

**Supplementary Information for
Heterolytic C–H activation routes in catalytic dehydrogenation of light
alkanes on Lewis acid-base pairs at ZrO₂ surfaces**

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S1. Surface area assessments

The surface areas of the ZrO_2 samples were measured from N_2 uptakes at its normal boiling point by nitrogen physisorption (77 K) using a 3Flex analyzer (Micromeritics) after evacuation in dynamic vacuum (10^{-5} bar) at 473 K for 4 h. Applying the Brunauer-Emmet-Teller equation to the isotherms showed that the synthesized $m\text{-ZrO}_2$ catalyst treated at 723 K in He expressed a surface area of $130 \text{ m}^2 \text{ g}^{-1}$. The commercial Saint-Gobain $m\text{-ZrO}_2$ expressed a surface area of $112 \text{ m}^2 \text{ g}^{-1}$.

S2. X-ray diffraction

The crystal structure and crystallite size of ZrO_2 were determined by X-ray diffraction (Rigaku Miniflex, $\text{Cu-K}\alpha$ radiation) in the 2θ range of $20\text{--}80^\circ$ with a step scan of $0.01^\circ \text{ s}^{-1}$. The diffractogram in Figure S1 illustrates the formation of $m\text{-ZrO}_2$ crystallites of 6.7 nm, assessed by Rietveld refinement and the Scherrer equation.

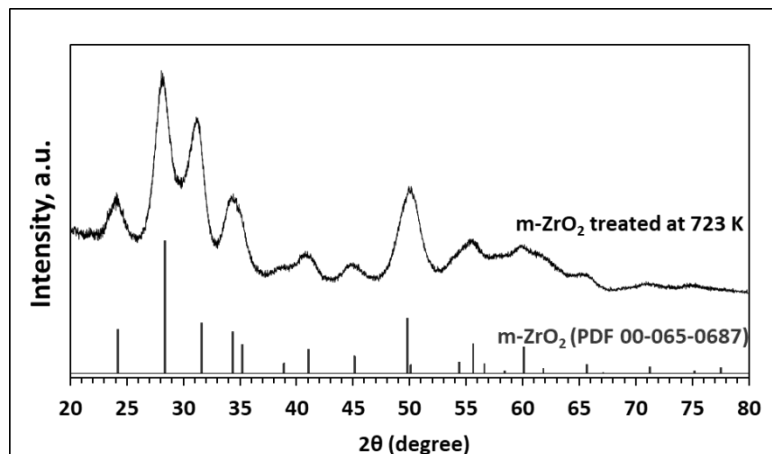


Figure S1. XRD pattern of $m\text{-ZrO}_2$ after treatment at 723 K compared to the PDF card of $m\text{-ZrO}_2$.

S3. Active site titrations by H_2O

Active sites were titrated by H_2O by flowing a He stream (99.999%, Praxair, $0.167\text{--}0.833 \text{ cm}^3 \text{ s}^{-1}$) through a H_2O -containing ($18.2 \text{ M}\Omega\text{-cm}$) vapor-liquid-equilibrium saturator, positioned within an ice-water bath. The gaseous stream passed through a sample loop (423 K , 1 cm^3), attached to a 6-way VICI valve. The $\text{H}_2\text{O}/\text{He}$ mixture charged within the loop was introduced onto the catalyst as pulse(s) into flowing reactant stream ($\text{C}_3\text{H}_8\text{-H}_2\text{-He}$ mixture, $0.833 \text{ cm}^3 \text{ g}^{-1} \text{ s}^{-1}$). The concentrations of all species in the inlet and outlet streams were measured by gas chromatography and also from fragmentation patterns in a mass spectrometer (MKS CirrusTM 3) using deconvolution methods. These analytical methods were used during chemical treatments, catalytic rate measurements, and site titrations.

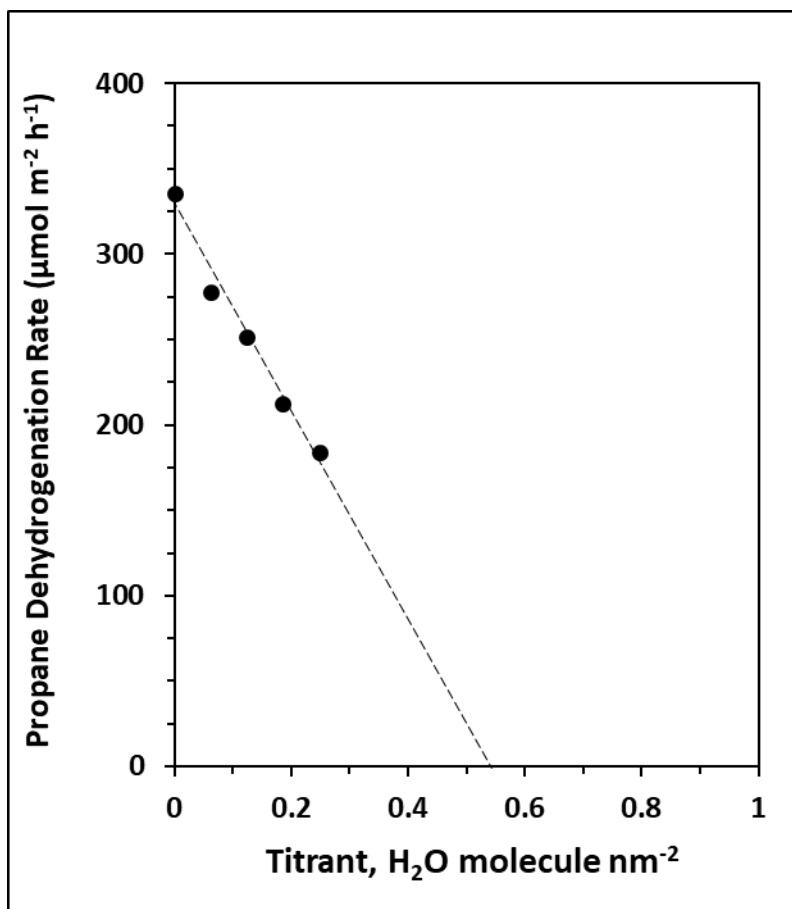


Figure S2. Propane dehydrogenation rates (15 kPa C₃H₈, 723 K) as a function of titrant molecules injected into the reactor via sample loop during reaction. The results implicate the presence of 0.56 active sites per nm² on the *m*-ZrO₂ sample.

S4. Additional supporting data

Mass dilution ratios of 1-to-20 catalyst-to-diluent (quartz sand) were sufficient to prevent observable effects of bed-scale temperature gradients on rates, as the measured rates become insensitive to further dilution. The potential for temperature gradients to impart effects on the bed scale was estimated from the data previously provided Chin criterion. Avoiding bed-scale temperature gradients requires that the ratio of the heat released in the bed to the external surface area of the catalyst bed be less than 0.4 W cm⁻² (the threshold computed from the data provided in the publication). Under the highest rates measured and under dilution typically utilized (1-to-50 catalyst-to-diluent), the maximum heat released in these experiments was 0.007 W cm⁻² which is less than the criterion previously determined.

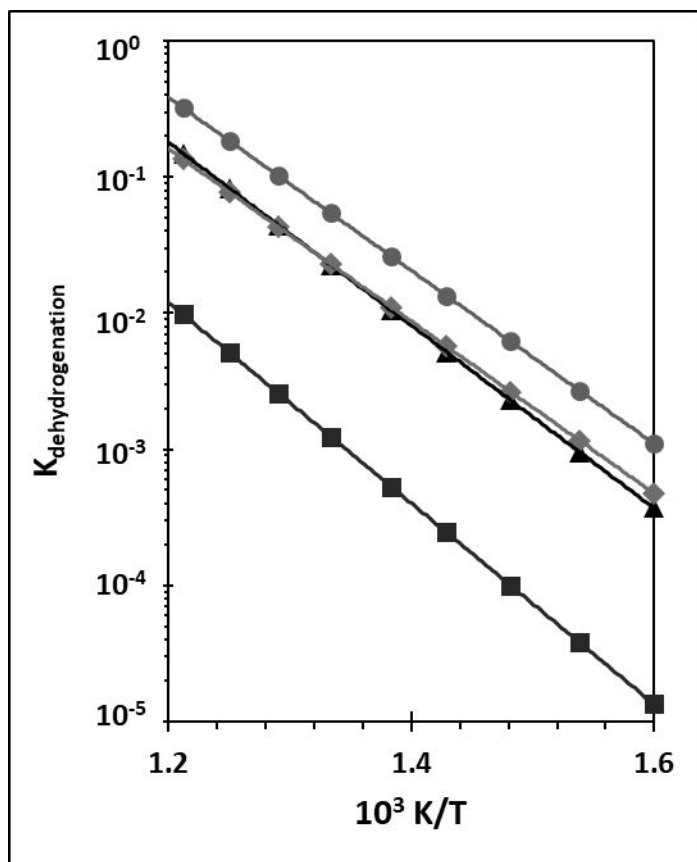


Figure S3. Alkane dehydrogenation equilibrium constants as a function of temperature for C_2H_6 (squares), C_3H_8 (triangles), $n\text{C}_4\text{H}_{10}$ (diamonds), and $i\text{C}_4\text{H}_{10}$ (circles)

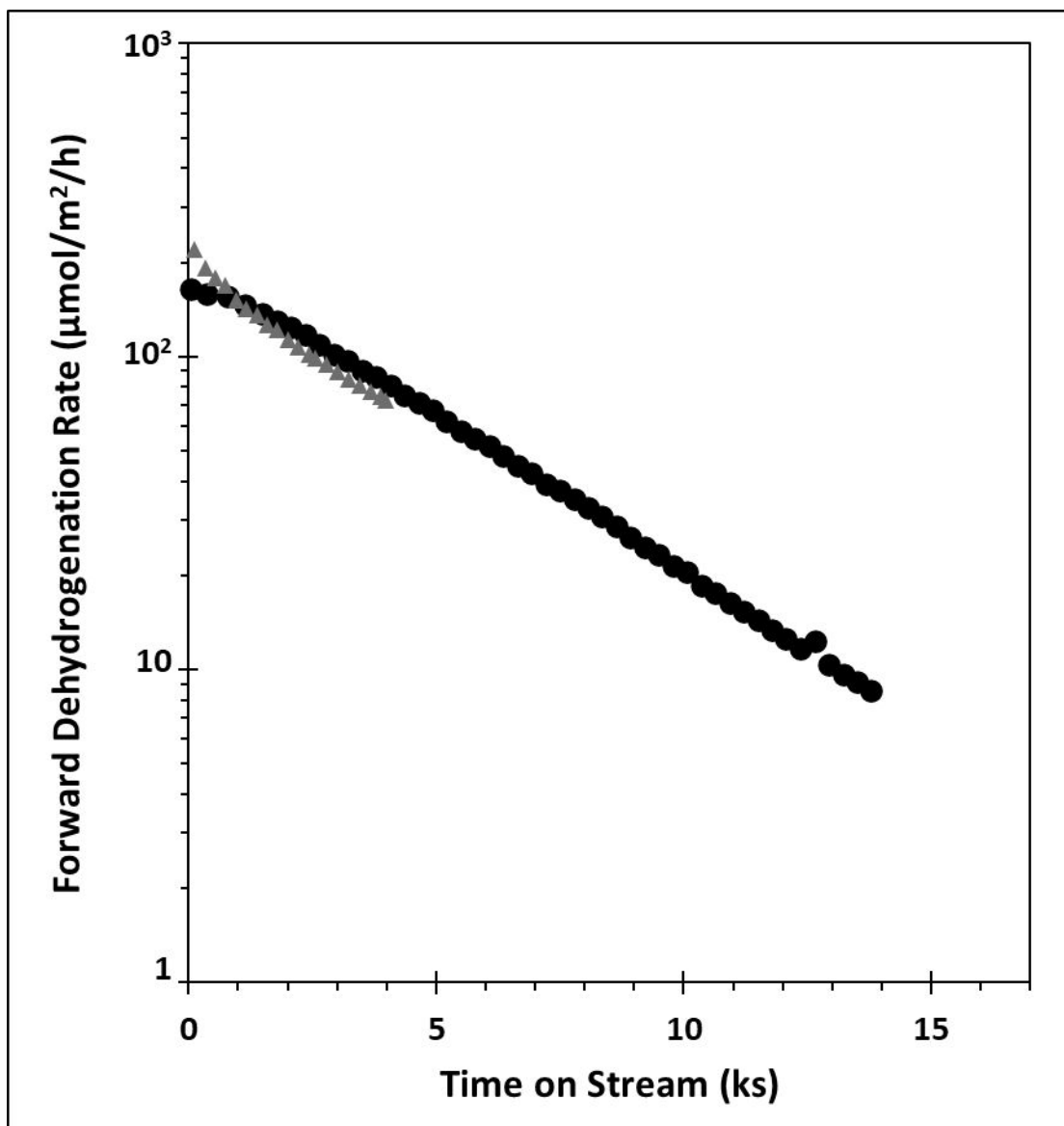


Figure S4. Propane dehydrogenation rate over time on stream after DME treatments on the Saint Gobain (black circles) and as-synthesized (grey triangles) ZrO_2 under 15.2 kPa C_3H_8 , 5.1 kPa H_2 , and 723 K. Rates are not corrected for deactivation imposed by trace O_2 or H_2O in the gas stream. The lower initial deactivation of the Saint Gobain test is due to residual DME-that was still being purged in the first several s of reaction and still activating the catalyst.

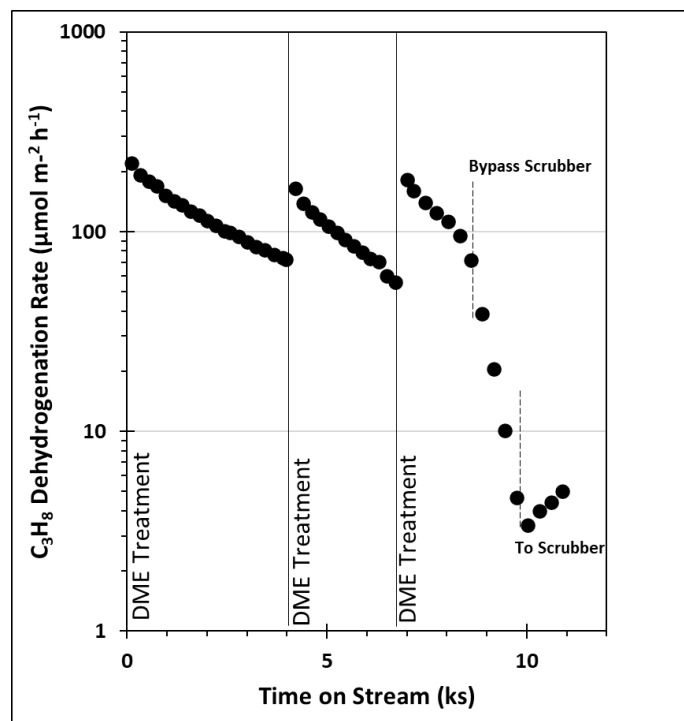


Figure S5. C_3H_8 dehydrogenation rates on $m\text{-ZrO}_2$ after successive DME treatments (723 K). The last panel depicts the faster deactivation induced by a higher concentration of influent impurities from bypassing the scrubber and self-activation from product propene molecules upon reduction of titrant concentration by passing through the scrubber. 15.2 kPa C_3H_8 , 5.1 kPa H_2 , 723 K.

Experiments with $\text{C}_3\text{H}_8\text{-D}_2$ reactant mixtures can be used to infer the extent to which the initial C–H activation step is reversible during dehydrogenation turnovers by comparing the rates of D-incorporation into C_3H_8 reactants and of their chemical conversion to propene. C_3H_8 dehydrogenation rates on DME-treated $m\text{-ZrO}_2$ (extrapolated to the time of initial contact with reactants) were about five-fold higher than for D-insertion into C_3H_8 (Fig. S6; 723 K), suggesting. In addition, D-introduction rates remained constant, or perhaps slightly increased, with time, while dehydrogenation rates decreased about 3.5-fold over a period of 0.9 ks (because of the titration of Zr–O site pairs by H_2O , CO_2 , O_2 trace impurities in the inlet stream). These data show that the deuteration of unreacted propane molecules occurs on sites distinct from those that activate C–H bonds most competently and that such sites do not interact strongly with titrants, thus rendering them unaffected by titrant presence in reactant streams. Such sites that facilitate deuteration may be surface carbonaceous species or hydroxyl groups. Therefore, the Zr–O pairs responsible for dehydrogenation turnovers mediate such routes through steps that preclude the re-introduction of a different hydrogen isotope in reversing C–H cleavage elementary steps. These results, however, do not unequivocally demonstrate the irreversible nature of C–H cleavage events, because the reverse steps may merely react the alkyl fragment with the same H-atom formed in the cleavage step before such an atom can isotopically exchange with D_2 .

$\text{H}_2\text{-D}_2$ exchange rates on $m\text{-ZrO}_2$ at 723 K (Fig. S6; SI) also show that exchange occurs via routes unrelated to those that activate C–H bonds and recombine H-atoms in catalytic

dehydrogenation turnovers. Forward (and background-subtracted) $\text{H}_2\text{-D}_2$ exchange rates on $m\text{-ZrO}_2$ are similar on samples treated in He or DME treatments at 723 K; these treatments led to 140-fold higher C_3H_8 dehydrogenation rates on DME-treated samples. The introduction of H_2O pulses (1, 3, or 5 pulses; each $0.3\ \mu\text{mol H}_2\text{O}$ or $0.05\ \text{H}_2\text{O}\cdot(\text{active site})^{-1}$ in this experiment with 50 mg ZrO_2 , as measured by H_2O titration experiments; SI, Section S3) or DME pulses (3 pulses of $2\ \mu\text{mol}$ each; $0.3\ \text{C}_2\text{H}_6\text{O}\cdot(\text{active site})^{-1}$) during reaction at 723 K did not influence $\text{H}_2\text{-D}_2$ exchange rates (on-stream pulses shown in Fig. S6). This contrasts C_3H_8 dehydrogenation experiments which decrease in proportion to the number of H_2O molecules in each pulse (see Section S3, SI).

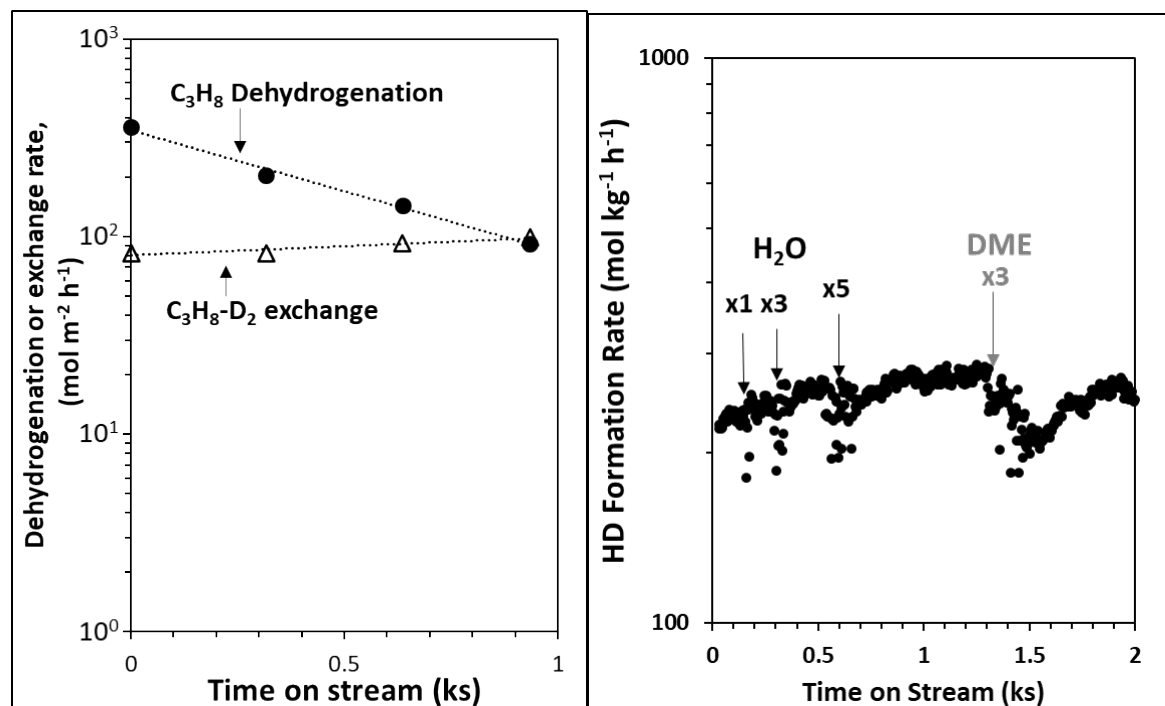


Figure S6. Left) C_3H_8 dehydrogenation (closed circles) and $\text{C}_3\text{H}_8\text{-D}_2$ exchange (open triangles) rate on DME-treated $m\text{-ZrO}_2$ as a function of time on stream at 15 kPa C_3H_8 , 2.5 kPa D_2 at 723 K. Dashed lines indicate exponential regression to guide the eye. Right) $\text{H}_2\text{-D}_2$ exchange rates on $m\text{-ZrO}_2$ as a function of time on stream during 1, 3, and 5 pulses of H_2O or 3 pulses of DME ($1\ \text{cm}^3$ sample loop) at 5 kPa H_2 , 5 kPa D_2 at 723 K.

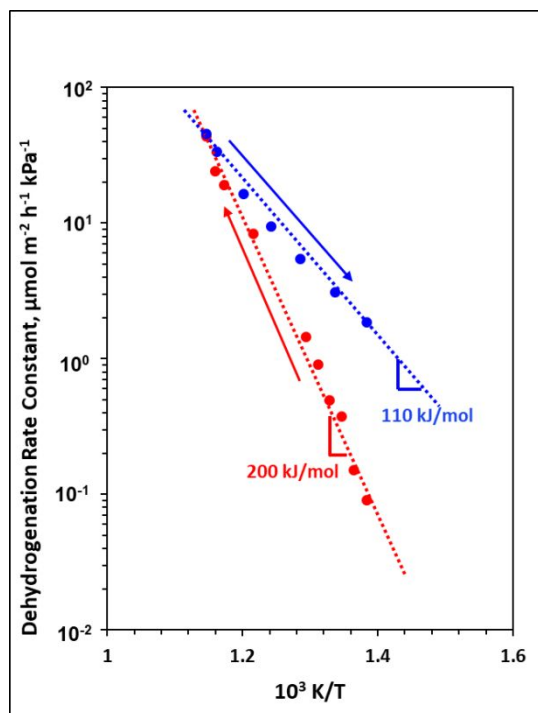


Figure S7. Arrhenius dependence of C_3H_8 dehydrogenation rate constants on thermally-treated yttria-stabilized ZrO_2 during an increasing temperature ramp (red) and subsequent decreasing temperature ramp (blue).

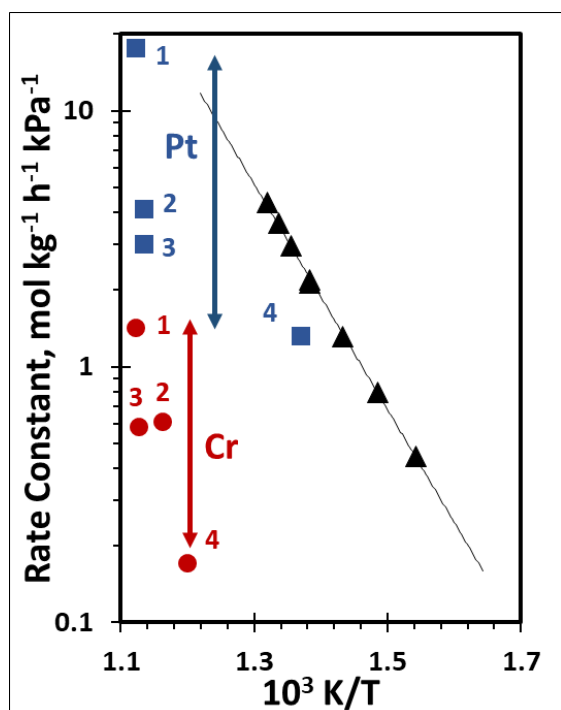


Figure S8. C_3H_8 dehydrogenation rate constants (per mass) of DME-treated $m-ZrO_2$ (black triangles) compared to several Cr- (red circles) and Pt-based (blue squares) catalysts from the literature.

Cr-based catalyst literature:

¹*RSC Adv.*, 4, 37107 (2014)

²*Molec. Catal.*, 493 111052 (2020)

³*J. Catal.*, 40, 184 (2019)

⁴*Int. Sci. J. Alt. Energy Ecol.*, 2, 98 (2009)

Pt-based catalyst literature:

¹*Appl. Catal. A*, 400, 25 (2011)

²*ACS Catal.*, 4, 1812 (2014)

³US6,756,340 B2

⁴*Nat. Mater.*, 18, 866 (2019)

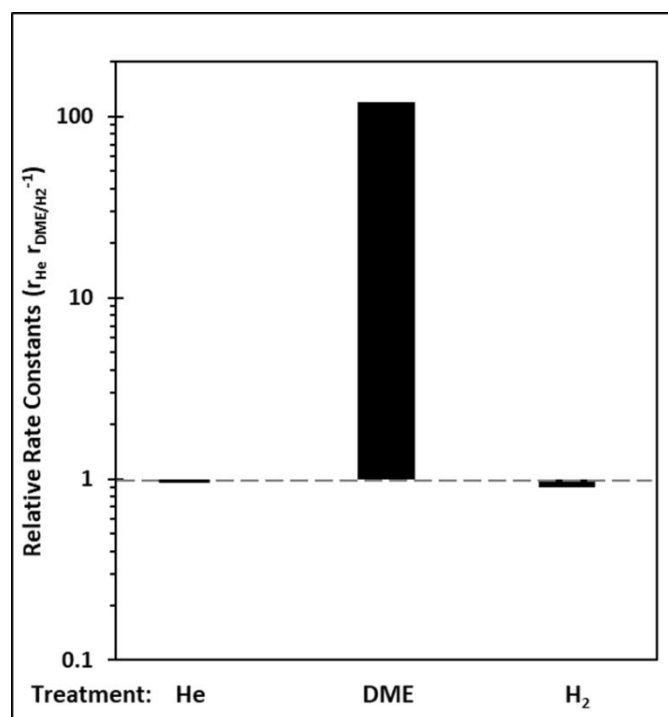


Figure S9. Relative rate constants for C_3H_8 dehydrogenation on ZrO_2 at 723 K after treatment in He, DME, and H_2 .

The same general trends are evident for other alkanes (e.g., $n\text{C}_4\text{H}_{10}$), which shows increasing selectivity to dehydrogenation at lower temperatures, but with a cracking barrier estimated at only 40 kJ mol^{-1} higher than for dehydrogenation. The smaller difference in β -scission and β -hydride elimination is expected from gas phase thermodynamics of $n\text{-C}_3\text{H}_7$ and $i\text{-C}_4\text{H}_9$ anionic fragments, where the difference in the two competing pathway reaction energies for each species are -26 and -22 kJ mol^{-1} , respectively. C–H bond heterolysis and the anionic nature of the alkyl fragments bound at Zr–O LAB pairs leads to relative rates of β -hydride abstraction and β -scission of C–C bonds that differ markedly from those in homolytic routes that form radical-like alkyls and heterolytic routes that form alkyl carbenium ions. As a result, reactions of C_3H_8 on $m\text{-ZrO}_2$ selectively forms C_3H_6 over $\text{CH}_4/\text{C}_2\text{H}_4$ (Fig. 5). Such preferences

are also evident from the reaction energies for cleaving C–H and C–C bonds in C_3H_8 when comparing homolytic and heterolytic cleavage in gaseous molecules (Table 2).

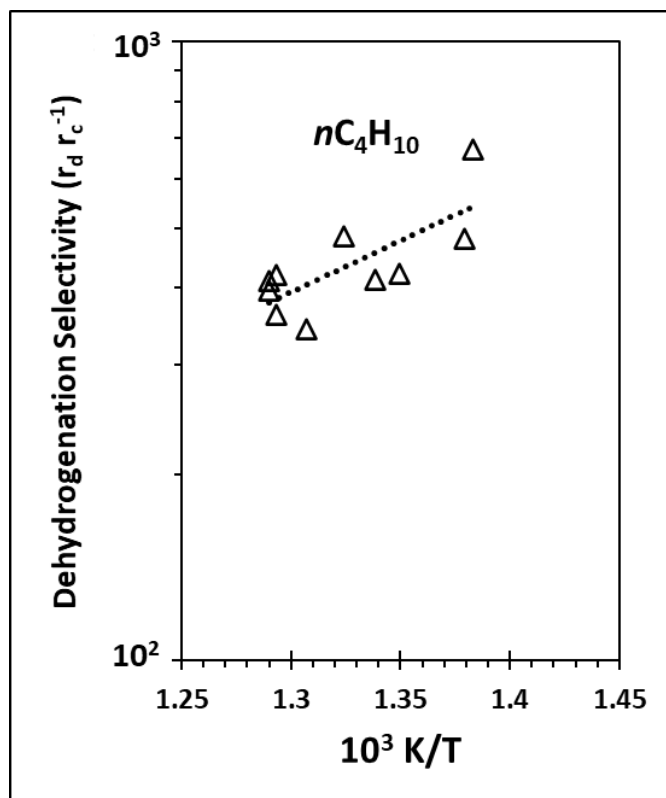


Figure S10. nC_4H_{10} (open triangles) dehydrogenation selectivity on DME-treated $m\text{-ZrO}_2$. 15 kPa nC_4H_{10} and 5.1 kPa H_2 . Dashed lines from exponential regression.

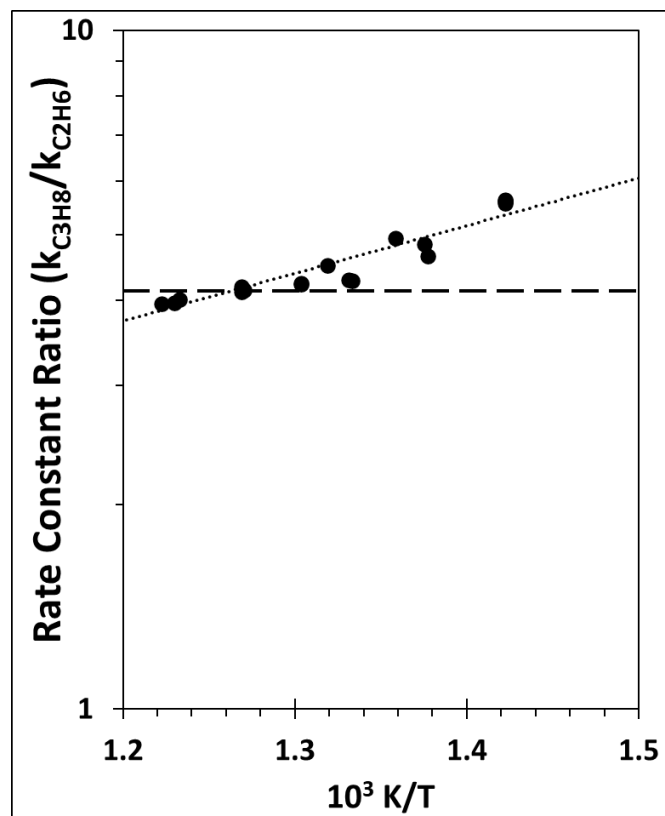


Figure S11. Relative rate constants for C_3H_8 and C_2H_6 dehydrogenation using mixtures of the two alkanes on $m\text{-ZrO}_2$ as a function of temperature (700-873 K, increasing and decreasing temperature cycles; 10 kPa C_2H_6 , 5 C_3H_8 , and 5 kPa H_2). Dotted line indicates exponential regression. The thick dashed line (- -) indicates the ratio from individual experiments.

S.5 Synthesis of Hf-doped ZrO_2

Hf-doped ZrO_2 catalysts were prepared in a fashion similar to the hydrothermal synthesis method of $m\text{-ZrO}_2$. Typically, a powdered mixture of 20.6 (12.1) g of $ZrO(NO_3)_2 \cdot xH_2O$ (Sigma-Aldrich, 99%) and 1.3 (1.0) g of $HfCl_4$ ($Hf(NO_3)_4$) and a separate 21.6 g of $CO(NH_2)_2$ (Sigma-Aldrich, 99.5%) were each dissolved in 30 cm^3 H_2O (18.2 $M\Omega\text{-cm}$) at 323 K. The solutions were mixed and placed within a 125 cm^3 Teflon liner and sealed within a Parr autoclave. The mixture was held at 393 K for 20 h as the $CO(NH_2)_2$ decomposed, resulting in an increase in pH and subsequent precipitation of Hf-Zr oxyhydroxides. The resulting material was rinsed with H_2O (18.2 $M\Omega\text{-cm}$) and centrifuged (8000 rpm) four times prior to treatment in stagnant ambient air at 393 K for 12 h. The resulting (1:11 atomic ratio) Hf- ZrO_2 made by either $HfCl_4$ (Hf- $ZrO_{2,Cl}$) or $Hf(NO_3)_4$ (Hf- ZrO_{2,NO_3}) were determined to have a surface area of 105.4 and 41.8 $m^2\text{ g}^{-1}$, respectively. In addition to low surface area, the Hf- ZrO_{2,NO_3} sample was tan in color and exhibited propane dehydrogenation reactivity nearly two orders of magnitude lower than the $m\text{-ZrO}_2$.

Impurity species were considered as potential active sites on ZrO_2 . Impurities are of particular interest due to the known challenges of separating Hf from Zr due to their similar chemical nature, where 2% Hf may be present in the Zr precursors. Though the chemical

properties of the two elements are similar, they exhibit notably different atomic radii (160 and 225 nm for Zr and Hf, respectively). The disruption of the lattice by elements of non-matching size can lead to unique reactive properties.⁶⁸⁻⁶⁹ Such site generation is not anticipated due to the similar areal rates achieved by ZrO₂ sourced from commercial suppliers and our synthesized material, but Hf-doped ZrO₂ catalysts were also synthesized to assess the potential impacts of Hf on the reactivity of ZrO₂. The 5% Hf-ZrO₂ 1:11 atomic ratio) material exhibited a surface area of 105.4 m² g⁻¹ and benefited from DME-treatments, resulting in C₃H₈ dehydrogenation rates of 14 mol kg⁻¹ h⁻¹ (723 K, 7 kPa C₃H₈, 5.1 kPa H₂) and a measured activation barrier of 85 kJ mol⁻¹, comparable to that of DME-treated *m*-ZrO₂. These nearly indistinguishable results preclude contributions to the rate by Hf.

69. Cleave, A. R. Atomic Scale Simulation for Waste Form Applications. Imperial College of Science, Technology and Medicine, 2006.

70. Zhang, Y. C., et al., Regulating the C-H Bond Activation Pathway over ZrO₂ Via Doping Engineering for Propane Dehydrogenation. *Acs Catal* **2023**, *13*, 6893-6904.

S6. H₂ temperature programmed reduction (TPR) measurements

H₂ TPR experiments were conducted with a Quantasorb QS-10 equipped with a cold trap (273 K) packed with molecular sieves. Approximately 0.2 g of ZrO₂ (123 m², corresponding to ~27 μmol sites in the sample, as measured by H₂O titration, which is comparable to the 58 μmol of H₂ shown to reduce the CuO/Al₂O₃ standard with well-defined and intense features), thermally treated in 20 kPa O₂ at 723 K for h (0.16 K s⁻¹), was placed in a quartz U-tube in the apparatus. The catalyst was subjected to flowing He treatments (6.67 cm³ g⁻¹ s⁻¹) at 723 K (0.33 K s⁻¹) for 0.5 h to remove physically adsorbed contaminants. The sample was then quickly cooled to ambient temperature and subjected to a flowing stream of 5 kPa H₂ (3.33 cm³ g⁻¹ s⁻¹), purified with an oxygen purifier, during TPR up to 723 K (0.67 K s⁻¹) and held there for 0.3 h. The catalyst was then subjected to flowing He treatments (6.67 cm³ g⁻¹ s⁻¹) at 893 K (0.33 K s⁻¹) for 30 mins to remove physically adsorbed contaminants and allow for particle sintering and annealing that occurs at elevated temperatures to discern any potential H₂ TPR signals from changes to catalyst surface area. The sample was then quickly cooled to 723 K and subjected to a flowing stream of 5 kPa H₂ (6.67 cm³ g⁻¹ s⁻¹) during TPR up to 893 K (0.67 K s⁻¹) and held there for 0.3 h. The Wheatstone bridge current was set at 90 mA during temperature ramps and treatments under He, and 150 mA during the same with H₂. No signals were observed during temperature ramp or treatments with He (detection limit of 0.04 μmol, over a 50 K temperature window). TCD signals collected during H₂ TPR are shown in Figure S12. The results show the absence of any consumption or formation of H₂ during the H₂ TPR experiment on the *m*-ZrO₂ up to 873 K. Given the TCD detection limit of 0.04 μmol and the anticipated presence of 27 μmol of active sites on ZrO₂, there does not appear to be any reduction of Zr, formation of O vacancies, or significant coverage of H₂ on the surface under these conditions, which are directly relevant to those of alkane dehydrogenation evaluated in this study, supporting the identity of the active centers as bare Lewis acid-base pairs.

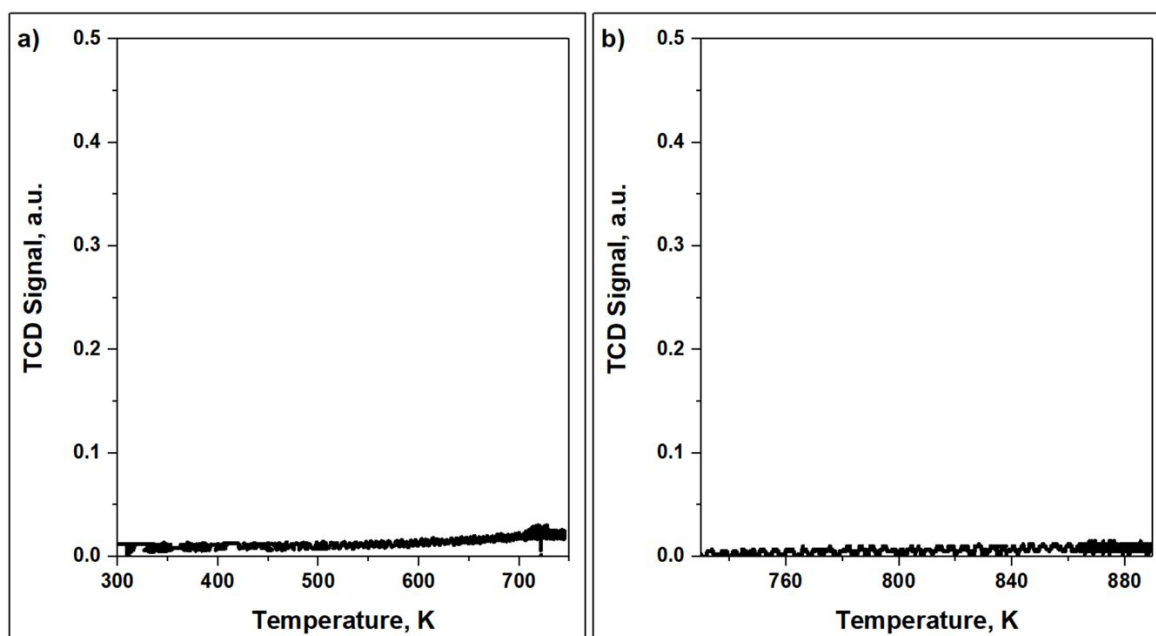


Figure S12. H₂ TPR profiles m-ZrO₂ a) after thermal treatment in He at 723 K and b) after thermal treatment in He at 893 K.

S7. Calculation of enthalpies and entropies using statistical mechanics formalisms

Free energies were computed for a given state as the difference of enthalpy and entropy contributions:

$$G = H - TS \quad (S1)$$

The enthalpy of a given step reflects the sum of contributions from the DFT electronic energy (E_0), the zero-point vibrational enthalpy (E_{ZPV}), and vibrational, translational, and rotational enthalpy (H_{vib} , H_{trans} , and H_{rot}):

$$H = E_0 + E_{ZPV} + H_{vib} + H_{trans} + H_{rot} \quad (S2)$$

DFT-derived vibrational frequencies were used to compute E_{ZPV} and H_{vib} :

$$E_{ZPV} = \sum \frac{1}{2} h \nu_i \quad (S3)$$

$$H_{vib} = \sum \frac{h \nu_i e^{\frac{-h \nu_i}{k_B T}}}{1 - e^{\frac{-h \nu_i}{k_B T}}} \quad (S4)$$

Where h is Planck's constant, ν_i is a vibrational frequency mode, k_B is Boltzmann's constant, and T is temperature. Translational and rotational entropies were computed by:

$$H_{trans} = \frac{1}{2} k_B T \quad (S5)$$

$$H_{rot,linear} = k_B T \text{ or } H_{rot,nonlinear} = \frac{3}{2} k_B T \quad (S6)$$

Entropic contributions can likewise be decomposed into vibrational, translational, and rotational components:

$$S = S_{elec} + S_{vib} + S_{trans} + S_{rot} \quad (S7)$$

Where the contributions are:

$$S_{elec} = R \ln[2S + 1] \quad (S8)$$

Where S is the spin multiplicity (0 for singlet, 0.5 for doublet, 1 for triplet, etc.).

$$S_{vib} = \sum_{i=1}^{3N-5} \left[\frac{h \nu_i e^{\frac{-h \nu_i}{k_B T}}}{T \left(e^{\frac{-h \nu_i}{k_B T}} - 1 \right)} - k_B \ln \left(1 - e^{\frac{-h \nu_i}{k_B T}} \right) \right] \quad (S9)$$

$$S_{trans}^{\circ} = R \left(\ln \left[\left(\frac{2\pi M k_B T}{h^2} \right)^{\frac{3}{2}} \cdot \frac{V^{\circ}}{N_A} \right] + \frac{5}{2} \right) \quad (\text{S10})$$

$$S_{rot} = R \left(\ln \left(\frac{\pi^{0.5}}{\sigma} \left(\frac{T^3}{\theta_x \theta_y \theta_z} \right)^{0.5} \right) + 1.5 \right) \quad (\text{S11})$$

where R is the ideal gas constant, M is the molecular mass of the gaseous molecule, V is the molar volume, and N_A is Avogadro's number. The value σ reports the rotational symmetry numbers for the point group. Values of θ_i were computed using the moments of inertia, I_i, about each axis:

$$\theta_{x,y,z} = \frac{h^2}{8\pi^2 I_{x,y,z} k_B} \quad (\text{S12})$$

S8. Reaction coordinate diagram at differing reaction conditions

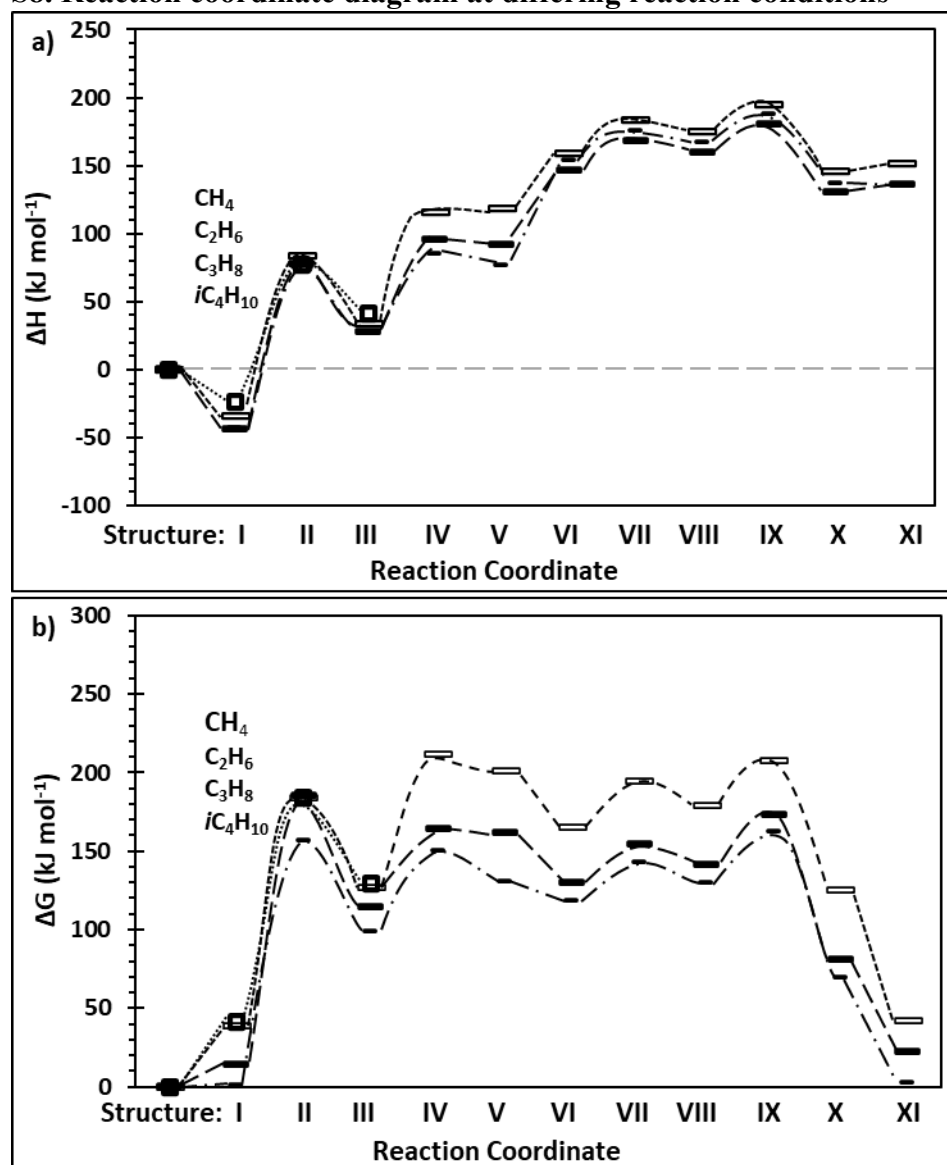


Figure S13. Reaction coordinate diagram showing the change in enthalpy (top) and free energy (bottom) for CH_4 (open squares, $\cdots$), C_2H_6 (open rectangles, $---$), C_3H_8 (large closed rectangles, $---$), and $i\text{C}_4\text{H}_{10}$ (small closed rectangles, $-\cdot-$) dehydrogenation referenced to bare $m\text{-ZrO}_2(-111)$ surface and gaseous alkane at 1 bar and 723 K. Free energies computed for 1 bar of alkanes, alkenes, and H_2 in the gas phase.

Table S1. DFT energies of C₂H₆, C₃H₈, and *i*C₄H₁₀ dehydrogenation on *m*-ZrO₂(-111) at 723 K, 1 bar.

Structure	Description	ΔE (kJ mol ⁻¹)	ΔH (kJ mol ⁻¹)	ΔS (J mol ⁻¹ K ⁻¹)	ΔG (kJ mol ⁻¹)
0	ZrO ₂ , bare	0	0	0	0
I _{C1}	ZrO ₂ , CH ₄ *	-18	-24	-91	+42
II [‡] _{C1}	(ZrO ₂ , CH ₃ *-H*) [‡]	88	77	-147	184
III _{C1}	ZrO ₂ , CH ₃ *-H*	+40	+42	-120	+129
0	ZrO ₂ , bare	0	0	0	0
I _{C2}	ZrO ₂ , C ₂ H ₆ *	-28	-22	-101	39
II [‡] _{C2}	(ZrO ₂ , C ₂ H ₅ *-H*) [‡]	88	84	-138	184
III _{C2}	ZrO ₂ , C ₂ H ₅ *-H*	32	33	-129	127
IV [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ *-2H*) [‡]	131	116	-115	199
V _{C2}	ZrO ₂ , C ₂ H ₄ *-2H*	127	11	-95	182
VI _{C2}	ZrO ₂ , C ₂ H ₄ -2H*	168	159	-8	165
VII [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ -2H**) [‡]	198	184	-15	195
VIII _{C2}	ZrO ₂ , C ₂ H ₄ -2H**	183	175	-5	179
IX [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ -H ₂ *) [‡]	221	195	-17	207
X _{C2}	ZrO ₂ , C ₂ H ₄ -H ₂ *	157	146	30	125
XI _{C2}	ZrO ₂ , C ₂ H ₄ -H ₂	171	152	152	42
0	ZrO ₂ , bare	0	0	0	0
I _{C3}	ZrO ₂ , C ₃ H ₈ *	-36	-44	-80	14
II [‡] _{C3}	(ZrO ₂ , C ₃ H ₇ *-H*) [‡]	90	78	-149	185
III _{C3}	ZrO ₂ , C ₃ H ₇ *-H*	28	27	-121	115
IV [‡] _{C3}	(ZrO ₂ , C ₃ H ₆ *-2H*) [‡]	107	96	-93	163
V _{C3}	ZrO ₂ , C ₃ H ₆ *-2H*	102	92	-95	160
VI _{C3}	ZrO ₂ , C ₃ H ₆ -2H*	156	147	23	130
VII [‡] _{C3}	(ZrO ₂ , C ₃ H ₆ -2H**) [‡]	184	168	20	154
VIII _{C3}	ZrO ₂ , C ₃ H ₆ -2H**	168	160	25	141
IX [‡] _{C3}	(ZrO ₂ , C ₃ H ₆ -H ₂ *) [‡]	204	180	9	173
X _{C3}	ZrO ₂ , C ₃ H ₆ -H ₂ *	145	130	68	81
XI _{C3}	ZrO ₂ , C ₃ H ₆ -H ₂	156	136	158	22
0	ZrO ₂ , bare	0	0	0	0
I _{C4}	ZrO ₂ , C ₄ H ₁₀ *	-40	-43	-60	1
II [‡] _{C4}	(ZrO ₂ , C ₄ H ₉ *-H*) [‡]	82	73	-116	157
III _{C4}	ZrO ₂ , C ₄ H ₉ *-H*	23	28	-98	99
IV [‡] _{C4}	(ZrO ₂ , C ₄ H ₈ *-2H*) [‡]	96	85	-90	150
V _{C4}	ZrO ₂ , C ₄ H ₈ *-2H*	81	77	-74	130
VI _{C4}	ZrO ₂ , C ₄ H ₈ -2H*	145	154	49	118
VII [‡] _{C4}	(ZrO ₂ , C ₄ H ₈ -2H**) [‡]	176	175	45	143
VIII _{C4}	ZrO ₂ , C ₄ H ₈ -2H**	160	167	51	130
IX [‡] _{C4}	(ZrO ₂ , C ₄ H ₈ -H ₂ *) [‡]	199	187	35	162
X _{C4}	ZrO ₂ , C ₄ H ₈ -H ₂ *	135	137	94	69

XI _{C4}	ZrO ₂ , C ₄ H ₈ -H ₂	149	135	183	2
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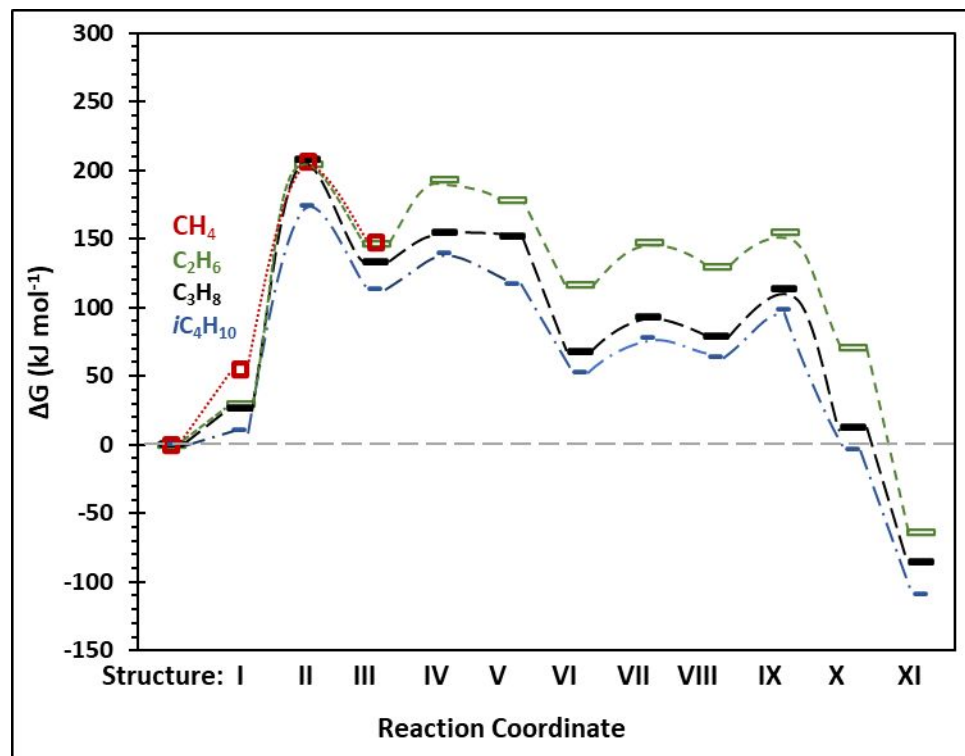


Figure S14. Reaction coordinate diagram (873 K) showing the change in free energy for CH₄ (red open squares, ···), C₂H₆ (green open rectangles, ---), C₃H₈ (black large closed rectangles, - · -), and iC₄H₁₀ (blue small closed rectangles, - · · -) dehydrogenation referenced to bare *m*-ZrO₂(-111) surface and gaseous alkane at 1 bar, 0.001 bar alkenes, and 0.01 bar H₂ in the gas phase.

S9. Sensitivity of the reaction coordinate on selection of entropy treatments

The selection of entropy treatment (potential source ii) also impacts the resulting free energies, particularly at the relatively high temperatures considered here (723 K). Vibrational frequencies calculated using harmonic oscillator formalisms often fail to accurately describe low frequencies modes, resulting in overestimations in the entropy of surface bound species. These matters are typically addressed by replacing the contributions from low frequency modes (typical threshold between 50 and 150 cm⁻¹) a fraction (typically ~0.7) of the corresponding rotational and translational entropy and enthalpy of the gaseous analogs of bound species. To show the potential ranges of free energies for various entropy treatments, our results (using a cutoff of 90 cm⁻¹, based on visual inspection of frequency modes) are compared to a less strict cutoff of 50 cm⁻¹, a treatment replacing the lowest 6 modes (or 5 for models without hydrocarbons) with 0.7 of the gas phase entropy, and a treatment whereby all models are expected to lose one-third of the gas phase translational entropy only. These different treatments (see reaction coordinate diagrams and summary table in Section S10; SI) show that a less strict cutoff allows for a greater propensity for overestimation to corrupt free energies, highlighted by the generally higher free energy of nearly every step and the more disparate C–H activation barriers in II[‡] and IV[‡] (209

and 250 kJ mol⁻¹, respectively). The replacement of all the lowest frequency modes by a portion of the gaseous analog reduces the overall energies, but not the disparities between the two C–H activation steps (147 and 190 kJ mol⁻¹, respectively). The final limiting treatment, using 0.7 of the gas phase S_{trans} for the entropy of adsorbed analogs results in a significant decrease in free energy, particularly after the alkene forms and desorbs, resulting in a decrease in free energy of later steps of the reaction coordinate. These results highlight the potential ranges of free energy expected by use of different treatments of entropy and their impact on the relative energies of intermediates and TS.

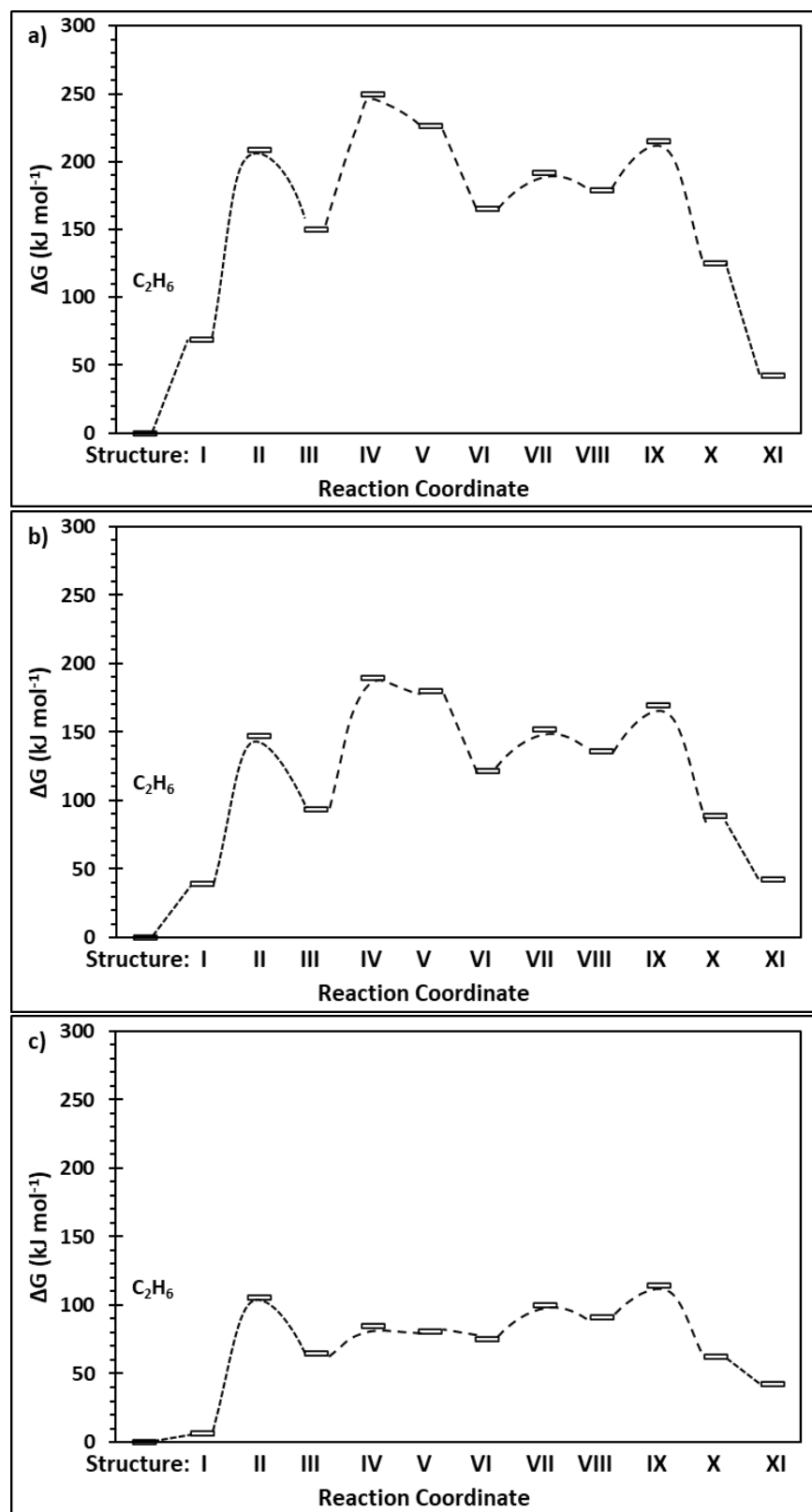


Figure S15. Reaction coordinate diagram showing the change in free energy for C_2H_6 (open rectangles,---) dehydrogenation referenced to bare $m\text{-ZrO}_2(-111)$ surface and gaseous alkane at 1 bar and 723 K using a) a 50 cm^{-1} frequency cutoff for entropy, b) replacing the 6 (or 5 for only adsorbed H_2) lowest frequency

modes with 0.7 of the gas phase rotational and translational entropy, irrespective of value, and c) by replacing ΔS with just -0.3 of the gas phase translational entropy of the adsorbed species.

Table S2. Free energies for C_2H_6 (open rectangles, ---) dehydrogenation using different entropy criteria, analogous to those in Figure S15.

Structure	Description	ΔG (^a 50 cm ⁻¹ cutoff) (kJ mol ⁻¹)	ΔG (^b 6 lowest modes) (kJ mol ⁻¹)	ΔG (^c $\Delta S = -0.3S_{trans, gas}$) (kJ mol ⁻¹)
0	ZrO ₂ , bare	0	0	0
I _{C2}	ZrO ₂ , C ₂ H ₆ *	69	39	7
II [‡] _{C2}	(ZrO ₂ , C ₂ H ₅ *-H*) [‡]	209	147	106
III _{C2}	ZrO ₂ , C ₂ H ₅ *-H*	150	93	65
IV [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ *-2H*) [‡]	250	190	85
V _{C2}	ZrO ₂ , C ₂ H ₄ *-2H*	227	180	81
VI _{C2}	ZrO ₂ , C ₂ H ₄ -2H*	165	121	75
VII [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ -2H**) [‡]	195	152	100
VIII _{C2}	ZrO ₂ , C ₂ H ₄ -2H**	179	136	92
IX [‡] _{C2}	(ZrO ₂ , C ₂ H ₄ -H ₂ *) [‡]	215	170	114
X _{C2}	ZrO ₂ , C ₂ H ₄ -H ₂ *	125	89	63
XI _{C2}	ZrO ₂ , C ₂ H ₄ -H ₂	42	42	42

S10. Supporting computational data

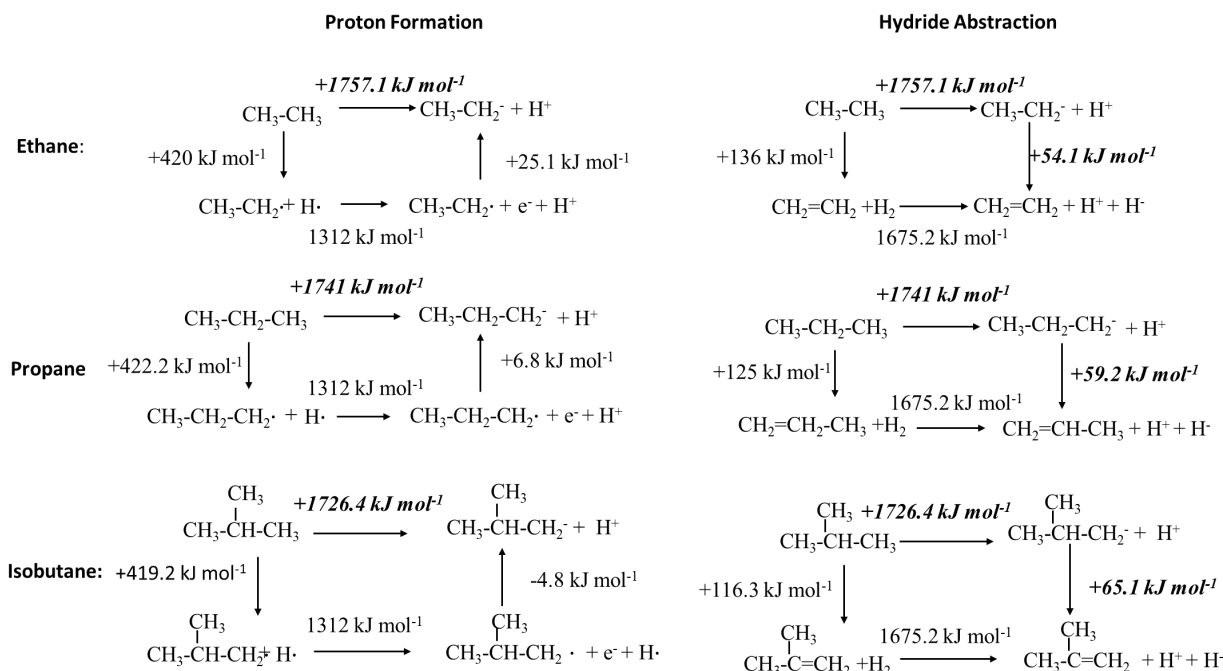


Figure S16. Thermochemical cycles for proton and hydride abstraction from alkane and carbanions, respectively. Data obtained from NIST or by difference (bold and italic).

Table S3. Heterolytic C–H dissociation energies of gaseous alkanes to form alkyl carbanions and protons from various C positions.

	C–H dissociation energy (kJ mol ⁻¹)		
Reactant	Primary C	Secondary C	Tertiary C
C ₂ H ₆	1757	-	-
C ₃ H ₈	1741	1753	-
iC ₄ H ₁₀	1726	-	1728

A theoretical description of the electronic state of Zr during alkane dehydrogenation can provide further insights into the nature of the active sites. Figure S17 illustrates the density of states (DOS) for the Zr atom in the participating LAB site pair. The integral below the fermi band (0 eV, integrated density of states (IDS)) describes the density of electrons associated with the atom or ensemble below the fermi level. The DOS for *d*-electrons of Zr in the bare ZrO₂ structure and the those of Zr in bound of carbanion-proton pair are nearly indistinguishable, indicating no significant change in electron distribution or electronic state of the Zr atom (Δ : 0.001 states in IDS). The difference in IDS for the transition state is likewise small (Δ : 0.06 states) and only small differences in the DOS are observed due to perturbations of the Zr–O bond distance imparted by the activated nature of the model. The absence of any new features in the conduction band further confirms that Zr is not reduced during C–H activation.

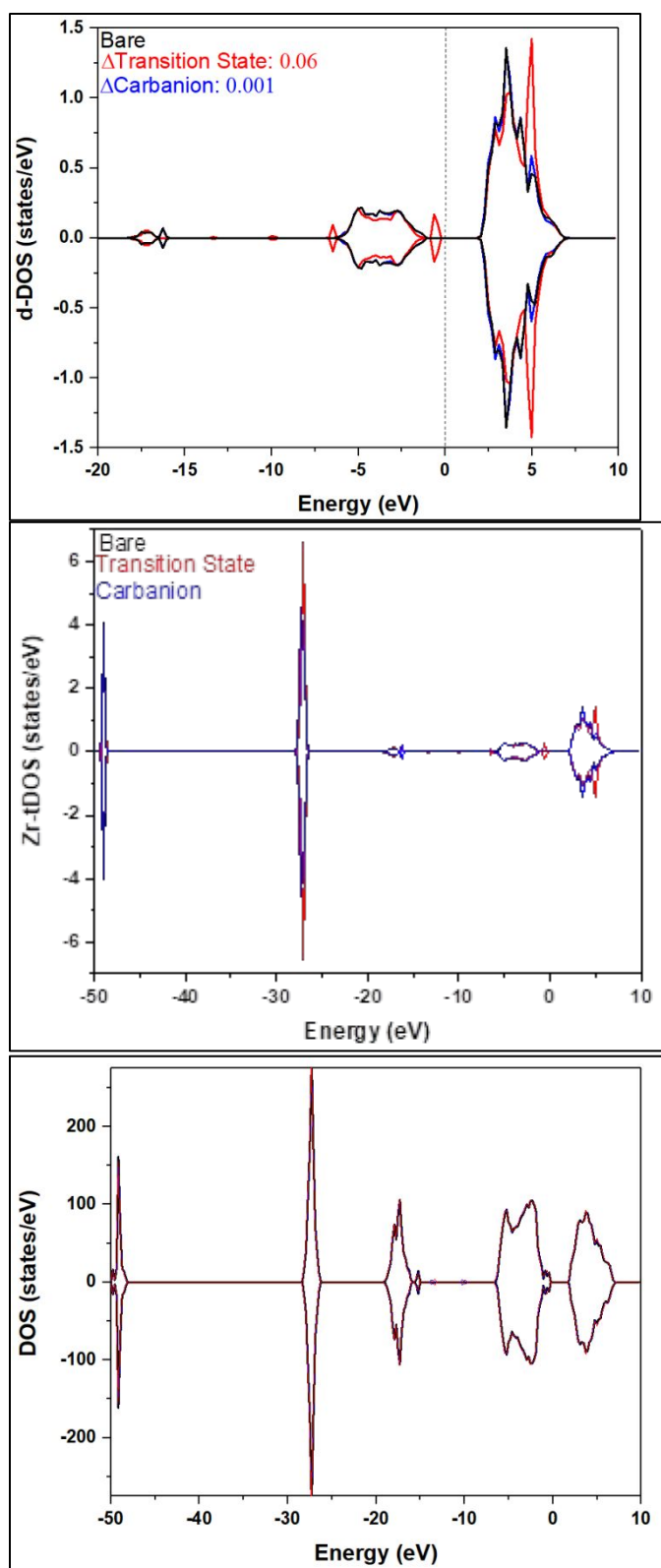


Figure S17. Top) Partial density of states (d-band) of the Zr atom which accommodates the carbanion for the bare ZrO_2 structure, the TS for the first C–H activation event, and for the adsorbed carbanion structure. Integrated residuals ($\int \text{structure} - \int \text{bare}$) of electronic state are shown as Δ . Middle) Total density of states of the Zr atom which accommodates the carbanion and Bottom) total model DOS for the bare

ZrO₂ structure (black), the TS for the first C–H activation event (red), and for the adsorbed carbanion structure (blue). Integrated residuals ($\int_{\text{structure}} - \int_{\text{bare}}$) of electronic states for models containing C₂H₆ are consistent with expected differences in electrons from the presence of the alkane.

Bader charges of bound carbanion ($n\text{C}_3\text{H}_7^{55}$ or C₂H₅) in structure III likewise demonstrate the absence of Zr reduction. The Bader charge of the carbanion in III is -0.5 e and H-atom exhibits a charge of +1 e, consistent with expectations for proton abstraction to form a bound carbanion and of the heterolytic nature of bond dissociation on ZrO₂.¹² In addition to these charges, that on the Zr atom to which C₂H₅ is bound was assessed on the bare surface, at the first C–H activation TS (structure II), and in structure III of the stable carbanion. The difference in charge of Zr at the TS and structure III to that of bare ZrO₂ was just -0.06 and -0.05 e, respectively, indicating no net change in the charge on Zr in spite of the genesis of coordination to a carbanion. This can be rationalized by increasing Zr–O bond distance to accommodate the carbanion-proton pair, which stabilize each other through space. The perturbation of the Zr–O bond to maintain constant charge is indicative of the Zr–O pair acting as a LAB site pair as they reconfigure to accept and donate electrons, respectively, with no net change in oxidation state. Taken together, this body of evidence implicates LAB site pairs of Zr⁴⁺ cations and O²⁻ anions in ZrO₂ as the active centers for alkane dehydrogenation.

To probe the potential for a more stable site for H⁻, the potential energy landscape was surveyed by displacing H⁻ along the surface in various locations around the Zr–O pair and optimizing the geometry to find a local energy minimum for the H⁻ fragment. For simplicity, the resulting weakly adsorbed C₃H₆ was excluded from the search as its presence is not expected to significantly impact the stability or geometry of $\beta\text{-H}^-$, evidenced by the comparable geometry of the H⁺–H⁻ pair after C₃H₆ desorption. The results in Figure S18 show the location of the initial position of H⁻ from the separate models (in yellow). The magenta atoms are the final locations of the H⁻ species after geometry optimization; note the significant overlap of final positions among these geometric configurations given the diverse starting locations. The white atoms are the H species locations of the surface model used in the reaction coordinate diagram. One of the final optimized geometries (magenta) in which several of the initial (yellow) geometries converge to corresponds well with the geometry utilized in the reaction coordinate diagram, indicating that the selected site is indeed a local, if not regional, minimum. The relative energies of final H⁻ positions with respect to the lowest energy configuration are shown as overlaid ovals. The hallow site with concerted interactions with two Zr atoms exhibits the lowest energy placement for the H⁻ species. Atop sites on Zr atoms (green) are higher in energy (20–70 kJ mol⁻¹), one of which reflects the migratory position of the H⁻ in the reaction coordinate diagram. All other converged configurations (orange and red) are significantly less stable (179–225 kJ mol⁻¹). As such, the abstraction of H⁻ to the concerted Zr hallow (blue) represents the structure which would lead to the most stable TS in this mechanism and on this surface.

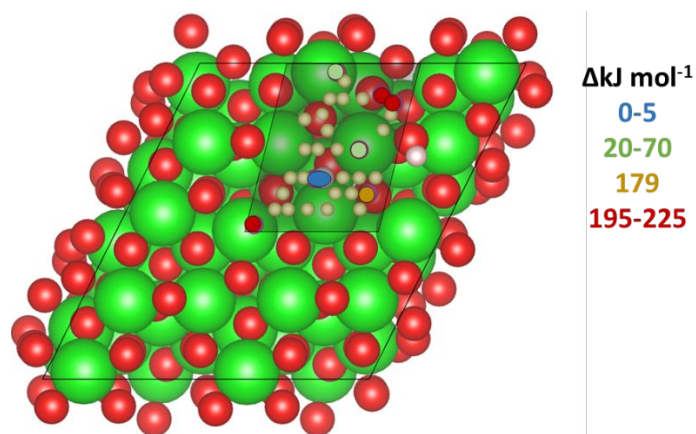


Figure S18. *m*-ZrO₂ surface with H⁺-H⁻ pairs. The position of the H⁻ was varied to survey the (111) surface of the most stable binding location of the H⁻. White are the H used in the reaction coordinate diagram, yellow are alternate H⁻ initial positions, magenta are optimized position. The lowest energy magenta positions are consistent with the location of H⁻ in white. The final optimized positions of the H⁻ species is color coded over the magenta to show the energy with respect that the lowest computed energy.

S11. DFT-optimized atomic coordinates

C₂H_{6(g)}

C	8.493095	5.668144	15.837319
C	9.812144	4.922773	16.040283
H	7.663986	4.970385	15.656517
H	10.646812	5.616195	16.221281
H	8.230842	6.273937	16.715958
H	8.544427	6.349095	14.975657
H	10.069822	4.320011	15.156588
H	9.761282	4.239109	16.901812

C₂H_{4(g)}

C	8.725495	5.805446	15.884843
C	9.578054	4.785503	15.991861
H	8.197742	6.206235	16.751820
H	8.524688	6.285354	14.925572
H	10.105536	4.386631	15.123817
H	9.781259	4.304685	16.950113

ZrO_{2, bare}

Zr	6.490613	4.027276	1.915198
Zr	9.800064	10.679861	1.915198
Zr	13.367713	4.027276	1.915198
Zr	16.677164	10.679861	1.915198
Zr	1.397412	1.046186	2.178894
Zr	4.706863	7.698771	2.178894
Zr	8.274511	1.046186	2.178894
Zr	11.583962	7.698771	2.178894
Zr	4.963430	0.369285	2.349170
Zr	8.272882	7.021871	2.349170
Zr	11.840529	0.369285	2.349170
Zr	15.149981	7.021871	2.349170
Zr	3.179680	4.040781	2.612866
Zr	6.489132	10.693367	2.612866
Zr	10.056781	4.040781	2.612866
Zr	13.366232	10.693367	2.612866
Zr	3.210353	1.561828	5.086616
Zr	6.519805	8.214415	5.086616
Zr	10.087454	1.561828	5.086616
Zr	13.396906	8.214415	5.086616
Zr	8.295355	5.213499	5.341621
Zr	11.604807	11.866084	5.341621
Zr	15.172456	5.213499	5.341621
Zr	18.481907	11.866084	5.341621
Zr	4.968449	4.570592	5.515699
Zr	8.277901	11.223179	5.515699
Zr	11.845549	4.570592	5.515699
Zr	15.155001	11.223179	5.515699
Zr	6.757049	1.582916	5.764459

Zr	10.066500	8.235501	5.764459
Zr	13.634149	1.582916	5.764459
Zr	16.943600	8.235501	5.764459
Zr	3.199092	5.756449	8.248093
Zr	6.508551	12.409035	8.248093
Zr	10.076200	5.756450	8.248088
Zr	13.385646	12.409033	8.248091
Zr	4.982064	2.777956	8.523219
Zr	8.291520	9.430543	8.523219
Zr	11.859166	2.777959	8.523221
Zr	15.168612	9.430540	8.523221
Zr	1.637617	2.143785	8.707086
Zr	4.947069	8.796359	8.707090
Zr	8.514720	2.143783	8.707079
Zr	11.824168	8.796367	8.707081
Zr	6.755073	5.771636	8.954039
Zr	10.064522	12.424218	8.954042
Zr	13.632169	5.771631	8.954040
Zr	16.941622	12.424220	8.954038
Zr	1.723483	0.350228	11.596232
Zr	5.032931	7.002813	11.596232
Zr	8.600576	0.350226	11.596231
Zr	11.910032	7.002815	11.596229
Zr	6.717912	3.331459	11.603924
Zr	10.027369	9.984048	11.603921
Zr	13.595015	3.331463	11.603926
Zr	16.904461	9.984044	11.603925
Zr	8.518157	6.279064	11.879636
Zr	11.827606	12.931643	11.879642
Zr	15.395255	6.279058	11.879637
Zr	18.704712	12.931647	11.879639
Zr	3.527948	3.339075	12.150968
Zr	6.837406	9.991664	12.150964
Zr	10.405048	3.339076	12.150964
Zr	13.714497	9.991659	12.150966
O	4.499074	3.908527	1.000000
O	7.808525	10.561112	1.000000
O	11.376174	3.908527	1.000000
O	14.685625	10.561112	1.000000
O	1.662866	3.094650	1.359833
O	4.972317	9.747235	1.359833
O	8.539967	3.094650	1.359833
O	11.849418	9.747235	1.359833
O	6.223626	6.241323	1.594743
O	9.533077	12.893909	1.594743
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O	9.592426	8.612969	2.053428
O	13.160075	1.960384	2.053428
O	16.469526	8.612969	2.053428

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O	6.696770	12.760260	2.474636	O	5.203217	4.837378	7.750842
O	10.264419	6.107673	2.474636	O	8.512667	11.489963	7.750844
O	13.573872	12.760260	2.474636	O	12.080315	4.837378	7.750844
O	3.446667	1.826733	2.933321	O	15.389770	11.489962	7.750845
O	6.756119	8.479319	2.933321	O	6.515152	1.343752	7.932779
O	10.323629	1.826733	2.933321	O	9.824604	7.996337	7.932778
O	13.633081	8.479319	2.933321	O	13.392302	1.343750	7.932760
O	8.007461	4.973473	3.168231	O	16.701710	7.996341	7.932770
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O	18.194012	11.626059	3.168231	O	9.860380	3.702196	8.378155
O	5.171220	4.159529	3.528064	O	13.169833	10.354781	8.378155
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O	12.048183	4.159529	3.528064	O	6.953960	7.844616	8.800887
O	15.357635	10.812116	3.528064	O	10.521610	1.192029	8.800883
O	1.215985	1.420527	4.156482	O	13.831060	7.844618	8.800882
O	4.525437	8.073112	4.156482	O	6.969513	3.531567	9.285176
O	8.093085	1.420527	4.156482	O	10.278967	10.184151	9.285175
O	11.402536	8.073112	4.156482	O	13.846614	3.531566	9.285172
O	5.222882	0.623746	4.476122	O	17.156067	10.184151	9.285174
O	8.532333	7.276332	4.476122	O	1.422600	0.065468	9.495368
O	12.099981	0.623746	4.476122	O	4.732053	6.718053	9.495367
O	15.409433	7.276332	4.476122	O	8.299705	0.065469	9.495364
O	2.942146	3.794435	4.821833	O	11.609149	6.718052	9.495368
O	6.251598	10.447021	4.821833	O	8.771176	5.978623	9.891722
O	9.819246	3.794435	4.821833	O	12.080634	12.631209	9.891723
O	13.128698	10.447021	4.821833	O	15.648279	5.978619	9.891720
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O	9.619469	12.809888	5.268025	O	4.722438	3.236154	10.523801
O	13.187117	6.157301	5.268025	O	8.031884	9.888742	10.523801
O	16.496569	12.809888	5.268025	O	11.599534	3.236153	10.523806
O	6.965536	3.643222	5.656374	O	14.908991	9.888741	10.523798
O	10.274988	10.295808	5.656374	O	1.880477	2.361461	10.884512
O	13.842637	3.643222	5.656374	O	5.189929	9.014049	10.884513
O	17.152088	10.295808	5.656374	O	8.757576	2.361465	10.884513
O	3.434196	6.015002	6.085457	O	12.067027	9.014047	10.884513
O	6.743647	12.667587	6.085457	O	6.511879	5.527299	11.076157
O	10.311296	6.015002	6.085457	O	9.821329	12.179883	11.076158
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O	8.064041	9.140186	6.281532	O	6.613245	1.242749	11.868469
O	11.631690	2.487601	6.281532	O	9.922689	7.895330	11.868465
O	14.941141	9.140186	6.281532	O	13.490337	1.242747	11.868465
O	1.848416	1.703394	6.660376	O	16.799789	7.895335	11.868460
O	5.157867	8.355980	6.660376	O	3.686434	5.494153	12.159203
O	8.725517	1.703394	6.660376	O	6.995884	12.146738	12.159206
O	12.034967	8.355980	6.660376	O	10.563530	5.494148	12.159202
O	8.105692	5.624776	7.378829	O	13.872985	12.146739	12.159201
O	11.415147	12.277360	7.378826	O	3.538826	1.041021	12.494611
O	14.982794	5.624772	7.378822	O	6.848281	7.693609	12.494608

O	10.415928	1.041022	12.494605
O	13.725381	7.693606	12.494606
O	8.358501	4.300589	12.590961
O	11.667955	10.953175	12.590961
O	15.235599	4.300590	12.590962
O	18.545055	10.953176	12.590963
O	12.195417	3.412201	13.050247
O	15.504877	10.064785	13.050241
O	5.318326	3.412204	13.050242
O	8.627773	10.064787	13.050242
O	15.417066	3.094650	1.359833
O	18.726517	9.747235	1.359833
O	-0.594125	1.960384	2.053428
O	2.914174	-0.411262	1.594743
O	0.077867	-0.544911	2.474636
O	2.715326	8.612969	2.053428
O	9.791272	-0.411262	1.594743
O	6.954968	-0.544911	2.474636
O	4.698009	-1.679112	3.168231
O	11.575109	-1.679112	3.168231
O	13.832067	-0.544911	2.474636
O	17.141518	6.107673	2.474636
O	1.130361	4.973473	3.168231
O	4.439812	11.626059	3.168231
O	3.000566	-0.495283	5.268025
O	9.877666	-0.495283	5.268025
O	11.841785	13.928917	4.476122
O	16.696346	3.794435	4.821833
O	17.188396	6.015002	6.085457
O	18.718884	13.928917	4.476122
O	20.005798	10.447021	4.821833
O	20.497847	12.667587	6.085457
O	7.001845	-0.637584	6.085457
O	13.878944	-0.637584	6.085457
O	14.970185	1.420527	4.156482
O	15.602615	1.703394	6.660376
O	18.279636	8.073112	4.156482
O	18.912067	8.355980	6.660376
O	1.228594	5.624772	7.378822
O	1.894079	5.978619	9.891720
O	2.947510	7.996341	7.932770
O	4.538044	12.277358	7.378825
O	5.203531	12.631207	9.891724
O	6.257005	14.648921	7.932760
O	8.041503	13.370640	9.495368
O	13.134055	14.648923	7.932779
O	14.918608	13.370640	9.495364
O	-0.361898	1.343750	7.932760
O	0.092414	3.531566	9.285172
O	3.401867	10.184151	9.285174
O	10.263416	14.497206	8.800885

O	17.140514	14.497200	8.800883
O	-0.263863	1.242747	11.868465
O	0.376981	-1.158433	12.159206
O	3.202426	-1.125288	11.076158
O	3.045589	7.895335	11.868460
O	7.254082	-1.158432	12.159201
O	10.079526	-1.125287	11.076154
O	15.634677	2.361461	10.884512
O	18.944130	9.014049	10.884513
O	10.157730	14.346192	12.494611
O	13.232148	14.547920	11.868469
O	17.440634	5.494153	12.159203
O	17.034832	14.346192	12.494605
O	20.109241	14.547918	11.868465
O	20.750084	12.146738	12.159206
O	1.481399	4.300590	12.590962
O	4.790855	10.953176	12.590963

ZrO₂, C₂H₆*

Zr	6.490611	4.027276	1.915200
Zr	9.800062	10.679861	1.915200
Zr	13.367708	4.027276	1.915200
Zr	16.677158	10.679861	1.915200
Zr	1.397412	1.046186	2.178900
Zr	4.706862	7.698771	2.178900
Zr	8.274508	1.046186	2.178900
Zr	11.583960	7.698771	2.178900
Zr	4.963428	0.369285	2.349180
Zr	8.272879	7.021871	2.349180
Zr	11.840524	0.369285	2.349180
Zr	15.149975	7.021871	2.349180
Zr	3.179680	4.040781	2.612880
Zr	6.489130	10.693365	2.612880
Zr	10.056777	4.040781	2.612880
Zr	13.366228	10.693365	2.612880
Zr	3.210352	1.561828	5.086620
Zr	6.519803	8.214414	5.086620
Zr	10.087448	1.561828	5.086620
Zr	13.396900	8.214414	5.086620
Zr	8.295352	5.213499	5.341620
Zr	11.604803	11.866083	5.341620
Zr	15.172449	5.213499	5.341620
Zr	18.481899	11.866083	5.341620
Zr	4.968447	4.570592	5.515710
Zr	8.277898	11.223178	5.515710
Zr	11.845544	4.570592	5.515710
Zr	15.154995	11.223178	5.515710
Zr	6.757046	1.582916	5.764470
Zr	10.066498	8.235501	5.764470
Zr	13.634143	1.582916	5.764470
Zr	16.943594	8.235501	5.764470

Zr	3.203643	5.749631	8.248085	O	13.573866	12.760258	2.474640
Zr	6.512005	12.401692	8.248018	O	3.446666	1.826733	2.933310
Zr	10.079936	5.748977	8.248722	O	6.756118	8.479319	2.933310
Zr	13.389839	12.401945	8.247636	O	10.323626	1.826733	2.933310
Zr	4.989792	2.767519	8.523607	O	13.633078	8.479319	2.933310
Zr	8.300048	9.419082	8.522669	O	8.007458	4.973473	3.168240
Zr	11.866023	2.766723	8.523787	O	11.316909	11.626059	3.168240
Zr	15.175257	9.419507	8.525038	O	14.884556	4.973473	3.168240
Zr	1.642993	2.134500	8.708142	O	18.194006	11.626059	3.168240
Zr	4.955441	8.784557	8.708392	O	5.171217	4.159529	3.528060
Zr	8.520877	2.132542	8.710129	O	8.480669	10.812115	3.528060
Zr	11.832819	8.785121	8.710226	O	12.048177	4.159529	3.528060
Zr	6.761401	5.759151	8.955952	O	15.357628	10.812115	3.528060
Zr	10.068708	12.415592	8.951451	O	1.215985	1.420527	4.156470
Zr	13.638102	5.758635	8.954452	O	4.525436	8.073112	4.156470
Zr	16.946854	12.413397	8.954377	O	8.093081	1.420527	4.156470
Zr	1.729218	0.327082	11.596898	O	11.402533	8.073112	4.156470
Zr	5.041526	6.978653	11.600237	O	5.222879	0.623746	4.476120
Zr	8.608939	0.325651	11.601284	O	8.532331	7.276332	4.476120
Zr	11.921248	6.977907	11.598624	O	12.099977	0.623746	4.476120
Zr	6.726478	3.300288	11.614934	O	15.409428	7.276332	4.476120
Zr	10.039637	9.952608	11.607006	O	2.942146	3.794435	4.821840
Zr	13.602735	3.299929	11.614594	O	6.251596	10.447021	4.821840
Zr	16.922655	9.951408	11.603216	O	9.819242	3.794435	4.821840
Zr	8.530159	6.246846	11.881498	O	13.128694	10.447021	4.821840
Zr	11.831528	12.906513	11.873755	O	6.310015	6.157300	5.268030
Zr	15.405121	6.245883	11.878200	O	9.619466	12.809886	5.268030
Zr	18.715477	12.897720	11.880733	O	13.187112	6.157300	5.268030
Zr	3.536529	3.303500	12.155286	O	16.496563	12.809886	5.268030
Zr	6.851783	9.953753	12.156451	O	6.965534	3.643222	5.656380
Zr	10.414012	3.301468	12.156061	O	10.274984	10.295807	5.656380
Zr	13.733763	9.959832	12.164923	O	13.842632	3.643222	5.656380
O	4.499073	3.908527	0.999990	O	17.152082	10.295807	5.656380
O	7.808524	10.561112	0.999990	O	3.434196	6.015002	6.085470
O	11.376169	3.908527	0.999990	O	6.743647	12.667587	6.085470
O	14.685621	10.561112	0.999990	O	10.311293	6.015002	6.085470
O	1.662866	3.094650	1.359840	O	13.620744	12.667587	6.085470
O	4.972317	9.747235	1.359840	O	4.754588	2.487601	6.281520
O	8.539963	3.094650	1.359840	O	8.064039	9.140186	6.281520
O	11.849415	9.747235	1.359840	O	11.631685	2.487601	6.281520
O	6.223625	6.241323	1.594740	O	14.941136	9.140186	6.281520
O	9.533075	12.893908	1.594740	O	1.848415	1.703394	6.660390
O	13.100722	6.241323	1.594740	O	5.157866	8.355980	6.660390
O	16.410173	12.893908	1.594740	O	8.725513	1.703394	6.660390
O	6.282972	1.960384	2.053440	O	12.034964	8.355980	6.660390
O	9.592424	8.612969	2.053440	O	8.111702	5.607398	7.381464
O	13.160070	1.960384	2.053440	O	11.421560	12.260361	7.379723
O	16.469521	8.612969	2.053440	O	14.988566	5.607394	7.380443
O	3.387318	6.107672	2.474640	O	18.297474	12.261240	7.380585
O	6.696769	12.760258	2.474640	O	5.206369	4.830237	7.750436
O	10.264415	6.107672	2.474640	O	8.514970	11.482449	7.750904

O	12.081594	4.830575	7.751315	O	11.665316	10.943926	12.577169
O	15.391897	11.482563	7.751194	O	15.242315	4.272619	12.602084
O	6.519761	1.336277	7.931301	O	18.557053	10.924712	12.598734
O	9.829561	7.987567	7.932026	O	12.199768	3.394949	13.058889
O	13.395199	1.335818	7.930020	O	15.531336	10.047394	13.048002
O	16.706215	7.987837	7.932068	O	5.322784	3.393114	13.058321
O	2.991949	3.698159	8.402951	O	8.639009	10.050428	13.057127
O	6.301366	10.350017	8.401573	C	12.017635	9.116920	15.268119
O	9.868020	3.697268	8.403638	C	13.213500	10.043292	15.485133
O	13.177586	10.350184	8.403704	H	11.879213	8.437902	16.119967
O	3.645052	1.179899	8.783577	H	11.086512	9.677208	15.114010
O	6.956739	7.830368	8.784481	H	12.166501	8.472674	14.385429
O	10.522263	1.178075	8.785539	H	14.170298	9.504611	15.465964
O	13.832336	7.830356	8.784733	H	13.265812	10.840634	14.723247
O	6.977757	3.519745	9.287603	H	13.143468	10.568613	16.447483
O	10.289458	10.171717	9.286550	O	15.417060	3.094650	1.359840
O	13.853325	3.518816	9.284961	O	18.726511	9.747235	1.359840
O	17.165380	10.172037	9.284556	O	-0.594124	1.960384	2.053440
O	1.425551	0.055377	9.494627	O	2.914173	-0.411263	1.594740
O	4.738998	6.703879	9.498227	O	0.077867	-0.544913	2.474640
O	8.304809	0.051825	9.499184	O	2.715326	8.612969	2.053440
O	11.615089	6.705431	9.499847	O	9.791271	-0.411263	1.594740
O	8.771523	5.979519	9.891325	O	6.954964	-0.544913	2.474640
O	12.080217	12.638837	9.885925	O	4.698007	-1.679112	3.168240
O	15.647291	5.978419	9.888032	O	11.575104	-1.679112	3.168240
O	18.957699	12.632504	9.890366	O	13.832061	-0.544913	2.474640
O	4.746155	3.164285	10.536347	O	17.141512	6.107672	2.474640
O	8.056590	9.818182	10.534982	O	1.130362	4.973473	3.168240
O	11.622211	3.163307	10.536819	O	4.439812	11.626059	3.168240
O	14.929832	9.821516	10.535716	O	3.000564	-0.495285	5.268030
O	1.885284	2.337252	10.885443	O	9.877661	-0.495285	5.268030
O	5.200995	8.988136	10.883775	O	11.841782	13.928917	4.476120
O	8.764374	2.335828	10.886515	O	16.696341	3.794435	4.821840
O	12.077861	8.988155	10.892665	O	17.188389	6.015002	6.085470
O	6.521101	5.498391	11.078740	O	18.718880	13.928917	4.476120
O	9.823404	12.155910	11.068356	O	20.005791	10.447021	4.821840
O	13.394461	5.491805	11.074712	O	20.497841	12.667587	6.085470
O	16.708231	12.151916	11.076471	O	7.001842	-0.637584	6.085470
O	6.634671	1.212391	11.907693	O	13.878939	-0.637584	6.085470
O	9.943223	7.863801	11.903155	O	14.970180	1.420527	4.156470
O	13.507369	1.211131	11.908058	O	15.602610	1.703394	6.660390
O	16.823168	7.861958	11.901701	O	18.279631	8.073112	4.156470
O	3.696650	5.447249	12.113238	O	18.912060	8.355980	6.660390
O	7.004208	12.101519	12.111439	O	1.234372	5.607394	7.380443
O	10.572010	5.449620	12.113158	O	1.893097	5.978419	9.888032
O	13.881184	12.102179	12.121998	O	2.952021	7.987837	7.932068
O	3.539401	1.011979	12.505632	O	4.543280	12.261240	7.380585
O	6.852583	7.666264	12.507604	O	5.203505	12.632504	9.890366
O	10.416553	1.011988	12.508804	O	6.259907	14.640989	7.930020
O	13.751842	7.653028	12.487909	O	8.044453	13.360548	9.494627
O	8.366355	4.273514	12.602060	O	13.138663	14.641448	7.931301

O	14.923711	13.356996	9.499184	Zr	15.154995	11.223178	5.515710
O	-0.358995	1.335818	7.930020	Zr	6.757046	1.582916	5.764470
O	0.099131	3.518816	9.284961	Zr	10.066498	8.235501	5.764470
O	3.411186	10.172037	9.284556	Zr	13.634143	1.582916	5.764470
O	10.263954	14.485070	8.783577	Zr	16.943594	8.235501	5.764470
O	17.141165	14.483246	8.785539	Zr	3.204735	5.758231	8.246191
O	-0.246825	1.211131	11.908058	Zr	6.511708	12.407820	8.243692
O	0.385306	-1.203652	12.111439	Zr	10.082058	5.756621	8.248225
O	3.204502	-1.149261	11.068356	Zr	13.393119	12.409602	8.246386
O	3.068974	7.861958	11.901701	Zr	4.991514	2.774458	8.520681
O	7.262281	-1.202992	12.121998	Zr	8.298686	9.423440	8.519044
O	10.089329	-1.153255	11.076471	Zr	11.865641	2.772699	8.521985
O	15.639478	2.337252	10.885443	Zr	15.174253	9.428373	8.577921
O	18.955189	8.988136	10.883775	Zr	1.640351	2.144210	8.703640
O	10.158303	14.317150	12.505632	Zr	4.956038	8.787291	8.701694
O	13.253573	14.517562	11.907693	Zr	8.523248	2.139769	8.707625
O	17.450844	5.447249	12.113238	Zr	11.835297	8.785452	8.705702
O	17.035454	14.317159	12.508804	Zr	6.764526	5.761220	8.956777
O	20.126270	14.516302	11.908058	Zr	10.064610	12.430065	8.941995
O	20.758402	12.101519	12.111439	Zr	13.638151	5.765913	8.952249
O	1.488121	4.272619	12.602084	Zr	16.947996	12.420032	8.951450
O	4.802858	10.924712	12.598734	Zr	1.724852	0.337912	11.587751
(ZrO ₂ , C ₂ H ₅ *-H*) [‡]				Zr	5.043530	6.975607	11.599296
Zr	6.490611	4.027276	1.915200	Zr	8.611783	0.322545	11.595690
Zr	9.800062	10.679861	1.915200	Zr	11.927507	6.972025	11.610441
Zr	13.367708	4.027276	1.915200	Zr	6.734451	3.300503	11.617992
Zr	16.677158	10.679861	1.915200	Zr	10.010278	9.959412	11.593816
Zr	1.397412	1.046186	2.178900	Zr	13.603879	3.307916	11.610361
Zr	4.706862	7.698771	2.178900	Zr	16.947706	9.936647	11.586559
Zr	8.274508	1.046186	2.178900	Zr	8.532521	6.253607	11.881549
Zr	11.583960	7.698771	2.178900	Zr	11.819490	12.936030	11.856015
Zr	4.963428	0.369285	2.349180	Zr	15.402069	6.253172	11.875817
Zr	8.272879	7.021871	2.349180	Zr	18.716003	12.905760	11.875171
Zr	11.840524	0.369285	2.349180	Zr	3.541968	3.312838	12.153748
Zr	15.149975	7.021871	2.349180	Zr	6.841124	9.965942	12.156932
Zr	3.179680	4.040781	2.612880	Zr	10.417145	3.304086	12.158136
Zr	6.489130	10.693365	2.612880	Zr	13.607624	9.978114	12.201447
Zr	10.056777	4.040781	2.612880	O	4.499073	3.908527	0.999990
Zr	13.366228	10.693365	2.612880	O	7.808524	10.561112	0.999990
Zr	3.210352	1.561828	5.086620	O	11.376169	3.908527	0.999990
Zr	6.519803	8.214414	5.086620	O	14.685621	10.561112	0.999990
Zr	10.087448	1.561828	5.086620	O	1.662866	3.094650	1.359840
Zr	13.396900	8.214414	5.086620	O	4.972317	9.747235	1.359840
Zr	8.295352	5.213499	5.341620	O	8.539963	3.094650	1.359840
Zr	11.604803	11.866083	5.341620	O	11.849415	9.747235	1.359840
Zr	15.172449	5.213499	5.341620	O	6.223625	6.241323	1.594740
Zr	18.481899	11.866083	5.341620	O	9.533075	12.893908	1.594740
Zr	4.968447	4.570592	5.515710	O	13.100722	6.241323	1.594740
Zr	8.277898	11.223178	5.515710	O	16.410173	12.893908	1.594740
Zr	11.845544	4.570592	5.515710	O	6.282972	1.960384	2.053440
				O	9.592424	8.612969	2.053440

O	13.160070	1.960384	2.053440	O	11.426888	12.253482	7.378455
O	16.469521	8.612969	2.053440	O	14.989484	5.610636	7.379013
O	3.387318	6.107672	2.474640	O	18.297934	12.271776	7.377748
O	6.696769	12.760258	2.474640	O	5.210120	4.832859	7.750898
O	10.264415	6.107672	2.474640	O	8.515929	11.484576	7.749191
O	13.573866	12.760258	2.474640	O	12.081240	4.838034	7.753633
O	3.446666	1.826733	2.933310	O	15.389503	11.479819	7.762536
O	6.756118	8.479319	2.933310	O	6.520456	1.343667	7.930401
O	10.323626	1.826733	2.933310	O	9.830197	7.992789	7.930769
O	13.633078	8.479319	2.933310	O	13.392180	1.342865	7.927104
O	8.007458	4.973473	3.168240	O	16.707214	7.997055	7.941932
O	11.316909	11.626059	3.168240	O	2.995184	3.707250	8.405880
O	14.884556	4.973473	3.168240	O	6.300291	10.354249	8.393987
O	18.194006	11.626059	3.168240	O	9.867485	3.704933	8.397467
O	5.171217	4.159529	3.528060	O	13.183504	10.358765	8.451725
O	8.480669	10.812115	3.528060	O	3.640702	1.189295	8.768652
O	12.048177	4.159529	3.528060	O	6.958779	7.836046	8.787484
O	15.357628	10.812115	3.528060	O	10.523829	1.186132	8.786257
O	1.215985	1.420527	4.156470	O	13.823524	7.834951	8.783415
O	4.525436	8.073112	4.156470	O	6.982587	3.525525	9.287519
O	8.093081	1.420527	4.156470	O	10.289724	10.169118	9.290052
O	11.402533	8.073112	4.156470	O	13.851360	3.522151	9.282331
O	5.222879	0.623746	4.476120	O	17.179043	10.184828	9.284040
O	8.532331	7.276332	4.476120	O	1.420890	0.070645	9.483740
O	12.099977	0.623746	4.476120	O	4.743506	6.707296	9.497159
O	15.409428	7.276332	4.476120	O	8.306927	0.061429	9.494140
O	2.942146	3.794435	4.821840	O	11.611811	6.724144	9.507429
O	6.251596	10.447021	4.821840	O	8.776134	5.981259	9.892434
O	9.819242	3.794435	4.821840	O	12.071543	12.676722	9.872765
O	13.128694	10.447021	4.821840	O	15.646428	5.986892	9.884856
O	6.310015	6.157300	5.268030	O	18.960459	12.638876	9.885799
O	9.619466	12.809886	5.268030	O	4.755198	3.151598	10.539044
O	13.187112	6.157300	5.268030	O	8.043936	9.834068	10.531149
O	16.496563	12.809886	5.268030	O	11.616351	3.176463	10.535305
O	6.965534	3.643222	5.656380	O	14.971087	9.748837	10.598693
O	10.274984	10.295807	5.656380	O	1.886337	2.347445	10.882376
O	13.842632	3.643222	5.656380	O	5.188912	8.991957	10.884897
O	17.152082	10.295807	5.656380	O	8.761493	2.332469	10.886655
O	3.434196	6.015002	6.085470	O	12.079651	9.006166	10.926137
O	6.743647	12.667587	6.085470	O	6.525646	5.497955	11.078641
O	10.311293	6.015002	6.085470	O	9.809286	12.174554	11.045851
O	13.620744	12.667587	6.085470	O	13.387161	5.485223	11.062825
O	4.754588	2.487601	6.281520	O	16.711828	12.154346	11.070399
O	8.064039	9.140186	6.281520	O	6.648957	1.208730	11.941533
O	11.631685	2.487601	6.281520	O	9.939587	7.871829	11.894694
O	14.941136	9.140186	6.281520	O	13.502796	1.220136	11.898229
O	1.848415	1.703394	6.660390	O	16.837486	7.855485	11.930068
O	5.157866	8.355980	6.660390	O	3.704650	5.441799	12.106848
O	8.725513	1.703394	6.660390	O	7.006573	12.114092	12.109186
O	12.034964	8.355980	6.660390	O	10.575512	5.458422	12.132387
O	8.114259	5.616128	7.380909	O	13.876919	12.073592	12.063221

O	3.541955	1.019150	12.495743	O	4.543739	12.271776	7.377748
O	6.854181	7.673653	12.497601	O	5.206264	12.638876	9.885799
O	10.418550	1.014842	12.502542	O	6.256888	14.648036	7.927104
O	13.766103	7.627414	12.467705	O	8.039792	13.375816	9.483740
O	8.373717	4.275701	12.600497	O	13.139359	14.648838	7.930401
O	11.616524	10.984344	12.546436	O	14.925829	13.366600	9.494140
O	15.241940	4.280877	12.600216	O	-0.362014	1.342865	7.927104
O	18.573147	10.931973	12.591423	O	0.097166	3.522151	9.282331
O	12.203573	3.398017	13.059140	O	3.424849	10.184828	9.284040
O	15.644060	10.086100	13.113478	O	10.259604	14.494467	8.768652
O	5.330840	3.396761	13.059389	O	17.142731	14.491303	8.786257
O	8.628003	10.059275	13.055714	O	-0.251398	1.220136	11.898229
C	12.462276	9.007285	15.047082	O	0.387671	-1.191079	12.109186
C	13.517464	10.046820	14.662939	O	3.190384	-1.130617	11.045851
H	11.927454	9.289735	15.969437	O	3.083292	7.855485	11.930068
H	11.668051	8.901880	14.284204	O	7.258017	-1.231579	12.063221
H	12.899583	8.012468	15.198238	O	10.092926	-1.150825	11.070399
H	14.250340	10.133307	15.484192	O	15.640532	2.347445	10.882376
H	14.794952	9.945272	13.925317	O	18.943106	8.991957	10.884897
H	13.060787	11.048016	14.602009	O	10.160858	14.324322	12.495743
O	15.417060	3.094650	1.359840	O	13.267859	14.513901	11.941533
O	18.726511	9.747235	1.359840	O	17.458843	5.441799	12.106848
O	-0.594124	1.960384	2.053440	O	17.037453	14.320013	12.502542
O	2.914173	-0.411263	1.594740	O	20.121698	14.525307	11.898229
O	0.077867	-0.544913	2.474640	O	20.760767	12.114092	12.109186
O	2.715326	8.612969	2.053440	O	1.487745	4.280877	12.600216
O	9.791271	-0.411263	1.594740	O	4.818953	10.931973	12.591423
O	6.954964	-0.544913	2.474640				
O	4.698007	-1.679112	3.168240	(ZrO ₂ , C ₂ H ₄ *-2H*) [‡] (			
O	11.575104	-1.679112	3.168240	Zr	6.490611	4.027276	1.915200
O	13.832061	-0.544913	2.474640	Zr	9.800062	10.679861	1.915200
O	17.141512	6.107672	2.474640	Zr	13.367708	4.027276	1.915200
O	1.130362	4.973473	3.168240	Zr	16.677158	10.679861	1.915200
O	4.439812	11.626059	3.168240	Zr	1.397412	1.046186	2.178900
O	3.000564	-0.495285	5.268030	Zr	4.706862	7.698771	2.178900
O	9.877661	-0.495285	5.268030	Zr	8.274508	1.046186	2.178900
O	11.841782	13.928917	4.476120	Zr	11.583960	7.698771	2.178900
O	16.696341	3.794435	4.821840	Zr	4.963428	0.369285	2.349180
O	17.188389	6.015002	6.085470	Zr	8.272879	7.021871	2.349180
O	18.718880	13.928917	4.476120	Zr	11.840524	0.369285	2.349180
O	20.005791	10.447021	4.821840	Zr	15.149975	7.021871	2.349180
O	20.497841	12.667587	6.085470	Zr	3.179680	4.040781	2.612880
O	7.001842	-0.637584	6.085470	Zr	6.489130	10.693365	2.612880
O	13.878939	-0.637584	6.085470	Zr	10.056777	4.040781	2.612880
O	14.970180	1.420527	4.156470	Zr	13.366228	10.693365	2.612880
O	15.602610	1.703394	6.660390	Zr	3.210352	1.561828	5.086620
O	18.279631	8.073112	4.156470	Zr	6.519803	8.214414	5.086620
O	18.912060	8.355980	6.660390	Zr	10.087448	1.561828	5.086620
O	1.235290	5.610636	7.379013	Zr	13.396900	8.214414	5.086620
O	1.892234	5.986892	9.884856	Zr	8.295352	5.213499	5.341620
O	2.953020	7.997055	7.941932	Zr	11.604803	11.866083	5.341620

Zr	15.172449	5.213499	5.341620	O	9.533075	12.893908	1.594740
Zr	18.481899	11.866083	5.341620	O	13.100722	6.241323	1.594740
Zr	4.968447	4.570592	5.515710	O	16.410173	12.893908	1.594740
Zr	8.277898	11.223178	5.515710	O	6.282972	1.960384	2.053440
Zr	11.845544	4.570592	5.515710	O	9.592424	8.612969	2.053440
Zr	15.154995	11.223178	5.515710	O	13.160070	1.960384	2.053440
Zr	6.757046	1.582916	5.764470	O	16.469521	8.612969	2.053440
Zr	10.066498	8.235501	5.764470	O	3.387318	6.107672	2.474640
Zr	13.634143	1.582916	5.764470	O	6.696769	12.760258	2.474640
Zr	16.943594	8.235501	5.764470	O	10.264415	6.107672	2.474640
Zr	3.199210	5.757319	8.249071	O	13.573866	12.760258	2.474640
Zr	6.511708	12.405069	8.245425	O	3.446666	1.826733	2.933310
Zr	10.077755	5.751720	8.249670	O	6.756118	8.479319	2.933310
Zr	13.390121	12.404809	8.253028	O	10.323626	1.826733	2.933310
Zr	4.987080	2.771392	8.523073	O	13.633078	8.479319	2.933310
Zr	8.301071	9.423093	8.520603	O	8.007458	4.973473	3.168240
Zr	11.864830	2.771708	8.522220	O	11.316909	11.626059	3.168240
Zr	15.163468	9.425105	8.615031	O	14.884556	4.973473	3.168240
Zr	1.636209	2.139884	8.704705	O	18.194006	11.626059	3.168240
Zr	4.968499	8.774782	8.682579	O	5.171217	4.159529	3.528060
Zr	8.517128	2.137303	8.712944	O	8.480669	10.812115	3.528060
Zr	11.832917	8.777796	8.714941	O	12.048177	4.159529	3.528060
Zr	6.760252	5.752690	8.959128	O	15.357628	10.812115	3.528060
Zr	10.063196	12.427523	8.945953	O	1.215985	1.420527	4.156470
Zr	13.631731	5.760635	8.952668	O	4.525436	8.073112	4.156470
Zr	16.944870	12.430527	8.946180	O	8.093081	1.420527	4.156470
Zr	1.719207	0.334416	11.590821	O	11.402533	8.073112	4.156470
Zr	5.037833	6.971180	11.606083	O	5.222879	0.623746	4.476120
Zr	8.602428	0.310537	11.602715	O	8.532331	7.276332	4.476120
Zr	11.924911	6.961100	11.616225	O	12.099977	0.623746	4.476120
Zr	6.727849	3.300187	11.620451	O	15.409428	7.276332	4.476120
Zr	10.012569	9.950007	11.586864	O	2.942146	3.794435	4.821840
Zr	13.597663	3.306410	11.609298	O	6.251596	10.447021	4.821840
Zr	17.014122	9.920934	11.488177	O	9.819242	3.794435	4.821840
Zr	8.525839	6.247201	11.878801	O	13.128694	10.447021	4.821840
Zr	11.809893	12.944348	11.862178	O	6.310015	6.157300	5.268030
Zr	15.390270	6.255672	11.877566	O	9.619466	12.809886	5.268030
Zr	18.709175	12.906065	11.878989	O	13.187112	6.157300	5.268030
Zr	3.532220	3.316583	12.152156	O	16.496563	12.809886	5.268030
Zr	6.849164	9.967572	12.165299	O	6.965534	3.643222	5.656380
Zr	10.409391	3.300680	12.159895	O	10.274984	10.295807	5.656380
Zr	13.544966	9.994282	12.290423	O	13.842632	3.643222	5.656380
O	4.499073	3.908527	0.999990	O	17.152082	10.295807	5.656380
O	7.808524	10.561112	0.999990	O	3.434196	6.015002	6.085470
O	11.376169	3.908527	0.999990	O	6.743647	12.667587	6.085470
O	14.685621	10.561112	0.999990	O	10.311293	6.015002	6.085470
O	1.662866	3.094650	1.359840	O	13.620744	12.667587	6.085470
O	4.972317	9.747235	1.359840	O	4.754588	2.487601	6.281520
O	8.539963	3.094650	1.359840	O	8.064039	9.140186	6.281520
O	11.849415	9.747235	1.359840	O	11.631685	2.487601	6.281520
O	6.223625	6.241323	1.594740	O	14.941136	9.140186	6.281520

O	1.848415	1.703394	6.660390	O	16.853016	7.882314	11.999605
O	5.157866	8.355980	6.660390	O	3.704425	5.445709	12.108438
O	8.725513	1.703394	6.660390	O	6.999897	12.117910	12.139479
O	12.034964	8.355980	6.660390	O	10.566118	5.456095	12.153709
O	8.108380	5.616885	7.380653	O	13.857929	12.099044	12.123998
O	11.427879	12.243228	7.381913	O	3.530497	1.021658	12.499874
O	14.987642	5.610550	7.380277	O	6.838892	7.676633	12.498019
O	18.297028	12.273612	7.376955	O	10.411176	1.000808	12.513220
O	5.206009	4.831955	7.752657	O	13.784053	7.581263	12.427842
O	8.516819	11.483544	7.750034	O	8.366203	4.267143	12.602618
O	12.076839	4.836184	7.754556	O	11.593794	10.999216	12.554854
O	15.385492	11.473935	7.773240	O	15.234419	4.284810	12.599169
O	6.519926	1.341338	7.931384	O	18.563519	10.919794	12.596733
O	9.829470	7.990139	7.932150	O	12.196981	3.386396	13.058573
O	13.391790	1.338491	7.926292	O	15.641087	10.218261	13.095051
O	16.710510	8.001244	7.944786	O	5.318750	3.392871	13.059512
O	2.989213	3.704901	8.404362	O	8.626717	10.043139	13.058964
O	6.302751	10.349056	8.382178	C	11.907852	8.885155	14.869964
O	9.864353	3.698257	8.390656	C	13.236336	9.558242	14.521147
O	13.183506	10.354202	8.483652	H	11.888697	8.455969	15.886202
O	3.639324	1.186136	8.772473	H	11.057764	9.576700	14.785718
O	6.960834	7.831689	8.793597	H	11.672368	8.025927	14.204858
O	10.521693	1.184917	8.786622	H	14.077003	8.939479	14.877207
O	13.814695	7.830556	8.788124	H	15.806337	10.040186	14.033960
O	6.976539	3.521880	9.291800	H	13.302723	10.535382	15.035309
O	10.286025	10.164650	9.294873	O	15.417060	3.094650	1.359840
O	13.847008	3.515617	9.276990	O	18.726511	9.747235	1.359840
O	17.201351	10.187736	9.279805	O	-0.594124	1.960384	2.053440
O	1.417314	0.066396	9.486343	O	2.914173	-0.411263	1.594740
O	4.741139	6.705247	9.502368	O	0.077867	-0.544913	2.474640
O	8.300620	0.057688	9.500581	O	2.715326	8.612969	2.053440
O	11.606493	6.718415	9.509535	O	9.791271	-0.411263	1.594740
O	8.771128	5.952915	9.891183	O	6.954964	-0.544913	2.474640
O	12.068415	12.667849	9.878409	O	4.698007	-1.679112	3.168240
O	15.643466	5.995128	9.886218	O	11.575104	-1.679112	3.168240
O	18.962362	12.626028	9.888809	O	13.832061	-0.544913	2.474640
O	4.745081	3.162068	10.536328	O	17.141512	6.107672	2.474640
O	8.035727	9.853952	10.529791	O	1.130362	4.973473	3.168240
O	11.608133	3.176184	10.534642	O	4.439812	11.626059	3.168240
O	15.023876	9.714460	10.633634	O	3.000564	-0.495285	5.268030
O	1.877326	2.347003	10.885262	O	9.877661	-0.495285	5.268030
O	5.184170	8.995550	10.870415	O	11.841782	13.928917	4.476120
O	8.764906	2.327538	10.888457	O	16.696341	3.794435	4.821840
O	12.061320	9.002164	10.955527	O	17.188389	6.015002	6.085470
O	6.522164	5.497386	11.083747	O	18.718880	13.928917	4.476120
O	9.801469	12.174146	11.046634	O	20.005791	10.447021	4.821840
O	13.372948	5.461376	11.051438	O	20.497841	12.667587	6.085470
O	16.715586	12.151184	11.062605	O	7.001842	-0.637584	6.085470
O	6.637570	1.218279	11.915391	O	13.878939	-0.637584	6.085470
O	9.909863	7.860378	11.839007	O	14.970180	1.420527	4.156470
O	13.490944	1.215027	11.883875	O	15.602610	1.703394	6.660390

O	18.279631	8.073112	4.156470
O	18.912060	8.355980	6.660390
O	1.233448	5.610550	7.380277
O	1.889272	5.995128	9.886218
O	2.956316	8.001244	7.944786
O	4.542833	12.273612	7.376955
O	5.208168	12.626028	9.888809
O	6.256498	14.643661	7.926292
O	8.036216	13.371567	9.486343
O	13.138828	14.646509	7.931384
O	14.919522	13.362860	9.500581
O	-0.362404	1.338491	7.926292
O	0.092813	3.515617	9.276990
O	3.447157	10.187736	9.279805
O	10.258226	14.491307	8.772473
O	17.140594	14.490088	8.786622
O	-0.263250	1.215027	11.883875
O	0.380994	-1.187261	12.139479
O	3.182567	-1.131025	11.046634
O	3.098822	7.882314	11.999605
O	7.239027	-1.206127	12.123998
O	10.096684	-1.153987	11.062605
O	15.631520	2.347003	10.885262
O	18.938364	8.995550	10.870415
O	10.149399	14.326830	12.499874
O	13.256472	14.523450	11.915391
O	17.458620	5.445709	12.108438
O	17.030079	14.305979	12.513220
O	20.109846	14.520198	11.883875
O	20.754091	12.117910	12.139479
O	1.480225	4.284810	12.599169
O	4.809324	10.919794	12.596733

(ZrO₂, C₂H₄*-2H*)[‡]

Zr	6.490611	4.027276	1.915200
Zr	9.800062	10.679861	1.915200
Zr	13.367708	4.027276	1.915200
Zr	16.677158	10.679861	1.915200
Zr	1.397412	1.046186	2.178900
Zr	4.706862	7.698771	2.178900
Zr	8.274508	1.046186	2.178900
Zr	11.583960	7.698771	2.178900
Zr	4.963428	0.369285	2.349180
Zr	8.272879	7.021871	2.349180
Zr	11.840524	0.369285	2.349180
Zr	15.149975	7.021871	2.349180
Zr	3.179680	4.040781	2.612880
Zr	6.489130	10.693365	2.612880
Zr	10.056777	4.040781	2.612880
Zr	13.366228	10.693365	2.612880
Zr	3.210352	1.561828	5.086620

Zr	6.519803	8.214414	5.086620
Zr	10.087448	1.561828	5.086620
Zr	13.396900	8.214414	5.086620
Zr	8.295352	5.213499	5.341620
Zr	11.604803	11.866083	5.341620
Zr	15.172449	5.213499	5.341620
Zr	18.481899	11.866083	5.341620
Zr	4.968447	4.570592	5.515710
Zr	8.277898	11.223178	5.515710
Zr	11.845544	4.570592	5.515710
Zr	15.154995	11.223178	5.515710
Zr	6.757046	1.582916	5.764470
Zr	10.066498	8.235501	5.764470
Zr	13.634143	1.582916	5.764470
Zr	16.943594	8.235501	5.764470
Zr	3.191072	5.754397	8.241092
Zr	6.511206	12.404613	8.246394
Zr	10.087992	5.752695	8.252120
Zr	13.390877	12.396754	8.246593
Zr	4.985070	2.765719	8.518849
Zr	8.297294	9.424553	8.521008
Zr	11.863626	2.777302	8.523096
Zr	15.140675	9.425126	8.605340
Zr	1.638482	2.139669	8.709180
Zr	4.964387	8.773790	8.679735
Zr	8.519814	2.134956	8.714146
Zr	11.821577	8.764326	8.703475
Zr	6.761342	5.747003	8.945526
Zr	10.063883	12.420013	8.948243
Zr	13.619518	5.767906	8.978128
Zr	16.942324	12.434516	8.945905
Zr	1.727815	0.337128	11.593798
Zr	5.052382	6.978267	11.590806
Zr	8.590407	0.280365	11.609026
Zr	11.921954	7.039671	11.686477
Zr	6.742274	3.293656	11.607287
Zr	10.023771	9.949626	11.582443
Zr	13.598382	3.324876	11.616063
Zr	17.008564	9.935488	11.475188
Zr	8.524814	6.258387	11.847375
Zr	11.845741	12.915434	11.856899
Zr	15.441681	6.239917	11.870749
Zr	18.709467	12.918803	11.880593
Zr	3.549775	3.292229	12.154359
Zr	6.853042	9.981084	12.152629
Zr	10.402247	3.317357	12.153650
Zr	13.523331	9.818848	12.301295
O	4.499073	3.908527	0.999990
O	7.808524	10.561112	0.999990
O	11.376169	3.908527	0.999990
O	14.685621	10.561112	0.999990

O	1.662866	3.094650	1.359840	O	13.620744	12.667587	6.085470
O	4.972317	9.747235	1.359840	O	4.754588	2.487601	6.281520
O	8.539963	3.094650	1.359840	O	8.064039	9.140186	6.281520
O	11.849415	9.747235	1.359840	O	11.631685	2.487601	6.281520
O	6.223625	6.241323	1.594740	O	14.941136	9.140186	6.281520
O	9.533075	12.893908	1.594740	O	1.848415	1.703394	6.660390
O	13.100722	6.241323	1.594740	O	5.157866	8.355980	6.660390
O	16.410173	12.893908	1.594740	O	8.725513	1.703394	6.660390
O	6.282972	1.960384	2.053440	O	12.034964	8.355980	6.660390
O	9.592424	8.612969	2.053440	O	8.109307	5.621519	7.373806
O	13.160070	1.960384	2.053440	O	11.424757	12.250710	7.380481
O	16.469521	8.612969	2.053440	O	14.983223	5.601011	7.385013
O	3.387318	6.107672	2.474640	O	18.297253	12.271584	7.380911
O	6.696769	12.760258	2.474640	O	5.200928	4.828881	7.750778
O	10.264415	6.107672	2.474640	O	8.511246	11.486221	7.749861
O	13.573866	12.760258	2.474640	O	12.080788	4.831613	7.754930
O	3.446666	1.826733	2.933310	O	15.391415	11.479596	7.768450
O	6.756118	8.479319	2.933310	O	6.521364	1.338962	7.930262
O	10.323626	1.826733	2.933310	O	9.821680	7.987592	7.930807
O	13.633078	8.479319	2.933310	O	13.395001	1.345419	7.931180
O	8.007458	4.973473	3.168240	O	16.708553	8.004015	7.940228
O	11.316909	11.626059	3.168240	O	2.992486	3.699740	8.407022
O	14.884556	4.973473	3.168240	O	6.296017	10.349526	8.375196
O	18.194006	11.626059	3.168240	O	9.867233	3.692937	8.383504
O	5.171217	4.159529	3.528060	O	13.183134	10.349122	8.427572
O	8.480669	10.812115	3.528060	O	3.635914	1.182016	8.773233
O	12.048177	4.159529	3.528060	O	6.958080	7.833871	8.801044
O	15.357628	10.812115	3.528060	O	10.521201	1.185411	8.788717
O	1.215985	1.420527	4.156470	O	13.823249	7.823384	8.761520
O	4.525436	8.073112	4.156470	O	6.974741	3.517704	9.286409
O	8.093081	1.420527	4.156470	O	10.277761	10.166482	9.288446
O	11.402533	8.073112	4.156470	O	13.843561	3.523067	9.303925
O	5.222879	0.623746	4.476120	O	17.169056	10.170669	9.295281
O	8.532331	7.276332	4.476120	O	1.419627	0.060455	9.490862
O	12.099977	0.623746	4.476120	O	4.741975	6.708668	9.493275
O	15.409428	7.276332	4.476120	O	8.302835	0.049565	9.503219
O	2.942146	3.794435	4.821840	O	11.610739	6.710912	9.506119
O	6.251596	10.447021	4.821840	O	8.759526	5.912317	9.871993
O	9.819242	3.794435	4.821840	O	12.073437	12.652142	9.874441
O	13.128694	10.447021	4.821840	O	15.646537	5.993992	9.881598
O	6.310015	6.157300	5.268030	O	18.956181	12.628801	9.892459
O	9.619466	12.809886	5.268030	O	4.755773	3.149819	10.536053
O	13.187112	6.157300	5.268030	O	8.025178	9.901917	10.521055
O	16.496563	12.809886	5.268030	O	11.600821	3.207116	10.534735
O	6.965534	3.643222	5.656380	O	14.954077	9.755363	10.643069
O	10.274984	10.295807	5.656380	O	1.886542	2.340159	10.881300
O	13.842632	3.643222	5.656380	O	5.189689	9.010356	10.862407
O	17.152082	10.295807	5.656380	O	8.756738	2.316171	10.891005
O	3.434196	6.015002	6.085470	O	12.144796	9.010683	10.826126
O	6.743647	12.667587	6.085470	O	6.525586	5.496326	11.075912
O	10.311293	6.015002	6.085470	O	9.815411	12.171010	11.057388

O	13.388105	5.519900	11.100736
O	16.713299	12.141460	11.066352
O	6.644881	1.198217	11.916156
O	9.860809	7.876626	11.645434
O	13.494506	1.228468	11.882363
O	16.876465	7.890572	11.982146
O	3.726282	5.445382	12.110804
O	6.997364	12.128789	12.166986
O	10.564362	5.512203	12.190269
O	13.867398	12.049482	12.152207
O	3.532993	1.021469	12.504247
O	6.847726	7.683414	12.483739
O	10.412349	0.999215	12.501020
O	13.935881	7.649545	12.447937
O	8.379531	4.267304	12.583823
O	11.623447	10.973853	12.553289
O	15.257262	4.266835	12.603052
O	18.554398	10.920472	12.587476
O	12.188410	3.403030	13.058594
O	15.621244	10.137997	13.120455
O	5.339239	3.382412	13.055247
O	8.644037	10.026493	13.054276
C	12.183244	9.197925	14.866571
C	13.381060	9.854147	14.944988
H	12.101249	8.156435	15.184375
H	11.246418	9.741801	14.729823
H	11.885614	8.535390	13.153822
H	14.271146	9.319879	15.281729
H	15.883417	9.703833	13.946724
H	13.445655	10.943330	14.865301
O	15.417060	3.094650	1.359840
O	18.726511	9.747235	1.359840
O	-0.594124	1.960384	2.053440
O	2.914173	-0.411263	1.594740
O	0.077867	-0.544913	2.474640
O	2.715326	8.612969	2.053440
O	9.791271	-0.411263	1.594740
O	6.954964	-0.544913	2.474640
O	4.698007	-1.679112	3.168240
O	11.575104	-1.679112	3.168240
O	13.832061	-0.544913	2.474640
O	17.141512	6.107672	2.474640
O	1.130362	4.973473	3.168240
O	4.439812	11.626059	3.168240
O	3.000564	-0.495285	5.268030
O	9.877661	-0.495285	5.268030
O	11.841782	13.928917	4.476120
O	16.696341	3.794435	4.821840
O	17.188389	6.015002	6.085470
O	18.718880	13.928917	4.476120
O	20.005791	10.447021	4.821840

O	20.497841	12.667587	6.085470
O	7.001842	-0.637584	6.085470
O	13.878939	-0.637584	6.085470
O	14.970180	1.420527	4.156470
O	15.602610	1.703394	6.660390
O	18.279631	8.073112	4.156470
O	18.912060	8.355980	6.660390
O	1.229029	5.601011	7.385013
O	1.892343	5.993992	9.881598
O	2.954359	8.004015	7.940228
O	4.543058	12.271584	7.380911
O	5.201986	12.628801	9.892459
O	6.259709	14.650590	7.931180
O	8.038529	13.365626	9.490862
O	13.140266	14.644134	7.930262
O	14.921738	13.354736	9.503219
O	-0.359193	1.345419	7.931180
O	0.089367	3.523067	9.303925
O	3.414862	10.170669	9.295281
O	10.254816	14.487186	8.773233
O	17.140102	14.490582	8.788717
O	-0.259688	1.228468	11.882363
O	0.378462	-1.176382	12.166986
O	3.196508	-1.134161	11.057388
O	3.122271	7.890572	11.982146
O	7.248496	-1.255689	12.152207
O	10.094397	-1.163711	11.066352
O	15.640737	2.340159	10.881300
O	18.943882	9.010356	10.862407
O	10.151896	14.326640	12.504247
O	13.263783	14.503387	11.916156
O	17.480476	5.445382	12.110804
O	17.031250	14.304386	12.501020
O	20.113407	14.533639	11.882363
O	20.751558	12.128789	12.166986
O	1.503068	4.266835	12.603052
O	4.800203	10.920472	12.587476

ZrO₂, C₂H₄*-2H*

Zr	6.490611	4.027276	1.915200
Zr	9.800062	10.679861	1.915200
Zr	13.367708	4.027276	1.915200
Zr	16.677158	10.679861	1.915200
Zr	1.397412	1.046186	2.178900
Zr	4.706862	7.698771	2.178900
Zr	8.274508	1.046186	2.178900
Zr	11.583960	7.698771	2.178900
Zr	4.963428	0.369285	2.349180
Zr	8.272879	7.021871	2.349180
Zr	11.840524	0.369285	2.349180
Zr	15.149975	7.021871	2.349180

Zr	3.179680	4.040781	2.612880	Zr	13.526505	9.826198	12.260306
Zr	6.489130	10.693365	2.612880	O	4.499073	3.908527	0.999990
Zr	10.056777	4.040781	2.612880	O	7.808524	10.561112	0.999990
Zr	13.366228	10.693365	2.612880	O	11.376169	3.908527	0.999990
Zr	3.210352	1.561828	5.086620	O	14.685621	10.561112	0.999990
Zr	6.519803	8.214414	5.086620	O	1.662866	3.094650	1.359840
Zr	10.087448	1.561828	5.086620	O	4.972317	9.747235	1.359840
Zr	13.396900	8.214414	5.086620	O	8.539963	3.094650	1.359840
Zr	8.295352	5.213499	5.341620	O	11.849415	9.747235	1.359840
Zr	11.604803	11.866083	5.341620	O	6.223625	6.241323	1.594740
Zr	15.172449	5.213499	5.341620	O	9.533075	12.893908	1.594740
Zr	18.481899	11.866083	5.341620	O	13.100722	6.241323	1.594740
Zr	4.968447	4.570592	5.515710	O	16.410173	12.893908	1.594740
Zr	8.277898	11.223178	5.515710	O	6.282972	1.960384	2.053440
Zr	11.845544	4.570592	5.515710	O	9.592424	8.612969	2.053440
Zr	15.154995	11.223178	5.515710	O	13.160070	1.960384	2.053440
Zr	6.757046	1.582916	5.764470	O	16.469521	8.612969	2.053440
Zr	10.066498	8.235501	5.764470	O	3.387318	6.107672	2.474640
Zr	13.634143	1.582916	5.764470	O	6.696769	12.760258	2.474640
Zr	16.943594	8.235501	5.764470	O	10.264415	6.107672	2.474640
Zr	3.190723	5.753960	8.240775	O	13.573866	12.760258	2.474640
Zr	6.513213	12.403972	8.246823	O	3.446666	1.826733	2.933310
Zr	10.091841	5.752069	8.251544	O	6.756118	8.479319	2.933310
Zr	13.392522	12.397738	8.245295	O	10.323626	1.826733	2.933310
Zr	4.984460	2.763407	8.522136	O	13.633078	8.479319	2.933310
Zr	8.299038	9.424510	8.527699	O	8.007458	4.973473	3.168240
Zr	11.864078	2.777636	8.526565	O	11.316909	11.626059	3.168240
Zr	15.142224	9.425220	8.594937	O	14.884556	4.973473	3.168240
Zr	1.638755	2.138071	8.714131	O	18.194006	11.626059	3.168240
Zr	4.965830	8.773735	8.681795	O	5.171217	4.159529	3.528060
Zr	8.520621	2.137059	8.716496	O	8.480669	10.812115	3.528060
Zr	11.818250	8.767508	8.698499	O	12.048177	4.159529	3.528060
Zr	6.764161	5.742860	8.946469	O	15.357628	10.812115	3.528060
Zr	10.064866	12.413730	8.953163	O	1.215985	1.420527	4.156470
Zr	13.619364	5.772605	8.982568	O	4.525436	8.073112	4.156470
Zr	16.944998	12.431745	8.951841	O	8.093081	1.420527	4.156470
Zr	1.730678	0.335600	11.599387	O	11.402533	8.073112	4.156470
Zr	5.053061	6.980935	11.594436	O	5.222879	0.623746	4.476120
Zr	8.592666	0.287798	11.611585	O	8.532331	7.276332	4.476120
Zr	11.910977	7.049140	11.687518	O	12.099977	0.623746	4.476120
Zr	6.744078	3.295717	11.613388	O	15.409428	7.276332	4.476120
Zr	10.034458	9.941834	11.598395	O	2.942146	3.794435	4.821840
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Zr	17.009583	9.941674	11.484040	O	9.819242	3.794435	4.821840
Zr	8.524055	6.262005	11.843036	O	13.128694	10.447021	4.821840
Zr	11.845848	12.916247	11.861198	O	6.310015	6.157300	5.268030
Zr	15.439526	6.244181	11.873724	O	9.619466	12.809886	5.268030
Zr	18.713072	12.922120	11.886749	O	13.187112	6.157300	5.268030
Zr	3.551505	3.294611	12.158325	O	16.496563	12.809886	5.268030
Zr	6.858794	9.983332	12.155526	O	6.965534	3.643222	5.656380
Zr	10.404013	3.323838	12.160757	O	10.274984	10.295807	5.656380

O	13.842632	3.643222	5.656380	O	5.189367	9.012215	10.866655
O	17.152082	10.295807	5.656380	O	8.756586	2.320843	10.891519
O	3.434196	6.015002	6.085470	O	12.168215	9.029356	10.802072
O	6.743647	12.667587	6.085470	O	6.525216	5.496919	11.081519
O	10.311293	6.015002	6.085470	O	9.818855	12.166965	11.066669
O	13.620744	12.667587	6.085470	O	13.390593	5.528160	11.107457
O	4.754588	2.487601	6.281520	O	16.711407	12.139812	11.077935
O	8.064039	9.140186	6.281520	O	6.645026	1.197594	11.925181
O	11.631685	2.487601	6.281520	O	9.843030	7.876465	11.559784
O	14.941136	9.140186	6.281520	O	13.489635	1.232212	11.870227
O	1.848415	1.703394	6.660390	O	16.876928	7.900304	12.005308
O	5.157866	8.355980	6.660390	O	3.727479	5.447728	12.111114
O	8.725513	1.703394	6.660390	O	7.003329	12.136699	12.197151
O	12.034964	8.355980	6.660390	O	10.564992	5.531812	12.216731
O	8.106380	5.631686	7.371626	O	13.883642	12.046132	12.153956
O	11.421122	12.259637	7.380296	O	3.537340	1.022455	12.508818
O	14.981153	5.605362	7.385802	O	6.853457	7.687813	12.482322
O	18.294685	12.278962	7.382504	O	10.415467	1.011867	12.502903
O	5.203447	4.825382	7.751832	O	13.947030	7.672724	12.442778
O	8.514146	11.484617	7.749425	O	8.381568	4.269312	12.589731
O	12.085994	4.829160	7.755794	O	11.637360	10.977392	12.561573
O	15.398491	11.481382	7.767906	O	15.256254	4.270572	12.606312
O	6.520491	1.339444	7.933535	O	18.554401	10.921112	12.591240
O	9.818452	7.987676	7.931189	O	12.192528	3.402476	13.061102
O	13.395263	1.344629	7.936890	O	15.601650	10.107175	13.143446
O	16.709688	8.005315	7.942141	O	5.341877	3.380537	13.060714
O	2.988744	3.699394	8.407194	O	8.653286	10.006217	13.059579
O	6.293640	10.348650	8.369336	C	12.274790	9.343830	15.079120
O	9.866508	3.690398	8.369776	C	13.468632	9.963518	15.154495
O	13.183356	10.350576	8.409644	H	12.172701	8.283688	15.309874
O	3.638821	1.179374	8.785691	H	11.358902	9.884442	14.842954
O	6.964487	7.833735	8.819253	H	11.816031	8.516632	13.062976
O	10.527944	1.184784	8.806282	H	14.361187	9.415582	15.458755
O	13.829885	7.824990	8.761054	H	15.850338	9.501847	13.861985
O	6.976276	3.518051	9.288233	H	13.578548	11.038498	14.999757
O	10.279400	10.169741	9.287745	O	15.417060	3.094650	1.359840
O	13.844957	3.523863	9.310150	O	18.726511	9.747235	1.359840
O	17.171251	10.171721	9.302675	O	-0.594124	1.960384	2.053440
O	1.419577	0.056677	9.497919	O	2.914173	-0.411263	1.594740
O	4.740306	6.709242	9.497942	O	0.077867	-0.544913	2.474640
O	8.302870	0.050003	9.506620	O	2.715326	8.612969	2.053440
O	11.612444	6.714923	9.499271	O	9.791271	-0.411263	1.594740
O	8.764421	5.876772	9.873142	O	6.954964	-0.544913	2.474640
O	12.081783	12.640265	9.881156	O	4.698007	-1.679112	3.168240
O	15.653059	5.995914	9.885691	O	11.575104	-1.679112	3.168240
O	18.964350	12.613251	9.902028	O	13.832061	-0.544913	2.474640
O	4.755337	3.154973	10.539576	O	17.141512	6.107672	2.474640
O	8.020348	9.931664	10.522966	O	1.130362	4.973473	3.168240
O	11.591805	3.232407	10.535045	O	4.439812	11.626059	3.168240
O	14.946648	9.770250	10.631776	O	3.000564	-0.495285	5.268030
O	1.889894	2.340248	10.885991	O	9.877661	-0.495285	5.268030

O	11.841782	13.928917	4.476120
O	16.696341	3.794435	4.821840
O	17.188389	6.015002	6.085470
O	18.718880	13.928917	4.476120
O	20.005791	10.447021	4.821840
O	20.497841	12.667587	6.085470
O	7.001842	-0.637584	6.085470
O	13.878939	-0.637584	6.085470
O	14.970180	1.420527	4.156470
O	15.602610	1.703394	6.660390
O	18.279631	8.073112	4.156470
O	18.912060	8.355980	6.660390
O	1.226959	5.605362	7.385802
O	1.898865	5.995914	9.885691
O	2.955494	8.005315	7.942141
O	4.540491	12.278962	7.382504
O	5.210155	12.613251	9.902028
O	6.259971	14.649800	7.936890
O	8.038480	13.361848	9.497919
O	13.139393	14.644615	7.933535
O	14.921772	13.355173	9.506620
O	-0.358932	1.344629	7.936890
O	0.090763	3.523863	9.310150
O	3.417057	10.171721	9.302675
O	10.257723	14.484545	8.785691
O	17.146847	14.489955	8.806282
O	-0.264560	1.232212	11.870227
O	0.384427	-1.168472	12.197151
O	3.199953	-1.138206	11.066669
O	3.122734	7.900304	12.005308
O	7.264740	-1.259039	12.153956
O	10.092505	-1.165359	11.077935
O	15.644088	2.340248	10.885991
O	18.943562	9.012215	10.866655
O	10.156242	14.327625	12.508818
O	13.263928	14.502765	11.925181
O	17.481674	5.447728	12.111114
O	17.034370	14.317038	12.502903
O	20.108536	14.537383	11.870227
O	20.757523	12.136699	12.197151
O	1.502060	4.270572	12.606312
O	4.800207	10.921112	12.591240

ZrO₂, C₂H₄-2H*

Zr	6.490611	4.027276	1.915200
Zr	9.800062	10.679861	1.915200
Zr	13.367708	4.027276	1.915200
Zr	16.677158	10.679861	1.915200
Zr	1.397412	1.046186	2.178900
Zr	4.706862	7.698771	2.178900
Zr	8.274508	1.046186	2.178900

Zr	11.583960	7.698771	2.178900
Zr	4.963428	0.369285	2.349180
Zr	8.272879	7.021871	2.349180
Zr	11.840524	0.369285	2.349180
Zr	15.149975	7.021871	2.349180
Zr	3.179680	4.040781	2.612880
Zr	6.489130	10.693365	2.612880
Zr	10.056777	4.040781	2.612880
Zr	13.366228	10.693365	2.612880
Zr	3.210352	1.561828	5.086620
Zr	6.519803	8.214414	5.086620
Zr	10.087448	1.561828	5.086620
Zr	13.396900	8.214414	5.086620
Zr	8.295352	5.213499	5.341620
Zr	11.604803	11.866083	5.341620
Zr	15.172449	5.213499	5.341620
Zr	18.481899	11.866083	5.341620
Zr	4.968447	4.570592	5.515710
Zr	8.277898	11.223178	5.515710
Zr	11.845544	4.570592	5.515710
Zr	15.154995	11.223178	5.515710
Zr	6.757046	1.582916	5.764470
Zr	10.066498	8.235501	5.764470
Zr	13.634143	1.582916	5.764470
Zr	16.943594	8.235501	5.764470
Zr	3.187673	5.752606	8.244014
Zr	6.516051	12.403450	8.249603
Zr	10.095418	5.755519	8.256564
Zr	13.392109	12.399848	8.246480
Zr	4.983374	2.763638	8.524661
Zr	8.302536	9.425733	8.539316
Zr	11.866348	2.781379	8.528997
Zr	15.150648	9.423937	8.566577
Zr	1.638843	2.136158	8.716405
Zr	4.968549	8.773787	8.686007
Zr	8.522207	2.140050	8.713853
Zr	11.814455	8.764966	8.700744
Zr	6.764549	5.742136	8.948424
Zr	10.067187	12.409265	8.960408
Zr	13.615718	5.778565	8.993587
Zr	16.949221	12.431116	8.954272
Zr	1.729495	0.337531	11.603231
Zr	5.054651	6.984101	11.598025
Zr	8.602649	0.305665	11.604733
Zr	11.912912	7.061132	11.728276
Zr	6.742262	3.301025	11.617702
Zr	10.036190	9.947402	11.637061
Zr	13.601469	3.338476	11.617357
Zr	17.010080	9.947377	11.504375
Zr	8.526114	6.269160	11.847400
Zr	11.846975	12.923167	11.868331

Zr	15.439869	6.251164	11.878974	O	9.619466	12.809886	5.268030
Zr	18.712835	12.930159	11.887790	O	13.187112	6.157300	5.268030
Zr	3.548819	3.298506	12.161898	O	16.496563	12.809886	5.268030
Zr	6.854304	9.986044	12.163299	O	6.965534	3.643222	5.656380
Zr	10.408160	3.336015	12.162045	O	10.274984	10.295807	5.656380
Zr	13.558304	9.869882	12.165122	O	13.842632	3.643222	5.656380
O	4.499073	3.908527	0.999990	O	17.152082	10.295807	5.656380
O	7.808524	10.561112	0.999990	O	3.434196	6.015002	6.085470
O	11.376169	3.908527	0.999990	O	6.743647	12.667587	6.085470
O	14.685621	10.561112	0.999990	O	10.311293	6.015002	6.085470
O	1.662866	3.094650	1.359840	O	13.620744	12.667587	6.085470
O	4.972317	9.747235	1.359840	O	4.754588	2.487601	6.281520
O	8.539963	3.094650	1.359840	O	8.064039	9.140186	6.281520
O	11.849415	9.747235	1.359840	O	11.631685	2.487601	6.281520
O	6.223625	6.241323	1.594740	O	14.941136	9.140186	6.281520
O	9.533075	12.893908	1.594740	O	1.848415	1.703394	6.660390
O	13.100722	6.241323	1.594740	O	5.157866	8.355980	6.660390
O	16.410173	12.893908	1.594740	O	8.725513	1.703394	6.660390
O	6.282972	1.960384	2.053440	O	12.034964	8.355980	6.660390
O	9.592424	8.612969	2.053440	O	8.107767	5.630108	7.374418
O	13.160070	1.960384	2.053440	O	11.421162	12.256437	7.383254
O	16.469521	8.612969	2.053440	O	14.979923	5.605854	7.388995
O	3.387318	6.107672	2.474640	O	18.297802	12.270746	7.385169
O	6.696769	12.760258	2.474640	O	5.200729	4.827410	7.753522
O	10.264415	6.107672	2.474640	O	8.514822	11.483923	7.752929
O	13.573866	12.760258	2.474640	O	12.087929	4.834083	7.757319
O	3.446666	1.826733	2.933310	O	15.402031	11.481435	7.762991
O	6.756118	8.479319	2.933310	O	6.518640	1.338058	7.932718
O	10.323626	1.826733	2.933310	O	9.818995	7.988543	7.932142
O	13.633078	8.479319	2.933310	O	13.395842	1.343180	7.939316
O	8.007458	4.973473	3.168240	O	16.709368	8.005703	7.938405
O	11.316909	11.626059	3.168240	O	2.987992	3.699800	8.413689
O	14.884556	4.973473	3.168240	O	6.298039	10.347196	8.380477
O	18.194006	11.626059	3.168240	O	9.869239	3.691465	8.369796
O	5.171217	4.159529	3.528060	O	13.184175	10.352613	8.414818
O	8.480669	10.812115	3.528060	O	3.636657	1.178466	8.789305
O	12.048177	4.159529	3.528060	O	6.964450	7.834534	8.825836
O	15.357628	10.812115	3.528060	O	10.531890	1.184957	8.808331
O	1.215985	1.420527	4.156470	O	13.832291	7.834156	8.764729
O	4.525436	8.073112	4.156470	O	6.974141	3.517846	9.286604
O	8.093081	1.420527	4.156470	O	10.282096	10.170053	9.295493
O	11.402533	8.073112	4.156470	O	13.847470	3.528482	9.310088
O	5.222879	0.623746	4.476120	O	17.174299	10.168383	9.312361
O	8.532331	7.276332	4.476120	O	1.421358	0.053135	9.503491
O	12.099977	0.623746	4.476120	O	4.738679	6.712864	9.500323
O	15.409428	7.276332	4.476120	O	8.308414	0.053042	9.500583
O	2.942146	3.794435	4.821840	O	11.614132	6.719456	9.504077
O	6.251596	10.447021	4.821840	O	8.765425	5.882621	9.876486
O	9.819242	3.794435	4.821840	O	12.081646	12.647648	9.884832
O	13.128694	10.447021	4.821840	O	15.652368	6.006646	9.889075
O	6.310015	6.157300	5.268030	O	18.964514	12.612990	9.902887

O	4.754225	3.154276	10.542571
O	8.022682	9.929390	10.535141
O	11.592035	3.246835	10.533926
O	14.958685	9.798081	10.607710
O	1.887506	2.341293	10.889550
O	5.183950	9.019563	10.876398
O	8.759547	2.329278	10.888041
O	12.160551	9.031925	10.814712
O	6.523786	5.499542	11.082891
O	9.822327	12.164716	11.079216
O	13.389070	5.532740	11.120438
O	16.711344	12.140656	11.084766
O	6.654029	1.201003	11.940532
O	9.847754	7.884041	11.565873
O	13.487390	1.235684	11.859808
O	16.876844	7.915040	12.022092
O	3.729575	5.456977	12.114552
O	6.997629	12.140437	12.204917
O	10.564161	5.537999	12.228907
O	13.901091	12.046544	12.108538
O	3.540144	1.028802	12.506607
O	6.854870	7.690714	12.482782
O	10.425929	1.019591	12.495047
O	13.971231	7.699500	12.408667
O	8.381785	4.273921	12.586631
O	11.665438	10.984843	12.574018
O	15.260434	4.272271	12.606611
O	18.543354	10.925636	12.600587
O	12.194932	3.405446	13.062162
O	15.526531	10.083523	13.196794
O	5.339691	3.388753	13.062767
O	8.641215	10.013213	13.074828
H	11.824696	8.485459	13.151917
H	15.748844	9.397551	13.851209
O	15.417060	3.094650	1.359840
O	18.726511	9.747235	1.359840
O	-0.594124	1.960384	2.053440
O	2.914173	-0.411263	1.594740
O	0.077867	-0.544913	2.474640
O	2.715326	8.612969	2.053440
O	9.791271	-0.411263	1.594740
O	6.954964	-0.544913	2.474640
O	4.698007	-1.679112	3.168240
O	11.575104	-1.679112	3.168240
O	13.832061	-0.544913	2.474640
O	17.141512	6.107672	2.474640
O	1.130362	4.973473	3.168240
O	4.439812	11.626059	3.168240
O	3.000564	-0.495285	5.268030
O	9.877661	-0.495285	5.268030
O	11.841782	13.928917	4.476120

O	16.696341	3.794435	4.821840
O	17.188389	6.015002	6.085470
O	18.718880	13.928917	4.476120
O	20.005791	10.447021	4.821840
O	20.497841	12.667587	6.085470
O	7.001842	-0.637584	6.085470
O	13.878939	-0.637584	6.085470
O	14.970180	1.420527	4.156470
O	15.602610	1.703394	6.660390
O	18.279631	8.073112	4.156470
O	18.912060	8.355980	6.660390
O	1.225729	5.605854	7.388995
O	1.898173	6.006646	9.889075
O	2.955173	8.005703	7.938405
O	4.543608	12.270746	7.385169
O	5.210320	12.612990	9.902887
O	6.260550	14.648352	7.939316
O	8.040260	13.358306	9.503491
O	13.137542	14.643229	7.932718
O	14.927317	13.358212	9.500583
O	-0.358353	1.343180	7.939316
O	0.093276	3.528482	9.310088
O	3.420105	10.168383	9.312361
O	10.255560	14.483637	8.789305
O	17.150791	14.490129	8.808331
O	-0.266805	1.235684	11.859808
O	0.378727	-1.164734	12.204917
O	3.203424	-1.140455	11.079216
O	3.122650	7.915040	12.022092
O	7.282188	-1.258627	12.108538
O	10.092442	-1.164515	11.084766
O	15.641700	2.341293	10.889550
O	18.938145	9.019563	10.876398
O	10.159046	14.333973	12.506607
O	13.272931	14.506174	11.940532
O	17.483768	5.456977	12.114552
O	17.044830	14.324762	12.495047
O	20.106293	14.540855	11.859808
O	20.751823	12.140437	12.204917
O	1.506240	4.272271	12.606611
O	4.789160	10.925636	12.600587

ZrO₂, C₂H₄-2H**

Zr	6.490611	4.027276	1.915200
Zr	9.800062	10.679861	1.915200
Zr	13.367708	4.027276	1.915200
Zr	16.677158	10.679861	1.915200
Zr	1.397412	1.046186	2.178900
Zr	4.706862	7.698771	2.178900
Zr	8.274508	1.046186	2.178900
Zr	11.583960	7.698771	2.178900

Zr	4.963428	0.369285	2.349180	Zr	18.720625	12.909516	11.880395
Zr	8.272879	7.021871	2.349180	Zr	3.541016	3.320703	12.157434
Zr	11.840524	0.369285	2.349180	Zr	6.858563	9.969405	12.173225
Zr	15.149975	7.021871	2.349180	Zr	10.422007	3.303484	12.162841
Zr	3.179680	4.040781	2.612880	Zr	13.567325	10.013179	12.256110
Zr	6.489130	10.693365	2.612880	O	4.499073	3.908527	0.999990
Zr	10.056777	4.040781	2.612880	O	7.808524	10.561112	0.999990
Zr	13.366228	10.693365	2.612880	O	11.376169	3.908527	0.999990
Zr	3.210352	1.561828	5.086620	O	14.685621	10.561112	0.999990
Zr	6.519803	8.214414	5.086620	O	1.662866	3.094650	1.359840
Zr	10.087448	1.561828	5.086620	O	4.972317	9.747235	1.359840
Zr	13.396900	8.214414	5.086620	O	8.539963	3.094650	1.359840
Zr	8.295352	5.213499	5.341620	O	11.849415	9.747235	1.359840
Zr	11.604803	11.866083	5.341620	O	6.223625	6.241323	1.594740
Zr	15.172449	5.213499	5.341620	O	9.533075	12.893908	1.594740
Zr	18.481899	11.866083	5.341620	O	13.100722	6.241323	1.594740
Zr	4.968447	4.570592	5.515710	O	16.410173	12.893908	1.594740
Zr	8.277898	11.223178	5.515710	O	6.282972	1.960384	2.053440
Zr	11.845544	4.570592	5.515710	O	9.592424	8.612969	2.053440
Zr	15.154995	11.223178	5.515710	O	13.160070	1.960384	2.053440
Zr	6.757046	1.582916	5.764470	O	16.469521	8.612969	2.053440
Zr	10.066498	8.235501	5.764470	O	3.387318	6.107672	2.474640
Zr	13.634143	1.582916	5.764470	O	6.696769	12.760258	2.474640
Zr	16.943594	8.235501	5.764470	O	10.264415	6.107672	2.474640
Zr	3.204493	5.760422	8.251172	O	13.573866	12.760258	2.474640
Zr	6.517231	12.407667	8.245866	O	3.446666	1.826733	2.933310
Zr	10.082227	5.756303	8.250580	O	6.756118	8.479319	2.933310
Zr	13.393518	12.410419	8.253997	O	10.323626	1.826733	2.933310
Zr	4.990963	2.775798	8.525805	O	13.633078	8.479319	2.933310
Zr	8.307198	9.425966	8.525352	O	8.007458	4.973473	3.168240
Zr	11.870146	2.775005	8.523360	O	11.316909	11.626059	3.168240
Zr	15.170424	9.426802	8.607309	O	14.884556	4.973473	3.168240
Zr	1.642632	2.141510	8.705499	O	18.194006	11.626059	3.168240
Zr	4.977100	8.775786	8.684565	O	5.171217	4.159529	3.528060
Zr	8.523835	2.140334	8.712508	O	8.480669	10.812115	3.528060
Zr	11.837068	8.782570	8.715209	O	12.048177	4.159529	3.528060
Zr	6.767344	5.754671	8.965199	O	15.357628	10.812115	3.528060
Zr	10.069483	12.429203	8.950508	O	1.215985	1.420527	4.156470
Zr	13.639124	5.764085	8.954496	O	4.525436	8.073112	4.156470
Zr	16.951826	12.431349	8.948987	O	8.093081	1.420527	4.156470
Zr	1.727425	0.338386	11.593916	O	11.402533	8.073112	4.156470
Zr	5.047970	6.975806	11.613150	O	5.222879	0.623746	4.476120
Zr	8.615693	0.320009	11.603483	O	8.532331	7.276332	4.476120
Zr	11.937510	6.966807	11.616727	O	12.099977	0.623746	4.476120
Zr	6.734696	3.304043	11.627275	O	15.409428	7.276332	4.476120
Zr	10.022003	9.954714	11.603642	O	2.942146	3.794435	4.821840
Zr	13.607566	3.311649	11.609747	O	6.251596	10.447021	4.821840
Zr	17.024595	9.924376	11.495852	O	9.819242	3.794435	4.821840
Zr	8.540437	6.249388	11.888755	O	13.128694	10.447021	4.821840
Zr	11.818640	12.946435	11.868906	O	6.310015	6.157300	5.268030
Zr	15.399960	6.262935	11.884442	O	9.619466	12.809886	5.268030

O	13.187112	6.157300	5.268030	O	8.047445	9.843175	10.539595
O	16.496563	12.809886	5.268030	O	11.617022	3.178487	10.535700
O	6.965534	3.643222	5.656380	O	15.031273	9.712216	10.627729
O	10.274984	10.295807	5.656380	O	1.884577	2.350042	10.888488
O	13.842632	3.643222	5.656380	O	5.192347	8.997093	10.873981
O	17.152082	10.295807	5.656380	O	8.772075	2.332200	10.891276
O	3.434196	6.015002	6.085470	O	12.071566	9.003238	10.948733
O	6.743647	12.667587	6.085470	O	6.530774	5.500219	11.090164
O	10.311293	6.015002	6.085470	O	9.809081	12.175990	11.052473
O	13.620744	12.667587	6.085470	O	13.382044	5.464794	11.052261
O	4.754588	2.487601	6.281520	O	16.720531	12.151898	11.066180
O	8.064039	9.140186	6.281520	O	6.648183	1.219087	11.926183
O	11.631685	2.487601	6.281520	O	9.936128	7.865654	11.893154
O	14.941136	9.140186	6.281520	O	13.498669	1.218742	11.879824
O	1.848415	1.703394	6.660390	O	16.863276	7.887490	12.005586
O	5.157866	8.355980	6.660390	O	3.712624	5.451194	12.116354
O	8.725513	1.703394	6.660390	O	7.008443	12.122509	12.144710
O	12.034964	8.355980	6.660390	O	10.577780	5.453392	12.146089
O	8.113612	5.618190	7.384235	O	13.873535	12.098197	12.105394
O	11.431377	12.244210	7.384027	O	3.542297	1.025689	12.499537
O	14.993307	5.610009	7.382210	O	6.848647	7.681741	12.505831
O	18.301414	12.272863	7.378897	O	10.423615	1.005187	12.512030
O	5.211884	4.835433	7.753913	O	13.785421	7.584238	12.439623
O	8.523306	11.483919	7.752622	O	8.375750	4.271811	12.608923
O	12.081639	4.840720	7.755600	O	11.613272	10.996866	12.559380
O	15.392275	11.477692	7.772066	O	15.245530	4.289696	12.600598
O	6.520640	1.343537	7.932919	O	18.576017	10.921321	12.594954
O	9.830036	7.992300	7.932821	O	12.210669	3.388434	13.060311
O	13.394217	1.338571	7.927739	O	15.645741	10.218064	13.093293
O	16.712561	8.001395	7.946702	O	5.329190	3.398866	13.064658
O	2.996268	3.707101	8.409031	O	8.634617	10.056629	13.066885
O	6.310767	10.351288	8.387458	H	13.394506	9.662904	14.094738
O	9.870046	3.702199	8.395617	H	15.734447	9.990551	14.030653
O	13.189220	10.358595	8.485260	O	15.417060	3.094650	1.359840
O	3.643906	1.189310	8.774045	O	18.726511	9.747235	1.359840
O	6.964410	7.834249	8.794197	O	-0.594124	1.960384	2.053440
O	10.527469	1.187720	8.789102	O	2.914173	-0.411263	1.594740
O	13.819942	7.834085	8.787470	O	0.077867	-0.544913	2.474640
O	6.984287	3.525765	9.293005	O	2.715326	8.612969	2.053440
O	10.292097	10.166597	9.299576	O	9.791271	-0.411263	1.594740
O	13.855515	3.518732	9.274567	O	6.954964	-0.544913	2.474640
O	17.208923	10.188536	9.283452	O	4.698007	-1.679112	3.168240
O	1.424372	0.069376	9.487912	O	11.575104	-1.679112	3.168240
O	4.748687	6.707778	9.506536	O	13.832061	-0.544913	2.474640
O	8.308438	0.063484	9.500501	O	17.141512	6.107672	2.474640
O	11.612107	6.724368	9.510802	O	1.130362	4.973473	3.168240
O	8.779420	5.971222	9.898589	O	4.439812	11.626059	3.168240
O	12.073543	12.676558	9.882360	O	3.000564	-0.495285	5.268030
O	15.651478	6.002591	9.891209	O	9.877661	-0.495285	5.268030
O	18.969095	12.629172	9.891032	O	11.841782	13.928917	4.476120
O	4.752438	3.166552	10.540905	O	16.696341	3.794435	4.821840

O	17.188389	6.015002	6.085470	Zr	8.272879	7.021871	2.349180
O	18.718880	13.928917	4.476120	Zr	11.840524	0.369285	2.349180
O	20.005791	10.447021	4.821840	Zr	15.149975	7.021871	2.349180
O	20.497841	12.667587	6.085470	Zr	3.179680	4.040781	2.612880
O	7.001842	-0.637584	6.085470	Zr	6.489130	10.693365	2.612880
O	13.878939	-0.637584	6.085470	Zr	10.056777	4.040781	2.612880
O	14.970180	1.420527	4.156470	Zr	13.366228	10.693365	2.612880
O	15.602610	1.703394	6.660390	Zr	3.210352	1.561828	5.086620
O	18.279631	8.073112	4.156470	Zr	6.519803	8.214414	5.086620
O	18.912060	8.355980	6.660390	Zr	10.087448	1.561828	5.086620
O	1.239113	5.610009	7.382210	Zr	13.396900	8.214414	5.086620
O	1.897284	6.002591	9.891209	Zr	8.295352	5.213499	5.341620
O	2.958366	8.001395	7.946702	Zr	11.604803	11.866083	5.341620
O	4.547220	12.272863	7.378897	Zr	15.172449	5.213499	5.341620
O	5.214901	12.629172	9.891032	Zr	18.481899	11.866083	5.341620
O	6.258924	14.643743	7.927739	Zr	4.968447	4.570592	5.515710
O	8.043274	13.374547	9.487912	Zr	8.277898	11.223178	5.515710
O	13.139543	14.648708	7.932919	Zr	11.845544	4.570592	5.515710
O	14.927341	13.368655	9.500501	Zr	15.154995	11.223178	5.515710
O	-0.359978	1.338571	7.927739	Zr	6.757046	1.582916	5.764470
O	0.101321	3.518732	9.274567	Zr	10.066498	8.235501	5.764470
O	3.454729	10.188536	9.283452	Zr	13.634143	1.582916	5.764470
O	10.262809	14.494481	8.774045	Zr	16.943594	8.235501	5.764470
O	17.146370	14.492891	8.789102	Zr	3.204029	5.753042	8.250459
O	-0.255526	1.218742	11.879824	Zr	6.515353	12.405205	8.249959
O	0.389541	-1.182662	12.144710	Zr	10.082869	5.753376	8.250924
O	3.190179	-1.129181	11.052473	Zr	13.392691	12.406438	8.250016
O	3.109081	7.887490	12.005586	Zr	4.987773	2.769451	8.527131
O	7.254633	-1.206974	12.105394	Zr	8.301866	9.423411	8.526466
O	10.101629	-1.153273	11.066180	Zr	11.867556	2.773966	8.527221
O	15.638771	2.350042	10.888488	Zr	15.175493	9.426078	8.529139
O	18.946541	8.997093	10.873981	Zr	1.643630	2.135257	8.712624
O	10.161199	14.330860	12.499537	Zr	4.959096	8.784107	8.709895
O	13.267086	14.524258	11.926183	Zr	8.523335	2.135705	8.714750
O	17.466818	5.451194	12.116354	Zr	11.835506	8.787547	8.712494
O	17.042517	14.310358	12.512030	Zr	6.763243	5.758978	8.959620
O	20.117571	14.523912	11.879824	Zr	10.072922	12.414331	8.958298
O	20.762638	12.122509	12.144710	Zr	13.639581	5.763933	8.962336
O	1.491336	4.289696	12.600598	Zr	16.950836	12.417684	8.958557
O	4.821823	10.921321	12.594954	Zr	1.734432	0.334089	11.602497
ZrO ₂ , C ₂ H ₄ -H ₂ *				Zr	5.043574	6.986659	11.604746
Zr	6.490611	4.027276	1.915200	Zr	8.610081	0.330865	11.604360
Zr	9.800062	10.679861	1.915200	Zr	11.920603	6.988986	11.607812
Zr	13.367708	4.027276	1.915200	Zr	6.727520	3.308361	11.615750
Zr	16.677158	10.679861	1.915200	Zr	10.042806	9.961564	11.613844
Zr	1.397412	1.046186	2.178900	Zr	13.604823	3.310214	11.617992
Zr	4.706862	7.698771	2.178900	Zr	16.929268	9.961093	11.598191
Zr	8.274508	1.046186	2.178900	Zr	8.534735	6.253481	11.885177
Zr	11.583960	7.698771	2.178900	Zr	11.845802	12.903109	11.885065
Zr	4.963428	0.369285	2.349180	Zr	15.413514	6.256169	11.886047
				Zr	18.722298	12.904773	11.885595

Zr	3.539166	3.308580	12.160918	O	16.496563	12.809886	5.268030
Zr	6.854627	9.963268	12.162044	O	6.965534	3.643222	5.656380
Zr	10.415369	3.308403	12.161820	O	10.274984	10.295807	5.656380
Zr	13.736298	9.956784	12.182080	O	13.842632	3.643222	5.656380
O	4.499073	3.908527	0.999990	O	17.152082	10.295807	5.656380
O	7.808524	10.561112	0.999990	O	3.434196	6.015002	6.085470
O	11.376169	3.908527	0.999990	O	6.743647	12.667587	6.085470
O	14.685621	10.561112	0.999990	O	10.311293	6.015002	6.085470
O	1.662866	3.094650	1.359840	O	13.620744	12.667587	6.085470
O	4.972317	9.747235	1.359840	O	4.754588	2.487601	6.281520
O	8.539963	3.094650	1.359840	O	8.064039	9.140186	6.281520
O	11.849415	9.747235	1.359840	O	11.631685	2.487601	6.281520
O	6.223625	6.241323	1.594740	O	14.941136	9.140186	6.281520
O	9.533075	12.893908	1.594740	O	1.848415	1.703394	6.660390
O	13.100722	6.241323	1.594740	O	5.157866	8.355980	6.660390
O	16.410173	12.893908	1.594740	O	8.725513	1.703394	6.660390
O	6.282972	1.960384	2.053440	O	12.034964	8.355980	6.660390
O	9.592424	8.612969	2.053440	O	8.112601	5.612424	7.383118
O	13.160070	1.960384	2.053440	O	11.421867	12.275038	7.380753
O	16.469521	8.612969	2.053440	O	14.988489	5.617656	7.383367
O	3.387318	6.107672	2.474640	O	18.299728	12.270210	7.382424
O	6.696769	12.760258	2.474640	O	5.206688	4.831209	7.754631
O	10.264415	6.107672	2.474640	O	8.518756	11.483804	7.751317
O	13.573866	12.760258	2.474640	O	12.084929	4.834369	7.754166
O	3.446666	1.826733	2.933310	O	15.396835	11.488160	7.753877
O	6.756118	8.479319	2.933310	O	6.521102	1.338935	7.936744
O	10.323626	1.826733	2.933310	O	9.830981	7.992126	7.935459
O	13.633078	8.479319	2.933310	O	13.397102	1.341811	7.934889
O	8.007458	4.973473	3.168240	O	16.709864	7.993773	7.935567
O	11.316909	11.626059	3.168240	O	2.989248	3.698627	8.392864
O	14.884556	4.973473	3.168240	O	6.302786	10.353037	8.399199
O	18.194006	11.626059	3.168240	O	9.869741	3.699856	8.400286
O	5.171217	4.159529	3.528060	O	13.178397	10.353260	8.391219
O	8.480669	10.812115	3.528060	O	3.647618	1.182431	8.798305
O	12.048177	4.159529	3.528060	O	6.959512	7.834345	8.795423
O	15.357628	10.812115	3.528060	O	10.526485	1.184873	8.795773
O	1.215985	1.420527	4.156470	O	13.834979	7.835042	8.793447
O	4.525436	8.073112	4.156470	O	6.976828	3.521567	9.291369
O	8.093081	1.420527	4.156470	O	10.291088	10.175259	9.291328
O	11.402533	8.073112	4.156470	O	13.854638	3.523823	9.295599
O	5.222879	0.623746	4.476120	O	17.164053	10.174382	9.290178
O	8.532331	7.276332	4.476120	O	1.429957	0.053712	9.498899
O	12.099977	0.623746	4.476120	O	4.742239	6.706810	9.501969
O	15.409428	7.276332	4.476120	O	8.308360	0.053273	9.502892
O	2.942146	3.794435	4.821840	O	11.617906	6.709631	9.502232
O	6.251596	10.447021	4.821840	O	8.777326	5.975709	9.895184
O	9.819242	3.794435	4.821840	O	12.086412	12.623904	9.895106
O	13.128694	10.447021	4.821840	O	15.652277	5.980337	9.895639
O	6.310015	6.157300	5.268030	O	18.964813	12.630746	9.894899
O	9.619466	12.809886	5.268030	O	4.740750	3.186772	10.538091
O	13.187112	6.157300	5.268030	O	8.054036	9.834925	10.537935

O	11.619158	3.188334	10.539344	O	18.718880	13.928917	4.476120
O	14.920166	9.829123	10.540533	O	20.005791	10.447021	4.821840
O	1.887549	2.340637	10.886712	O	20.497841	12.667587	6.085470
O	5.199955	8.991687	10.887951	O	7.001842	-0.637584	6.085470
O	8.763708	2.340496	10.888160	O	13.878939	-0.637584	6.085470
O	12.078321	8.994683	10.892154	O	14.970180	1.420527	4.156470
O	6.523861	5.506388	11.083676	O	15.602610	1.703394	6.660390
O	9.830488	12.159721	11.081779	O	18.279631	8.073112	4.156470
O	13.401764	5.510496	11.086360	O	18.912060	8.355980	6.660390
O	16.714081	12.161641	11.079897	O	1.234295	5.617656	7.383367
O	6.632770	1.218047	11.904638	O	1.898083	5.980337	9.895639
O	9.943254	7.872984	11.907919	O	2.955669	7.993773	7.935567
O	13.508421	1.219765	11.903481	O	4.545534	12.270210	7.382424
O	16.821371	7.871996	11.899303	O	5.210619	12.630746	9.894899
O	3.698659	5.463156	12.135935	O	6.261810	14.646982	7.934889
O	7.008322	12.115157	12.136681	O	8.048859	13.358884	9.498899
O	10.572795	5.461720	12.134427	O	13.140004	14.644106	7.936744
O	13.883995	12.110703	12.142484	O	14.927262	13.358444	9.502892
O	3.543661	1.023583	12.507789	O	-0.357092	1.341811	7.934889
O	6.858626	7.674932	12.508365	O	0.100444	3.523823	9.295599
O	10.419876	1.024956	12.505060	O	3.409859	10.174382	9.290178
O	13.735507	7.678172	12.518665	O	10.266520	14.487602	8.798305
O	8.368343	4.277405	12.604057	O	17.145388	14.490044	8.795773
O	11.675220	10.932919	12.602541	O	-0.245773	1.219765	11.903481
O	15.249481	4.280577	12.598970	O	0.389420	-1.190014	12.136681
O	18.562252	10.929985	12.598979	O	3.211586	-1.145450	11.081779
O	12.204672	3.400943	13.063213	O	3.067177	7.871996	11.899303
O	15.547054	10.062724	13.051055	O	7.265093	-1.194468	12.142484
O	5.329420	3.399884	13.060688	O	10.095179	-1.143530	11.079897
O	8.641423	10.053016	13.062583	O	15.641744	2.340637	10.886712
H	13.147390	9.954911	14.964406	O	18.954149	8.991687	10.887951
H	13.896271	9.908025	14.858006	O	10.162563	14.328754	12.507789
O	15.417060	3.094650	1.359840	O	13.251673	14.523217	11.904638
O	18.726511	9.747235	1.359840	O	17.452852	5.463156	12.135935
O	-0.594124	1.960384	2.053440	O	17.038778	14.330127	12.505060
O	2.914173	-0.411263	1.594740	O	20.127323	14.524936	11.903481
O	0.077867	-0.544913	2.474640	O	20.762516	12.115157	12.136681
O	2.715326	8.612969	2.053440	O	1.495287	4.280577	12.598970
O	9.791271	-0.411263	1.594740	O	4.808058	10.929985	12.598979
O	6.954964	-0.544913	2.474640				
O	4.698007	-1.679112	3.168240				
O	11.575104	-1.679112	3.168240				
O	13.832061	-0.544913	2.474640				
O	17.141512	6.107672	2.474640				
O	1.130362	4.973473	3.168240				
O	4.439812	11.626059	3.168240				
O	3.000564	-0.495285	5.268030				
O	9.877661	-0.495285	5.268030				
O	11.841782	13.928917	4.476120				
O	16.696341	3.794435	4.821840				
O	17.188389	6.015002	6.085470				