The Influence of Chemical Modification on Linker Rotational Dynamics in Metal–Organic Frameworks

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Supporting Information

Table of Contents

SI 1. Sample Preparation and Synthesis

Reagents:
Zirconium tetrachloride (Stem, sublimed grade), terephthalic acid acid (Fisher Scientific, 98%), 2-aminoterephthalic acid (Acros Organics, >99%), 2-bromoterephthalic acid (Acros Organics, 95%), 2,5-dimethylterephthalic acid (TCI, >97%), 2,5-dihydroxylterephthalic acid, biphenyl-4,4'-dicarboxylic acid (Acros Organics, 98%), dimethylformamide (DMF, Fisher Scientific, >99.5%) and concentrated HCl (Fisher Scientific, ACS grade) were used as received

MOF synthesis:
All UiO series MOFs in this paper were synthesized according to a published procedure.[1]

MOF activation:
All synthesized UiO MOFs were first washed with DMF (3 × 20 mL) and then with acetone three times (3 × 20 mL) over 3 days before activation. Approximately 50 mg of samples in a sample cell were evacuated under a dynamic vacuum (10^{-2} torr) at 150 °C for 12 hours using a MasterPrep™ Degasser.

Instrumental analysis
Powder X-ray diffraction:
The powder X-ray data of all activated MOFs were collected with a Bruker D8 advance diffractometer equipped with a 60 mm sealed Göbel mirror and a LynxEye linear position sensitive detector. The Cu-Kα X-ray source was operated at 40 kV and 40 mA. Samples were evenly dispersed on a low-background quartz plate before measurements.
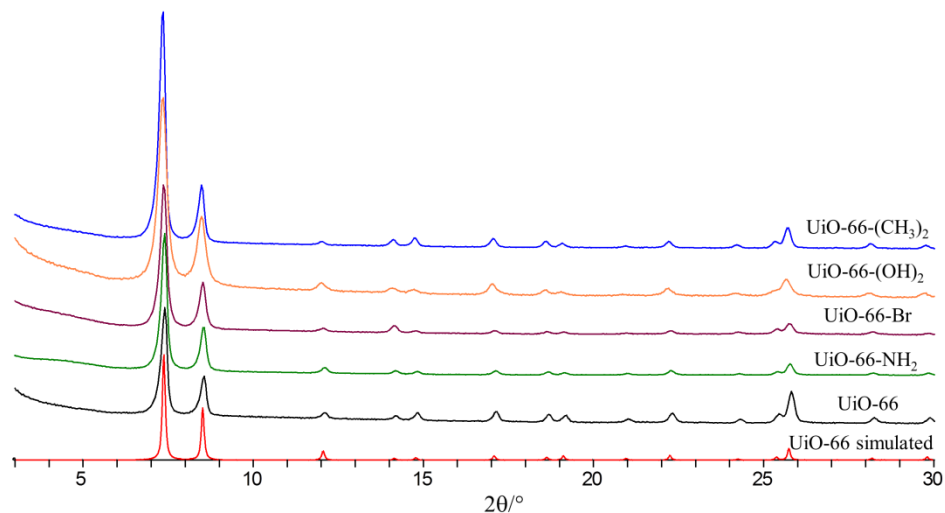
Figure S1. Simulated and experimental powder X-ray diffraction patterns for UiO-66 series MOFs investigated in the study.
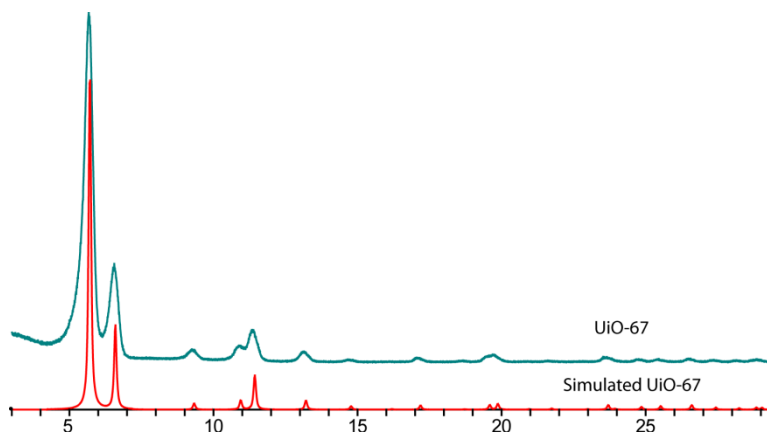
Figure S2. Simulated and experimental powder X-ray diffraction patterns for UiO-67.

Gas sorption measurements:

Gas sorption experiments were carried out at 77 K using a NOVA 4200 by Quantachrome Instruments (Boynton Beach, Florida, USA). Ultra-high purity N_2 (99,999%) was 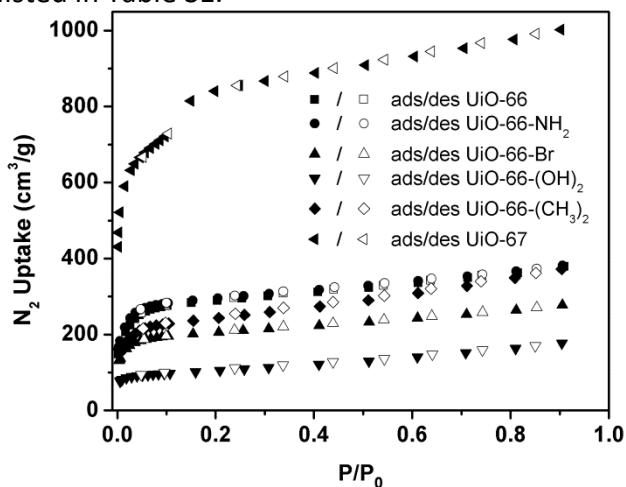purchased from Cryogenic Gasses and used as received. The obtained isotherm was analyzed using NOVAwin software. The relative pressure range for calculating the surface area satisfies the criteria for applying BET theory.[2] A summary of the obtained BET surface area and literature values for the UiO series of MOFs are listed in Table S1.

Figure S3. N_2 isotherm plot for UiO series of MOFs used in this study.

	BET surface area (m^2/g)	Calculated geometric surface area with no missing linker defects (m^2/g)
UiO-66	1160	800[1]
UiO-66-NH$_2$	1160	700[1]
UiO-66-Br	790	800[3]
UiO-66-(OH)$_2$	390	400[1]
UiO-66-(CH$_3$)$_2$	945	N.A.
UiO-67	3120	2700[1]

Table S1. Brunauer-Emmett-Teller (BET) surface area of UiO series of MOFs used in this study.
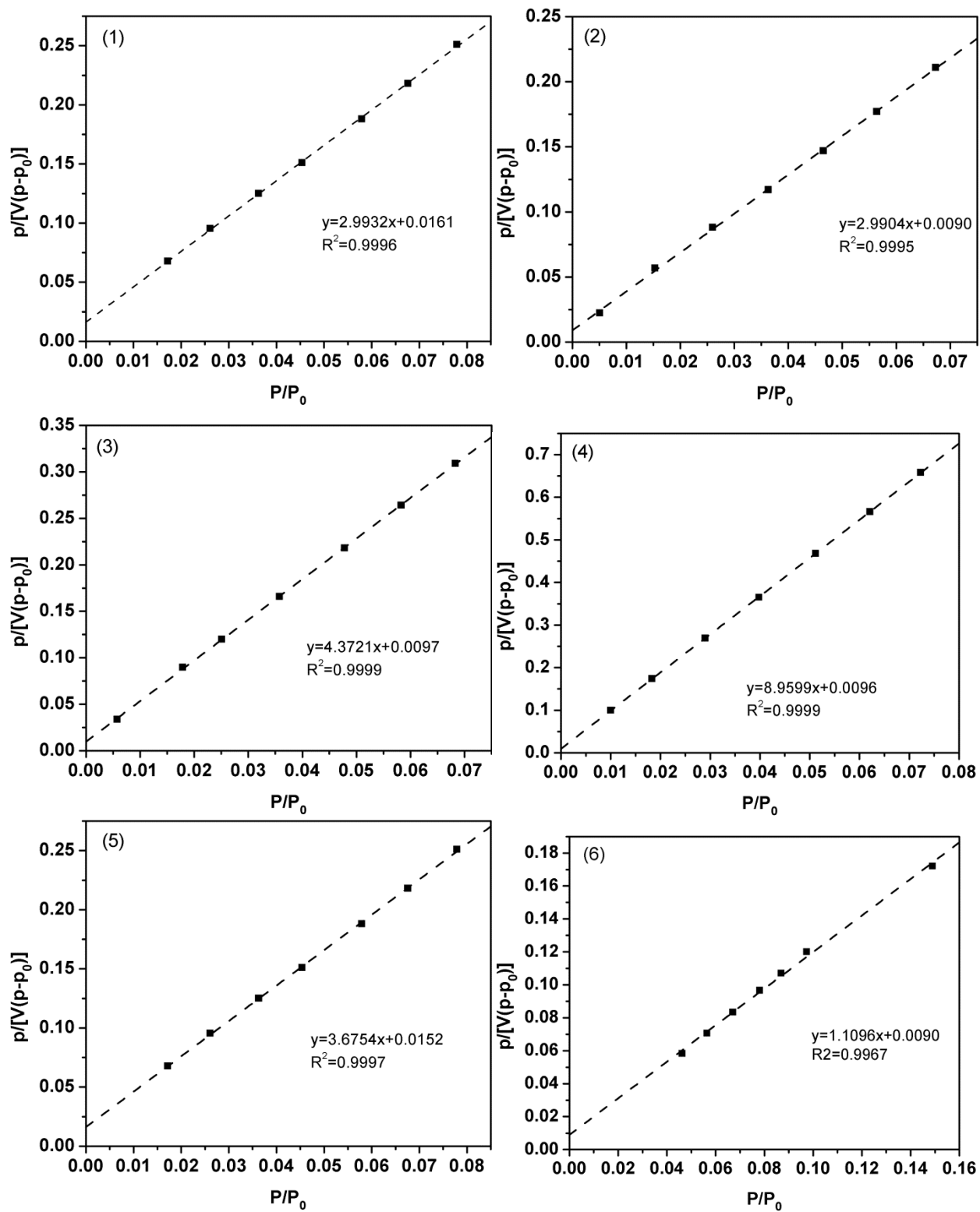
Figure S4. BET fit for the N_2 adsorption isotherm of (1) UiO-66, (2) UiO-66-NH_2, (3) UiO-66-Br, (4) UiO-66-$(OH)_2$, (5) UiO-66-$(CH_3)_2$ and (6) UiO-67.

SI 2. Model complex simulation

Single cluster model complex simulation

All DFT calculations were performed using Gaussian 09 with B3LYP functions and the LANL2DZ basis set. All model complexes were initially constructed by modifying a UiO-66 crystal structure[4] leaving only one Zr_6 cluster and a single phenyl rotor with a general formula $Zr_6O_4(OH)_4(COOH)_{11}(COOC_6H_5)$. Functional groups were then added to the phenyl rotor if required. The model structure was geometry optimized and used as the starting conformation for energy surface scan calculation. Potential energy surfaces were constructed by varying one C_{Ar}-C_{Ar}-C-O dihedral angle 10° a step while allowing the remaining coordinates to relax.
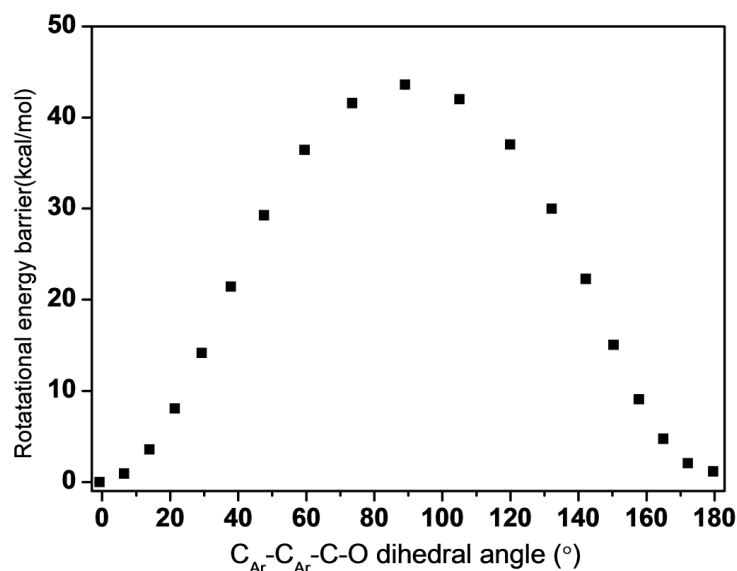

Figure S5. Results of rotational energy barrier calculation for $Zr_6O_4(OH)_4(COOH)_{11}(COOC_6H_5)$.
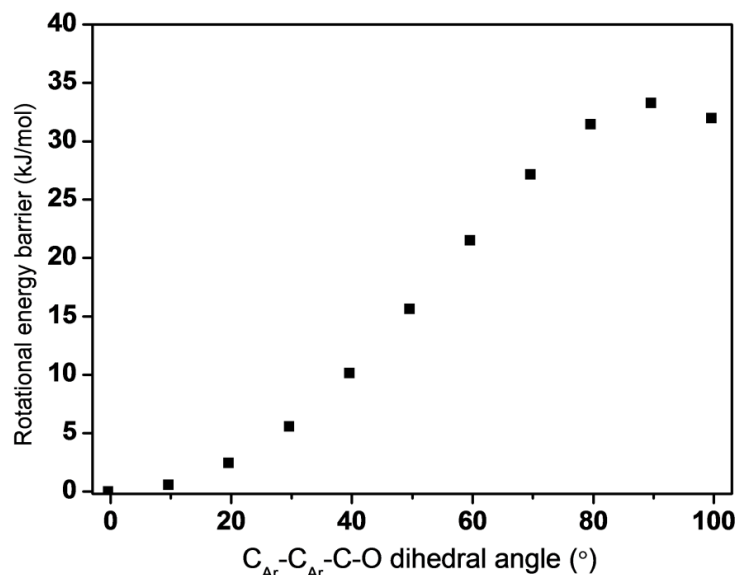

Figure S6. Results of rotational energy barrier calculation for $Zr_6O_4(OH)_4(COOH)_{11}(COOC_6H_4$-$o$-$CH_3)$.

Two cluster model simulations

All model complexes were initially constructed by modifying a UiO-66 crystal structure leaving only two Zr_6 cluster bridging a terephthalate linker.[4] Functional groups were then added to the linker if required to give a general formula $Zr_6O_4(OH)_4(COOH)_{11}$(terephthalate) $Zr_6O_4(OH)_4(COOH)_{11}$. All coordinates for $Zr_6O_4(OH)_4(COOH)_{11}CO_2$ were fixed to mimic the geometric constraint imposed on the linker. Model complexes were geometry optimized by a semi empirical method (PM6) and used as the starting conformation for energy surface scans. Potential energy surfaces were constructed by varying one C_{Ar}-C_{Ar}-C-O dihedral angle by 5° steps spanning 180° while allowing the remaining linker coordinates to relax. To give an accurate energy barrier, DFT single point energy calculations were performed on highest and lowest energy conformation obtained from the energy surface scan using the B3LYP functional and the LANL2DZ basis set. The obtained energy barriers for all the model complexes are listed below in the table.

	Energy barrier from the single cluster model (kJ/mol)	Energy barrier from the dicluster model (kJ/mol)
UiO-66-$(CH_3)_2$	33.5	23.4
UiO-66	43.5	65.8
UiO-66-$(OH)_2$	75.3	91.6

Table S2. Energy barriers for all model complex simulations.

SI 3. Solid-state NMR

Most NMR measurements were performed on a Bruker Avance III spectrometer at 400 MHz [1]H Larmor frequency with a 4 mm Bruker double-resonance MAS probe, using 90° pulse lengths of 3.5 μs for ^{1}H and 4.0 μs for ^{13}C under 5 kHz MAS. The UiO-66-$(CH_3)_2$ and UiO-66-Br data were collected on a Bruker Avance III spectrometer at 500 MHz [1]H Larmor frequency with a 3.2 mm Bruker triple-resonance MAS probe, using 90° pulse lengths of 2.8 μs for ^{1}H and 4.0 μs for ^{13}C under 5.5 kHz and 6.5 kHz MAS, respectively to avoid overlap with spinning sidebands. Temperature calibrations were done with $PbNO_3$. The DIPSHIFT pulse sequence[5,6] used in this study to measure C-H dipolar couplings is depicted below in Figure S6. After preparation of the proton magnetization, it is transferred to carbon-13 nuclei through ramped-CP, which is then followed by an optional 'rotor directed exchange of orientations' (RODEO) delay[7] to correct for inhomogeneous cross polarization effects when using short CP times.[6] Next the CH dipolar coupling is expressed under frequency switched Lee-Goldberg homonuclear decoupling[8] on the proton channel during the t_1 period, ranging from 0 to t_{rot}, where t_{rot} is the rotor period. Heteronuclear decoupling is then applied while a spin-echo is implemented on the ^{13}C channel before acquisition of ^{13}C magnetization. The resultant 2D spectrum correlates the chemical shift with dipolar-dephased intensity mapping out the DIPSHIFT curves. All DIPSHIFT curves in this report were selected from the projections of the aromatic CH group. [13]C spectral assignments were given in a previous report.[9]
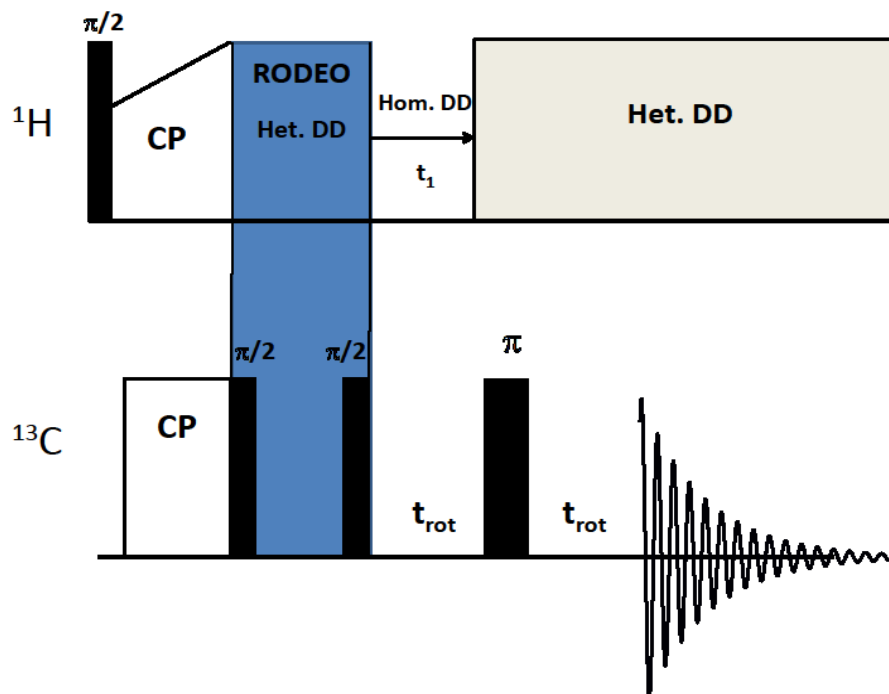
Figure S7. Radio-frequency pulse sequence for the DIPSHIFT experiment featuring the RODEO delay. See the text for details.

For all samples, cross polarization times were kept under 1 ms to avoid the loss of magnetization due to $T_{1\rho}$ relaxation. Due to spectral overlap in certain cases, shorter CP times were used to filter out magnetization from non-CH bonded resonances. For UiO-66-$(CH_3)_2$ and UiO-66-Br it was kept to 500 µs, which was the shortest reasonable time for signal intensity. For UiO-66-$(OH)_2$, the aromatic CH and quaternary aromatic carbon are also overlapped, but the rigid nature of this sample required a very short CP filter (< 100 µs). A side-effect of such short CP times is the induction of inhomogeneous cross polarization effects distorting the DIPSHIFT curves, requiring the RODEO delay. For all other samples, the usual DIPSHIFT sequence without the RODEO period was employed. ^1H and ^{13}C assignments were previously reported for the samples.[9] We note that while the short CP times mostly select for CH bonded carbons, this process may not be completely selective and some small contributions from other carbons could artificially reduce the extracted dipolar coupling value. This is one reason why comparing the intermediate T2 regime is so important as it gives a secondary dynamic metric regardless of the absolute dipolar coupling value. The aromatic CH peak was monitored over a regular increment of t_1 to give a 2D correlation between the chemical shift and a modulation in the peak intensity from the heteronuclear ^{13}C-^1H dipole-dipole interaction, resulting in the depicted DIPSHIFT curves. The curves can be described by $F(t) = S(t) * e^{(-t/T2)}$ with

$$S(t) = \cos\left\{\frac{D}{\omega_r}\left[\frac{1}{4}\sin^2\alpha(\sin 2\gamma(t) - \sin 2\gamma_0) + \frac{1}{\sqrt{2}}\sin 2\alpha(\sin 2\gamma(t) - \sin 2\gamma_0)\right]\right\}$$

.

for the signal under MAS for the dipolar tensor.[10,11]

T$_2$ is similar to the usual relaxation constant which becomes effective once the motional reorientation of the CH bond is on the order of the inverse coupling constant. S(t) describes the MAS-dependent dipolar fid of an individual CH pair with D the coupling constant, ω_r the MAS frequency, α the angle between the CH bond vector and the rotor axis, and $\gamma(t)$ is the time-dependent angle describing the rotor rotation. γ and α are the Euler angles relating the dipolar tensor the fixed rotor frame. The DIPSHIFT curves can then be fit by F(t) after suitable powder averaging of γ and α between $0 \leq 2\pi$ and $0 \leq \pi$, respectively, along with accounting for the Lee-Goldberg scaling factor in the coupling constant.
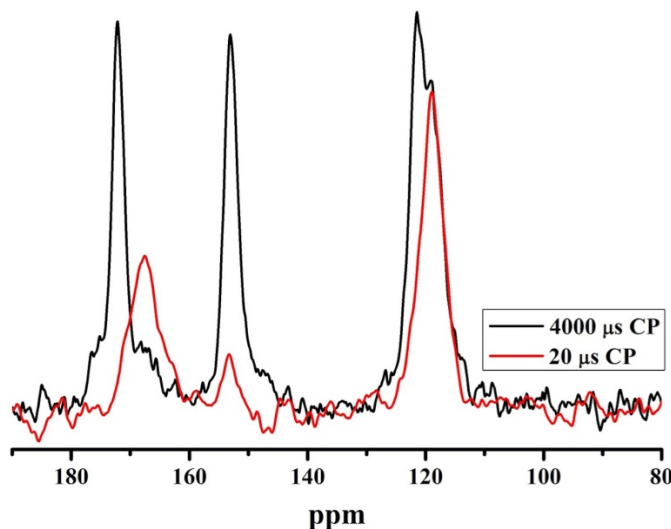
Figure S8. ^{13}C CPMAS spectra of UiO-66-(OH)$_2$ employing long and short CP times to extract the CH resonance only for UiO-66-(OH)$_2$.

SI 4. Anderson-Weiss Approximation for Diffusive Anisotropic Motions

As shown in detail elsewhere,[12,13] adopting the Anderson-Weiss approximation for anisotropic diffusive motions can be used as an approximate model for the effect molecular motion on dipolar coupled spins under MAS. The dipolar modulated FID accounting for such motions was found to be

$$S(t) = exp\left\{-M_2^{rigid}\left[S^2\left(\frac{2}{3}f(\omega_r, 0, t) + \frac{1}{3}f(2\omega_r, 0, t)\right)\right.\right.$$
$$\left.\left. + (1-S^2)\left(\frac{2}{3}f(\omega_r, 1/\tau_c, t) + \frac{1}{3}f(2\omega_r, 1/\tau_c, t)\right)\right]\right\}$$

with

$$f(\omega_r, 1/\tau_c, t) = \frac{t\tau_c}{1+(\omega_r\tau_c)^2} - \frac{\tau_c^2[1-(\omega_r\tau_c)^2]}{[1-(\omega_r\tau_c)^2]^2} \times [1 - exp(-^t/_{\tau_c})\cos(\omega_r t)] -$$
$$\frac{2\omega_r\tau_c^3}{[1-(\omega_r\tau_c)^2]^2} exp(-^t/_{\tau_c})\sin(\omega_r t),$$

where τ_c is the correlation time of motion, ω_r the MAS frequency, S^2 is the order parameter defined as $S^2 = M_2^{fast}/M_2^{rigid}$, and M_2 is the second moment of the dipolar field. To approximate τ_c for UiO-66, the parameters were determined with the following procedure. First, $M_2^{rigid} = 8.1 \times 10^8$ was determined by fitting t_c (~6ms) and M_2^{rigid} to the 23 °C data (slow limit) while keeping S^2 constant (S^2 does not contribute to curve in the slow limit regime). Thereafter, $S^2 = 0.66$ was determined from the high temperature data (155 °C) by using the M_2^{rigid} value and setting τ_c=1.0$\times 10^{-8}s$ in the fast limit regime. The determined S = 0.66 is comparable that of a 180° ring flip for a phenylene ring (S2=0.62).[10] The fact that the value is somewhat larger is reasonable given that other small amplitude motions are present as shown by Kolokolov and co-workers.[14] These parameters were then used to approximate τ_c for UiO-66 over the temperature range shown in the figure below. The determined values are comparable to the values obtained via extensive simulations shown by deAzevedo et. al.[12]
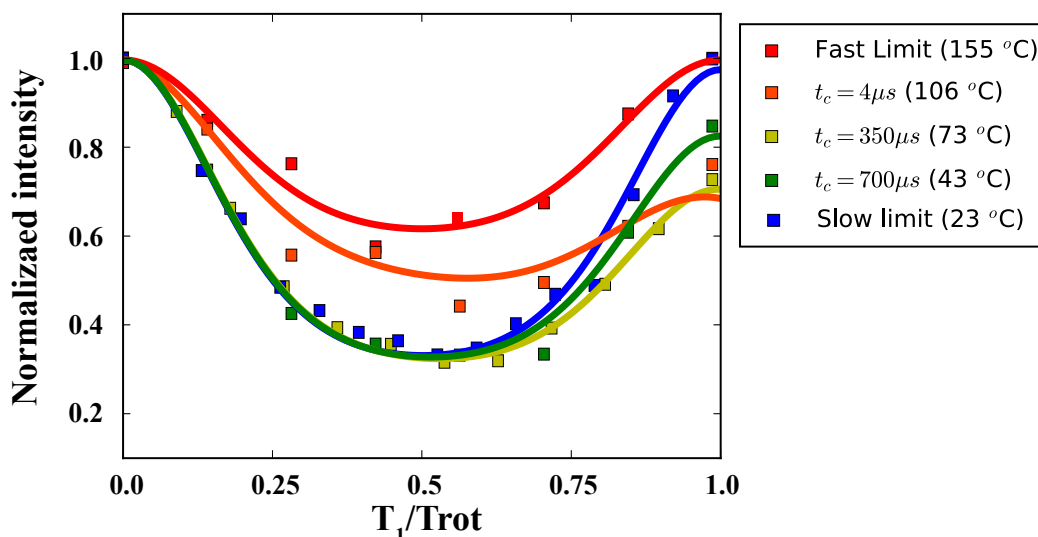
Figure S9. Model fits of experimentally measured data for UiO-66 at the indicated sample temperature using the Anderson-Weiss formulation for anisotropic diffusive motions. This data is reproduced with the fits for the dipolar coupling constant in Figure S10.

As a general comment, M_2^{rigid} and S^2 can be determined *a priori* when the precise geometry and amplitude of motion is known.[10] However, the curve shape is also highly dependent on the distribution of parameters[12] from a mixture in motional modes, such as librations and rotations, making it difficult to model, as was already previously demonstrated for UiO-66.[14] Any attempt to model the precise nature and distribution of motions or extend to the functionalized versions Ui0-66 is interesting but outside the scope of this paper. As such, we took an empirical approach for these parameters here, which is sufficient for capturing the general trend.

SI 5. Temperature Dependent DIPSHIFT Measurements

DIPSHIFT curves as a function of temperature were measured for different samples. For UiO-66 and UiO-66-(OH)$_2$. The curves display typical asymmetric behavior marking 'intermediate' dynamic timescales coinciding with the coupling constants upon heating. For UiO-66 the intermediate regime is immediately achieved upon heating to 43 °C and is pushed into the fast limit by 155 °C. The intermediate regime for UiO-66-(OH)$_2$, however, does not begin until 100 °C and up to 211 °C is still not quite achieved the fast limit as marked by some residual T$_2$ relaxation at this temperature. For UiO-66-(CH$_3$) and UiO-66-Br, only upon cooling is the intermediate regime obtained suggesting fast limit dynamics at room temperature.
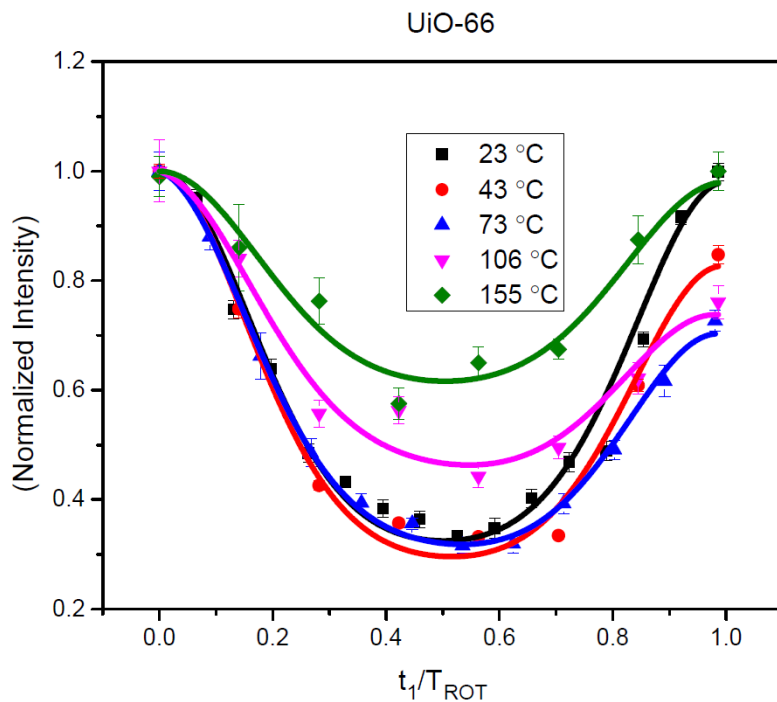
Figure S10. DIPSHIFT curves for UiO-66 at various temperatures spanning the intermediate motional regime. Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.
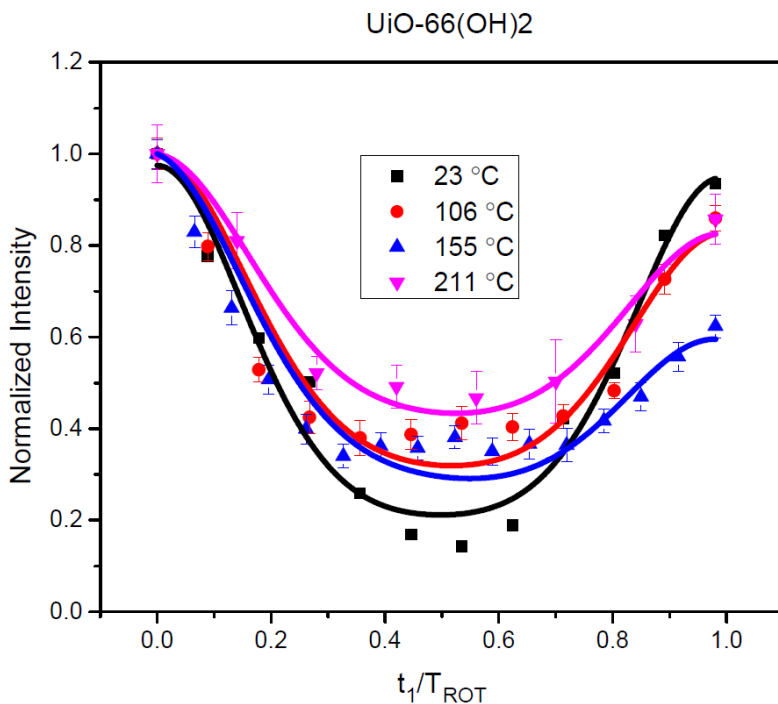
Figure S11. DIPSHIFT curves for UiO-66-(OH)$_2$ at various temperatures. The intermediate regime occurs at much higher temperatures than UiO-66. Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.
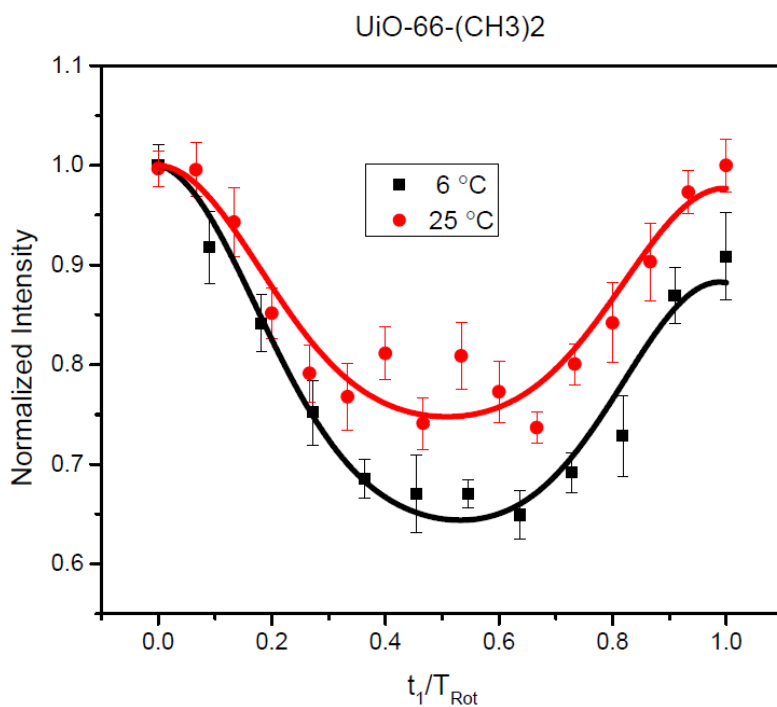
Figure S12. DIPSHIFT curves for UiO-66-(CH$_3$)$_2$ at 6 °C and 25 °C. Upon cooling the curve displays typical intermediate dynamic behavior. Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.
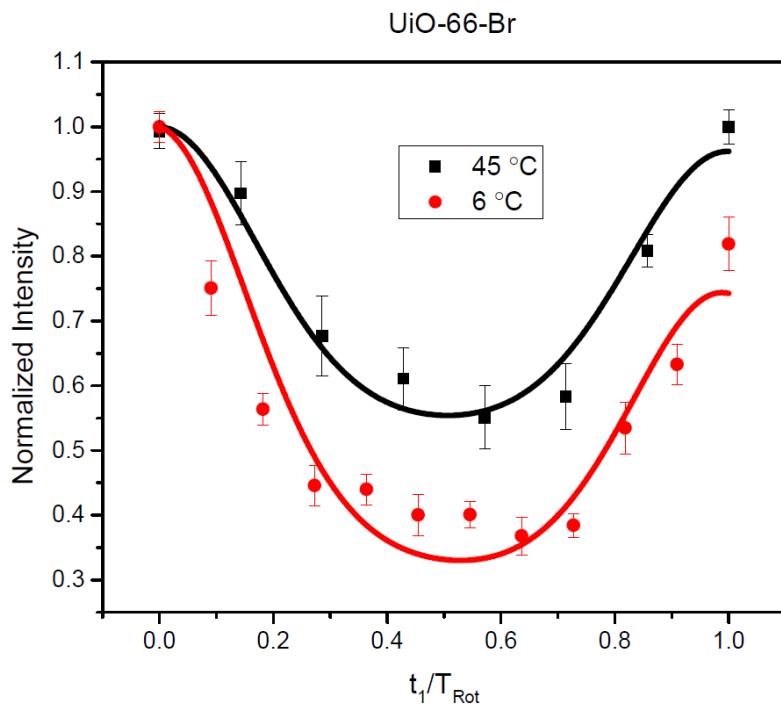
Figure S13. DIPSHIFT curves for UiO-66-Br at various temperatures. Upon cooling the curve displays typical intermediate dynamic behavior. Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.
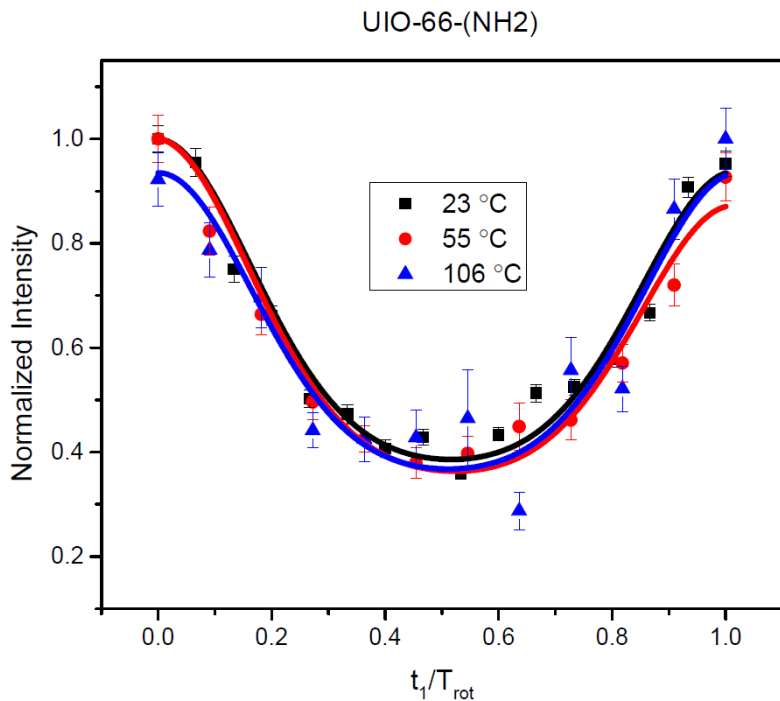
Figure S14. DIPSHIFT curves for UiO-66-NH_2 at various temperatures. The DIPSHIFT curves are fairly constant over a wide temperature range. Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.
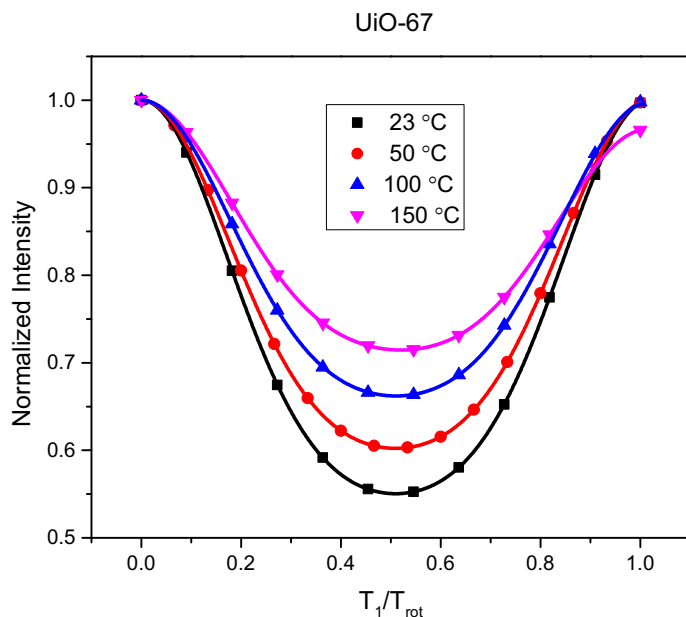
UiO-67

Figure S15. DIPSHIFT curves of UiO-67 at elevated temperatures. It is particularly notable that the curves depths decrease dramatically from a corresponding 12 kHz D_{ch} at ambient conditions to 9 kHz at 150 °C without exhibiting intermediate motions (Error bars are within the symbols). Symbols are the experimental data and lines are simulated curves from best fit parameters of the dipolar coupling constants from the equation in section SI 3.

SI 6. References

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SI 7. Cartesian coordinates and electronic energies for all models used in the calculation of energy barriers.

All Cartesian coordinates for model complexes used in the manuscript for the calculation of energy barriers are provided below together with the electronic energy calculated from B3LYP/LANL2DZ.

1. $Zr_6O_4(OH)_4(COOH)_{11}(COOC_6H_5)$ (lowest energy geometry)
   3386.51056639 A.U.

	X	Y	Z
C	-0.01161	-0.00608	0.016424
C	0.007506	0.01042	6.423581
C	6.407112	0.007965	6.389587
C	6.367193	0.495513	0.012555
C	2.954675	3.198004	6.52315
C	3.460166	-3.17516	6.291831
C	3.174722	-2.95236	-0.10607
C	3.176594	3.442712	0.135057
C	6.504485	-2.95165	3.208937
C	0.117957	-3.19064	2.956899
C	-0.13124	3.182274	3.46813
C	6.258969	3.445809	3.190092
O	5.145023	0.398532	-0.38753
O	5.183918	0.013616	6.797664
O	1.235237	-0.01905	6.817446
O	1.20799	0.122712	-0.38324
O	3.098727	3.793738	1.373691
O	3.262289	-3.39982	1.100012
O	3.403941	-3.53399	5.05453
O	2.998897	3.645115	5.314274
O	6.708341	2.237187	3.211295
O	-0.48452	1.946986	3.355422
O	-0.3049	-1.96703	3.088913
O	6.857164	-1.71115	3.188233
O	1.075232	3.634535	3.412463
O	1.376684	-3.51483	3.026921
O	5.297396	-3.39863	3.130231
O	5.020496	3.795775	3.275291
O	3.15899	2.233333	-0.31226
O	3.07099	1.963936	6.8792
O	3.349021	-1.97015	6.737812
O	3.192813	-1.71143	-0.45787

O	-0.41246	-0.00042	1.24202
O	6.775238	0.39671	1.231913
O	6.798643	0.131989	5.166871
O	-0.39747	-0.02709	5.199823
O	2.18907	-0.91241	2.133426
O	2.114801	1.0875	4.293629
O	4.275463	-0.91065	4.211116
O	4.187017	1.244128	2.204627
O	4.561139	1.547025	4.676866
O	4.656955	-1.18602	1.735908
O	1.838241	-1.39278	4.587373
O	1.711054	1.53985	1.848213
Zr	3.18034	0.219938	0.674479
Zr	3.202683	0.034339	5.747513
Zr	3.090288	2.656905	3.304362
Zr	3.282491	-2.40706	3.118046
Zr	5.723965	0.221802	3.203322
Zr	0.65631	0.019978	3.218464
H	1.123051	2.101095	1.309722
H	1.292588	-2.00466	5.115278
H	5.238619	-1.70728	1.15224
H	5.104941	2.111446	5.256911
H	7.131024	0.668105	-0.75622
H	7.187153	-0.10214	7.153572
H	-0.77963	-0.12081	-0.75909
H	-0.76386	0.061812	7.202531
H	2.815548	3.936383	7.32295
H	3.60636	-3.9694	7.034953
H	3.087072	-3.69539	-0.90897
H	3.254444	4.24761	-0.60678
H	-0.93234	3.917938	3.614783
H	7.307139	-3.69566	3.290452
H	6.999126	4.251243	3.102047
C	-0.87991	-4.26861	2.727603
C	-2.76461	-6.30841	2.290517
C	-2.25555	-3.95296	2.657225
C	-0.4484	-5.60603	2.577909
C	-1.39169	-6.62287	2.359658
C	-3.19477	-4.97372	2.439092
H	-2.56334	-2.91806	2.772023
H	0.61389	-5.82347	2.633115
H	-1.06299	-7.65238	2.243647
H	-4.2536	-4.73452	2.384486

H	-3.49371	-7.09756	2.121499
H	-3.49371	-7.09756	2.121499

2. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(COOC$_6$H$_5$)(Highest energy geometry) -3386.49395991 A.U.

	X	Y	Z
C	-0.11596	0.101957	0.120008
C	0.120747	-0.11112	6.515616
C	6.514977	-0.08432	6.267215
C	6.256868	0.628356	-0.08338
C	3.057881	3.082101	6.630032
C	3.580862	-3.27516	6.154569
C	3.079713	-2.82847	-0.21535
C	3.063537	3.552029	0.249154
C	6.517639	-2.92658	2.982002
C	0.120571	-3.1966	2.950775
C	-0.12693	3.161657	3.681557
C	6.246165	3.464542	3.198599
O	5.021858	0.538637	-0.44388
O	5.306085	-0.09935	6.71589
O	1.361222	-0.15224	6.866696
O	1.088294	0.245213	-0.31933
O	3.026319	3.858868	1.501319
O	3.203185	-3.31435	0.972261
O	3.480571	-3.58896	4.907952
O	3.059818	3.571987	5.43709
O	6.700033	2.257917	3.161816
O	-0.47803	1.929084	3.538407
O	-0.30735	-1.9864	3.129363
O	6.864648	-1.68425	2.992774
O	1.075519	3.621202	3.600651
O	1.375762	-3.52067	2.954403
O	5.309868	-3.37531	2.929069
O	5.009877	3.80516	3.336932
O	3.034351	2.358859	-0.23942
O	3.190102	1.836457	6.937451
O	3.476729	-2.08796	6.647762
O	3.075896	-1.57625	-0.52571
O	-0.46996	0.053672	1.358874
O	6.707127	0.489808	1.11709
O	6.864251	0.085266	5.037193
O	-0.32449	-0.11105	5.305468
O	2.158104	-0.87603	2.127474
O	2.150115	1.047376	4.35536
O	4.313959	-0.93546	4.130263

O	4.149792	1.286882	2.206928
O	4.606518	1.506486	4.673899
O	4.613839	-1.12198	1.635428
O	1.890501	-1.44489	4.570132
O	1.662834	1.584418	1.942239
Zr	3.096184	0.313323	0.675994
Zr	3.291093	-0.05008	5.734298
Zr	3.086733	2.657015	3.390771
Zr	3.293452	-2.3982	3.019468
Zr	5.725249	0.239789	3.115492
Zr	0.659296	0.014107	3.294766
H	1.055879	2.162704	1.444282
H	1.370013	-2.07392	5.102852
H	5.178558	-1.6193	1.015319
H	5.167306	2.052419	5.255477
H	6.992686	0.831618	-0.87163
H	7.320735	-0.21814	6.999989
H	-0.91368	0.023131	-0.62959
H	-0.62424	-0.0849	7.320958
H	2.944325	3.790825	7.460041
H	3.760961	-4.09464	6.861889
H	2.977919	-3.54581	-1.03969
H	3.114022	4.382663	-0.46611
H	-0.92545	3.887495	3.880763
H	7.324865	-3.66941	3.00921
H	6.980081	4.275983	3.114424
C	-0.89192	-4.28787	2.739866
C	-2.77705	-6.3415	2.335776
C	-1.32069	-4.60316	1.435305
C	-1.40508	-4.99948	3.842045
C	-2.34671	-6.02439	3.638479
C	-2.26222	-5.62881	1.235696
H	-0.92471	-4.05471	0.584042
H	-1.07457	-4.7598	4.850128
H	-2.74052	-6.57163	4.491201
H	-2.59113	-5.86969	0.22793
H	-3.50424	-7.13452	2.17972

3. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(COOC$_6$H$_5$-*o*-OH)(lowest energy geometry) -3461.73353729 A.U.

	X	Y	Z
C	3.105471	0.57938	-2.42902
C	-3.27385	0.871368	-2.40219
C	-3.25908	0.632466	3.997329
C	3.135141	0.850422	3.975156
C	-3.25136	3.953291	0.670027
C	-3.29242	-2.43727	0.928183
C	3.10771	-2.47292	0.647667
C	3.143286	3.917646	0.897138
C	-0.20798	-2.45724	3.986159
C	0.056362	-2.49531	-2.40805
C	-0.19551	3.924816	-2.41142
C	0.085837	3.935874	3.982363
O	3.531495	0.783059	2.749543
O	-3.66439	0.70056	2.774772
O	-3.67233	0.821641	-1.17697
O	3.510618	0.657556	-1.20841
O	1.920912	4.324237	0.83685
O	1.882828	-2.8688	0.723196
O	-2.07171	-2.84746	0.861715
O	-2.02458	4.34632	0.732779
O	0.012687	2.712529	4.383784
O	-0.13703	2.699033	-2.80861
O	-0.00212	-1.23532	-2.80028
O	-0.13386	-1.23316	4.385284
O	-0.12191	4.328833	-1.18875
O	-0.05061	-2.83605	-1.16286
O	-0.14771	-2.85998	2.762272
O	0.017539	4.336283	2.758115
O	3.53701	2.691073	0.831687
O	-3.65941	2.731708	0.738717
O	-3.68367	-1.20999	0.862303
O	3.513673	-1.25001	0.713359
O	1.877474	0.647204	-2.82455
O	1.912123	0.789714	4.379587
O	-2.03293	0.691133	4.392734
O	-2.0502	0.79208	-2.80434
O	0.962415	-0.30821	-0.24921
O	-1.11274	1.784956	-0.24642
O	-1.11778	-0.29555	1.833794

O	0.978677	1.774801	1.825334
O	-1.47931	2.166945	2.212797
O	1.343527	-0.68753	2.205422
O	-1.50522	-0.67122	-0.62216
O	1.349936	2.146834	-0.63717
Zr	2.466992	0.725512	0.780867
Zr	-2.61282	0.753142	0.798008
Zr	-0.05812	3.275842	0.787525
Zr	-0.08865	-1.79859	0.788858
Zr	-0.06427	0.739144	3.324881
Zr	-0.08244	0.730786	-1.73498
H	1.913157	2.705381	-1.20431
H	-2.05582	-1.24129	-1.19022
H	1.90406	-1.25414	2.76726
H	-2.03605	2.733563	2.77839
H	3.910087	0.95907	4.744341
H	-4.0284	0.525033	4.772316
H	3.870915	0.45221	-3.20456
H	-4.04576	0.981177	-3.17417
H	-4.0186	4.729706	0.558355
H	-4.07074	-3.20258	1.040728
H	3.876033	-3.24677	0.526241
H	3.919775	4.685501	1.003797
H	-0.30796	4.694844	-3.18498
H	-0.32258	-3.22743	4.759323
H	0.206965	4.707404	4.753109
C	0.293697	-3.52927	-3.42889
C	0.872378	-5.55358	-5.30411
C	0.744972	-3.18747	-4.74036
C	0.157986	-4.89802	-3.07799
C	0.430882	-5.90592	-4.00457
C	1.033158	-4.21227	-5.66812
H	-0.15895	-5.13475	-2.06665
H	0.313675	-6.95012	-3.73047
H	1.374756	-3.92514	-6.65742
H	1.092368	-6.33263	-6.03032
O	0.925701	-1.89061	-5.16238
H	0.650568	-1.2565	-4.44717

4. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(COOC$_6$H$_5$-o-OH)(Highest energy geometry) -3461.70485549 A.U.

	X	Y	Z
C	2.971781	0.722411	-2.57276
C	-3.45125	0.809922	-2.27293
C	-3.13846	0.57313	4.109369
C	3.241936	0.949915	3.802711
C	-3.36444	3.882081	0.774103
C	-3.22147	-2.51	1.051867
C	3.141439	-2.37922	0.454518
C	3.024642	4.018467	0.737741
C	-0.01001	-2.4313	3.973591
C	-0.05816	-2.46538	-2.44086
C	-0.4291	3.916387	-2.44897
C	0.108851	3.965244	3.933787
O	3.583948	0.881594	2.560411
O	-3.59992	0.625556	2.906096
O	-3.79089	0.732894	-1.0306
O	3.42793	0.819646	-1.37085
O	1.788871	4.388872	0.708469
O	1.935129	-2.80141	0.623105
O	-1.99355	-2.884	0.924308
O	-2.14613	4.306165	0.775398
O	0.089056	2.741907	4.341962
O	-0.34293	2.690485	-2.84397
O	-0.21137	-1.23141	-2.82023
O	0.052445	-1.20385	4.365157
O	-0.32976	4.327871	-1.23136
O	-0.05095	-2.83526	-1.20141
O	0.002375	-2.83614	2.74919
O	-0.02456	4.358204	2.712426
O	3.450828	2.804054	0.670618
O	-3.73705	2.65118	0.868995
O	-3.65117	-1.29513	1.00471
O	3.517982	-1.14435	0.494261
O	1.725528	0.651036	-2.90644
O	2.03949	0.870811	4.261185
O	-1.89754	0.666287	4.448774
O	-2.2474	0.767106	-2.73214
O	0.917239	-0.28008	-0.32904
O	-1.21108	1.764927	-0.23458
O	-1.06966	-0.30581	1.854909

O	0.963999	1.816297	1.747261
O	-1.48227	2.147613	2.240348
O	1.413641	-0.63307	2.116567
O	-1.55992	-0.69933	-0.57891
O	1.225156	2.187474	-0.72925
Zr	2.434411	0.803493	0.645912
Zr	-2.63651	0.69914	0.884548
Zr	-0.15466	3.286508	0.749414
Zr	-0.04992	-1.78668	0.772042
Zr	0.019131	0.762389	3.296996
Zr	-0.22147	0.734056	-1.76813
H	1.750195	2.768894	-1.30979
H	-2.1278	-1.27727	-1.1211
H	2.012873	-1.18835	2.649197
H	-2.03003	2.701732	2.826693
H	4.048741	1.077318	4.535197
H	-3.86864	0.448259	4.918764
H	3.708597	0.697296	-3.38626
H	-4.26203	0.909601	-3.00558
H	-4.15544	4.638365	0.695343
H	-3.96917	-3.29856	1.203835
H	3.915393	-3.1329	0.268946
H	3.780334	4.810119	0.815415
H	-0.59258	4.677882	-3.22185
H	-0.06762	-3.20126	4.753077
H	0.240382	4.743248	4.696247
C	0.238935	-3.50157	-3.48854
C	0.894623	-5.60413	-5.2417
C	1.587938	-3.78289	-3.79551
C	-0.77932	-4.27119	-4.08115
C	-0.45734	-5.31664	-4.96357
C	1.918879	-4.83638	-4.66315
H	-1.81937	-4.06161	-3.84252
H	-1.24847	-5.90466	-5.41978
H	2.96621	-5.02643	-4.87611
H	1.151209	-6.41806	-5.91502
O	2.648013	-3.03596	-3.25621
H	2.365277	-2.13857	-2.98321

5. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(COOC$_6$H$_5$-*o*-CH$_3$)(lowest energy geometry) -3425.81883957 A.U.

	X	Y	Z
C	3.124965	0.75605	-2.41328
C	-3.28037	1.033291	-2.40873
C	-3.26687	0.852407	3.98674
C	3.124278	1.085479	3.977194
C	-3.26127	4.138989	0.621984
C	-3.28475	-2.25266	0.95239
C	3.121187	-2.27403	0.68922
C	3.129629	4.123804	0.866275
C	-0.20756	-2.23516	4.006389
C	0.047182	-2.31398	-2.38224
C	-0.19615	4.081734	-2.45831
C	0.067782	4.162507	3.938958
O	3.525352	1.008222	2.753982
O	-3.67073	0.907674	2.763414
O	-3.67915	0.983643	-1.18295
O	3.523978	0.837499	-1.18912
O	1.90646	4.525756	0.793632
O	1.897519	-2.67763	0.752512
O	-2.06319	-2.66111	0.884022
O	-2.03518	4.535006	0.680101
O	-0.00284	2.943757	4.35508
O	-0.13044	2.853037	-2.84453
O	-0.03062	-1.06663	-2.75969
O	-0.13895	-1.00741	4.394977
O	-0.12911	4.499051	-1.23973
O	-0.03438	-2.65655	-1.12958
O	-0.14036	-2.65047	2.787041
O	-9.8E-05	4.54934	2.710582
O	3.528496	2.898252	0.818036
O	-3.66758	2.917947	0.704822
O	-3.68081	-1.02791	0.877504
O	3.520708	-1.04967	0.747446
O	1.902742	0.821715	-2.81824
O	1.900231	1.022818	4.378555
O	-2.04134	0.916928	4.383854
O	-2.05813	0.958762	-2.81219
O	0.966745	-0.12029	-0.24387
O	-1.11495	1.963061	-0.26979
O	-1.1189	-0.0948	1.836986

O	0.971322	1.982028	1.811167
O	-1.48857	2.370928	2.18651
O	1.343424	-0.47686	2.215009
O	-1.5069	-0.49187	-0.6111
O	1.347971	2.329075	-0.65532
Zr	2.464152	0.926786	0.781317
Zr	-2.61322	0.940696	0.785897
Zr	-0.06809	3.465312	0.748746
Zr	-0.08174	-1.60155	0.802404
Zr	-0.07226	0.957689	3.316694
Zr	-0.07709	0.891058	-1.75527
H	1.909739	2.884086	-1.22727
H	-2.05295	-1.06831	-1.17695
H	1.903924	-1.03528	2.784826
H	-2.04739	2.94305	2.744318
H	3.895977	1.205269	4.748163
H	-4.03697	0.751708	4.762026
H	3.898987	0.629326	-3.18094
H	-4.05446	1.138694	-3.17955
H	-4.02968	4.913083	0.501311
H	-4.06038	-3.01942	1.075586
H	3.895705	-3.04491	0.585845
H	3.902818	4.895836	0.968237
H	-0.30902	4.84413	-3.23968
H	-0.32346	-2.99817	4.78673
H	0.186148	4.94304	4.70126
C	0.218799	-3.35532	-3.43271
C	0.539984	-5.1711	-5.56456
C	0.2908	-2.8967	-4.773
C	0.311215	-4.75167	-3.14356
C	0.471756	-5.63167	-4.23856
C	0.449795	-3.79212	-5.83681
H	0.220233	-1.82851	-4.94967
H	0.543805	-6.69873	-4.04178
H	0.502932	-3.42584	-6.85835
H	0.663334	-5.88293	-6.37769
C	0.24951	-5.3471	-1.74873
H	1.030044	-4.93805	-1.09813
H	0.363339	-6.43597	-1.79945
H	-0.70007	-5.11615	-1.25241

6. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(COOC$_6$H$_5$-*o*-CH$_3$)(Highest energy geometry) -3425.80616245 A.U.

	X	Y	Z
C	3.054239	0.933183	-2.51365
C	-3.33511	0.587468	-2.22317
C	-3.03232	0.615227	4.168101
C	3.299028	1.460222	3.858045
C	-3.48961	3.775428	0.716456
C	-2.87842	-2.57154	1.229652
C	3.478282	-1.99038	0.677666
C	2.879305	4.378878	0.668818
C	0.309174	-2.15956	4.139375
C	0.288917	-2.42483	-2.25667
C	-0.57154	3.916627	-2.49351
C	-0.04046	4.226556	3.875958
O	3.651065	1.379621	2.620038
O	-3.49078	0.592142	2.963029
O	-3.67393	0.538974	-0.97977
O	3.500366	1.085339	-1.31298
O	1.620757	4.659516	0.641911
O	2.302208	-2.50109	0.810673
O	-1.62737	-2.86179	1.112699
O	-2.30703	4.289923	0.708192
O	0.024864	3.020662	4.328573
O	-0.40632	2.687271	-2.84643
O	0.086345	-1.21619	-2.68018
O	0.277046	-0.91819	4.488161
O	-0.48942	4.377482	-1.29172
O	0.311108	-2.74697	-1.00068
O	0.360183	-2.6059	2.930536
O	-0.1958	4.565038	2.641121
O	3.392497	3.196179	0.635345
O	-3.77011	2.523697	0.850401
O	-3.39581	-1.39421	1.133605
O	3.762008	-0.73182	0.671487
O	1.813679	0.85998	-2.85727
O	2.105522	1.295489	4.318062
O	-1.80302	0.809153	4.507114
O	-2.12939	0.608368	-2.68025
O	1.086249	-0.08633	-0.22277
O	-1.18088	1.788088	-0.21202
O	-0.89623	-0.19075	1.948134

O	0.977996	2.071276	1.769788
O	-1.48881	2.239867	2.247332
O	1.604594	-0.32511	2.227942
O	-1.34632	-0.70781	-0.47202
O	1.216388	2.377199	-0.71911
Zr	2.521058	1.131735	0.703007
Zr	-2.52646	0.66207	0.939998
Zr	-0.24239	3.417393	0.717452
Zr	0.236926	-1.62891	0.916538
Zr	0.105288	1.004557	3.352112
Zr	-0.11111	0.777848	-1.71241
H	1.696942	2.966005	-1.32996
H	-1.86862	-1.34773	-0.98994
H	2.239734	-0.80932	2.787314
H	-2.07722	2.772906	2.813343
H	4.088817	1.679213	4.587666
H	-3.75547	0.466495	4.979922
H	3.798623	0.869781	-3.31755
H	-4.14795	0.600746	-2.96047
H	-4.33494	4.466976	0.610097
H	-3.56776	-3.40453	1.417914
H	4.316732	-2.69013	0.569324
H	3.577503	5.22424	0.71359
H	-0.79227	4.638459	-3.29001
H	0.303263	-2.90381	4.945741
H	0.032523	5.03908	4.609884
C	0.499557	-3.51281	-3.27322
C	0.95002	-5.5383	-5.16526
C	1.808414	-3.79431	-3.70651
C	-0.60661	-4.23855	-3.77899
C	-0.35668	-5.25087	-4.72823
C	2.037735	-4.80792	-4.65362
H	2.644236	-3.22523	-3.30664
H	-1.19451	-5.81842	-5.12743
H	3.050051	-5.02248	-4.98584
H	1.116	-6.3244	-5.89792
C	-2.02097	-3.9412	-3.31363
H	-2.12601	-4.11313	-2.23308
H	-2.7462	-4.58284	-3.8247
H	-2.29442	-2.89699	-3.52048

7. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(terephthalate)Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(lowest energy geometry) -6539.56235309 A.U.

	X	Y	Z
Zr	-5.581	-1.76899	-0.0046
Zr	-9.12	1.768994	0.004589
Zr	-5.581	1.768994	0.004589
Zr	-9.12	-1.76899	-0.0046
Zr	-7.35	-0.0065	2.501986
Zr	-7.35	0.006498	-2.502
Zr	9.12	-1.76899	-0.0046
Zr	5.581	1.768994	0.004588
Zr	9.12	1.768994	0.004588
Zr	5.581	-1.76899	-0.0046
Zr	7.35	-0.0065	2.501986
Zr	7.35	0.006498	-2.502
O	-4.813	-2.54215	1.9814
O	-9.887	2.531829	1.994577
O	-9.887	2.542152	-1.98041
O	-4.814	-2.53183	-1.99459
O	-3.408	1.130997	0.002932
C	-0.70133	1.203708	-0.00205
O	-8.481	-3.94199	-0.01024
O	-11.293	-1.131	-0.00294
O	-6.219	3.941987	0.010232
O	-5.944	1.395678	3.591631
O	-5.945	1.415311	-3.58334
O	-8.756	-1.39568	-3.59164
O	-8.756	-1.41531	3.584332
O	-4.814	2.542154	-1.98141
O	-9.887	-2.53183	-1.99359
O	-9.887	-2.54215	1.9814
O	-4.813	2.531829	1.994576
O	-3.408	-1.131	-0.00294
C	-0.70132	-1.20372	-0.00203
O	-8.481	3.941987	0.010232
O	-11.293	1.130997	0.002932
O	-6.219	-3.94199	-0.01024
O	-5.945	-1.39668	-3.59064
O	-5.944	-1.41431	3.584334
O	-8.756	1.396678	3.591634
O	-8.756	1.414313	-3.58434
O	9.887	-2.54215	1.981399

O	4.813	2.531829	1.994576
O	4.814	2.542154	-1.98141
O	9.887	-2.53183	-1.99359
O	11.293	1.130997	0.002931
O	6.219	-3.94199	-0.01024
O	3.408	-1.131	-0.00294
C	0.701323	-1.20372	-0.00199
O	8.481	3.941987	0.010231
O	8.756	1.396678	3.591634
O	8.756	1.414313	-3.58435
O	5.945	-1.39668	-3.59065
O	5.944	-1.41431	3.584334
O	9.887	2.542152	-1.98041
O	4.814	-2.53183	-1.99459
O	4.813	-2.54215	1.981399
O	9.887	2.531829	1.994576
O	11.293	-1.131	-0.00294
O	6.219	3.941987	0.010231
O	3.408	1.130997	0.002932
C	0.701325	1.203708	-0.00195
O	8.481	-3.94199	-0.01024
O	8.756	-1.39568	-3.59164
O	8.756	-1.41531	3.584331
O	5.944	1.395678	3.591631
O	5.945	1.415311	-3.58334
O	-7.35	-1.64597	-1.17028
O	-7.35	1.652023	-1.16172
O	-8.999	-0.00303	1.165991
O	-5.701	-0.00303	1.165991
O	-7.35	1.644967	1.170271
O	-7.35	-1.65102	1.161711
O	-8.999	0.003026	-1.165
O	-5.702	0.003028	-1.166
O	7.35	-1.64597	-1.17028
O	7.35	1.652023	-1.16172
O	5.701	-0.00303	1.165991
O	8.999	-0.00303	1.16599
O	7.35	1.644967	1.17027
O	7.35	-1.65102	1.161711
O	5.702	0.003028	-1.166
O	8.999	0.003026	-1.165
C	-5.177	-2.18097	3.066341
C	-9.522	2.164013	3.078625

C	-9.523	2.180971	-3.06635
C	-5.178	-2.16401	-3.07864
C	-3.006	0	-5E-06
C	-1.41757	-4E-06	0.00062
C	-7.35	-4.34499	-0.01129
C	-11.695	0	-5E-06
C	-7.35	4.344986	0.011278
C	-5.177	2.165015	3.077628
C	-5.178	2.179973	-3.06735
C	-9.523	-2.16502	-3.07764
C	-9.522	-2.17997	3.067344
C	9.522	-2.17997	3.067344
C	5.177	2.165015	3.077627
C	5.178	2.179973	-3.06736
C	9.523	-2.16502	-3.07764
C	11.695	0	-6E-06
C	7.35	-4.34499	-0.01129
C	3.006	0	-5E-06
C	1.417575	-4E-06	0.000742
C	7.35	4.344986	0.011278
C	9.522	2.164013	3.078624
C	9.523	2.180971	-3.06635
C	5.178	-2.16401	-3.07864
C	5.177	-2.18097	3.066341
H	-1.24674	2.150967	-0.00884
H	-1.24672	-2.15098	-0.00916
H	1.246722	-2.15098	-0.00909
H	1.246737	2.150967	-0.00874
H	-4.634	-2.72496	3.831931
H	-10.065	2.705019	3.847033
H	-10.066	2.724961	-3.83194
H	-4.635	-2.70402	-3.84704
H	-7.35	-5.42998	-0.01311
H	-12.781	0	-5E-06
H	-7.35	5.429979	0.015096
H	-4.634	2.705022	3.846032
H	-4.635	2.723963	-3.83294
H	-10.066	-2.70502	-3.84604
H	-10.065	-2.72496	3.832931
H	10.065	-2.72496	3.832931
H	4.634	2.705022	3.846032
H	4.635	2.723963	-3.83295
H	10.066	-2.70502	-3.84604

H	12.781	0	-6E-06
H	7.35	-5.42998	-0.01311
H	7.35	5.429979	0.015096
H	10.065	2.705019	3.847032
H	10.066	2.724961	-3.83194
H	4.635	-2.70402	-3.84704
H	4.634	-2.72496	3.831931
H	-7.35	-2.44948	-1.74237
H	-7.35	2.4585	-1.72963
H	7.35	-2.44948	-1.74237
H	7.35	2.4585	-1.72963
H	-4.895	-0.00451	1.734989
H	-9.804	-0.00451	1.735989
H	4.895	-0.00451	1.734989
H	9.804	-0.00451	1.735989

8. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(terephthalate)Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(Highest energy geometry) -6539.53730445 A.U.

	X	Y	Z
Zr	-5.581	0.000022	1.769001
Zr	-9.12	-0.00017	-1.769
Zr	-5.581	-0.00017	-1.769
Zr	-9.12	0.000022	1.769001
Zr	-7.35	2.501926	-0.00013
Zr	-7.35	-2.50207	0.000137
Zr	9.120001	0.000022	1.769001
Zr	5.581001	-0.00017	-1.769
Zr	9.120001	-0.00017	-1.769
Zr	5.581001	0.000021	1.769001
Zr	7.350001	2.501926	-0.00013
Zr	7.350001	-2.50207	0.000137
O	-4.813	1.988064	2.536894
O	-9.887	1.987789	-2.53711
O	-9.887	-1.98721	-2.53689
O	-4.814	-1.98794	2.537109
O	-3.408	-0.00014	-1.131
C	-0.70226	1.203371	-0.00029
O	-8.481	0.00014	3.942001
O	-11.293	-1.3E-05	1.131001
O	-6.219	-0.00029	-3.942
O	-5.944	3.58785	-1.40519
O	-5.945	-3.58715	-1.40581
O	-8.756	-3.588	1.405196
O	-8.756	3.588002	1.405807
O	-4.814	-1.98821	-2.53689
O	-9.887	-1.98694	2.537109
O	-9.887	1.988064	2.536894
O	-4.813	1.987789	-2.53711
O	-3.408	0.000002	1.131001
C	-0.7029	-1.20285	0.000088
O	-8.481	-0.00029	-3.942
O	-11.293	-0.00014	-1.131
O	-6.219	0.00014	3.942001
O	-5.945	-3.587	1.406195
O	-5.944	3.588002	1.404807
O	-8.756	3.58785	-1.40619
O	-8.756	-3.58815	-1.4048
O	9.887001	1.988064	2.536894

O	4.813001	1.987789	-2.53711
O	4.814001	-1.98821	-2.53689
O	9.887001	-1.98694	2.537109
O	11.293	-0.00014	-1.131
O	6.219001	0.00014	3.942001
O	3.408001	-1.9E-05	1.131001
C	0.702685	-1.20291	-0.00017
O	8.481001	-0.00029	-3.942
O	8.756001	3.58785	-1.40619
O	8.756001	-3.58815	-1.4048
O	5.945001	-3.587	1.406196
O	5.944001	3.588002	1.404807
O	9.887001	-1.98721	-2.53689
O	4.814001	-1.98794	2.537109
O	4.813001	1.988064	2.536894
O	9.887001	1.987789	-2.53711
O	11.293	-1.2E-05	1.131001
O	6.219001	-0.00029	-3.942
O	3.408001	-0.00013	-1.131
C	0.70238	1.203234	0.000111
O	8.481001	0.00014	3.942001
O	8.756001	-3.588	1.405196
O	8.756001	3.588002	1.405807
O	5.944001	3.58785	-1.40519
O	5.945001	-3.58715	-1.4058
O	-7.35	-1.16599	1.649064
O	-7.35	-1.16616	-1.64894
O	-8.999	1.165926	-6.2E-05
O	-5.701	1.165926	-6.2E-05
O	-7.35	1.165837	-1.64806
O	-7.35	1.166015	1.647938
O	-8.999	-1.16507	0.000064
O	-5.702	-1.16607	0.000064
O	7.350001	-1.16598	1.649065
O	7.350001	-1.16616	-1.64894
O	5.701001	1.165926	-6.2E-05
O	8.999001	1.165926	-6.2E-05
O	7.350001	1.165837	-1.64806
O	7.350001	1.166015	1.647938
O	5.702001	-1.16607	0.000065
O	8.999001	-1.16507	0.000064
C	-5.177	3.072044	2.172835
C	-9.522	3.072809	-2.17217

C	-9.523	-3.07219	-2.17283
C	-5.178	-3.07296	2.172168
C	-3.006	-8.9E-05	0.000003
C	-1.41728	-7.6E-05	-3.4E-05
C	-7.35	0.000161	4.345001
C	-11.695	-7.4E-05	0.000001
C	-7.35	-0.00031	-4.345
C	-5.177	3.071809	-2.17317
C	-5.178	-3.07319	-2.17183
C	-9.523	-3.07196	2.173168
C	-9.522	3.073044	2.171835
C	9.522001	3.073044	2.171835
C	5.177001	3.071809	-2.17317
C	5.178001	-3.07319	-2.17183
C	9.523001	-3.07196	2.173168
C	11.695	-7.4E-05	0.000001
C	7.350001	0.000161	4.345001
C	3.005999	-7.4E-05	0.000001
C	1.417255	-0.00038	-6E-06
C	7.350001	-0.00031	-4.345
C	9.522001	3.072809	-2.17217
C	9.523001	-3.07219	-2.17283
C	5.178001	-3.07296	2.172168
C	5.177001	3.072044	2.172835
H	-1.23363	2.152574	-5E-06
H	-1.23849	-2.15157	0.000459
H	1.238103	-2.15181	-0.00056
H	1.233904	2.15241	0.00025
H	-4.634	3.839073	2.714794
H	-10.065	3.839779	-2.71521
H	-10.066	-3.83922	-2.71479
H	-4.635	-3.83993	2.714209
H	-7.35	0.00122	5.430001
H	-12.781	-7.4E-05	0.000001
H	-7.35	0.000632	-5.43
H	-4.634	3.838779	-2.71521
H	-4.635	-3.84022	-2.71379
H	-10.066	-3.83893	2.715209
H	-10.065	3.840073	2.714794
H	10.065	3.840073	2.714794
H	4.634001	3.838779	-2.71521
H	4.635001	-3.84022	-2.71379
H	10.066	-3.83893	2.715209

H	12.781	-7.4E-05	0.000001
H	7.350001	0.00122	5.430001
H	7.350001	0.000632	-5.43
H	10.065	3.839779	-2.71521
H	10.066	-3.83922	-2.71479
H	4.635001	-3.83993	2.714209
H	4.634001	3.839073	2.714794
H	-7.35	-1.73594	2.454095
H	-7.35	-1.73621	-2.45391
H	7.350001	-1.73594	2.454095
H	7.350001	-1.73621	-2.45391
H	-4.895	1.734926	-9.2E-05
H	-9.804	1.735926	-9.3E-05
H	4.895001	1.734926	-9.2E-05
H	9.804001	1.735926	-9.3E-05

9. $Zr_6O_4(OH)_4(COOH)_{11}$(2,4-dihydroxyterephthalate)
$Zr_6O_4(OH)_4(COOH)_{11}$(lowest energy geometry)-
6689.98670133 A.U.

	X	Y	Z
Zr	-5.58237	1.678248	-0.54555
Zr	-9.11857	-1.69042	0.544989
Zr	-5.57957	-1.68749	0.544975
Zr	-9.12137	1.675317	-0.54553
Zr	-7.34934	-0.77728	-2.38046
Zr	-7.3506	0.765107	2.379904
Zr	9.118628	1.690424	-0.54561
Zr	5.582422	-1.67825	0.544928
Zr	9.121421	-1.67532	0.544913
Zr	5.57963	1.687493	-0.54559
Zr	7.350654	-0.76511	-2.38052
Zr	7.349397	0.777281	2.379841
O	-4.81447	1.796728	-2.67348
O	-9.88447	-3.03443	-1.10949
O	-9.88547	-1.80921	2.67197
O	-4.81647	3.022253	1.108937
O	-3.40708	-1.07875	0.348309
C	-0.67503	1.207609	0.0045
O	-8.48408	3.743045	-1.21532
O	-11.2939	1.06658	-0.34887
O	-6.21586	-3.75522	1.214763
O	-5.94196	-2.44745	-2.98053
O	-5.94476	-0.23684	3.845443
O	-8.75798	2.435273	2.97997
O	-8.75618	0.22436	-3.84695
O	-4.81247	-1.8047	2.6729
O	-9.88947	3.017743	1.108007
O	-9.88847	1.792527	-2.67346
O	-4.81047	-3.03023	-1.10952
O	-3.40886	1.073115	-0.3489
C	-0.73731	-1.18922	0.005308
O	-8.47786	-3.75709	1.214772
O	-11.2921	-1.08529	0.348348
O	-6.22208	3.744919	-1.21533
O	-5.94698	2.438245	2.978697
O	-5.94418	0.225738	-3.84666
O	-8.75396	-2.45073	-2.98021
O	-8.75576	-0.23791	3.846098

O	9.885522	1.808903	-2.67354
O	4.815527	-3.02225	-1.10956
O	4.815529	-1.79673	2.672859
O	9.884523	3.03412	1.107923
O	11.29392	-1.06658	0.348253
O	6.215914	3.75522	-1.21538
O	3.407139	1.078755	-0.34893
C	0.672109	-1.20631	0.00934
O	8.484136	-3.74304	1.214701
O	8.758036	-2.43622	-2.98028
O	8.756232	-0.22341	3.846025
O	5.943015	2.448092	2.978648
O	5.943819	0.235584	-3.84671
O	9.888527	-1.79283	2.671887
O	4.811525	3.030227	1.108896
O	4.811523	1.804701	-2.67352
O	9.889526	-3.01805	-1.10958
O	11.29213	1.085287	-0.34897
O	6.222137	-3.74492	1.214711
O	3.408919	-1.07311	0.348303
C	0.737369	1.189633	0.003971
O	8.477914	3.757094	-1.21539
O	8.754015	2.449776	2.979895
O	8.755816	0.238865	-3.84702
O	5.946036	-2.4376	-2.98058
O	5.945234	-0.227	3.845393
O	-7.35156	1.922023	0.600678
O	-7.34896	-1.2154	1.617224
O	-8.99868	-0.36685	-1.1095
O	-5.70068	-0.36412	-1.10952
O	-7.34838	-1.93325	-0.60154
O	-7.35098	1.202278	-1.61747
O	-8.99926	0.351636	1.108007
O	-5.70226	0.354676	1.108944
O	7.348431	1.934197	0.600617
O	7.351034	-1.20323	1.617162
O	5.701319	-0.35467	-1.10956
O	8.999318	-0.35194	-1.10958
O	7.351619	-1.92107	-0.6016
O	7.349018	1.214452	-1.61753
O	5.701733	0.364121	1.108897
O	8.998732	0.366543	1.107932
C	-5.17791	1.116027	-3.5925

C	-9.51948	-3.02133	-2.25417
C	-9.52203	-1.1282	3.591947
C	-5.18046	3.009153	2.253616
C	-3.00596	-0.0025	-0.0003
C	-1.43424	0.019186	0.000427
C	-7.3534	4.127361	-1.33954
C	-11.695	-0.00969	-0.00026
C	-7.34654	-4.13954	1.338986
C	-5.17448	-3.01837	-2.25293
C	-5.17703	-1.12334	3.592571
C	-9.52546	3.006198	2.252375
C	-9.52291	1.111169	-3.59313
C	9.521083	1.126943	-3.59321
C	5.179513	-3.0098	-2.25297
C	5.178968	-1.11477	3.592527
C	9.520538	3.021972	2.252294
C	11.69502	0.009687	-0.00036
C	7.346596	4.139535	-1.3396
C	3.006018	0.002489	-0.00035
C	1.432906	-0.01725	0.001145
C	7.353454	-4.12736	1.338923
C	9.524511	-3.00555	-2.25425
C	9.523968	-1.11243	3.591866
C	5.17554	3.01773	2.253573
C	5.176083	1.124603	-3.59255
H	-1.27773	-2.14088	0.025427
H	1.278028	2.141807	-0.00346
H	-4.63515	1.395675	-4.48922
H	-10.0619	-3.77475	-2.81646
H	-10.0648	-1.40785	4.488666
H	-4.63808	3.761626	2.816208
H	-7.35425	5.159225	-1.67492
H	-12.781	-0.01059	-0.00026
H	-7.34568	-5.17202	1.672464
H	-4.63086	-3.76995	-2.81553
H	-4.63379	-1.40209	4.489285
H	-10.0691	3.757771	2.814972
H	-10.0661	1.390869	-4.49015
H	10.06385	1.407541	-4.49024
H	4.637134	-3.76227	-2.81557
H	4.636203	-1.39441	4.489247
H	10.06292	3.774445	2.814887
H	12.78102	0.010586	-0.00036

H	7.345741	5.1714	-1.67498
H	7.354311	-5.15984	1.672402
H	10.06813	-3.75808	-2.81654
H	10.0672	-1.39118	4.48858
H	4.631919	3.769304	2.81617
H	4.632848	1.403351	-4.48926
H	-7.35234	2.863519	0.8948
H	-7.34847	-1.80552	2.407597
H	7.347652	2.875694	0.894739
H	7.351526	-1.79334	2.407536
H	-4.89454	-0.53883	-1.65081
H	-9.80353	-0.54321	-1.65175
H	4.895462	-0.53073	-1.65086
H	9.80446	-0.52697	-1.65183
O	-1.1964	2.470727	0.020802
H	-2.20213	2.4766	-0.04739
O	1.197832	-2.47018	-0.00652
H	2.183064	-2.47954	0.201425

10. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(2,4-dihydroxyterephthalate)
    Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(Highest energy geometry)-
    6689.95176223 A.U.

	X	Y	Z
Zr	-5.58109	-0.13086	1.765564
Zr	-9.1198	0.144311	-1.76201
Zr	-5.5808	0.141313	-1.76195
Zr	-9.12009	-0.12786	1.765504
Zr	-7.34783	2.50131	0.194249
Zr	-7.35206	-2.48786	-0.1907
Zr	9.119904	-0.14332	1.76581
Zr	5.581196	0.131855	-1.76176
Zr	9.120195	0.128855	-1.76171
Zr	5.580906	-0.14032	1.765752
Zr	7.352161	2.488854	0.194496
Zr	7.34794	-2.50032	-0.19045
O	-4.81148	1.791517	2.684233
O	-9.88506	2.18615	-2.37482
O	-9.88841	-1.77707	-2.68061
O	-4.81583	-2.1727	2.378367
O	-3.40785	0.090397	-1.12581
C	-0.68354	-1.20543	-0.03784
O	-8.48127	-0.29557	3.932075
O	-11.293	-0.07694	1.129358
O	-6.21862	0.309017	-3.92852
O	-5.9408	3.690984	-1.12302
O	-5.94786	-3.46267	-1.67598
O	-8.75909	-3.67753	1.12657
O	-8.75303	3.477122	1.679603
O	-4.81541	-1.78237	-2.6806
O	-9.88883	-2.1674	2.378359
O	-9.88548	1.795817	2.684149
O	-4.81106	2.18185	-2.37473
O	-3.40804	-0.08363	1.129491
C	-0.72935	1.190596	-0.00139
O	-8.48062	0.310934	-3.92856
O	-11.2929	0.097072	-1.12594
O	-6.21927	-0.29748	3.932113
O	-5.94809	-3.679	1.127693
O	-5.94103	3.474817	1.678653
O	-8.7528	3.693443	-1.12406
O	-8.75886	-3.46137	-1.6751
O	9.888519	1.779061	2.68448

O	4.814936	2.173693	-2.37457
O	4.812582	-1.79052	-2.68043
O	9.885165	-2.18416	2.378691
O	11.29314	0.077933	-1.12556
O	6.218727	-0.30802	3.932321
O	3.407963	-0.08942	1.129605
C	0.675375	1.180581	-0.01984
O	8.481373	0.29656	-3.92828
O	8.759192	3.678604	-1.12377
O	8.753139	-3.47621	-1.67481
O	5.94191	-3.68907	1.127892
O	5.946963	3.464743	1.678853
O	9.885581	-1.79383	-2.68027
O	4.812167	-2.18086	2.378529
O	4.81452	1.783361	2.684395
O	9.888935	2.169394	-2.37448
O	11.29296	-0.09608	1.129738
O	6.219374	0.298477	-3.92832
O	3.408144	0.084578	-1.1257
C	0.731012	-1.21243	-0.05188
O	8.480727	-0.30994	3.93236
O	8.752908	-3.69237	1.126865
O	8.758961	3.462283	1.679898
O	5.947193	3.68091	-1.12282
O	5.94214	-3.47275	-1.67578
O	-7.35106	-1.28267	1.556191
O	-7.35079	-1.02897	-1.73204
O	-8.99796	1.170667	0.091446
O	-5.69996	1.167872	0.091502
O	-7.34883	1.296047	-1.55164
O	-7.3491	1.042492	1.73459
O	-8.99993	-1.15343	-0.08787
O	-5.70293	-1.15722	-0.08789
O	7.348932	-1.29513	1.556438
O	7.349202	-1.04142	-1.73179
O	5.702034	1.158211	0.091694
O	9.000033	1.155415	0.091749
O	7.351169	1.28359	-1.5514
O	7.350899	1.030036	1.734837
O	5.701067	-1.16688	-0.0877
O	8.998067	-1.16868	-0.08757
C	-5.17453	2.900615	2.404695
C	-9.51917	3.239546	-1.92743

C	-9.52536	-2.88717	-2.40115
C	-5.18072	-3.2261	1.930976
C	-3.00595	0.00304	0.001848
C	-1.43048	-0.01696	-0.00371
C	-7.3503	-0.32753	4.3339
C	-11.6949	0.010407	0.001703
C	-7.34959	0.340977	-4.33035
C	-5.17418	3.234945	-1.92843
C	-5.18036	-2.89192	-2.40015
C	-9.52571	-3.22149	1.931978
C	-9.51953	2.905371	2.403702
C	9.524464	2.889234	2.404023
C	5.179821	3.22617	-1.92825
C	5.175637	-2.9007	-2.39998
C	9.52028	-3.23763	1.932297
C	11.69505	-0.00941	0.002096
C	7.349694	-0.33998	4.334147
C	3.006051	-0.00199	0.001954
C	1.427157	-0.01004	-0.00225
C	7.350406	0.32852	-4.3301
C	9.52482	3.223408	-1.92711
C	9.520637	-2.9033	-2.40082
C	5.175281	-3.23487	1.93115
C	5.179465	2.891841	2.404869
H	-1.24884	2.14755	0.002341
H	1.25221	-2.17006	-0.07694
H	-4.63093	3.623187	3.004102
H	-10.0615	4.046505	-2.40982
H	-10.069	-3.60974	-3.00055
H	-4.63841	-4.03298	2.412375
H	-7.35039	-0.41	5.415761
H	-12.7809	0.011327	0.001684
H	-7.3495	0.425441	-5.41206
H	-4.63048	4.040905	-2.40981
H	-4.63796	-3.61541	-2.99954
H	-10.0694	-4.02746	2.413358
H	-10.0619	3.628785	3.004088
H	10.06807	3.611729	3.004427
H	4.637512	4.033052	-2.40965
H	4.632035	-3.62327	-2.99938
H	10.06259	-4.04451	2.413696
H	12.78105	-0.01033	0.002114
H	7.349607	-0.42245	5.416008

H	7.350496	0.412985	-5.41181
H	10.06851	4.029447	-2.40948
H	10.06303	-3.6268	-3.00021
H	4.631589	-4.04083	2.412531
H	4.637067	3.615333	3.004258
H	-7.35161	-1.91291	2.314956
H	-7.35121	-1.53535	-2.5785
H	7.348385	-1.92537	2.315203
H	7.348787	-1.54781	-2.57825
H	-4.89348	1.734503	0.135287
H	-9.80248	1.739659	0.135282
H	4.896515	1.726207	0.135452
H	9.805514	1.723045	0.13561
O	-1.24503	-2.46105	-0.06841
H	-2.23562	-2.42629	-0.02213
O	1.259151	2.437798	-0.04301
H	2.116364	2.415529	-0.53121

11. $Zr_6O_4(OH)_4(COOH)_{11}$(2,4-dimethylterephthalate)
$Zr_6O_4(OH)_4(COOH)_{11}$(lowest energy geometry) -
6618.16882441 A.U.

	X	Y	Z
Zr	5.582703	1.763683	0.006227
Zr	9.11829	-1.77772	-0.00613
Zr	5.579291	-1.77431	-0.00613
Zr	9.121701	1.76027	0.006224
Zr	7.349989	-0.01612	2.502539
Zr	7.350002	0.001081	-2.50145
Zr	-9.11829	1.777859	0.006238
Zr	-5.5827	-1.76354	-0.00612
Zr	-9.1217	-1.76013	-0.00612
Zr	-5.57929	1.774447	0.006234
Zr	-7.35	-0.00195	2.50255
Zr	-7.34999	0.015256	-2.50144
O	4.815439	2.525422	1.996857
O	9.884543	-2.55345	1.979228
O	9.884554	-2.53946	-1.99576
O	4.816449	2.539419	-1.97913
O	3.406915	-1.13421	-0.00426
C	0.729391	-1.17332	-0.00084
O	8.484797	3.933882	0.01334
O	11.29409	1.120174	0.004372
O	6.215195	-3.94792	-0.01324
O	5.942633	-1.42331	3.583058
O	5.943651	-1.39901	-3.59193
O	8.75736	1.409277	-3.58296
O	8.757342	1.384966	3.593022
O	4.811556	-2.53457	-1.99676
O	9.889447	2.534521	-1.97814
O	9.889436	2.520529	1.996853
O	4.810546	-2.54856	1.979232
O	3.409096	1.127776	0.004381
C	0.677774	1.237172	-0.00083
O	8.477194	-3.9501	-0.01325
O	11.2919	-1.14181	-0.00428
O	6.222798	3.936063	0.013342
O	5.946362	1.412982	-3.58195
O	5.945342	1.386678	3.593018
O	8.75463	-1.42702	3.58305
O	8.75465	-1.40071	-3.59292
O	-9.88455	2.539598	1.996868

O	-4.81545	-2.53928	1.979239
O	-4.81644	-2.52528	-1.99675
O	-9.88454	2.553589	-1.97812
O	-11.2941	-1.12003	-0.00426
O	-6.2152	3.948057	0.013351
O	-3.40692	1.134348	0.004389
C	-0.72939	1.173423	0.001354
O	-8.4848	-3.93374	-0.01323
O	-8.75736	-1.41014	3.583063
O	-8.75734	-1.38383	-3.59291
O	-5.94363	1.424448	-3.58195
O	-5.94265	1.398142	3.593027
O	-9.88944	-2.52039	-1.99575
O	-4.81155	2.548703	-1.97912
O	-4.81056	2.534705	1.996864
O	-9.88945	-2.53439	1.979243
O	-11.2919	1.141955	0.004389
O	-6.2228	-3.93592	-0.01323
O	-3.4091	-1.12763	-0.00428
C	-0.67776	-1.23706	-0.00287
O	-8.4772	3.950239	0.013353
O	-8.75463	1.426165	-3.58295
O	-8.75465	1.401853	3.593035
O	-5.94536	-1.41185	3.583067
O	-5.94634	-1.38754	-3.59192
O	7.35159	1.646017	-1.1605
O	7.348409	-1.65198	-1.1714
O	8.998993	-0.01265	1.166544
O	5.700994	-0.00947	1.166547
O	7.348404	-1.65905	1.160599
O	7.351583	1.636942	1.171492
O	8.998999	-0.00458	-1.16445
O	5.702	-0.00139	-1.16545
O	-7.3484	1.660192	-1.16049
O	-7.35158	-1.6378	-1.17139
O	-5.701	0.001528	1.166555
O	-8.999	0.004708	1.166557
O	-7.35159	-1.64488	1.16061
O	-7.34841	1.651117	1.171503
O	-5.702	0.009604	-1.16544
O	-8.99899	0.012777	-1.16444
C	5.179085	2.157529	3.079658
C	9.519893	-2.19165	3.06543

44

C	9.520908	-2.17156	-3.07956
C	5.1801	2.177617	-3.06533
C	3.005966	-0.00283	0.000533
C	1.421504	0.038899	0.002789
C	7.354186	4.337971	0.014773
C	11.69499	-0.01121	0.000545
C	7.345806	-4.35201	-0.01468
C	5.174894	-2.18846	3.064427
C	5.175911	-2.16637	-3.08055
C	9.525099	2.174421	-3.06433
C	9.524082	2.152333	3.080648
C	-9.51991	2.170698	3.080663
C	-5.1791	-2.17847	3.064435
C	-5.18008	-2.15638	-3.08054
C	-9.52089	2.192788	-3.06432
C	-11.695	0.011345	0.000563
C	-7.34581	4.352147	0.014784
C	-3.00597	0.002966	0.000558
C	-1.4215	-0.03879	0.002739
C	-7.35419	-4.33783	-0.01467
C	-9.5241	-2.17329	3.065444
C	-9.52508	-2.1532	-3.07955
C	-5.1759	2.187604	-3.06533
C	-5.17491	2.167514	3.079665
H	1.306702	-2.1039	-0.00852
H	-1.30671	2.104025	-0.00439
H	4.636606	2.697426	3.847928
H	10.06237	-2.73781	3.83115
H	10.06339	-2.71146	-3.84783
H	4.637625	2.722766	-3.83006
H	7.355233	5.422963	0.019322
H	12.78099	-0.01226	0.000544
H	7.34476	-5.43701	-0.01723
H	4.63137	-2.73256	3.830154
H	4.63239	-2.70522	-3.84882
H	10.06862	2.718523	-3.82906
H	10.0676	2.692182	3.848924
H	-10.0624	2.711594	3.848938
H	-4.63663	-2.72363	3.830161
H	-4.63761	-2.69628	-3.84881
H	-10.0634	2.737937	-3.82904
H	-12.781	0.012393	0.000563
H	-7.34476	5.437138	0.019333

H	-7.35523	-5.42283	-0.01721
H	-10.0676	-2.7184	3.831165
H	-10.0686	-2.69205	-3.84782
H	-4.63237	2.731705	-3.83005
H	-4.63139	2.706363	3.847934
H	7.352367	2.452454	-1.72764
H	7.347634	-2.45553	-1.74426
H	-7.34763	2.46663	-1.72763
H	-7.35236	-2.44136	-1.74425
H	4.894993	-0.01113	1.735543
H	9.80399	-0.01587	1.736539
H	-4.895	-0.00168	1.73555
H	-9.804	0.003044	1.736554
C	-1.30563	-2.59091	-0.01566
H	-1.96785	-2.71156	-0.89084
H	-1.95105	-2.74266	0.864748
H	-0.57532	-3.40674	-0.03797
C	1.305654	2.591024	-0.01152
H	0.575392	3.406855	-0.03537
H	1.970298	2.712177	-0.88477
H	1.948667	2.742286	0.870765

12. Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(2,4-dimethylterephthalate)
Zr$_6$O$_4$(OH)$_4$(COOH)$_{11}$(Highest energy geometry) -
6618.15990954 A.U.

	X	Y	Z
Zr	-5.58093	-0.00048	1.769069
Zr	-9.11992	0.014988	-1.76892
Zr	-5.58093	0.011345	-1.76892
Zr	-9.11993	0.003161	1.769072
Zr	-7.34735	2.509746	0.008075
Zr	-7.3525	-2.49424	-0.00892
Zr	9.120058	-0.01561	1.769057
Zr	5.581069	-0.00014	-1.76893
Zr	9.120067	-0.00378	-1.76893
Zr	5.58106	-0.01197	1.76906
Zr	7.352638	2.494621	0.008063
Zr	7.34749	-2.50936	-0.00894
O	-4.81089	1.98411	2.543656
O	-9.88488	2.006385	-2.53033
O	-9.88897	-1.9686	-2.54351
O	-4.81598	-1.99188	2.530478
O	-3.40793	0.006611	-1.13093
C	-0.70891	1.198275	0.001227
O	-8.48094	-0.00523	3.942066
O	-11.2929	0.007907	1.131076
O	-6.21892	0.01974	-3.94192
O	-5.94023	3.598419	-1.39306
O	-5.94862	-3.57656	-1.41779
O	-8.75962	-3.58391	1.393206
O	-8.75224	3.592066	1.41794
O	-4.81597	-1.97482	-2.54351
O	-9.88898	-1.98566	2.530483
O	-9.88489	1.989331	2.54366
O	-4.81088	2.001165	-2.53033
O	-3.40794	-0.0002	1.131069
C	-0.70144	-1.21479	-0.001
O	-8.48092	0.022067	-3.94191
O	-11.2929	0.014714	-1.13092
O	-6.21894	-0.00756	3.942064
O	-5.94862	-3.58581	1.394204
O	-5.94024	3.589174	1.416938
O	-8.75223	3.601313	-1.39405
O	-8.75962	-3.57467	-1.41679
O	9.889101	1.968984	2.543643

O	4.815117	1.99126	-2.53034
O	4.812026	-1.98473	-2.54352
O	9.885011	-2.006	2.530467
O	11.29306	-0.00853	-1.13094
O	6.219053	-0.02036	3.942054
O	3.408063	-0.00722	1.131064
C	0.709299	-1.19418	-0.001
O	8.481074	0.004614	-3.94193
O	8.759758	3.583294	-1.39407
O	8.752374	-3.59269	-1.4168
O	5.94137	-3.59804	1.394194
O	5.947753	3.576942	1.416928
O	9.885024	-1.98895	-2.54352
O	4.812013	-2.00178	2.53047
O	4.815104	1.974205	2.543648
O	9.889114	1.986039	-2.53035
O	11.29306	-0.01533	1.131057
O	6.219075	0.006942	-3.94193
O	3.40807	-0.00041	-1.13093
C	0.700307	1.217939	0.001194
O	8.481052	-0.02269	3.942052
O	8.752367	-3.60193	1.393191
O	8.759751	3.574047	1.417926
O	5.94776	3.586187	-1.39307
O	5.941377	-3.58879	-1.4178
O	-7.35113	-1.16456	1.645139
O	-7.35112	-1.15293	-1.65285
O	-8.99773	1.175447	0.004009
O	-5.69973	1.172053	0.004006
O	-7.34872	1.179067	-1.64399
O	-7.34873	1.167433	1.652003
O	-9.00013	-1.15555	-0.00385
O	-5.70313	-1.15994	-0.00386
O	7.348859	-1.17969	1.645127
O	7.348868	-1.16805	-1.65287
O	5.702265	1.160321	0.003996
O	9.000263	1.156928	0.003994
O	7.351268	1.163941	-1.644
O	7.351259	1.152308	1.651991
O	5.700865	-1.17167	-0.00387
O	8.997864	-1.17407	-0.00387
C	-5.17378	3.069772	2.183523
C	-9.51876	3.089715	-2.16146

C	-9.52608	-3.05527	-2.18337
C	-5.1811	-3.07521	2.161613
C	-3.00593	0.003267	0.000074
C	-1.41783	-0.00529	0.000012
C	-7.34994	-0.00772	4.345065
C	-11.6949	0.012224	0.000079
C	-7.34992	0.022225	-4.34491
C	-5.17376	3.084245	-2.16247
C	-5.18109	-3.06074	-2.18238
C	-9.52609	-3.06974	2.162617
C	-9.51877	3.075244	2.182527
C	9.525219	3.055648	2.182512
C	5.180231	3.073591	-2.16248
C	5.174908	-3.07139	-2.18239
C	9.519896	-3.08934	2.162601
C	11.69506	-0.01184	0.00006
C	7.350052	-0.02284	4.345052
C	3.006061	-0.0029	0.000065
C	1.41771	0.00848	0.000087
C	7.350075	0.0071	-4.34493
C	9.52523	3.07012	-2.16148
C	9.519907	-3.07486	-2.18339
C	5.174897	-3.08586	2.161604
C	5.18022	3.059118	2.183514
H	-1.25194	2.141065	0.002069
H	1.25621	-2.13667	-0.00178
H	-4.62999	3.833778	2.728134
H	-10.061	3.859705	-2.70185
H	-10.0699	-3.81927	-2.72798
H	-4.63889	-3.8442	2.700998
H	-7.34994	-0.01059	5.430063
H	-12.7809	0.013342	0.00008
H	-7.34991	0.027092	-5.42991
H	-4.62997	3.853117	-2.70185
H	-4.63887	-3.82586	-2.72699
H	-10.0699	-3.83761	2.702004
H	-10.061	3.840366	2.728139
H	10.06901	3.819653	2.728122
H	4.638023	3.843581	-2.70186
H	4.631121	-3.8354	-2.727
H	10.06211	-3.85833	2.701987
H	12.78106	-0.01296	0.000059
H	7.35005	-0.02571	5.43005

H	7.350079	0.011967	-5.42992
H	10.06902	3.838993	-2.70186
H	10.06212	-3.83999	-2.728
H	4.631107	-3.85374	2.700991
H	4.638007	3.824242	2.728126
H	-7.35172	-1.7372	2.447682
H	-7.35171	-1.72028	-2.46031
H	7.348271	-1.75233	2.44767
H	7.348284	-1.73541	-2.46032
H	-4.89314	1.740223	0.00546
H	-9.80214	1.746274	0.005465
H	4.896851	1.730149	0.005452
H	9.805849	1.726098	0.005448
C	1.429716	2.524324	0.002084
H	2.066909	2.615639	-0.89007
H	2.06907	2.613608	0.892799
H	0.753316	3.387877	0.004001
C	-1.43431	-2.51652	-0.00204
H	-0.76783	-3.3859	-0.00067
H	-2.08431	-2.59878	-0.88816
H	-2.08745	-2.59843	0.881832