Targeted Single-Site MOF Node Modification: Trivalent Metal Loading via Atomic Layer Deposition

In Soo Kim,[a] Joshua Borycz,[b] Ana E. Platero-Prats,[c] Samat Tussupbayev,[b] Timothy C. Wang,[d] Omar K. Farha,[d,e] Joseph T. Hupp,[a,d] Laura Gagliardi,[b] Karena W. Chapman,[c] Christopher J. Cramer,*[b] Alex B. F. Martinson*[a]

[a]Materials Science Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, Illinois 60439, USA
[b]Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota, Minneapolis, Minnesota 55455, United States
[c]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, Illinois 60439, USA
[d]Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA
[e]Department of Chemistry, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

ABSTRACT

Post-synthetic functionalization of metal organic frameworks (MOFs) enables the controlled, high-density incorporation of new atoms on a crystallographically precise framework. Leveraging the broad palette of known atomic layer deposition (ALD) chemistries, ALD in MOFs (AIM) is one such targeted approach to construct diverse, highly functional, few-atom clusters. We here demonstrate the saturating reaction of trimethylindium ($InMe_3$) with the node hydroxyls and ligated water of NU-1000, which takes place without significant loss of MOF crystallinity or internal surface area. We computationally identify the elementary steps by which trimethylated trivalent metal compounds (ALD precursors) react with this Zr-based MOF node to generate a uniform and well characterized new surface layer on the node itself, and we predict a final structure that is fully consistent with experimental X-ray pair distribution function (PDF) analysis. We further demonstrate tunable metal loading through controlled number density of the reactive handles (–OH and $–OH_2$) achieved through node dehydration at elevated temperatures.

INTRODUCTION

Metal-organic frameworks (MOFs) are attractive systems for catalytic studies,[1-2] in part because they exhibit uniform mesoscale and/or microscale porosity, generated by periodic and atomically well-defined structures. Importantly, these structures, comprising organic linkers and inorganic, metal-containing nodes, are amenable to full experimental structural characterization and rigorous computational modeling.[3-6] While the vast majority of MOF catalysis work focuses on linkers as catalysts[7] for condensed-phase reactions, a few reports of node-based catalysis have also appeared,[8-16] including at least one for high temperature (350 ^{o}C) heterogeneous catalysis of a gas-phase oxidation reaction.[17] Increasingly popular as nodes for these types of studies are

hexa-zirconium(IV)oxo/hydroxo/aqua species and their hafnium(IV) analogues. The lability and reactivity of the nodes' oxygen-rich ligands—specifically, aqua and terminal hydroxo ligands—allows for site-specific functionalization, both with nonstructural organic ligands[18-22] and, in principle, with nonstructural metal ions. We have shown that the latter can be accomplished in reproducible fashion with a suitably porous MOF, NU-1000 (aperture width > 3 nm), via chemistry akin to atomic-layer deposition (ALD), a materials synthesis technique typically applied to hydroxyl-presenting surfaces of purely inorganic surfaces.[23-25] We reasoned that the nodes within NU-1000 and related MOFs could be viewed chemically as tiny fragments of zirconia, and therefore, be subjected to the self-limiting, conformal functionalization chemistry that characterizes conventional ALD.[26] Indeed, with vapor-phase organometallic precursors such as diethyl zinc, and as previously described in preliminary fashion, **A**LD **i**n **M**OFs (AIM)[26] is readily accomplished specifically with NU-1000. Here, with the ultimate goal of arbitrary, single-atom precision for MOF post-metalation, we investigate and report on the details of AIM using two well-known ALD precursors, trimethylindium ($InMe_3$) and trimethyaluminum ($AlMe_3$).

Recent advances in both MOF and ALD science make their potential union both feasible and versatile. While the stability ranges of early MOFs and process ranges of early ALD procedures occupied different temperature windows – generally below and above 200 °C, respectively – advances in both fields now permit significant overlap of these ranges. For example, selected MOFs based on Zr_6O_{16} nodes (**Figure 1**), retain their mesoporosity at temperatures above 400 °C, and in some case above 500 °C.[12, 26-27] In addition, an ever growing number of ALD processes for oxides, sulfides, nitrides, and pure metals have been identified at temperatures as low as 100 °C.[28-32] Appropriately chosen MOFs exhibit the high porosity and large pore apertures (> 3 nm) desirable to minimize the influence of mass transport limitations that would otherwise practically inhibit vapor-phase loading. Such characteristics allow for AIM, where precise surface chemical control is retained through self-limiting reactions that allow uniform reaction throughout an arbitrarily complex framework. Recently, the platform MOF material NU-1000 has been modified with Al, Zn, and their combination.[26] In order to provide mechanistic insight and establish universal applicability of the AIM approach, we take trimethylated trivalent metal precursors as model reactants, and examine the extent to which uniform and self-limiting (ALD-like) reactions can be achieved in MOFs. Furthermore, we determine the exact locations of the trivalent metals, obtaining results that are consistent with a mechanism that we derive from-first principles computation. Finally, we assess one of the most chemically aggressive ALD precursors, $AlMe_3$, for compatibility with the MOF framework.

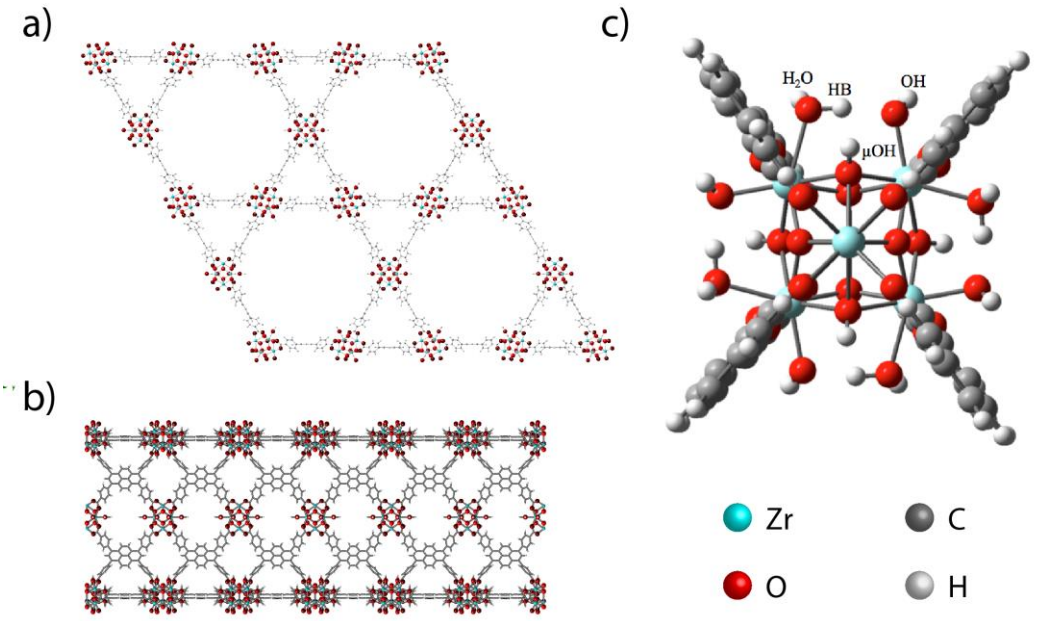


Figure 1. a) and b) Zr_6-based framework NU-1000. c) Cluster used to model the Zr_6-node in NU-1000.

RESULTS AND DISCUSSION

A Zr_6-based framework, NU-1000 nodes are octahedral Zr_6 clusters including four each bridging μ–O and μ–OH groups. The 3D structure of the MOF results from bridging of the nodes by tetra-carboxylate linkers (**Figure 1a,b**).[26] Importantly, under ambient conditions, four each aquo and hydroxo groups can occupy remaining open metal coordination sites of the node. The detailed structure of NU-1000 was previously investigated both computationally and experimentally to reveal a staggered mixed proton topology for the $[Zr_6(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4(OH)_4(H_2O)_4]^{8+}$ cluster (**Figure 1c**) at room temperature.[33]

The –OH and $–OH_2$ functional groups at the surface of the node present in a manner making them likely to be amenable to many conventional oxide ALD half-reactions. Using density functional theory (DFT) calculations, we have identified highly exothermic reaction pathways for reaction of the node with two trimethylated trivalent metal compounds, $AlMe_3$ and $InMe_3$, as illustrated in **Figure 2**. This chemistry is in close analogy to that previously hypothesized for planar surface modification in traditional thin film ALD growth.[34] Based on the reaction pathways, a maximum of 8 metal atoms are predicted to bind to each Zr_6 node with the release of up to twelve methane (CH_4) molecules.

Computational Results. There are four chemically distinct protons on each of the four faces of the Zr_6-node in NU-1000, one that engages in a hydrogen bond between the aquo and hydroxo ligands (HB; see Figure 1c), two that are *non*-hydrogen bonded on the aquo (H_2O) and hydroxo

(OH) ligands, respectively, and one that is on the core itself (μOH). To test which of the four protons on each face is most likely to be replaced with either $AlMe_3$ or $InMe_3$, each proton was individually substituted for an $AlMe_2$ or $InMe_2$ group and the structure of the cluster was then optimized with fixed linker positions. Replacement of hydrogen HB with $AlMe_2$ or $InMe_2$ results in the most stable product (**Table 1**). We subsequently located the transition-state (TS) structure leading to this intermediate, and we characterized all of the elementary steps involved in the further reaction of the node face under operating conditions. The full reaction coordinate, shown in **Figure 2**, indicates that each face of the Zr_6-node will react with two ALD precursors to generate four CH_4 product molecules, i.e., our model predicts that every O-H bond on each node will react with $AlMe_3$ and $InMe_3$ to lead to a final structure with eight tetrahedrally coordinated $(RO)_3AlMe$ or $(RO)_3InMe$ groups disposed at the surface.

	Relative Energy (kcal/mol)			
	ΔE		ΔG	
	$AlMe_3$	$InMe_3$	$AlMe_3$	$InMe_3$
HB	0.0	0.0	0.0	0.0
H_2O	18.5	15.7	19.2	17.3
OH	22.3	21.6	22.9	23.0
μOH	24.4	22.6	24.9	24.0

Table 1. Relative reaction energies for substitution of $AlMe_2$ and $InMe_2$ (and generation of CH_4) at the positions of the labeled hydrogens in the bare Zr_6 cluster shown in **Figure 1c**.

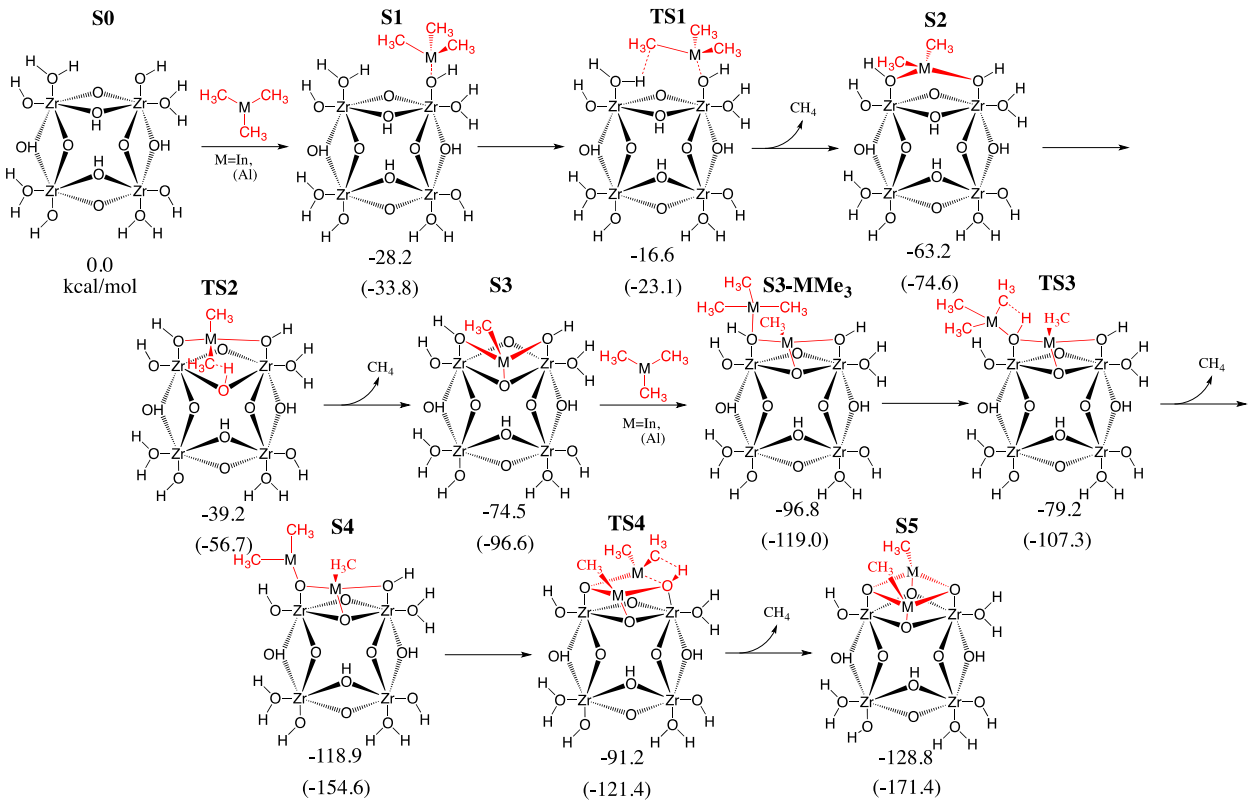


Figure 2. M06-L relative enthalpies (kcal mol^{-1}) for intermediates and TS structures on the reaction coordinate for one face of the NU-1000 node reacting with two equivalents of $AlMe_3$ or $InMe_3$ (in parentheses) and liberating 4 equivalents of CH_4. Subsequent reaction coordinates for the remaining faces of the node (not shown) were found to be entirely equivalent, with negligible differences in enthalpies relative to analogous precursors, i.e., there is no significant influence of one face upon another over the course of reaction.

Experimental Results. To verify the self-limiting nature of the precursor with hydroxyl and water groups, a full saturation study including exploration of mole-limited and diffusion-time limited variable space was undertaken (**Figure 3**). In each experiment, 10 mg of microcrystalline NU-1000 powder was warmed to 125 °C under vacuum with 0.5 Torr of flowing nitrogen for 20 minutes in order to remove any physisorbed water or solvent. Next, the powder was soaked at the desired temperature (75 and 125 °C for $InMe_3$ and $AlMe_3$, respectively) prior to a 60 second exposure to water vapor. Further soaking under flowing N_2 at temperature establishes an equilibrium –OH and $–OH_2$ population. Finally, the metal precursor ($InMe_3$ or $AlMe_3$) was delivered to the reaction chamber under its own vapor pressure and exposed without pumping (quasi-static mode) for the indicated time for a given number of repetitions. The results of the AIM process with $InMe_3$ (**Figure 3**) reveal many of the characteristics of archetypal ALD surface reactions, albeit with much large doses and exposures, as predicted for a large surface area powder with high aspect ratio pores. Clearly, a stoichiometric number of precursor

molecules must be delivered with respect to the available reaction sites in order to achieve a saturating reaction. The number of sites in 10 mg of powder is estimated to be 3.7 x 10^{-5} moles based on 8 sites per Zr_6 node. Based on the vapor pressure of $InMe_3$, an equal or greater number of moles are expected to be delivered in a single 0.4 second dose. Therefore, under these processing conditions the reaction is never mole-limited. Still, due to the very high aspect ratio of the channels through which the vapor is required to traverse (~10,000), a non-trivial time for precursor diffusion to all points within the microcrystals must also be considered. An empirical formula[35] based on Monte Carlo simulations assuming Knudsen diffusion was used to calculate a total exposure time of at least 20 seconds required to traverse the long, narrow channels with this aspect ratio. This is roughly consistent with a 600 second exposure time required to achieve the complete loading of the longest crystals. As evidenced by the saturating In ratio in the limit of large dose and long diffusion time, the process shows ideal self-limiting behavior. Based on the saturation studies under these optimized ALD conditions, the number of In per Zr_6 node obtained by inductively coupled plasma-optical emission spectroscopy (ICP-OES) saturates at ~6 (In:Zr_6=1), in reasonable agreement with the computational prediction. Several factors account for the deviation from the computationally predicted loading of 8 In per Zr_6 node. First, the NU-1000 structure is known to contain a fraction (perhaps 25 %) of "secondary" nodes within the largest pores.[26] This secondary node is connected to the framework through additional linkers, each one of which reduces the potential number of deposition sites on neighboring nodes by 2. Furthermore, the computationally predicted reaction assumes full initial ligation of the node (4 OH_2, 4 OH, 4 μ-OH), which may be slightly reduced via dehydration under continuous heating (75 °C) in vacuum. Finally, there is the possibility that only a subset of the potential reaction sites are reasonably accessible by $InMe_3$. This possibility, however, was minimized by performing saturation studies in excess of both diffusion time and moles of $InMe_3$ (**Figure 3**). Furthermore, the possibility of a minority of clogged pores, through which the metal precursor will never pass, has not been rigorously excluded.

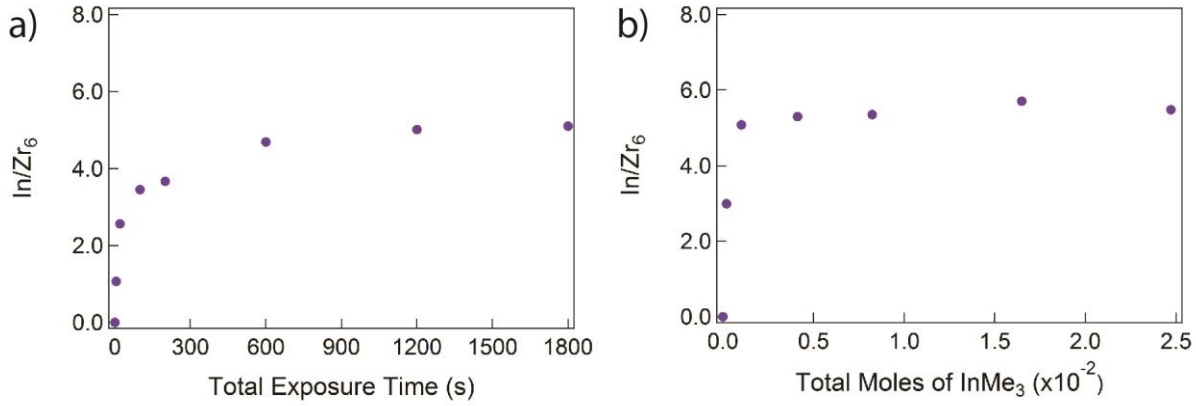


Figure 3. In to Zr_6 node ratio as a function of the ALD process conditions. Sub-saturating In loading is observed upon delivery of a non-stoichiometric $InMe_3$ dose or insufficient exposure time. In the limit of exceptionally large and long exposures, the process exhibits self-limiting behavior.

While the AIM process with $AlMe_3$ shows, with moderate exposures, apparent self-limiting behavior with ~6 Al per Zr_6 (**Figure 4a**), larger exposures reveal non-self-limiting behavior (~14 metal per Zr_6 node) as shown in **Figure 4b**.

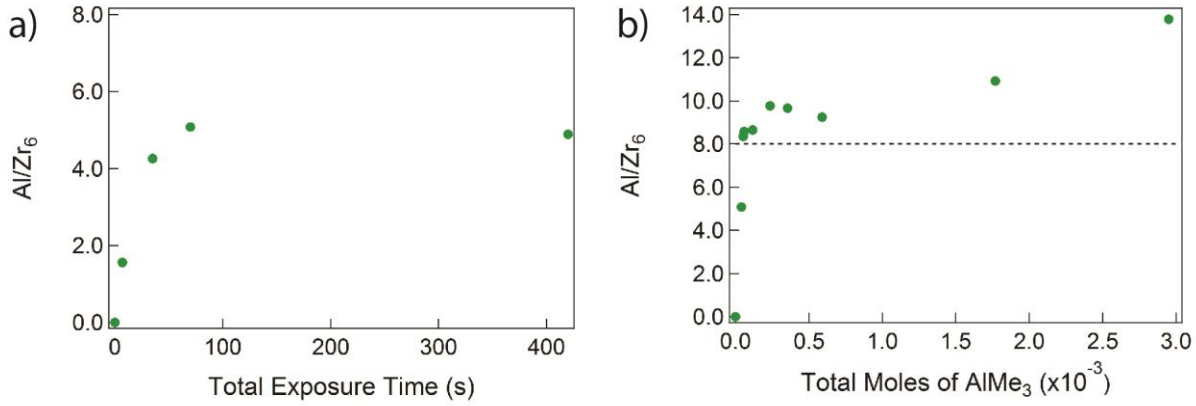


Figure 4. ALD metal to Zr_6 node ratio as a function of ALD process conditions. The delivery of a non-stoichiometic $AlMe_3$ dose or insufficient diffusion time produce sub-saturating Al loading. In the limit of exceptionally large and long doses, the process does not exhibit self-limiting behavior.

Consistent with its strong Lewis acidity, $AlMe_3$ is known to aggressively react with many functional groups beyond -OH. In extreme cases, for example, $AlMe_3$ preferentially attacks and abstracts oxygen anions from surface oxides of GaAs and $In_{0.2}Ga_{0.8}As$ substrates.[36-37] As such, reaction with components in the MOF framework beyond the hydroxylated node is not extraordinary. The extra-nodal reactivity of this aggressive precursor is further corroborated by the significant loss of sample crystallinity evident in powder x-ray diffraction (PXRD) data obtained following large $AlMe_3$ exposures, **Figure S1**. Although $InMe_3$ is also Lewis acidic (albeit not as much as $AlMe_3$), the strong diffraction peaks of the parent MOF are retained even after total exposures in excess of ~2 hours. Furthermore, the large specific surface area that is associated with the mesoporosity of NU-1000 is significantly degraded upon large $AlMe_3$ exposures, whereas the surface area is retained even after exposure to a ten-fold larger $InMe_3$ dose (**Figure S2**).

The exothermic reaction pathway for trivalent metal binding derived from theory predicts metal atom placement at high-symmetry nodal sites. Each atom is expected to bridge three oxygen

atoms, two deriving from previously terminal $–OH_2$ and –OH groups, and one deriving from the previously bridging μ-OH ligand. Experimental confirmation of ALD metal installation location was obtained from X-ray pair distribution function (PDF) analyses. This method yields atomic scale structural information with crystallographic resolution at a length scale suitable for analysis of few-atom clusters like the Zr_6 node. A differential data plots reveals the new pair correlations present after $InMe_3$ AIM, **Figure 5**.

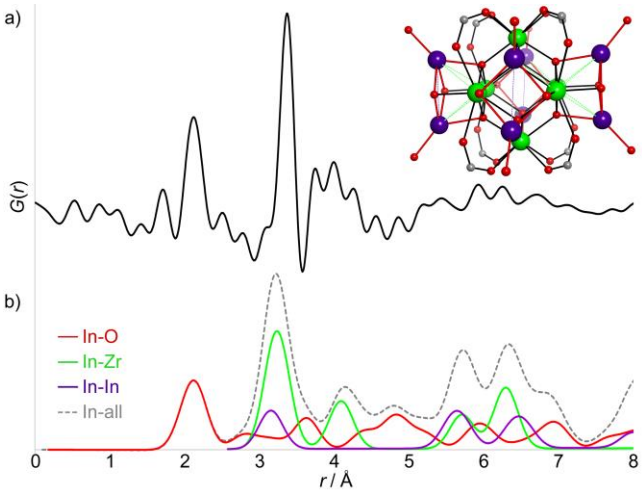


Figure 5. a) The differential PDF corresponding to the new atom-atom distances formed upon $InMe_3$-ALD treatment of NU-1000 at 75 °C following dehydration at 125 °C. b) Partial pair PDFs calculated based on the model for In-loaded NU-1000 structure predicted by DFT. A representation of DFT-derived model of the Zr_6 node, highlighting the new In-node distances, is inset.

The experimental differential PDF reflects the new atom-atom distances formed upon In-loading; the distances are consistent with those derived from first principles calculations. The differential PDF is dominated by features at short distances, suggesting that the In-siting is well defined only locally. Two sharp peaks, centered at 2.12 Å and 3.33 Å, correspond to the In-O bond and In…Zr next-nearest neighbor distances, respectively (*cf.* 2.18 and 3.27 Å from theory, respectively). A broader feature at ~4 Å reflects longer range In…Zr distances within the Zr-node, for which a distribution of distances and increased local disorder are evident. Peaks associated with well-defined In…In distances are not readily evident in the experimental data, suggesting that the In atoms do not order relative to each other.

Having established the location and bonding environment of In upon exposure to $InMe_3$, we sought to further control the number of metal atoms installed on each node. In principle, the room temperature population of terminal –OH, terminal $–OH_2$, and μ-OH on the NU-1000 node support the installation of up to 8 metal atoms. However, under conditions in which the node is

dehydrated (*e.g.* following heating in medium vacuum), a diminished number of presenting functional groups is anticipated to yield a lower degree of metal incorporation under the same AIM conditions. Like many oxide surfaces, the Zr_6O_{16} node releases water through water desorption and hydroxyl recombination at increased temperatures under vacuum. *In situ* Fourier transform infrared spectroscopy (conventional FTIR) studies of NU-1000 as a function of temperature clearly reveal dynamics of node dehydration. At elevated temperatures (> 125 °C), the intensity of –OH, -OH_2, and μ-OH stretches located at ~3673 cm^{-1} decrease continuously with time and temperature (**Figure S3**). Based on these findings, we performed node dehydration at elevated temperatures prior to AIM to provide control over the number of metals to be installed on the nodes. While we do not expect a 1:1 correlation between –OH population as inferred from IR and the In:Zr_6 ratio, the integrated intensity of the –OH stretches (*i.e.*, a measure of –OH population) and the ICP-OES derived ratios of In:Zr_6 do trend together (**Figure 6**). This confirms an ability to control metal loading via node dehydration. Such ability to tune metal loading should allow further customization of node decoration, with the potential for mixed-metal attachment directly to the Zr_6 node in the future through cycles of partial dehydration, deposition, rehydration, and alternative deposition.

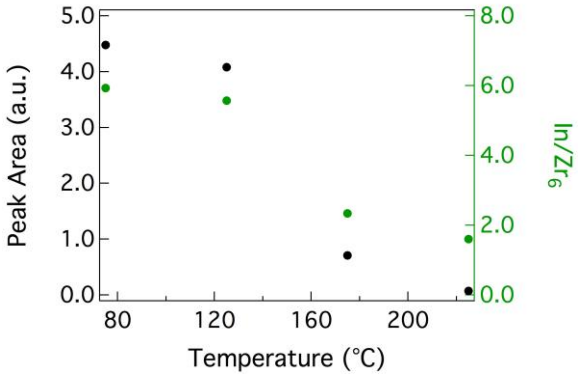


Figure 6. The In AIM loading as a function of node dehydration temperature is correlated to the integrated intensity of FTIR peaks associated with –OH stretches.

CONCLUSIONS

We demonstrate that the Zr_6-node present in the NU-1000 framework reacts with the trimethylated trivalent metal compounds $InMe_3$ and $AlMe_3$ to form stable structures with up to eight metals per Zr_6 node. $InMe_3$ exhibits strict self-limiting behavior in the limit of both excess diffusion time and moles without significant loss of crystallinity or internal surface area. Differential PDF analysis of In-loaded NU-1000 is consistent with theoretical prediction of a highly symmetric structure having two metals deposited on each of four faces of the Zr_6 node; a fully characterized reaction coordinate rationalizes the elementary reaction steps that lead to this

structure and confirms that it is highly exothermic. In practice, the number of In per Zr_6 node saturates at a slightly less than 8:1 stoichiometric ratio, which we attribute to the presence of secondary nodes and unintentional dehydration, both of which reduce the total number of reactive sites. In contrast to $InMe_3$, which displays ideal self-limiting behavior, reactions with $AlMe_3$ evidence extra-nodal reactions with NU-1000 for large exposures, as judged by noticeable degradation of crystallinity and loss of internal surface area. These combined results begin to demarcate process variable space for AIM - *i.e.* temperature and choice of precursors - that must be carefully considered to achieve targeted metal loading while retaining the benefits of mesoporosity and crystallinity. We anticipate reporting soon on using these insights to achieve more ideal functionalization of NU-1000 with Al(III). Importantly, deliberate partial node dehydration at elevated AIM temperatures enables reproducible modulation of the stoichiometry for a single ALD cycle of the saturating reaction of $InMe_3$ with NU-1000, and this control should prove useful for the design of multistep ALD procedures that may involve different metal-containing precursors.

EXPERIMENTAL SECTION

Computational Methods. The periodic structures were computed with the generalized gradient approximation exchange-correlation functional PBE using the Vienna *ab initio* simulation package (VASP).[38-44] The VASP calculations were performed with projector-augmented wave potentials to describe the interaction between the valence and core electrons. A full gamma-point only geometry optimization was performed with a plane-wave kinetic energy cutoff of 520 eV. The energy and force convergence criteria were 10^{-6} eV and 0.05 eV, respectively.

The initial structures for the cluster models were taken from reference (12). The bare Zr_6-node cluster model is provided in **Figure 1**. For the structures shown in the reaction pathway in **Figure 2**, the core zirconium and oxygen atoms were optimized with Gaussian 09[45-46] using the M06-L[47] density functional and the 6-31G(d) basis set[48] on Al, O, C, and H, and the Stuttgart/Dresden effective core potential (SDD)[49] on Zr and In, and the linker atoms were fixed. Frequency calculations at 298 K were then performed at the same level of theory. A singlepoint calculation with the 6-311+G(df,p) basis set[48] was then performed to verify the nature of all stationary points. The enthalpies shown in **Figure 2** were then computed by adding the enthalpy correction at the 6-31G(d) level to the 6-311+G(df,p) energies ($\Delta H = \Delta E_{6\text{-}311G(df,p)} + \Delta H_{6\text{-}31G(d)} - \Delta E_{6\text{-}31G(d)}$).

NU-1000 Synthesis. $ZrOCl_2 \cdot 8H_2O$ (97 mg, 0.30 mmol) and benzoic acid (2.70 g, 22 mmol) were mixed in 8 mL of DMF (in a 6-dram vial) and dissolved using sonication. The clear solution was incubated in an oven at 80 ˚C for 1h. After cooling down to room temperature, **H_4TBAPy** (40 mg, 0.06 mmol) was added to this solution and the mixture was sonicated for 10 mins. The yellow suspension was heated in an oven at 100 ˚C for 18 h. After cooling down to

room temperature, yellow **NU-1000** precipitate was collected by centrifuge. (7800 rpm, 5 mins) and washed with fresh DMF for two times. As synthesized **NU-1000** was then suspended in 13 mL of DMF and 0.5 mL of 8M HCl was added to acid-activate the zirconium node. This mixture was heated in an oven at 100 ˚C for 24 h. After cooling down to room temperature, the supernatant was removed by centrifuge, and the material was washed twice with fresh DMF. Subsequently the solid materials were washed twice with acetone and soaked in acetone for additional 12 h. Then the acetone was removed by centrifuge, and the solid was briefly dried in an oven at 80 °C. The solid material was activated on a SmartVacPrep station (Micromeritics) under dynamic vacuum at 120 ˚C until an outgassing rate of ≤ 0.002 mm Hg min^{-1} was reached.

ALD in MOFs (AIM). AIM process was performed in a Savannah S200 system (Cambridge Nanotech, Cambridge, MA). In-line Entegris Ni filtered nitrogen (N_2) was continuously introduced to the ALD chamber at a flow rate of 20 sccm to maintain a chamber base pressure of ~0.5 Torr. Typically, 10 mg of NU-1000 powder was heated to 125 °C to remove physisorbed water followed by soaking at the desired AIM temperature. All ALD reactions were carried out in quasi-static mode. Standard pulse times for water vapor, $InMe_3$, and $AlMe_3$ were 1 s, 5 s, and 0.015 s, respectively.

PDF Analysis. X-ray total scattering data suitable for PDF analysis were collected at beamline 11-ID-B at the Advanced Photon Source (APS). High energy X-rays (λ = 0.2114 Å) were used in combination with a large amorphous-silicon based area detector to collect data to high values of momentum transfer (Q).[50] Borosilicate capillary-loaded samples of NU-1000 and $InMe_3$-AIM treated NU-1000 (125 °C dehydration followed by AIM at 75 °C followed by exposure to room ambient) were heated at 125 °C under vacuum in a flow-cell furnace[51] during the measurements. The two-dimensional X-ray scattering images were reduced to one-dimensional diffraction data within fit2D. The data were corrected for background, Compton scattering and detector effects within pdfgetX2[52] to obtain the structure function $S(Q)$. Fourier transformation of $S(Q)$ to Q_{max} = 24 $Å^{-1}$, yielded the total PDFs, $G(r)$. Subtraction of the PDF for pristine NU-1000 from that obtained for $InMe_3$-AIM treated NU-1000 yielded the differential PDF.[53] The bond lengths of features of interest were estimated by fitting Gaussian functions to the differential PDF data within fityk.[54] For comparison with the experimental differential data, partial pair PDFs for the DFT-optimized model were calculated within PDFgui.[55] The partial pair PDFs are given by $G(r) = \frac{1}{r}\sum_i \sum_j \left[\frac{b_i b_j}{\langle b \rangle^2}\delta\left(r - r_{ij}\right)\right] - 4\pi r \rho_0$, where the sum goes over pairs of atoms i and j within the model separated by r_{ij}. The scattering power of atom i is b_i and $\langle b \rangle$ is the average scattering power of the sample.

ASSOCIATED CONTENT

PXRD, BET, in-situ FTIR data, predicted structures and energetics for the 8:1 decorated nodes having either CH_3 or OH groups on the Group 13 metal atoms, and the complete citation for

reference 42 can be found in the Supporting Information. This material is available free of charge via the Internet at http://pubs.acs.org.

AUTHOR INFORMATION

Corresponding Author

*E-mail: martinson@anl.gov, cramer@umn.edu

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

This work was supported as part of the Inorganometallic Catalysis Design Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0012702. Work done at Argonne made use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. DOE/Office of Science by Argonne National Laboratory, and was supported by the US DOE, Contract No. DE-AC02-06CH11357. We thank Dr. J. W. Elam and Dr. J. A. Libera for technical assistance and the use of their *in situ* FTIR system. We also thank Dr. L. M. Utschig-Johnson and Dr. S. R. Soltau for the use of their ICP-OES system. Finally, we thank Prof. D. G. Truhlar and Dr. L. Fernandez for helpful discussions.

REFERENCES

1. Lee, J.; Farha, O. K.; Roberts, J.; Scheidt, K. A.; Nguyen, S. T. and Hupp, J. T. Metal-Organic Framework Materials as Catalysts. *Chem. Soc. Rev.* **2009,** *38*, 1450-1459.

2. Ma, L.; Abney, C. and Lin, W. Enantioselective Catalysis with Homochiral Metal-Organic Frameworks. *Chem. Soc. Rev.* **2009,** *38*, 1248-1256.

3. Roy, S.; George, C. B. and Ratner, M. A. Catalysis by a Zinc-Porphyrin-Based Metal–Organic Framework: From Theory to Computational Design. *J. Phys. Chem. C* **2012,** *116*, 23494-23502.

4. Planas, N.; Dzubak, A. L.; Poloni, R.; Lin, L.-C.; McManus, A.; McDonald, T. M.; Neaton, J. B.; Long, J. R.; Smit, B. and Gagliardi, L. The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal–Organic Framework. *J. Am. Chem. Soc.* **2013,** *135*, 7402-7405.

5. Oxford, G. A. E.; Dubbeldam, D.; Broadbelt, L. J. and Snurr, R. Q. Elucidating Steric Effects on Enantioselective Epoxidation Catalyzed by (Salen)Mn in Metal-Organic Frameworks. *J. Mol. Catal. A: Chem.* **2011,** *334*, 89-97.

6. Odoh, S. O.; Cramer, C. J.; Truhlar, D. G. and Gagliardi, L. Quantum-Chemical Characterization of the Properties and Reactivities of Metal–Organic Frameworks. *Chem. Rev.* [Article ASAP]. DOI:10.1021/cr500551h. Published Online: Apr 15, 2015. http://pubs.acs.org/doi/abs/10.1021/cr500551h.

7. Mondloch, J. E.; Farha, O. K. and Hupp, J. T., Catalysis at the Organic Ligands. In *Metal Organic Frameworks as Heterogeneous Catalysts*, Xamena, F. L. i.; Gascon, J., Eds. The Royal Society of Chemistry: 2013. pp 289-309.

8. Indeed, the earliest report of catalysis by a MOF material entails node catalysis. See: *J. Am. Chem. Soc.* **1994,** 116, 1151.

9. Vermoortele, F.; Valvekens, P. and De Vos, D., Catalysis at the Metallic Nodes of Mofs. In *Metal Organic Frameworks as Heterogeneous Catalysts*, Xamena, F. L. i.; Gascon, J., Eds. The Royal Society of Chemistry: 2013. pp 268-288.

10. Corma, A.; Iglesias, M.; Llabrés i Xamena, F. X. and Sánchez, F. Cu and Au Metal–Organic Frameworks Bridge the Gap between Homogeneous and Heterogeneous Catalysts for Alkene Cyclopropanation Reactions. *Chem. Eur. J.* **2010,** *16*, 9789-9795.

11. Henschel, A.; Gedrich, K.; Kraehnert, R. and Kaskel, S. Catalytic Properties of MIL-101. *Chem. Commun.* **2008**. 10.1039/B718371B 4192-4194.

12. Beyzavi, M. H.; Klet, R. C.; Tussupbayev, S.; Borycz, J.; Vermeulen, N. A.; Cramer, C. J.; Stoddart, J. F.; Hupp, J. T. and Farha, O. K. A Hafnium-Based Metal–Organic Framework as an Efficient and Multifunctional Catalyst for Facile CO_2 Fixation and Regioselective and Enantioretentive Epoxide Activation. *J. Am. Chem. Soc.* **2014,** *136*, 15861-15864.

13. Katz, M. J.; Mondloch, J. E.; Totten, R. K.; Park, J. K.; Nguyen, S. T.; Farha, O. K. and Hupp, J. T. Simple and Compelling Biomimetic Metal–Organic Framework Catalyst for the Degradation of Nerve Agent Simulants. *Angew. Chem.* **2014,** *126*, 507-511.

14. Mondloch, J. E.; Katz, M. J.; Isley Iii, W. C.; Ghosh, P.; Liao, P.; Bury, W.; Wagner, G. W.; Hall, M. G.; DeCoste, J. B.; Peterson, G. W.; et al. Destruction of Chemical Warfare Agents Using Metal–Organic Frameworks. *Nat. Mater.* **2015,** *14*, 512-516.

15. Vermoortele, F.; Vandichel, M.; Van de Voorde, B.; Ameloot, R.; Waroquier, M.; Van Speybroeck, V. and De Vos, D. E. Electronic Effects of Linker Substitution on Lewis Acid Catalysis with Metal–Organic Frameworks. *Angew. Chem. Int. Ed.* **2012,** *51*, 4887-4890.

16. Phan, A.; Czaja, A. U.; Gándara, F.; Knobler, C. B. and Yaghi, O. M. Metal–Organic Frameworks of Vanadium as Catalysts for Conversion of Methane to Acetic Acid. *Inorg. Chem.* **2011,** *50*, 7388-7390.

17. Nguyen, H. G. T.; Schweitzer, N. M.; Chang, C.-Y.; Drake, T. L.; So, M. C.; Stair, P. C.; Farha, O. K.; Hupp, J. T. and Nguyen, S. T. Vanadium-Node-Functionalized UiO-66: A Thermally Stable Mof-Supported Catalyst for the Gas-Phase Oxidative Dehydrogenation of Cyclohexene. *ACS Catal.* **2014,** *4*, 2496-2500.

18. Deria, P.; Mondloch, J. E.; Tylianakis, E.; Ghosh, P.; Bury, W.; Snurr, R. Q.; Hupp, J. T. and Farha, O. K. Perfluoroalkane Functionalization of NU-1000 Via Solvent-Assisted Ligand Incorporation: Synthesis and Co_2 Adsorption Studies. *J. Am. Chem. Soc.* **2013,** *135*, 16801-16804.

19. Deria, P.; Bury, W.; Hupp, J. T. and Farha, O. K. Versatile Functionalization of the NU-1000 Platform by Solvent-Assisted Ligand Incorporation. *Chem. Commun.* **2014,** *50*, 1965-1968.

20. Deria, P.; Bury, W.; Hod, I.; Kung, C.-W.; Karagiaridi, O.; Hupp, J. T. and Farha, O. K. MOF Functionalization via Solvent-Assisted Ligand Incorporation: Phosphonates vs Carboxylates. *Inorg. Chem.* **2015,** *54*, 2185-2192.

21. Hod, I.; Bury, W.; Gardner, D. M.; Deria, P.; Roznyatovskiy, V.; Wasielewski, M. R.; Farha, O. K. and Hupp, J. T. Bias-Switchable Permselectivity and Redox Catalytic Activity of a Ferrocene-Functionalized, Thin-Film Metal–Organic Framework Compound. *J. Phys. Chem. Lett.* **2015,** *6*, 586-591.

22. Deria, P.; Mondloch, J. E.; Karagiaridi, O.; Bury, W.; Hupp, J. T. and Farha, O. K. Beyond Post-Synthesis Modification: Evolution of Metal-Organic Frameworks Via Building Block Replacement. *Chem. Soc. Rev.* **2014,** *43*, 5896-5912.

23. Ritala, M. and Niinisto, J., Atomic Layer Deposition. In *Chemical Vapour Deposition: Precursors, Processes and Applications*, Jones, A. C.; Hitchman, M. L., Eds. The Royal Society of Chemistry: Cambridge, UK, 2009.

24. George, S. M. Atomic Layer Deposition: An Overview. *Chem. Rev.* **2010,** *110*, 111-131.

25. Leskelä, M. and Ritala, M. Atomic Layer Deposition (ALD): From Precursors to Thin Film Structures. *Thin Solid Films* **2002,** *409*, 138-146.

26. Mondloch, J. E.; Bury, W.; Fairen-Jimenez, D.; Kwon, S.; DeMarco, E. J.; Weston, M. H.; Sarjeant, A. A.; Nguyen, S. T.; Stair, P. C.; Snurr, R. Q.; et al. Vapor-Phase Metalation by Atomic Layer Deposition in a Metal–Organic Framework. *J. Am. Chem. Soc.* **2013,** *135*, 10294-10297.

27. Cavka, J. H.; Jakobsen, S.; Olsbye, U.; Guillou, N.; Lamberti, C.; Bordiga, S. and Lillerud, K. P. A New Zirconium Inorganic Building Brick Forming Metal Organic Frameworks with Exceptional Stability. *J. Am. Chem. Soc.* **2008,** *130*, 13850-13851.

28. Groner, M. D.; Fabreguette, F. H.; Elam, J. W. and George, S. M. Low-Temperature Al_2O_3 Atomic Layer Deposition. *Chem. Mater.* **2004,** *16*, 639-645.

29. Heil, S. B. S.; Langereis, E.; Roozeboom, F.; van de Sanden, M. C. M. and Kessels, W. M. M. Low-Temperature Deposition of Tin by Plasma-Assisted Atomic Layer Deposition. *J. Electrochem. Soc.* **2006,** *153*, G956-G965.

30. Bakke, J. R.; King, J. S.; Jung, H. J.; Sinclair, R. and Bent, S. F. Atomic Layer Deposition of ZnS via in situ Production of H_2S. *Thin Solid Films* **2010,** *518*, 5400-5408.

31. Ten Eyck, G. A.; Senkevich, J. J.; Tang, F.; Liu, D.; Pimanpang, S.; Karaback, T.; Wang, G. C.; Lu, T. M.; Jezewski, C. and Lanford, W. A. Plasma-Assisted Atomic Layer Deposition of Palladium. *Chem. Vapor Depos.* **2005,** *11*, 60-66.

32. Miikkulainen, V.; Leskelä, M.; Ritala, M. and Puurunen, R. L. Crystallinity of Inorganic Films Grown by Atomic Layer Deposition: Overview and General Trends. *J. Appl. Phys.* **2013,** *113*, 021301.

33. Planas, N.; Mondloch, J. E.; Tussupbayev, S.; Borycz, J.; Gagliardi, L.; Hupp, J. T.; Farha, O. K. and Cramer, C. J. Defining the Proton Topology of the Zr_6-Based Metal–Organic Framework NU-1000. *J. Phys. Chem. Lett.* **2014,** *5*, 3716-3723.

34. Goldstein, D. N.; McCormick, J. A. and George, S. M. Al_2O_3 Atomic Layer Deposition with Trimethylaluminum and Ozone Studied by in Situ Transmission Ftir Spectroscopy and Quadrupole Mass Spectrometry. *J. Phys. Chem. C* **2008,** *112*, 19530-19539.

35. Elam, J. W.; Routkevitch, D.; Mardilovich, P. P. and George, S. M. Conformal Coating on Ultrahigh-Aspect-Ratio Nanopores of Anodic Alumina by Atomic Layer Deposition. *Chem. Mater*. **2003,** *15*, 3507-3517.

36. Hinkle, C. L.; Sonnet, A. M.; Vogel, E. M.; McDonnell, S.; Hughes, G. J.; Milojevic, M.; Lee, B.; Aguirre-Tostado, F. S.; Choi, K. J.; Kim, H. C.; et al. GaAs Interfacial Self-Cleaning by Atomic Layer Deposition. *Appl. Phys. Lett.* **2008,** *92*, 071901.

37. Milojevic, M.; Aguirre-Tostado, F. S.; Hinkle, C. L.; Kim, H. C.; Vogel, E. M.; Kim, J. and Wallace, R. M. Half-Cycle Atomic Layer Deposition Reaction Studies of Al_2O_3 on $In_{0.2}Ga_{0.8}As$ (100) Surfaces. *Appl. Phys. Lett.* **2008,** *93*, 202902.

38. Perdew, J. P. and Wang, Y. Accurate and Simple Analytic Representation of the Electron-Gas Correlation Energy. *Phys. Rev. B* **1992,** *45*, 13244-13249.

39. Perdew, J. P.; Burke, K. and Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996,** *77*, 3865-3868.

40. Perdew, J. P.; Ernzerhof, M. and Burke, K. Rationale for Mixing Exact Exchange with Density Functional Approximations. *J. Chem. Phys.* **1996,** *105*, 9982-9985.

41. Kresse, G. and Furthmüller, J. Efficient Iterative Schemes for *Ab Initio* Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys. Rev. B* **1996,** *54*, 11169-11186.

42. Kresse, G. and Furthmüller, J. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a Plane-Wave Basis Set. *Comp. Mater. Sci.* **1996,** *6*, 15-50.

43. Kresse, G. and Hafner, J. *Ab Initio* Molecular-Dynamics Simulation of the Liquid-Metal-Amorphous-Semiconductor Transition in Germanium. *Phys. Rev. B* **1994,** *49*, 14251-14269.

44. Kresse, G. and Hafner, J. *Ab Initio* Molecular Dynamics for Liquid Metals. *Phys. Rev. B* **1993,** *47*, 558-561.

45. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; et al. *Gaussian 09*, Revisions A.02, B.01 and C.01; Gaussian Inc.: Wallinfgord, CT, 2009.

46. Zhao, Y.; Peverari, R.; Yang, K. and Truhlar, D. G. *Mn-Gfm*, 6.4; University of Minnesota, Minneapolis, MN, 2012.

47. Zhao, Y. and Truhlar, D. G. A New Local Density Functional for Main-Group Thermochemistry, Transition Metal Bonding, Thermochemical Kinetics, and Noncovalent Interactions. *J. Chem. Phys.* **2006,** *125*, 194101.

48. Hehre, W. J.; Radom, L.; Schleyer, P. v. R. and Pople, J. A., *Ab Initio Molecular Orbital Theory*. Wiley: New York, 1986.

49. Nicklass, A.; Dolg, M.; Stoll, H. and Preuss, H. Ab Initio Energy-Adjusted Pseudopotentials for the Noble Gases Ne through Xe: Calculation of Atomic Dipole and Quadrupole Polarizabilities. *J. Chem. Phys.* **1995,** *102*, 8942-8952.

50. Chupas, P. J.; Lee, P. L. and Chapman, K. W. Applications of an Amorphous Silicon-Based Area Detector for High-Resolution, High-Sensitivity and Fast Time-Resolved Pair Distribution Function Measurements. *J. Appl. Crystallogr.* **2007,** *40*, 463-470.

51. Chupas, P. J.; Chapman, K. W.; Kurtz, C.; Hanson, J. C.; Lee, P. L. and Grey, C. P. A Versatile Sample-Environment Cell for Non-Ambient X-Ray Scattering Experiments. *J. Appl. Crystallogr.* **2008,** *41*, 822-824.

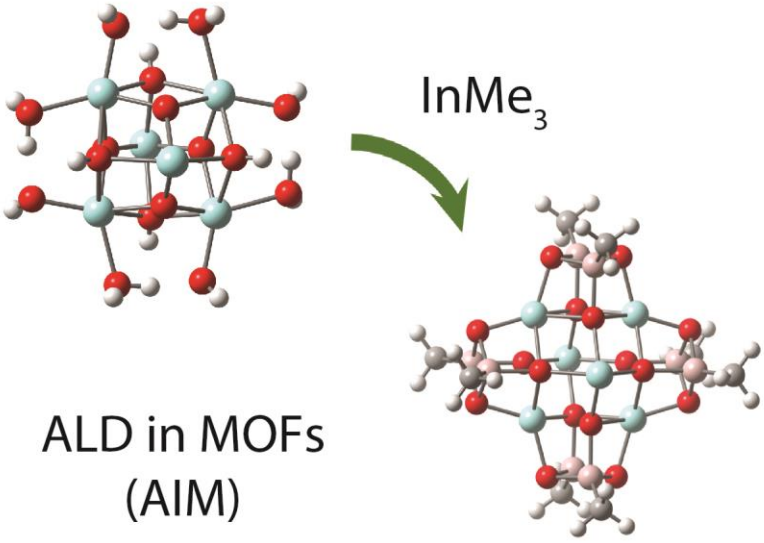
52. Qiu, X.; Thompson, J. W. and Billinge, S. J. L. PDFgetX2: A Gui-Driven Program to Obtain the Pair Distribution Function from X-Ray Powder Diffraction Data. *J. Appl. Crystallogr.* **2004,** *37*, 678-678.

53. Chapman, K. W.; Chupas, P. J. and Kepert, C. J. Selective Recovery of Dynamic Guest Structure in a Nanoporous Prussian Blue through in Situ X-Ray Diffraction: A Differential Pair Distribution Function Analysis. *J. Am. Chem. Soc.* **2005,** *127*, 11232-11233.

54. Wojdyr, M. Fityk: A General-Purpose Peak Fitting Program. *J. Appl. Crystallogr.* **2010,** *43*, 1126-1128.

55. Farrow, C. L.; Juhas, P.; Liu, J. W.; Bryndin, D.; Božin, E. S.; Bloch, J.; Th, P. and Billinge, S. J. L. PDFfit2 and PDFgui: Computer Programs for Studying Nanostructure in Crystals. *J. Phys.: Condens. Matter* **2007,** *19*, 335219.

TOC Figure



Supporting information for:

Targeted Single-Site MOF Node Modification: Trivalent Metal Loading via ALD

In Soo Kim,[a] Joshua Borycz,[b] Ana E. Platero-Prats,[c] Samat Tussupbayev,[b] Timothy C. Wang,[d] Omar K. Farha,[d,e] Joseph T. Hupp,[a,d] Laura Gagliardi,[b] Karena W. Chapman,[c] Christopher J. Cramer,*[b] Alex B. F. Martinson*[a]

[a]Materials Science Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, Illinois 60439, USA

[b]Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota, Minneapolis, Minnesota 55455, United States

[c]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, Illinois 60439, USA

[d]Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

[e]Department of Chemistry, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

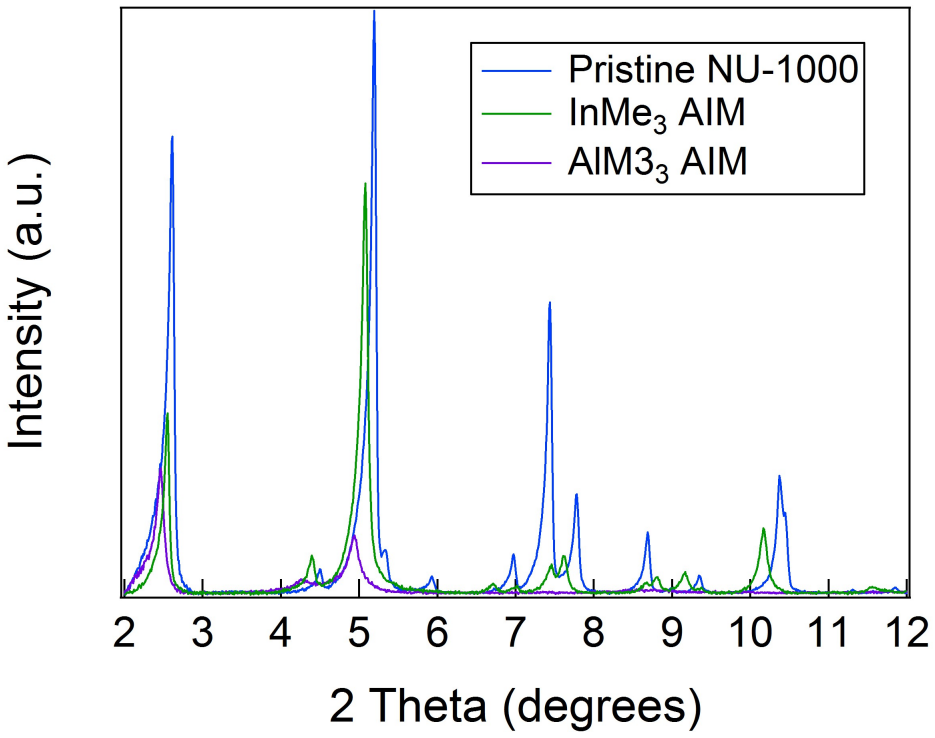


Figure S1. PXRD spectra of pristine MOF, $InMe_3$ AIM, and $AlMe_3$ AIM samples. $InMe_3$ and $AlMe_3$ AIM samples had total $InMe_3$ and $AlMe_3$ exposures of 7200 and 400 seconds, respectively.

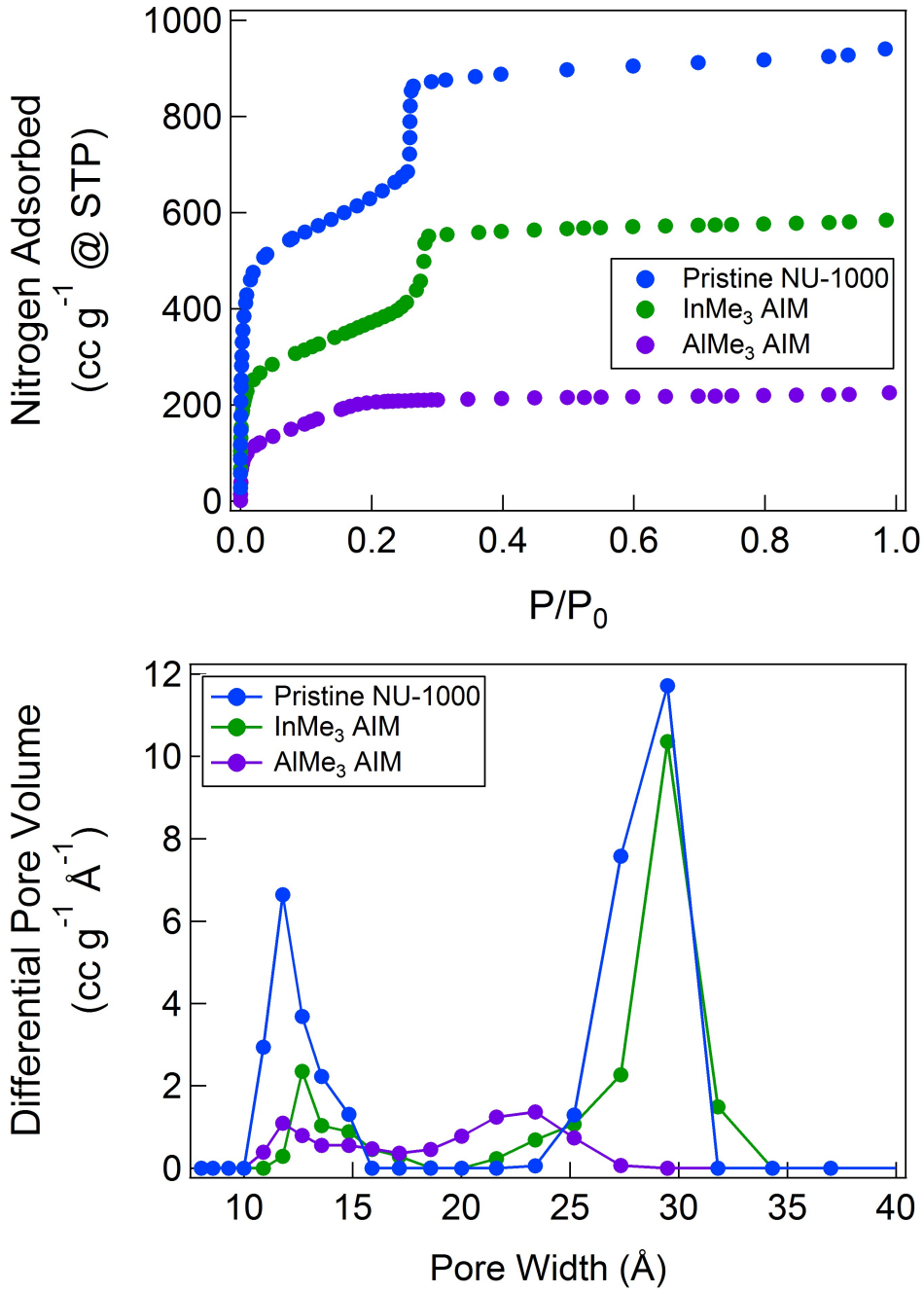
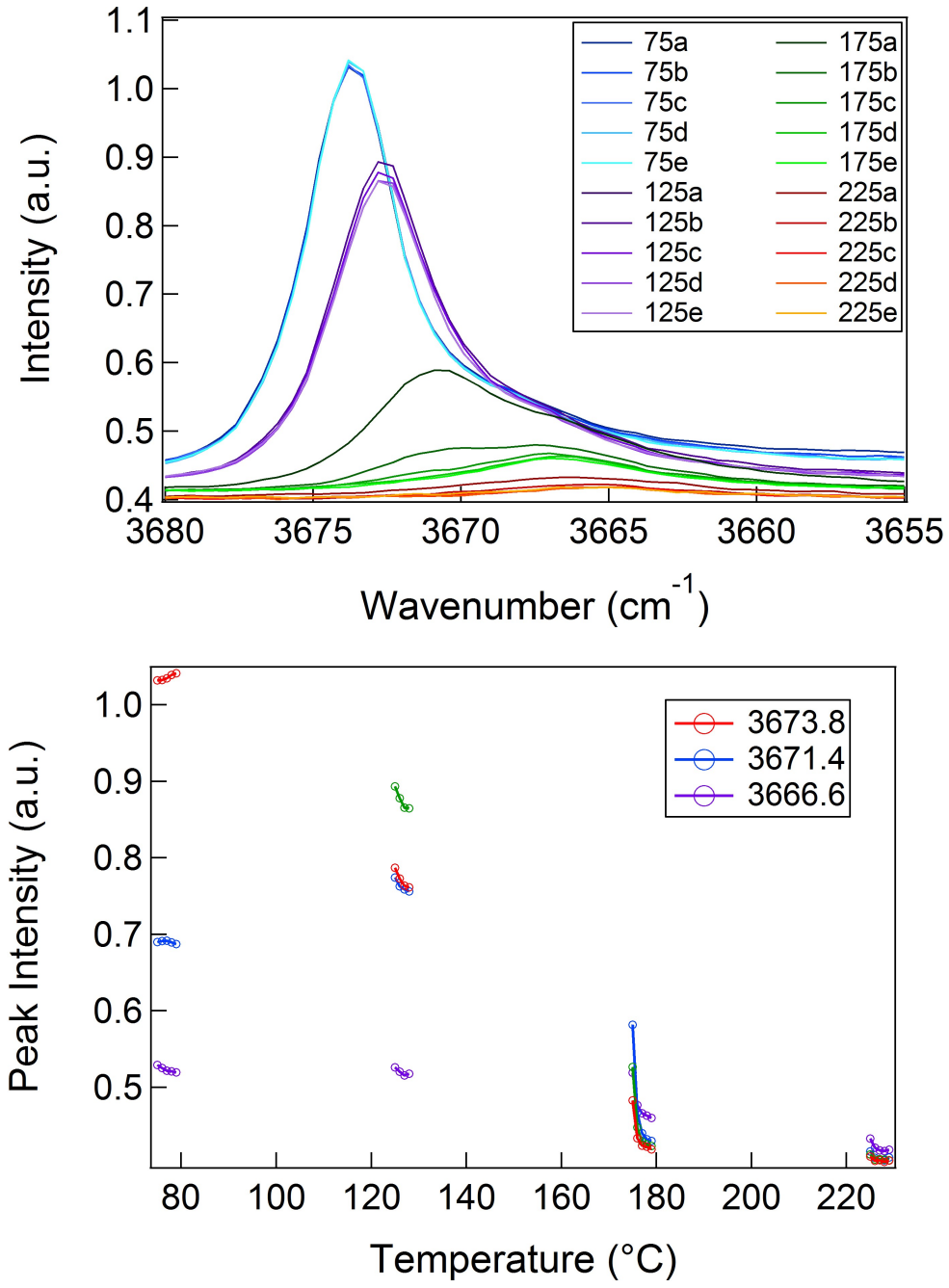


Figure S2. N_2 adsorption isotherms and DFT pore size distributions for pristine MOF, $InMe_3$ AIM, and $AlMe_3$ AIM samples.



vi

Figure S3. a) Changes in the intensity of the peak enclosing –OH, -OH_2, and μ-OH stretches with temperature. Five spectra are acquired at each temperature at 5 minute intervals. b) Evolution of the intensity of selected peaks indicating decrease in –OH population.

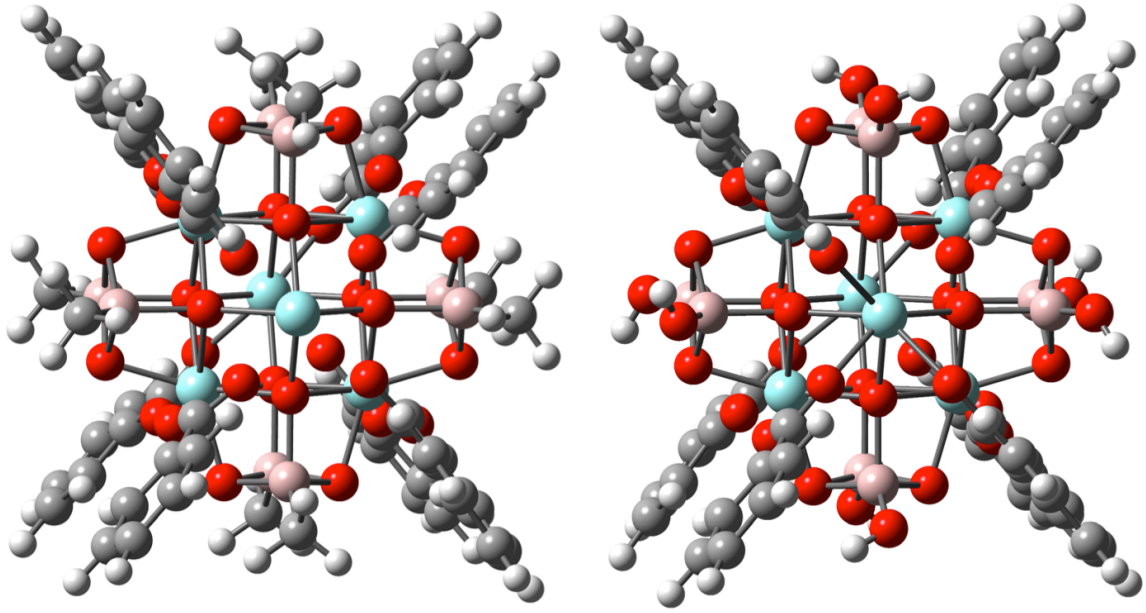


Figure S4. Cluster models of the Zr_6-node in $AlMe_3$ saturated NU-1000 before (left) and after (right) exposure to water. The same topologies are observed with In (not shown).

	ΔE		ΔH	
Structure	Al	In	Al	In
S5 (one face)	-286.9	-66.7	-278.5	-58.7
Saturated Node	-1142.7	-262.9	-1106.4	-230.8

Table S1. Reaction enthalpies of methyl/hydroxyl exchange (see **Figure S4**) computed with M06-L, the 6-31G(d) basis set on C, H, and O, and SDD on Zr and In.

Alternate Reaction Paths

Several other reaction pathways were explored for the addition of $AlMe_3$ to the Zr_6-node. These calculations were all performed at the M06L/6-31G(d) SDD level of theory. The Zr_6-node within NU-1000 has two faces that point towards small pores (~8 Å) and two faces that point towards large pores (~30 Å). S2 and TS1 were computed with the attached $AlMe_3$ cluster in the large and small pore regions of the model clusters. The resulting energies were within about 1 kJ/mol of each other, indicating that the differences between the faces are unimportant at the cluster level. To discern the location at which the metal clusters would bind to the node the

binding energy upon addition to both the terminal –OH and –OH_2 ligands computed. The metal cluster always shifted back to its binding location over the terminal –OH groups. The possibility of binding to a linker oxygen was tested by placing $AlMe_2$ in between the terminal –OH and the nearest carboxylate oxygen. This position was 37.9 kcal/mol higher in energy than the original S2 location. The $AlMe_2$ in S2 can lean towards the muO or the muOH, but the muOH position is energetically favored by 6.0 kcal/mol. The attached $AlMe_2$ may then react with either the muOH hydrogen or one of the terminating –OH groups. In this case the structure resulting from the reaction with the muOH structure is favored by 29.3 kcal/mol.

Periodic Coordinates (Fractional)

The primitive cell of bare NU-1000 was optimized with PBE and a 520 eV energy cutoff. Electronic energy is provided in eV. The unit cell vector lengths are represented by a, b, and c. The angles are represented by alpha, beta, and gamma.

E = -3987.86364661 eV

a	39.973500		
b	39.999690		
c	16.584460		
alpha	89.995890		
beta	90.072890		
gamma	120.021820		
C	0.495179	0.216645	0.327646
C	0.504455	0.782739	0.671664
C	0.782789	0.278534	0.328490
C	0.217181	0.721694	0.672678
C	0.721647	0.504452	0.327860
C	0.278844	0.495497	0.671436
C	0.504400	0.782847	0.327799
C	0.495440	0.216988	0.672019
C	0.217025	0.721539	0.328621
C	0.783143	0.278248	0.672639
C	0.277997	0.495293	0.327095
C	0.721623	0.504319	0.671849
C	0.217425	0.495589	0.671732
C	0.783287	0.504818	0.327767
C	0.278669	0.783195	0.672827
C	0.721320	0.216997	0.328349
C	0.504550	0.721384	0.671668
C	0.495541	0.278266	0.327701
C	0.783265	0.504658	0.672089
C	0.216651	0.495584	0.327720
C	0.721645	0.216753	0.672530

C	0.278435	0.782987	0.328647
C	0.495595	0.278479	0.671763
C	0.504396	0.721411	0.327314
C	0.496342	0.216936	0.413374
C	0.503136	0.782406	0.586013
C	0.782631	0.279367	0.414174
C	0.217412	0.720758	0.587015
C	0.720787	0.503324	0.413511
C	0.279603	0.496667	0.585706
C	0.503100	0.782439	0.413400
C	0.496469	0.217112	0.586319
C	0.217360	0.720645	0.414300
C	0.782790	0.279227	0.586944
C	0.279188	0.496526	0.412779
C	0.720779	0.503239	0.586177
C	0.217604	0.496798	0.586097
C	0.783065	0.503688	0.413458
C	0.279458	0.782845	0.587140
C	0.720511	0.217219	0.414023
C	0.503260	0.720418	0.585956
C	0.496697	0.279188	0.413371
C	0.783059	0.503626	0.586399
C	0.217239	0.496790	0.413423
C	0.720675	0.217056	0.586846
C	0.279394	0.782763	0.414350
C	0.496657	0.279242	0.586073
C	0.503193	0.720458	0.413027
C	0.517200	0.163500	0.166017
C	0.479730	0.835932	0.827971
C	0.835889	0.353866	0.167191
C	0.163000	0.644626	0.830182
C	0.644207	0.480569	0.170377
C	0.353411	0.517071	0.834322
C	0.481574	0.837065	0.170317
C	0.517794	0.163686	0.832779
C	0.163612	0.643333	0.172690
C	0.836751	0.353365	0.834024
C	0.354024	0.517649	0.167209
C	0.644271	0.479561	0.829430
C	0.164224	0.520532	0.827549
C	0.836557	0.483053	0.166127
C	0.355310	0.836519	0.832043
C	0.646441	0.164516	0.165722

C	0.482015	0.645458	0.831760
C	0.520374	0.355691	0.170236
C	0.835448	0.481850	0.834402
C	0.163473	0.518976	0.168468
C	0.646603	0.163178	0.833922
C	0.356646	0.836277	0.172939
C	0.519598	0.355976	0.829005
C	0.482999	0.646871	0.164480
C	0.490050	0.124776	0.182233
C	0.506474	0.874653	0.810719
C	0.874532	0.364555	0.181953
C	0.124401	0.633363	0.813121
C	0.632927	0.507895	0.186916
C	0.364221	0.489252	0.819527
C	0.508914	0.875622	0.187457
C	0.490014	0.125000	0.817320
C	0.124893	0.631345	0.190095
C	0.875404	0.364766	0.817485
C	0.365406	0.490397	0.183885
C	0.631976	0.506056	0.812249
C	0.125480	0.493891	0.809858
C	0.875292	0.510269	0.182529
C	0.366753	0.875193	0.815936
C	0.635629	0.125853	0.179975
C	0.509304	0.634081	0.815503
C	0.493941	0.368048	0.187548
C	0.874175	0.509615	0.820419
C	0.124738	0.491743	0.184359
C	0.635272	0.124531	0.817472
C	0.368656	0.875000	0.190412
C	0.492243	0.367258	0.812556
C	0.510841	0.636074	0.179633
C	0.490303	0.093329	0.134008
C	0.505833	0.906331	0.857347
C	0.906095	0.395869	0.133045
C	0.092642	0.601866	0.861216
C	0.601284	0.507932	0.139015
C	0.395035	0.488574	0.869549
C	0.509213	0.907307	0.139039
C	0.489994	0.093460	0.865533
C	0.093231	0.598929	0.143502
C	0.906923	0.396656	0.865353
C	0.397617	0.490851	0.137106

C	0.599739	0.505346	0.859161
C	0.093789	0.495001	0.855446
C	0.906703	0.509808	0.134603
C	0.397879	0.906755	0.865398
C	0.604577	0.094448	0.130263
C	0.508996	0.602090	0.862757
C	0.494716	0.400343	0.140799
C	0.905502	0.509819	0.870115
C	0.093196	0.491177	0.134489
C	0.603495	0.093062	0.865508
C	0.401320	0.906688	0.144557
C	0.492130	0.398767	0.860772
C	0.511444	0.605074	0.130154
C	0.464154	0.116273	0.246283
C	0.533524	0.883094	0.749050
C	0.882938	0.346476	0.244918
C	0.116449	0.651920	0.750440
C	0.651548	0.534754	0.248991
C	0.346921	0.463384	0.755227
C	0.535385	0.883588	0.250320
C	0.463437	0.116768	0.754477
C	0.116506	0.650006	0.251751
C	0.883740	0.347232	0.753398
C	0.347140	0.463972	0.246785
C	0.650076	0.532875	0.750000
C	0.117032	0.466650	0.748522
C	0.883752	0.536219	0.246552
C	0.348856	0.883646	0.752652
C	0.653220	0.117084	0.243347
C	0.535696	0.652172	0.752517
C	0.467096	0.349939	0.249787
C	0.883116	0.536113	0.757317
C	0.116174	0.465512	0.247848
C	0.652886	0.116227	0.753487
C	0.349858	0.883406	0.251721
C	0.465358	0.348653	0.750455
C	0.536755	0.653545	0.243854
C	0.465801	0.145790	0.293721
C	0.533202	0.853523	0.704234
C	0.853473	0.319060	0.293128
C	0.146319	0.680418	0.704897
C	0.680204	0.533733	0.294792
C	0.319777	0.465616	0.706272

C	0.534034	0.853722	0.295885
C	0.465344	0.146327	0.706836
C	0.146169	0.679334	0.296381
C	0.854065	0.319421	0.706064
C	0.318991	0.465526	0.293296
C	0.679192	0.532574	0.704663
C	0.146658	0.466845	0.704188
C	0.854192	0.534426	0.294045
C	0.320494	0.854086	0.705976
C	0.680508	0.146300	0.292346
C	0.534211	0.680256	0.705615
C	0.467326	0.320750	0.294952
C	0.853979	0.534351	0.708263
C	0.145690	0.466781	0.294804
C	0.680581	0.145886	0.706066
C	0.320487	0.853790	0.296167
C	0.466369	0.320009	0.704661
C	0.534475	0.680726	0.292466
C	0.493312	0.184740	0.278712
C	0.505810	0.814602	0.719702
C	0.814622	0.308477	0.279388
C	0.185110	0.691394	0.720665
C	0.691212	0.505931	0.279727
C	0.308841	0.493543	0.720489
C	0.506241	0.814969	0.279937
C	0.493573	0.185110	0.720977
C	0.185095	0.690878	0.280797
C	0.815184	0.308175	0.721476
C	0.307970	0.493334	0.278220
C	0.691072	0.505451	0.720052
C	0.185597	0.494257	0.719772
C	0.815232	0.506808	0.278857
C	0.309082	0.815158	0.721217
C	0.691330	0.185191	0.278946
C	0.506412	0.691317	0.720405
C	0.494401	0.308819	0.279457
C	0.815018	0.506355	0.721452
C	0.184671	0.494177	0.279618
C	0.691723	0.184744	0.721343
C	0.308997	0.814877	0.280736
C	0.494167	0.308960	0.719772
C	0.506462	0.691558	0.278086
C	0.518688	0.192952	0.213290

C	0.479516	0.806395	0.783238
C	0.806442	0.326132	0.214834
C	0.192828	0.673252	0.784867
C	0.673025	0.479750	0.215922
C	0.326072	0.519061	0.785751
C	0.480362	0.807251	0.215698
C	0.519430	0.193217	0.785565
C	0.193223	0.672700	0.217323
C	0.807143	0.325426	0.786974
C	0.325670	0.518957	0.213405
C	0.673443	0.479387	0.784138
C	0.193791	0.520598	0.783257
C	0.807070	0.481465	0.213337
C	0.326839	0.807001	0.785596
C	0.674018	0.193697	0.214207
C	0.480726	0.673701	0.785130
C	0.520500	0.326461	0.215437
C	0.806335	0.480410	0.785927
C	0.192919	0.520048	0.215232
C	0.674464	0.192755	0.786849
C	0.327177	0.806722	0.217338
C	0.520402	0.327171	0.783525
C	0.480974	0.674259	0.212750
C	0.499782	0.188434	0.458779
C	0.499431	0.810841	0.540944
C	0.811275	0.311314	0.459473
C	0.188931	0.688622	0.541789
C	0.688690	0.499695	0.458613
C	0.311486	0.500000	0.540212
C	0.499435	0.810864	0.458627
C	0.499870	0.188524	0.541130
C	0.188916	0.688565	0.459463
C	0.811334	0.311263	0.541822
C	0.311279	0.500000	0.457844
C	0.688674	0.499606	0.540934
C	0.189060	0.500426	0.541164
C	0.811658	0.500312	0.458809
C	0.311540	0.811269	0.541977
C	0.688564	0.188565	0.459188
C	0.499860	0.688479	0.540592
C	0.500373	0.311306	0.458534
C	0.811654	0.500265	0.541171
C	0.188895	0.500461	0.458874

C	0.688657	0.188500	0.541532
C	0.311514	0.811235	0.459651
C	0.500295	0.311301	0.540831
C	0.499780	0.688470	0.458217
C	0.752414	0.504658	0.287443
C	0.248133	0.495477	0.711910
C	0.495273	0.247429	0.287352
C	0.504641	0.752145	0.712020
C	0.752031	0.247798	0.288173
C	0.247905	0.752459	0.713141
C	0.247185	0.495339	0.287031
C	0.752440	0.504530	0.712278
C	0.504482	0.752238	0.287183
C	0.495491	0.247762	0.712269
C	0.247667	0.752294	0.288264
C	0.752450	0.247488	0.712881
C	0.752028	0.503679	0.456656
C	0.248439	0.496556	0.542718
C	0.496327	0.247984	0.456525
C	0.503311	0.751475	0.542835
C	0.751693	0.248184	0.457239
C	0.248315	0.751888	0.543939
C	0.248235	0.496508	0.456248
C	0.752026	0.503658	0.543151
C	0.503285	0.751490	0.456363
C	0.496347	0.248038	0.543020
C	0.248281	0.751830	0.457502
C	0.751755	0.248094	0.543754
H	0.456776	0.400368	0.004005
H	0.599713	0.543244	0.995898
H	0.056533	0.457321	0.992514
H	0.055954	0.599278	0.004871
H	0.543428	0.943891	0.995738
H	0.400849	0.943916	0.006270
H	0.470071	0.525557	0.827538
H	0.474402	0.529926	0.172379
H	0.943568	0.473489	0.827022
H	0.944493	0.470161	0.172269
H	0.529883	0.056372	0.172599
H	0.526368	0.055233	0.827128
H	0.537425	0.169998	0.116470
H	0.458879	0.829517	0.876192
H	0.829445	0.368062	0.118464

H	0.169078	0.630206	0.879014
H	0.629693	0.459834	0.121935
H	0.367166	0.537323	0.883900
H	0.461112	0.831027	0.121357
H	0.538415	0.170015	0.881556
H	0.169970	0.628843	0.124486
H	0.830456	0.367238	0.883596
H	0.368283	0.538156	0.118343
H	0.630204	0.458857	0.878064
H	0.170613	0.541480	0.875589
H	0.830129	0.462817	0.116594
H	0.369344	0.830094	0.881166
H	0.632541	0.171177	0.116711
H	0.461495	0.631316	0.880650
H	0.541084	0.369765	0.121615
H	0.828673	0.461194	0.883208
H	0.169977	0.539376	0.119252
H	0.632711	0.169470	0.883441
H	0.371217	0.829901	0.124953
H	0.540377	0.370459	0.877437
H	0.462723	0.633047	0.114935
H	0.442989	0.086199	0.258882
H	0.554903	0.913164	0.737093
H	0.912941	0.354562	0.256033
H	0.086528	0.643905	0.738443
H	0.643461	0.556623	0.260300
H	0.355283	0.441720	0.743907
H	0.557276	0.913495	0.262340
H	0.441617	0.086791	0.742907
H	0.086435	0.641300	0.263833
H	0.913786	0.356058	0.740616
H	0.355781	0.442617	0.259417
H	0.641145	0.554060	0.738054
H	0.086936	0.445335	0.736342
H	0.913832	0.557446	0.259211
H	0.357085	0.913634	0.741260
H	0.644908	0.087031	0.254112
H	0.557053	0.643493	0.740183
H	0.445957	0.358928	0.261805
H	0.913237	0.557797	0.746808
H	0.086135	0.443766	0.259039
H	0.644193	0.086218	0.740823
H	0.358557	0.913463	0.263787

H	0.443450	0.356708	0.739093
H	0.558476	0.645266	0.255464
H	0.445185	0.138727	0.342795
H	0.554639	0.860448	0.656961
H	0.860449	0.305097	0.341548
H	0.139726	0.694941	0.657031
H	0.694800	0.555059	0.342307
H	0.306221	0.445014	0.657097
H	0.555124	0.860273	0.343862
H	0.444375	0.139483	0.658460
H	0.139293	0.693914	0.343592
H	0.860914	0.305757	0.656868
H	0.304940	0.444680	0.341791
H	0.693375	0.553899	0.657047
H	0.139759	0.445327	0.657060
H	0.861186	0.555016	0.343193
H	0.306347	0.861017	0.657843
H	0.694204	0.139121	0.341013
H	0.555090	0.694215	0.657131
H	0.445993	0.306553	0.342550
H	0.861265	0.555298	0.659771
H	0.138676	0.445753	0.343027
H	0.694262	0.139038	0.656915
H	0.305869	0.860682	0.343268
H	0.444998	0.305443	0.657170
H	0.555094	0.694352	0.341632
H	0.540392	0.222903	0.200783
H	0.458047	0.776401	0.795997
H	0.776550	0.318448	0.203308
H	0.222688	0.681248	0.797877
H	0.681146	0.457960	0.203560
H	0.318220	0.541113	0.797293
H	0.458518	0.777399	0.202677
H	0.541562	0.223093	0.797411
H	0.223216	0.681223	0.204459
H	0.777219	0.317254	0.799613
H	0.317618	0.540781	0.200738
H	0.682210	0.458107	0.796890
H	0.223812	0.542045	0.796182
H	0.777113	0.459713	0.200763
H	0.318608	0.777057	0.797990
H	0.681888	0.223645	0.203162
H	0.458901	0.681793	0.797482

H	0.541748	0.317652	0.202642
H	0.776317	0.458378	0.796727
H	0.222923	0.541700	0.202911
H	0.682558	0.222645	0.799506
H	0.318664	0.776740	0.204485
H	0.542222	0.319071	0.795962
H	0.458876	0.682047	0.200927
H	0.833554	0.496940	0.573485
H	0.167131	0.504083	0.426796
H	0.503881	0.336604	0.573089
H	0.496438	0.663269	0.425892
H	0.663456	0.166593	0.573778
H	0.336821	0.832956	0.427400
H	0.167409	0.504018	0.573652
H	0.833548	0.496975	0.426619
H	0.496550	0.663263	0.572783
H	0.504041	0.336622	0.426227
H	0.336870	0.833006	0.574288
H	0.663322	0.166699	0.426819
H	0.495844	0.832569	0.426332
H	0.503260	0.166701	0.573480
H	0.336439	0.503334	0.425395
H	0.663338	0.495953	0.573145
H	0.167198	0.663222	0.427192
H	0.833217	0.336475	0.574182
H	0.503146	0.166549	0.426638
H	0.495836	0.832525	0.573278
H	0.663386	0.496135	0.426256
H	0.336792	0.503356	0.572248
H	0.833129	0.336542	0.427192
H	0.167231	0.663342	0.574113
H	0.753322	0.506613	0.221760
H	0.247218	0.493497	0.777596
H	0.493296	0.246471	0.221658
H	0.506691	0.753167	0.777708
H	0.752983	0.246871	0.222478
H	0.246920	0.753415	0.778836
H	0.246042	0.493320	0.221343
H	0.753357	0.506405	0.777979
H	0.506562	0.753378	0.221518
H	0.493632	0.246880	0.777965
H	0.246683	0.753224	0.222552
H	0.753539	0.246419	0.778541

H	0.399684	0.001539	0.019225
H	0.602218	0.001449	0.981478
H	0.979577	0.601695	0.903426
H	0.378689	0.399432	0.905450
H	0.622288	0.022225	0.095670
H	0.998651	0.600604	0.019544
H	0.974926	0.380689	0.894673
H	0.381082	0.407747	0.102409
H	0.600378	0.601581	0.979928
H	0.998671	0.398278	0.978656
H	0.973683	0.593399	0.101610
H	0.592399	0.618929	0.897620
H	0.398410	0.399700	0.020195
H	0.620042	0.025776	0.898698
H	0.406929	0.026537	0.101326
H	0.600490	0.621238	0.094603
H	0.528473	0.978502	0.734062
H	0.023372	0.554968	0.740279
H	0.509224	0.507711	0.244429
H	0.470536	0.444137	0.744209
H	0.508152	-0.000114	0.244054
H	0.021474	0.548535	0.266536
H	0.471546	0.450236	0.268418
H	0.021114	0.472411	0.733049
H	0.491558	0.998524	0.756349
H	0.531023	0.975988	0.259110
H	0.549813	0.528488	0.731731
H	0.999907	0.508255	0.755843
H	0.000561	0.491837	0.243595
H	0.451131	0.979241	0.266534
H	0.492278	0.490811	0.755582
H	0.555937	0.529480	0.255923
H	0.021574	0.466156	0.264778
H	0.975854	0.378358	0.090022
H	0.444566	0.974228	0.741102
H	0.398891	0.020222	0.902166
O	0.517349	0.103706	0.082105
O	0.480578	0.896281	0.913199
O	0.895934	0.412840	0.081349
O	0.102883	0.587517	0.918609
O	0.586739	0.483051	0.082337
O	0.411840	0.515327	0.922100
O	0.484538	0.897034	0.081758

0	0.516953	0.103634	0.917769
0	0.103329	0.583992	0.087235
0	0.896542	0.413280	0.917279
0	0.414918	0.518185	0.085995
0	0.585027	0.480400	0.915465
0	0.103819	0.520172	0.911483
0	0.896311	0.482638	0.083105
0	0.412344	0.896473	0.922290
0	0.587662	0.104543	0.078544
0	0.481677	0.584868	0.913922
0	0.519695	0.415092	0.084536
0	0.895318	0.482485	0.921038
0	0.103520	0.516180	0.078170
0	0.586500	0.103390	0.916561
0	0.416630	0.896610	0.089072
0	0.517006	0.413251	0.917536
0	0.484590	0.588127	0.077772
0	0.464464	0.058443	0.149110
0	0.530294	0.941191	0.838240
0	0.940759	0.403270	0.145020
0	0.057722	0.591118	0.841787
0	0.591065	0.532586	0.157296
0	0.403317	0.462085	0.855428
0	0.533508	0.942227	0.158197
0	0.463125	0.058711	0.852427
0	0.058334	0.588348	0.162787
0	0.941831	0.405910	0.849840
0	0.406151	0.464563	0.151534
0	0.588918	0.529352	0.838925
0	0.058902	0.470829	0.835546
0	0.941679	0.535701	0.149585
0	0.408612	0.941584	0.845665
0	0.596882	0.059803	0.143546
0	0.535371	0.593654	0.848636
0	0.470746	0.411195	0.161083
0	0.940149	0.536889	0.857385
0	0.058294	0.466470	0.152864
0	0.594633	0.058152	0.851004
0	0.411683	0.941570	0.163510
0	0.467441	0.408984	0.842539
0	0.537906	0.596757	0.144577
0	0.402035	0.001413	0.082251
0	0.599520	0.000926	0.918315

0	0.998867	0.400753	0.068895
0	0.000216	0.598991	0.927927
0	0.598850	0.598252	0.070710
0	0.401742	0.401198	0.929439
0	0.599273	0.000448	0.072763
0	0.401377	0.999699	0.927787
0	0.998714	0.598034	0.082512
0	0.999527	0.401305	0.915223
0	0.400985	0.402300	0.083527
0	0.597817	0.599022	0.916598
0	0.471628	0.001001	0.237608
0	0.529359	0.000105	0.762937
0	0.999150	0.464498	0.237705
0	0.999060	0.534269	0.761564
0	0.535308	0.534066	0.238089
0	0.465918	0.464748	0.761864
0	0.534939	0.000519	0.238489
0	0.465150	0.998741	0.761938
0	-0.000382	0.528060	0.237600
0	0.999070	0.470709	0.761619
0	0.470880	0.470733	0.238203
0	0.529305	0.529177	0.761836
0	0.522250	0.040593	0.124168
0	0.483309	0.969451	0.911811
0	0.959971	0.478093	0.123496
0	0.029859	0.516884	0.910943
0	0.516968	0.486060	0.088522
0	0.478209	0.517675	0.875630
0	0.487052	0.970157	0.088783
0	0.518534	0.039718	0.875880
0	0.030258	0.513376	0.087917
0	0.959382	0.481453	0.875447
0	0.482279	0.521775	0.124354
0	0.513976	0.483053	0.911418
0	0.478849	0.030331	0.002921
0	0.532059	0.960397	0.996258
0	0.969690	0.448303	0.996056
0	0.039434	0.571396	0.004344
0	0.571768	0.531470	0.995790
0	0.448668	0.478426	0.004032
0	0.039817	0.468452	0.993612
0	0.969457	0.521219	0.003021
0	0.428761	0.960336	0.005585

O	0.552021	0.030460	0.997148
O	0.521567	0.551311	0.995966
O	0.468569	0.428294	0.004187
Zr	0.457939	0.999674	0.112840
Zr	0.542184	0.999418	0.887885
Zr	0.999492	0.452378	0.101365
Zr	0.998691	0.546819	0.897344
Zr	0.546868	0.547205	0.101747
Zr	0.452786	0.453165	0.898260
Zr	0.548248	0.001315	0.103031
Zr	0.453203	0.000370	0.897672
Zr	0.000317	0.542158	0.112732
Zr	0.000417	0.458169	0.886190
Zr	0.458497	0.457223	0.113900
Zr	0.542817	0.541525	0.886149
Zr	0.536326	0.072268	0.999828
Zr	0.464466	0.928451	0.000684
Zr	0.927651	0.463704	0.999672
Zr	0.071445	0.535914	0.999147
Zr	0.536261	0.463749	0.000000
Zr	0.464224	0.535705	0.000000

Cluster Model Coordinates (xyz format)

The cartesian coordinates and total electronic energies (Hartree) provided were optimized by fixing the linker positions from the PBE optimized crystal structure provided and relaxing the remaining atoms with M06-L/6-31G(d) SDD.

Bare Zr6-node
150
Bare Node (E = -4859.0506356)
C 5.668384 2.752686 2.581489
C -5.704996 2.819603 -2.482672
C 5.663897 2.789915 -2.556609
C -5.670285 2.831817 2.480715
C 4.329553 2.997375 2.921080
C -4.361341 3.105374 -2.767477
C 4.324145 3.058129 -2.875230
C -4.332363 3.106005 2.801205
C 4.030526 4.064521 3.781492
C -4.060262 4.137889 -3.668078
C 4.035511 4.101787 -3.767167
C -4.047600 4.137260 3.708085

C	5.046828	4.877834	4.277438
C	-5.080208	4.887790	-4.245877
C	5.059080	4.879951	-4.300962
C	-5.076361	4.896512	4.258793
C	6.393737	4.642752	3.938232
C	-6.431220	4.631835	-3.940395
C	6.405576	4.636060	-3.965877
C	-6.421684	4.644504	3.924666
C	6.683005	3.559606	3.086167
C	-6.722432	3.569501	-3.064217
C	6.686150	3.563569	-3.097513
C	-6.697597	3.585876	3.038728
C	-5.659335	-2.835572	-2.487625
C	5.675448	-2.768924	2.571272
C	-5.698635	-2.828206	2.484774
C	5.687051	-2.728906	-2.590910
C	-4.321321	-3.109241	-2.807927
C	4.337188	-3.046257	2.889320
C	-4.354481	-3.114053	2.766805
C	4.348984	-2.981713	-2.931008
C	-4.033796	-4.139544	-3.714717
C	4.055559	-4.088862	3.785452
C	-4.050778	-4.145190	3.668009
C	4.058635	-4.048031	-3.795716
C	-5.060497	-4.900622	-4.265188
C	5.085387	-4.859001	4.318970
C	-5.069265	-4.894601	4.248943
C	5.080796	-4.854030	-4.291669
C	-6.405613	-4.651442	-3.929921
C	6.430459	-4.608182	3.982584
C	-6.420770	-4.638882	3.945715
C	6.426018	-4.614115	-3.948934
C	-6.684655	-3.592455	-3.045500
C	6.703930	-3.533756	3.113709
C	-6.714878	-3.578212	3.068621
C	6.707523	-3.529318	-3.096153
C	3.241144	2.253285	-2.237661
C	3.245895	2.173931	2.316189
C	3.249064	-2.251071	2.245596
C	-3.261074	-2.349951	2.107456
C	-3.232679	-2.308812	-2.176764
C	-3.266123	2.340974	-2.110365
C	3.258901	-2.169783	-2.319085
C	-3.242173	2.303586	2.173315
H	5.892151	1.929599	1.909986
H	-5.929816	2.011828	-1.792908

H	5.882577	1.976710	-1.871760
H	-5.882715	2.025363	1.785828
H	2.992042	4.258505	4.032220
H	-3.019739	4.341937	-3.900624
H	2.997351	4.308979	-4.009969
H	-3.012311	4.331869	3.972206
H	4.794211	5.707243	4.932922
H	-4.828631	5.689538	-4.935466
H	4.812073	5.694494	-4.976930
H	-4.836246	5.696063	4.954865
H	7.714341	3.354726	2.810389
H	-7.757606	3.339086	-2.825559
H	7.717558	3.343606	-2.833527
H	-7.728153	3.361736	2.775218
H	-5.872944	-2.029216	-1.793128
H	5.888212	-1.955626	1.884683
H	-5.924826	-2.020920	1.794924
H	5.905523	-1.905971	-1.917510
H	-2.997843	-4.331901	-3.977783
H	3.019065	-4.302699	4.029565
H	-3.009647	-4.348505	3.898372
H	3.021850	-4.248481	-4.048575
H	-4.819284	-5.700047	-4.961016
H	4.844296	-5.673920	4.996707
H	-4.816411	-5.695371	4.939171
H	4.833519	-5.683341	-4.949373
H	-7.715960	-3.370863	-2.782766
H	7.733631	-3.306518	2.849323
H	-7.750677	-3.348572	2.832077
H	7.737131	-3.318281	-2.818515
H	7.203075	5.247137	-4.376098
H	-7.225384	5.223524	-4.384261
H	7.231608	-5.214078	4.393299
H	7.221336	-5.244831	-4.332807
H	-7.213784	-5.230366	4.391992
H	-7.222967	5.239105	4.351560
H	-7.205750	-5.248274	-4.355938
H	7.185212	5.277894	4.322882
H	-1.964671	0.054934	-2.855780
H	1.952522	2.868453	0.062863
H	0.960312	-1.652393	4.221632
H	0.025274	-0.379824	4.056608
H	0.762387	-1.631701	-4.397193
H	-0.013665	-4.063738	-0.373493
H	-0.755737	-4.396112	1.625958
H	-0.937211	-4.232973	-1.652860

H	-1.967410	-0.061490	2.854521
H	1.961671	-2.869937	-0.061186
H	0.750571	1.628174	4.399337
H	0.027689	0.373938	-4.057274
H	0.958127	1.649306	-4.223301
H	-0.949256	4.225752	1.651316
H	-0.766321	4.388701	-1.627223
H	-0.024447	4.058498	0.372678
O	1.061742	-0.059846	1.475251
O	3.608145	-1.425484	1.347914
O	3.608085	-1.309431	-1.452717
O	3.600076	1.310807	1.454920
O	2.051191	2.410339	2.679648
O	-0.049959	3.966790	1.387607
O	-2.042323	2.621689	2.441862
O	-2.070015	2.668676	-2.388193
O	-3.602676	1.351403	1.414237
O	-3.616279	1.415686	-1.315028
O	-3.613162	-1.425808	1.311726
O	-3.595551	-1.358595	-1.416493
O	-2.032369	-2.626818	-2.443010
O	-2.064498	-2.676805	2.384144
O	-1.061606	-1.487239	-0.058414
O	-1.387678	-0.071402	2.079288
O	-0.020966	1.253451	3.950213
O	0.059540	-1.394573	3.962198
O	0.058349	1.388772	-3.963394
O	-1.066550	1.482507	0.057566
O	1.391310	2.079615	0.071564
O	2.044963	2.464444	-2.606993
O	0.013721	3.947551	-1.260581
O	3.603625	1.426456	-1.342780
O	0.022977	-3.952661	1.259272
O	-0.038835	-3.971645	-1.388482
O	1.397896	-2.082918	-0.070649
O	2.052929	-2.468074	2.611809
O	2.064859	-2.412426	-2.680848
O	-0.011767	-1.259764	-3.950186
O	-1.384984	0.064629	-2.080532
O	1.063445	0.056134	-1.474243
Zr	-2.502381	-0.003790	-0.000644
Zr	0.026411	1.697426	1.891540
Zr	-0.023970	-1.891685	1.698296
Zr	0.033974	-1.702555	-1.891688
Zr	2.512696	-0.001497	0.001290
Zr	-0.027748	1.886310	-1.698924

$AlMe_3$ Reaction Path Structures

163

S1 (E = -5221.2026696)

C	5.434856	-3.024598	-2.866238
C	-5.985400	-2.979376	2.091553
C	5.357852	-3.735490	2.221999
C	-5.883937	-2.342377	-2.829880
C	4.087392	-3.130650	-3.241410
C	-4.667926	-3.391060	2.342490
C	3.998918	-3.951150	2.496195
C	-4.563154	-2.662721	-3.177514
C	3.729265	-4.052738	-4.236414
C	-4.449032	-4.550974	3.100448
C	3.628851	-5.080702	3.241344
C	-4.335820	-3.583088	-4.211072
C	4.695435	-4.861357	-4.830518
C	-5.524727	-5.298864	3.569526
C	4.590591	-5.990209	3.672646
C	-5.405554	-4.191508	-4.861908
C	6.050322	-4.765291	-4.456969
C	-6.851256	-4.913443	3.294142
C	5.954848	-5.796900	3.378960
C	-6.735390	-3.894327	-4.503769
C	6.399897	-3.825634	-3.468163
C	-7.058642	-3.727927	2.564356
C	6.318485	-4.641382	2.660936
C	-6.951778	-2.944799	-3.487265
C	-5.560875	2.609814	2.842444
C	5.811850	2.434441	-2.127923
C	-5.532802	3.257842	-2.087629
C	5.750383	1.716531	2.983896
C	-4.212023	2.747071	3.202359
C	4.499647	2.841781	-2.412887
C	-4.168794	3.485836	-2.323213
C	4.427759	2.013207	3.348104
C	-3.868469	3.627463	4.238378
C	4.300773	4.009754	-3.165007
C	-3.784405	4.603194	-3.079125
C	4.197774	2.974127	4.344498
C	-4.849259	4.377975	4.879593
C	5.387079	4.771173	-3.587475
C	-4.742360	5.490106	-3.560921
C	5.264802	3.636417	4.947191
C	-6.203355	4.267326	4.508098
C	6.707606	4.387180	-3.280808

C	-6.111972	5.289622	-3.300397
C	6.595466	3.352332	4.582114
C	-6.540669	3.355113	3.490451
C	6.896581	3.191873	-2.559938
C	-6.488439	4.145572	-2.572224
C	6.815227	2.372190	3.595053
C	2.981087	-2.997595	1.965248
C	3.053225	-2.321659	-2.538312
C	3.352007	2.045122	-1.884751
C	-3.138162	2.568784	-1.765602
C	-3.170922	1.962535	2.477580
C	-3.515029	-2.623130	1.797679
C	3.294152	1.364805	2.629405
C	-3.429936	-2.024325	-2.445595
H	5.704114	-2.313970	-2.091015
H	-6.146151	-2.074616	1.513291
H	5.639859	-2.856267	1.651404
H	-6.051289	-1.621504	-2.035714
H	2.683627	-4.140815	-4.515395
H	-3.427792	-4.854301	3.308925
H	2.575927	-5.246641	3.449839
H	-3.312398	-3.811536	-4.493698
H	4.396753	-5.578370	-5.590830
H	-5.336876	-6.199467	4.148533
H	4.280353	-6.867657	4.234129
H	-5.210104	-4.907286	-5.656207
H	7.438790	-3.729579	-3.162947
H	-8.072695	-3.398086	2.353322
H	7.365818	-4.459570	2.433096
H	-7.968490	-2.687389	-3.201327
H	-5.818564	1.918059	2.046682
H	5.960246	1.525457	-1.553594
H	-5.821975	2.384330	-1.511331
H	5.922365	0.976125	2.208884
H	-2.825635	3.712486	4.529361
H	3.284366	4.324005	-3.383639
H	-2.728946	4.763464	-3.275786
H	3.173404	3.209931	4.616724
H	-4.564513	5.060818	5.675889
H	5.210411	5.682531	-4.152949
H	-4.427019	6.355406	-4.138330
H	5.064724	4.387152	5.707350
H	-7.580828	3.240815	3.195964
H	7.905037	2.862172	-2.323010
H	-7.540428	3.958091	-2.372882
H	7.832062	2.129658	3.296833

H	6.703930	-6.509515	3.708744
H	-7.689268	-5.502690	3.652379
H	7.553087	4.985649	-3.604278
H	7.425962	3.871455	5.049530
H	-6.857402	5.987286	-3.668485
H	-7.568832	-4.371680	-5.009094
H	-6.967422	4.856275	5.005349
H	6.802615	-5.396965	-4.918307
H	-2.069509	-0.543541	2.838821
H	1.687792	-3.215445	-0.404654
H	1.028947	1.905535	-3.970346
H	0.047959	0.648077	-3.957495
H	0.728537	0.732097	4.618158
H	-0.701880	4.273162	-0.998167
H	-0.754609	3.788063	2.327063
H	-1.968840	0.330562	-2.815109
H	2.093357	2.456963	0.468130
H	0.635236	-1.340149	-4.542301
H	-0.124059	-1.162735	4.003448
H	0.714819	-2.510941	4.001039
H	-1.278433	-4.168414	-2.174540
H	-1.149531	-4.758980	1.060304
H	-0.365691	-4.224868	-0.875495
O	1.014367	-0.075446	-1.422917
O	3.642651	1.086270	-1.102117
O	3.596639	0.603849	1.658773
O	3.452689	-1.605264	-1.569090
O	1.850390	-2.426507	-2.935186
O	-0.370888	-3.997800	-1.870374
O	-2.250943	-2.387498	-2.746542
O	-2.347508	-3.065822	2.034825
O	-3.736932	-1.161167	-1.565828
O	-3.791544	-1.580494	1.128160
O	-3.562122	1.574648	-1.099817
O	-3.586407	1.150481	1.594090
O	-1.955767	2.162182	2.787245
O	-1.918684	2.847063	-1.990569
O	-1.027551	1.298655	0.269900
O	-1.414411	0.183466	-2.034928
O	-0.113781	-0.973206	-4.050180
O	0.129715	1.636697	-3.716183
O	-0.159304	-2.153927	3.769221
O	-1.228347	-1.628709	-0.231954
O	1.178423	-2.397067	-0.312817
O	1.768539	-3.173280	2.297900
O	-0.342562	-4.321579	0.751967

O	3.410333	-2.087129	1.188939
O	0.165409	3.909086	-0.748360
O	0.120753	3.499260	2.014008
O	1.451899	1.730454	0.376215
O	2.178210	2.389342	-2.224705
O	2.114221	1.639136	3.014154
O	-0.052756	0.470561	4.109370
O	-1.482163	-0.493390	2.070638
O	0.967910	-0.569706	1.477357
Zr	-2.572261	-0.077123	0.019864
Zr	-0.134869	-1.700572	-2.074049
Zr	0.071301	1.799014	-1.415043
Zr	0.057078	1.177161	2.133257
Zr	2.450967	-0.420566	0.044655
Zr	-0.245961	-2.340875	1.461474
Al	1.423818	5.399332	-0.702306
H	0.155317	3.758681	1.055281
C	2.968810	4.647073	0.317225
H	3.532821	3.790298	-0.081151
H	3.732881	5.429430	0.445117
H	2.664506	4.392816	1.347190
C	1.506692	5.973243	-2.605636
H	1.347010	5.139598	-3.307800
H	0.704762	6.699585	-2.809652
H	2.441441	6.465117	-2.910805
C	0.380049	6.662930	0.433571
H	0.807142	7.676697	0.420813
H	-0.663668	6.788068	0.100464
H	0.337671	6.374050	1.494885

158
S2 (E=-5180.8014345)

C	-5.537575	-3.150412	2.543650
C	5.829079	-2.778714	-2.522414
C	-5.534897	-3.114804	-2.594461
C	5.797685	-2.862239	2.440308
C	-4.191350	-3.356557	2.879570
C	4.495175	-3.103631	-2.811062
C	-4.187376	-3.335120	-2.917020
C	4.469491	-3.183955	2.757057
C	-3.857550	-4.425562	3.724752
C	4.227033	-4.132482	-3.726150
C	-3.865747	-4.356203	-3.823676
C	4.218674	-4.236584	3.649286
C	-4.846797	-5.278173	4.209268
C	5.270301	-4.840838	-4.314636

C	-4.863994	-5.159358	-4.368302
C	5.271714	-4.969962	4.189059
C	-6.200786	-5.081897	3.873596
C	6.612532	-4.545774	-4.005735
C	-6.217460	-4.963800	-4.029625
C	6.608012	-4.669980	3.858359
C	-6.525343	-3.996705	3.036986
C	6.869835	-3.487095	-3.114646
C	-6.531977	-3.913310	-3.146131
C	6.849112	-3.590577	2.987459
C	5.601009	2.871547	-2.447312
C	-5.722762	2.367687	2.611591
C	5.643436	2.795128	2.524479
C	-5.736089	2.400330	-2.550639
C	4.254676	3.106407	-2.763537
C	-4.393959	2.683527	2.933361
C	4.290925	3.033441	2.810700
C	-4.407074	2.700961	-2.887296
C	3.933533	4.139619	-3.655615
C	-4.145587	3.721897	3.844125
C	3.954644	4.041394	3.726449
C	-4.151780	3.788215	-3.736862
C	4.934827	4.941135	-4.195390
C	-5.199409	4.450786	4.388623
C	4.948766	4.814983	4.317802
C	-5.199699	4.567749	-4.221225
C	6.287476	4.730766	-3.863857
C	-6.535887	4.161484	4.048893
C	6.307639	4.607316	4.010810
C	-6.536281	4.279734	-3.881746
C	6.601053	3.668932	-2.994549
C	-6.775065	3.091190	3.164932
C	6.635297	3.569199	3.118753
C	-6.782146	3.174466	-3.044370
C	-3.130529	-2.504850	-2.268261
C	-3.135173	-2.490105	2.286257
C	-3.281127	1.933047	2.278306
C	3.222351	2.243861	2.140742
C	3.192791	2.262425	-2.143627
C	3.376252	-2.384336	-2.143055
C	-3.291008	1.916051	-2.287067
C	3.353616	-2.408328	2.140728
H	-5.788171	-2.325558	1.883893
H	6.028128	-1.973942	-1.821313
H	-5.779295	-2.318845	-1.898142
H	5.983582	-2.039604	1.756878

H	-2.813201	-4.589464	3.972577
H	3.193498	-4.366686	-3.961426
H	-2.821587	-4.526336	-4.069521
H	3.190356	-4.468211	3.910758
H	-4.567172	-6.108188	4.852913
H	5.044316	-5.640452	-5.015472
H	-4.591233	-5.955866	-5.055763
H	5.057925	-5.786609	4.873775
H	-7.562912	-3.821327	2.764267
H	7.897177	-3.226801	-2.872883
H	-7.569789	-3.730494	-2.878925
H	7.871748	-3.329599	2.727015
H	5.840926	2.062762	-1.764326
H	-5.909582	1.557740	1.913586
H	5.895148	2.005398	1.823243
H	-5.927507	1.561332	-1.888926
H	2.891760	4.302153	-3.915799
H	-3.116388	3.965591	4.091107
H	2.907632	4.207733	3.959800
H	-3.122148	4.025568	-3.986991
H	4.667543	5.742123	-4.879802
H	-4.984336	5.263392	5.077796
H	4.670615	5.597337	5.019328
H	-4.979688	5.413825	-4.867156
H	7.639122	3.477035	-2.735111
H	-7.797055	2.834610	2.897489
H	7.677826	3.376466	2.878849
H	-7.804247	2.926414	-2.769614
H	-6.995071	-5.594426	-4.448352
H	7.425110	-5.105195	-4.458034
H	-7.355924	4.735347	4.468246
H	-7.351756	4.889827	-4.256552
H	7.081420	5.217707	4.465314
H	7.428309	-5.244398	4.276691
H	7.067694	5.359069	-4.281486
H	-6.971134	-5.747620	4.249319
H	2.003945	-0.119465	-2.842765
H	-1.819943	-3.109714	0.017507
H	-0.972442	1.365323	4.258525
H	-0.004256	0.115403	4.073759
H	-0.767440	1.502705	-4.372537
H	0.755522	4.178115	1.742255
H	0.741885	4.124730	-1.806044
H	1.995843	-0.091754	2.869906
H	-2.086229	2.566934	-0.009152
H	-0.659665	-1.908698	4.375582

H	0.016831	-0.478728	-4.052705
H	-0.864223	-1.787507	-4.250102
H	1.124041	-4.416029	1.578895
H	0.939541	-4.507903	-1.692596
H	0.195203	-4.241258	0.300859
O	-1.025618	-0.187165	1.495024
O	-3.613914	1.109083	1.369074
O	-3.611749	1.032714	-1.432920
O	-3.517517	-1.626763	1.437337
O	-1.933252	-2.692962	2.646180
O	0.219471	-4.170919	1.320706
O	2.164809	-2.768744	2.404899
O	2.191177	-2.746496	-2.425341
O	3.682771	-1.434369	1.395157
O	3.696843	-1.459574	-1.334746
O	3.603602	1.342905	1.331966
O	3.586572	1.313752	-1.396928
O	1.982691	2.545272	-2.405190
O	2.016016	2.527993	2.422184
O	1.046747	1.346856	-0.017116
O	1.422502	-0.100875	2.089811
O	0.101665	-1.503180	3.935610
O	-0.068389	1.131615	3.987255
O	0.022468	-1.498455	-3.976321
O	1.150051	-1.622358	0.043692
O	-1.285362	-2.302905	0.045019
O	-1.928375	-2.672061	-2.640698
O	0.149497	-4.096013	-1.313621
O	-3.518970	-1.702886	-1.361719
O	-0.090114	3.816394	1.433124
O	-0.113793	3.790487	-1.492917
O	-1.417451	1.861218	-0.020904
O	-2.092400	2.183327	2.647400
O	-2.105627	2.202184	-2.645512
O	0.007412	1.136351	-3.922165
O	1.423074	-0.159099	-2.069268
O	-1.021206	-0.240185	-1.461500
Zr	2.541196	-0.095291	-0.003805
Zr	0.071703	-1.924463	1.869734
Zr	-0.008153	1.634131	1.729792
Zr	-0.048465	1.589608	-1.865347
Zr	-2.472932	-0.262958	-0.008640
Zr	0.122865	-2.025078	-1.726458
Al	-0.748181	4.750630	-0.044908
C	-2.726477	4.765299	0.000108
H	-3.337987	3.849516	-0.044422

H -3.057238 5.276751 0.916590
H -3.092235 5.377002 -0.838148
C 0.204605 6.475007 -0.045990
H 1.300360 6.369632 -0.058771
H -0.048070 7.094503 -0.917804
H -0.030178 7.087959 0.835558

153
S3 (E= -5140.3353401)
C 5.487386 3.132180 2.543691
C -5.872828 2.619363 -2.524497
C 5.486349 3.090848 -2.594377
C -5.843607 2.708757 2.438135
C 4.138720 3.322625 2.879088
C -4.542817 2.959675 -2.813395
C 4.136374 3.294722 -2.917482
C -4.519410 3.046308 2.755248
C 3.791997 4.388515 3.723001
C -4.286752 3.990801 -3.729378
C 3.802808 4.310893 -3.825344
C -4.281382 4.103171 3.645938
C 4.770892 5.253398 4.206790
C -5.338253 4.686015 -4.318884
C 4.791537 5.125289 -4.370638
C -5.343219 4.824538 4.184661
C 6.127205 5.072908 3.871639
C -6.676943 4.375310 -4.009956
C 6.147158 4.946259 -4.031442
C -6.675766 4.508277 3.853996
C 6.464876 3.990736 3.036308
C -6.921816 3.314627 -3.117749
C 6.473968 3.900573 -3.146710
C -6.903774 3.425112 2.984242
C -5.577422 -3.027691 -2.443067
C 5.738338 -2.383240 2.617805
C -5.621935 -2.946272 2.528627
C 5.753276 -2.421443 -2.544382
C -4.228323 -3.246611 -2.759012
C 4.413320 -2.714532 2.939641
C -4.266748 -3.168106 2.815436
C 4.428020 -2.738256 -2.881020
C -3.894659 -4.277129 -3.649587
C 4.177129 -3.754793 3.851491
C -3.918688 -4.170980 3.732358
C 4.185908 -3.829434 -3.729416
C -4.886197 -5.091124 -4.188695

C	5.239439	-4.470461	4.397033
C	-4.903655	-4.955712	4.324348
C	5.243162	-4.596954	-4.212678
C	-6.241337	-4.896532	-3.857698
C	6.572453	-4.165620	4.057282
C	-6.264835	-4.764603	4.016822
C	6.576135	-4.292646	-3.873222
C	-6.567758	-3.837548	-2.989641
C	6.799061	-3.093530	3.172185
C	-6.604636	-3.731456	3.123539
C	6.808606	-3.183599	-3.037019
C	3.089344	2.452633	-2.268024
C	3.093084	2.443032	2.286447
C	3.291770	-1.978083	2.283500
C	-3.207158	-2.366078	2.145246
C	-3.176010	-2.388305	-2.140630
C	-3.415287	2.254439	-2.144371
C	3.302532	-1.966064	-2.281877
C	-3.393621	2.282804	2.140457
H	5.747955	2.309642	1.884908
H	-6.062433	1.813053	-1.822547
H	5.740056	2.298632	-1.897119
H	-6.019521	1.883206	1.755578
H	2.745710	4.540229	3.970410
H	-3.256027	4.237052	-3.964684
H	2.756752	4.468292	-4.071611
H	-3.255960	4.347332	3.907383
H	4.481239	6.080732	4.849450
H	-5.121651	5.487490	-5.020558
H	4.509461	5.917726	-5.059045
H	-5.139344	5.644434	4.868517
H	7.504527	3.827440	2.764016
H	-7.946039	3.042370	-2.875926
H	7.513823	3.730441	-2.879070
H	-7.923163	3.151671	2.723860
H	-5.827127	-2.221067	-1.761033
H	5.915652	-1.571897	1.918943
H	-5.882879	-2.160377	1.826457
H	5.934519	-1.579490	-1.883559
H	-2.850961	-4.427518	-3.909358
H	3.150850	-4.010467	4.098513
H	-2.869822	-4.324564	3.966129
H	3.159239	-4.079324	-3.979512
H	-4.609220	-5.889626	-4.872157
H	5.033906	-5.284809	5.087061
H	-4.616363	-5.733916	5.026805

H	5.033408	-5.446309	-4.857718
H	-7.608103	-3.657756	-2.730649
H	7.817982	-2.825080	2.904686
H	-7.649333	-3.551433	2.883188
H	7.827611	-2.923073	-2.762310
H	6.917294	5.585648	-4.450695
H	-7.496026	4.924501	-4.463058
H	7.399174	-4.729199	4.477455
H	7.398915	-4.893388	-4.247166
H	-7.031391	-5.383672	4.471830
H	-7.502953	5.073337	4.271506
H	-7.013909	-5.534555	-4.274803
H	6.889472	5.748185	4.246795
H	-2.016418	0.021988	-2.849741
H	1.790132	3.031936	0.021114
H	0.980893	-1.429029	4.247949
H	-0.001579	-0.189677	4.075936
H	0.777384	-1.560931	-4.370030
H	-0.529118	-4.398182	1.442331
H	-0.583295	-4.288768	-1.503006
H	-2.005232	-0.013204	2.871794
H	0.629084	1.844692	4.366413
H	-0.032297	0.410176	-4.057286
H	0.828889	1.733420	-4.245790
H	-1.191811	4.329844	1.573001
H	-1.009846	4.419471	-1.694446
H	-0.255563	4.165047	0.298628
O	1.012537	0.121048	1.501365
O	3.614882	-1.151154	1.373396
O	3.612476	-1.077956	-1.428601
O	3.485837	1.583310	1.438523
O	1.888775	2.631975	2.645875
O	-0.284047	4.093541	1.318331
O	-2.209832	2.658086	2.404008
O	-2.234784	2.630266	-2.426612
O	-3.712157	1.305280	1.390651
O	-3.725329	1.325810	-1.332366
O	-3.599643	-1.469773	1.332270
O	-3.582897	-1.445278	-1.389285
O	-1.963253	-2.657887	-2.400848
O	-1.997905	-2.635853	2.426808
O	-1.089785	-1.467406	-0.021372
O	-1.440022	0.013235	2.086312
O	-0.133347	1.434402	3.932633
O	0.072237	-1.202877	3.985970
O	-0.054531	1.430462	-3.976086

O	-1.177759	1.520456	0.042090
O	1.245307	2.232135	0.045884
O	1.885399	2.605079	-2.641017
O	-0.214186	4.018946	-1.314994
O	3.487080	1.656296	-1.360435
O	0.285780	-3.883476	1.392923
O	0.281108	-3.857979	-1.496832
O	1.401566	-1.983680	-0.012748
O	2.106034	-2.242215	2.652562
O	2.120746	-2.266880	-2.640111
O	-0.000958	-1.196639	-3.924361
O	-1.443260	0.070162	-2.071104
O	1.007262	0.173806	-1.465144
Zr	-2.565539	-0.018447	-0.002230
Zr	-0.106280	1.851611	1.866844
Zr	0.010167	-1.685121	1.716052
Zr	0.040964	-1.635337	-1.861315
Zr	2.454016	0.166167	-0.005710
Zr	-0.155725	1.949317	-1.724320
Al	1.410984	-3.772005	-0.063670
C	3.047115	-4.816485	-0.057664
H	3.139071	-5.474669	-0.930860
H	3.926340	-4.156277	-0.071973
H	3.145781	-5.446310	0.835839

161

S4 (E = -5462.0630874)

C	-5.734504	-3.319277	2.069862
C	5.701201	-2.703768	-2.813762
C	-5.664940	-2.525143	-3.006157
C	5.603141	-3.518073	2.081527
C	-4.402664	-3.631817	2.379992
C	4.358454	-2.923271	-3.155890
C	-4.324031	-2.754469	-3.349326
C	4.258532	-3.824029	2.339242
C	-4.125474	-4.827601	3.059547
C	4.058397	-3.793028	-4.214807
C	-4.034672	-3.643556	-4.395213
C	3.951777	-4.985116	3.063620
C	-5.156219	-5.698071	3.406183
C	5.077953	-4.451886	-4.895178
C	-5.059209	-4.312726	-5.059070
C	4.965674	-5.835808	3.495391
C	-6.496241	-5.394970	3.094798
C	6.427493	-4.265046	-4.537552
C	-6.407318	-4.109982	-4.703665

C	6.317634	-5.549357	3.221179
C	-6.763615	-4.184871	2.426167
C	6.718294	-3.361987	-3.497858
C	-6.688024	-3.188729	-3.676284
C	6.615549	-4.364804	2.521331
C	5.713042	2.877902	-1.903853
C	-5.685359	2.130981	2.953380
C	5.688918	2.066029	3.001922
C	-5.631605	2.926453	-2.147031
C	4.382071	3.215742	-2.190546
C	-4.348513	2.337026	3.326735
C	4.344252	2.318701	3.311812
C	-4.286818	3.214731	-2.427105
C	4.116594	4.382699	-2.921407
C	-4.067748	3.217518	4.382815
C	4.039580	3.194141	4.364631
C	-3.974660	4.403279	-3.104582
C	5.157902	5.210316	-3.330186
C	-5.096415	3.903627	5.022658
C	5.058142	3.827377	5.070294
C	-4.982181	5.291165	-3.474684
C	6.496037	4.893963	-3.024990
C	-6.439571	3.726781	4.635435
C	6.410734	3.607750	4.744463
C	-6.334028	5.015254	-3.190020
C	6.753021	3.702594	-2.320631
C	-6.712848	2.810394	3.601182
C	6.705204	2.699410	3.710531
C	-6.637377	3.810308	-2.527186
C	-3.241117	-2.076472	-2.578095
C	-3.303076	-2.734589	1.928161
C	-3.260411	1.643354	2.574722
C	3.251249	1.684020	2.525897
C	3.276648	2.336135	-1.710171
C	3.262509	-2.261928	-2.395758
C	-3.212909	2.301379	-1.942760
C	3.184062	-2.917003	1.838117
H	-5.941328	-2.395787	1.538025
H	5.925408	-2.020951	-1.999937
H	-5.884057	-1.830812	-2.201150
H	5.832585	-2.612484	1.528690
H	-3.092292	-5.072112	3.286908
H	3.018902	-3.944196	-4.488669
H	-2.995662	-3.821284	-4.656988
H	2.911283	-5.207353	3.281431
H	-4.920411	-6.625557	3.921505

H	4.827052	-5.128463	-5.708146
H	-4.811894	-5.010156	-5.855220
H	4.708604	-6.734442	4.050212
H	-7.789219	-3.925643	2.175930
H	7.752630	-3.185727	-3.213754
H	-7.720424	-3.001906	-3.391465
H	7.651601	-4.113469	2.308850
H	5.909587	1.967326	-1.346730
H	-5.897609	1.442053	2.141927
H	5.915668	1.378258	2.193022
H	-5.866984	2.008149	-1.618130
H	3.086084	4.627569	-3.161178
H	-3.032330	3.376523	4.669631
H	2.997718	3.370090	4.613472
H	-2.932755	4.629440	-3.310318
H	4.933704	6.114602	-3.890047
H	-4.855713	4.595242	5.825949
H	4.804662	4.508982	5.878222
H	-4.718136	6.212873	-3.986750
H	7.778590	3.428986	-2.085973
H	-7.741353	2.641363	3.292267
H	7.741548	2.498547	3.451272
H	-7.672527	3.569606	-2.298633
H	-7.205691	-4.636994	-5.216070
H	7.221197	-4.786718	-5.062625
H	-7.239691	4.267917	5.130018
H	-7.117945	5.709310	-3.475418
H	7.203964	4.109651	5.289228
H	7.107334	-6.214807	3.554938
H	7.307556	5.542121	-3.340022
H	-7.298961	-6.074345	3.362907
H	1.964802	0.101154	-2.780069
H	-2.001292	-3.084613	-0.389264
H	-1.011508	0.674366	4.462858
H	-0.100428	-0.582255	4.108609
H	-0.636498	2.126279	-4.045930
H	0.725355	3.882672	1.963774
H	1.910915	-0.691175	2.902008
H	-0.836207	-2.604126	4.096958
H	0.005994	0.042135	-4.020890
H	-0.935552	-1.178388	-4.398922
H	0.887776	-4.741380	0.975665
H	0.740316	-4.347309	-2.285085
H	-0.023365	-4.348399	-0.264352
O	-1.092999	-0.461749	1.510064
O	-3.616368	0.978109	1.551268

O	-3.581768	1.316515	-1.230974
O	-3.637438	-1.739242	1.214029
O	-2.115603	-3.041099	2.261572
O	-0.004464	-4.426439	0.753042
O	1.978266	-3.260194	2.037944
O	2.067002	-2.525838	-2.735867
O	3.565068	-1.859414	1.241792
O	3.612202	-1.481173	-1.454523
O	3.604744	0.896106	1.591770
O	3.621805	1.271892	-1.103825
O	2.083788	2.708158	-1.933532
O	2.055000	1.976749	2.838401
O	1.111680	1.216015	0.247692
O	1.355107	-0.568856	2.118815
O	-0.049104	-2.176813	3.728708
O	-0.116723	0.435308	4.167177
O	-0.035000	-0.975198	-4.093431
O	1.035989	-1.746592	-0.131271
O	-1.418496	-2.325248	-0.245129
O	-2.042568	-2.239550	-2.963780
O	-0.036377	-3.964328	-1.852055
O	-3.606495	-1.400882	-1.565192
O	-0.148267	3.464340	1.975412
O	-0.055119	3.763855	-0.843288
O	-1.369263	1.823725	0.325072
O	-2.066789	1.784036	2.984421
O	-2.012049	2.584853	-2.247016
O	0.088552	1.631749	-3.637355
O	1.403030	-0.012397	-2.000327
O	-1.078162	-0.095863	-1.445308
Zr	2.496696	-0.301128	0.068667
Zr	-0.076860	-2.277455	1.623665
Zr	-0.000448	1.248030	1.998813
Zr	-0.038620	1.684080	-1.527135
Zr	-2.526423	-0.194261	0.013328
Zr	0.013083	-1.859395	-1.946879
Al	-1.242870	3.614820	0.483876
C	-2.813194	4.749087	0.634791
H	-2.853210	5.529428	-0.136251
H	-3.734108	4.158029	0.525966
H	-2.878410	5.251295	1.608688
Al	1.440934	4.569834	-1.332013
C	1.047199	5.754946	-2.849057
H	0.123794	6.308385	-2.624094
H	1.809487	6.503068	-3.103010
H	0.836496	5.182462	-3.764561

C	2.639315	4.953523	0.179266
H	2.189048	5.647334	0.905694
H	2.869908	4.025810	0.728086
H	3.605565	5.395003	-0.097037

156

S5 (E = -5421.5921032)

C	5.655689	2.991955	2.539153
C	-5.718689	2.936507	-2.522906
C	5.650224	2.947186	-2.598884
C	-5.683210	3.028036	2.439647
C	4.316029	3.237135	2.875097
C	-4.376134	3.222605	-2.812531
C	4.309449	3.205381	-2.921452
C	-4.346248	3.312183	2.755430
C	4.013241	4.316776	3.718437
C	-4.078980	4.241713	-3.729558
C	4.016854	4.233619	-3.829856
C	-4.065109	4.358815	3.645674
C	5.026643	5.141606	4.201119
C	-5.101757	4.978568	-4.319021
C	5.037483	5.006901	-4.376226
C	-5.096549	5.122993	4.184426
C	6.374347	4.906065	3.865406
C	-6.451774	4.722584	-4.009194
C	6.384917	4.773309	-4.037592
C	-6.440997	4.860771	3.854661
C	6.667435	3.810527	3.030668
C	-6.738956	3.673307	-3.116115
C	6.669552	3.715842	-3.152289
C	-6.713181	3.787143	2.985786
C	-5.652347	-2.717823	-2.437645
C	5.682944	-2.529051	2.617027
C	-5.690860	-2.631268	2.534011
C	5.693557	-2.571358	-2.545139
C	-4.313394	-2.991657	-2.753862
C	4.345759	-2.806169	2.939752
C	-4.345622	-2.907643	2.820294
C	4.356366	-2.834448	-2.880861
C	-4.022250	-4.035259	-3.644139
C	4.068094	-3.835361	3.852470
C	-4.038002	-3.923176	3.737742
C	4.069778	-3.915479	-3.728385
C	-5.046252	-4.808768	-4.182169
C	5.100818	-4.593121	4.397978
C	-5.053647	-4.666939	4.330783

C	5.094798	-4.725547	-4.211643
C	-6.392215	-4.559187	-3.850622
C	6.444909	-4.342788	4.057336
C	-6.406128	-4.421031	4.023814
C	6.439191	-4.475281	-3.873077
C	-6.674983	-3.487252	-2.983146
C	6.714306	-3.281368	3.171368
C	-6.704257	-3.375572	3.129975
C	6.716866	-3.375995	-3.037775
C	3.229492	2.406900	-2.270855
C	3.235305	2.400238	2.283637
C	3.254642	-2.025171	2.283822
C	-3.255138	-2.150070	2.148772
C	-3.227604	-2.177184	-2.135999
C	-3.278023	2.472725	-2.143622
C	3.263446	-2.016715	-2.281880
C	-3.253223	2.503787	2.140230
H	5.882355	2.159082	1.880816
H	-5.940441	2.139023	-1.820292
H	5.871989	2.145816	-1.901198
H	-5.892803	2.209826	1.757761
H	2.974095	4.510938	3.966269
H	-3.039248	4.445826	-3.965561
H	2.977903	4.433115	-4.075702
H	-3.030495	4.561395	3.906426
H	4.771102	5.980438	4.843343
H	-4.853228	5.770126	-5.021368
H	4.787386	5.809648	-5.065048
H	-4.859247	5.934419	4.867601
H	7.699468	3.605044	2.757964
H	-7.773241	3.442950	-2.873580
H	7.701802	3.503890	-2.885057
H	-7.742955	3.555062	2.726115
H	-5.868790	-1.901275	-1.756054
H	5.892620	-1.726039	1.917503
H	-5.920114	-1.835923	1.831421
H	5.909127	-1.736990	-1.885003
H	-2.985644	-4.228002	-3.904333
H	3.032428	-4.049062	4.100194
H	-2.996098	-4.118983	3.971088
H	3.033691	-4.123726	-3.977784
H	-4.802231	-5.618307	-4.865209
H	4.862820	-5.397998	5.088685
H	-4.797753	-5.455667	5.033643
H	4.850448	-5.566144	-4.855978
H	-7.707048	-3.265266	-2.723753

H	7.743126	-3.054617	2.903163
H	-7.740927	-3.153522	2.890028
H	7.745740	-3.156793	-2.763767
H	7.180108	5.380674	-4.457686
H	-7.248170	5.304211	-4.462268
H	7.248335	-4.939122	4.477486
H	7.236747	-5.109131	-4.247016
H	-7.196900	-5.008213	4.479648
H	-7.244379	5.459176	4.272193
H	-7.190233	-5.165661	-4.266885
H	7.163557	5.550151	4.239699
H	-1.995355	0.129753	-2.802884
H	1.946421	3.044462	0.014826
H	0.947576	-1.354602	4.375607
H	0.033877	-0.073559	4.106579
H	0.700287	-1.524179	-4.493805
H	-1.981647	0.091415	2.822417
H	0.744864	1.909772	4.371384
H	0.019165	0.511278	-4.087684
H	0.937560	1.794281	-4.247069
H	-0.968954	4.465571	1.579080
H	-0.791749	4.538618	-1.694276
H	-0.046589	4.257616	0.298651
O	1.063894	0.185185	1.520899
O	3.610565	-1.212887	1.372850
O	3.609704	-1.141481	-1.429237
O	3.592643	1.524673	1.436204
O	2.039816	2.637998	2.643622
O	-0.076303	4.183399	1.318320
O	-2.054496	2.830522	2.403336
O	-2.083181	2.800350	-2.426862
O	-3.610498	1.538471	1.396360
O	-3.624745	1.559232	-1.333341
O	-3.610832	-1.240033	1.338336
O	-3.593913	-1.216310	-1.390729
O	-2.026144	-2.495369	-2.396806
O	-2.057283	-2.468497	2.429764
O	-1.196510	-1.577711	-0.017713
O	-1.381832	0.125011	2.062652
O	-0.034695	1.529281	3.940414
O	0.076143	-1.094887	4.035421
O	0.039301	1.527357	-3.986699
O	-1.062336	1.598491	0.040258
O	1.367756	2.268767	0.042295
O	2.032511	2.607730	-2.643295
O	-0.017617	4.103884	-1.307994

O	3.595242	1.595671	-1.363116
O	0.019256	-3.662564	1.215199
O	0.043197	-3.643656	-1.329886
O	1.397924	-1.820645	-0.007552
O	2.059394	-2.240896	2.653331
O	2.070233	-2.269737	-2.639023
O	-0.001981	-1.107377	-3.975890
O	-1.391897	0.181582	-2.046998
O	1.054798	0.234675	-1.492596
Zr	-2.520352	0.148948	0.001272
Zr	0.014334	1.939756	1.873960
Zr	0.051595	-1.621283	1.794772
Zr	0.068656	-1.561127	-1.928334
Zr	2.492060	0.156149	-0.007168
Zr	-0.033749	2.036750	-1.734247
Al	1.352600	-3.626721	-0.058968
C	2.972021	-4.698162	-0.014822
H	3.044865	-5.301500	0.899435
H	3.050257	-5.389874	-0.862999
H	3.867419	-4.060902	-0.043710
Al	-1.289469	-3.492189	-0.086863
C	-2.948831	-4.493305	-0.002530
H	-2.986134	-5.107090	0.906754
H	-3.843202	-3.855871	0.010718
H	-3.059706	-5.167506	-0.861437

174
Saturated Node (E = -7110.78840085)

C	-5.666968	-2.748225	2.588002
C	5.706194	-2.824855	-2.476512
C	-5.662707	-2.797281	-2.549997
C	5.671710	-2.825650	2.486892
C	-4.328083	-2.991885	2.928113
C	4.362575	-3.111521	-2.760584
C	-4.322921	-3.066017	-2.868043
C	4.333849	-3.099324	2.808076
C	-4.028832	-4.057014	3.790946
C	4.061631	-4.146147	-3.658805
C	-4.034152	-4.111658	-3.757606
C	4.049304	-4.128540	3.717338
C	-5.044972	-4.869357	4.288810
C	5.081680	-4.897202	-4.234922
C	-5.057613	-4.891223	-4.289563
C	5.078219	-4.886347	4.269745
C	-6.391936	-4.635287	3.949125
C	6.432662	-4.640313	-3.930092

C	-6.404135	-4.646792	-3.954978
C	6.423484	-4.634879	3.934977
C	-6.681428	-3.554154	3.094582
C	6.723732	-3.575915	-3.056375
C	-6.684852	-3.572353	-3.089072
C	6.699176	-3.578246	3.046592
C	5.659565	2.830286	-2.494480
C	-5.674977	2.773345	2.565074
C	5.699092	2.834373	2.477920
C	-5.686807	2.721442	-2.597002
C	4.321490	3.103002	-2.815333
C	-4.336750	3.051637	2.882423
C	4.354901	3.120627	2.759367
C	-4.348799	2.973694	-2.937742
C	4.033747	4.131152	-3.724497
C	-4.055260	4.096352	3.776139
C	4.051062	4.153796	3.658196
C	-4.058672	4.038068	-3.804916
C	5.060294	4.891136	-4.276765
C	-5.085194	4.867541	4.307929
C	5.069448	4.904716	4.237357
C	-5.080992	4.842749	-4.302676
C	6.405467	4.642958	-3.940987
C	-6.430239	4.615719	3.972183
C	6.420982	4.648530	3.934656
C	-6.426158	4.603394	-3.959328
C	6.684731	3.586058	-3.054143
C	-6.703566	3.539248	3.105796
C	6.715232	3.585894	3.059993
C	-6.707439	3.520515	-3.104040
C	-3.240047	-2.259522	-2.232437
C	-3.244597	-2.169649	2.321248
C	-3.248522	2.255168	2.240488
C	3.261632	2.354887	2.101830
C	3.233047	2.303843	-2.182329
C	3.267300	-2.345862	-2.105223
C	-3.258563	2.163378	-2.324023
C	3.243528	-2.298522	2.178450
H	-5.890906	-1.926724	1.914616
H	5.930907	-2.015456	-1.788619
H	-5.881495	-1.982539	-1.867012
H	5.883971	-2.020760	1.790140
H	-2.990302	-4.250242	4.042073
H	3.021132	-4.350909	-3.890832
H	-2.995968	-4.319230	-3.999979
H	3.014059	-4.322718	3.981953

H	-4.792184	-5.697211	4.946190
H	4.830209	-5.700578	-4.922652
H	-4.810495	-5.707279	-4.963664
H	4.838273	-5.684334	4.967667
H	-7.712811	-3.350087	2.818380
H	7.758877	-3.344776	-2.818295
H	-7.716286	-3.351959	-2.825546
H	7.729682	-3.354536	2.782520
H	5.873344	2.025567	-1.798139
H	-5.887633	1.958433	1.880369
H	5.925390	2.025540	1.789921
H	-5.905108	1.900022	-1.921699
H	2.997749	4.322725	-3.987958
H	-3.018791	4.310928	4.019711
H	3.009907	4.357462	3.888138
H	-3.021932	4.238114	-4.058283
H	4.818912	5.688915	-4.974421
H	-4.844212	5.684059	4.983778
H	4.816488	5.707030	4.925751
H	-4.833887	5.670586	-4.962299
H	7.716085	3.365248	-2.790947
H	-7.733241	3.311226	2.841981
H	7.751060	3.355888	2.823931
H	-7.736998	3.309941	-2.825869
H	-7.201548	-5.258947	-4.363755
H	7.226907	-5.232887	-4.372631
H	-7.231473	5.222421	4.381539
H	-7.221602	5.233088	-4.344616
H	7.213915	5.241175	4.379535
H	7.224888	-5.228359	4.363202
H	7.205482	5.238944	-4.368413
H	-7.183285	-5.269676	4.335272
O	-1.252632	0.036800	1.860806
O	-3.607514	1.427404	1.344681
O	-3.607514	1.304933	-1.455614
O	-3.598899	-1.308552	1.458009
O	-2.049842	-2.405227	2.685210
O	-0.065307	-3.853187	1.326386
O	2.043588	-2.616183	2.447586
O	2.071314	-2.673929	-2.381994
O	3.603682	-1.348026	1.417091
O	3.617186	-1.418639	-1.312007
O	3.613663	1.428929	1.308152
O	3.596022	1.355387	-1.419862
O	2.032633	2.620874	-2.449201
O	2.065021	2.681909	2.377544

O	1.251920	1.879459	-0.034019
O	1.315090	0.036947	1.860561
O	0.062835	-1.186968	3.883699
O	0.064701	1.332286	3.840771
O	0.065414	-1.327253	-3.841019
O	1.259710	-1.874115	0.032838
O	-1.320519	-1.872919	0.037942
O	-2.043777	-2.471091	-2.601189
O	-0.058004	-3.891263	-1.194644
O	-3.602576	-1.430640	-1.339380
O	-0.067970	3.895621	1.194403
O	-0.077559	3.856913	-1.326689
O	-1.328428	1.876163	-0.036526
O	-2.052314	2.473212	2.606091
O	-2.064542	2.405234	-2.686255
O	0.054185	1.191819	-3.883627
O	1.312473	-0.030428	-1.861307
O	-1.255015	-0.033820	-1.859624
Zr	2.504044	0.003591	-0.000883
Zr	-0.002287	-1.805972	1.865969
Zr	0.001044	1.872665	1.800448
Zr	-0.011749	1.810360	-1.866032
Zr	-2.510917	0.000673	0.001266
Zr	0.006377	-1.867743	-1.800330
Al	-1.396908	3.747274	-0.061192
C	-3.097234	4.670945	-0.062575
H	-3.196571	5.347738	-0.920518
H	-3.940836	3.969606	-0.111555
H	-3.236789	5.273473	0.843986
Al	1.273247	3.776050	-0.071067
C	2.917556	4.795606	-0.070736
H	2.988237	5.448263	0.808548
H	3.806163	4.149242	-0.054947
H	3.008024	5.430669	-0.960819
Al	-1.289736	-0.072574	-3.753577
Al	1.386399	-0.060292	-3.730774
C	3.092377	-0.059135	-4.642946
H	3.926552	-0.086645	-3.929213
H	3.208302	-0.925666	-5.305958
H	3.228026	0.839562	-5.258065
C	-2.950428	-0.090009	-4.745172
H	-3.819761	-0.095413	-4.072874
H	-3.054131	0.790798	-5.391160
H	-3.038281	-0.978431	-5.382976
Al	-1.385750	-3.744620	0.062281
Al	1.283886	-3.770615	0.069697

C -3.085920 -4.668975 0.064081
H -3.929646 -3.966123 0.078463
H -3.211108 -5.297739 -0.826605
H -3.199612 -5.320087 0.939937
C 2.930027 -4.787168 0.065818
H 3.022475 -5.424198 0.954287
H 3.001341 -5.437466 -0.815158
H 3.817312 -4.138968 0.050977
Al -1.285866 0.072522 3.754738
Al 1.390166 0.069862 3.729801
C -2.945401 0.081267 4.748380
H -3.037440 0.968724 5.386905
H -3.815746 0.082055 4.077395
H -3.043074 -0.800592 5.393918
C 3.096364 0.078990 4.641483
H 3.227376 -0.805769 5.277392
H 3.930584 0.086034 3.927329
H 3.216770 0.960099 5.284218

158
Saturated Node Upon Exposure to Water (E = -7396.83882954)
C 5.667684 2.771559 2.563310
C -5.705416 2.802161 -2.501835
C 5.663489 2.774469 -2.574922
C -5.670997 2.847534 2.461362
C 4.328782 3.018201 2.901201
C -4.361805 3.086329 -2.788453
C 4.323694 3.040274 -2.895387
C -4.333154 3.124146 2.780093
C 4.029469 4.091022 3.754430
C -4.060899 4.112860 -3.695926
C 4.034887 4.077870 -3.794308
C -4.048670 4.161500 3.680078
C 5.045564 4.907852 4.244992
C -5.080975 4.858662 -4.278778
C 5.058319 4.852675 -4.333232
C -5.077627 4.924189 4.225644
C 6.392543 4.670804 3.907440
C -6.431950 4.604455 -3.971671
C 6.404848 4.611322 -3.996447
C -6.422877 4.669661 3.893129
C 6.682098 3.582054 3.062644
C -6.722981 3.547935 -3.088434
C 6.685604 3.544717 -3.120923
C -6.698507 3.605077 3.014267
C -5.658517 -2.852911 -2.469011

C	5.675954	-2.749993	2.589973
C	-5.698112	-2.812342	2.503223
C	5.687851	-2.744453	-2.572361
C	-4.320424	-3.128434	-2.787385
C	4.337736	-3.025488	2.909792
C	-4.353910	-3.095993	2.787247
C	4.349859	-2.999818	-2.910839
C	-4.032622	-4.164694	-3.687277
C	4.056283	-4.062148	3.812850
C	-4.050035	-4.121032	3.695323
C	4.059794	-4.071952	-3.768422
C	-5.059125	-4.929656	-4.232709
C	5.086247	-4.828481	4.351557
C	-5.068392	-4.866769	4.281192
C	5.082159	-4.881022	-4.258922
C	-6.404314	-4.678537	-3.899190
C	6.431284	-4.579620	4.013582
C	-6.419935	-4.613377	3.976184
C	6.427309	-4.638529	-3.917720
C	-6.683641	-3.613727	-3.021878
C	6.704572	-3.510960	3.137565
C	-6.714224	-3.558653	3.092009
C	6.708527	-3.547999	-3.072189
C	3.240850	2.239468	-2.252576
C	3.245342	2.190497	2.301732
C	3.249479	-2.234867	2.260715
C	-3.260669	-2.336137	2.122874
C	-3.232029	-2.323570	-2.161570
C	-3.266503	2.326638	-2.126227
C	3.259577	-2.184075	-2.304437
C	-3.242786	2.317773	2.157698
H	5.891669	1.944054	1.897333
H	-5.930098	1.998962	-1.806704
H	5.882305	1.965903	-1.884644
H	-5.883211	2.036409	1.771865
H	2.990927	4.286449	4.003798
H	-3.020406	4.315579	-3.929770
H	2.996697	4.283208	-4.038549
H	-3.013437	4.358096	3.942951
H	4.792728	5.741564	4.894907
H	-4.829533	5.655840	-4.973692
H	4.811171	5.662630	-5.014638
H	-4.837729	5.728423	4.916373
H	7.713495	3.375564	2.788299
H	-7.758117	3.318894	-2.848301
H	7.717045	3.326747	-2.855414

H	-7.728999	3.378957	2.752201
H	-5.872344	-2.041981	-1.779930
H	5.888579	-1.941253	1.897979
H	-5.924439	-2.009732	1.807985
H	5.906104	-1.916990	-1.904458
H	-2.996610	-4.358577	-3.948992
H	3.019821	-4.274577	4.058327
H	-3.008873	-4.322576	3.927097
H	3.023067	-4.274315	-4.019996
H	-4.817696	-5.733657	-4.923169
H	4.845295	-5.638906	5.034710
H	-4.815403	-5.662857	4.976767
H	4.835102	-5.714761	-4.911086
H	-7.715008	-3.390611	-2.760689
H	7.734240	-3.285267	2.871727
H	-7.750059	-3.330826	2.853877
H	7.738072	-3.334886	-2.795906
H	7.202236	5.219819	-4.410697
H	-7.226217	5.192994	-4.419525
H	7.232542	-5.182582	4.428380
H	7.222789	-5.271620	-4.297327
H	-7.212846	-5.202041	4.426358
H	-7.224314	5.266924	4.315996
H	-7.204295	-5.278376	-4.321257
H	7.183857	5.308674	4.287883
O	1.249502	-0.023563	1.864934
O	3.608443	-1.415166	1.357515
O	3.608476	-1.317848	-1.443768
O	3.599697	1.321698	1.446266
O	2.050572	2.429276	2.663548
O	0.061894	3.869096	1.290955
O	-2.042865	2.637896	2.423986
O	-2.070529	2.652262	-2.405919
O	-3.602885	1.360460	1.404902
O	-3.616355	1.406559	-1.324721
O	-3.612733	-1.417361	1.320906
O	-3.595059	-1.368322	-1.407658
O	-2.031595	-2.642929	-2.425569
O	-2.064046	-2.660613	2.401529
O	-1.244409	-1.877096	-0.017888
O	-1.314156	-0.020121	1.863002
O	-0.059145	1.213127	3.881685
O	-0.067707	-1.295235	3.858118
O	-0.067889	1.290334	-3.858119
O	-1.252303	1.871277	0.016651
O	1.321400	1.874279	0.023610

O	2.044574	2.447661	-2.623230
O	0.054631	3.885428	-1.218216
O	3.603407	1.418657	-1.352107
O	0.065620	-3.889726	1.217866
O	0.075008	-3.872918	-1.291290
O	1.329106	-1.876816	-0.022198
O	2.053276	-2.449676	2.628247
O	2.065572	-2.429231	-2.664497
O	-0.050173	-1.217891	-3.881708
O	-1.311723	0.013423	-1.864211
O	1.251843	0.020716	-1.863419
Zr	-2.517326	-0.003874	-0.001012
Zr	0.004799	1.823285	1.856322
Zr	-0.001708	-1.865832	1.824138
Zr	0.014207	-1.827659	-1.856473
Zr	2.528085	-0.000768	0.001350
Zr	-0.007096	1.861007	-1.823741
Al	1.383575	-3.728573	-0.033228
H	3.714940	-4.074750	0.063377
Al	-1.260561	-3.752113	-0.037785
H	-3.149314	-4.958312	-0.758891
Al	1.275363	0.051314	-3.735974
Al	-1.373845	0.025883	-3.714112
H	-3.696607	0.095359	-4.001284
H	3.096466	-0.684048	-5.014033
Al	1.371538	3.726343	0.034339
Al	-1.271993	3.746307	0.036244
H	3.702300	4.082248	-0.063131
H	-3.164965	4.947222	0.755393
Al	1.271060	-0.051148	3.737573
Al	-1.378188	-0.035357	3.712719
H	3.088421	0.691564	5.016732
H	-3.701350	-0.103893	3.994526
O	2.757584	-0.093064	4.569200
O	-2.887778	0.009190	4.497140
O	2.864736	4.538023	0.067828
O	-2.763471	4.565597	-0.030986
O	-2.882312	-0.028550	-4.500139
O	2.762690	0.098974	-4.565867
O	2.879624	-4.535010	-0.066373
O	-2.750404	-4.574592	0.027780

$AlMe_3$ Transition States

163

TS1 (E = -5221.216608)

C	5.385446	-3.260203	-2.712478

C	-6.001651	-2.775070	2.297778
C	5.335931	-3.614099	2.413316
C	-5.927175	-2.483462	-2.656612
C	4.034782	-3.380989	-3.071337
C	-4.685843	-3.179153	2.568993
C	3.977158	-3.798872	2.709944
C	-4.611231	-2.838174	-2.988891
C	3.662978	-4.367183	-3.997466
C	-4.471130	-4.285195	3.404687
C	3.603095	-4.870645	3.534240
C	-4.397841	-3.830183	-3.957075
C	4.618897	-5.223208	-4.539454
C	-5.549587	-4.989649	3.931157
C	4.560456	-5.755811	4.022207
C	-5.476520	-4.473608	-4.557533
C	5.976894	-5.112558	-4.181562
C	-6.874814	-4.613392	3.637442
C	5.924249	-5.594736	3.707662
C	-6.801629	-4.141196	-4.213107
C	6.340244	-4.109199	-3.262788
C	-7.077635	-3.479943	2.827997
C	6.292263	-4.495116	2.908653
C	-7.003956	-3.121377	-3.264033
C	-5.528442	2.849157	2.654510
C	5.810024	2.233709	-2.358933
C	-5.527322	3.151771	-2.308834
C	5.776145	1.874328	2.790782
C	-4.176244	2.999996	2.995964
C	4.499231	2.631045	-2.663819
C	-4.163126	3.351496	-2.567835
C	4.458282	2.206600	3.141256
C	-3.819073	3.947575	3.966003
C	4.304640	3.745368	-3.494370
C	-3.774907	4.410238	-3.402102
C	4.242318	3.236494	4.069555
C	-4.789760	4.749040	4.559124
C	5.394115	4.466477	-3.975352
C	-4.728989	5.269313	-3.938885
C	5.318400	3.930324	4.618247
C	-6.147068	4.623980	4.204294
C	6.713555	4.093875	-3.650494
C	-6.098409	5.098814	-3.656889
C	6.644395	3.610485	4.265981
C	-6.498129	3.645886	3.254764
C	6.897831	2.950190	-2.849151
C	-6.479096	4.011447	-2.848480

C	6.850045	2.562151	3.348394
C	2.963407	-2.876248	2.119838
C	3.011581	-2.516434	-2.420246
C	3.348836	1.882654	-2.074607
C	-3.136116	2.467037	-1.953752
C	-3.146059	2.158268	2.321499
C	-3.530524	-2.460626	1.965119
C	3.314980	1.519091	2.476267
C	-3.468310	-2.159721	-2.310015
H	5.665298	-2.499529	-1.990315
H	-6.159056	-1.911510	1.658790
H	5.621111	-2.779143	1.781128
H	-6.083705	-1.707635	-1.913675
H	2.614891	-4.465833	-4.263415
H	-3.450967	-4.581697	3.627746
H	2.550279	-5.012932	3.760045
H	-3.378101	-4.086233	-4.229149
H	4.309668	-5.988968	-5.246123
H	-5.365046	-5.849234	4.570439
H	4.247001	-6.589397	4.645348
H	-5.291854	-5.244595	-5.301126
H	7.381819	-4.000708	-2.971186
H	-8.090420	-3.157231	2.600496
H	7.339487	-4.338298	2.662477
H	-8.016739	-2.836261	-2.990714
H	-5.796712	2.105782	1.910473
H	5.955017	1.365765	-1.723499
H	-5.819585	2.322968	-1.671312
H	5.937276	1.080314	2.068287
H	-2.773736	4.044038	4.244154
H	3.289330	4.052018	-3.728350
H	-2.719524	4.547672	-3.615721
H	3.221619	3.499166	4.330748
H	-4.494501	5.483338	5.304155
H	5.220928	5.337641	-4.601951
H	-4.410631	6.089629	-4.577096
H	5.129158	4.733840	5.325372
H	-7.541045	3.519955	2.975144
H	7.905189	2.629468	-2.595795
H	-7.531205	3.847027	-2.630308
H	7.862989	2.291019	3.061785
H	6.669848	-6.288809	4.081890
H	-7.715076	-5.169285	4.040869
H	7.561584	4.661328	-4.019927
H	7.481956	4.154030	4.691118
H	-6.840722	5.775274	-4.068306

H	-7.642054	-4.645692	-4.678954
H	-6.903246	5.252455	4.663786
H	6.721197	-5.781051	-4.602179
H	-2.064073	-0.308136	2.837353
H	1.646785	-3.247248	-0.208294
H	1.028236	1.574754	-4.112521
H	0.014844	0.350053	-4.025905
H	0.753942	1.076521	4.498631
H	-0.561489	4.248068	-1.490074
H	-0.696180	3.848287	2.198862
H	-2.002332	0.138017	-2.855485
H	2.090581	2.451750	0.255225
H	0.585915	-1.673478	-4.472107
H	-0.103546	-0.828799	4.022419
H	0.713473	-2.191038	4.139056
H	-1.337725	-4.298506	-1.878348
H	-1.182789	-4.638171	1.373902
H	-0.411013	-4.261015	-0.586088
O	0.997938	-0.191027	-1.471528
O	3.637031	0.978304	-1.228746
O	3.605177	0.689864	1.559292
O	3.422939	-1.737565	-1.505734
O	1.805407	-2.638729	-2.801695
O	-0.424294	-4.116832	-1.599582
O	-2.294182	-2.552729	-2.591893
O	-2.364994	-2.895361	2.225628
O	-3.762806	-1.234839	-1.490782
O	-3.803198	-1.464932	1.226168
O	-3.563523	1.525261	-1.217751
O	-3.573630	1.290083	1.499275
O	-1.927389	2.368947	2.609269
O	-1.915981	2.718860	-2.204813
O	-1.032905	1.328820	0.137148
O	-1.441100	0.044755	-2.072287
O	-0.163150	-1.269797	-4.009876
O	0.115926	1.352977	-3.860671
O	-0.155134	-1.842746	3.877331
O	-1.252205	-1.631347	-0.145574
O	1.150381	-2.416424	-0.181843
O	1.751706	-3.018282	2.471123
O	-0.371774	-4.236483	1.029934
O	3.394727	-2.025681	1.279388
O	0.287663	3.845229	-1.248070
O	0.196351	3.611132	1.894182
O	1.457057	1.717731	0.196287
O	2.175590	2.212047	-2.430767

O	2.139761	1.829324	2.847944
O	-0.029183	0.776759	4.014832
O	-1.480442	-0.314685	2.064971
O	0.961954	-0.455772	1.469420
Zr	-2.576854	-0.055959	0.012035
Zr	-0.170941	-1.846894	-1.980944
Zr	0.059581	1.673903	-1.567210
Zr	0.067641	1.403173	1.999410
Zr	2.425775	-0.437928	0.038584
Zr	-0.256877	-2.202384	1.598601
Al	1.550902	5.025211	-0.606384
H	0.523489	4.697137	1.307070
C	0.552731	6.053479	1.005130
H	0.430565	6.193635	2.086100
H	1.349919	6.778188	0.771904
H	-0.368107	6.430404	0.539619
C	3.150632	4.302496	0.299301
H	3.829813	5.165425	0.386754
H	2.937558	4.006583	1.337829
H	3.772924	3.515321	-0.146915
C	1.711561	6.463411	-1.936538
H	2.463397	7.215720	-1.659345
H	2.003489	6.086921	-2.926467
H	0.769024	7.010985	-2.083818

158

TS2 (E = -5180.7686361)

C	-5.482729	-3.216005	2.541326
C	5.877979	-2.685364	-2.523921
C	-5.480357	-3.176274	-2.596755
C	5.847553	-2.773260	2.438731
C	-4.133830	-3.404047	2.877144
C	4.548638	-3.028204	-2.812889
C	-4.129948	-3.377943	-2.919427
C	4.523857	-3.113304	2.755163
C	-3.785519	-4.469075	3.721490
C	4.294577	-4.059885	-3.728807
C	-3.794398	-4.393825	-3.826881
C	4.287381	-4.169963	3.646543
C	-4.763068	-5.335478	4.205282
C	5.347425	-4.753486	-4.317809
C	-4.781585	-5.210079	-4.372191
C	5.350302	-4.889348	4.185781
C	-6.119595	-5.157409	3.869705
C	6.685498	-4.440398	-4.008612
C	-6.137603	-5.033260	-4.033421

C	6.682398	-4.570915	3.855381
C	-6.458886	-4.076076	3.033943
C	6.928315	-3.379020	-3.116669
C	-6.466441	-3.987857	-3.149105
C	6.908792	-3.487633	2.985351
C	5.572905	2.961202	-2.444335
C	-5.743122	2.299001	2.613648
C	5.616197	2.881410	2.527395
C	-5.756713	2.335568	-2.548555
C	4.223507	3.177939	-2.760435
C	-4.418759	2.632669	2.935730
C	4.260553	3.101037	2.813744
C	-4.431907	2.654556	-2.884912
C	3.888340	4.207387	-3.651706
C	-4.184596	3.673603	3.847331
C	3.910531	4.103582	3.730279
C	-4.191428	3.745865	-3.733601
C	4.878634	5.022907	-4.190797
C	-5.248275	4.387626	4.392360
C	4.893995	4.890180	4.322292
C	-5.249859	4.511427	-4.217391
C	6.234014	4.830733	-3.859369
C	-6.580674	4.080402	4.052340
C	6.255583	4.701301	4.015198
C	-6.582403	4.204949	-3.878203
C	6.562005	3.772580	-2.990892
C	-6.805208	3.007651	3.167516
C	6.597393	3.668456	3.122330
C	-6.813208	3.095767	-3.041718
C	-3.084539	-2.533860	-2.269960
C	-3.089542	-2.522806	2.284568
C	-3.295777	1.897950	2.280129
C	3.202864	2.297497	2.143110
C	3.173204	2.319067	-2.141245
C	3.419991	-2.324760	-2.144361
C	-3.305267	1.884455	-2.285256
C	3.397534	-2.352469	2.139401
H	-5.744522	-2.394119	1.882214
H	6.066014	-1.878512	-1.822172
H	-5.735607	-2.384275	-1.899814
H	6.022243	-1.947623	1.755964
H	-2.739042	-4.618923	3.969232
H	3.264339	-4.307970	-3.964317
H	-2.748007	-4.549514	-4.072813
H	3.262307	-4.415794	3.907784
H	-4.472177	-6.162115	4.848280

H	5.132385	-5.555548	-5.019291
H	-4.497968	-6.002248	-5.060273
H	5.147641	-5.709378	4.869837
H	-7.498740	-3.914641	2.761317
H	7.952005	-3.104938	-2.874652
H	-7.506658	-3.819419	-2.881802
H	7.927784	-3.212532	2.725161
H	5.823801	2.155218	-1.761982
H	-5.918859	1.487139	1.914991
H	5.878675	2.095743	1.825542
H	-5.936699	1.493513	-1.887518
H	2.844458	4.355912	-3.911808
H	-3.158823	3.931107	4.094554
H	2.861340	4.255447	3.963715
H	-3.165119	3.997430	-3.983494
H	4.600481	5.820721	-4.874584
H	-5.044323	5.202539	5.082190
H	4.605181	5.668111	5.024428
H	-5.041380	5.360938	-4.862639
H	7.602585	3.594645	-2.731560
H	-7.823596	2.737377	2.899823
H	7.642461	3.490144	2.882321
H	-7.831842	2.833586	-2.767206
H	-6.906530	-5.674093	-4.452684
H	7.505642	-4.988331	-4.461319
H	-7.408472	4.642699	4.472112
H	-7.406106	4.804168	-4.252560
H	7.020956	5.321820	4.470222
H	7.510434	-5.134430	4.273293
H	7.005609	5.469945	-4.276462
H	-6.880811	-5.833870	4.244863
H	2.001806	-0.071461	-2.844843
H	-1.783952	-3.114669	0.018191
H	-0.991688	1.350481	4.229107
H	0.005046	0.128704	4.057728
H	-0.804177	1.487938	-4.331718
H	0.664113	4.236044	1.797001
H	0.673648	4.175534	-1.845760
H	1.990711	-0.039647	2.864336
H	-2.138751	3.004772	-0.012931
H	-0.624995	-1.912969	4.367399
H	0.031498	-0.457218	-4.034449
H	-0.829818	-1.778290	-4.242500
H	1.202989	-4.405683	1.569142
H	1.021554	-4.495901	-1.696043
H	0.264471	-4.242029	0.296720

O	-1.022040	-0.213928	1.517091
O	-3.617269	1.070250	1.370227
O	-3.613966	0.996148	-1.431827
O	-3.483590	-1.664081	1.436318
O	-1.884980	-2.709546	2.644384
O	0.293785	-4.173010	1.316582
O	2.213741	-2.729266	2.403231
O	2.239972	-2.702816	-2.426989
O	3.713408	-1.373521	1.394620
O	3.727918	-1.396358	-1.335302
O	3.596390	1.402466	1.333634
O	3.579854	1.375256	-1.395283
O	1.959370	2.585600	-2.402638
O	1.992758	2.564935	2.424722
O	1.101457	1.398044	-0.022865
O	1.431892	-0.082167	2.075090
O	0.141453	-1.509778	3.934113
O	-0.079952	1.139076	3.967058
O	0.055450	-1.480490	-3.973388
O	1.179919	-1.595420	0.041292
O	-1.238140	-2.315698	0.044433
O	-1.880205	-2.684373	-2.642475
O	0.223707	-4.098012	-1.318579
O	-3.483908	-1.737988	-1.362798
O	-0.155316	3.847012	1.455983
O	-0.164927	3.820656	-1.512442
O	-1.381118	1.874241	-0.012749
O	-2.110585	2.164117	2.649476
O	-2.123884	2.187005	-2.643420
O	-0.009272	1.148989	-3.895860
O	1.437770	-0.137800	-2.060994
O	-1.010742	-0.264113	-1.476937
Zr	2.565419	-0.055308	-0.002946
Zr	0.111632	-1.930343	1.869869
Zr	-0.039980	1.612900	1.678707
Zr	-0.064629	1.570977	-1.819104
Zr	-2.437525	-0.253200	-0.006993
Zr	0.162148	-2.026606	-1.727909
Al	-0.882156	4.556435	-0.039938
C	-2.921509	4.063172	-0.013869
H	-3.743165	3.335202	-0.011749
H	-3.086581	4.670796	0.887257
H	-3.096876	4.671776	-0.912516
C	-0.806277	6.505302	-0.037612
H	-1.299203	6.940221	0.841839
H	0.221620	6.893203	-0.037302

H -1.297183 6.939969 -0.918252

153
TS3 (E = -5502.48450288)
C 5.487386 3.132180 2.543691
C -5.872828 2.619363 -2.524497
C 5.486349 3.090848 -2.594377
C -5.843607 2.708757 2.438135
C 4.138720 3.322625 2.879088
C -4.542817 2.959675 -2.813395
C 4.136374 3.294722 -2.917482
C -4.519410 3.046308 2.755248
C 3.791997 4.388515 3.723001
C -4.286752 3.990801 -3.729378
C 3.802808 4.310893 -3.825344
C -4.281382 4.103171 3.645938
C 4.770892 5.253398 4.206790
C -5.338253 4.686015 -4.318884
C 4.791537 5.125289 -4.370638
C -5.343219 4.824538 4.184661
C 6.127205 5.072908 3.871639
C -6.676943 4.375310 -4.009956
C 6.147158 4.946259 -4.031442
C -6.675766 4.508277 3.853996
C 6.464876 3.990736 3.036308
C -6.921816 3.314627 -3.117749
C 6.473968 3.900573 -3.146710
C -6.903774 3.425112 2.984242
C -5.577422 -3.027691 -2.443067
C 5.738338 -2.383240 2.617805
C -5.621935 -2.946272 2.528627
C 5.753276 -2.421443 -2.544382
C -4.228323 -3.246611 -2.759012
C 4.413320 -2.714532 2.939641
C -4.266748 -3.168106 2.815436
C 4.428020 -2.738256 -2.881020
C -3.894659 -4.277129 -3.649587
C 4.177129 -3.754793 3.851491
C -3.918688 -4.170980 3.732358
C 4.185908 -3.829434 -3.729416
C -4.886197 -5.091124 -4.188695
C 5.239439 -4.470461 4.397033
C -4.903655 -4.955712 4.324348
C 5.243162 -4.596954 -4.212678
C -6.241337 -4.896532 -3.857698
C 6.572453 -4.165620 4.057282

C	-6.264835	-4.764603	4.016822
C	6.576135	-4.292646	-3.873222
C	-6.567758	-3.837548	-2.989641
C	6.799061	-3.093530	3.172185
C	-6.604636	-3.731456	3.123539
C	6.808606	-3.183599	-3.037019
C	3.089344	2.452633	-2.268024
C	3.093084	2.443032	2.286447
C	3.291770	-1.978083	2.283500
C	-3.207158	-2.366078	2.145246
C	-3.176010	-2.388305	-2.140630
C	-3.415287	2.254439	-2.144371
C	3.302532	-1.966064	-2.281877
C	-3.393621	2.282804	2.140457
H	5.747955	2.309642	1.884908
H	-6.062433	1.813053	-1.822547
H	5.740056	2.298632	-1.897119
H	-6.019521	1.883206	1.755578
H	2.745710	4.540229	3.970410
H	-3.256027	4.237052	-3.964684
H	2.756752	4.468292	-4.071611
H	-3.255960	4.347332	3.907383
H	4.481239	6.080732	4.849450
H	-5.121651	5.487490	-5.020558
H	4.509461	5.917726	-5.059045
H	-5.139344	5.644434	4.868517
H	7.504527	3.827440	2.764016
H	-7.946039	3.042370	-2.875926
H	7.513823	3.730441	-2.879070
H	-7.923163	3.151671	2.723860
H	-5.827127	-2.221067	-1.761033
H	5.915652	-1.571897	1.918943
H	-5.882879	-2.160377	1.826457
H	5.934519	-1.579490	-1.883559
H	-2.850961	-4.427518	-3.909358
H	3.150850	-4.010467	4.098513
H	-2.869822	-4.324564	3.966129
H	3.159239	-4.079324	-3.979512
H	-4.609220	-5.889626	-4.872157
H	5.033906	-5.284809	5.087061
H	-4.616363	-5.733916	5.026805
H	5.033408	-5.446309	-4.857718
H	-7.608103	-3.657756	-2.730649
H	7.817982	-2.825080	2.904686
H	-7.649333	-3.551433	2.883188
H	7.827611	-2.923073	-2.762310

H	6.917294	5.585648	-4.450695
H	-7.496026	4.924501	-4.463058
H	7.399174	-4.729199	4.477455
H	7.398915	-4.893388	-4.247166
H	-7.031391	-5.383672	4.471830
H	-7.502953	5.073337	4.271506
H	-7.013909	-5.534555	-4.274803
H	6.889472	5.748185	4.246795
H	-2.016418	0.021988	-2.849741
H	1.790132	3.031936	0.021114
H	0.980893	-1.429029	4.247949
H	-0.001579	-0.189677	4.075936
H	0.777384	-1.560931	-4.370030
H	-0.529118	-4.398182	1.442331
H	-0.583295	-4.288768	-1.503006
H	-2.005232	-0.013204	2.871794
H	0.629084	1.844692	4.366413
H	-0.032297	0.410176	-4.057286
H	0.828889	1.733420	-4.245790
H	-1.191811	4.329844	1.573001
H	-1.009846	4.419471	-1.694446
H	-0.255563	4.165047	0.298628
O	1.012537	0.121048	1.501365
O	3.614882	-1.151154	1.373396
O	3.612476	-1.077956	-1.428601
O	3.485837	1.583310	1.438523
O	1.888775	2.631975	2.645875
O	-0.284047	4.093541	1.318331
O	-2.209832	2.658086	2.404008
O	-2.234784	2.630266	-2.426612
O	-3.712157	1.305280	1.390651
O	-3.725329	1.325810	-1.332366
O	-3.599643	-1.469773	1.332270
O	-3.582897	-1.445278	-1.389285
O	-1.963253	-2.657887	-2.400848
O	-1.997905	-2.635853	2.426808
O	-1.089785	-1.467406	-0.021372
O	-1.440022	0.013235	2.086312
O	-0.133347	1.434402	3.932633
O	0.072237	-1.202877	3.985970
O	-0.054531	1.430462	-3.976086
O	-1.177759	1.520456	0.042090
O	1.245307	2.232135	0.045884
O	1.885399	2.605079	-2.641017
O	-0.214186	4.018946	-1.314994
O	3.487080	1.656296	-1.360435

O	0.285780	-3.883476	1.392923
O	0.281108	-3.857979	-1.496832
O	1.401566	-1.983680	-0.012748
O	2.106034	-2.242215	2.652562
O	2.120746	-2.266880	-2.640111
O	-0.000958	-1.196639	-3.924361
O	-1.443260	0.070162	-2.071104
O	1.007262	0.173806	-1.465144
Zr	-2.565539	-0.018447	-0.002230
Zr	-0.106280	1.851611	1.866844
Zr	0.010167	-1.685121	1.716052
Zr	0.040964	-1.635337	-1.861315
Zr	2.454016	0.166167	-0.005710
Zr	-0.155725	1.949317	-1.724320
Al	1.410984	-3.772005	-0.063670
C	3.047115	-4.816485	-0.057664
H	3.139071	-5.474669	-0.930860
H	3.926340	-4.156277	-0.071973
H	3.145781	-5.446310	0.835839

161

TS4 (E = -5462.00856053)

C	5.676482	3.016220	2.561195
C	-5.695964	3.066852	-2.505252
C	5.672851	3.012380	-2.577037
C	-5.661978	3.118674	2.457884
C	4.338126	3.266458	2.898602
C	-4.351661	3.347312	-2.792293
C	4.333722	3.280889	-2.898016
C	-4.323530	3.392233	2.776820
C	4.041240	4.341090	3.750396
C	-4.048247	4.372116	-3.700882
C	4.047445	4.317994	-3.798318
C	-4.036702	4.430431	3.675052
C	5.059197	5.156177	4.239996
C	-5.066507	5.119542	-4.284829
C	5.072751	5.089685	-4.338145
C	-5.063926	5.196248	4.219500
C	6.405654	4.915525	3.902906
C	-6.418106	4.868914	-3.977538
C	6.418674	4.845615	-4.000895
C	-6.409732	4.944441	3.887171
C	6.692743	3.824987	3.059577
C	-6.711713	3.814241	-3.092945
C	6.696831	3.779507	-3.123936
C	-6.687766	3.879354	3.009679

C	-5.662344	-2.588266	-2.464987
C	5.671789	-2.505298	2.595121
C	-5.702381	-2.541063	2.507187
C	5.684258	-2.506576	-2.567214
C	-4.324871	-2.867116	-2.783141
C	4.332894	-2.777220	2.915161
C	-4.358881	-2.827485	2.791743
C	4.345710	-2.759229	-2.905523
C	-4.039400	-3.905464	-3.681342
C	4.048910	-3.812036	3.819543
C	-4.057510	-3.852049	3.701189
C	4.053219	-3.831822	-3.761710
C	-5.067637	-4.668730	-4.225884
C	5.077015	-4.580075	4.359372
C	-5.077678	-4.594622	4.287925
C	5.073736	-4.643934	-4.251031
C	-6.412269	-4.414016	-3.892846
C	6.422670	-4.334817	4.021220
C	-6.428590	-4.338460	3.982435
C	6.419415	-4.404150	-3.909999
C	-6.689190	-3.347400	-3.016965
C	6.698559	-3.267955	3.143828
C	-6.720306	-3.284214	3.096841
C	6.703101	-3.313172	-3.065870
C	3.248908	2.483474	-2.254209
C	3.252803	2.440566	2.300069
C	3.246566	-1.984925	2.264907
C	-3.263378	-2.070526	2.126894
C	-3.233864	-2.062982	-2.159041
C	-3.257907	2.585774	-2.128944
C	3.257253	-1.940080	-2.300262
C	-3.234383	2.581923	2.155960
H	5.898598	2.187317	1.896331
H	-5.922609	2.265099	-1.809089
H	5.889696	2.204212	-1.885671
H	-5.876020	2.307143	1.769430
H	3.003134	4.539281	3.999392
H	-3.007256	4.572084	-3.934877
H	3.009767	4.525447	-4.042943
H	-3.001040	4.624942	3.937783
H	4.808249	5.991335	4.888786
H	-4.813119	5.915215	-4.980763
H	4.827579	5.899323	-5.020644
H	-4.822215	6.000826	4.909199
H	7.723681	3.615715	2.785618
H	-7.747411	3.587945	-2.852625

H	7.727728	3.559467	-2.858027
H	-7.718756	3.655308	2.747795
H	-5.874342	-1.775931	-1.776995
H	5.886389	-1.697969	1.902088
H	-5.926748	-1.738839	1.810868
H	5.904380	-1.678750	-1.900377
H	-3.003820	-4.102121	-3.942689
H	3.011926	-4.021709	4.065183
H	-3.016849	-4.055730	3.933346
H	3.016047	-4.032081	-4.013132
H	-4.828022	-5.474203	-4.915259
H	4.834087	-5.389034	5.043563
H	-4.826635	-5.390387	4.984575
H	4.824793	-5.477949	-4.902126
H	-7.720059	-3.121521	-2.756186
H	7.728782	-3.045031	2.877808
H	-7.755579	-3.054268	2.858294
H	7.733112	-3.102114	-2.789754
H	7.217534	5.451695	-4.415853
H	-7.210942	5.458724	-4.426253
H	7.222463	-4.939114	4.436899
H	7.213446	-5.039606	-4.288683
H	-7.222928	-4.924668	4.433293
H	-7.209812	5.544140	4.309163
H	-7.213611	-5.012531	-4.314212
H	7.198421	5.552035	4.282601
H	-1.986301	0.265302	-2.822265
H	1.973586	3.101493	0.036549
H	0.962643	-1.325812	4.267034
H	0.034137	-0.046315	4.079770
H	0.728797	-1.420940	-4.411560
H	-0.105882	-4.875730	1.177968
H	-1.967125	0.192436	2.856543
H	0.761946	1.942442	4.381437
H	0.027275	0.589451	-4.055725
H	0.955520	1.867076	-4.232995
H	-0.939181	4.535883	1.600641
H	-0.754231	4.627433	-1.663250
H	-0.014326	4.328411	0.321952
O	1.059616	0.231109	1.519252
O	3.607515	-1.167194	1.360614
O	3.608084	-1.073557	-1.440782
O	3.605244	1.569763	1.445677
O	2.058592	2.682436	2.661402
O	-0.045856	4.252915	1.342770
O	-2.034443	2.900055	2.421648

O	-2.061294	2.908603	-2.409048
O	-3.597951	1.625671	1.399214
O	-3.610498	1.666620	-1.323573
O	-3.614047	-1.151110	1.320628
O	-3.596557	-1.107602	-1.400685
O	-2.034868	-2.386478	-2.421652
O	-2.067908	-2.398136	2.405967
O	-1.125084	-1.344460	-0.020542
O	-1.385700	0.214051	2.082559
O	-0.021020	1.573295	3.947044
O	0.069327	-1.063798	3.987871
O	0.056403	1.608548	-3.968565
O	-1.053027	1.711228	0.053897
O	1.390723	2.328775	0.059371
O	2.053270	2.694229	-2.625559
O	0.019834	4.186965	-1.283373
O	3.609434	1.663010	-1.352680
O	0.134673	-3.731346	1.203065
O	0.093002	-3.672455	-1.367614
O	1.396184	-1.786139	-0.023588
O	2.049810	-2.196695	2.632747
O	2.062843	-2.183094	-2.659879
O	-0.016358	-1.021632	-3.940709
O	-1.392823	0.292171	-2.057630
O	1.051375	0.297535	-1.479508
Zr	-2.508595	0.242286	-0.001454
Zr	0.023454	2.006793	1.884453
Zr	-0.000767	-1.537522	1.723136
Zr	0.011500	-1.492167	-1.886948
Zr	2.494538	0.224077	-0.010890
Zr	-0.020884	2.119085	-1.716498
Al	1.463732	-3.545807	-0.170051
C	3.055373	-4.649947	-0.097171
H	3.089221	-5.395620	-0.901327
H	3.971099	-4.048933	-0.181181
H	3.125891	-5.196101	0.853235
Al	-1.155463	-4.173189	-0.186552
C	-3.085630	-4.313236	-0.088214
H	-3.479344	-4.901157	-0.928563
H	-3.342299	-4.861884	0.828209
H	-3.642375	-3.371631	-0.069594
C	-0.578103	-6.139601	0.469978
H	0.403577	-6.610187	0.621290
H	-1.290655	-6.617559	1.152297
H	-0.865795	-6.476060	-0.541472

$InMe_3$ Reaction Path Structures

163

S1 (E = -4980.6713554)

C	4.892416	-3.876652	-2.898119
C	-6.445160	-2.381983	2.024210
C	4.692001	-4.662067	2.175777
C	-6.231392	-1.676071	-2.884206
C	3.545047	-3.793417	-3.279346
C	-5.196559	-2.971925	2.271508
C	3.314900	-4.697508	2.441724
C	-4.963868	-2.165180	-3.233632
C	3.071558	-4.640756	-4.292434
C	-5.140106	-4.164175	3.008508
C	2.791920	-5.780113	3.164597
C	-4.856804	-3.089054	-4.283392
C	3.923317	-5.561387	-4.898452
C	-6.309327	-4.768593	3.460277
C	3.619984	-6.818537	3.581917
C	-5.995091	-3.535960	-4.948728
C	5.276692	-5.655518	-4.518984
C	-7.570304	-4.203033	3.187985
C	4.999461	-6.805593	3.296105
C	-7.274760	-3.068768	-4.589258
C	5.744119	-4.789476	-3.511818
C	-7.612059	-2.987453	2.479701
C	5.519410	-5.696895	2.600793
C	-7.366956	-2.117174	-3.555974
C	-5.275928	3.084596	2.880078
C	5.997090	1.467617	-2.057391
C	-5.133347	3.811480	-2.037003
C	5.810994	0.672733	3.040000
C	-3.922911	3.032316	3.246676
C	4.753314	2.053135	-2.338810
C	-3.749768	3.857773	-2.264086
C	4.538366	1.138322	3.405567
C	-3.469692	3.839621	4.299910
C	4.717755	3.250588	-3.069725
C	-3.214184	4.926552	-2.997916
C	4.434345	2.103418	4.418899
C	-4.344025	4.703807	4.951906
C	5.899052	3.866142	-3.474609
C	-4.041257	5.942988	-3.466129
C	5.577474	2.604925	5.037093
C	-5.698593	4.783348	4.574222
C	7.154099	3.302242	-3.171031
C	-5.426824	5.924255	-3.213621

C	6.859767	2.150719	4.670932
C	-6.150014	3.943362	3.538770
C	7.176343	2.079605	-2.471900
C	-5.957998	4.828465	-2.507991
C	6.951018	1.167813	3.666527
C	2.437747	-3.606134	1.925427
C	2.625367	-2.865178	-2.564569
C	3.505932	1.409116	-1.829137
C	-2.855171	2.800365	-1.720368
C	-2.992940	2.127839	2.510672
C	-3.947705	-2.356656	1.744683
C	3.331763	0.661577	2.671441
C	-3.759107	-1.698609	-2.486442
H	5.250603	-3.222848	-2.109002
H	-6.479364	-1.453562	1.462354
H	5.093031	-3.818749	1.622485
H	-6.304554	-0.953621	-2.077314
H	2.025157	-4.582086	-4.576245
H	-4.170202	-4.606060	3.214483
H	1.725094	-5.806366	3.366708
H	-3.871916	-3.448217	-4.567034
H	3.535030	-6.217819	-5.672871
H	-6.247714	-5.696562	4.023041
H	3.191269	-7.656126	4.126045
H	-5.893399	-4.257147	-5.755572
H	6.784766	-4.839805	-3.201651
H	-8.571256	-2.520224	2.271684
H	6.582942	-5.653817	2.379618
H	-8.341315	-1.730282	-3.268460
H	-5.619996	2.448301	2.070811
H	6.018506	0.536747	-1.499584
H	-5.540740	2.974685	-1.477924
H	5.886008	-0.070038	2.251909
H	-2.426548	3.778087	4.595655
H	3.754167	3.702826	-3.285635
H	-2.145676	4.946633	-3.188293
H	3.449566	2.470184	4.692278
H	-3.974351	5.327617	5.761624
H	5.849893	4.803014	-4.023608
H	-3.609035	6.768142	-4.026388
H	5.476095	3.361982	5.810437
H	-7.194432	3.975594	3.238986
H	8.129869	1.612802	-2.238008
H	-7.026747	4.780909	-2.315428
H	7.927570	0.795865	3.367011
H	5.643891	-7.618469	3.614920

H	-8.482026	-4.680319	3.532618
H	8.074270	3.787032	-3.480708
H	7.749994	2.544698	5.150482
H	-6.069435	6.722515	-3.571001
H	-8.162069	-3.420284	-5.105944
H	-6.379138	5.460855	5.079951
H	5.939616	-6.374412	-4.989635
H	-2.243362	-0.511771	2.831459
H	1.137311	-3.605049	-0.452332
H	1.202316	1.601741	-3.915169
H	0.048311	0.504344	-3.932839
H	0.697110	0.344374	4.637011
H	-0.163823	4.161428	-0.930882
H	-0.332187	3.623817	2.384979
H	-2.003293	0.440620	-2.800550
H	2.303923	1.929537	0.540864
H	0.368463	-1.531747	-4.559209
H	-0.401018	-1.406542	3.989218
H	0.251077	-2.853856	3.961970
H	-1.917469	-4.112532	-2.244814
H	-1.887184	-4.777491	0.975438
H	-1.026194	-4.318417	-0.946365
H	0.515065	3.451362	1.076088
O	0.901729	-0.384724	-1.415383
O	3.660499	0.405865	-1.063604
O	3.534422	-0.115520	1.687684
O	3.112278	-2.226706	-1.581081
O	1.421620	-2.799810	-2.967223
O	-0.996020	-4.074936	-1.936737
O	-2.638060	-2.211831	-2.790490
O	-2.851782	-2.956883	1.977284
O	-3.951861	-0.817953	-1.591761
O	-4.077595	-1.274357	1.093833
O	-3.412783	1.860600	-1.074447
O	-3.509072	1.395167	1.611012
O	-1.763759	2.156313	2.827668
O	-1.608065	2.915681	-1.936422
O	-0.948381	1.215918	0.299110
O	-1.470664	0.209213	-2.025717
O	-0.326771	-1.077070	-4.061630
O	0.269366	1.467774	-3.676859
O	-0.567783	-2.379977	3.737670
O	-1.539390	-1.646686	-0.257750
O	0.745110	-2.726168	-0.346017
O	1.210787	-3.622606	2.250847
O	-1.025371	-4.449460	0.679883

O	2.989954	-2.747963	1.167355
O	0.610890	3.637478	-0.665864
O	0.480329	3.209661	2.045600
O	1.568781	1.303063	0.421150
O	2.391067	1.914011	-2.165980
O	2.197259	1.085699	3.057597
O	-0.112200	0.200207	4.125214
O	-1.650032	-0.527349	2.066504
O	0.770451	-0.924272	1.478414
Zr	-2.660793	0.069076	0.017390
Zr	-0.451547	-1.825622	-2.096813
Zr	0.215568	1.607874	-1.370838
Zr	0.099250	0.919810	2.161066
Zr	2.266359	-0.948082	0.050895
Zr	-0.669664	-2.511597	1.425906
In	2.350300	5.084265	-0.412059
C	3.730229	3.777433	0.672810
H	3.290923	3.506281	1.646643
H	4.087953	2.856254	0.190048
H	4.646900	4.334062	0.917216
C	2.532852	5.824303	-2.447344
H	1.984003	6.770540	-2.551085
H	3.563055	6.015416	-2.774841
H	2.089226	5.119898	-3.166845
C	1.252635	6.403558	0.940576
H	1.394863	6.128178	1.994888
H	1.546837	7.457820	0.844439
H	0.167825	6.376798	0.748385

158

S2 (E = -4940.2213262)

C	5.280656	3.671372	2.539922
C	-6.042355	2.607894	-2.525887
C	5.280700	3.628334	-2.598133
C	-6.016604	2.700243	2.436710
C	3.924415	3.796463	2.875516
C	-4.730432	3.012218	-2.814970
C	3.922385	3.766552	-2.921042
C	-4.710255	3.101890	2.753038
C	3.526685	4.844608	3.719156
C	-4.524699	4.054058	-3.731519
C	3.539887	4.765096	-3.829165
C	-4.523451	4.169001	3.643759
C	4.462679	5.755996	4.202476
C	-5.608707	4.697393	-4.321045
C	4.487961	5.626191	-4.374915

C	-5.618846	4.838334	4.182456
C	5.826076	5.641221	3.867119
C	-6.930743	4.322391	-4.011756
C	5.850717	5.513065	-4.035925
C	-6.934593	4.457868	3.852153
C	6.215555	4.576375	3.032071
C	-7.123857	3.251400	-3.119158
C	6.227891	4.484707	-3.150920
C	-7.110088	3.364652	2.982793
C	-5.474089	-3.018229	-2.442693
C	5.798150	-1.825425	2.615766
C	-5.521598	-2.937410	2.528983
C	5.813995	-1.864572	-2.546412
C	-4.116011	-3.171952	-2.758545
C	4.490768	-2.220340	2.937951
C	-4.157213	-3.093347	2.815579
C	4.505557	-2.245258	-2.882668
C	-3.733068	-4.185196	-3.649138
C	4.305344	-3.270490	3.850198
C	-3.760881	-4.077886	3.732778
C	4.316366	-3.347133	-3.730686
C	-4.684162	-5.046385	-4.187790
C	5.401129	-3.933747	4.395765
C	-4.706626	-4.909153	4.325212
C	5.409426	-4.062768	-4.213907
C	-6.047070	-4.917469	-3.856592
C	6.717774	-3.564888	4.055654
C	-6.075512	-4.784221	4.017890
C	6.726177	-3.694217	-3.874808
C	-6.424184	-3.875230	-2.988813
C	6.892093	-2.483384	3.170168
C	-6.465057	-3.769018	3.124340
C	6.904872	-2.574945	-3.039009
C	2.917448	2.875017	-2.271119
C	2.922466	2.867080	2.283411
C	3.334781	-1.539247	2.281777
C	-3.138097	-2.241746	2.144502
C	-3.106993	-2.264615	-2.139800
C	-3.570263	2.362637	-2.145915
C	3.344122	-1.528198	-2.283572
C	-3.549592	2.394062	2.137860
H	5.580594	2.862184	1.881353
H	-6.192605	1.793588	-1.823640
H	5.572559	2.849551	-1.900669
H	-6.152496	1.866922	1.754454
H	2.474327	4.945609	3.966720

H	-3.507136	4.349806	-3.967105
H	2.487396	4.871624	-4.075279
H	-3.510995	4.462571	3.904925
H	4.133455	6.568561	4.844925
H	-5.431258	5.508175	-5.023019
H	4.167756	6.403825	-5.063522
H	-5.454752	5.667360	4.866008
H	7.261840	4.463476	2.759629
H	-8.133665	2.929992	-2.877049
H	7.274807	4.365169	-2.883427
H	-8.115102	3.042129	2.722697
H	-5.762402	-2.224403	-1.760870
H	5.935881	-1.006686	1.916607
H	-5.820382	-2.165292	1.826611
H	5.954413	-1.014618	-1.885896
H	-2.683362	-4.285004	-3.909063
H	3.292679	-3.575432	4.097502
H	-2.705772	-4.180471	3.966393
H	3.302943	-3.646481	-3.980501
H	-4.369002	-5.830779	-4.871048
H	5.235357	-4.756856	5.086095
H	-4.381897	-5.672314	5.027865
H	5.240892	-4.921489	-4.858632
H	-7.471963	-3.745891	-2.729675
H	7.896786	-2.166044	2.902383
H	-7.517282	-3.639826	2.884134
H	7.910130	-2.265335	-2.764582
H	6.588944	6.188823	-4.455534
H	-7.775517	4.831164	-4.464875
H	7.570867	-4.087673	4.475849
H	7.576989	-4.254576	-4.248719
H	-6.811141	-5.439498	4.473247
H	-7.788072	4.982387	4.269642
H	-6.787946	-5.592259	-4.273340
H	6.554849	6.352708	4.241908
H	-2.067776	0.184103	-2.839514
H	1.570215	3.403437	0.014908
H	0.993314	-1.116420	4.265282
H	-0.043476	0.076888	4.077394
H	0.790095	-1.277400	-4.379128
H	-0.558766	-4.006515	1.837421
H	-0.545154	-3.968699	-1.865412
H	-2.056422	0.164862	2.869201
H	2.234285	-2.203167	0.002349
H	0.485252	2.141594	4.374363
H	-0.100239	0.658073	-4.054295

H	0.697011	2.020347	-4.253747
H	-1.449021	4.518149	1.572507
H	-1.271359	4.617489	-1.697790
H	-0.508907	4.405436	0.295800
O	0.959329	0.436654	1.497964
O	3.617323	-0.698003	1.371399
O	3.610876	-0.625907	-1.430718
O	3.356258	2.027134	1.435722
O	1.710461	2.997603	2.643047
O	-0.529176	4.335995	1.315624
O	-2.384684	2.825885	2.401621
O	-2.409132	2.795201	-2.428766
O	-3.819365	1.400962	1.393663
O	-3.834633	1.421381	-1.336283
O	-3.572846	-1.366553	1.334459
O	-3.557307	-1.340326	-1.394506
O	-1.881998	-2.474360	-2.400620
O	-1.916845	-2.452196	2.426055
O	-1.014829	-1.228265	-0.014777
O	-1.482245	0.203028	2.090685
O	-0.249750	1.688507	3.936139
O	0.077747	-0.933700	3.994118
O	-0.169526	1.676733	-3.978935
O	-1.300272	1.735334	0.042444
O	1.087128	2.564852	0.042599
O	1.707434	2.968910	-2.643865
O	-0.453801	4.261796	-1.319928
O	3.353435	2.099216	-1.363407
O	0.287234	-3.607659	1.578739
O	0.309817	-3.587239	-1.610049
O	1.472116	-1.602999	-0.016731
O	2.163264	-1.860225	2.650895
O	2.178232	-1.885780	-2.641316
O	0.002465	-0.946366	-3.923939
O	-1.486666	0.255762	-2.068589
O	0.949485	0.484512	-1.461274
Zr	-2.593556	0.127912	-0.003539
Zr	-0.242665	2.101855	1.868376
Zr	0.048673	-1.453226	1.738704
Zr	0.085331	-1.412564	-1.869057
Zr	2.388530	0.603926	-0.008236
Zr	-0.299309	2.194664	-1.729951
In	1.225066	-4.671127	-0.031503
C	3.351401	-4.302614	0.033315
H	3.719412	-3.267454	-0.022805
H	3.765052	-4.713988	0.963944

H	3.841448	-4.830353	-0.795721
C	0.217382	-6.569336	-0.027990
H	-0.873159	-6.438388	-0.033420
H	0.470229	-7.175454	-0.906678
H	0.463780	-7.169971	0.856322

153

S3 (E = -4899.7389132)

C	5.207445	3.625193	2.532502
C	-6.096255	2.394280	-2.538512
C	5.213018	3.557873	-2.605288
C	-6.076491	2.510404	2.423613
C	3.849403	3.734659	2.866267
C	-4.789266	2.813678	-2.828491
C	3.853374	3.677330	-2.930082
C	-4.775619	2.929758	2.739636
C	3.437599	4.781653	3.704568
C	-4.595885	3.853857	-3.749602
C	3.459130	4.666637	-3.843277
C	-4.603248	4.003668	3.625047
C	4.361495	5.707111	4.184414
C	-5.687389	4.480601	-4.343156
C	4.396742	5.537095	-4.392238
C	-5.707563	4.661594	4.159569
C	5.726562	5.608051	3.850846
C	-7.004864	4.090331	-4.033296
C	5.760493	5.442863	-4.051476
C	-7.018059	4.262917	3.829875
C	6.130318	4.544294	3.021208
C	-7.185251	3.021208	-3.135810
C	6.149813	4.423566	-3.161264
C	-7.178839	3.163466	2.965546
C	-5.456796	-3.223729	-2.428141
C	5.794505	-1.864180	2.634864
C	-5.510149	-3.120020	2.543051
C	5.815852	-1.927523	-2.527053
C	-4.096602	-3.361465	-2.742345
C	4.491923	-2.274069	2.957770
C	-4.144180	-3.257241	2.831674
C	4.512673	-2.326308	-2.862745
C	-3.699951	-4.374214	-3.627458
C	4.318939	-3.322208	3.874771
C	-3.736285	-4.232373	3.753837
C	4.338286	-3.434538	-3.705651
C	-4.639529	-5.249931	-4.162888
C	5.422515	-3.968930	4.424471

C	-4.671989	-5.072757	4.349344
C	5.440799	-4.138529	-4.184480
C	-6.004283	-5.136745	-3.833545
C	6.734708	-3.585016	4.083816
C	-6.042051	-4.966648	4.040187
C	6.752442	-3.751712	-3.845934
C	-6.395421	-4.095280	-2.971058
C	6.896162	-2.505586	3.193373
C	-6.443567	-3.960702	3.141483
C	6.916124	-2.626326	-3.015285
C	2.859180	2.776210	-2.276839
C	2.859877	2.789904	2.277609
C	3.328065	-1.610785	2.297376
C	-3.135004	-2.395468	2.157943
C	-3.099152	-2.437452	-2.127855
C	-3.621320	2.181962	-2.155329
C	3.341711	-1.621239	-2.268131
C	-3.604832	2.233279	2.129291
H	5.518256	2.816770	1.878049
H	-6.236852	1.581463	-1.832551
H	5.514051	2.786159	-1.903876
H	-6.201147	1.672211	1.745190
H	2.383806	4.870470	3.950693
H	-3.581925	4.161369	-3.985661
H	2.405613	4.758645	-4.090851
H	-3.594849	4.311284	3.885740
H	4.021375	6.518464	4.822706
H	-5.519551	5.290241	-5.048803
H	4.067373	6.307343	-5.084814
H	-5.554654	5.495856	4.839334
H	7.178214	4.443386	2.750257
H	-8.191139	2.688169	-2.893099
H	7.197900	4.318579	-2.892256
H	-8.179430	2.826999	2.706067
H	-5.755810	-2.430409	-1.750351
H	5.922524	-1.047074	1.931960
H	-5.818015	-2.355081	1.836755
H	5.944843	-1.072744	-1.870445
H	-2.648814	-4.461929	-3.885953
H	3.309983	-3.638795	4.122596
H	-2.680186	-4.320465	3.988897
H	3.328982	-3.747890	-3.954967
H	-4.313789	-6.033486	-4.842135
H	5.266521	-4.790803	5.118543
H	-4.338294	-5.828409	5.055900
H	5.283789	-5.002357	-4.825282

H	-7.445005	-3.978016	-2.713491
H	7.897011	-2.176800	2.925003
H	-7.497112	-3.846000	2.899710
H	7.917109	-2.302700	-2.741414
H	6.490501	6.125938	-4.473611
H	-7.855580	4.586202	-4.489590
H	7.593951	-4.094949	4.507259
H	7.610652	-4.302997	-4.216411
H	-6.769755	-5.629041	4.497975
H	-7.878524	4.778538	4.244097
H	-6.736141	-5.822837	-4.247766
H	6.445894	6.330486	4.222923
H	-2.092213	0.030792	-2.846484
H	1.524267	3.288201	0.009023
H	0.982282	-1.196113	4.254800
H	-0.072298	-0.020787	4.074010
H	0.789879	-1.385919	-4.360258
H	-0.384726	-4.234956	1.563143
H	-0.425933	-4.166554	-1.571202
H	-2.081684	0.023446	2.870057
H	0.432322	2.053669	4.361688
H	-0.130404	0.537260	-4.053525
H	0.647217	1.910253	-4.249664
H	-1.537145	4.403409	1.550398
H	-1.357388	4.489714	-1.714848
H	-0.588089	4.294383	0.279770
O	0.925739	0.349661	1.519915
O	3.600710	-0.770282	1.383191
O	3.596057	-0.711550	-1.419228
O	3.305048	1.951436	1.434251
O	1.645993	2.906752	2.635500
O	-0.614592	4.227678	1.299812
O	-2.446368	2.681449	2.391593
O	-2.465737	2.627716	-2.439004
O	-3.862525	1.234376	1.384320
O	-3.874769	1.240285	-1.338746
O	-3.580747	-1.528859	1.340206
O	-3.563373	-1.517167	-1.381520
O	-1.871947	-2.633863	-2.385716
O	-1.911710	-2.589554	2.441053
O	-1.085203	-1.392955	-0.014130
O	-1.518140	0.084153	2.085423
O	-0.306900	1.599033	3.932035
O	0.062400	-1.027224	3.990443
O	-0.218015	1.556022	-3.983635
O	-1.343879	1.593821	0.036421

O	1.025832	2.458955	0.038021
O	1.648466	2.852955	-2.651209
O	-0.536252	4.145234	-1.334542
O	3.304057	2.010203	-1.364991
O	0.426535	-3.709674	1.538097
O	0.422875	-3.703545	-1.602568
O	1.435150	-1.683442	-0.002719
O	2.160333	-1.945014	2.666759
O	2.180761	-1.995495	-2.624909
O	-0.003182	-1.059445	-3.911993
O	-1.523159	0.120408	-2.068629
O	0.916673	0.388959	-1.477891
Zr	-2.636595	-0.024439	-0.001218
Zr	-0.299270	2.001671	1.863180
Zr	0.032363	-1.530183	1.717770
Zr	0.059268	-1.495372	-1.844819
Zr	2.341850	0.471091	-0.002314
Zr	-0.351426	2.078861	-1.734199
In	1.809524	-3.683491	-0.050971
C	3.634705	-4.745940	-0.023512
H	3.744664	-5.375345	-0.912659
H	4.472581	-4.038431	-0.008589
H	3.715376	-5.380222	0.865470

161
S4 (E = -4980.8829055)

C	5.865111	3.542563	1.895179
C	-5.660561	3.111910	-2.792827
C	5.692353	2.625768	-3.157652
C	-5.461723	4.043651	2.078403
C	4.547146	3.898020	2.218095
C	-4.318244	3.287046	-3.161224
C	4.352534	2.882219	-3.485540
C	-4.105540	4.319930	2.307388
C	4.312509	5.117151	2.871699
C	-4.012680	4.122162	-4.246134
C	4.069681	3.752673	-4.548738
C	-3.756692	5.489913	2.997600
C	5.371241	5.968118	3.180325
C	-5.025495	4.790997	-4.926839
C	5.100525	4.377747	-5.245025
C	-4.740765	6.377700	3.423658
C	6.697614	5.621836	2.855803
C	-6.373493	4.649053	-4.543673
C	6.448436	4.147965	-4.905688
C	-6.104052	6.120711	3.177794

C	6.922240	4.388939	2.213617
C	-6.670991	3.779949	-3.477279
C	6.721496	3.245146	-3.860044
C	-6.444282	4.927638	2.512567
C	-5.804169	-2.443354	-1.743288
C	5.687239	-1.881032	2.915627
C	-5.679126	-1.511815	3.139636
C	5.529852	-2.800185	-2.161798
C	-4.487353	-2.823553	-2.042022
C	4.351687	-2.042077	3.314826
C	-4.336703	-1.792489	3.434808
C	4.173595	-3.059317	-2.413618
C	-4.264502	-4.014768	-2.747558
C	4.065071	-2.888534	4.396850
C	-4.038076	-2.649569	4.504332
C	3.819384	-4.255470	-3.056131
C	-5.333676	-4.824160	-3.119209
C	5.085619	-3.585843	5.037586
C	-5.061325	-3.237862	5.241414
C	4.797108	-5.178737	-3.419516
C	-6.657915	-4.464838	-2.801235
C	6.426494	-3.454445	4.625186
C	-6.412795	-2.990360	4.931284
C	6.160175	-4.932021	-3.162939
C	-6.872068	-3.250055	-2.123029
C	6.706914	-2.571421	3.564169
C	-6.700057	-2.100240	3.879630
C	6.505770	-3.719625	-2.535305
C	3.264853	2.252521	-2.680791
C	3.417187	3.019624	1.805977
C	3.270143	-1.338440	2.562711
C	-3.240324	-1.206721	2.616363
C	-3.351855	-1.962632	-1.601593
C	-3.227846	2.615654	-2.401913
C	3.132069	-2.106055	-1.935629
C	-3.063513	3.372495	1.812487
H	6.038961	2.601069	1.383489
H	-5.889380	2.455565	-1.958758
H	5.906201	1.945885	-2.339012
H	-5.723805	3.131155	1.552068
H	3.289928	5.394635	3.108923
H	-2.974156	4.238783	-4.539850
H	3.031584	3.951524	-4.798673
H	-2.707325	5.689641	3.193546
H	5.168259	6.913971	3.675858
H	-4.770144	5.440416	-5.760311

H	4.858717	5.061696	-6.054451
H	-4.451221	7.282558	3.951720
H	7.936488	4.096386	1.954014
H	-7.704851	3.638367	-3.172776
H	7.753121	3.037950	-3.586744
H	-7.489887	4.698844	2.322608
H	-5.967673	-1.514416	-1.206160
H	5.904305	-1.218202	2.083961
H	-5.900839	-0.838380	2.317388
H	5.797811	-1.875731	-1.659800
H	-3.244803	-4.292845	-2.997136
H	3.030627	-3.012777	4.703648
H	-2.997291	-2.847037	4.741250
H	2.768699	-4.458785	-3.239887
H	-5.142412	-5.747616	-3.659662
H	4.839911	-4.250800	5.861603
H	-4.812749	-3.905871	6.062120
H	4.500680	-6.105416	-3.904155
H	-7.886157	-2.943516	-1.879358
H	7.734354	-2.437520	3.235138
H	-7.734841	-1.878278	3.631589
H	7.550456	-3.501038	-2.329001
H	7.251949	4.640732	-5.443505
H	-7.161644	5.178599	-5.069228
H	7.220052	-4.004364	5.120652
H	6.920865	-5.653541	-3.443031
H	-7.209982	-3.457373	5.500738
H	-6.870488	6.814989	3.507032
H	-7.491177	-5.098703	-3.087254
H	7.522139	6.285977	3.094275
H	-2.015272	0.188001	-2.721759
H	2.090147	3.325183	-0.506999
H	1.073147	-0.259514	4.465286
H	0.189606	1.007650	4.087991
H	0.557574	-1.904572	-3.973315
H	-0.789707	-3.450511	2.233745
H	-1.841160	1.132710	2.908788
H	0.981523	3.009196	4.017863
H	-0.063460	0.151325	-3.988282
H	0.895798	1.336294	-4.441853
H	-0.729479	5.110546	0.850997
H	-0.651160	4.610463	-2.379427
H	0.150555	4.646308	-0.388070
O	1.143647	0.807927	1.506007
O	3.626596	-0.708326	1.517489
O	3.537972	-1.114163	-1.254548

O	3.713692	1.998374	1.111817
O	2.243733	3.365658	2.150128
O	0.149571	4.761517	0.628267
O	-1.846061	3.688256	1.984985
O	-2.031526	2.839182	-2.767097
O	-3.481806	2.311116	1.248823
O	-3.582583	1.867959	-1.436072
O	-3.588126	-0.432863	1.668385
O	-3.658809	-0.874320	-1.016593
O	-2.171753	-2.370348	-1.832814
O	-2.047269	-1.523648	2.917019
O	-1.143266	-0.881159	0.308966
O	-1.296226	0.979854	2.123573
O	0.172495	2.600778	3.676797
O	0.180177	-0.007240	4.176931
O	-0.002036	1.167530	-4.109818
O	-0.979358	2.089632	-0.156537
O	1.484478	2.592056	-0.326474
O	2.064865	2.437963	-3.051712
O	0.127062	4.222371	-1.953889
O	3.628753	1.592533	-1.657071
O	0.105717	-3.079267	2.234070
O	0.005698	-3.531901	-0.800321
O	1.341289	-1.470415	0.353053
O	2.079876	-1.437250	2.994001
O	1.919191	-2.364890	-2.213840
O	-0.171954	-1.408546	-3.575474
O	-1.427105	0.309543	-1.963134
O	1.051819	0.336325	-1.470228
Zr	-2.468651	0.690903	0.096929
Zr	0.173508	2.640830	1.568686
Zr	0.010731	-0.877202	2.027488
Zr	-0.038605	-1.464539	-1.454377
Zr	2.512458	0.459182	-0.035964
Zr	0.014521	2.111112	-1.995207
In	1.444940	-3.494976	0.637302
C	3.150592	-4.715549	0.912329
H	3.145059	-5.580480	0.240577
H	4.055630	-4.133770	0.698168
H	3.220802	-5.075715	1.944276
In	-1.739146	-4.550090	-0.991930
C	-1.484729	-6.049532	-2.505018
H	-0.663596	-6.727719	-2.240440
H	-2.380211	-6.660315	-2.671453
H	-1.211353	-5.579436	-3.458652
C	-2.984989	-4.344545	0.743009

H	-2.666637	-4.952611	1.600704
H	-2.956264	-3.289699	1.049030
H	-4.032814	-4.600177	0.542427

156
S5 (E = -4940.4028004)

C	5.617703	3.337907	2.525451
C	-5.754680	3.152321	-2.537991
C	5.613684	3.265752	-2.612276
C	-5.721036	3.270573	2.424010
C	4.275806	3.572705	2.859880
C	-4.414718	3.449039	-2.828934
C	4.270686	3.510051	-2.936419
C	-4.386770	3.568513	2.738486
C	3.963065	4.654027	3.697414
C	-4.126636	4.465913	-3.751321
C	3.968958	4.530743	-3.850329
C	-4.115319	4.622377	3.623185
C	4.968845	5.490575	4.175855
C	-5.155937	5.190310	-4.344854
C	4.982640	5.310336	-4.400650
C	-5.153759	5.380021	4.157704
C	6.318698	5.265489	3.841608
C	-6.503639	4.923740	-4.033877
C	6.332069	5.090784	-4.060570
C	-6.495705	5.103861	3.829132
C	6.621882	4.168229	3.012757
C	-6.781470	3.876668	-3.135270
C	6.626108	4.040669	-3.169608
C	-6.757962	4.023198	2.965943
C	-5.637059	-2.500640	-2.422626
C	5.695031	-2.182132	2.632714
C	-5.677360	-2.387985	2.548494
C	5.707070	-2.251808	-2.529152
C	-4.295613	-2.763990	-2.737178
C	4.360351	-2.469642	2.956711
C	-4.329729	-2.650612	2.836454
C	4.372393	-2.528780	-2.863700
C	-3.994833	-3.809632	-3.621839
C	4.091849	-3.496448	3.874844
C	-4.013093	-3.658420	3.759338
C	4.095793	-3.616884	-3.705477
C	-5.011666	-4.595252	-4.155902
C	5.131295	-4.241893	4.424537
C	-5.022068	-4.408201	4.356173
C	5.128218	-4.420179	-4.184259

C	-6.359905	-4.356134	-3.825896
C	6.473129	-3.981191	4.082773
C	-6.376662	-4.176212	4.047692
C	6.470216	-4.155927	-3.846823
C	-6.652562	-3.282208	-2.964180
C	6.733064	-2.922100	3.191210
C	-6.684083	-3.138272	3.148255
C	6.737738	-3.049737	-3.017341
C	3.197909	2.705285	-2.281732
C	3.202839	2.722884	2.272705
C	3.262335	-1.702078	2.296453
C	-3.246031	-1.886786	2.161049
C	-3.217381	-1.936452	-2.123453
C	-3.309985	2.712738	-2.155872
C	3.271945	-1.717826	-2.269234
C	-3.286342	2.766817	2.127776
H	5.852049	2.503634	1.871591
H	-5.969330	2.356609	-1.831177
H	5.842568	2.470150	-1.910300
H	-5.923060	2.446879	1.746457
H	2.922151	4.840068	3.944050
H	-3.088751	4.678193	-3.988247
H	2.928290	4.719492	-4.097393
H	-3.082638	4.835722	3.883015
H	4.705575	6.330459	4.813566
H	-4.914457	5.980343	-5.051367
H	4.725410	6.107104	-5.093774
H	-4.923966	6.197191	4.836587
H	7.655791	3.970670	2.741310
H	-7.813671	3.638229	-2.891672
H	7.660184	3.839516	-2.901092
H	-7.785535	3.780405	2.707352
H	-5.861039	-1.682474	-1.745424
H	5.897555	-1.380984	1.928958
H	-5.913679	-1.598503	1.841645
H	5.914929	-1.412018	-1.873433
H	-2.956468	-3.994343	-3.880844
H	3.058115	-3.718216	4.123543
H	-2.969502	-3.843521	3.993883
H	3.061688	-3.835847	-3.953923
H	-4.760172	-5.406167	-4.834586
H	4.900470	-5.045210	5.119481
H	-4.759171	-5.190824	5.063261
H	4.891634	-5.266375	-4.824148
H	-7.686651	-3.068218	-2.706131
H	7.759839	-2.687454	2.921960

H	-7.722677	-2.926917	2.906969
H	7.764525	-2.819754	-2.744345
H	7.121803	5.703095	-4.483769
H	-7.305187	5.495698	-4.490163
H	7.281847	-4.567967	4.506215
H	7.273565	-4.784494	-4.217260
H	-7.162167	-4.768111	4.506522
H	-7.304567	5.697164	4.243350
H	-7.152304	-4.972030	-4.239047
H	7.101956	5.918691	4.212589
H	-1.996448	0.387112	-2.806401
H	1.911245	3.342686	0.000028
H	0.946203	-1.053273	4.362204
H	0.021315	0.214172	4.092649
H	0.706520	-1.274282	-4.446099
H	-1.985377	0.388025	2.834751
H	0.713107	2.217352	4.372373
H	0.009102	0.746127	-4.066805
H	0.914228	2.036581	-4.254042
H	-1.021082	4.738526	1.550348
H	-0.839738	4.801270	-1.717173
H	-0.090919	4.533700	0.277115
O	1.060071	0.491358	1.542682
O	3.610881	-0.891413	1.381233
O	3.609699	-0.835014	-1.421326
O	3.568225	1.846018	1.429951
O	2.005116	2.951686	2.631162
O	-0.122128	4.470212	1.297164
O	-2.090647	3.105877	2.389383
O	-2.118067	3.049731	-2.440677
O	-3.634600	1.794270	1.388961
O	-3.648445	1.800371	-1.340798
O	-3.609657	-0.984353	1.345711
O	-3.592386	-0.974999	-1.383383
O	-2.012955	-2.245075	-2.381950
O	-2.045336	-2.192694	2.443491
O	-1.182279	-1.246191	-0.003797
O	-1.394535	0.408858	2.068052
O	-0.065145	1.833559	3.942322
O	0.070117	-0.804579	4.026735
O	0.016959	1.767537	-3.993166
O	-1.086374	1.889965	0.035285
O	1.338358	2.563103	0.032614
O	1.999162	2.893230	-2.655413
O	-0.057898	4.378103	-1.333890
O	3.570863	1.902170	-1.369369

O	0.087654	-3.422206	1.364266
O	0.098074	-3.428226	-1.410872
O	1.399802	-1.483731	0.000800
O	2.069000	-1.926528	2.666500
O	2.081160	-1.983561	-2.624810
O	-0.006447	-0.862329	-3.939294
O	-1.403524	0.440794	-2.042892
O	1.047093	0.524753	-1.505207
Zr	-2.516310	0.424847	0.004389
Zr	-0.009956	2.225925	1.872188
Zr	0.057430	-1.348797	1.776126
Zr	0.070743	-1.312836	-1.879735
Zr	2.462576	0.471445	-0.004723
Zr	-0.059109	2.304731	-1.746911
In	1.653086	-3.531239	-0.039460
C	3.479383	-4.597603	0.018762
H	3.551744	-5.217412	0.918965
H	3.596756	-5.243587	-0.857755
H	4.316324	-3.888595	0.028919
In	-1.465240	-3.440468	-0.048860
C	-3.314679	-4.454336	0.058435
H	-3.377204	-5.046463	0.978016
H	-4.145837	-3.738939	0.063060
H	-3.452890	-5.120434	-0.800027

174
Saturated Node (E = -5184.4805881)

C	5.663054	2.739910	2.603702
C	-5.709045	2.833044	-2.462921
C	5.659891	2.815739	-2.533972
C	-5.675664	2.808002	2.500428
C	4.323882	2.980630	2.944775
C	-4.365614	3.122354	-2.745192
C	4.319942	3.084966	-2.850915
C	-4.338114	3.081158	2.823340
C	4.023512	4.040987	3.813079
C	-4.065371	4.161909	-3.637939
C	4.030461	4.134975	-3.735084
C	-4.054667	4.105872	3.738015
C	5.038834	4.851608	4.315400
C	-5.085946	4.915069	-4.210365
C	5.053361	4.918192	-4.262739
C	-5.084364	4.859894	4.294130
C	6.386076	4.620483	3.974805
C	-6.436771	4.655420	-3.907184
C	6.400021	4.673191	-3.929127

C	-6.429335	4.609005	3.957751
C	6.676699	3.544070	3.114705
C	-6.727108	3.586231	-3.039092
C	6.681481	3.594499	-3.068769
C	-6.703910	3.556777	3.063810
C	-5.657488	-2.821884	-2.510349
C	5.675876	-2.781456	2.552001
C	-5.698116	-2.851919	2.461953
C	5.688807	-2.702641	-2.609731
C	-4.319105	-3.091757	-2.832319
C	4.337821	-3.062564	2.867590
C	-4.353739	-3.138466	2.742210
C	4.351095	-2.954277	-2.952084
C	-4.030265	-4.114908	-3.746760
C	4.057043	-4.112165	3.755788
C	-4.049200	-4.176042	3.635710
C	4.062087	-4.014369	-3.824859
C	-5.056027	-4.872895	-4.303214
C	5.087530	-4.885219	4.283785
C	-5.067060	-4.930856	4.210719
C	5.085218	-4.815556	-4.326574
C	-6.401491	-4.627640	-3.966452
C	6.432429	-4.630481	3.949661
C	-6.418750	-4.674271	3.909051
C	6.430099	-4.576824	-3.981679
C	-6.681872	-3.575620	-3.074175
C	6.705011	-3.549272	3.088957
C	-6.713731	-3.607347	3.039871
C	6.710247	-3.498173	-3.120696
C	3.237626	2.274218	-2.219768
C	3.241242	2.160620	2.333386
C	3.249039	-2.263696	2.229570
C	-3.260986	-2.368360	2.088912
C	-3.231493	-2.294964	-2.194902
C	-3.269813	2.354242	-2.093573
C	3.260012	-2.148112	-2.334396
C	-3.246949	2.284599	2.189786
H	5.887857	1.922125	1.926095
H	-5.933206	2.019876	-1.779306
H	5.879237	1.997639	-1.855193
H	-5.887070	2.006570	1.799443
H	2.984758	4.232001	4.064975
H	-3.024999	4.368782	-3.868660
H	2.992150	4.342905	-3.976607
H	-3.019650	4.299568	4.003873
H	4.785179	5.675805	4.977028

H	-4.835022	5.722237	-4.893842
H	4.805682	5.737535	-4.932634
H	-4.845268	5.654442	4.996256
H	7.708321	3.342342	2.837677
H	-7.762104	3.352954	-2.802455
H	7.713048	3.373631	-2.806161
H	-7.734162	3.333550	2.798342
H	-5.872123	-2.020991	-1.809872
H	5.887974	-1.962802	1.871601
H	-5.924965	-2.039709	1.778127
H	5.906243	-1.884562	-1.930107
H	-2.994042	-4.304204	-4.010981
H	3.020707	-4.328908	3.998004
H	-3.007919	-4.379998	3.864824
H	3.025578	-4.213993	-4.079500
H	-4.813796	-5.666817	-5.004963
H	4.847109	-5.705457	4.955315
H	-4.813555	-5.736526	4.894980
H	4.838980	-5.640158	-4.990559
H	-7.713476	-3.357082	-2.810066
H	7.734546	-3.318983	2.826568
H	-7.749706	-3.377015	2.804776
H	7.739560	-3.288156	-2.841198
H	7.196991	5.288162	-4.334528
H	-7.231434	5.249602	-4.346809
H	7.234100	-5.238611	4.356031
H	7.226176	-5.203809	-4.370063
H	-7.211265	-5.269916	4.350656
H	-7.231350	5.199548	4.388882
H	-7.200891	-5.222086	-4.397159
H	7.176787	5.253539	4.364432
O	1.243816	-0.043765	1.815643
O	3.607590	-1.430906	1.338118
O	3.608104	-1.293855	-1.461384
O	3.596568	1.304296	1.465689
O	2.046221	2.393131	2.698143
O	0.074210	3.894712	1.467969
O	-2.047373	2.601739	2.460699
O	-2.074076	2.684624	-2.368217
O	-3.606184	1.337716	1.423343
O	-3.619142	1.422533	-1.305227
O	-3.613722	-1.438525	1.299937
O	-3.595542	-1.350757	-1.427524
O	-2.030774	-2.609398	-2.463004
O	-2.064177	-2.695609	2.363046
O	-1.247164	-1.843502	-0.042795

O	-1.310077	-0.046502	1.821702
O	-0.081209	1.287838	3.935565
O	-0.078483	-1.475075	3.874970
O	-0.080016	1.470456	-3.875292
O	-1.257837	1.836742	0.041102
O	1.317177	1.844680	0.047610
O	2.041273	2.486533	-2.587530
O	0.068790	3.949450	-1.298614
O	3.600760	1.440952	-1.330907
O	0.085920	-3.952828	1.298080
O	0.094879	-3.897420	-1.468291
O	1.327752	-1.844336	-0.045575
O	2.052958	-2.484552	2.593609
O	2.066299	-2.388986	-2.697997
O	-0.068081	-1.292270	-3.935454
O	-1.306864	0.038560	-1.823082
O	1.246979	0.043732	-1.813850
Zr	-2.438390	-0.005440	-0.001425
Zr	-0.001123	1.796290	1.869458
Zr	0.000269	-1.880780	1.785898
Zr	0.012236	-1.799783	-1.869525
Zr	2.442586	0.001909	0.001895
Zr	-0.007423	1.876691	-1.785809
In	1.644713	-3.936305	-0.083647
C	3.547273	-4.857464	-0.084750
H	3.688199	-5.479393	-0.975325
H	4.327391	-4.086985	-0.082378
H	3.685732	-5.482827	0.803900
In	-1.476970	-3.976195	-0.092443
C	-3.321883	-5.004610	-0.087515
H	-3.413614	-5.642155	0.798540
H	-4.153215	-4.288906	-0.072315
H	-3.434417	-5.627886	-0.981048
In	1.499004	0.097916	-3.938598
In	-1.630762	0.084357	-3.910272
C	-3.542704	0.095404	-4.807639
H	-4.309111	0.085573	-4.023566
H	-3.691822	0.992011	-5.418540
H	-3.692250	-0.784924	-5.441714
C	3.369195	0.122736	-4.917706
H	4.173103	0.102751	-4.171211
H	3.492601	-0.748595	-5.569646
H	3.492740	1.029065	-5.520049
In	1.625201	3.938821	0.085490
In	-1.495756	3.968476	0.089971
C	3.521332	4.873416	0.086865

H	4.307899	4.109616	0.081548
H	3.653398	5.502081	-0.800453
H	3.658274	5.494305	0.978802
C	-3.343085	4.992502	0.080865
H	-3.458090	5.616900	0.973302
H	-3.434680	5.628520	-0.806306
H	-4.173034	4.275236	0.065528
In	1.493212	-0.094090	3.940687
In	-1.636500	-0.096857	3.908196
C	3.362469	-0.107602	4.921765
H	3.491629	-1.013811	5.523095
H	4.166796	-0.081477	4.175912
H	3.479453	0.763821	5.574769
C	-3.549985	-0.119518	4.802067
H	-3.701523	0.753307	5.445951
H	-4.314828	-0.101380	4.016618
H	-3.699581	-1.023464	5.401952

158

Saturated Node Upon Exposure to Water (E = -5471.8658269)

C	5.664287	2.757711	2.585402
C	-5.707671	2.816127	-2.482057
C	5.661269	2.799065	-2.552665
C	-5.674432	2.824390	2.481349
C	4.325090	3.000627	2.924817
C	-4.364249	3.103623	-2.766222
C	4.321313	3.066070	-2.871450
C	-4.336908	3.099796	2.802455
C	4.024628	4.066770	3.785975
C	-4.064046	4.137182	-3.665918
C	4.031790	4.110109	-3.762649
C	-4.053553	4.130638	3.710246
C	5.039884	4.880807	4.282875
C	-5.084652	4.886420	-4.243414
C	5.054656	4.889832	-4.295518
C	-5.083313	4.888310	4.261260
C	6.387151	4.647487	3.943877
C	-6.435470	4.628725	-3.938537
C	6.401321	4.647161	-3.960231
C	-6.428259	4.635084	3.926534
C	6.677867	3.565346	3.091027
C	-6.725765	3.565366	-3.063298
C	6.682825	3.574283	-3.092646
C	-6.702741	3.576864	3.039664
C	-5.655756	-2.838989	-2.491539
C	5.677459	-2.763877	2.570750

C	-5.696526	-2.835663	2.480852
C	5.690535	-2.719697	-2.591395
C	-4.317346	-3.110936	-2.811648
C	4.339413	-3.042941	2.888185
C	-4.352139	-3.120239	2.763062
C	4.352849	-2.973707	-2.932092
C	-4.028415	-4.140177	-3.719200
C	4.058675	-4.086581	3.783393
C	-4.047560	-4.151775	3.663514
C	4.063933	-4.039652	-3.797740
C	-5.054113	-4.901946	-4.270584
C	5.089195	-4.856009	4.316594
C	-5.065390	-4.902778	4.243546
C	5.087129	-4.844122	-4.294039
C	-6.399602	-4.654522	-3.935514
C	6.434088	-4.603434	3.980807
C	-6.417086	-4.648309	3.940124
C	6.431985	-4.602996	-3.950714
C	-6.680075	-3.596556	-3.050324
C	6.706627	-3.528008	3.112876
C	-6.712109	-3.587260	3.063797
C	6.712040	-3.518575	-3.096980
C	3.239028	2.259498	-2.234895
C	3.242520	2.176454	2.318904
C	3.250598	-2.248433	2.244775
C	-3.259416	-2.354456	2.104637
C	-3.229804	-2.309808	-2.179550
C	-3.268420	2.339962	-2.109428
C	3.261697	-2.163475	-2.319850
C	-3.245677	2.299067	2.174280
H	5.889161	1.935412	1.913304
H	-5.931801	2.007550	-1.793008
H	5.880646	1.985552	-1.868406
H	-5.885767	2.018259	1.785751
H	2.985855	4.259404	4.036553
H	-3.023681	4.342568	-3.897992
H	2.993473	4.316348	-4.005591
H	-3.018556	4.326179	3.974828
H	4.786158	5.709409	4.938950
H	-4.833759	5.688999	-4.932285
H	4.806945	5.704646	-4.970903
H	-4.844288	5.687566	4.958045
H	7.709509	3.361829	2.815388
H	-7.760753	3.333617	-2.825130
H	7.714398	3.355248	-2.828533
H	-7.732972	3.351796	2.775671

H	-5.870461	-2.033427	-1.796458
H	5.889525	-1.949793	1.884878
H	-5.923407	-2.028073	1.791585
H	5.907899	-1.897063	-1.917269
H	-2.992173	-4.331176	-3.982115
H	3.022345	-4.301760	4.027027
H	-3.006273	-4.354124	3.894021
H	3.027444	-4.241046	-4.051066
H	-4.811811	-5.700543	-4.966984
H	4.848806	-5.671739	4.993606
H	-4.811853	-5.703823	4.933205
H	4.840963	-5.673177	-4.952482
H	-7.711701	-3.376316	-2.787717
H	7.736155	-3.299419	2.848976
H	-7.748093	-3.358576	2.827132
H	7.741332	-3.306622	-2.818868
H	7.198265	5.259448	-4.369726
H	-7.230157	5.219893	-4.382161
H	7.235786	-5.208773	4.391271
H	7.228113	-5.232523	-4.334860
H	-7.209577	-5.241027	4.385693
H	-7.230324	5.228456	4.353669
H	-7.198953	-5.251895	-4.362246
H	7.177810	5.283193	4.329270
O	1.240002	-0.031804	1.811841
O	3.609012	-1.421649	1.347791
O	3.609600	-1.303381	-1.452607
O	3.597813	1.314373	1.457011
O	2.047465	2.411238	2.681958
O	0.077090	3.914188	1.442170
O	-2.046112	2.617987	2.443006
O	-2.072681	2.668467	-2.386156
O	-3.604724	1.347061	1.414232
O	-3.617606	1.413569	-1.314883
O	-3.612081	-1.429985	1.309456
O	-3.593828	-1.360516	-1.418570
O	-2.029038	-2.625853	-2.445413
O	-2.062580	-2.679681	2.380903
O	-1.237812	-1.837291	-0.031772
O	-1.308067	-0.034289	1.819670
O	-0.079500	1.312476	3.936481
O	-0.079821	-1.446639	3.895736
O	-0.081139	1.442202	-3.896046
O	-1.248752	1.830556	0.030164
O	1.318849	1.844508	0.034585
O	2.042662	2.469167	-2.603994

O	0.061722	3.951280	-1.321477
O	3.602079	1.432266	-1.340481
O	0.079610	-3.954647	1.320781
O	0.098055	-3.916665	-1.442613
O	1.329725	-1.844011	-0.032570
O	2.054510	-2.466817	2.610137
O	2.068003	-2.406766	-2.681760
O	-0.066390	-1.316673	-3.936423
O	-1.304710	0.026384	-1.820935
O	1.243275	0.031921	-1.810054
Zr	-2.466341	-0.005614	-0.001442
Zr	0.002497	1.809074	1.859174
Zr	-0.000351	-1.871920	1.800784
Zr	0.016054	-1.812445	-1.859243
Zr	2.476010	0.002089	0.001941
Zr	-0.008261	1.867830	-1.800577
In	1.633047	-3.916173	-0.056204
H	4.096926	-4.214499	0.179450
In	-1.464700	-3.952200	-0.064090
H	-3.656387	-4.881728	-0.833143
In	1.485868	0.081428	-3.918378
In	-1.621867	0.053851	-3.887857
H	-4.094041	0.141674	-4.050463
H	3.644775	-0.676576	-4.925376
In	1.613120	3.918704	0.057543
In	-1.483862	3.944483	0.061749
H	4.075034	4.233915	-0.183143
H	-3.681349	4.864523	0.825705
In	1.480016	-0.077543	3.920462
In	-1.627715	-0.066111	3.885934
H	3.633849	0.691882	4.929512
H	-4.099697	-0.162856	4.046067
O	3.370642	-4.782086	-0.117262
O	-3.199788	-4.822268	0.017945
O	-3.396133	0.001379	4.690994
O	3.215545	-0.168387	4.790013
O	-3.221448	4.809148	-0.023904
O	3.345551	4.794816	0.118418
O	3.222289	0.181538	-4.785166
O	-3.389448	-0.024367	-4.693814

$InMe_3$ Transition States

163

TS1 (E = -4980.6453719)

C	4.872542	-3.965337	-2.792386
C	-6.421900	-2.290611	2.170965
C	4.727224	-4.511981	2.314621

C	-6.261170	-1.815534	-2.767155
C	3.521012	-3.906037	-3.163210
C	-5.167996	-2.862735	2.432863
C	3.353064	-4.540944	2.596116
C	-4.994869	-2.314962	-3.106260
C	3.041446	-4.802220	-4.130373
C	-5.098283	-4.018745	3.224440
C	2.842711	-5.590609	3.374465
C	-4.893903	-3.286730	-4.112475
C	3.891524	-5.746591	-4.701199
C	-6.259916	-4.606375	3.716166
C	3.680008	-6.604590	3.831574
C	-6.036656	-3.769460	-4.744284
C	5.249108	-5.816801	-4.331710
C	-7.526325	-4.059812	3.430614
C	5.056448	-6.599036	3.531248
C	-7.314896	-3.291507	-4.393991
C	5.722450	-4.902273	-3.371250
C	-7.581169	-2.879106	2.666434
C	5.563929	-5.522011	2.779255
C	-7.401296	-2.292757	-3.405688
C	-5.270792	3.215285	2.756779
C	5.959543	1.417386	-2.215278
C	-5.181434	3.710588	-2.190246
C	5.828827	0.862451	2.915494
C	-3.913897	3.186287	3.111432
C	4.710142	1.983531	-2.511063
C	-3.800460	3.752237	-2.433513
C	4.557699	1.339143	3.271864
C	-3.454014	4.044233	4.120832
C	4.661356	3.145094	-3.297058
C	-3.277541	4.787642	-3.222273
C	4.459207	2.350367	4.239741
C	-4.325925	4.934287	4.740467
C	5.835482	3.746105	-3.742602
C	-4.114257	5.777268	-3.729191
C	5.606058	2.885439	4.821845
C	-5.684612	4.990001	4.373460
C	7.096271	3.202648	-3.425817
C	-5.497093	5.764336	-3.461798
C	6.886790	2.420155	4.464230
C	-6.142361	4.100239	3.383355
C	7.131545	2.014375	-2.670246
C	-6.015756	4.700640	-2.699988
C	6.972689	1.391482	3.506257
C	2.465421	-3.478909	2.038155

C	2.604066	-2.949282	-2.483396
C	3.471109	1.358644	-1.958812
C	-2.895256	2.725488	-1.849983
C	-2.986997	2.252237	2.409222
C	-3.927561	-2.267489	1.864785
C	3.346106	0.823126	2.573447
C	-3.784901	-1.808426	-2.394334
H	5.235484	-3.273552	-2.038617
H	-6.466310	-1.389818	1.566467
H	5.118523	-3.693879	1.718185
H	-6.329706	-1.056241	-1.994406
H	1.991958	-4.761579	-4.405816
H	-4.124202	-4.446173	3.440941
H	1.778122	-5.612019	3.588584
H	-3.910188	-3.654504	-4.389068
H	3.498646	-6.440442	-5.439853
H	-6.188092	-5.506551	4.321267
H	3.260906	-7.417523	4.418871
H	-5.939599	-4.527364	-5.517339
H	6.766409	-4.933369	-3.069814
H	-8.544688	-2.426411	2.446592
H	6.624949	-5.484705	2.545338
H	-8.374578	-1.897057	-3.126641
H	-5.619905	2.540102	1.981914
H	5.991137	0.513902	-1.614576
H	-5.579069	2.899244	-1.588271
H	5.899502	0.083755	2.162462
H	-2.407647	4.001279	4.408363
H	3.693441	3.582423	-3.524036
H	-2.211122	4.803446	-3.424397
H	3.475460	2.725253	4.505724
H	-3.951142	5.597132	5.516106
H	5.776206	4.655879	-4.334502
H	-3.691749	6.577035	-4.332054
H	5.508800	3.677597	5.559749
H	-7.189899	4.113731	3.093182
H	8.089653	1.563299	-2.424520
H	-7.082261	4.657494	-2.494385
H	7.947972	1.010153	3.214496
H	5.708028	-7.393163	3.881259
H	-8.432179	-4.524359	3.806693
H	8.010890	3.676373	-3.767422
H	7.779881	2.840179	4.915516
H	-6.147172	6.542058	-3.849660
H	-8.205651	-3.670852	-4.884395
H	-6.363314	5.687554	4.853775

H	5.910747	-6.554121	-4.774861
H	-2.219060	-0.341828	2.831711
H	1.140788	-3.592123	-0.310585
H	1.143089	1.420659	-4.031559
H	-0.005646	0.319282	-3.991645
H	0.728650	0.619044	4.561597
H	-0.122157	4.163455	-1.274271
H	-0.338276	3.661424	2.340310
H	-2.052246	0.311428	-2.836396
H	2.294807	1.949945	0.406144
H	0.316244	-1.741689	-4.515358
H	-0.349587	-1.150310	4.005606
H	0.297998	-2.603852	4.067168
H	-1.931438	-4.204429	-2.039817
H	-1.858052	-4.689161	1.197131
H	-1.022165	-4.331252	-0.741385
O	0.882513	-0.432676	-1.457297
O	3.638218	0.393283	-1.148541
O	3.542603	0.001398	1.625382
O	3.097753	-2.263084	-1.535984
O	1.395991	-2.908237	-2.876062
O	-1.006116	-4.146115	-1.747644
O	-2.664539	-2.330496	-2.685401
O	-2.826431	-2.851236	2.113926
O	-3.973000	-0.887462	-1.540097
O	-4.069245	-1.217643	1.165103
O	-3.441803	1.814735	-1.154906
O	-3.508611	1.475810	1.550331
O	-1.754784	2.301006	2.711918
O	-1.650998	2.836087	-2.084004
O	-0.967884	1.262681	0.206219
O	-1.509291	0.122867	-2.057487
O	-0.380747	-1.265646	-4.040914
O	0.210656	1.296263	-3.788360
O	-0.521482	-2.143599	3.819804
O	-1.541407	-1.637501	-0.197297
O	0.746523	-2.709821	-0.252058
O	1.241871	-3.485600	2.376790
O	-0.999094	-4.377966	0.876429
O	3.005822	-2.654978	1.235059
O	0.678457	3.623811	-1.186766
O	0.522030	3.312408	2.051941
O	1.551575	1.336024	0.295685
O	2.350478	1.842626	-2.307816
O	2.213648	1.259704	2.950894
O	-0.079844	0.436186	4.061615

O	-1.632682	-0.391994	2.063031
O	0.777287	-0.808428	1.477774
Zr	-2.666848	0.080365	0.014778
Zr	-0.475647	-1.908560	-2.034699
Zr	0.168679	1.548507	-1.486763
Zr	0.112403	1.122938	2.073246
Zr	2.242442	-0.915114	0.051054
Zr	-0.645653	-2.397140	1.527126
In	2.386288	4.646918	-0.449931
H	1.045939	4.336809	1.588334
C	1.288869	5.736081	1.389488
H	1.168225	5.808845	2.478819
H	2.136234	6.423275	1.220171
H	0.407169	6.225559	0.950634
C	3.880625	3.496344	0.593434
H	4.806506	4.088495	0.578482
H	3.582432	3.412122	1.647372
H	4.174681	2.498802	0.244826
C	2.659830	6.265311	-1.831220
H	3.706954	6.585663	-1.899307
H	2.339408	5.980375	-2.841207
H	2.067143	7.141701	-1.538309

158

TS2 (E = -4940.1780293)

C	5.231109	3.713709	2.538639
C	-6.079392	2.524063	-2.527058
C	5.231897	3.667566	-2.599388
C	-6.054914	2.619689	2.435484
C	3.873569	3.824245	2.874091
C	-4.771930	2.942461	-2.816321
C	3.872176	3.790808	-2.922443
C	-4.753029	3.035718	2.751623
C	3.464416	4.868510	3.717081
C	-4.577492	3.985920	-3.733494
C	3.478887	4.784581	-3.831190
C	-4.577890	4.105332	3.641714
C	4.390416	5.790317	4.199892
C	-5.668402	4.617069	-4.323460
C	4.417568	5.655606	-4.377417
C	-5.680531	4.763036	4.179953
C	5.754998	5.690177	3.864669
C	-6.986298	4.227897	-4.014006
C	5.781456	5.557516	-4.038294
C	-6.992043	4.368080	3.849819
C	6.156082	4.629126	3.030284

C	-7.167798	3.155408	-3.120770
C	6.169746	4.533857	-3.152649
C	-7.155589	3.272494	2.981112
C	-5.449966	-3.095494	-2.440430
C	5.808360	-1.777086	2.617836
C	-5.498619	-3.012190	2.531193
C	5.824907	-1.819182	-2.544316
C	-4.090280	-3.234625	-2.756128
C	4.505334	-2.186001	2.940202
C	-4.132633	-3.153103	2.817948
C	4.520705	-2.214278	-2.880406
C	-3.696289	-4.244184	-3.646087
C	4.331294	-3.237557	3.853073
C	-3.725665	-4.132717	3.735761
C	4.343556	-3.318662	-3.727763
C	-4.637930	-5.115994	-4.184262
C	5.434200	-3.888525	4.399092
C	-4.662344	-4.973864	4.328654
C	5.444362	-4.022656	-4.210499
C	-6.002178	-5.001710	-3.853206
C	6.746773	-3.505572	4.058821
C	-6.032491	-4.864015	4.021192
C	6.757008	-3.639600	-3.871561
C	-6.390653	-3.963109	-2.986076
C	6.909365	-2.422772	3.172688
C	-6.433008	-3.853650	3.127009
C	6.923473	-2.517944	-3.036431
C	2.876952	2.888779	-2.272031
C	2.881812	2.883652	2.282508
C	3.342051	-1.517919	2.283580
C	-3.122814	-2.290869	2.146419
C	-3.091236	-2.315984	-2.137902
C	-3.604793	2.305945	-2.146809
C	3.351522	-1.509534	-2.281818
C	-3.584694	2.340186	2.136917
H	5.539867	2.907434	1.880574
H	-6.220813	1.708596	-1.824325
H	5.532173	2.892426	-1.901439
H	-6.181697	1.784526	1.753726
H	2.411008	4.958208	3.964534
H	-3.563194	4.292577	-3.969211
H	2.425314	4.879504	-4.077418
H	-3.568701	4.410055	3.902750
H	4.052338	6.599642	4.841835
H	-5.499745	5.429309	-5.025917
H	4.088961	6.429295	-5.066510

H	-5.525501	5.594210	4.863011
H	7.203547	4.527449	2.757961
H	-8.174064	2.823182	-2.878513
H	7.217886	4.425875	-2.885034
H	-8.157022	2.938901	2.721165
H	-5.746933	-2.304439	-1.759103
H	5.937214	-0.957321	1.918188
H	-5.805746	-2.243793	1.828340
H	5.956035	-0.967351	-1.884308
H	-2.645547	-4.332724	-3.905902
H	3.321993	-3.553347	4.100514
H	-2.669515	-4.223678	3.969488
H	3.333463	-3.629167	-3.977445
H	-4.314220	-5.897326	-4.867030
H	5.277354	-4.712971	5.089913
H	-4.329370	-5.733022	5.031784
H	5.285213	-4.883550	-4.854712
H	-7.439791	-3.845019	-2.727067
H	7.910562	-2.094684	2.904759
H	-7.486563	-3.736057	2.886676
H	7.925289	-2.197252	-2.762145
H	6.512311	6.241010	-4.458278
H	-7.836531	4.727176	-4.467474
H	7.605480	-4.018792	4.479372
H	7.613885	-4.190896	-4.245093
H	-6.760973	-5.526980	4.476911
H	-7.851200	4.883537	4.266949
H	-6.735648	-5.684771	-4.269581
H	6.475969	6.409776	4.239062
H	-2.058880	0.133559	-2.840959
H	1.542306	3.393271	0.015259
H	1.006164	-1.119862	4.233647
H	-0.052520	0.048113	4.058740
H	0.825813	-1.272241	-4.332309
H	-0.536661	-4.039250	1.922743
H	-0.535696	-4.000963	-1.948449
H	-2.043505	0.108975	2.863152
H	2.390905	-2.634378	-0.003258
H	0.455540	2.129156	4.367009
H	-0.108640	0.624627	-4.033610
H	0.670332	1.997326	-4.246168
H	-1.513312	4.496997	1.564346
H	-1.339900	4.593418	-1.699417
H	-0.565438	4.393587	0.292606
O	0.954816	0.446214	1.512743
O	3.615544	-0.674216	1.372681

O	3.608458	-0.603885	-1.429462
O	3.324757	2.047974	1.435364
O	1.668441	3.001222	2.641974
O	-0.590370	4.324776	1.312413
O	-2.424585	2.784794	2.400395
O	-2.448432	2.750917	-2.429791
O	-3.843595	1.343768	1.393321
O	-3.858932	1.362363	-1.336629
O	-3.567046	-1.420961	1.335794
O	-3.551641	-1.396213	-1.393153
O	-1.864034	-2.512560	-2.398845
O	-1.899373	-2.487893	2.428482
O	-1.068300	-1.289132	-0.021140
O	-1.487526	0.177815	2.073793
O	-0.283360	1.678757	3.932493
O	0.085207	-0.955936	3.970173
O	-0.193853	1.646231	-3.973384
O	-1.323999	1.702728	0.040459
O	1.046631	2.562352	0.042299
O	1.666017	2.969291	-2.644850
O	-0.515759	4.250714	-1.324016
O	3.321296	2.118322	-1.363842
O	0.303236	-3.657432	1.622862
O	0.318319	-3.640407	-1.660972
O	1.443488	-1.659447	-0.008818
O	2.174074	-1.851378	2.653141
O	2.189564	-1.879995	-2.639722
O	0.018165	-0.968292	-3.894151
O	-1.496932	0.228989	-2.058649
O	0.939156	0.491081	-1.469359
Zr	-2.614901	0.087581	-0.002645
Zr	-0.275924	2.095555	1.867856
Zr	0.079173	-1.444989	1.683874
Zr	0.100481	-1.405468	-1.819757
Zr	2.361636	0.575994	-0.005906
Zr	-0.330976	2.185433	-1.730418
In	1.231460	-4.474142	-0.030060
C	3.350896	-3.567035	0.004311
H	4.035886	-2.709423	-0.009166
H	3.631824	-4.117198	0.914440
H	3.646445	-4.148935	-0.881392
C	1.421984	-6.594073	-0.008451
H	0.446667	-7.093100	0.017264
H	1.950422	-6.950821	-0.899665
H	1.986795	-6.929208	0.868776

160
TS3 (E = -5021.3192921)

C	4.737841	5.085066	1.500389
C	-6.266746	1.453090	-3.050633
C	4.903004	3.544420	-3.398650
C	-6.405476	2.992025	1.666251
C	3.366009	5.165228	1.782013
C	-4.991180	1.885364	-3.443412
C	3.548482	3.444655	-3.750377
C	-5.154163	3.597924	1.853607
C	2.843387	6.368281	2.280066
C	-4.857694	2.629709	-4.624914
C	3.100660	4.090752	-4.912314
C	-5.098566	4.891888	2.391672
C	3.672090	7.470585	2.476251
C	-5.979378	2.960212	-5.379292
C	3.978449	4.846070	-5.685071
C	-6.269423	5.575278	2.708155
C	5.050046	7.401024	2.191843
C	-7.268413	2.560498	-4.975952
C	5.334479	4.974843	-5.325329
C	-7.531635	4.984314	2.501698
C	5.565789	6.183764	1.706887
C	-7.385835	1.782914	-3.808638
C	5.780586	4.293103	-4.176750
C	-7.574190	3.673082	1.991242
C	-5.164613	-3.816455	-1.318491
C	5.777293	-0.068738	3.187448
C	-5.375409	-2.293223	3.410323
C	5.958559	-1.611132	-1.735764
C	-3.788863	-3.917779	-1.573167
C	4.504341	-0.482130	3.608999
C	-4.012016	-2.220273	3.732564
C	4.703824	-2.203294	-1.947859
C	-3.282791	-5.102955	-2.126043
C	4.391955	-1.233401	4.788983
C	-3.552054	-2.849031	4.899075
C	4.647806	-3.517926	-2.435371
C	-4.129596	-6.175187	-2.389886
C	5.528645	-1.594495	5.507208
C	-4.431845	-3.562117	5.707710
C	5.819040	-4.229399	-2.685233
C	-5.508291	-6.093341	-2.113604
C	6.813870	-1.210162	5.076199
C	-5.796099	-3.671037	5.374762
C	7.083119	-3.647099	-2.466870

C	-6.010592	-4.886781	-1.590701
C	6.911363	-0.422400	3.912562
C	-6.252986	-3.005551	4.221855
C	7.127411	-2.320557	-1.996139
C	2.613764	2.685054	-2.869191
C	2.476803	4.007426	1.486941
C	3.309516	-0.142406	2.779702
C	-3.058464	-1.502747	2.843166
C	-2.890792	-2.771592	-1.247325
C	-3.795333	1.579779	-2.611040
C	3.460813	-1.463552	-1.587746
C	-3.911616	2.861865	1.475983
H	5.134461	4.153451	1.108924
H	-6.360167	0.868409	-2.140557
H	5.246183	3.036712	-2.502769
H	-6.439408	1.986591	1.258433
H	1.778956	6.430483	2.485158
H	-3.866291	2.944853	-4.935087
H	2.051036	4.014100	-5.180770
H	-4.127600	5.349438	2.556994
H	3.246516	8.397755	2.851262
H	-5.858568	3.544365	-6.288025
H	3.606902	5.352411	-6.572201
H	-6.207062	6.579849	3.118523
H	6.626099	6.102372	1.481495
H	-8.367268	1.446052	-3.484681
H	6.825242	4.363059	-3.884048
H	-8.535009	3.189057	1.835457
H	-5.548923	-2.891490	-0.900266
H	5.857736	0.519799	2.279000
H	-5.724684	-1.793986	2.511694
H	5.996080	-0.595767	-1.353604
H	-2.220726	-5.167897	-2.343308
H	3.405941	-1.553374	5.113066
H	-2.499809	-2.772012	5.154432
H	3.676077	-3.977757	-2.588148
H	-3.719435	-7.088892	-2.812204
H	5.420998	-2.192593	6.408449
H	-4.057625	-4.050138	6.604024
H	5.753892	-5.251329	-3.049776
H	-7.073546	-4.793788	-1.382856
H	7.888901	-0.097416	3.565247
H	-7.304705	-3.058895	3.952393
H	8.089262	-1.844607	-1.822862
H	6.017305	5.569540	-5.923480
H	-8.143457	2.826955	-5.559997

H	7.699566	-1.498718	5.632897
H	7.995030	-4.203409	-2.658262
H	-6.479423	-4.235557	6.001078
H	-8.444130	5.518987	2.745264
H	-6.167639	-6.931503	-2.315250
H	5.695149	8.260623	2.342584
H	-2.079904	-0.544263	-2.621455
H	1.169637	3.708184	-0.837756
H	0.877704	0.622037	4.538575
H	-0.264114	1.595379	4.011560
H	0.985695	-2.048525	-3.633599
H	-0.124982	-3.201589	2.729728
H	-0.084957	-4.319253	0.063600
H	-2.238664	1.108477	2.836272
H	0.052479	3.699873	3.689220
H	-0.130011	-0.243708	-3.908791
H	0.551869	1.065156	-4.498455
H	-2.011174	4.955788	0.302163
H	-1.739261	4.110942	-2.847794
H	-1.019891	4.561618	-0.876203
O	0.772279	1.299659	1.468730
O	3.538514	0.420518	1.662931
O	3.612989	-0.329453	-1.036800
O	3.015416	3.004788	0.923943
O	1.247222	4.114365	1.790161
O	-1.070831	4.792224	0.119085
O	-2.802940	3.467174	1.602830
O	-2.672963	2.025631	-3.006004
O	-4.062653	1.672240	1.050299
O	-3.993712	0.893995	-1.558340
O	-3.550276	-0.950842	1.807860
O	-3.452359	-1.720524	-0.800922
O	-1.644347	-2.924508	-1.432146
O	-1.832354	-1.498042	3.176303
O	-1.039250	-0.989605	0.500165
O	-1.654670	0.989130	2.073574
O	-0.631007	3.075393	3.405406
O	-0.042446	0.623690	4.226305
O	-0.294302	0.736822	-4.150394
O	-1.547924	1.852410	-0.327819
O	0.742377	2.882489	-0.567953
O	1.412636	2.543529	-3.255339
O	-0.907633	3.958353	-2.376126
O	3.093436	2.256040	-1.772867
O	0.637584	-2.609425	2.658102
O	0.742392	-3.505199	-0.283901

O	1.497141	-1.009041	0.597171
O	2.163192	-0.458099	3.224924
O	2.346357	-2.025863	-1.826984
O	0.134212	-1.725162	-3.305247
O	-1.537974	-0.177269	-1.908466
O	0.850182	0.460670	-1.420808
Zr	-2.698829	0.181671	0.096722
Zr	-0.594402	2.860860	1.308329
Zr	0.034065	-0.516744	2.202368
Zr	0.164502	-1.519819	-1.194178
Zr	2.214532	1.099428	-0.024901
Zr	-0.545926	1.887180	-2.158163
In	2.103055	-2.866151	1.165765
C	4.053832	-3.602729	1.511487
H	4.387627	-4.240248	0.685771
H	4.753916	-2.762358	1.594315
H	4.108872	-4.181177	2.439889
In	0.925787	-5.372889	-1.398999
C	2.603761	-6.411197	-0.547100
H	2.614527	-6.309673	0.546371
H	2.577314	-7.485324	-0.768997
H	3.563737	-6.031579	-0.921192
C	0.237739	-5.190001	-3.412263
H	-0.366934	-6.050321	-3.726588
H	-0.367992	-4.282746	-3.521535
H	1.082840	-5.118595	-4.109370
C	-0.791124	-5.572617	0.302778
H	-1.653295	-4.974345	0.634988
H	-1.274606	-6.363605	-0.294896
H	-0.368134	-6.066136	1.189786

161
TS4 (E = -4980.8393947)

C	5.689509	3.282111	2.552289
C	-5.678247	3.346746	-2.524514
C	5.690314	3.246022	-2.585819
C	-5.648352	3.429595	2.438228
C	4.351882	3.539853	2.886925
C	-4.332575	3.619980	-2.812111
C	4.352557	3.517903	-2.909671
C	-4.309087	3.699757	2.756633
C	4.058596	4.621000	3.731693
C	-4.024242	4.637827	-3.726843
C	4.071248	4.550479	-3.816719
C	-4.018852	4.742410	3.648588
C	5.079408	5.435037	4.217075

C	-5.038972	5.385668	-4.316376
C	5.100125	5.314628	-4.360463
C	-5.043449	5.515764	4.187303
C	6.425175	5.186851	3.882703
C	-6.391837	5.142422	-4.008723
C	6.444760	5.067260	-4.020489
C	-6.389971	5.267298	3.855362
C	6.708593	4.089891	3.046491
C	-6.690462	4.094516	-3.117791
C	6.717854	4.005567	-3.136609
C	-6.671539	4.197851	2.984323
C	-5.667477	-2.308098	-2.448729
C	5.662511	-2.239021	2.620862
C	-5.711630	-2.229512	2.523013
C	5.679447	-2.272766	-2.541350
C	-4.330865	-2.594326	-2.763934
C	4.322254	-2.503531	2.941408
C	-4.369544	-2.519553	2.810559
C	4.340184	-2.522142	-2.879261
C	-4.048807	-3.639435	-3.655346
C	4.033313	-3.531496	3.852013
C	-4.073096	-3.539591	3.726686
C	4.044110	-3.598904	-3.728960
C	-5.079643	-4.401956	-4.196004
C	5.057844	-4.300266	4.397568
C	-5.096760	-4.274349	4.317160
C	5.061766	-4.418178	-4.212264
C	-6.423525	-4.139741	-3.865770
C	6.404769	-4.062559	4.059083
C	-6.446362	-4.014670	4.008864
C	6.408105	-4.181681	-3.871544
C	-6.696899	-3.066539	-2.996847
C	6.685720	-3.002348	3.175260
C	-6.733055	-2.964839	3.116411
C	6.695459	-3.086575	-3.034026
C	3.263978	2.728923	-2.261839
C	3.263755	2.714599	2.292619
C	3.239694	-1.710965	2.285226
C	-3.270420	-1.771203	2.141949
C	-3.237164	-1.790690	-2.143921
C	-3.242477	2.858222	-2.143021
C	3.254517	-1.694831	-2.280123
C	-3.222681	2.881182	2.141843
H	5.908855	2.448161	1.892838
H	-5.908727	2.550300	-1.823535
H	5.903297	2.441344	-1.889202

H	-5.865069	2.614626	1.754690
H	3.021083	4.824931	3.978515
H	-2.982251	4.832127	-3.961159
H	3.034627	4.760571	-4.063566
H	-2.982641	4.934393	3.911016
H	4.831270	6.275257	4.860387
H	-4.781773	6.175928	-5.017063
H	4.858813	6.120945	-5.048249
H	-4.799092	6.323676	4.872154
H	7.738915	3.874751	2.774770
H	-7.727273	3.873908	-2.876979
H	7.747624	3.783050	-2.868405
H	-7.703198	3.976321	2.722931
H	-5.876791	-1.490611	-1.766038
H	5.880967	-1.436931	1.922967
H	-5.932155	-1.430779	1.821474
H	5.902329	-1.441662	-1.879526
H	-3.013802	-3.841900	-3.914530
H	2.995280	-3.735442	4.098039
H	-3.033467	-3.746001	3.961043
H	3.006357	-3.796557	-3.980045
H	-4.842682	-5.212702	-4.880097
H	4.811061	-5.103927	5.086605
H	-4.849533	-5.066728	5.019014
H	4.810025	-5.255254	-4.858334
H	-7.727074	-2.834876	-2.738410
H	7.717065	-2.785251	2.908764
H	-7.767185	-2.732226	2.875503
H	7.726074	-2.877938	-2.758322
H	7.246418	5.667498	-4.438530
H	-7.181898	5.732592	-4.461838
H	7.201758	-4.667451	4.479259
H	7.199894	-4.822695	-4.245525
H	-7.243449	-4.594830	4.462684
H	-7.187991	5.872855	4.272868
H	-7.226909	-4.737656	-4.284086
H	7.220174	5.822533	4.259102
H	-1.977317	0.508811	-2.803877
H	1.987134	3.373911	0.023489
H	0.945235	-1.032460	4.312963
H	0.035068	0.254521	4.087320
H	0.703166	-1.192802	-4.425541
H	-0.315008	-4.448459	1.397696
H	-1.965243	0.471826	2.843302
H	0.766419	2.241841	4.380294
H	0.038573	0.828712	-4.050943

H	0.968154	2.104357	-4.237323
H	-0.921661	4.825128	1.576666
H	-0.734046	4.892517	-1.687936
H	0.003988	4.604478	0.300538
O	1.074189	0.527848	1.543629
O	3.604723	-0.900389	1.376141
O	3.608097	-0.824348	-1.425785
O	3.613420	1.837034	1.444024
O	2.070217	2.963542	2.651363
O	-0.029242	4.536944	1.321921
O	-2.021698	3.196139	2.406599
O	-2.044329	3.174462	-2.424078
O	-3.589449	1.921670	1.390789
O	-3.599471	1.945571	-1.332211
O	-3.616679	-0.855462	1.329616
O	-3.596655	-0.829114	-1.391899
O	-2.039255	-2.120657	-2.403427
O	-2.076523	-2.101868	2.424139
O	-1.182015	-1.156547	-0.004749
O	-1.378196	0.496972	2.073713
O	-0.020285	1.877695	3.948403
O	0.064658	-0.763224	4.004310
O	0.067310	1.850596	-3.973955
O	-1.037102	1.975507	0.048480
O	1.399964	2.604759	0.051854
O	2.069523	2.942157	-2.635571
O	0.037875	4.452632	-1.303183
O	3.620411	1.912690	-1.354858
O	0.122901	-3.405117	1.378436
O	0.034793	-3.373320	-1.433702
O	1.379580	-1.465984	-0.000310
O	2.041775	-1.915598	2.653320
O	2.059448	-1.935284	-2.639272
O	-0.012866	-0.773444	-3.929009
O	-1.384109	0.547439	-2.039566
O	1.063683	0.572324	-1.485978
Zr	-2.497525	0.525115	0.002520
Zr	0.035784	2.293713	1.883431
Zr	0.025224	-1.260728	1.742181
Zr	0.033341	-1.241647	-1.870002
Zr	2.487132	0.493221	-0.001473
Zr	-0.004348	2.381407	-1.728617
In	1.640342	-3.495400	-0.144565
C	3.418747	-4.631571	-0.059530
H	3.575851	-5.199210	-0.982510
H	4.278049	-3.964513	0.079536

H	3.394882	-5.334837	0.780074
In	-1.554636	-3.608336	-0.143136
C	-3.633603	-4.023092	-0.028700
H	-3.934994	-4.666407	-0.864045
H	-3.806395	-4.574893	0.902415
H	-4.274646	-3.137045	-0.032644
C	-0.951977	-5.771416	0.898755
H	-0.047177	-6.333257	1.181207
H	-1.732624	-6.049947	1.620502
H	-1.253613	-6.232931	-0.057639

Full Citation for Reference 45: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revisions A.02, B.01, and C.01*; Gaussian, Inc.: Wallingford, CT, 2010.