

Supplementary Information: Computational Details and Results

Organozinc hydroxylamides –

On the bulk-dependent interplay of nuclearity, structure and dynamics

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Introduction

General Information

This supplementary information provides a detailed background to the computations of the parent publication. It outlists the results from the individual calculations on all chemical entities of interest, *i.e.* the coordinates of fully converged geometries of all these species as addressed at different levels of theory. Furthermore, insight is given into the specific reasonings behind the different computational approaches at a breadth unsuitable within the scope and conciseness of the main manuscript itself.

The first chapter of the computational work focuses on the coordination isomerism at the central Zn atom of the pentazinc complexes $Zn(RZn)_4(O-NR'_2)_6$ between the tetra- and hexacoordinate, *i.e.* fenestranoïd and octahedroid aggregation motifs **A** and **B**, respectively (see main manuscript, Scheme 1, upper part).^[1] Concerning this isomerism, a decreasing energy barrier with growing size/ α -branch of the zinc-bound alkyl residues was initially observed with the O-NMe₂-substituted species $Zn(RZn)_4(O-NMe_2)_6$ (**3–6**; R = Me, Et, *i*Pr and *t*Bu) by ¹H NMR spectroscopy (stacked NMR plot, see main manuscript, Fig. 1).

The second chapter deals with judging on the likelihood of the two most apparent pathways of aggregate conversion from the pentanuclear, Zn-centered species $Zn(RZn)_4(O-NR'_2)_6$ (dynamic between motifs **A** and **B**) to their tetranuclear analogues $(RZn)_4(O-NR'_2)_4$ which do not build around a central metal atom, since an example of the latter species (**13**; R = Me, R' = Et; tetrahedroid motif **D**) was obtained from the reaction of excess R₂Zn with HO-NR'₂ in the presence of an excess of a secondary amine, HNR"₂ (R" = *i*Pr) under reflux (see main manuscript, experimental section and Fig. 5, Tables 3 and 6). Particular attention herein was thus paid on the assumable role of the excess R₂Zn as a reaction partner in an isodesmic transformation, with the bulky amine merely acting passively as a polar co-solvent; alternatively though, the latter could actively serve as a competitive complexation agent, likely interconnected with hydroxylamine ligands via hydrogen bonding.

Methodical Details

Geometry optimisations were carried out using the Turbomole^[2] program package, Version 5.10, employing Turbomole's DSCF^[3] and RI-DFT^[4–6] program decks. The DFT^[7,8] calculations were done with the PBE^[9–13] functional and a multipole-accelerated RI-method utilising the 'RI two-electron-integral' evaluation routine, and a standard grid of M4 size.^[6,14] The all-electron SV(P) basis sets^[15] (def2-TZVP^[16] plus auxiliary basis) for all elements including Zn were employed, since relativistic effects are expected to be negligible. For all geometry optimisation procedures, redundant internal coordinates were used.^[17] In order to characterise each converged geometry as a local minimum on the Potential Energy Surface (PES), the three lowest eigenvalues of its Hessian were determined by the Lowest Eigenvalue Search (LES) procedure, as implemented in Turbomole's Aoforce deck.^[18,19]

In addition, for all molecular geometries featured herein, their electrostatic interaction with a solvent medium was considered by comparing the individual relative energies with and without the COSMO solvation model,^[20] which addresses such effects well. One possible inaccuracy that may result at applying COSMO is that "textured" structures in the surface polarity of rather crowded molecules may end up being accounted for at a sub-optimal level of precision. As the program constructs a "supersurface" of a molecule by combining the spherical surfaces about the individual atoms, "polar spots" expected to exist on that supersurface may thus accidentally be "swallowed" underneath the perimeter of bulky, unpolar regiments. Though this phenomenon is exactly the one assumed to effect the experimentally observed behaviour of the complexes $\text{Zn}(\text{RZn})_4(\text{O}-\text{NMe}_2)_6$ (**3–6**), the associated values obtained by computations may suffer from some uncertainty at turning to bulkier peripheral groups, *i.e.* dipole interactions with the "shell" of solvent molecules may be under- or overestimated in certain embodiments. Nevertheless to our view, the COSMO solvation model provides the most efficient approach to factor in solvent effects at judging on the stabilities of the aggregation motifs **A** and **B** relative to one another.

Starting Geometries

As the starting points for the calculations, atomic coordinates obtained from crystal structure determinations were used whenever possible. Thus for the $\text{O}-\text{NMe}_2$ complexes $\text{Zn}(\text{RZn})_4(\text{O}-\text{NMe}_2)_6$ (**3–6**) featured in Chapter 1, the starting geometries were constructed by mutual replacement of β -methyl groups by hydrogen atoms, where needed, from the solid-state structures of $\text{Zn}(\text{MeZn})_4(\text{O}-\text{NMe}_2)_6^{[1]}$ (**3**), $\text{Zn}(\text{EtZn})_4(\text{O}-\text{NEt}_2)_6^{[1]}$ (**8**) and $\text{Zn}(\text{iPrZn})_4(\text{O}-\text{NEt}_2)_6$ (**9**; main manuscript, Fig. 2, Table 2) for the four RZn analogues in aggregation motif **A** (**3-A–6-A**); alike, the crystal structure of $\text{Zn}(\text{iPrZn})_4(\text{O}-\text{NMe}_2)_6^{[1]}$ (**5**) was used as the starting point for the four homologues in motif **B** (**3-B–6-B**). With each of the geometries, substituent conformation effects were addressed by comparing all possible RZn rotamers to one another during optimisation; along suggestions from crystallography, this was done whilst maintaining that pairs of RZn groups "opposite to one another" resided in the same rotameric form (molecular C₂-symmetry). Each optimisation was then finalised towards its end without this symmetry restraint, as a deliberate test run on the species $\text{Zn}(\text{EtZn})_4(\text{O}-\text{NEt}_2)_6$ with a tetracoordinated central zinc atom (**4-A**) had revealed that the relative energies obtained were near identical, with and without such restraining.

The optimisation of the key molecule of Chapter 2, the minimum-alkylated tetranuclear hydroxylamide $(\text{MeZn})_4(\text{O}-\text{NMe}_2)_4$ (**13-Me**), was approached similarly. As the starting point, the coordinates of its $\text{O}-\text{NEt}_2$ homologue **13** were taken, and the ethyl residues shortened to methyl. Here, applying symmetry restraints was judged unnecessary: First, compound **13** adopts the tetrahedroid motif **D** which has no element of higher symmetry, and second, the all-methyl substituent pattern of **13-Me** renders rotamer-based energy discrepancies from different positionings of hydrogen atoms relative to one another negligible.

At accessing a likely molecular geometry of an assumed disproportionation side-product of the general kind $\text{Zn}(\text{O}-\text{NR}'_2)_2(\text{HNR}''_2)_2$ by comparison to analogous complexes, we found that mononuclear zinc compounds with an O_2N_2 donor set of non-chelate nature were scarcely described.^[21] To complement the all-methyl starting geometries **3** and **13-Me**, we thus derived the respective $\text{O}-\text{NMe}_2$ compound stabilised by diisopropylamine units, the hypothetical bis(amine) complex $\text{Zn}(\text{O}-\text{NMe}_2)_2(\text{HNiPr}_2)_2$ (**14**), in a straightforward fashion. Taking the parent inorganic zinc hydroxylamine complex, the 2:1 adduct of unsubstituted hydroxylamine and zinc chloride, $\text{ZnCl}_2(\text{HO}-\text{NH}_2)_2$ ('Crismer's Salt'^[22]), and simply formally replacing the chloride by amide ligands, furnishes the desired species after tautomerism. In addition, the argument of strong hydrogen bonds between two additional amine ligands and the two deprotonated hydroxylamide units as a key stability factor is thus reinterpreted and manifested along. The target molecule **14** thus formally constructed was now optimised by taking the coordinates of the zinc environment in the crystal structure of a macrocyclic dinuclear analogue to Crismer's Salt, $(\text{ZnCl}_2)_2[-(\text{CH}_2)_3\text{N}(\text{H})-\text{O}(\text{CH}_2)_3\text{O}-\text{N}(\text{H})-]_2$.^[23] On the basis of this structural fundament, the crucial orientation of the two NH-protons was then set relative towards each one of the dangling nitrogen atoms of the two $\text{O}-\text{NMe}_2$ ligands. This was viewed as the by far most likely scenario as it fosters the formation of stabilising inter-ligand hydrogen bonds, with the NH-protons acidified upon coordination to the metal, the uncoordinated nitrogen donor atoms well within proximity, and thus two five-membered, *i.e.* unstrained rings to form the detailed molecular scaffold of **14** (see Scheme 1, page 35).

Finally, the geometry optimisation of HNiPr_2 (DIPA) was done from scratch, whereas the one of the structurally simple precursor Me_2Zn (**1a**) was based on data from X-ray diffraction experiments on single-crystalline material obtained by *in situ* methods.^[24]

1 Coordination Isomerism of Pentanuclear Zinc Hydroxylamides

1.1 Scientific Stimulus

The goal of this part was to provide a quantifying body to the understanding of the coordination isomerism of pentanuclear zinc hydroxylamides, $\text{Zn}(\text{RZn})_4(\text{O}-\text{NR}'_2)_6$. In earlier work, we had shown that such compounds adopt either of the two aggregation motifs **A** or **B** in the solid state, which centre around a tetra- or hexacoordinate zinc atom, respectively (see main manuscript, Scheme 1, upper part). In solution though, both motifs represent the "resting states" of a highly dynamic isomerisation process, with the mechanism of this ligand redistribution proceeding in a three-dimensional, carroussel-type fashion.^[1]

Beyond the concise scope of that communication, comparing the ^1H NMR spectra of the full series $\text{Zn}(\text{RZn})_4(\text{O}-\text{NMe}_2)_6$ (**3–6**; R = Me, Et, *i*Pr and *t*Bu) in the region of the N-Me groups qualitatively shows that, as the Zn-bound R units increase in size/ α -branch, this Me

resonance increasingly simplifies, collapsing from a complex set of peaks (**3**; R = Me) to a sharp singlet (**6**; R = *t*Bu). As the six types of O-NMe₂ ligands are magnetically inequivalent in principle (three types for each, motif **A** and **B** – both contain six ligand units and are C₂-symmetric) thus become unresolved on the ¹H NMR time scale with R growing and branching from methyl to *tert*-butyl, we wondered if such dependence of the "isomerisation speed" on the spherical nature of the peripheral R groups would be reflected by a trend within the relative energy gaps ΔE between the two aggregation motifs of each of these four differently alkylated analogues. Therefore, the relative energies of Zn(RZn)₄(O-NMe₂)₆ (**3–6**) in both, aggregation motif **A** and **B**, were desirable. Furthermore, in order to judge on the effect of a possible interaction of the molecule with a dielectric field, *i.e.* the influence of solvation onto its overall relative energy, the whole calculation efforts were undertaken with and without the COSMO solvation model^[20] applied.

1.2 Results

The calculations reveal that without COSMO, motif **B** is slightly favoured overall (Fig. 1.1, blue line). By contrast, factoring in solvation renders motif **A** distinctly more stable (red line), with a maximum energy gain ΔE relative to motif **B** of 11.5 kJ·mol⁻¹ in case of the smallest representative, Zn(MeZn)₄(O-NMe₂)₆ (**3**; geometries **3-A**_{COSMO} vs. **3-B**_{COSMO}), a finding that matches with the crystal structure of **3**. One exception is Zn(*i*PrZn)₄(O-NMe₂)₆ (**5**), which is predicted to be more stable in motif **A** by 9.3 kJ·mol⁻¹ (geometry **5-A**_{COSMO}), but indeed was found to crystallise in motif **B** from Et₂O.^[1] All in all, the results can be summarised in two notes. First, it is obvious that solvation seems to play a non-negligible role, as the trends in the change of the relative energy gap ΔE with growing R group size are opposite with or without COSMO. Second, this influence annihilates in both cases with growing R group size: ΔE sharply approaches zero with R being *tert*-butyl – the coordination isomerism (**A** ↔ **B**) is facilitated with increasing size/ branch of the peripheral RZn units.

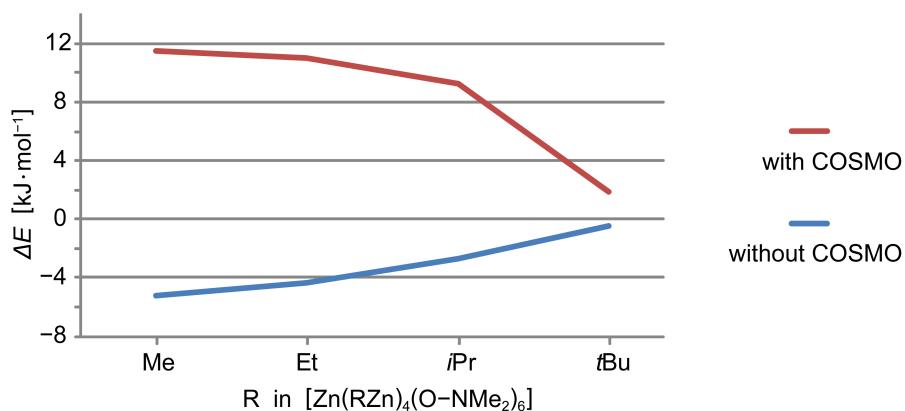


Fig. 1.1 Plot of the relative energy gap ΔE (motif transition **A** → **B**) of Zn(RZn)₄(O-NMe₂)₆ (**3–6**) (R = Me (**3**), Et (**4**), *i*Pr (**5**) and *t*Bu (**6**)) as a function of the size of the peripheral RZn units.

1.3 Coordinates of All Optimised Geometries in Bohr Units

Zn(MeZn)₄(O-NMe₂)₆ Aggregation motif: **A**

Level of theory: PBE def2-TZVP

Compound geometry #: **3-A**

0.00055746936574	0.00028156927286	-1.73300974157875	Zn
3.17668154398076	-5.03220226515488	0.29616552161199	Zn
-3.17648312268109	5.03265390982746	0.29505814178717	Zn
3.44456541634666	4.71284601792829	-0.28332860838677	Zn
-3.44483942671287	-4.71182178607667	-0.28479314655099	Zn
0.32767860345269	5.05096536119687	1.91649842115227	O
-0.32858945170450	-5.05316689275986	1.91542127695407	O
0.96845278969576	3.35922347049587	-3.20962325917907	O
-0.96700903852484	-3.35864521413683	-3.20986136473868	O
3.22320472470972	-1.05828661582571	-0.21118829300726	O
-3.22263591698401	1.05904628594444	-0.21185158706615	O
0.93342103680760	6.40888325733546	4.21780377252181	N
-0.93632743641608	-6.41199752687692	4.21565326357874	N
1.24701361771049	-4.98590396189888	-3.44055541636669	N
-1.24573049330596	4.98601356604536	-3.44140201391194	N
4.76313542389763	0.88884805399539	0.88772177690393	N
-4.76204505161278	-0.88786917558369	0.88794854410356	N
6.25459841361982	7.11692415389284	-0.95225783218948	C
-6.33675994949592	7.01043427695071	0.77066832791278	C
-2.79603201242321	3.94953250618989	-5.50109258326504	C
-0.31707156769041	7.50408757325951	-4.16087575678356	C
0.58298256541960	9.10042661335319	3.75439366173583	C
-0.76909229587541	5.50946974156438	6.17621066189075	C
7.36407961448669	0.47191954995177	-0.00042707822595	C
4.61717104668143	0.64562889404163	3.65043412879614	C
-6.25548091597168	-7.11432200027719	-0.95670246930205	C
6.33699616532886	-7.00973696781187	0.77237664081659	C
2.79811827065973	-3.95022414614874	-5.50003811578680	C
0.31805611528209	-7.50398363829301	-4.15965121390561	C
-0.58724956822580	-9.10319695264190	3.74901738937814	C
0.76457773887628	-5.51637858224618	6.17719520948244	C
-7.36357127801421	-0.47052871112742	0.00164028274393	C
-4.61403032096667	-0.64477284786306	3.65058341720255	C
7.55947546176699	7.22754686304807	0.66365310695819	H
5.56471590057211	9.04462109525307	-1.31775931481232	H
7.35541521773450	6.52932309650762	-2.61616593886364	H
-7.20898218830574	6.61616170587591	2.61726953923513	H
-7.74010120544530	6.55223225284936	-0.69592018973763	H
-5.97897044138686	9.05713108576551	0.68177369593459	H
-1.69013940249035	3.83640968865884	-7.26499746606552	H
-4.44193480344745	5.18651734449713	-5.77525601733378	H
-3.47001625505081	2.06331506509371	-4.96780793936910	H
0.81332890734152	7.39941750309433	-5.90977809960243	H
0.85785275726049	8.27159249873757	-2.63530131105834	H
-1.95300038138464	8.75124103074310	-4.44481852633597	H
1.89415429308292	9.71093304762682	2.26607517718172	H
1.04284943871150	10.13954006245093	5.49575977462062	H
-1.38192498367182	9.56684138953416	3.18207293415176	H
-0.47754715595570	3.47577236246787	6.46584717788031	H
-2.78922710670791	5.84389088975248	5.70104267180441	H
-0.32945494651639	6.50304644725151	7.94827916387759	H
8.04141056303537	-1.41656934259395	0.56680083599996	H
8.58854312392151	1.94014079143945	0.80830034468992	H
7.40307601391489	0.63208711277091	-2.06575470221631	H

5.31180622228787	-1.22369439068277	4.26396601545804	H
2.64549827613465	0.89825133387301	4.22620360754111	H
5.76352459420671	2.14489456515745	4.51779410090075	H
-7.56606304891599	-7.21944749456826	0.65495091567272	H
-5.56655649434237	-9.04372536481457	-1.31495685017034	H
-7.34987831861041	-6.52954419452725	-2.62583378047416	H
7.20996484617077	-6.61371450984667	2.61824652792016	H
7.73976672382586	-6.55292767226153	-0.69518508606552	H
5.97909894279998	-9.05649991705990	0.68555503898827	H
1.69271887938604	-3.83729030128404	-7.26426047266675	H
4.44382075065763	-5.18762472432195	-5.77347778454342	H
3.47236518529356	-2.06403127149918	-4.96701236444377	H
-0.81139571696475	-7.39963293193397	-5.90918661515675	H
-0.85788299288711	-8.27064763540581	-2.63441880870649	H
1.95379784603664	-8.75167377814904	-4.44228440288020	H
-1.89787894433670	-9.71102753396000	2.25913421114664	H
-1.04856586186862	-10.14434374762957	5.48877912432561	H
1.37771845211884	-9.56983849602248	3.17715775509997	H
0.47393210884841	-3.48289096280931	6.46924112696798	H
2.78503569296825	-5.85148381148646	5.70384702617305	H
0.32231177972832	-6.51201886944986	7.94744957387231	H
-8.04073971006982	1.41752365455902	0.57053304616039	H
-8.58744330300335	-1.93940190831402	0.81009747474692	H
-7.40373363879379	-0.62931866320887	-2.06377426867295	H
-5.30794362098765	1.22466382046115	4.26464820678357	H
-2.64197771536053	-0.89765795970067	4.22492804204324	H
-5.75994356217936	-2.14388923057247	4.51878242794576	H

Zn(MeZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

3-Acosmo

-0.00005102261991	0.00005858152657	-1.77764508537086	Zn
3.11312814656025	-5.06757038938914	0.24756553127983	Zn
-3.11334357539989	5.06763086064237	0.24722915993373	Zn
3.48634349342354	4.64249338397246	-0.21912325526734	Zn
-3.48623199955040	-4.64219858661296	-0.21900042303421	Zn
0.37005572388191	5.12861045034719	1.92803709215966	O
-0.37044500757459	-5.12844415440080	1.92832811006584	O
1.03893203533804	3.36022313590086	-3.20025399438139	O
-1.03847472148547	-3.36022691535419	-3.20056768900753	O
3.18026068628145	-1.10613827439912	-0.20976721855630	O
-3.18086728854044	1.10610614904584	-0.21060058801491	O
0.93830598023278	6.60248953346542	4.16835151546441	N
-0.93874250709205	-6.60306401037112	4.16816821197805	N
1.16244268033841	-5.01498496552364	-3.45561086869488	N
-1.16211197817230	5.01467127089750	-3.45567889885476	N
4.72394249289642	0.80895985929549	0.94627306784614	N
-4.72407477376287	-0.80896552847548	0.94612188971306	N
6.34616511910021	7.00695529016318	-0.87913863839827	C
-6.26945355492167	7.06745866874879	0.72404121221732	C
-2.70684069335885	3.99454579531471	-5.53042303080939	C
-0.20147887741014	7.52413568343269	-4.16762775015228	C
0.46056796188406	9.25860996317565	3.60475565588576	C
-0.71644073157669	5.70816505159918	6.17663774011670	C
7.33935443082132	0.36163888132263	0.11041861867557	C
4.51655066075616	0.53023084560771	3.70345041034092	C
-6.34567567989436	-7.00687781136998	-0.88022523122979	C
6.26926080280200	-7.06739630776890	0.72440970891671	C
2.70791594783039	-3.99495964545402	-5.52984288472369	C

0.20197965497597	-7.52437945817228	-4.16795845231840	C
-0.46005395623159	-9.25891231944181	3.60410936936684	C
0.71538815382511	-5.70859401955179	6.17688529430962	C
-7.33967001517413	-0.36197147321541	0.11069262904178	C
-4.51620106132341	-0.52976408312182	3.70319907669467	C
7.74054340148456	6.95392200107843	0.66481339912958	H
5.68824922229244	8.97134127469547	-1.07327403799401	H
7.33159899259427	6.49001111272662	-2.63783543451411	H
-7.13285454966623	6.66329337859052	2.57360173549473	H
-7.66596155925580	6.60405422714280	-0.74844892180322	H
-5.89171987160592	9.11159111848121	0.63189436065123	H
-1.58770676869477	3.86444756316534	-7.28372087784758	H
-4.32653486528687	5.25910930454922	-5.82796994261240	H
-3.42116682079907	2.12155077168311	-5.00114271771343	H
0.93014425077308	7.41120750774797	-5.91483122870065	H
0.96808996217637	8.28167230076073	-2.63305442605543	H
-1.82216704556316	8.78621042265135	-4.46707194752547	H
1.71968149942101	9.87309994125596	2.07342132329017	H
0.88215086269991	10.38547098016683	5.30052833356004	H
-1.52877564269320	9.60677698311412	3.03693436748751	H
-0.33727652517666	3.70264160732893	6.54575804930017	H
-2.74760398721744	5.93618702972498	5.69271086694499	H
-0.31876287305425	6.79478622901756	7.90338492753257	H
7.97288340503649	-1.54051840418026	0.67990475626438	H
8.56976302033954	1.79460916162919	0.97056739383223	H
7.43053941151569	0.53603797564467	-1.95218401946600	H
5.15108685928298	-1.36453571891419	4.30030545919734	H
2.54191857825432	0.82473907693580	4.25027116632758	H
5.69890728067464	1.97407083368278	4.61499408156506	H
-7.74802482934540	-6.94328472968953	0.65612632565743	H
-5.68916573972424	-8.97318753764572	-1.05926549423741	H
-7.32131698981812	-6.49913093360472	-2.64701383691878	H
7.13492946954277	-6.66025280838894	2.57225625011031	H
7.66413230384552	-6.60669984447172	-0.75050305468646	H
5.89112082825359	-9.11160623629452	0.63605742849095	H
1.58911083560576	-3.86400725685274	-7.28328435098831	H
4.32724729223901	-5.25997668908777	-5.82745782668659	H
3.42273151447646	-2.12233311852180	-4.99988793920885	H
-0.92892915652844	-7.41135301670106	-5.91561168581268	H
-0.96830350128934	-8.28173466174063	-2.63384622152744	H
1.82259601351578	-8.78671686939717	-4.46680927551924	H
-1.71869884155598	-9.87361583663510	2.07248401886507	H
-0.88147812000770	-10.38624576809887	5.29960992640157	H
1.52948429019202	-9.60626297746165	3.03649406117491	H
0.33548506429965	-3.70327844521454	6.54638921800578	H
2.74669502869229	-5.93572782614575	5.69312849653762	H
0.31788981933571	-6.79577644578924	7.90331689737269	H
-7.97282293378326	1.54062989805340	0.67906382789912	H
-8.57002191289245	-1.79426334164977	0.97202815254312	H
-7.43146726730747	-0.53775951663513	-1.95176261042004	H
-5.15141378199577	1.36481350873373	4.29996341867125	H
-2.54130441708868	-0.82325564150494	4.24957574691541	H
-5.69768840697667	-1.97398201652959	4.61526053302462	H

Zn(MeZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP

Compound geometry #: **3-B**

0.00140217718432	-0.00149288406417	0.01434680482937	Zn
2.83197272383652	5.45246802648626	-0.00733024972776	Zn
-2.83979619222345	-5.44802338937368	-0.00926721955785	Zn
4.32519504908244	-3.76824535817936	-0.01728344006447	Zn
-4.31604310285106	3.76915620643117	0.01101710644827	Zn
1.59667919089312	-2.84970780857356	2.63812834214696	O
-1.59031081203709	2.84790311960991	2.65403984065371	O
1.59904512867583	-2.84170481615360	-2.64982952964741	O
-1.60092540670603	2.83251885484227	-2.63798283319387	O
3.49221298444041	1.68545854954483	0.00627011306953	O
-3.49354524173818	-1.68154681535137	0.01545229492752	O
0.22120384432386	4.78602757269939	-3.20580034213879	N
-0.22003977269914	-4.81384056973294	3.18577301895891	N
0.23542403746678	4.80299542841105	3.20576443733219	N
-0.23984032867940	-4.78005414671603	-3.21612580862821	N
5.69803611668276	0.13022484383582	-0.00529690383782	N
-5.69907546634769	-0.12529643669739	0.02392960874003	N
-1.12999418379928	7.11404232073099	3.93189001805936	C
1.66542366745830	3.87326880723061	5.40498108515891	C
-1.14774816580295	7.09402255645776	-3.93539546102017	C
1.64237845079679	3.84762332668011	-5.40688781936239	C
-7.19249810261994	-0.68414341317063	-2.24985754295547	C
-7.16798834779422	-0.67620467145722	2.31564081783893	C
5.04743913124276	8.49346152684699	-0.02832322323269	C
-7.00602554464474	6.40149253635447	-0.00391740337346	C
1.10678645064470	-7.09745052062537	-3.95424926394202	C
-1.66066911517291	-3.82394694131299	-5.40993216901730	C
1.15545069168342	-7.12802440831430	3.88314451877411	C
-1.63919426136878	-3.90640327454860	5.40111659413203	C
7.17944765028174	0.66768389393146	2.28186006400202	C
7.17994653812091	0.70210904456062	-2.28310161441994	C
-5.05911008311660	-8.48616340247251	-0.01534647023437	C
7.01547795741561	-6.39989760705046	0.08483360937831	C
-2.24735743457965	7.80713925883333	2.32895583191002	H
0.25468602134794	8.56594010329926	4.47154493053799	H
-2.41652198604376	6.72830942444860	5.52836511847282	H
0.38890952680375	3.64377284230726	7.03858931451035	H
3.17259217548093	5.22832187774731	5.86842710075149	H
2.48532693386217	2.03807209632254	4.92060067758795	H
-2.43850706604704	6.70273575351131	-5.52715947286150	H
0.23464924953474	8.54513043328069	-4.48310249881202	H
-2.26139810368953	7.79132413638641	-2.33161467732558	H
2.46023892267741	2.01210536223925	-4.91989014036247	H
3.15014600217175	5.19876655273001	-5.87975979155257	H
0.36015922534510	3.615287110258151	-7.03567346626855	H
-6.07500068124646	-0.19685471626453	-3.92353364675332	H
-8.90978153890496	0.48393065262504	-2.22356010670606	H
-7.71825218576179	-2.70364705529752	-2.31066516753391	H
-7.69077556007435	-2.69599366231030	2.39047966289393	H
-8.88687805174321	0.48975856965531	2.30251099698086	H
-6.03342102546925	-0.17994922153277	3.97533294432680	H
6.40926876157481	8.45889275699139	1.54320937494910	H
3.93716235545056	10.24356573582385	0.15009531970263	H
6.14166645848178	8.62997349129231	-1.79192763949367	H
-8.26472712176903	6.18554024242850	1.63912434148223	H
-8.17878424283925	6.25004039290743	-1.71622140990012	H
-6.26273179717957	8.34378572646365	0.05328462273100	H

2.20294696826049	-7.81761779318249	-2.34896614754993	H
-0.28891653013077	-8.52980475003962	-4.51711757875521	H
2.40930511991582	-6.71069150276469	-5.53758698459075	H
-0.38245044106787	-3.59873309700916	-7.04286009676988	H
-3.18171577581235	-5.16105705715966	-5.88016230333189	H
-2.46116299901587	-1.98253680913530	-4.91552487176976	H
2.44849049201037	-6.75437064486507	5.47731604238476	H
-0.22280822226118	-8.58892862816087	4.41497974231914	H
2.26859796227750	-7.80322941436653	2.26891543635697	H
-2.46921890378241	-2.07087208202109	4.93541802435654	H
-3.13841079959135	-5.27038530355038	5.86437363705827	H
-0.35313889079016	-3.68388984964692	7.02818258977439	H
6.05045313188746	0.16930628096388	3.94457953260483	H
8.89356390467871	-0.50519763649619	2.25697614329691	H
7.70992605008237	2.68521844087497	2.36194479027492	H
7.70298886350062	2.72254432193263	-2.33624072819786	H
8.89932001209576	-0.46313799014644	-2.27065398488740	H
6.05616199613793	0.22145328824345	-3.95445335442168	H
-3.94723459856707	-10.23912298843793	-0.15056019246186	H
-6.38224567028661	-8.46457327534191	-1.61983590142778	H
-6.19614349873746	-8.60512358566715	1.72223452014341	H
8.78391818420851	-5.69149010352036	-0.75428061828682	H
7.43993135303333	-6.95163354208892	2.04521526311061	H
6.50927876578777	-8.12929419124858	-0.95361087648055	H

Zn(MeZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

3-Bcosmo

0.00118485861802	-0.00380401977365	0.00794252116673	Zn
2.80809980689639	5.44620547232338	-0.00228656926285	Zn
-2.81505022156478	-5.44275294170915	-0.00388527802018	Zn
4.32640636387375	-3.74230885972268	-0.01964748812052	Zn
-4.31530044027230	3.74249027348238	0.00822220071293	Zn
1.60244663667015	-2.85668845886857	-2.65526060407834	O
-1.59960259804157	2.85594768601647	2.65500360125210	O
1.60265261687648	-2.85470991505187	2.63568492557104	O
-1.60682324362284	2.85122714881102	-2.64489923278231	O
3.47952724934826	1.68766952974114	-0.00362638546728	O
-3.48345977053503	-1.68363685304121	0.00598665407000	O
0.21586347677278	4.81135179971709	-3.19929401323633	N
-0.21357690750994	-4.82165647921321	3.18527980029973	N
0.22768560677790	4.81333979216711	3.20460036570746	N
-0.23409555962233	-4.80425587609561	-3.20888626578030	N
5.69531491028731	0.14129864208399	-0.01163126761391	N
-5.69851043807530	-0.13616992391923	0.01689793582511	N
-1.13655153532166	7.12698127919604	3.92689736021437	C
1.65627172122692	3.88629658284885	5.40704655640212	C
-1.15295247303426	7.12390480418785	-3.91678165338460	C
1.63922827644872	3.88705436324092	-5.40606956771709	C
-7.19061404513642	-0.70433325284358	-2.25708952689673	C
-7.16561863055817	-0.69982247529778	2.30821230232467	C
5.04610120476500	8.48351211596361	-0.01384224781021	C
-7.02166303278528	6.37545966183795	-0.00329379357450	C
1.11672263344144	-7.12411645357416	-3.93462823199479	C
-1.65774759775112	-3.86466299200498	-5.40907045365874	C
1.16425681793538	-7.13625605766055	3.87894932558112	C
-1.62917682032551	-3.91611646959904	5.40490927554569	C
7.17375957302458	0.69225600973708	2.27556727421253	C
7.17614062862060	0.72072663164953	-2.28970242965559	C

-5.05831072873794	-8.47616296896921	-0.00039495287267	C
7.03018570003772	-6.37620988332336	0.08489597035820	C
-2.22945227444289	7.83579507395880	2.31365849456891	H
0.24564556898971	8.57033371779193	4.49370764484764	H
-2.43726362590245	6.73765412279965	5.51084357284875	H
0.37513719888009	3.65557985450087	7.03639723158067	H
3.15665044134755	5.24554862601187	5.87776046074257	H
2.48325201398564	2.05423492847555	4.92235056447836	H
-2.45581129310481	6.73488567323761	-5.49909325245505	H
0.22650830706834	8.56975357170623	-4.48408326695039	H
-2.24426962121147	7.82954574788257	-2.30097275947676	H
2.46857639671682	2.05528183704713	-4.92401730339558	H
3.13764735001929	5.24732685880223	-5.87997711011887	H
0.35400627532872	3.65698581113853	-7.03236266515408	H
-6.07988562467164	-0.21277566340461	-3.93424272775543	H
-8.92087423441976	0.44377585075211	-2.22598084656202	H
-7.70217439130865	-2.72692848779197	-2.31611702895813	H
-7.67479981086104	-2.72273140487231	2.37791109085492	H
-8.89712414971276	0.44672760380051	2.29276000739715	H
-6.03718914043628	-0.20248799144846	3.97189742125254	H
6.42511034019502	8.40726920399762	1.54269347956996	H
3.93703007458411	10.23112377547129	0.20555690755000	H
6.10908946052953	8.62601829338558	-1.79718296934489	H
-8.28351667398432	6.13906430486613	1.63629353094029	H
-8.18741840396483	6.21718749486231	-1.72148051920467	H
-6.26512986031556	8.31306066064164	0.06340977819409	H
2.19150467331294	-7.85094879207349	-2.31761180274897	H
-0.27331116734350	-8.55308618253407	-4.51846306413963	H
2.43228041669078	-6.73665823684798	-5.50665404883575	H
-0.37601214232529	-3.63978551904725	-7.03881041252998	H
-3.16711196815675	-5.21341193437221	-5.88123377835010	H
-2.47300969546941	-2.02817370805908	-4.92024918842854	H
2.47873934671318	-6.75424403317861	5.45313321027181	H
-0.20881479631789	-8.58792329357588	4.44682730577928	H
2.24689067209376	-7.82986511168871	2.25154506886599	H
-2.47146956823865	-2.08666263802138	4.93663122887451	H
-3.11766349055267	-5.286737110836974	5.88053646921127	H
-0.33597072405217	-3.68553769129750	7.02476596396677	H
6.05216900369793	0.18742686994028	3.94150305759664	H
8.90325442300919	-0.45708330591655	2.24610832525507	H
7.68631958460180	2.71399141905358	2.35291189682334	H
7.68550700213649	2.74413066960990	-2.34254863580065	H
8.90798818830129	-0.42525463972304	-2.27126814605304	H
6.05903060121314	0.23394816094258	-3.96391899527920	H
-3.94665256275470	-10.22857642392889	-0.16054172869852	H
-6.39561548643095	-8.42494570720809	-1.59388806461112	H
-6.16832483252392	-8.58688772336427	1.75635731450642	H
8.83372004069867	-5.61135057517421	-0.62263470000003	H
7.34429417631974	-7.01940858887572	2.03943836870026	H
6.56593466088647	-8.04768823501155	-1.06414098902927	H

Zn(EtZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP

Compound geometry #: **4-A**

-0.00627956170284	-1.76290332766881	-0.00353567858743	Zn
3.17384317453217	0.21187804323944	5.07488552130359	Zn
-3.17471244879738	0.23256110157156	-5.07266887192729	Zn
3.46576814951124	-0.33050941399463	-4.70901554198136	Zn
-3.46959484600485	-0.33187379664568	4.70826154104261	Zn
0.32863669487109	1.86129572585781	-5.07011585120489	O
-0.32363080893945	1.84586043847025	5.08759771256902	O
0.99153769061720	-3.25538676978930	-3.34959720287195	O
-1.00633802984581	-3.25797569531831	3.34187577972484	O
3.20727621866299	-0.24384843893271	1.07465353845838	O
-3.22452942310084	-0.24783009301272	-1.07625602666903	O
0.94981252588689	4.15263465880399	-6.43191335618366	N
-0.93609877948980	4.14102795763671	6.44591623076027	N
1.19718530504705	-3.52386401632754	4.97781026259906	N
-1.21161903730294	-3.50924320113196	-4.98810360373520	N
4.76736085271724	0.83436156510639	-0.86753193723099	N
-4.76159718639353	0.85793212578036	0.86934040564797	N
4.64732730477772	3.59910726288853	-0.62951330505521	C
0.77824235238013	6.10176487998176	5.57554025490069	C
7.35649047220603	-0.07956127198711	-0.43318204307647	C
0.61486414395968	3.68129336521126	-9.12189957743066	C
6.27679136355609	-0.93492147977843	-7.17292431383930	C
7.91221750995782	1.37409017692490	-7.81933555471963	C
-2.76173914266049	-5.56350647550746	-3.94059787852482	C
-7.3659823841684	-0.01397263895000	0.44114346150984	C
-6.44696502905852	0.60949732023531	-6.94417479094804	C
-6.42289747027205	0.05230385459264	-9.78988204817495	C
0.24760143608644	-4.27104493153955	7.47977057055346	C
2.73983154145042	-5.57938395893427	3.92242626692850	C
6.46818665948974	0.54314712735280	6.91561535188241	C
6.44289077837199	0.15205874570602	9.78851766552390	C
-6.28682392241266	-0.93536367581769	7.16561674083151	C
-7.90741949395917	1.37855938048410	7.83142602591276	C
-4.59751410992759	3.62019850217997	0.63017848884077	C
-0.26107329747060	-4.25180373465169	-7.49117507096774	C
-0.61917650020581	3.66526848310469	9.13736510044483	C
-0.74458254104968	6.12562267910858	-5.55045602316926	C
5.82181132341602	4.45349237172148	-2.11445106860830	H
7.37585639105369	-2.14543124752989	-0.59030147678737	H
4.37784850310783	-5.88023600267177	5.16374046902184	H
-5.75147947645350	4.49386071270739	2.11998418827906	H
0.89042975521274	-5.98504969206337	-7.35547001980774	H
-1.07939297293046	5.40338993530823	10.18164884169393	H
-0.46181140202865	6.42322250325817	-3.51684557149926	H
0.50943251394911	6.40268495387914	3.540548411303967	H
-7.41767604211717	-2.07949490478669	0.59496154273959	H
1.09020787862573	5.41439003421653	-10.16778202743709	H
-4.39940650488515	-5.85530861825341	-5.18452557259379	H
-0.90266195590565	-6.00504677961664	7.34255184833598	H
5.32437857378020	4.20721752375283	1.24830619074833	H
2.68486128253557	4.19570908837205	-0.90604456663333	H
8.02898183076946	0.48204092596153	1.45876504926347	H
8.60128744054022	0.71720229142208	-1.89086238923509	H
2.79356969858066	5.61541537722743	5.92721649725330	H
0.33500885318045	7.86953614353578	6.57491653171814	H
1.33812111961165	3.07951368866972	9.62269604052753	H
-1.93934521651411	2.17697078554388	9.72890245847014	H

-8.03462833404003	0.56150771161547	-1.44798982782814	H
-8.59375499005947	0.80034837488987	1.90349332225399	H
-5.27243565698029	4.23888367345327	-1.24501806635382	H
-2.62448640536307	4.18491874912340	0.89835904829283	H
-1.35122637402309	3.11804899479203	-9.59880044686744	H
1.91554221946053	2.17846366960805	-9.71977696841205	H
-2.76549591926755	5.65574592368006	-5.89099232684047	H
-0.29320998911026	7.89075021506034	-6.55102282778471	H
-3.44919713639892	-5.01342216157292	-2.06398402833260	H
-1.65181007657437	-7.32326718773486	-3.80251177176879	H
0.89866518401232	-2.72199819092687	-8.27357293228093	H
-1.88447700283909	-4.57403803558680	-8.74511453689999	H
-0.91266616886227	-2.74301384115177	8.26479704165559	H
1.87192732806672	-4.59415228619321	8.73248549360775	H
3.42706087826256	-5.02563924445251	2.04675161088805	H
1.62449407765333	-7.33535010002134	3.77954781335381	H
-7.49723920383094	-2.44933897928228	6.39659247511599	H
-5.46950958153779	-1.73219715911344	8.91117237772930	H
-6.76738519239666	2.92249063101866	8.63430285507841	H
-9.40435135264556	0.93631609805610	9.21741959109112	H
-8.86756315551547	2.17013375447530	6.16019900787083	H
-7.15756461551829	2.54274060935295	-6.61696672943457	H
-7.81763102126914	-0.65160232002498	-6.00393751006516	H
-5.11011380576475	1.29753923951276	-10.81996071409445	H
-8.29931289916460	0.30160226522291	-10.66853313709404	H
-5.82876173808441	-1.90166028739039	-10.19676476527535	H
7.47723266764436	-2.46357429023851	-6.41748529310776	H
5.45324848359829	-1.71097363895555	-8.92488234467307	H
6.78146554576648	2.93255342550185	-8.60713047538380	H
9.40516960429086	0.93461723378561	-9.21049941204934	H
8.87897710456307	2.14398182717898	-6.14172504000835	H
7.77071288766750	-0.83228286577653	6.04042246275755	H
7.26586485060407	2.41892949781308	6.47363285173397	H
8.33851716852579	0.35142868815969	10.63824648785796	H
5.20833612855402	1.52322173602915	10.75294722715304	H
5.74930251133713	-1.74014534946016	10.31264847346179	H

Zn(EtZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

4-Acosmo

0.00097509895837	1.74974327118413	0.00116029217140	Zn
4.70177977858677	0.22192949936265	-3.43596149084770	Zn
-4.70186670601330	0.22048385846507	3.43869592532979	Zn
5.04602750542512	-0.24173005534291	3.18192742519867	Zn
-5.04432864115463	-0.24230075279529	-3.18317086534326	Zn
1.06982339710644	0.19866129495485	3.20181679833211	O
-1.06846846308871	0.18926746371054	-3.19455835821757	O
3.36488698130641	3.19200533749517	-1.00096742666812	O
-3.36406117075445	3.19359837707251	0.99897565476478	O
5.13039435231754	-1.92834700733248	-0.30561415492954	O
-5.13561377736216	-1.92447306767228	0.30633980996833	O
0.86887931234207	-0.96955072088726	-4.70644173426565	N
-0.86715777135162	-0.97600224771648	4.70342573051069	N
4.97739263300643	3.47533772533526	1.22774785437600	N
-4.97576557834914	3.47613896944059	-1.22959600705291	N
6.61053976905197	-4.17033572846109	-0.84672982611907	N
-6.61453087176530	-4.16629738258117	0.84942079688791	N
0.60390939849131	-3.72673751201535	-4.47569099083774	C
7.49726377027757	4.20381223630518	0.30926510684344	C

7.05655116644701	-0.76942866722152	6.35608618408364	C
7.17964418185475	1.48429903594082	8.18161505338119	C
0.43989057273193	-0.15863499449504	-7.33168969947412	C
-7.05531717493574	-0.77317032601527	-6.35653026984957	C
-7.12165980891160	0.89605925094334	6.28010027494389	C
-3.90377088530633	5.55139143786770	-2.73805708811338	C
-9.27759037778395	-3.56671734787596	0.46923991754291	C
-5.78512605969730	-6.13481619932656	-0.88442231414945	C
5.78414718128560	-6.13585932844481	0.89111572599160	C
7.12697749974271	0.88859294089581	-6.27545343707832	C
9.27391485942342	-3.56805716408039	-0.46785852735188	C
7.92199306598816	-1.43749239621234	-7.82122150192981	C
3.90540549887026	5.55182229554698	2.73490502403865	C
-0.59749944564868	-3.73081176270188	4.45607373834383	C
-0.44347538421261	-0.17996055989275	7.33414256468336	C
-7.49601277122633	4.20424687343779	-0.31196552624560	C
-7.18133926667192	1.47876591627007	-8.18407358777042	C
-7.93500194433976	-1.42812691086798	7.81891225594700	C
-6.24823759367044	-2.43181743365822	-7.33317880408497	H
-6.24630440329367	2.30580101110203	7.54533085769062	H
6.24905017613575	-2.42740681162558	7.33333943085137	H
-8.98592807481110	-1.33605753809509	-5.80380789749276	H
2.05477916975464	-4.64117435476133	-5.64729884549417	H
0.60424954929074	1.90383347305342	-7.43910932193470	H
-5.13778507329853	5.88598266145551	-4.37358716948161	H
-2.05096759107434	-4.65415299748632	5.61748462792397	H
7.38955501963747	5.93755141237604	-0.84396137655703	H
-10.40773196026298	-5.26393944590115	0.87712985895496	H
3.77396556078980	-6.53905707855137	0.57564664651185	H
-3.77350446748391	-6.53545714925738	-0.56678760791331	H
-0.61475265008653	1.88132682849102	7.45398525022986	H
10.40503343058749	-5.26577248076476	-0.87161374682417	H
5.13979763219517	5.88765695927938	4.37000235800093	H
-7.38925455309797	5.93889500803379	0.84000617865030	H
-1.28687173249725	-4.33922815928566	-5.10697496977666	H
0.90157347334747	-4.25487454047989	-2.49639128347703	H
-1.45383853185170	-0.74400617441731	-7.97646254733718	H
1.88450912819237	-1.02136135682072	-8.54680095165123	H
-6.05594089811830	-5.58895353475829	-2.89720797798756	H
-6.88261127570420	-7.86049947063087	-0.51163404551210	H
-9.68409325982498	-2.93606075818933	-1.49005703308454	H
-9.83779984718158	-2.06607217629578	1.79160449623421	H
1.45141968172241	-0.76325870966515	7.97727701952915	H
-1.88651790763568	-1.05500227088453	8.54230529191874	H
1.29214029043511	-4.34523937980229	5.08891485205349	H
-0.88915985889487	-4.24681107680669	2.47256183025016	H
9.67792897144861	-2.93483432558471	1.49112094919610	H
9.83260498858360	-2.06975714328962	-1.79157237088093	H
6.05588420631839	-5.58697499094160	2.90268440585841	H
6.88319142178990	-7.86093221803681	0.52072174103692	H
2.02965903321659	5.00300220875032	3.42762779626161	H
3.76584729504336	7.29005713135033	1.59310949722575	H
8.29331490673462	2.66390799329056	-0.82730154629152	H
8.72534610627301	4.53457676339938	1.95024704963590	H
-8.29151966640428	2.66462608942270	0.82524552368162	H
-8.72419526273493	4.53349772947452	-1.95312510334443	H
-2.02787702097290	5.00216883929171	-3.42970271613815	H
-3.76429204999930	7.29053712192286	-1.59765617957815	H
-8.80775708606870	1.83142103703437	5.48380914320058	H
-8.85216944211452	-2.86255606015877	6.62183088586644	H
-9.28014150877969	-0.95772859088034	9.34736286565408	H
-6.31187602879082	-2.36844167054407	8.72513256716003	H

8.98762126990161	-1.33303208570681	5.80595462698251	H
8.82058455066061	1.80796574968688	-5.47623889818655	H
8.84549114808567	-2.87402103182629	-6.63133054180391	H
9.25645189532592	-0.97092077271830	-9.36013174871942	H
6.29003834746729	-2.37467965826032	-8.71469371707080	H
8.26739163636459	1.06251582409865	9.91504431427923	H
8.08055625086998	3.14224316526495	7.30075298426580	H
5.28519698113898	2.09339195467014	8.79494473929010	H
-8.27235783803629	1.05540667239052	-9.91502730673926	H
-8.07996665615097	3.13811789195851	-7.30344962421463	H
-5.28791062862778	2.08663996130142	-8.80176098336538	H
6.26228204223365	2.30875654360376	-7.53643024510549	H

Zn(EtZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP

Compound geometry #:

4-B

-0.00736993398769	0.05335832207088	-0.04377173870689	Zn
0.18576768992972	-2.92755320875021	-5.41188614638737	Zn
-0.08822377901264	3.02987245894597	5.34150138707827	Zn
0.39390974355540	4.26241643959396	-3.92504164863080	Zn
-0.28893920685073	-4.16441521482432	3.84597737475619	Zn
0.05626850113268	3.58666908198931	1.54652395551689	O
-0.14927328860401	-3.48438573660015	-1.63773728211121	O
2.48358649560508	-1.57771011464480	2.91961446703680	O
-2.41992538376475	1.68307938367548	-3.07368010245947	O
2.86193245035981	1.46171113313189	-2.74560087695411	O
-2.79959414718393	-1.36108885747995	2.74782697496373	O
0.19858570588831	5.75111286948077	-0.06020291204611	N
-0.28133872621009	-5.64702105567464	-0.02817960400627	N
3.04239945699838	0.27753848588977	4.84467523970143	N
-2.94667913231159	-0.16708018295426	-5.01267194008750	N
3.46923957739211	-0.45423737756130	-4.59286916178868	N
-3.37043332906381	0.53167648650529	4.63049550938584	N
4.41779543504777	0.79275356342922	-6.88979979593220	C
5.52852574523922	-1.94244247851560	-3.45755917688495	C
-2.65504328551204	-6.99309792453966	-0.55120303211934	C
5.31224274914714	1.61157023700158	3.94043914148508	C
0.73728063722188	6.81181266625579	-6.71261146505482	C
-5.25932284366220	-1.46999758455138	-4.17590097348513	C
-0.05715100348454	5.51361580186413	8.20683912488572	C
-0.52489425750995	-6.73199250171578	6.62771738442328	C
-5.47431893589643	2.01362659220337	3.56932517067161	C
0.36556762305607	-5.16004605339468	-8.46765919898342	C
-1.62627042071703	-7.26090620783902	-8.66522634220009	C
2.48626612801394	7.18869219311963	0.58508961064941	C
-3.47745610892505	1.16925325523370	-7.39283558512533	C
-2.07142766166016	7.29987426136726	0.34748293888628	C
-1.50503500661952	8.61684556016090	-7.08118186377921	C
-4.25097225491974	-0.75443935532655	6.93430663831119	C
3.66589020317699	-1.06036153570225	7.20237381416345	C
1.90160926477047	-7.28014740472688	-0.55516578893273	C
-0.23710211474398	4.44290045377251	10.89866593990299	C
1.75777271977738	-8.49836914699213	6.93126417838294	C
2.46970645326160	7.91308489449637	-6.33841157059983	H
-1.62034612762692	6.85806372634520	7.88964661468885	H
-2.24588911696210	-7.86220211435469	6.28824121741029	H
2.27196356546522	-6.00263548839400	-8.54227694601879	H
2.91562336432346	1.94031842574582	-7.74001238829212	H
5.00623364134492	-0.66572424738140	-8.24765722081755	H

6.03349472480912	2.03129742623386	-6.43234988304293	H
7.20553721659816	-0.73540791809834	-3.17012230273172	H
6.00583857508865	-3.52870927549278	-4.71406300189959	H
4.88670654015123	-2.65266978882267	-1.62395550555423	H
-5.03850639330435	2.52887379509611	-7.13198338567435	H
-3.99146554085319	-0.22584879246277	-8.84418723668785	H
-1.78833148965301	2.19963616714602	-8.01408700520767	H
-4.90803210554894	-2.28487795748364	-2.30910803276317	H
-5.73077374140141	-2.97542565431691	-5.53031909584289	H
-6.83520748235005	-0.10926966486416	-4.04872236903089	H
-3.73762800677716	6.21622562399058	-0.23331321278364	H
-1.93814146062945	9.00843471937351	-0.82551953404783	H
-2.24101551189691	7.84240722755442	2.35640411169751	H
2.45910508667931	7.75971278875921	2.59317552427537	H
2.57519477507207	8.87865585103028	-0.61924264063903	H
4.14767034685895	6.01076698222708	0.21163048904652	H
0.24632587058857	-3.93023272777546	-10.14829705580964	H
-1.42623529447781	-8.39619918520278	-10.40551153143335	H
-3.56598413393052	-6.50286314376515	-8.66753558818291	H
-1.51319484635256	-8.59370963661955	-7.06907249531943	H
1.11639760045532	5.81925830269362	-8.50821273318235	H
-1.87785729033681	9.75695356106329	-5.37922222100860	H
-3.26791754729504	7.59249087630518	-7.50124542435759	H
-1.20252945205146	9.96543198603507	-8.64551460337302	H
-2.71347930312777	-1.88378914233357	7.74449293021130	H
-4.84158553660659	0.67846856400011	8.31779631566040	H
-5.85286520167749	-2.01645740274531	6.49314050008139	H
-7.14055707554670	0.78886261622906	3.29728200991933	H
-5.94261776956091	3.57049680120298	4.86519200208717	H
-4.88027580031531	2.77006338861326	1.73929308273492	H
5.22294182593629	-2.41124775892591	6.87939874037624	H
4.22907221261632	0.33397706242217	8.63578629050927	H
2.00647397678199	-2.10070330713127	7.88390751481177	H
4.90724031007693	2.38901134527638	2.06789765225273	H
5.78345743105342	3.14325227930326	5.26496745720610	H
6.91051875907092	0.27884239728759	3.79741328923064	H
3.63915057088832	-6.26710651440559	-0.06511620137124	H
1.76283907696226	-8.98708836698250	0.61935980369217	H
1.94446448604556	-7.82137834924288	-2.57179515680442	H
-2.75831306821955	-7.56382183309307	-2.55683041135608	H
-2.74689722944528	-8.67903457493036	0.65859619840664	H
-4.24442246230402	-5.74818946233232	-0.08944832189060	H
1.68135595295835	6.65305483952762	8.02890813142958	H
-1.99026012200907	3.36032518114069	11.19405100440295	H
1.33483488494380	3.14940522931965	11.33328606497039	H
-0.20347442876681	5.93630608250479	12.35643510321479	H
-0.87875691361224	-5.75706550847083	8.43809253560614	H
2.11463059264134	-9.61655631859779	5.21152220770870	H
3.51008601922389	-7.44465566969211	7.32175729613071	H
1.51459891326355	-9.86490230698965	8.49028300659896	H

Zn(EtZn)₄(O-NMe₂)₆

Level of theory: PBE def2-TZVP + COSMO

Compound geometry #: **4-Bcosmo**

0.00334670592108	0.05839444362913	-0.04916690833121	Zn
0.15391445728959	-2.88757037200365	-5.42844771086638	Zn
-0.06611775650290	2.99668885873473	5.34510131637226	Zn
0.38416253342501	4.28653691072701	-3.88942597020362	Zn
-0.32001576183216	-4.17248245795084	3.80356245979370	Zn
0.10044653107223	3.57454081626290	1.56151326741186	O
-0.14134777497724	-3.46576248033125	-1.65997369576073	O
2.47530382363892	-1.60399999198756	2.92959033409347	O
-2.42963668908853	1.71389515637734	-3.06019501298866	O
2.85714577272114	1.46965932347861	-2.77774890695375	O
-2.80801665892320	-1.35003773595174	2.73748828038766	O
0.26675192609445	5.75353360933673	-0.02738402908093	N
-0.28823811825857	-5.63876295015510	-0.06233452372255	N
3.03493692640418	0.23340202993682	4.87388096528599	N
-2.95821780331899	-0.12323285518083	-5.01362814177924	N
3.44092580279274	-0.43624151054469	-4.64573615492705	N
-3.36293300393634	0.54214368249448	4.62873617386211	N
4.36516465774234	0.82545717306793	-6.94502138849330	C
5.51226653702638	-1.93521994320767	-3.54507241867212	C
-2.65458975111279	-6.98695820260992	-0.61567861615165	C
5.32757977074819	1.55095536454282	4.00083480565087	C
0.69392085892763	6.88086327854046	-6.64936987253378	C
-5.27247723096689	-1.43081977136348	-4.18665729765383	C
-0.03532277079433	5.48323655602153	8.21723073180837	C
-0.58293910170634	-6.77581337331592	6.55951525941053	C
-5.45107718766191	2.04948793509681	3.56967288037769	C
0.27305416451726	-5.10445407440753	-8.50918972186738	C
-1.32477020073395	-7.52695893506797	-8.44091389751476	C
2.59653734800976	7.13377673627802	0.59650355969701	C
-3.48968075071130	1.22915381101365	-7.38486849751197	C
-1.96032685165906	7.35030917628969	0.43307243892999	C
-1.61745106637843	8.59147408997661	-7.05037176025733	C
-4.26061741981030	-0.74316713577871	6.92657765625744	C
3.62413669254673	-1.12598607354597	7.22879408264599	C
1.90285459464173	-7.26634673090326	-0.57653859749703	C
-0.22791237397933	4.40469018063633	10.90648940828992	C
1.73854097152284	-8.48177923661317	6.92113335373986	C
2.36478315972351	8.05170957335150	-6.20610613770748	H
-1.59880135393624	6.82639379719144	7.88998865521495	H
-2.25662087468418	-7.95041833446068	6.13762433314853	H
2.26979982843550	-5.59221520297951	-8.86762740622203	H
2.84631952866589	1.95852405242208	-7.78582125234227	H
4.96475603080753	-0.62193550113454	-8.30957411494746	H
5.97404581370175	2.07379170971621	-6.49069330405214	H
7.18922887549207	-0.72768082577125	-3.26134129850602	H
5.98339996068613	-3.50471730577285	-4.82407721906917	H
4.88425934412198	-2.66967732879426	-1.71613070302027	H
-5.03704563459346	2.60055490689638	-7.10696529437614	H
-4.03164868862607	-0.15203228953273	-8.83888655339670	H
-1.79269297879239	2.24181486627557	-8.01533233507893	H
-4.91900385855729	-2.26456339585091	-2.32831143511777	H
-5.75069901934147	-2.92011146514930	-5.55594189967343	H
-6.84517390077340	-0.06778827487344	-4.04819513529177	H
-3.66340899206780	6.31473140577938	-0.12862424535183	H
-1.80094730485860	9.07311628361214	-0.71513304072554	H
-2.08454047497826	7.87363685039559	2.45007975213438	H
2.61581255997756	7.67566341594626	2.61229388893011	H

2.69653223440941	8.84338410285586	-0.57830171247408	H
4.22704831535970	5.92770593645915	0.17766076254326	H
-0.31342628495649	-3.92943148367014	-10.13119313977821	H
-1.20021264716199	-8.63179140834261	-10.21096417142497	H
-3.34327606718250	-7.11862868734332	-8.12962678314136	H
-0.73533610848513	-8.79877521523703	-6.90050131802766	H
1.15823047960545	5.91598018251207	-8.44039611240895	H
-2.08409638921234	9.67802912696178	-5.33654463403988	H
-3.31741137833904	7.48951778068384	-7.53210277104605	H
-1.34464823550741	9.98306691525895	-8.58585593260600	H
-2.72807366215006	-1.87023413297621	7.75000715261542	H
-4.86561530085979	0.68877891267622	8.30463436944905	H
-5.86219667194190	-2.00080101733813	6.47259728152237	H
-7.12490257986618	0.83819393077999	3.28527657642605	H
-5.91506933426026	3.59913560878848	4.87505448554403	H
-4.84126617280046	2.81412236577300	1.74778173490741	H
5.16002148694805	-2.50032002521047	6.90504044147341	H
4.21117461138622	0.24978596010946	8.67025679457836	H
1.94211366607615	-2.13655709111805	7.90098875412324	H
4.94040690274820	2.36087898443670	2.13828241156183	H
5.81323007463702	3.05648925900151	5.34922469995204	H
6.90817171855484	0.19832492360874	3.85109664428764	H
3.63551851624105	-6.25584374349107	-0.06308852466129	H
1.74882108457234	-8.98605846595089	0.57678804141661	H
1.96785174323316	-7.79428722779480	-2.59578145734435	H
-2.73831976011961	-7.54001883603949	-2.62646305945311	H
-2.74847893066264	-8.68813171908850	0.57175003013169	H
-4.25367267432190	-5.75245457541187	-0.15898081447446	H
1.71133079729495	6.61176998110991	8.04007830573759	H
-1.98468164889839	3.32237191083075	11.18426788946596	H
1.34050784438766	3.10438438128818	11.33557830341323	H
-0.19723266159724	5.88912338717026	12.37752634250623	H
-1.02256322297871	-5.81758400486975	8.36047390262911	H
2.18586572894902	-9.55788786460245	5.19560504002195	H
3.44125272550552	-7.37704313939837	7.38638594802277	H
1.48931248077912	-9.88177756609480	8.45293822827467	H

Zn(*i*PrZn)₄(O–NMe₂)₆ Aggregation motif: **A**

Level of theory: PBE def2-TZVP

Compound geometry #: **5-A**

0.00159114985068	1.60874131618631	-0.00098265786503	Zn
3.28761983748880	-0.30504156775050	-4.99173754810913	Zn
-3.28659371591051	-0.30859425387790	4.99147109664958	Zn
3.38543019986543	0.27850791566815	4.79295720037448	Zn
-3.38444187282041	0.27709251039718	-4.79312349632087	Zn
0.24217603083550	-1.93440169156237	4.99700421632034	O
-0.24099495167081	-1.93556198373376	-4.99129913152320	O
0.94721226199790	3.16351014913609	3.33571716052846	O
-0.94850483503574	3.16447579946115	-3.33614423875442	O
3.26339732111592	0.13929931127400	-1.01068251144522	O
-3.25281485180027	0.12387725197309	1.00952410900049	O
0.85457408149930	-4.29211727356435	6.24199015732088	N
-0.85535831806466	-4.29307347525609	-6.23601106215753	N
1.30014139312842	3.45285186776615	-4.90601387747232	N
-1.30179112450566	3.45113788568235	4.90485736475425	N
4.85236453749526	-0.80243274339972	0.97686774252837	N
-4.85401615859917	-0.79717930327516	-0.97741765298745	N
-4.95198147856220	-3.56629215937667	-0.77997901118389	C
-0.71833045824020	-6.25056951637322	5.13485032779010	C

-7.37121333264144	0.30848464973142	-0.57332795189572	C
-0.34720892852007	-4.01936357558659	-8.92764890450844	C
-5.96731838677965	0.82456900153608	-7.54912542883095	C
-7.76191621004886	-1.42584979023845	-7.89252466839738	C
2.77647901063587	5.52646405344933	-3.79092396786815	C
7.38008937877995	0.28085873563756	0.57831305083406	C
-0.42912291020325	4.19666340033712	7.43472137662203	C
-2.77926446773789	5.52337246062783	3.78880747400501	C
-6.35869022742596	-0.69105603330575	7.23537600061499	C
5.96896055925024	0.82812546711681	7.54782151743313	C
7.75931405643321	-1.42456666583393	7.89825054018782	C
6.35715010019520	-0.68608416245406	-7.23945781020818	C
7.90729288227271	-3.08305692616381	-6.75168723300288	C
4.92538168604663	-3.57243377103308	0.77343488774816	C
0.42670028062063	4.19704134566982	-7.43591001469338	C
0.35184253829900	-4.01448619106807	8.93425916837741	C
0.71437148088014	-6.25202271617746	-5.12493115253333	C
7.45782328508345	3.30047186852733	7.28484526521237	C
8.08253668441334	1.64293969961585	-7.22511856428546	C
-7.45174592413360	3.30023376296773	-7.29252322464621	C
-8.06977913970798	1.64856730561979	7.24239822489660	C
-7.92357476720552	-3.07419221838528	6.72710755829060	C
-5.55031240394283	-0.87697679109521	9.15377170733743	H
-6.15945634529207	-4.30583668914144	-2.29954790557248	H
-7.23221637763360	2.37133862151923	-0.70272131599960	H
-4.45430306446013	5.85913153529369	4.96896634181383	H
6.12119882898930	-4.32652163720022	2.29508815064659	H
-0.73730520366850	5.92450473949116	-7.33613244686004	H
0.83068226729254	-5.79876610675451	9.88820263675073	H
0.30969974397605	-6.39872597651909	-3.09536471592325	H
-0.31829233111503	-6.39781512826728	3.10443351418143	H
7.25928482236173	2.34474827763698	0.70883458175606	H
-0.82696328521875	-5.80423686544538	-9.88026011558400	H
4.45113399284542	5.86265776524780	-4.97151369335625	H
0.73451596711316	5.92458221828437	7.33464523197585	H
-5.71197474055281	-4.14688044111360	1.07471589943827	H
-3.03600462196906	-4.30705934229273	-1.02546395340720	H
-8.11509289537230	-0.22212981038898	1.30185915466555	H
-8.65384073905244	-0.37822690197493	-2.05366801047649	H
-2.77071723403883	-5.87131649282000	5.38801889862724	H
-0.26228272253525	-8.06648345640682	6.03789211875511	H
-1.65559708880804	-3.54790322921406	9.33261921822537	H
1.56276993564309	-2.51592160854441	9.70499741617673	H
8.12248928553328	-0.25515278383383	-1.29594431020876	H
8.65372546572597	-0.41858012514753	2.06044834974517	H
5.68568864266338	-4.15600404144503	-1.08025846774235	H
3.00202544683248	-4.29631435648401	1.01144785074395	H
1.66155539697809	-3.55603094359381	-9.32296271497483	H
-1.55471970005654	-2.52011302228407	-9.70242738791436	H
2.76734218221780	-5.87364652579611	-5.37371744723779	H
0.25981851896603	-8.06797445074433	-6.02854553067739	H
3.40561248063172	4.97629848126825	-1.89396721014324	H
1.62588113702435	7.26135596278493	-3.67615519841317	H
-0.69551389850497	2.66153827605452	-8.26160151386759	H
2.08907581897069	4.53399094813369	-8.63419703038526	H
0.69333882311527	2.66181228642073	8.26130860623475	H
-2.09172332602626	4.53364134870094	8.63270036686776	H
-3.40749086893525	4.97207305244865	1.89195843069993	H
-1.62965870062470	7.25910718805536	3.67307305422499	H
4.82826863280884	0.97856660679887	9.29484547194846	H
6.73364790227301	-3.20724598303638	8.21021228698009	H
9.04558674557813	-1.14531419786035	9.52608943403556	H

8.98635515303706	-1.70913493491196	6.23590901691770	H
5.54801827577333	-0.85007275258682	-9.15953915311446	H
8.76543287798606	-3.08526412690679	-4.85125715767044	H
9.48946653129673	-3.26543066700586	-8.10926686806870	H
6.76629104065849	-4.81708900986751	-6.90707756681667	H
-4.82703653102423	0.96800303474984	-9.29704700351145	H
-6.73957030563645	-3.21122763711639	-8.19999453491049	H
-9.04844023284003	-1.14893869360097	-9.52056765272478	H
-8.98875699562638	-1.70348087273473	-6.22881120356956	H
-8.73990645021536	3.59967607061425	-8.91518426743593	H
-8.64508941487373	3.31556511538879	-5.58454858190565	H
-6.20587559105453	4.96248457935799	-7.17673778224627	H
8.74566444735908	3.60240294618969	8.90730599697576	H
8.65214187478195	3.30863548771370	5.57750368090408	H
6.21488391805949	4.96451603552127	7.16349646751505	H
-9.50482245016441	-3.26020179332793	8.08525600108213	H
-8.78452478646750	-3.05323325996029	4.82810422658911	H
-6.79248643166807	-4.81624997122891	6.86416187428835	H
9.69886147370032	1.40925987985949	-8.53409442956579	H
7.08551878647196	3.37672422912664	-7.80332012124637	H
8.89713548807275	2.00447086651867	-5.34110832393226	H
-9.68900465942345	1.41181856976189	8.54723747851050	H
-7.06258506368360	3.37013853170430	7.83917390523316	H
-8.88013172755448	2.03395249219609	5.36123013344532	H

Zn(*i*PrZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

5-Acosmo

0.00163272383727	1.62625719263038	-0.00123399151127	Zn
3.24540712327930	-0.27902003159396	-5.00846729826119	Zn
-3.24609687351149	-0.28357994203301	5.00731456499645	Zn
3.41104544478931	0.24798127114581	4.75573714400998	Zn
-3.41045207061697	0.2437350553290	-4.75702971704782	Zn
0.26916699677042	-1.94581186115664	5.00657379214435	O
-0.26709774607388	-1.94766190356022	-4.99991250565548	O
0.98543576322073	3.15950770806278	3.34020526135430	O
-0.98687195548499	3.15860630844429	-3.34091579857978	O
3.24619702902465	0.14575839700988	-1.03261278937526	O
-3.23529708562952	0.13064814260845	1.03211201180943	O
0.84176173472070	-4.29740283904219	6.28392130225751	N
-0.84062033981594	-4.29930768351901	-6.27694443141583	N
1.25580084669581	3.45733807886532	-4.92819737877526	N
-1.25845591265804	3.45756673579161	4.92611489999207	N
4.85114944325062	-0.80931134845490	0.93837778984599	N
-4.85215855728894	-0.80452278108957	-0.93825495761286	N
-4.94374793948929	-3.57382460985743	-0.71931689555855	C
-0.75984208385753	-6.24099427136921	5.18396243404807	C
-7.36899857299181	0.29862972518121	-0.51635080326422	C
-0.31303889099047	-3.99234615347838	-8.96328725965559	C
-6.00707256659992	0.78279281418586	-7.50903109821125	C
-7.80075009298400	-1.47030183054420	-7.84060631804410	C
2.72939269136119	5.54251161227586	-3.82783221933317	C
7.37856625908916	0.27083184596097	0.52114881926288	C
-0.37147490860620	4.1907485558033	7.45541388358747	C
-2.73240680538949	5.54070881303887	3.82324963217415	C
-6.30819484125030	-0.65952783365175	7.27549678740798	C
6.00882623294366	0.78988306862735	7.50640815760230	C
7.78840639841795	-1.47194400301479	7.85407817942826	C
6.30665282429288	-0.65562932754492	-7.27762084017777	C

7.87020699650132	-3.04748093199656	-6.80559924498617	C
4.91741270870661	-3.57887773895565	0.71470407277292	C
0.36696602078707	4.18945031366250	-7.45740565549081	C
0.32472685040429	-3.98410883495214	8.97149812200854	C
0.75542768237157	-6.24414444571728	-5.17045088840397	C
7.51392171081641	3.25155440411570	7.23099750393564	C
8.02407987980431	1.68015408680036	-7.26596689584390	C
-7.49687070713156	3.25530551154277	-7.24818645766693	C
-8.01053053962695	1.68732559948838	7.28476589669250	C
-7.88758303317230	-3.03720081894706	6.78465351464782	C
-5.48292475112205	-0.84152173943443	9.18771875712073	H
-6.19107714155258	-4.32498339969612	-2.20018607760510	H
-7.23891734838241	2.36178983268851	-0.64848238130353	H
-4.38626345594044	5.89600010249877	5.02607388158512	H
6.15408196266104	-4.34402995473764	2.19736282596982	H
-0.79918241353849	5.91535279325978	-7.36032283787963	H
0.76223447781353	-5.76690342548107	9.94818067132389	H
0.33547183621301	-6.42030854474304	-3.14658008795771	H
-0.34236933853482	-6.42251196603269	3.16006706715518	H
7.26756560460123	2.33492358871339	0.65561420973162	H
-0.75081485958594	-5.77630292590537	-9.93779284385457	H
4.38203424766750	5.89793329287555	-5.03224761859480	H
0.79410282826697	5.91715181304345	7.35897168331522	H
-5.66931605085073	-4.13956908865248	1.15290334014101	H
-3.03357254375313	-4.32120016691578	-0.99216885932281	H
-8.09425487945377	-0.23136679432022	1.36577915905878	H
-8.66727669563000	-0.40206202438178	-1.97581127193987	H
-2.80430712548273	-5.81024619623534	5.41022696637681	H
-0.35694857974380	-8.05317033206239	6.11937713248567	H
-1.67843065608324	-3.48105981767237	9.34466244625192	H
1.54735732497550	-2.49185404975794	9.73660120489728	H
8.10119206603552	-0.26371891479952	-1.36070146351393	H
8.66834250146822	-0.44393836724517	1.98134439161063	H
5.64198682384304	-4.14813144016485	-1.15682830242112	H
2.99974832620295	-4.30882434699645	0.98216464636619	H
1.69256581152630	-3.49452789960321	-9.33025139071599	H
-1.52947484155870	-2.49909737205917	-9.73631396644443	H
2.80091884557505	-5.81823029138867	-5.39539828124825	H
0.34921014905673	-8.05742788623528	-6.10216928148775	H
3.39195731576119	4.99580990906900	-1.94118203083104	H
1.56953326737179	7.26982949714411	-3.70154367613743	H
-0.74719792275198	2.64478018000251	-8.27693664574198	H
2.02171084286987	4.53675750796907	-8.66218577199851	H
0.74271549110613	2.64663211213275	8.27591052416369	H
-2.02708333577423	4.53772126856746	8.65913764289026	H
-3.39309493121263	4.99231202501484	1.93638779428572	H
-1.57389853596450	7.26891675916564	3.69612016061316	H
4.86863886352141	0.95142446273087	9.25241165971934	H
6.74798714819573	-3.24134043149943	8.19701443596214	H
9.09828555304344	-1.19045976785161	9.46613974536236	H
8.98625121807056	-1.78437629174628	6.17605570430434	H
5.48183626856387	-0.81605578291697	-9.19200465719357	H
8.73501583761020	-3.04822548430198	-4.90821540903531	H
9.44748247401352	-3.21947629400262	-8.17382937952753	H
6.73401261951907	-4.78555325130685	-6.95586841954185	H
-4.86754660150990	0.92598685211336	-9.25706794621823	H
-6.77138196428999	-3.24833997906107	-8.17203791865052	H
-9.10951052942469	-1.19166352373627	-9.45405116389588	H
-8.99991205212108	-1.76380661701397	-6.16011585989763	H
-8.80797818408833	3.54406897381379	-8.85786507827834	H
-8.66512051750694	3.27673312218032	-5.52271672547559	H
-6.25035597726024	4.91986557391585	-7.16122690579217	H

8.82496115761329	3.54298805016227	8.84026983331439	H
8.68426344860830	3.25453828251739	5.50686947767539	H
6.27755103367482	4.92300063045061	7.13164134514826	H
-9.46313885942070	-3.21192494625523	8.15442944559993	H
-8.75630738792796	-3.01479621962449	4.88920286907373	H
-6.76194466933242	-4.78364462737670	6.91634856582785	H
9.63601294432529	1.45519346586944	-8.58564050376636	H
7.01548551632227	3.41184101971465	-7.82823238785143	H
8.84468423480035	2.03411878814248	-5.38289962909579	H
-9.62357854287939	1.46125003982599	8.60285969312426	H
-6.99066206687040	3.40744740522199	7.86207172321491	H
-8.82931319811936	2.06301459855422	5.40508879957873	H

Zn(*i*PrZn)₄(O–NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP

Compound geometry #:

5-B

-0.00085226672524	-0.00096376059839	0.00293852496176	Zn
3.07806993749880	-5.33353052001158	0.18208083320921	Zn
-3.07786017783915	5.33289557185264	-0.18395733178608	Zn
4.14935031386281	3.97360951360968	0.03165292161380	Zn
-4.15180506879871	-3.97398556921572	-0.03379209219689	Zn
1.39033804677776	2.95472558844482	2.62072962875602	O
-1.39121487994963	-2.95161887781001	-2.61954665986466	O
1.54867257473330	2.82795327522323	-2.66778571240409	O
-1.55085142957633	-2.83448039111900	2.66890821004221	O
3.57350713577796	-1.52685757012974	0.10537304848400	O
-3.57490175405563	1.52614136372427	-0.09713572995776	O
0.35075783519414	-4.67992697944994	3.32767448384856	N
-0.35305007363698	4.67168399174371	-3.33093804179645	N
0.52696917738649	-4.83076874118466	-3.11695673278052	N
-0.52760601527209	4.83473905690470	3.11566227001601	N
5.70642083388876	0.12861857617184	0.12007134247278	N
-5.70835024481220	-0.12851653093201	-0.11077388728831	N
-0.73741102836166	-7.18921942685875	-3.87571789298652	C
1.96758907122694	-3.84869480169832	-5.28824699997388	C
-0.92415759670308	-7.02122839565268	4.11601553551849	C
1.69043419984986	-3.60567973222422	5.51778453888383	C
-7.22579130697767	0.36553549770279	2.16480472528420	C
-7.19396642023749	0.37168088881253	-2.40421419628432	C
5.43572882770088	-8.31840669737271	0.58368554373842	C
4.21976341907187	-10.85624535576051	-0.11676243108498	C
7.97071966800677	-8.02006799009768	-0.78868120246936	C
-6.59906912820446	-6.91458545085080	-0.04937666799086	C
-8.30587214041365	-6.99067907441037	2.29294898006350	C
-8.19529667442500	-7.05026215611085	-2.46597802255449	C
0.73649451092986	7.19467128828298	3.87025091374898	C
-1.96772135209338	3.85613276584590	5.28901044954594	C
0.92278187569204	7.00975964451383	-4.12739735921281	C
-1.69392641472402	3.59104568894200	-5.51728187159133	C
7.23132631637509	-0.37232528560478	-2.14922014949023	C
7.18443841840007	-0.36325270789327	2.42023151948423	C
-5.44007141957363	8.31455543443248	-0.58203392263451	C
-4.20371963969867	10.86225279682381	0.04319159262119	C
-7.93972059181855	8.04414688724413	0.85943445847785	C
6.59547486809047	6.91498985235679	0.04107509875806	C
8.30096452026851	6.98812038450798	-2.30230123732121	C
8.19305734832874	7.05454238700370	2.45656529404355	C
-1.82970894467723	-7.94932607244917	-2.28654847585419	H
0.70369074577798	-8.57832159239858	-4.42882010040269	H

-2.02720616800736	-6.83218391968843	-5.47615952966669	H
0.71841360621339	-3.67757249341081	-6.94982318394528	H
3.53952796064138	-5.14131886215929	-5.71463169624171	H
2.69941028811793	-1.97992520688633	-4.79336160188048	H
-2.26408340527838	-6.63317113557417	5.66793844011303	H
0.50964416333543	-8.38417296471620	4.75123959455083	H
-1.96523447180420	-7.83084210037374	2.51637325321699	H
2.42999573715459	-1.74973760200414	4.98471910328086	H
3.25219880090796	-4.86798690782250	6.05673269359031	H
0.37321723658996	-3.38326646283571	7.12002708507432	H
-6.10428766507755	-0.11921529629421	3.83662511749848	H
-8.91628219862743	-0.83970571211080	2.11817383013542	H
-7.80001120985857	2.36982306073510	2.25032430544136	H
-7.77090752951385	2.37655426711052	-2.48513040228917	H
-8.88238806119071	-0.83717347838170	-2.39006392302796	H
-6.04837065310427	-0.09468664420185	-4.06449024831122	H
5.84420836383195	-8.37277791293523	2.63416747506024	H
3.78251657394219	-10.96810394615368	-2.15117790631363	H
2.44328429505240	-11.20956755003703	0.90775287953714	H
5.49879845509554	-12.46084439110040	0.29623544149854	H
9.22565124043737	-9.66215164353496	-0.45471169895384	H
9.01441003508353	-6.32637779120660	-0.17753415085680	H
7.72523661551013	-7.87594609637840	-2.85389544285990	H
-5.41901041590881	-8.64150649311971	0.00000755890665	H
-9.57158838291289	-5.33672982725291	2.38016175531116	H
-7.22213657561044	-7.01999818359473	4.06869489013753	H
-9.54556684675636	-8.67708626674029	2.29346109598931	H
-9.43875571628143	-8.73388200161209	-2.47981271145805	H
-7.03017625140440	-7.12890880039282	-4.18786861244514	H
-9.4499958992931	-5.39647353571978	-2.65601082556375	H
1.82839747437276	7.95241955499734	2.27967931943233	H
-0.70505134897571	8.58425155466868	4.42129709855526	H
2.02646350542860	6.84090878769386	5.47129348350815	H
-0.71769173062793	3.68656948205578	6.95008396622484	H
-3.53886655630915	5.14998892809148	5.71445973111533	H
-2.70088238518881	1.98727246415406	4.79673098452151	H
2.26352971536597	6.61503164933113	-5.67691464176471	H
-0.51018273543453	8.37049701285237	-4.76907672452770	H
1.96294979226802	7.82542425402945	-2.53023061884051	H
-2.43206498785114	1.73605031178033	-4.97888362734394	H
-3.25644690644753	4.85141022553018	-6.05857139763390	H
-0.37764108670924	3.36485107649980	-7.11977008224809	H
6.11526508726588	0.10662404753524	-3.82630532018905	H
8.92130131264572	0.83354898264108	-2.10107180383065	H
7.80660446618756	-2.37665631235035	-2.22648729330784	H
7.76219777932173	-2.36746846131236	2.50989338048781	H
8.87221377283437	0.84639345477296	2.40780656667165	H
6.03277662867699	0.10827377891249	4.07490075250050	H
-5.90026332585165	8.33368513744719	-2.62210534976705	H
-3.71200898239996	11.00808678290023	2.06293523003435	H
-2.45493823938627	11.19611269619284	-1.03397528229965	H
-5.49197276238694	12.46126391041970	-0.36281807076066	H
-9.20078621699890	9.68231124758129	0.52927086446264	H
-9.00063770715987	6.34186977039405	0.30445575248481	H
-7.64203572996910	7.93525705743934	2.91996217674288	H
5.41478876654253	8.64142334514652	-0.01016861917635	H
9.56626880235511	5.33381775846444	-2.38849167044392	H
7.21618960580037	7.01573118078853	-4.07744621431624	H
9.54091811916412	8.67433860417154	-2.30538527123606	H
9.43573971252647	8.73875182722396	2.46756728267850	H
7.02893470098647	7.13476317359638	4.17906059646652	H
9.44870701689147	5.40161926142452	2.64787933173067	H

Zn(*i*PrZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

5-Bcosmo

-0.00078234683869	-0.00024377473959	0.00479045709200	Zn
3.06389131834248	-5.32854920052657	0.17908939590087	Zn
-3.06396690740902	5.32732654737528	-0.18553714327677	Zn
4.14748893309925	3.95813454196219	0.03566481132043	Zn
-4.15019880113473	-3.95849359002826	-0.03201385940653	Zn
1.39271721264712	2.96352982497012	2.62539347416156	O
-1.39487339077019	-2.95954628116344	-2.62047829510977	O
1.55311721184588	2.83533454757090	-2.66655550034614	O
-1.55337610439878	-2.84174261068687	2.67414653235346	O
3.56549847417800	-1.52947484155870	0.10143863757057	O
-3.56692710753561	1.52844305080043	-0.09686171959155	O
0.35186332529229	-4.68886538656835	3.32422006350767	N
-0.34948226969627	4.68130270046098	-3.32831132173417	N
0.52349585977896	-4.84171403801971	-3.11577754334249	N
-0.52831277304424	4.84457697391493	3.11340215692645	N
5.70590871796294	0.12241271380887	0.11901876472121	N
-5.70532857187725	-0.12157556489694	-0.11421130008924	N
-0.74106009054890	-7.20090927599923	-3.87293054615784	C
1.96538942939061	-3.86389387325293	-5.28895375774604	C
-0.91749631021420	-7.03486655298323	4.10869473442405	C
1.69702367672552	-3.62139091970465	5.51457389328252	C
-7.22607854543052	0.37981616209894	2.15803005519551	C
-7.18606358333069	0.38213107726174	-2.41071674573346	C
5.41742682496479	-8.32290235710520	0.58254981801365	C
4.19680135038356	-10.85534773559534	-0.12789859031304	C
7.95630861247084	-8.02951473368857	-0.78485450597575	C
-6.60398241752959	-6.90113248673327	-0.04261333626216	C
-8.30682456265206	-6.97306871163312	2.30282658133367	C
-8.20580544440078	-7.03346815525223	-2.45582641091812	C
0.73423628756696	7.20487203281261	3.87133183740051	C
-1.97603614941283	3.86999958010274	5.28383826766791	C
0.92310123949817	7.02264947010364	-4.12083055905711	C
-1.69163228655452	3.60500132035202	-5.51656188573254	C
7.22655286682306	-0.37811729782844	-2.15396336341564	C
7.18700466720912	-0.38216887179501	2.41512358831277	C
-5.42387457234068	8.31658311114242	-0.58673934202666	C
-4.17960294801895	10.85982260833453	0.04160611195051	C
-7.92506765126969	8.05400748097433	0.85452494860605	C
6.59869496232509	6.90286725581037	0.04517580561788	C
8.30146718756100	6.97595432424830	-2.30029056815123	C
8.19979800333748	7.03840223157066	2.45864210364675	C
-1.81795106537687	-7.96986173210154	-2.27695433358355	H
0.69764739990808	-8.58378479218279	-4.44661943584629	H
-2.04146793513687	-6.84093902332047	-5.46402181530696	H
0.71364015666136	-3.69243708334598	-6.94851171364080	H
3.53059522270296	-5.16253860286385	-5.71993993843951	H
2.70396452937699	-1.99757525392352	-4.79437260564545	H
-2.26381695381882	-6.65016355773245	5.65595001415972	H
0.51680433766347	-8.39161092886377	4.75521368972419	H
-1.94639956614899	-7.85079383448708	2.50399743329766	H
2.44263611880681	-1.76761252651428	4.98141208161971	H
3.25404317413155	-4.88914995672715	6.05325748625611	H
0.38053236850441	-3.40060281524675	7.11770839045820	H
-6.11430888557414	-0.11061326052191	3.83501884983450	H
-8.93037766981055	-0.80493096204888	2.10103400929738	H
-7.78504268495690	2.38827246215095	2.24337200104630	H
-7.75070446175426	2.39015651963447	-2.49662560958330	H

-8.88675899896341	-0.80877466608246	-2.39057981840709	H
-6.04410554002473	-0.09255692225207	-4.07134617664643	H
5.81768038092959	-8.37942408161079	2.63493848353895	H
3.74963155054378	-10.95227370589345	-2.16117645009026	H
2.42268816414680	-11.20548574044385	0.90276589087214	H
5.47594788028037	-12.46668553621731	0.27429004575520	H
9.20973407275062	-9.67717874996320	-0.45241946051101	H
8.99971552054808	-6.33653696174963	-0.17008295862258	H
7.71153231774635	-7.87792464019510	-2.85015189433949	H
-5.41801830941046	-8.62394715296238	0.00493029686510	H
-9.55693544236404	-5.30743339478850	2.39703323496298	H
-7.21289392249921	-7.01409089804460	4.07303181283028	H
-9.55979648853259	-8.65356105950625	2.30450276888420	H
-9.46176502813633	-8.71174385374906	-2.46656572754684	H
-7.03782964439161	-7.12316025188242	-4.17622600647126	H
-9.44645824216190	-5.36903659429228	-2.64726895001836	H
1.81446451968269	7.97191397525811	2.27679181709048	H
-0.70607369110067	8.58805179498900	4.44070648111617	H
2.03122561662064	6.84615844836509	5.46547312538454	H
-0.72884300766930	3.69937993910772	6.94692434324345	H
-3.54191846487072	5.16961184976537	5.70908534848431	H
-2.71512336532502	2.00419307669913	4.78775478286984	H
2.27281394246379	6.62947860967367	-5.66303459942122	H
-0.50865583629041	8.37694287050160	-4.77765419385338	H
1.94907919855785	7.84569157249560	-2.51777920985464	H
-2.43974294728498	1.75445624948292	-4.97596966882880	H
-3.24590034193848	4.87228414625532	-6.06393633163161	H
-0.37229504997817	3.37305626967276	-7.11594716520780	H
6.11332244825579	0.11164316155353	-3.83014524476930	H
8.93026239648408	0.80750099031126	-2.09742652109674	H
7.78652989984109	-2.38629580806092	-2.23969837241244	H
7.75194979162551	-2.39004880521465	2.49993452097111	H
8.88742985192896	0.80911670660856	2.39601089283802	H
6.04494457866333	0.09140796844066	4.07612151592512	H
-5.87865241172775	8.33428796025285	-2.62842459572983	H
-3.67490797881526	10.99440516185641	2.05918223288062	H
-2.43455564759364	11.18734814392748	-1.04453885434867	H
-5.46663719700926	12.46632270869792	-0.35440689738138	H
-9.18422654224656	9.69790527200858	0.52539125562246	H
-8.98768363088151	6.35211208891028	0.30055913610465	H
-7.62455953778495	7.94101127512973	2.91493172436462	H
5.41079955355586	8.62428730376181	-0.00338827990767	H
9.55314276095037	5.31151331465502	-2.39410982781453	H
7.20774819679447	7.01559889992208	-4.07066209559424	H
9.55278749233763	8.65766743554605	-2.30238060584108	H
9.45377148434968	8.71813112987173	2.46840065213711	H
7.03159354640203	7.12764268352827	4.17894343341338	H
9.44227627705555	5.37548434166817	2.65125816300503	H

Zn(*t*BuZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP, M4 grid

Compound geometry #:

6-A

-0.00056880772572	-0.96277038161858	0.00040251177933	Zn
3.37893898877627	0.30474677039099	4.89986281718259	Zn
-3.37792231583130	0.30572186934936	-4.90228733649187	Zn
3.39040773989712	-0.32744994652640	-4.90532034778681	Zn
-3.38984649107805	-0.32600241590216	4.90575876437274	Zn
0.20435693111867	1.84549950067752	-5.00416061119505	O
-0.20374276995303	1.84761410481399	4.99923409378328	O
0.96554450036062	-3.00359580968986	-3.11271996560093	O
-0.96631172938600	-3.00294574371761	3.11413726059856	O
3.20945696323268	0.66634029827370	0.88741186173112	O
-3.21071174173726	0.66341689112525	-0.88868553750232	O
0.76182818658088	4.49574288046424	-5.39260337551291	N
-0.75829817717344	4.49892895961892	5.38712883736873	N
1.34974482831890	-3.45151583101505	4.53358465690104	N
-1.35016056818487	-3.45166700914813	-4.53299884163535	N
5.04820824999481	0.82076687148910	-1.11884479648456	N
-5.04782085602879	0.82401909107700	1.11851031486512	N
5.85035753439501	3.48233538317024	-1.25241067706147	C
-0.61510035979262	-4.36468088771649	-7.04820235404762	C
-6.44033019874293	0.44937322112943	-7.24573926163768	C
-8.05754693901508	-1.94322293562763	-6.97993597832831	C
7.19513616104220	-0.80472309211590	-0.44457520513077	C
6.44151883681428	0.44868536062391	7.24339600057493	C
8.10419673143050	2.74655707864585	6.64988576791292	C
-6.04460253813724	-1.07368788813332	7.61609356233243	C
-4.89606446658893	-1.12014303870240	10.27908692791785	C
2.70018129659664	-5.46985162206389	3.18354314149597	C
-0.57805793773449	5.03836655353125	8.07915218395899	C
1.07613508416257	5.96585951779542	3.96733184163350	C
-1.04478829826826	5.96369767049237	-3.93834910379524	C
6.04365200562549	-1.07090243103131	-7.61792470746937	C
4.89398198780575	-1.10094152607447	-10.28062705514861	C
0.54116480408278	5.04616923492488	-8.07918430931227	C
8.12507632133562	0.95107108384479	-7.58676689424141	C
7.25106073192213	-3.66467132947902	-7.13096293327606	C
-5.84064433934457	3.48839195712679	1.25293602107393	C
-2.70334280930470	-5.46729293216150	-3.18168554018574	C
-7.20061636836638	-0.79364362468774	0.44459977157740	C
-8.09237649115024	2.75765355361398	-6.66280204965801	C
-5.54918612685138	0.63066603831995	-10.00091538359580	C
0.61566727779167	-4.36097135427602	7.05036798080401	C
5.55004784220994	0.64804774417092	9.99714159944877	C
8.04849136884354	-1.95219157837265	6.98978901315186	C
-8.12053152870988	0.95405496224647	7.59359069722335	C
-7.25875002971595	-3.66207673477002	7.11706966284593	C
7.33904640537517	3.65689510425868	-2.68957237110770	H
6.56259740359871	-2.77439464212602	-0.33868248181431	H
4.49290829046898	-5.85030840150176	4.16027671343123	H
-7.32826173530652	3.66770434077396	2.69072699409910	H
0.64934976584208	-6.01662891433729	-6.89300099290018	H
-1.05469991461837	7.03900505437632	8.38546553775404	H
-0.91504533473163	5.43562489273439	-1.93946804874724	H
0.97477959456519	5.44757741388109	1.96430094683243	H
-6.57435717262574	-2.76506128213494	0.33442303791476	H
1.02436791194237	7.04519579892598	-8.38584348308674	H
-4.49531013305830	-5.84773081433273	-4.15980428176535	H
-0.64942535490862	-6.01270206233052	6.89808813707835	H

6.58181592376661	4.11777109158889	0.59463273030014	H
4.23494548308651	4.63943958568423	-1.83515702664813	H
8.00486135963641	-0.23306376886405	1.39036261322439	H
8.64912020184700	-0.64665123616659	-1.91692549937822	H
3.04553451353315	5.64476661176507	4.63547304941752	H
0.62705288093932	7.98432003080406	4.18321610539958	H
1.34111066719332	4.67276302566857	8.84308741576969	H
-1.94414323251276	3.86974635672983	9.11206543987375	H
-8.01108800899268	-0.21635669543196	-1.38825556799458	H
-8.65212675696864	-0.63338724471541	1.91915348711450	H
-6.57100668725133	4.12642037052778	-0.59366141079509	H
-4.22091615233661	4.63974761113038	1.83532710204785	H
-1.39264918248724	4.69529990585760	-8.81287068642016	H
1.88288585298841	3.87320455652405	-9.13862365840273	H
-3.02538624784680	5.65306818099787	-4.57741686686116	H
-0.59103091127949	7.98139284420228	-4.15201104900503	H
-3.09906858018373	-4.85497991919756	-1.24121404658017	H
-1.54653718360354	-7.20164437967133	-3.11221918803510	H
0.34754718959284	-2.84806563610297	-8.08169575604808	H
-2.33217214669132	-4.89197887754242	-8.09080045911287	H
-0.34588611985561	-2.84261377467874	8.08230802748706	H
2.33310378193643	-4.88741140819672	8.09280734882952	H
3.09404946616545	-4.86052248750163	1.24174694949928	H
1.54200183961111	-7.20341883300837	3.11763514465272	H
-7.37158560879415	2.86070601775519	7.96390909311148	H
-9.54815577228537	0.55696669844305	9.07847554842986	H
-9.15535907773478	1.02552064520711	5.78818741689218	H
-8.87277502165343	2.71315427014164	-4.73242169643559	H
-9.72726784490620	2.84572048531355	-7.97404369720789	H
-7.04979350389830	4.54759509038430	-6.87364830213917	H
7.38087739479863	2.86148080568723	-7.94689966341322	H
9.55055572514803	0.55752983698878	-9.07467152865621	H
9.16156494009774	1.01034802982578	-5.78185494284276	H
7.19566528450799	0.69773621706126	11.29673497184477	H
4.44787988353085	2.37666576098367	10.34947924613361	H
4.37103981793920	-0.96798224775654	10.57317186047332	H
-6.39308892188184	-1.47021679284435	11.70614236376762	H
-3.48892486004590	-2.63326796516841	10.52165224244603	H
-3.98251012619481	0.67700969501588	10.79378988953149	H
-8.70025809508825	-4.09328590320979	8.57917385912383	H
-8.22245582603297	-3.75288188040502	5.27508883321586	H
-5.86381238823920	-5.20584357908485	7.16228515272374	H
9.70879576677039	-1.86246924611585	8.26837051477628	H
6.99104568138309	-3.66926714472468	7.51170695116678	H
8.78889383451354	-2.23170104917246	5.06468666650062	H
9.73848715210746	2.83373772854024	7.96189842394151	H
8.88583114317163	2.68898088666202	4.72038791704236	H
7.06973012019833	4.54229062763983	6.85119079047002	H
8.69193951831548	-4.09270764685075	-8.59464883077131	H
8.21393693823387	-3.76642555140240	-5.28905580298587	H
5.85231151176508	-5.20474564789335	-7.18376756543453	H
6.38896742802872	-1.45048048757064	-11.70997850889455	H
3.48029258864698	-2.60692517547907	-10.52977617737247	H
3.98791852390578	0.70255502005321	-10.78618940889086	H
-9.71774551224877	-1.85244046671260	-8.25859117929262	H
-7.00762614312873	-3.66734718243455	-7.49380746021001	H
-8.79864860355058	-2.21035847623478	-5.05340877777279	H
-7.19517962475546	0.67605916250413	-11.30018750245901	H
-4.44341445942498	2.35469579879370	-10.36397533936940	H
-4.37394621754768	-0.99131848232423	-10.56786361827552	H

Zn(*t*BuZn)₄(O-NMe₂)₆

Aggregation motif: **A**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #:

6-Acosmo

0.00262483033562	-1.06725336884407	0.00335048537440	Zn
3.32240214645737	0.26484519189097	4.96056083761454	Zn
-3.31993794288815	0.25761320794972	-4.96800636066877	Zn
3.43938378583531	-0.26841488555834	-4.86717054590386	Zn
-3.44121115151893	-0.27954726533308	4.86628993327867	Zn
0.24086833998435	1.84186177685027	-5.13223305636114	O
-0.24406386777235	1.84681286070866	5.11827742495111	O
1.01679577720168	-3.00606190298574	-3.14403462614196	O
-1.01272719569514	-3.00542884455347	3.15296358462704	O
3.15763876839257	0.63330976592220	0.94903773795485	O
-3.17483339130385	0.57960940332523	-0.95462376997219	O
0.78090497724901	4.48144709825479	-5.60381623496680	N
-0.77456305456627	4.48865640547608	5.58972265351034	N
1.28566419715926	-3.45544835220181	4.61206689496329	N
-1.28030493234155	-3.45872513823634	-4.60475176304884	N
5.01718838681329	0.82628298361989	-1.03803630489954	N
-5.01623974402821	0.84107954339517	1.03881865173823	N
5.82500685120402	3.48771732470792	-1.10268007460490	C
-0.49772943672199	-4.37700379528924	-7.10497919165279	C
-6.37539919058472	0.39872854654735	-7.33252495865939	C
-8.08719297091223	-1.91161158800043	-6.95595534696837	C
7.15744934219182	-0.81543406284467	-0.37676992271736	C
6.39012960992678	0.39481114317389	7.31205165998692	C
8.01354276392858	2.73590279971698	6.78283748732419	C
-6.16231550173396	-0.97138942493085	7.53311755426435	C
-5.05835608217786	-1.01547863771721	10.21440158422589	C
2.65003928930706	-5.49047420914278	3.29906024270969	C
-0.40186549280878	4.99031458393151	8.27070810665905	C
0.96090711112836	5.98222077124810	4.07213608239178	C
-0.83421794587997	5.97942208605944	-3.96081795382438	C
6.14762476665183	-0.96183874637347	-7.54552172008363	C
5.04050950356767	-0.87587885990372	-10.22461366711550	C
0.24285255298104	5.02362668555587	-8.24850003890947	C
8.25774080229404	1.02561513154028	-7.41038358692268	C
7.30883345547897	-3.58786716869397	-7.12955886636507	C
-5.73956852929339	3.52681765910261	1.10265739788493	C
-2.66125103760167	-5.47363863429756	-3.27768743414539	C
-7.21014059075048	-0.73105020841228	0.38553258525606	C
-7.93417991324114	2.79775355341367	-6.87209116736844	C
-5.47671321957910	0.39950522420605	-10.09156179219107	C
0.50858591640386	-4.34427183975057	7.12456620852008	C
5.50558068409088	0.49552034625235	10.07339584977474	C
8.03578673648476	-1.97171245480671	6.99110426290966	C
-8.20186347458070	1.09150990029689	7.46121912389777	C
-7.41049508079583	-3.54312600020870	7.03431097334416	C
7.30801331410700	3.70320096642133	-2.53945248495844	H
6.52605386937975	-2.78711061284478	-0.31118128968024	H
4.40655534085321	-5.89630056903827	4.32770649581824	H
-7.21101742392234	3.78941785571733	2.54383476109112	H
0.74731886525844	-6.04019947501126	-6.92623939518467	H
-0.86376949144394	6.98327134588941	8.64272347709101	H
-0.47855815972068	5.46104927526526	-1.98669609752169	H
0.71772196625455	5.50124376139812	2.07176403300627	H
-6.63990234194959	-2.72080199394887	0.30761915491953	H
0.72463647611633	7.01002987544471	-8.62992624812572	H
-4.40835436063687	-5.88945408933637	-4.31858100576015	H
-0.75351527898810	-5.99687749125028	6.96742220836255	H

6.57098778998470	4.07148412669287	0.75520091517195	H
4.20711736823966	4.66916876555458	-1.62255710782323	H
7.95042211391401	-0.27502136997397	1.47398490781139	H
8.63096748751732	-0.62589636822125	-1.82500163555843	H
2.96902515010760	5.63685243649829	4.59380457648712	H
0.53931476167920	7.99775220792829	4.35737142498203	H
1.57278926641302	4.63069204095884	8.88038873038072	H
-1.67508583988883	3.79202756823964	9.38514984001763	H
-7.99637081773726	-0.15856507460849	-1.45857040741713	H
-8.66876580024085	-0.50043741503080	1.84280097100203	H
-6.47385772920693	4.13045115750104	-0.75363433176790	H
-4.08441174679794	4.65689688060174	1.61880789012283	H
-1.77686462825883	4.71779899151335	-8.72653096489103	H
1.40935814564600	3.80893873215139	-9.45796100836268	H
-2.87494132871141	5.67506648908779	-4.36519867282229	H
-0.39428012998145	7.99206224094446	-4.23956397505213	H
-3.14887988530720	-4.83742624822021	-1.36589443238526	H
-1.49353035069207	-7.19565205642134	-3.14708842443019	H
0.49453390893400	-2.86371257287684	-8.11499651931246	H
-2.19430146877493	-4.89786159664593	-8.18219897892021	H
-0.46248225499420	-2.81243672958915	8.12712100558554	H
2.20627477691493	-4.87242587575508	8.19657223992287	H
3.11846284493134	-4.88207859955229	1.37339853696606	H
1.47742421033897	-7.21142749460833	3.20168451746567	H
-7.42117014671800	2.98422611138888	7.84032096931791	H
-9.66516386783660	0.72456655622978	8.92270726928337	H
-9.19673275330567	1.17800079995909	5.63484932623497	H
-8.70924185564658	2.88105837392120	-4.94064689803447	H
-9.56797333580560	2.88101868966126	-8.18928356418171	H
-6.81957944284282	4.53133777189812	-7.17205314984743	H
7.54288366166137	2.95611831699583	-7.72168014992940	H
9.70306989497995	0.65760220218163	-8.88935548339907	H
9.26050724874582	1.01317317118773	-5.58642697020918	H
7.15951859288836	0.53347172683563	11.36691375094756	H
4.37430148616042	2.19295598339051	10.48204168185219	H
4.35850715070680	-1.16004461720242	10.60017605449488	H
-6.58527790301416	-1.34292669451695	11.61889746316668	H
-3.66705049534838	-2.53857565178657	10.48567184677280	H
-4.13777006886882	0.77855604700627	10.72893636016648	H
-8.88823487548761	-3.93538601238686	8.47495732335789	H
-8.33810709783980	-3.63338690456461	5.17399790535138	H
-6.03967413099880	-5.10752865968907	7.12426196252725	H
9.69481367918708	-1.88648200282907	8.27574044876397	H
7.00438715162747	-3.71875530658869	7.46062385999877	H
8.77976645472878	-2.18410639342529	5.05935385785620	H
9.65116855216664	2.81022763911950	8.09566650527141	H
8.78801700134167	2.74444814368937	4.84956585230660	H
6.94794857509507	4.50747619331798	7.03579818822834	H
8.77726067717297	-3.98190352393583	-8.57929858108362	H
8.22733699000482	-3.76697735158814	-5.27075757970310	H
5.88858292534450	-5.10341850419593	-7.27181559986746	H
6.55077338386513	-1.21990548872243	-11.64323147341270	H
3.58572232893089	-2.32947928619582	-10.54257718579109	H
4.19461304690721	0.97104738440476	-10.67578968748192	H
-9.73556563468568	-1.81763737075073	-8.25372891258741	H
-7.10120729723242	-3.69887916154189	-7.36846189061937	H
-8.84801015372813	-2.04836543745868	-5.02415391929499	H
-7.12330009165552	0.45915633606642	-11.39367417022953	H
-4.28608526605443	2.04564045160990	-10.53886009344396	H
-4.38554913926163	-1.30780990392894	-10.56974767575904	H

Zn(*t*BuZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP

Compound geometry #: **6-B**

0.000000000000000	-0.00000755890665	0.13840736028882	Zn
3.06278393851767	-5.35405484130397	0.08324623898096	Zn
-3.06284818922423	5.35410019474389	0.08303458959464	Zn
4.21681733520346	4.02146306190975	-0.02164303947718	Zn
-4.21676820231021	-4.02163691676279	-0.02213625813636	Zn
1.46847068540726	2.81042039123918	-2.56400948295075	O
-1.46820423394771	-2.81027677201276	-2.56417955835047	O
1.55259375756009	3.03758065400643	2.68411295077682	O
-1.55284131175301	-3.03757498482644	2.68390508084383	O
3.54233420473669	-1.54573216004488	0.27046901844158	O
-3.54223026977020	1.54578129293813	0.27066366028792	O
0.35702605853700	-4.89151967396319	3.28454903166059	N
-0.35695991810378	4.89205257688230	3.28409549726135	N
0.50466473357708	-4.59216807319652	-3.19133826398295	N
-0.50443418692413	4.59221153690978	-3.19139306605619	N
5.68870086696502	0.09151190340715	0.38132038452309	N
-5.68844008468546	-0.09166119181357	0.38192698678208	N
-0.68706493059242	-6.91656399466749	-4.13445737802769	C
1.92859834097873	-3.40694473792949	-5.27198779176104	C
6.90152554987928	-0.24256909398151	2.86049058891555	C
-1.65250171653321	3.90488204458447	5.54085054253864	C
-7.01908733534292	-6.67326168674054	-0.48106204754983	C
-7.87605947997822	-6.63647437778199	-3.25591211380176	C
1.65226928015360	-3.90359514072662	5.54115856798479	C
-5.46379315838068	8.37722821922779	-0.07776036247679	C
-7.43578340300693	8.21232122193657	2.04266413211487	C
7.01907221752961	6.67311806751411	-0.48087685433681	C
9.30369884136701	6.00448742052424	1.18171222312623	C
5.46335096234141	-8.37743419943412	-0.07752603637051	C
6.85729649731982	-8.43723270997424	-2.62016460048363	C
-7.42902574045821	0.62350019481192	-1.65829750821020	C
-0.92045751189592	-7.26548312581804	3.95264488600470	C
-6.90037659606786	0.24206075750903	2.86155450502711	C
4.01589403743239	-10.87504057715578	0.21470129487472	C
-9.30347396389405	-6.00476710007044	1.18189552661259	C
-1.92819204974607	3.40700709890939	-5.27215975688742	C
0.92086758258191	7.26596689584390	3.95164711032636	C
0.68731437451200	6.916671710908731	-4.13439312732113	C
7.42854386015902	-0.62350586399191	-1.65960708878801	C
-4.01660079520454	10.87494987027593	0.21485625246113	C
7.87558326885901	6.63647815723531	-3.25587431926849	C
7.43515790348130	-8.21286735294232	2.04310254870081	C
-6.24528206116871	-9.38490606527804	0.18839440999200	C
-6.85751192615946	8.43715334145437	-2.62051419991638	C
6.24535387078193	9.38471142343170	0.18883849575792	C
-1.77857294116264	-7.81106800056677	-2.61589381822409	H
0.79587350215068	-8.22967836134091	-4.76109829855436	H
-1.96304238887453	-6.48481814385529	-5.72713790730082	H
0.68431537829701	-3.15753861287940	-6.92754141685583	H
3.54309198512876	-4.61460101841905	-5.77672433495133	H
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-2.34884142559014	-6.92381865532871	5.43539434608144	H
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4.62328053298456	10.07492274891886	-0.92062380784231	H
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-5.55775603727040	8.66298701610383	-4.23218648215779	H
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Zn(*t*BuZn)₄(O-NMe₂)₆

Aggregation motif: **B**

Level of theory:

PBE def2-TZVP + COSMO

Compound geometry #: **6-Bcosmo**

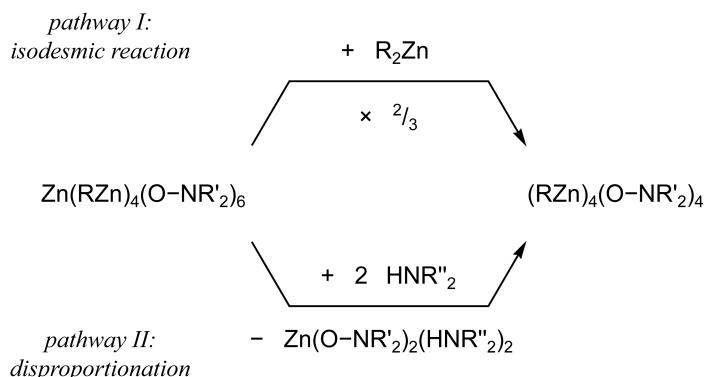
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-4.23195593550484	-3.99653000831140	-0.02643916574917	Zn
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-8.18692707503232	10.09145218804458	-2.61434991154001	H
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-7.98418963966428	6.74926271369360	-2.89707191766778	H

2 Conversion Pathways from Penta- to Tetranuclear Zinc Hydroxylamides

2.1 Scientific Stimulus

As outlined in the main manuscript, two conversion routes of $\text{Zn}(\text{RZn})_4(\text{O}-\text{NR}'_2)_6$ to $(\text{RZn})_4(\text{O}-\text{NR}'_2)_4$ can be envisioned: an isodesmic one with R_2Zn (**1**) to give 1.5 equivalents of the tetranuclear product (pathway I, Scheme 2.1), or a disproportionation by withdrawal of the central Zn^{2+} and two of the six anionic $\text{O}-\text{NR}'_2$ ligands, *i.e.* the extrusion of the binary hydroxylamide $\text{Zn}(\text{O}-\text{NR}'_2)_2$ (pathway II). Since the reaction that resulted in the isolation of $(\text{MeZn})_4(\text{O}-\text{NEt}_2)_4$ (**13**) was performed using an excess of the bulky secondary amine $\text{HN}i\text{Pr}_2$, one could thus envision the "masking" or complexation of the $\text{Zn}(\text{O}-\text{NR}'_2)_2$ unit by two equivalents of amine. The presence of a generic non-tertiary amine, HNR''_2 , should thus yield an inorganic coordination compound of the formula $\text{Zn}(\text{O}-\text{NR}'_2)_2(\text{HNR}''_2)_2$, assumably stabilised by intramolecular hydrogen bonding. Branched secondary amines such as $\text{HN}i\text{Pr}_2$ should foster good solubility of this disproportionation side-product in organic media, as well as a better "shielded" Zn^{2+} centre.



Scheme 2.1 The two possible conversion routes of pentanuclear hydroxylamides $\text{Zn}(\text{RZn})_4(\text{O}-\text{NR}'_2)_6$ to their tetranuclear analogues, $(\text{RZn})_4(\text{O}-\text{NR}'_2)_4$. Pathway I: isodesmic incorporation of R_2Zn ; pathway II: disproportionation driven by amine complexation of $\text{Zn}(\text{O}-\text{NR}'_2)_2$; $\text{R} = \text{Me}, \text{Et}, i\text{Pr}; \text{R}' = \text{Me}, \text{Et}; \text{R}'' = i\text{Pr}$.

2.2 Results

As with the investigations on the energy thresholds of coordination isomerisation of pentanuclear aggregates (Chapter 1 of this supplementary information), the two possible pathways of penta- to tetranuclear aggregate conversion were addressed with and without solvation effects factored in, *i.e.* the respective DFT calculations were conducted with and without COSMO.²⁰ To minimize conformational issues, the two all-methyl representatives $\text{Zn}(\text{MeZn})_4(\text{O}-\text{NMe}_2)_6$ (**3**) and $(\text{MeZn})_4(\text{O}-\text{NMe}_2)_4$ (**13-Me**) were chosen (for details, see

Starting Geometries, page 2), wherein the geometries of **3** in its more stable isomer **A** were taken (**3-A** and **3-Acosmo**, Chapter 1). The optimisation of **13-Me**, Me₂Zn (**1a**) and HNiPr₂ (DIPA) gave the respective pairs **13-Me / 13-Mecosmo**, **1a / 1acosmo** and **DIPA / DIPAcosmo**. Concerning the hypothetical (bis)amine adduct Zn(O-NMe₂)₂(HNiPr₂)₂ (**14**), computational efforts were not extended beyond dealing with the described and least sophisticated, *i.e.* mononuclear case. Computations on any kind of higher-order derivative / oligomer of **14** were considered to be of little additional value due to the lack of reliable starting factors (*e.g.* the order and nature of aggregation of such species). The geometries **14 / 14cosmo** were thus accessed as described; a depiction of the mononuclear species **14** as obtained from the optimisation procedure including COSMO is given in Fig. 2.1, selected geometrical parameters thereof are given in Table 2.1.

The calculated energetics of the two alternative pathways reveal without any doubt that the isodesmic reaction of complexes Zn(RZn)₄(O-NR'₂)₆ to their (RZn)₄(O-NR'₂)₄ analogues (pathway I, Scheme 2.1) is highly favoured. The formal uptake of a further equivalent of R₂Zn to yield 1.5 equivalents of the tetranuclear product is by far lower in relative energy with respect to the formal extrusion of binary Zn(O-NR'₂)₂ from the starting compound Zn(RZn)₄(O-NR'₂)₆ with its concurrent complexation by two equivalents of a secondary amine to give a complex of the type Zn(O-NR'₂)₂(HNR''₂)₂ (pathway II, Scheme 2.1).

For the specific calculated case of the reaction of Zn(MeZn)₄(O-NMe₂)₆ (**3**) with Me₂Zn (**1a**) to give 1.5 equivalents of (MeZn)₄(O-NMe₂)₄ (**13-Me**), the computations reveal a distinct drop in energy by 15.7 kJ·mol⁻¹. This result is even much more pronounced with solvation factored in, with the relative energy dropping by a sharp 50.1 kJ·mol⁻¹. By contrast, the complexation of the Zn(O-NMe₂)₂ entity by two diisopropylamine units as ligands to give **13-Me** and the side-product Zn(O-NMe₂)₂(HNiPr₂)₂ (**14**) is unfavoured by about the same magnitude, being 53.8 kJ·mol⁻¹ and 35.0 kJ·mol⁻¹ with COSMO applied, respectively.

Altogether, these numbers clearly show that the isodesmic rearrangement of pentanuclear zinc hydroxylamides with additional zinc dialkyl under thermodynamic conditions to their tetranuclear analogues is strongly preferred with respect to the formation of a (bis)amine complex of binary zinc hydroxylamide, Zn(O-NR'₂)₂. In the investigated, all-methyl situation with the species **3**, **1a** and **13-Me** and HNiPr₂ as the amine, the energy gap is substantial at 69.5 kJ·mol⁻¹, and even 85.1 kJ·mol⁻¹ with solvation considered.

With the disproportionation / amine complexation (pathway II) thus clearly disclosed to be the less viable route, the role of the bulky secondary amine in the reaction mixture remains a matter of scrutiny in ongoing work. One option may be that, apart from acting as a polar co-solvent, it might serve with its protic function as a facilitating agent in the redistribution of the O-NR'₂ ligand units about the scaffold of the organozinc moieties.

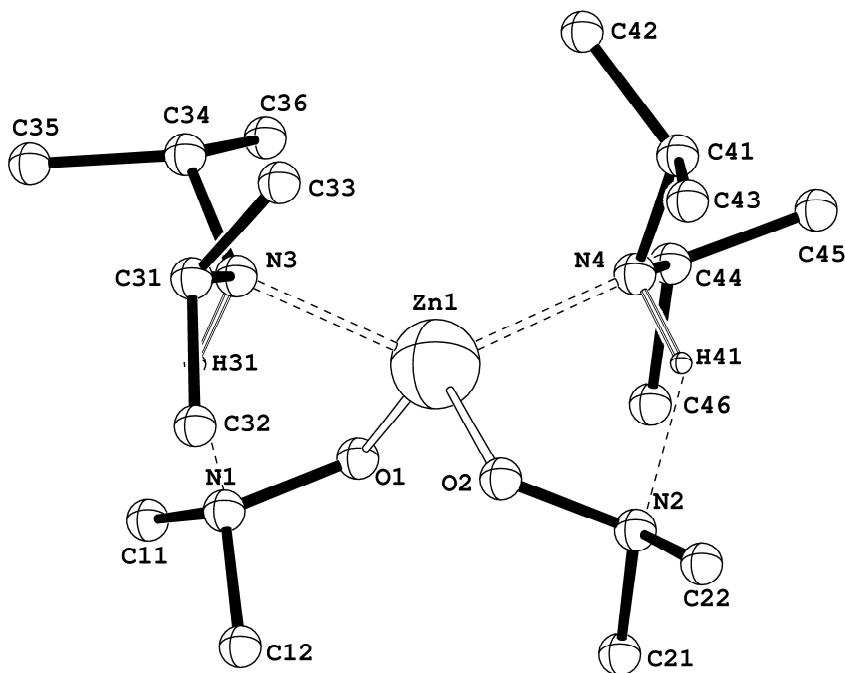


Fig. 2.1 Graphical representation of the converged geometry of $\text{Zn}(\text{O}-\text{NMe}_2)_2(\text{HNiPr}_2)_2$ (**14**) as obtained by DFT calculations at the PBE^[9–13] def2-TZVP^[16] level of theory (+ COSMO^[20]). Alkyl hydrogen atoms have been omitted for clarity.

Table 2.1 Selected parameters [\AA , $^\circ$] of the converged geometry of $\text{Zn}(\text{O}-\text{NMe}_2)_2(\text{HNiPr}_2)_2$ (**14**) as obtained by DFT calculations at the PBE^[9–13] def2-TZVP^[16] level of theory (+ COSMO^[20]).

Zn1-O1	1.967
Zn1-N3	2.190
O1-N1	1.442
N1-C12	1.462
N3-C34	1.499
N3-H31	1.044
N1-H31	2.089

O1-Zn1-O2	123.0
N3-Zn1-N4	130.8
O1-Zn1-N3	95.1
Zn1-O1-N1	110.8
Zn1-N3-H31	90.1
O1-N1-H31	91.8
N1-H31-N3	141.5

2.3 Coordinates of All Optimised Geometries in Bohr Units

Me₂Zn

Level of theory: PBE def2-TZVP

Compound geometry #: **1a**

-0.00000337956395	-0.00000228143924	-0.00000174811714	Zn
0.00000568447480	0.00000593748313	3.68052192613472	C
0.00000762140350	0.00000275879805	-3.68051359977571	C
1.38026028161888	-1.36467390844528	4.42531778602978	H
1.27278858292287	1.46541929968412	-4.42533841370252	H
0.63270014029113	-1.83495580733636	-4.42535492963802	H
0.49175024802090	1.87766656143082	4.42534163560915	H
-1.90548241873929	0.36957948486452	-4.42533281798540	H
-1.87195621406106	-0.51299129817862	4.42538089216205	H

Me₂Zn

Level of theory: PBE def2-TZVP + COSMO

Compound geometry #: **1a_{COSMO}**

0.00003070747635	-0.00002059958851	-0.00001161204648	Zn
-0.00006565654654	0.00003785597849	-3.68528793023409	C
-0.00006061986025	0.00003941176553	3.68533500762167	C
-0.99741185848212	1.67132607951970	-4.41904914151976	H
-0.09617065447444	-1.94378358735869	4.41928608851037	H
-0.94872847656065	-1.69928204845051	-4.41927326965572	H
1.94593903294549	0.02819563680206	-4.41918810325077	H
1.73136284992501	0.88876887648091	4.41927241363818	H
-1.63547763687326	1.05519025440920	4.41914410719549	H

HN*i*Pr₂

Level of theory: PBE def2-TZVP

Compound geometry #: **DIPA**

0.02276243401448	1.05260647975434	-0.33184994914129	N
2.34663822963398	-0.25292403446025	0.44202296559787	C
-2.34631382196779	-0.39754127094847	-0.30083583399153	C
3.20483207308906	-2.10088367787300	-1.61165063108033	C
-3.19368728490405	-1.28070375619541	2.33481620087044	C
4.38142614278322	1.73452177284332	0.94383175943635	C
-4.40224644646869	1.19238180839594	-1.56513277394531	C
-0.20817862536637	2.63224774417354	0.76235843451704	H
-2.02863291945802	-2.08740508488998	-1.48071079592936	H
2.07963558754805	-1.34725641836658	2.21811451618775	H
-6.19895287540328	0.15400302891178	-1.67100685427804	H
-4.74886171136577	2.93494136328097	-0.47652186968591	H
-3.82708649437708	1.73912457282671	-3.48274040964191	H
-4.91402911291383	-2.44363625021336	2.21778973203241	H
-1.73455847555780	-2.41909272324675	3.27951512846610	H
-3.61714885422752	0.35870666313593	3.54815027240245	H
4.95551403243088	-3.06279021247447	-1.03716192631758	H
1.78195971260231	-3.56818511433520	-1.98330452752429	H
3.55471357351061	-1.08015994535046	-3.38905426810364	H
6.17731456875006	0.83807916818480	1.47653549032447	H
4.69764015359563	2.88487721852962	-0.75978073271588	H
3.82579527760110	3.00873388430825	2.49294069455731	H

HN*i*Pr₂

Level of theory: PBE def2-TZVP + COSMO

Compound geometry #: **DIPA_{COSMO}**

0.02144317716747	1.11864895902113	0.06272417850429	N
2.34904644863139	-0.38967223380336	0.31556533325751	C
-2.34429664355307	-0.28114757377704	-0.40593039828982	C
3.19626414003594	-1.40572305974976	-2.25614357638891	C
-3.19453966396761	-1.94592679225871	1.81686721039605	C
4.39480511474799	1.28137787706910	1.48386569996828	C
-4.40954911500969	1.61027872673447	-1.12180359329363	C
-0.21324334886575	2.14228508354444	1.69157717560836	H
-2.00049223763170	-1.51233277900231	-2.05161439163382	H
2.06678597498855	-2.03266257341196	1.59239523071821	H
-6.19466432686206	0.63766246348128	-1.55498324451228	H
-4.77015122628324	2.92511754889752	0.45369564143095	H
-3.84203358463587	2.72784995810434	-2.77848822435100	H
-4.91317943937737	-3.01300373509816	1.33303621363198	H
-1.73224773529045	-3.31961847132344	2.35805591065918	H
-3.62013215165913	-0.76488832489220	3.47951465410963	H
4.93665282124973	-2.52388661822298	-2.05031635523379	H
1.76168664940756	-2.63541213112680	-3.12048321205918	H
3.57134891369868	0.16971189963736	-3.56330137380899	H
6.17657397571866	0.23254472077497	1.68511785278199	H
4.74514412779467	2.94359743313914	0.28084077078864	H
3.82852173082437	1.95331605038988	3.37024641675958	H

(MeZn)₄(O-NMe₂)₄

Level of theory: PBE def2-TZVP

Compound geometry #: **13-Me**

-1.01085258892350	0.28561835670628	3.75724067920922	Zn
-2.03571731523691	-3.31714861756322	-1.43250229539202	Zn
-1.71214993872689	3.25389260974980	-1.83892715606943	Zn
4.29932800780684	-0.16925776101073	-0.14933038134932	Zn
-3.77423567455008	-0.88714266031951	1.11833720398404	O
-0.41034798853450	-0.19333961689423	-3.27907545934105	O
0.24002152981546	3.33554677193846	1.61760741850679	O
1.87857393832966	-2.05590495077358	2.30146458742541	O
-4.84096890392019	1.30717680031234	-0.12601439469670	N
2.26313751659819	-0.39692418354627	-3.78252770224143	N
2.97184789844902	3.38225521370199	1.48867479609301	N
0.79584698856627	-4.40714117553788	1.42077066606224	N
-1.81188086719580	0.45388028265465	7.42220453869581	C
-3.66122932601854	-6.11383193850847	-3.35762953386787	C
-2.23657910642496	6.37005428687843	-3.88806266123617	C
8.02411913280313	-0.73539122968914	-0.41067102500868	C
-6.71137601305929	0.40401209513446	-1.97774609558564	C
-6.12816605943840	2.81698058167144	1.82718823173129	C
2.97544948799977	1.68944886259396	-5.48466360597276	C
2.66153852346765	-2.77686495061212	-5.17475947677247	C
3.69266936433569	5.77148039553546	0.25573291464588	C
3.93154426820759	3.43607722425931	4.11076123330964	C
-0.59545782252612	-5.54629670893836	3.55412638252989	C
2.89720189056267	-6.10042806630322	0.75715443566839	C
-0.28175111544116	-0.36520024399889	8.56867128523548	H
-3.55599505344607	-0.58992043009134	7.86210423617698	H
-2.08124876794117	2.41874634861826	8.04914938071268	H
-5.36451931178354	-6.80237822998599	-2.38362067713898	H

-2.38599761243012	-7.73915425504635	-3.60814450806270	H
-4.23274840187147	-5.48094227405161	-5.25453692290396	H
-2.46928318833236	8.02981900004875	-2.65691303676873	H
-3.94975818838873	6.21100374079006	-5.05783323527618	H
-0.65831888256021	6.76805464653768	-5.18319832277603	H
8.95766394952031	-0.43824281098534	1.42388542996278	H
8.91040545415135	0.56004319081145	-1.77689909934650	H
8.47627198144552	-2.67385583335285	-1.01604342616701	H
-7.00920662949504	4.46282463633656	0.91758130748185	H
-7.57495892510253	1.67033695749559	2.79410373566454	H
-4.74210653975457	3.48565982330408	3.21816599178411	H
-7.60016430911336	2.05021033456133	-2.87881130778998	H
-5.76053849377487	-0.72424301794435	-3.43599268279154	H
-8.15774239106304	-0.76517286557685	-1.03679873213996	H
-1.32490517890706	-7.39345405873149	2.94700064831863	H
0.66252575935367	-5.77761578066046	5.19962241368431	H
-2.20217644346724	-4.34399248027582	4.08100504194348	H
2.11909573049320	-7.87189286613739	0.00172226370256	H
4.09456088810211	-5.21279012169977	-0.68154144319568	H
4.06912167206195	-6.49636554725797	2.43569437536282	H
4.69442834665151	-3.01469930480209	-5.52813865177888	H
1.97138228489094	-4.37711408339573	-4.05562250954298	H
1.61969355058591	-2.73924200067947	-6.97990857694636	H
5.00596111922467	1.54667010977990	-5.89654293579233	H
1.87564970656056	1.58937748634637	-7.25284054837828	H
2.59140592912067	3.50635782495091	-4.57316609229715	H
5.75688485150833	5.81577214759660	0.03214703173009	H
2.78988926522304	5.90168304739306	-1.60251323560308	H
3.06267006017573	7.39405385552787	1.40300422929994	H
5.99835334933372	3.62965596778809	4.05123161567282	H
3.09057751210270	5.03497251638016	5.14902335816220	H
3.45743433692840	1.66155238702857	5.07469595793218	H

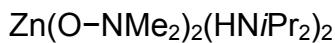
(MeZn)₄(O-NMe₂)₄

Level of theory: PBE def2-TZVP + COSMO

Compound geometry #: **13-Me_{cosmo}**

-0.96915013867601	0.26251231461064	3.74152113189379	Zn
-2.01076483849419	-3.31099122952978	-1.41907459690326	Zn
-1.74131621267814	3.23304809336248	-1.80660225803463	Zn
4.28905517296447	-0.14405145997133	-0.19288574823133	Zn
-3.77889320789234	-0.89823317561296	1.16309798105408	O
-0.42446463610388	-0.18684368910458	-3.28179135661631	O
0.24222617976319	3.34542364111278	1.62896483468563	O
1.89182066446302	-2.07571651548843	2.29223409663803	O
-4.85939341603654	1.30267543804046	-0.07473019094248	N
2.26003356183153	-0.37715003258057	-3.79066658893711	N
2.98225733230912	3.39612602287913	1.46384087159550	N
0.80067836277280	-4.42322907850825	1.38698342024102	N
-1.74300845686493	0.44154404789794	7.42456590913346	C
-3.77080943640249	-6.03392992102190	-3.34965447873029	C
-2.31650489158774	6.34865244978020	-3.85724054503222	C
8.01810266659098	-0.75960937901780	-0.33448015761055	C
-6.74904337648843	0.40546285062477	-1.91158557440181	C
-6.13279888684408	2.81722609849899	1.88488453464146	C
2.96282942705418	1.71811818333586	-5.49009017874117	C
2.66524603272449	-2.75232345712701	-5.19429194301231	C
3.69103140720453	5.78172450241559	0.21284073204445	C
3.97432101626546	3.46406198546366	4.07331658384855	C
-0.56636299247507	-5.59693765194042	3.51898395337488	C

2.89852325494997	-6.10862782865931	0.68003281027108	C
-0.20142019077001	-0.38637506035415	8.55122195456145	H
-3.48940235543184	-0.59751349514097	7.87286745211707	H
-1.99662121964514	2.41179084348280	8.04508095350445	H
-5.47982534086601	-6.67346229728173	-2.34953809065356	H
-2.53782965415523	-7.68786078381875	-3.62453082643017	H
-4.34943922197825	-5.35334582645954	-5.22911573005866	H
-2.54985430539100	8.00319222803765	-2.61685796621671	H
-4.04568477100018	6.16803826671992	-5.00235697530258	H
-0.74105517464964	6.74525013427648	-5.15629360699388	H
8.88230492659021	-0.51135124797565	1.54219177934589	H
8.94760963795961	0.56566884497128	-1.64250776112911	H
8.44647990451638	-2.69104718566490	-0.97965068761609	H
-7.01800911029902	4.46164874142531	0.97872015810595	H
-7.58587081740345	1.68043113063400	2.85339981343359	H
-4.74046661445743	3.48529164024384	3.26991217957617	H
-7.64312004138934	2.05486877365909	-2.79937898230766	H
-5.81794945762323	-0.72566997225311	-3.37979197373761	H
-8.19769240507406	-0.75082957231030	-0.95901738643576	H
-1.29048906130788	-7.44064720072425	2.89825003785228	H
0.71102862255370	-5.85552461859545	5.14445697974391	H
-2.17209736499057	-4.40875670479630	4.08000233301814	H
2.11327825633603	-7.86983942198079	-0.08861720524182	H
4.08236302608690	-5.20794341281010	-0.76034050865433	H
4.07673846429001	-6.53405236422475	2.34564255928383	H
4.69712630101567	-2.98070691154653	-5.55197092378086	H
1.98892124830849	-4.36369862714052	-4.08318750611072	H
1.63288103453564	-2.70306265109414	-7.00333610370076	H
4.98958165205979	1.57434549675632	-5.91436213626084	H
1.86448356493059	1.61467994943088	-7.25778460106183	H
2.59108741323719	3.53404575682018	-4.57273733097703	H
5.75217635612692	5.82348140862000	-0.02821388144088	H
2.78056982668611	5.90427844376950	-1.64157735992770	H
3.08364974472813	7.40916742614992	1.36432647171596	H
6.03824334266159	3.66628637181461	3.98677759536561	H
3.15338585299998	5.07159421471203	5.11353855305466	H
3.51934060332470	1.69346542760758	5.05362930117568	H



Level of theory: PBE def2-TZVP

Compound geometry #: **14**

-0.00002066451271	-0.48036178890162	0.07957161202259	Zn
1.10222099721483	-2.38885517908543	-2.87451103593978	O
-0.85836898774876	-1.69446103159235	3.44976030241278	O
3.74163846135454	-3.04668425140507	-2.74327011409057	N
3.67868270951979	1.55715869971545	0.49009345984986	N
-3.43044741590359	-2.57326325918249	3.60966469862098	N
-3.85141417942986	0.87037602855810	-0.80677546710379	N
-4.96625914111803	-0.09006178706011	-3.21678956655301	C
-4.35202900380259	3.59124144063235	-0.22618116691550	C
-3.60811957408483	1.00817635414258	-5.51386169375822	C
-4.90755455605090	-2.97564902194553	-3.24794445314562	C
-7.03688575972177	4.49204022611924	-0.85005904872701	C
-3.79849801913028	4.07855768248900	2.56738159366753	C
-3.38696599761521	-5.30612272094373	3.18933060763210	C
-4.26305007402666	-2.03974311485174	6.18632041150842	C
3.98726782500965	4.04088569174686	-0.80529307973399	C
4.98074945248483	1.37629776982750	3.00174703251863	C
2.82306006658646	3.94871950299649	-3.43979640584690	C

2.87535261448969	6.20912948628296	0.74198048694103	C
7.70465619339259	2.37732620016652	2.96768235940165	C
4.96247710902606	-1.35804433264159	3.92427754403086	C
3.90945700372546	-5.54964952520433	-1.57980259081421	C
4.63512436063595	-3.16873648247317	-5.35114054378058	C
-4.55917564801353	-0.22149854165056	0.67905740010539	H
4.45736724300841	0.16332146959122	-0.67702107103049	H
-6.96977265029435	0.49439071354971	-3.28293747501443	H
-3.02238734666994	4.71248881595854	-1.37744102343472	H
-3.74142336122526	6.11955200397222	2.94774781821514	H
-5.29614900102511	3.25372726732549	3.75185734799958	H
-2.00156310479292	3.22832482977785	3.16962740010558	H
-7.26149971466590	6.45604274269331	-0.20845832672902	H
-7.45621652962469	4.45182947941586	-2.88174068968462	H
-8.46045228933941	3.33956566223781	0.13771802806749	H
-4.54410470774942	0.36776896858832	-7.25530832276311	H
-3.63297189496669	3.08738929039031	-5.52439977980361	H
-1.63692765903073	0.34814579384259	-5.54982996106194	H
-5.85851460990934	-3.66623602634457	-4.96164320009612	H
-2.94907608669614	-3.67960889936663	-3.26665290328115	H
-5.90766867861044	-3.76374216636339	-1.60547009581225	H
-6.20996366921771	-2.73012727308313	6.43616369420423	H
-3.01874989165042	-2.95907544184768	7.59993669556836	H
-4.22243541279832	0.00704683647997	6.51350318391620	H
-5.31939931168408	-6.06373655529145	3.35167082406391	H
-2.67147647645437	-5.69467269611085	1.28156584982066	H
-2.14754463531405	-6.27180880242637	4.57536465786031	H
6.03025051827672	4.40865602250653	-1.04892212269548	H
3.86307392778038	2.51765451981264	4.33799844517776	H
3.58241059894690	2.37565033774959	-4.55867595822107	H
0.76146585872457	3.70784243303390	-3.34797787581323	H
3.12822805746903	7.99977341924096	-0.28059310109849	H
0.84106666012670	5.92968420343631	1.05504712272024	H
3.78492535576146	6.41326514790922	2.59676990944952	H
8.56456025228520	2.08398323726404	4.83578688241429	H
8.85583378140965	1.34113547003412	1.57668830189696	H
7.83703803580937	4.40444863370056	2.53994924778621	H
5.84075755710286	-1.45794560321478	5.80465902074243	H
3.03007722447483	-2.10836961519248	4.08414240596048	H
6.07223599893530	-2.56619974182748	2.64471556299995	H
3.21950943402912	5.72195507907801	-4.44793046304996	H
6.63469912142893	-3.74228363082211	-5.36647493105237	H
3.51594035426964	-4.53205814923027	-6.48315265387873	H
4.46577880647809	-1.29791011603372	-6.23173335406817	H
5.90380601799975	-6.13998232014049	-1.48722807629359	H
3.14554329966863	-5.46090620015679	0.34678053836693	H
2.81720692575589	-6.96988710652951	-2.66597860913487	H

Zn(O-NMe₂)₂(HN*i*Pr₂)₂

Level of theory: PBE def2-TZVP + COSMO

Compound geometry #: **14cosmo**

0.00129136941063	-0.45263339325773	0.05774225911896	Zn
1.08690023218336	-2.40360184315110	-2.91326494750996	O
-0.91565487493913	-2.03806785886627	3.30875310798443	O
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-4.91092379106545	0.28936381405434	-3.22609474500937	C

-4.29071446647270	3.66191570000700	0.10587312388680	C
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-4.47401321058796	-2.74421881712708	5.79855467552159	C
3.96911016381802	4.09478127901751	-0.57504213804562	C
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2.81993544636588	6.19058322805991	1.04030856849188	C
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4.05118202495394	-5.48060926350833	-1.78027383593997	C
4.64588595525701	-2.90109355705459	-5.43935862580042	C
-4.54613171571202	-0.21946699609667	0.62351457268958	H
4.45213020631215	0.21966959218058	-0.62489537868387	H
-6.90714470581251	0.89245869801052	-3.23828994642683	H
-2.98957097603312	4.88616323776543	-0.96696584508228	H
-3.66935835792080	5.89774682790308	3.48185083206282	H
-5.12630789593037	2.92358675227695	4.05526915723487	H
-1.84304109938024	3.05880545245165	3.39220993330499	H
-7.21865866392315	6.47716588563446	0.45882317397646	H
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-8.38872991325536	3.32594036794692	0.50454445737815	H
-4.49213220343880	1.12867519160659	-7.19904438061643	H
-3.53168171653201	3.65442564730850	-5.21594807554354	H
-1.57896184326768	0.90269571947031	-5.51047640600794	H
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-2.91384710258111	-3.28318040712971	-3.54986032899410	H
-5.91557186577867	-3.50793526245172	-1.98639903777784	H
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-3.28570132002522	-3.77640378825667	7.18753380844343	H
-4.53641322356633	-0.74297671846487	6.34187833936425	H
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-2.51503868471792	-5.78661169124240	0.62013985554958	H
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3.71585390756880	2.28113085195037	4.49457864772842	H
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8.77827004132317	1.42191665996717	1.75218757309190	H
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3.02187041235662	-2.37407933579244	3.84160315169150	H
6.16035997598910	-2.62033078172884	2.58632542238843	H
6.66767137629482	-3.38835688772841	-5.48758810175663	H
3.58404730866257	-4.26109919405891	-6.63354382950733	H
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6.07136908878303	-5.97803848363269	-1.71308391837601	H
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3.02995029154523	-6.90493890025805	-2.93291883717376	H

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