41.390000	22.590000	49.410000
C	41.720000	21.420000	47.360000
C	41.440000	23.800000	48.790000
H	41.410000	22.510000	50.490000

C	41.660000	22.670000	46.680000
H	41.980000	20.520000	46.820000
C	41.500000	23.820000	47.410000
H	41.260000	24.740000	49.300000
H	41.930000	22.580000	45.640000
C	41.340000	25.110000	46.770000
C	41.140000	26.290000	46.300000
C	40.890000	27.680000	45.900000
C	39.570000	28.210000	45.750000
C	41.940000	28.400000	45.400000
C	39.330000	29.410000	45.040000
H	38.730000	27.750000	46.250000
C	41.690000	29.590000	44.660000
H	42.970000	28.130000	45.590000
C	40.380000	30.090000	44.450000
H	38.320000	29.770000	44.960000
H	42.470000	30.170000	44.190000
C	40.210000	31.260000	43.710000
O	41.200000	31.920000	43.310000
N	38.970000	31.620000	43.430000
C	38.700000	32.910000	42.930000
H	38.160000	31.030000	43.560000
C	37.460000	33.120000	43.710000
O	36.560000	33.850000	43.220000
N	37.310000	32.200000	44.670000
H	38.170000	31.880000	45.090000
C	36.270000	32.360000	45.630000
C	37.030000	32.140000	46.840000
O	37.930000	31.260000	46.770000
C	37.940000	33.220000	48.640000
H	38.910000	33.490000	48.240000
H	37.660000	34.020000	49.320000
H	38.000000	32.310000	49.240000
O	36.960000	33.170000	47.640000
H	35.770000	33.320000	45.630000
H	39.500000	33.620000	43.160000
C	38.490000	33.010000	41.430000
H	38.820000	32.060000	41.020000
H	37.430000	32.950000	41.150000
C	35.270000	31.250000	45.590000
H	34.630000	31.320000	44.710000
H	35.830000	30.310000	45.620000
C	39.170000	34.250000	40.770000
C	38.390000	35.180000	40.130000
C	40.570000	34.350000	40.710000
C	39.000000	36.260000	39.500000
H	37.320000	35.150000	40.240000
C	41.190000	35.380000	40.050000
H	41.150000	33.580000	41.210000
C	40.370000	36.360000	39.410000
H	38.430000	37.120000	39.160000
H	42.270000	35.450000	40.110000
H	40.830000	37.160000	38.840000
C	34.350000	31.370000	46.820000
C	33.290000	32.220000	46.820000
C	34.460000	30.360000	47.800000
C	32.290000	32.120000	47.790000
H	33.210000	32.990000	46.070000
C	33.470000	30.290000	48.760000
H	35.280000	29.660000	47.740000
C	32.400000	31.170000	48.810000
H	31.410000	32.740000	47.660000

H	33.550000	29.490000	49.490000
H	31.700000	31.140000	49.630000

5: $\Delta E = -11502.28965$ a.u.

P	51.02000000	8.17000000	64.27000000
W	53.70000000	10.36000000	63.04000000
W	51.16000000	9.89000000	67.58000000
W	48.14000000	6.18000000	65.46000000
W	54.06000000	6.54000000	62.89000000
W	51.43000000	6.30000000	67.41000000
W	47.91000000	9.77000000	65.46000000
W	50.68000000	10.19000000	61.18000000
W	50.78000000	11.93000000	64.34000000
W	47.78000000	8.04000000	62.38000000
W	51.31000000	4.47000000	64.04000000
W	54.08000000	8.34000000	66.28000000
O	51.60000000	6.90000000	63.38000000
O	51.40000000	9.63000000	63.51000000
O	51.62000000	8.18000000	65.78000000
O	49.36000000	8.05000000	64.37000000
O	48.86000000	9.45000000	61.53000000
O	54.42000000	7.21000000	64.78000000
O	48.96000000	11.28000000	64.79000000
O	51.65000000	5.10000000	65.90000000
O	54.11000000	9.72000000	64.90000000
O	49.44000000	5.00000000	64.58000000
O	51.17000000	11.26000000	66.19000000
O	49.01000000	6.90000000	61.44000000
O	49.27000000	9.86000000	66.91000000
O	51.04000000	8.40000000	60.68000000
O	49.51000000	6.25000000	66.88000000
O	54.13000000	8.50000000	62.61000000
O	53.20000000	4.88000000	63.51000000
O	50.35000000	11.78000000	62.46000000
O	53.33000000	6.91000000	67.43000000
O	47.06000000	9.37000000	63.74000000
O	51.02000000	4.65000000	62.16000000
O	53.08000000	9.53000000	67.47000000
O	47.22000000	6.68000000	63.76000000
O	52.67000000	11.88000000	63.75000000
O	52.62000000	10.65000000	61.48000000
O	47.39000000	7.93000000	66.05000000
O	53.08000000	6.27000000	61.28000000
O	51.19000000	8.05000000	68.32000000
O	55.13000000	11.18000000	62.42000000
O	46.99000000	5.08000000	66.16000000
O	55.65000000	5.94000000	62.41000000
O	51.49000000	5.25000000	68.78000000
O	46.54000000	10.70000000	66.18000000
O	50.36000000	10.96000000	59.64000000
O	50.44000000	13.66000000	64.65000000
O	46.39000000	8.11000000	61.36000000
O	51.37000000	2.78000000	64.43000000
O	55.74000000	8.48000000	66.87000000
Sn	51.02000000	6.39000000	61.08000000
C	50.92000000	5.56000000	59.12000000
C	51.54000000	4.35000000	58.96000000
C	50.30000000	6.24000000	58.09000000
C	51.50000000	3.75000000	57.74000000
H	51.94000000	3.81000000	59.81000000
C	50.24000000	5.59000000	56.79000000
H	49.84000000	7.20000000	58.25000000

C	50.82000000	4.30000000	56.69000000
H	52.14000000	2.89000000	57.60000000
H	49.85000000	6.18000000	55.98000000
C	50.86000000	3.68000000	55.41000000
C	50.74000000	3.17000000	54.31000000
C	50.71000000	2.59000000	53.01000000
C	51.37000000	3.20000000	51.95000000
C	49.96000000	1.45000000	52.74000000
C	51.34000000	2.73000000	50.65000000
H	52.00000000	4.06000000	52.11000000
C	49.97000000	1.01000000	51.44000000
H	49.37000000	0.88000000	53.44000000
C	50.55000000	1.69000000	50.34000000
H	52.02000000	3.19000000	49.94000000
H	49.30000000	0.17000000	51.28000000
C	50.32000000	1.24000000	49.02000000
O	49.79000000	0.18000000	48.77000000
N	50.87000000	1.97000000	48.04000000
C	50.58000000	1.74000000	46.63000000
H	51.48000000	2.71000000	48.36000000
C	51.91000000	2.30000000	46.07000000
O	52.02000000	2.87000000	44.97000000
N	52.76000000	2.45000000	47.01000000
H	52.64000000	1.96000000	47.88000000
C	53.94000000	3.26000000	46.84000000
C	54.81000000	2.65000000	47.88000000
O	54.21000000	2.30000000	48.88000000
C	56.44000000	1.06000000	48.24000000
H	55.77000000	0.38000000	48.77000000
H	57.18000000	0.49000000	47.67000000
H	57.01000000	1.56000000	49.02000000
O	55.77000000	1.92000000	47.34000000
H	54.48000000	3.15000000	45.91000000
H	50.49000000	0.66000000	46.46000000
C	49.29000000	2.46000000	46.19000000
H	48.44000000	2.11000000	46.77000000
H	49.47000000	3.52000000	46.39000000
C	53.79000000	4.71000000	47.27000000
H	53.04000000	5.22000000	46.65000000
H	53.38000000	4.80000000	48.27000000
C	49.00000000	2.28000000	44.74000000
C	48.78000000	3.41000000	43.96000000
C	48.99000000	1.05000000	44.11000000
C	48.70000000	3.39000000	42.56000000
H	48.76000000	4.37000000	44.46000000
C	48.82000000	0.92000000	42.74000000
H	49.15000000	0.14000000	44.68000000
C	48.79000000	2.13000000	41.99000000
H	48.59000000	4.25000000	41.92000000
H	48.99000000	-0.01000000	42.22000000
H	48.86000000	2.08000000	40.91000000
C	55.04000000	5.59000000	47.31000000
C	55.55000000	6.12000000	48.54000000
C	55.65000000	5.78000000	46.10000000
C	56.65000000	6.97000000	48.51000000
H	55.18000000	5.78000000	49.50000000
C	56.75000000	6.66000000	46.04000000
H	55.25000000	5.39000000	45.18000000
C	57.29000000	7.12000000	47.26000000
H	57.00000000	7.41000000	49.43000000
H	57.16000000	6.94000000	45.08000000
H	58.19000000	7.73000000	47.28000000

P	57.27000000	5.17000000	31.51000000
W	57.89000000	1.52000000	31.64000000
W	59.77000000	5.45000000	28.71000000
W	56.51000000	8.73000000	31.17000000
W	58.33000000	3.69000000	34.76000000
W	60.19000000	7.49000000	31.51000000
W	56.12000000	6.71000000	28.32000000
W	54.51000000	2.67000000	31.31000000
W	56.79000000	2.97000000	28.61000000
W	53.86000000	6.45000000	31.05000000
W	57.71000000	7.22000000	34.52000000
W	60.74000000	3.97000000	31.79000000
O	57.08000000	5.17000000	33.16000000
O	56.81000000	3.67000000	31.04000000
O	58.85000000	5.41000000	31.07000000
O	56.32000000	6.30000000	30.79000000
O	53.79000000	4.48000000	30.92000000
O	59.95000000	3.82000000	33.54000000
O	56.14000000	4.80000000	28.09000000
O	59.27000000	7.49000000	33.25000000
O	59.63000000	2.40000000	31.37000000
O	56.96000000	8.32000000	33.04000000
O	58.55000000	3.89000000	28.39000000
O	54.08000000	6.09000000	32.91000000
O	58.10000000	6.46000000	28.26000000
O	54.41000000	3.33000000	33.08000000
O	58.53000000	8.54000000	31.14000000
O	58.08000000	2.16000000	33.53000000
O	58.52000000	5.57000000	35.30000000
O	55.11000000	2.38000000	29.42000000
O	61.27000000	5.89000000	32.06000000
O	54.37000000	6.81000000	29.14000000
O	56.06000000	6.61000000	35.17000000
O	61.04000000	4.51000000	29.92000000
O	54.63000000	8.26000000	31.27000000
O	57.62000000	1.55000000	29.70000000
O	55.92000000	1.33000000	31.72000000
O	56.33000000	8.47000000	29.22000000
O	56.54000000	3.85000000	35.35000000
O	60.55000000	6.97000000	29.65000000
O	58.33000000	-0.19000000	31.72000000
O	56.33000000	10.49000000	31.32000000
O	59.07000000	2.90000000	36.13000000
O	61.40000000	8.79000000	31.69000000
O	55.88000000	7.29000000	26.68000000
O	53.06000000	1.67000000	31.34000000
O	56.71000000	2.20000000	27.04000000
O	52.14000000	6.81000000	30.90000000
O	58.02000000	8.47000000	35.73000000
O	62.26000000	3.19000000	32.08000000
Sn	55.05000000	4.92000000	34.37000000
C	53.40000000	4.99000000	35.72000000
C	52.17000000	4.75000000	35.27000000
C	53.59000000	5.19000000	37.14000000
C	51.11000000	4.75000000	36.13000000
H	52.11000000	4.46000000	34.23000000
C	52.55000000	5.07000000	38.04000000
H	54.60000000	5.29000000	37.49000000
C	51.21000000	5.01000000	37.53000000
H	50.15000000	4.53000000	35.69000000
H	52.62000000	5.05000000	39.12000000
C	50.08000000	4.98000000	38.34000000

C	49.01000000	5.01000000	38.94000000
C	47.68000000	5.09000000	39.57000000
C	47.40000000	6.05000000	40.50000000
C	46.58000000	4.31000000	39.12000000
C	46.18000000	5.95000000	41.21000000
H	48.18000000	6.76000000	40.75000000
C	45.33000000	4.23000000	39.72000000
H	46.72000000	3.67000000	38.26000000
C	45.18000000	5.01000000	40.88000000
H	46.02000000	6.63000000	42.04000000
H	44.57000000	3.57000000	39.33000000
C	43.98000000	4.98000000	41.54000000
O	43.14000000	4.23000000	41.01000000
N	43.69000000	5.82000000	42.52000000
C	42.38000000	6.11000000	43.07000000
H	44.41000000	6.36000000	42.97000000
C	42.61000000	7.50000000	43.55000000
O	42.33000000	7.85000000	44.71000000
N	43.55000000	8.07000000	42.82000000
H	43.68000000	7.78000000	41.86000000
C	43.94000000	9.49000000	43.02000000
C	44.43000000	9.82000000	41.68000000
O	44.27000000	8.98000000	40.81000000
C	44.77000000	11.30000000	40.15000000
H	43.78000000	11.11000000	39.74000000
H	45.08000000	12.33000000	39.95000000
H	45.53000000	10.67000000	39.69000000
O	44.65000000	11.08000000	41.52000000
H	43.11000000	10.15000000	43.30000000
H	41.66000000	6.16000000	42.25000000
C	41.97000000	5.24000000	44.20000000
H	41.92000000	4.21000000	43.83000000
H	42.64000000	5.25000000	45.06000000
C	45.01000000	9.70000000	44.06000000
H	45.22000000	10.77000000	44.06000000
H	44.67000000	9.40000000	45.06000000
C	40.57000000	5.62000000	44.68000000
C	40.30000000	5.90000000	46.05000000
C	39.42000000	5.56000000	43.85000000
C	39.04000000	6.31000000	46.55000000
H	41.19000000	5.90000000	46.65000000
C	38.15000000	5.93000000	44.32000000
H	39.50000000	5.32000000	42.80000000
C	38.03000000	6.43000000	45.61000000
H	38.87000000	6.72000000	47.53000000
H	37.33000000	5.88000000	43.62000000
H	37.06000000	6.66000000	46.02000000
C	46.29000000	8.83000000	43.98000000
C	47.42000000	9.20000000	43.19000000
C	46.26000000	7.58000000	44.62000000
C	48.54000000	8.32000000	43.14000000
H	47.52000000	10.17000000	42.74000000
C	47.33000000	6.69000000	44.43000000
H	45.43000000	7.24000000	45.21000000
C	48.49000000	7.06000000	43.75000000
H	49.49000000	8.63000000	42.73000000
H	47.31000000	5.70000000	44.88000000
H	49.31000000	6.36000000	43.81000000
O	50.98577991	10.87447399	68.97959220
O	60.57255489	5.45429227	27.18872185

6: $\Delta E = -11502,28459$ a.u.

P	38.28000000	6.70000000	82.95000000
W	41.12000000	5.01000000	84.64000000
W	35.95000000	5.35000000	85.48000000
W	35.48000000	8.58000000	81.41000000
W	40.32000000	4.41000000	80.86000000
W	35.29000000	4.82000000	81.99000000
W	36.18000000	9.13000000	84.82000000
W	41.36000000	8.53000000	84.01000000
W	39.14000000	7.32000000	86.51000000
W	38.44000000	10.33000000	82.32000000
W	37.65000000	6.12000000	79.34000000
W	37.93000000	3.08000000	83.66000000
O	39.00000000	6.45000000	81.51000000
O	39.49000000	6.84000000	84.09000000
O	37.29000000	5.48000000	83.35000000
O	37.46000000	8.12000000	82.89000000
O	40.03000000	9.89000000	83.40000000
O	39.04000000	3.31000000	82.01000000
O	37.65000000	8.53000000	85.97000000
O	36.32000000	5.05000000	80.38000000
O	39.63000000	3.72000000	84.51000000
O	36.52000000	7.61000000	80.06000000
O	37.57000000	6.05000000	86.40000000
O	39.46000000	9.56000000	80.95000000
O	35.56000000	7.31000000	85.43000000
O	41.55000000	8.23000000	82.16000000
O	34.93000000	6.74000000	81.77000000
O	41.17000000	4.55000000	82.69000000
O	38.97000000	4.65000000	79.44000000
O	40.57000000	8.44000000	85.89000000
O	36.31000000	3.19000000	82.55000000
O	37.29000000	10.45000000	83.98000000
O	39.19000000	7.21000000	78.95000000
O	36.77000000	3.64000000	85.12000000
O	36.65000000	10.16000000	81.42000000
O	40.53000000	5.88000000	86.31000000
O	42.11000000	6.74000000	84.54000000
O	34.99000000	9.20000000	83.25000000
O	41.20000000	5.93000000	80.25000000
O	34.85000000	4.93000000	83.92000000
O	42.38000000	3.94000000	85.27000000
O	35.03000000	4.85000000	86.89000000
O	34.12000000	9.27000000	80.51000000
O	41.29000000	3.15000000	80.18000000
O	33.86000000	4.13000000	81.33000000
O	35.35000000	10.11000000	86.01000000
O	42.79000000	9.54000000	84.31000000
O	39.21000000	7.44000000	88.26000000
O	38.62000000	12.04000000	82.04000000
O	36.93000000	6.01000000	77.74000000
O	37.97000000	1.38000000	83.97000000
Sn	40.56000000	7.88000000	80.36000000
C	41.97000000	8.89000000	79.09000000
C	42.24000000	8.46000000	77.80000000
C	42.67000000	9.96000000	79.63000000
C	43.13000000	9.22000000	77.02000000
H	41.70000000	7.67000000	77.29000000
C	43.72000000	10.54000000	78.92000000
H	42.64000000	10.24000000	80.67000000
C	44.00000000	10.11000000	77.67000000
H	43.26000000	9.00000000	75.97000000
H	44.24000000	11.32000000	79.45000000

C	45.03000000	10.78000000	77.05000000
C	46.07000000	11.29000000	76.55000000
C	47.20000000	11.97000000	75.87000000
C	46.98000000	13.22000000	75.26000000
C	48.52000000	11.46000000	75.74000000
C	47.93000000	13.85000000	74.43000000
H	46.02000000	13.69000000	75.42000000
C	49.58000000	12.16000000	75.13000000
H	48.74000000	10.48000000	76.15000000
C	49.27000000	13.37000000	74.43000000
H	47.62000000	14.64000000	73.76000000
H	50.56000000	11.71000000	75.11000000
C	50.31000000	14.10000000	73.77000000
O	51.41000000	13.62000000	73.82000000
N	49.98000000	15.29000000	73.18000000
C	51.00000000	16.08000000	72.60000000
H	49.01000000	15.55000000	73.09000000
C	50.33000000	17.37000000	72.60000000
O	50.22000000	18.06000000	71.60000000
N	49.31000000	17.43000000	73.45000000
H	49.25000000	16.71000000	74.15000000
C	48.41000000	18.53000000	73.55000000
C	47.93000000	18.35000000	74.91000000
O	48.43000000	17.39000000	75.48000000
C	46.26000000	18.48000000	76.50000000
H	45.30000000	18.95000000	76.68000000
H	46.13000000	17.40000000	76.52000000
H	46.90000000	18.73000000	77.34000000
O	46.75000000	18.88000000	75.25000000
H	48.96000000	19.45000000	73.37000000
H	51.86000000	16.25000000	73.26000000
C	51.35000000	15.75000000	71.11000000
H	51.73000000	14.74000000	70.99000000
H	50.44000000	15.80000000	70.51000000
C	47.30000000	18.47000000	72.54000000
H	46.66000000	19.35000000	72.58000000
H	47.82000000	18.59000000	71.59000000
C	52.41000000	16.62000000	70.43000000
C	53.37000000	17.47000000	70.98000000
C	52.32000000	16.64000000	68.99000000
C	54.32000000	18.10000000	70.15000000
H	53.51000000	17.41000000	72.05000000
C	53.28000000	17.37000000	68.21000000
H	51.47000000	16.20000000	68.49000000
C	54.30000000	18.07000000	68.76000000
H	55.23000000	18.47000000	70.60000000
H	53.25000000	17.29000000	67.13000000
H	55.04000000	18.52000000	68.12000000
C	46.52000000	17.14000000	72.42000000
C	47.04000000	16.13000000	71.58000000
C	45.28000000	16.95000000	73.01000000
C	46.30000000	15.05000000	71.27000000
H	47.92000000	16.31000000	70.98000000
C	44.54000000	15.83000000	72.60000000
H	44.95000000	17.68000000	73.73000000
C	45.04000000	14.92000000	71.70000000
H	46.76000000	14.38000000	70.55000000
H	43.54000000	15.63000000	72.94000000
H	44.43000000	14.10000000	71.35000000
P	40.37000000	25.03000000	75.11000000
W	43.63000000	25.94000000	76.45000000
W	38.76000000	27.77000000	76.97000000

W	37.10000000	24.23000000	73.53000000
W	42.28000000	22.39000000	76.85000000
W	37.47000000	24.47000000	77.39000000
W	38.43000000	27.55000000	73.16000000
W	43.29000000	25.70000000	72.95000000
W	41.82000000	28.43000000	74.70000000
W	39.91000000	24.79000000	71.45000000
W	39.05000000	21.56000000	75.51000000
W	40.65000000	25.32000000	78.74000000
O	40.73000000	23.41000000	75.11000000
O	41.75000000	25.93000000	74.90000000
O	39.63000000	25.45000000	76.52000000
O	39.31000000	25.28000000	73.85000000
O	41.68000000	25.58000000	71.79000000
O	41.44000000	23.60000000	78.23000000
O	40.23000000	28.31000000	73.50000000
O	38.13000000	22.75000000	76.83000000
O	42.32000000	25.94000000	77.96000000
O	37.87000000	22.58000000	74.24000000
O	40.45000000	28.44000000	76.20000000
O	40.62000000	23.12000000	72.03000000
O	38.17000000	27.81000000	75.11000000
O	43.03000000	23.80000000	73.01000000
O	36.84000000	24.47000000	75.47000000
O	43.39000000	24.03000000	76.53000000
O	40.64000000	21.27000000	76.68000000
O	42.98000000	27.65000000	73.35000000
O	38.83000000	24.59000000	78.82000000
O	38.93000000	26.58000000	71.54000000
O	40.19000000	20.99000000	74.09000000
O	39.64000000	27.05000000	78.55000000
O	38.03000000	24.22000000	71.84000000
O	43.20000000	27.79000000	75.93000000
O	44.36000000	25.74000000	74.62000000
O	37.05000000	26.18000000	73.19000000
O	42.82000000	21.67000000	75.18000000
O	37.37000000	26.48000000	77.54000000
O	45.06000000	26.24000000	77.40000000
O	38.06000000	29.24000000	77.63000000
O	35.53000000	23.67000000	73.05000000
O	43.31000000	21.45000000	77.88000000
O	36.01000000	24.05000000	78.30000000
O	37.58000000	28.92000000	72.43000000
O	44.55000000	25.83000000	71.71000000
O	42.26000000	30.13000000	74.61000000
O	39.91000000	24.57000000	69.74000000
O	38.12000000	20.15000000	75.59000000
O	40.98000000	25.28000000	80.44000000
Sn	41.87000000	22.14000000	73.39000000
C	42.72000000	20.61000000	72.12000000
C	42.42000000	19.29000000	72.22000000
C	43.63000000	21.06000000	71.18000000
C	42.90000000	18.36000000	71.34000000
H	41.65000000	19.13000000	72.97000000
C	44.09000000	20.14000000	70.18000000
H	43.75000000	22.13000000	71.07000000
C	43.69000000	18.83000000	70.32000000
H	42.56000000	17.34000000	71.39000000
H	44.54000000	20.36000000	69.22000000
C	44.17000000	17.92000000	69.38000000
C	44.54000000	17.17000000	68.50000000
C	44.77000000	16.29000000	67.41000000

C	43.86000000	16.23000000	66.41000000
C	45.93000000	15.53000000	67.38000000
C	44.17000000	15.32000000	65.38000000
H	42.95000000	16.81000000	66.45000000
C	46.27000000	14.78000000	66.26000000
H	46.57000000	15.55000000	68.25000000
C	45.34000000	14.61000000	65.29000000
H	43.57000000	15.31000000	64.48000000
H	47.18000000	14.21000000	66.31000000
C	45.53000000	13.68000000	64.22000000
O	46.54000000	13.03000000	64.12000000
N	44.51000000	13.52000000	63.36000000
C	44.42000000	12.57000000	62.30000000
H	43.72000000	14.15000000	63.44000000
C	43.51000000	13.34000000	61.46000000
O	42.55000000	12.80000000	60.92000000
N	43.63000000	14.71000000	61.67000000
H	44.57000000	14.90000000	61.98000000
C	43.12000000	15.55000000	60.67000000
C	44.45000000	15.90000000	60.14000000
O	45.43000000	15.73000000	60.87000000
C	45.65000000	16.59000000	58.37000000
H	46.35000000	15.76000000	58.49000000
H	45.65000000	16.88000000	57.32000000
H	46.02000000	17.47000000	58.90000000
O	44.37000000	16.17000000	58.86000000
H	42.49000000	15.02000000	59.95000000
H	45.36000000	12.26000000	61.84000000
C	43.70000000	11.28000000	62.72000000
H	44.11000000	10.94000000	63.68000000
H	42.68000000	11.53000000	63.04000000
C	42.38000000	16.80000000	61.07000000
H	43.08000000	17.33000000	61.72000000
H	42.36000000	17.48000000	60.22000000
C	43.65000000	10.13000000	61.77000000
C	44.74000000	9.32000000	61.57000000
C	42.44000000	9.84000000	61.13000000
C	44.70000000	8.28000000	60.66000000
H	45.74000000	9.51000000	61.95000000
C	42.35000000	8.77000000	60.25000000
H	41.56000000	10.44000000	61.32000000
C	43.53000000	7.99000000	59.99000000
H	45.65000000	7.77000000	60.58000000
H	41.42000000	8.57000000	59.74000000
H	43.48000000	7.22000000	59.24000000
C	40.93000000	16.61000000	61.56000000
C	39.92000000	16.84000000	60.59000000
C	40.54000000	16.47000000	62.91000000
C	38.58000000	16.82000000	60.99000000
H	40.17000000	17.10000000	59.58000000
C	39.17000000	16.41000000	63.31000000
H	41.32000000	16.44000000	63.66000000
C	38.20000000	16.42000000	62.30000000
H	37.82000000	17.07000000	60.27000000
H	38.94000000	16.26000000	64.36000000
H	37.19000000	16.33000000	62.69000000

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