

## ELECTRONIC SUPPORTING INFORMATION 2

# Exploring Enantiopure Zinc-Scorpionates as Catalysts for the Preparation of Polylactides, Cyclic Carbonates, and Polycarbonates

*Marta Navarro,<sup>a,b</sup> Sonia Sobrino,<sup>a</sup> Israel Fernández,<sup>c</sup> Agustín Lara-Sánchez,<sup>a</sup> Andrés Garcés,<sup>\*b</sup> Luis F. Sánchez-Barba<sup>\*b</sup>*

*<sup>a</sup>Universidad de Castilla-La Mancha, Departamento de Química Inorgánica, Orgánica y Bioquímica-Centro de Innovación en Química Avanzada (ORFEO-CINQA), Campus Universitario, 13071-Ciudad Real, Spain.*

*<sup>b</sup>Universidad Rey Juan Carlos, Departamento de Biología y Geología, Física y Química Inorgánica, Móstoles-28933-Madrid, Spain. E-mail: [luisfernando.sanchezbarba@urjc.es](mailto:luisfernando.sanchezbarba@urjc.es); [andres.garces@urjc.es](mailto:andres.garces@urjc.es)*

*<sup>c</sup>Universidad Complutense de Madrid. Departamento de Química Orgánica I and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Facultad de Ciencias Químicas, 28040, Madrid, Spain.*

# TABLE OF CONTENTS

## 1. DFT calculations

1.1. Computational Details .....	S2
Input coordinates .....	S2
1.2. References.....	S22

## 1.1. Computational Details

Density Functional Theory (DFT) calculations reported in this paper were performed with the Gaussian 16 package.<sup>1</sup> Electron correlation was partially taken into account using the hybrid functional usually denoted as B3LYP<sup>2</sup> in conjunction with the D3 dispersion correction suggested by Grimme et al.<sup>3</sup> using the double- $\zeta$  quality def2-SVP<sup>4</sup> basis set for all atoms. All species were characterized by frequency calculations and have positive definite Hessian matrices. The energetic diagrams are based on electronic energies corrected with zero-point vibrational energies. Transition states (TSs) showed only one negative eigenvalue in their diagonalized force constant matrices. Solvent effects (solvent = toluene) were taken into account using the Polarizable Continuum Model (PCM)<sup>5</sup> during the geometry optimizations. This level is therefore denoted PCM-(toluene)-B3LYP-D3/def2-SVP. The computed thermochemistry data were corrected following Grimme's quasi-harmonic (QHA) model for entropy<sup>6</sup> with a frequency cutoff value of 100.0 cm<sup>-1</sup> using the GoodVibes<sup>7</sup> program at 353.15 K

### 1.1.1. Cartesian coordinates and energies.

Cartesian coordinates (in Å) and total energies (in a.u., noncorrected ZVPE included) of all the stationary points discussed in the text.

#### 5a

ZVPE at 353.15 K: -1631.541265

Gibbs Energy at 353.15 K: -1631.635236

N	-0.344234000	-3.246324000	-0.255816000
N	-0.955529000	-2.269200000	-0.955270000
N	-0.354996000	-0.708515000	1.851010000
N	-1.398855000	-1.165608000	1.125281000
C	-1.050103000	-2.551331000	-2.290058000
C	-0.450135000	-3.791016000	-2.451168000
H	-0.342326000	-4.341848000	-3.383423000
C	-0.030400000	-4.180625000	-1.149944000
C	-1.681478000	-1.623609000	-3.276233000
H	-2.715333000	-1.365464000	-2.991615000
H	-1.709753000	-2.093689000	-4.268427000
H	-1.115664000	-0.681395000	-3.351005000
C	0.673103000	-5.437082000	-0.736875000
H	0.086871000	-6.332722000	-1.000824000
H	0.837043000	-5.435831000	0.350028000
H	1.652170000	-5.529083000	-1.235604000
C	-2.357233000	-1.762384000	1.895193000
C	-1.897079000	-1.672588000	3.197678000
H	-2.401863000	-2.031341000	4.092143000
C	-0.643484000	-1.006877000	3.113870000
C	-3.613014000	-2.326969000	1.320872000
H	-4.229751000	-1.537404000	0.857841000
H	-4.209410000	-2.800298000	2.112249000
H	-3.394720000	-3.086321000	0.552695000
C	0.295299000	-0.665291000	4.231804000
H	0.727083000	0.337166000	4.093361000
H	1.133547000	-1.380257000	4.280378000
H	-0.224952000	-0.690493000	5.200456000

C	-1.418521000	-1.037270000	-0.311075000
H	-2.469812000	-0.916923000	-0.600277000
C	-0.697904000	0.241871000	-0.747079000
C	-1.387788000	1.414046000	-0.618431000
C	-0.718005000	2.738687000	-0.706002000
C	0.415612000	3.007359000	0.088893000
C	1.046747000	4.251791000	0.047080000
H	1.926155000	4.431746000	0.671264000
C	0.547626000	5.265868000	-0.779265000
H	1.038185000	6.242078000	-0.811479000
C	-0.591936000	5.023483000	-1.554276000
H	-0.994965000	5.812599000	-2.194918000
C	-1.219684000	3.775016000	-1.515812000
H	-2.112850000	3.595022000	-2.119491000
C	-2.844565000	1.415038000	-0.271407000
C	-3.251646000	1.525008000	1.070082000
H	-2.488405000	1.609769000	1.847257000
C	-4.606068000	1.492978000	1.412355000
H	-4.901956000	1.565961000	2.462162000
C	-5.580619000	1.355669000	0.416892000
H	-6.639957000	1.327899000	0.684948000
C	-5.191604000	1.253710000	-0.922777000
H	-5.946522000	1.148003000	-1.706508000
C	-3.834574000	1.284902000	-1.262375000
H	-3.528649000	1.194568000	-2.308213000
H	0.785051000	2.222993000	0.752831000
C	1.590932000	-0.838983000	-0.919623000
H	1.461026000	-1.757919000	-1.514483000
H	1.473745000	-1.120362000	0.134352000
C	3.009385000	-0.321166000	-1.197587000
H	3.036123000	-0.058903000	-2.272421000
C	4.049832000	-1.461692000	-0.949847000
H	4.321841000	-1.916717000	-1.914334000
H	3.552528000	-2.266451000	-0.386870000
C	5.341858000	-1.037368000	-0.183085000
H	5.515052000	-1.724623000	0.661283000
H	6.221318000	-1.134581000	-0.841606000
C	5.292670000	0.409599000	0.324475000
H	6.210905000	0.668436000	0.879266000
C	4.861112000	1.318640000	-0.852623000
H	5.188936000	1.017512000	-1.861642000
H	5.109171000	2.378213000	-0.707951000
C	3.402953000	0.965951000	-0.453891000
H	2.646976000	1.753529000	-0.583148000
C	3.923798000	0.738019000	1.012577000
C	3.278894000	-0.310054000	1.922217000
H	3.287577000	-1.324910000	1.507966000
H	2.227892000	-0.056005000	2.123999000
H	3.810168000	-0.346870000	2.888615000
C	3.963277000	2.064891000	1.787657000
H	4.572744000	1.960342000	2.700777000
H	2.945105000	2.353120000	2.098383000
H	4.378979000	2.898729000	1.203626000
N	0.567221000	0.144149000	-1.281222000
H	0.921905000	1.021865000	-1.642781000

[5a-ZnMe<sub>2</sub>]

ZVPE at 353.15 K: -3490.462884

Gibbs Energy at 353.15 K: -3490.56514

C	3.528215000	-1.057027000	1.457052000
C	4.637624000	-1.278539000	0.658788000
H	5.635426000	-1.551876000	0.993732000
C	4.205485000	-1.057606000	-0.672708000
C	5.004799000	-1.126360000	-1.935390000
H	4.372945000	-1.444185000	-2.777607000
H	5.839684000	-1.833814000	-1.830672000
H	5.423912000	-0.138831000	-2.188090000
C	3.348332000	-1.123823000	2.937747000
H	3.088731000	-0.135527000	3.353243000
H	4.279873000	-1.458592000	3.412318000
H	2.542434000	-1.820221000	3.218683000
C	0.555750000	-3.066991000	0.625246000
C	-0.352131000	-3.885297000	1.280890000
H	-0.553299000	-4.929289000	1.050337000
C	-0.926297000	-3.092239000	2.307052000
C	1.496091000	-3.426605000	-0.481810000
H	1.430441000	-2.764390000	-1.356125000
H	1.273611000	-4.448883000	-0.815438000
H	2.543899000	-3.396098000	-0.143197000
C	-1.964534000	-3.478821000	3.313651000
H	-1.612260000	-4.300678000	3.958202000
H	-2.885883000	-3.825529000	2.818468000
H	-2.215153000	-2.618508000	3.949637000
C	1.129268000	-0.555159000	1.022662000
C	0.317184000	0.390562000	0.140106000
C	0.032704000	1.643076000	0.605916000
C	-0.588944000	2.741130000	-0.187546000
C	-0.223044000	3.003478000	-1.521448000
H	0.526394000	2.376102000	-1.999538000
C	-0.802299000	4.055771000	-2.231481000
H	-0.494479000	4.239166000	-3.264301000
C	-1.764707000	4.872736000	-1.627928000
H	-2.220867000	5.694190000	-2.186305000
C	-2.130332000	4.633315000	-0.299083000
H	-2.877614000	5.266083000	0.186905000
C	-1.541820000	3.587693000	0.415195000
H	-1.828864000	3.416157000	1.454775000
C	0.365580000	2.029311000	2.016681000
C	-0.314489000	1.472765000	3.114774000
H	-1.067022000	0.701658000	2.938724000
C	0.001507000	1.863504000	4.420256000
H	-0.532025000	1.414850000	5.262276000
C	0.994287000	2.821402000	4.647983000
H	1.240556000	3.126775000	5.668247000
C	1.669774000	3.389859000	3.561008000
H	2.447264000	4.139470000	3.730262000
C	1.352922000	3.001494000	2.257230000
H	1.876130000	3.447963000	1.407769000
N	2.913686000	-0.731421000	-0.688917000
N	2.509706000	-0.723385000	0.604347000
N	-0.411776000	-1.867383000	2.286159000
N	0.482629000	-1.853329000	1.266880000
N	0.004771000	-0.136729000	-1.118764000

H	1.168674000	-0.102371000	2.013314000
C	-1.262375000	0.093130000	-1.832898000
H	-1.025603000	0.287100000	-2.892006000
H	-1.737531000	0.994201000	-1.441964000
C	-2.224120000	-1.098350000	-1.731212000
H	-1.646522000	-1.995132000	-2.025384000
C	-3.415525000	-0.942852000	-2.726457000
H	-3.197549000	-1.512066000	-3.642805000
H	-3.463515000	0.108064000	-3.051100000
C	-4.808834000	-1.356893000	-2.158920000
H	-5.549389000	-0.574106000	-2.391861000
H	-5.164334000	-2.273287000	-2.659236000
C	-4.788380000	-1.624076000	-0.646841000
H	-5.798486000	-1.863301000	-0.272136000
C	-3.634653000	-2.612979000	-0.344191000
H	-3.409020000	-3.369503000	-1.113994000
H	-3.726232000	-3.120524000	0.624072000
C	-2.715018000	-1.364680000	-0.301069000
H	-1.883204000	-1.370518000	0.412092000
C	-3.977596000	-0.528107000	0.123825000
C	-4.141478000	0.938196000	-0.284905000
H	-4.044375000	1.119366000	-1.361386000
H	-3.396902000	1.571223000	0.222281000
H	-5.138760000	1.300536000	0.017066000
C	-4.182111000	-0.605605000	1.645367000
H	-5.185775000	-0.240166000	1.919990000
H	-3.439719000	0.028301000	2.157894000
H	-4.073976000	-1.622162000	2.047802000
H	0.240409000	-1.121402000	-1.176461000
Zn	1.986125000	0.128992000	-2.633666000
C	1.410381000	-1.450762000	-3.753062000
H	0.452214000	-1.903550000	-3.435369000
H	1.280143000	-1.175307000	-4.815547000
H	2.158579000	-2.265475000	-3.733845000
C	2.877266000	1.929117000	-2.517769000
H	2.489861000	2.693679000	-3.214313000
H	3.953182000	1.812216000	-2.748833000
H	2.816213000	2.351568000	-1.498808000

**TS-[5a-ZnMe<sub>2</sub>]**

ZVPE at 353.15 K: -3490.462884

Gibbs Energy at 353.15 K: -3490.56514

C	3.829429000	0.152449000	0.646368000
C	4.725257000	-0.054698000	-0.392701000
H	5.778726000	0.213175000	-0.403962000
C	3.986966000	-0.663649000	-1.429889000
C	4.462894000	-1.123613000	-2.770243000
H	5.331728000	-0.534743000	-3.095724000
H	3.665432000	-1.031288000	-3.520608000
H	4.768841000	-2.182519000	-2.733759000
C	4.030108000	0.777282000	1.987526000
H	3.432596000	1.697593000	2.094654000
H	5.088299000	1.038245000	2.117909000
H	3.741823000	0.093714000	2.802140000
C	1.702474000	-2.739812000	1.723111000
C	0.874950000	-3.538828000	2.498651000
H	1.093542000	-4.551499000	2.831218000
C	-0.293608000	-2.774879000	2.740777000
C	3.059304000	-3.074760000	1.190626000
H	3.094830000	-3.019311000	0.093471000
H	3.311476000	-4.101104000	1.489582000
H	3.844459000	-2.408911000	1.580253000
C	-1.533663000	-3.168254000	3.482092000
H	-2.207998000	-3.756685000	2.836808000
H	-2.083483000	-2.275227000	3.810326000
H	-1.294571000	-3.784642000	4.361978000
C	1.376502000	-0.275833000	0.956610000
C	0.291106000	0.396783000	0.102818000
C	0.172673000	1.772626000	0.236437000
C	-0.290121000	2.642197000	-0.874842000
C	0.138307000	2.414322000	-2.200103000
H	0.793026000	1.565777000	-2.409854000
C	-0.268189000	3.245519000	-3.244263000
H	0.078372000	3.041854000	-4.261203000
C	-1.110842000	4.335284000	-2.994330000
H	-1.431629000	4.985136000	-3.812530000
C	-1.534559000	4.585071000	-1.684051000
H	-2.192727000	5.432712000	-1.474008000
C	-1.126405000	3.753050000	-0.639509000
H	-1.465219000	3.955868000	0.379092000
C	0.562744000	2.458134000	1.496966000
C	0.123196000	1.981168000	2.751793000
H	-0.524626000	1.100883000	2.781318000
C	0.522803000	2.600745000	3.939436000
H	0.174806000	2.205299000	4.897672000
C	1.348701000	3.729184000	3.905081000
H	1.655334000	4.218486000	4.833097000
C	1.768932000	4.233650000	2.667377000
H	2.411169000	5.117844000	2.627432000
C	1.379477000	3.608726000	1.481233000
H	1.718977000	4.003627000	0.520641000
N	2.715123000	-0.820758000	-1.044537000
N	2.628881000	-0.335001000	0.220732000
N	-0.192269000	-1.585105000	2.157189000
N	1.000951000	-1.575339000	1.523044000
N	-0.305319000	-0.415691000	-0.818858000

H	1.581114000	0.386198000	1.799114000
C	-1.566067000	-0.036069000	-1.457845000
H	-1.413728000	0.098144000	-2.544487000
H	-1.896163000	0.936563000	-1.083245000
C	-2.694782000	-1.055583000	-1.230075000
H	-2.337712000	-2.032389000	-1.595920000
C	-3.959824000	-0.657480000	-2.055018000
H	-3.998137000	-1.259025000	-2.976267000
H	-3.838198000	0.381158000	-2.401335000
C	-5.316212000	-0.773881000	-1.291147000
H	-5.893410000	0.157532000	-1.415353000
H	-5.932307000	-1.575747000	-1.732228000
C	-5.142263000	-1.082650000	0.202406000
H	-6.119396000	-1.121756000	0.715200000
C	-4.186011000	-2.294312000	0.339673000
H	-4.231436000	-3.056567000	-0.456290000
H	-4.252014000	-2.802635000	1.311052000
C	-3.029865000	-1.261087000	0.255335000
H	-2.117462000	-1.447265000	0.835560000
C	-4.026113000	-0.197836000	0.852532000
C	-3.938909000	1.284063000	0.473921000
H	-3.968518000	1.475231000	-0.604860000
H	-3.007447000	1.728851000	0.860580000
H	-4.780591000	1.836146000	0.926312000
C	-4.041974000	-0.274813000	2.387732000
H	-4.898480000	0.288986000	2.794725000
H	-3.119366000	0.167928000	2.797823000
H	-4.110386000	-1.303311000	2.768770000
H	-0.091404000	-1.725547000	-0.830682000
Zn	1.089789000	-1.437491000	-2.239544000
C	0.132140000	-3.133392000	-1.118945000
H	-0.407920000	-3.311499000	-0.174016000
H	-0.479454000	-3.577334000	-1.922985000
H	1.064459000	-3.718999000	-1.027819000
C	1.036492000	-1.136423000	-4.208234000
H	-0.003767000	-1.166874000	-4.576621000
H	1.602830000	-1.898908000	-4.771357000
H	1.450208000	-0.149589000	-4.482136000



[κ<sup>2</sup>-5a-ZnMe]

ZVPE at 353.15 K: -3450.041113

Gibbs Energy at 353.15 K: -3450.138091

C	-3.948443000	0.262231000	-0.007353000
C	-4.596234000	0.860090000	-1.081218000
H	-5.653135000	0.780644000	-1.323516000
C	-3.602516000	1.573100000	-1.791465000
C	-3.727828000	2.397763000	-3.031593000
H	-2.789602000	2.934512000	-3.230292000
H	-4.541628000	3.132557000	-2.933654000
H	-3.958445000	1.764370000	-3.903497000
C	-4.467106000	-0.624242000	1.076131000
H	-3.982092000	-1.613960000	1.050645000
H	-5.548819000	-0.765416000	0.954429000
H	-4.286983000	-0.191128000	2.073274000
C	-1.496406000	2.639946000	1.784423000
C	-0.652589000	3.167547000	2.751620000
H	-0.714047000	4.168590000	3.173832000
C	0.274585000	2.144581000	3.065237000
C	-2.656506000	3.329093000	1.133831000
H	-2.440331000	3.600795000	0.089998000
H	-2.864941000	4.255181000	1.686547000
H	-3.572822000	2.721340000	1.132003000
C	1.423451000	2.192505000	4.023741000
H	1.152505000	2.734953000	4.942489000
H	2.287989000	2.710990000	3.575576000
H	1.746033000	1.176954000	4.290565000
C	-1.538374000	0.232906000	0.754940000
C	-0.454657000	-0.470727000	-0.083613000
C	-0.460784000	-1.864793000	-0.072518000
C	0.041594000	-2.656520000	-1.222052000
C	-0.218194000	-2.259616000	-2.551787000
H	-0.774980000	-1.335462000	-2.724605000
C	0.223337000	-3.018719000	-3.636300000
H	0.003712000	-2.685259000	-4.654644000
C	0.936877000	-4.204956000	-3.427357000
H	1.285054000	-4.798823000	-4.276358000
C	1.195824000	-4.621380000	-2.116195000
H	1.753238000	-5.544940000	-1.935893000
C	0.752091000	-3.861643000	-1.032314000
H	0.962943000	-4.196671000	-0.013941000
C	-1.029351000	-2.632308000	1.065099000
C	-0.715330000	-2.312223000	2.405044000
H	-0.023007000	-1.489826000	2.599550000
C	-1.290801000	-3.012410000	3.470004000
H	-1.034542000	-2.735759000	4.496719000
C	-2.173199000	-4.070337000	3.229746000
H	-2.615943000	-4.623142000	4.062365000
C	-2.474079000	-4.421057000	1.906646000
H	-3.159822000	-5.248518000	1.703250000
C	-1.910902000	-3.714525000	0.843116000
H	-2.159394000	-3.991609000	-0.184350000
N	-2.424521000	1.414622000	-1.185188000
N	-2.639808000	0.631069000	-0.102887000
N	0.024018000	1.060623000	2.339162000
N	-1.032594000	1.363444000	1.552409000
N	0.298218000	0.366741000	-0.836320000

H	-1.957756000	-0.492536000	1.454438000
C	1.575037000	-0.063957000	-1.385109000
H	1.510765000	-0.192176000	-2.483805000
H	1.842698000	-1.051042000	-0.991728000
C	2.707819000	0.925257000	-1.063600000
H	2.351157000	1.927647000	-1.367035000
C	3.996451000	0.594412000	-1.878914000
H	4.051235000	1.255751000	-2.757644000
H	3.893617000	-0.420229000	-2.294839000
C	5.330814000	0.672465000	-1.073934000
H	5.926514000	-0.238073000	-1.253465000
H	5.944490000	1.515059000	-1.435431000
C	5.112016000	0.862229000	0.433315000
H	6.073615000	0.867562000	0.975924000
C	4.141657000	2.052875000	0.639913000
H	4.201854000	2.876327000	-0.091652000
H	4.178932000	2.482655000	1.650062000
C	2.997416000	1.022451000	0.442050000
H	2.061717000	1.156657000	1.000730000
C	3.986686000	-0.078781000	0.981099000
C	3.923938000	-1.527165000	0.484822000
H	3.970107000	-1.632532000	-0.604983000
H	2.994115000	-2.013121000	0.823419000
H	4.767269000	-2.101857000	0.904911000
C	3.967496000	-0.125367000	2.517156000
H	4.824774000	-0.707540000	2.895756000
H	3.044327000	-0.614298000	2.868824000
H	4.009779000	0.869037000	2.982007000
Zn	-0.419810000	2.033430000	-1.567685000
C	-0.107127000	3.724613000	-2.551919000
H	0.924330000	4.094815000	-2.425703000
H	-0.789631000	4.522002000	-2.208031000
H	-0.277699000	3.597109000	-3.636089000

[ $\kappa^3$ -5a-ZnMe]

ZVPE at 353.15 K: -3450.062353

Gibbs Energy at 353.15 K: -3490.56514

Zn	-1.298256000	-1.831414000	-1.211544000
N	-1.251880000	-2.067944000	0.921990000
N	-0.087506000	-1.697874000	1.504507000
N	0.682876000	-2.723584000	-1.146286000
N	1.503008000	-2.201790000	-0.205851000
N	-0.444529000	-0.016453000	-0.899867000
C	-0.114960000	-1.928492000	2.851738000
C	-1.378895000	-2.432380000	3.130113000
H	-1.754384000	-2.724343000	4.107958000
C	-2.055330000	-2.504151000	1.889470000
C	1.052795000	-1.713160000	3.755989000
H	1.898473000	-2.363419000	3.477306000
H	0.768768000	-1.955263000	4.788461000
H	1.414720000	-0.675586000	3.730894000
C	-3.451959000	-2.938716000	1.582059000
H	-4.175760000	-2.170837000	1.902494000
H	-3.704471000	-3.873755000	2.104434000
H	-3.573461000	-3.087251000	0.499464000
C	2.773952000	-2.678876000	-0.325864000
C	2.748572000	-3.569125000	-1.392285000
H	3.589619000	-4.143075000	-1.774058000
C	1.416807000	-3.564398000	-1.874636000
C	3.895136000	-2.239714000	0.557382000
H	4.050929000	-1.150474000	0.498273000
H	4.824751000	-2.738825000	0.254543000
H	3.705071000	-2.490505000	1.613912000
C	0.808034000	-4.327952000	-3.006699000
H	-0.243514000	-4.034854000	-3.137404000
H	0.848098000	-5.413265000	-2.820131000
H	1.347678000	-4.135406000	-3.947408000
C	0.996739000	-1.158225000	0.688242000
H	1.808533000	-0.911539000	1.373002000
C	0.657104000	0.095398000	-0.151883000
C	-1.075875000	1.158887000	-1.466095000
H	-0.977249000	1.169278000	-2.569269000
H	-0.575443000	2.070266000	-1.116910000
C	-2.572735000	1.222800000	-1.101384000
H	-3.046737000	0.333585000	-1.555397000
C	-3.247488000	2.500116000	-1.695011000
H	-3.832885000	2.220740000	-2.584194000
H	-2.458125000	3.168690000	-2.074193000
C	-4.152954000	3.300941000	-0.704211000
H	-3.844291000	4.359287000	-0.686551000
H	-5.197258000	3.294350000	-1.059373000
C	-4.138591000	2.734088000	0.722200000
H	-4.785777000	3.327222000	1.391651000
C	-4.365772000	1.203527000	0.637836000
H	-5.017608000	0.839841000	-0.173970000
H	-4.701871000	0.753130000	1.581684000
C	-2.834546000	1.096688000	0.407294000
H	-2.312229000	0.219442000	0.811074000
C	-2.680461000	2.437790000	1.212097000
C	-1.573319000	3.443233000	0.881476000
H	-1.692556000	4.348461000	1.501202000

H	-1.563480000	3.765280000	-0.166261000
H	-0.580288000	3.019000000	1.101843000
C	-2.613622000	2.153312000	2.720926000
H	-2.744175000	3.082888000	3.300164000
H	-1.628349000	1.730929000	2.981849000
H	-3.375358000	1.437531000	3.061857000
C	-2.761450000	-2.585838000	-2.335466000
H	-2.846686000	-3.681509000	-2.217996000
H	-2.607670000	-2.388632000	-3.411582000
H	-3.744678000	-2.156782000	-2.070834000
C	1.624238000	1.119749000	-0.165222000
C	1.863646000	1.929944000	-1.378655000
C	1.756606000	1.366294000	-2.672023000
H	1.461022000	0.318809000	-2.767431000
C	2.017486000	2.116689000	-3.818056000
H	1.928223000	1.645726000	-4.801385000
C	2.399655000	3.460586000	-3.718354000
H	2.603005000	4.048433000	-4.617092000
C	2.514991000	4.037994000	-2.448743000
H	2.805981000	5.087884000	-2.350072000
C	2.251089000	3.287637000	-1.301281000
H	2.336775000	3.759334000	-0.319644000
C	2.435301000	1.411223000	1.033108000
C	1.844032000	1.487359000	2.314965000
H	0.760836000	1.365882000	2.398136000
C	2.606364000	1.742703000	3.460662000
H	2.113419000	1.798678000	4.435563000
C	3.984280000	1.950634000	3.360216000
H	4.580572000	2.159771000	4.251831000
C	4.589095000	1.905025000	2.094892000
H	5.666212000	2.069425000	1.999957000
C	3.830440000	1.643288000	0.955497000
H	4.315069000	1.608123000	-0.023279000

## 6c

ZVPE at 353.15 K: -1631.583545

Gibbs Energy at 353.15 K: -1631.677195

C	3.073204000	-2.160797000	-0.359816000
C	3.988836000	-2.269792000	-1.392336000
H	4.974773000	-2.727436000	-1.341141000
C	3.372598000	-1.649936000	-2.515443000
C	3.928798000	-1.479076000	-3.895900000
H	3.197986000	-0.969917000	-4.540259000
H	4.174990000	-2.452759000	-4.350760000
H	4.856277000	-0.882862000	-3.882729000
C	3.137709000	-2.566495000	1.074884000
H	3.039752000	-1.686332000	1.731107000
H	4.096485000	-3.058643000	1.287104000
H	2.316924000	-3.249585000	1.341841000
C	-0.642686000	-3.177669000	-0.683643000
C	-1.375191000	-4.019873000	0.136489000
H	-1.986629000	-4.862628000	-0.179353000
C	-1.148920000	-3.555878000	1.461920000
C	-0.438652000	-3.174529000	-2.162019000
H	-0.388102000	-2.151272000	-2.558628000
H	-1.254467000	-3.718794000	-2.657850000
H	0.514879000	-3.658668000	-2.430423000
C	-1.716177000	-4.092178000	2.740166000
H	-1.494184000	-5.165011000	2.860012000
H	-2.813347000	-3.981486000	2.764980000
H	-1.294868000	-3.549140000	3.598095000
C	0.786455000	-1.176094000	-0.205872000
C	0.504554000	0.120003000	0.123146000
C	1.606307000	1.174059000	-0.019606000
H	2.355549000	0.761171000	-0.704812000
C	2.331342000	1.433802000	1.301401000
C	1.951538000	0.835266000	2.511996000
H	1.092130000	0.163480000	2.543638000
C	2.678038000	1.077785000	3.684677000
H	2.367331000	0.599482000	4.617244000
C	3.792446000	1.919417000	3.666063000
H	4.357820000	2.107071000	4.582457000
C	4.182639000	2.516717000	2.461329000
H	5.057351000	3.171759000	2.431374000
C	3.459437000	2.272618000	1.292843000
H	3.769358000	2.740824000	0.354542000
C	1.045132000	2.418600000	-0.706878000
C	0.758076000	2.339223000	-2.080276000
H	1.003601000	1.417721000	-2.616541000
C	0.153791000	3.408337000	-2.743372000
H	-0.065552000	3.330367000	-3.811391000
C	-0.175302000	4.575933000	-2.043000000
H	-0.652406000	5.411780000	-2.560820000
C	0.111569000	4.665598000	-0.678973000
H	-0.139005000	5.573513000	-0.124270000
C	0.721092000	3.593397000	-0.014613000
H	0.948191000	3.674769000	1.050964000
C	-1.991909000	0.040479000	0.615241000
H	-1.892939000	-1.040704000	0.542631000
C	-2.845057000	0.401204000	1.867855000
H	-3.017217000	-0.486922000	2.492747000

H	-2.332989000	1.139751000	2.503996000
C	-4.145030000	0.968724000	1.259711000
H	-5.008346000	0.941195000	1.942274000
C	-3.812420000	2.378386000	0.719176000
H	-3.281313000	2.983349000	1.470738000
H	-4.723424000	2.934534000	0.452551000
C	-2.938281000	2.071433000	-0.533113000
H	-3.393433000	2.462447000	-1.454993000
H	-1.935209000	2.518537000	-0.490260000
C	-2.881784000	0.523620000	-0.578469000
C	-4.308606000	0.129000000	-0.044988000
C	-4.516925000	-1.377067000	0.201035000
H	-5.502542000	-1.547481000	0.664111000
H	-3.765422000	-1.843197000	0.851254000
H	-4.502641000	-1.928757000	-0.752601000
C	-5.465094000	0.588687000	-0.948444000
H	-5.481756000	-0.000281000	-1.879708000
H	-5.418219000	1.647689000	-1.233227000
H	-6.429558000	0.426074000	-0.439747000
C	-2.448684000	-0.045311000	-1.918051000
H	-1.417567000	0.261738000	-2.154399000
H	-3.099140000	0.310914000	-2.733037000
H	-2.478152000	-1.145364000	-1.911156000
N	2.160365000	-1.203204000	-2.201969000
N	1.984015000	-1.515983000	-0.887204000
N	-0.330751000	-2.507557000	1.461605000
N	-0.034780000	-2.274289000	0.152672000
N	-0.653562000	0.599663000	0.661673000
H	-0.629051000	1.593096000	0.858278000

**6c-ZnMe<sub>2</sub>**

ZVPE at 353.15 K: -3490.498996

Gibbs Energy at 353.15 K: -3490.602689

C	-3.107068000	-0.851860000	1.529690000
C	-3.899294000	-0.398019000	2.568958000
H	-4.933491000	-0.674191000	2.763348000
C	-3.085218000	0.510013000	3.301132000
C	-3.451552000	1.308398000	4.514299000
H	-2.582875000	1.880839000	4.869635000
H	-3.799107000	0.656329000	5.332297000
H	-4.267985000	2.016463000	4.294405000
C	-3.389202000	-1.793016000	0.411848000
H	-3.155551000	-1.328838000	-0.556939000
H	-4.449046000	-2.079628000	0.412150000
H	-2.780241000	-2.706859000	0.479426000
C	0.205737000	-2.447693000	1.991734000
C	0.694444000	-3.652939000	1.506858000
H	1.102247000	-4.472825000	2.093322000
C	0.544985000	-3.595120000	0.102851000
C	0.056897000	-1.945906000	3.388360000
H	0.270444000	-0.870854000	3.456500000
H	0.728825000	-2.497778000	4.059723000
H	-0.978256000	-2.082219000	3.742960000
C	0.926598000	-4.613706000	-0.924973000
H	1.190280000	-5.568814000	-0.450474000
H	1.793970000	-4.272399000	-1.513939000
H	0.096167000	-4.786532000	-1.627450000
C	-0.727940000	-0.411087000	0.887092000
C	-0.142106000	0.650098000	0.242419000
C	-0.961923000	1.959773000	0.152989000
H	-1.219027000	2.191555000	1.194448000
C	-2.277419000	1.753833000	-0.587071000
C	-2.339176000	1.023471000	-1.783237000
H	-1.433271000	0.574830000	-2.190948000
C	-3.555368000	0.833678000	-2.444607000
H	-3.579853000	0.248964000	-3.367817000
C	-4.732641000	1.373972000	-1.916621000
H	-5.686804000	1.219728000	-2.426906000
C	-4.681006000	2.105277000	-0.725452000
H	-5.596748000	2.522156000	-0.298223000
C	-3.461633000	2.293868000	-0.067882000
H	-3.431388000	2.847960000	0.873888000
C	-0.144478000	3.144094000	-0.355082000
C	0.543790000	3.941105000	0.575049000
H	0.447555000	3.720094000	1.641730000
C	1.357452000	4.996659000	0.156158000
H	1.884770000	5.602780000	0.897140000
C	1.499582000	5.273176000	-1.207735000
H	2.137437000	6.096388000	-1.539045000
C	0.816542000	4.491056000	-2.143849000
H	0.916670000	4.701338000	-3.211665000
C	-0.002003000	3.437792000	-1.721184000
H	-0.533455000	2.839558000	-2.463382000
C	2.237220000	-0.179568000	-0.116252000
H	1.872253000	-1.136429000	0.250482000
C	3.100890000	-0.409496000	-1.392560000
H	2.993098000	-1.440774000	-1.756366000

H	2.785388000	0.242137000	-2.219503000
C	4.532349000	-0.079736000	-0.918408000
H	5.322623000	-0.533548000	-1.535805000
C	4.622248000	1.458422000	-0.807465000
H	4.252481000	1.952087000	-1.719390000
H	5.659627000	1.794461000	-0.662358000
C	3.739282000	1.762251000	0.438943000
H	4.310645000	2.267868000	1.231679000
H	2.888694000	2.423008000	0.220582000
C	3.274066000	0.364172000	0.922013000
C	4.518540000	-0.533365000	0.573644000
C	4.305324000	-2.046782000	0.762520000
H	5.200230000	-2.594469000	0.425332000
H	3.447396000	-2.459430000	0.216248000
H	4.155438000	-2.287013000	1.827372000
C	5.789529000	-0.168517000	1.358586000
H	5.688934000	-0.471364000	2.413397000
H	6.030599000	0.902261000	1.348604000
H	6.657669000	-0.706450000	0.943601000
C	2.763336000	0.337661000	2.351458000
H	1.850035000	0.946860000	2.451207000
H	3.512989000	0.738987000	3.051993000
H	2.516590000	-0.687369000	2.666506000
N	-1.872047000	0.592315000	2.765726000
N	-1.891370000	-0.232157000	1.679781000
N	-0.011374000	-2.433552000	-0.252214000
N	-0.200934000	-1.729737000	0.899113000
N	1.086027000	0.677345000	-0.335880000
H	1.284597000	1.529291000	-0.847057000
Zn	-0.885637000	-2.138814000	-2.318974000
C	0.240125000	-0.868561000	-3.387912000
H	0.562343000	0.012516000	-2.812383000
H	1.162167000	-1.363800000	-3.744810000
H	-0.294963000	-0.505498000	-4.284524000
C	-2.350434000	-3.517128000	-2.338073000
H	-2.264841000	-4.193207000	-3.209421000
H	-2.349941000	-4.148992000	-1.432466000
H	-3.351170000	-3.051854000	-2.402987000



**TS-[6c-ZnMe<sub>2</sub>]**

ZVPE at 353.15 K: -3490.450043

Gibbs Energy at 353.15 K: -3490.547115

C	-3.162764000	-1.185289000	1.348574000
C	-3.976337000	-0.955375000	2.443479000
H	-5.017791000	-1.250952000	2.552551000
C	-3.173602000	-0.228362000	3.367506000
C	-3.562299000	0.295302000	4.716206000
H	-2.709329000	0.807221000	5.183986000
H	-3.888761000	-0.519779000	5.383075000
H	-4.399215000	1.009465000	4.642654000
C	-3.427047000	-1.827342000	0.029154000
H	-3.152936000	-1.144085000	-0.790769000
H	-4.492820000	-2.072986000	-0.066851000
H	-2.842405000	-2.751460000	-0.107232000
C	0.063828000	-2.921528000	1.510097000
C	0.428811000	-4.047038000	0.771618000
H	0.748327000	-5.007786000	1.167442000
C	0.307578000	-3.681390000	-0.581000000
C	0.001071000	-2.690628000	2.980504000
H	0.386268000	-1.691978000	3.235856000
H	0.583803000	-3.457121000	3.508645000
H	-1.038711000	-2.724988000	3.343616000
C	0.616077000	-4.462441000	-1.816539000
H	0.520702000	-5.541586000	-1.633367000
H	1.647942000	-4.267389000	-2.154540000
H	-0.065430000	-4.184259000	-2.636238000
C	-0.783565000	-0.649235000	0.851805000
C	-0.183545000	0.471692000	0.300725000
C	-1.022144000	1.778470000	0.318790000
H	-1.332199000	1.865541000	1.368731000
C	-2.317647000	1.676664000	-0.482450000
C	-2.333073000	1.428860000	-1.864826000
H	-1.394539000	1.324543000	-2.408392000
C	-3.535974000	1.296807000	-2.563620000
H	-3.515257000	1.085886000	-3.635204000
C	-4.755689000	1.420159000	-1.891150000
H	-5.698093000	1.312959000	-2.434227000
C	-4.756917000	1.676304000	-0.516554000
H	-5.702370000	1.766442000	0.024692000
C	-3.549817000	1.803009000	0.176601000
H	-3.561551000	1.973977000	1.255756000
C	-0.208282000	3.029668000	0.027500000
C	-0.022192000	3.970893000	1.050508000
H	-0.471968000	3.789541000	2.030875000
C	0.740148000	5.126551000	0.845587000
H	0.872721000	5.841248000	1.662205000
C	1.332095000	5.360926000	-0.397402000
H	1.932583000	6.259262000	-0.562940000
C	1.149227000	4.433477000	-1.429855000
H	1.610939000	4.603031000	-2.406243000
C	0.387881000	3.282663000	-1.218093000
H	0.274827000	2.567863000	-2.030249000
C	2.126799000	-0.256984000	0.376378000
H	1.756499000	-0.678603000	1.321857000
C	2.836417000	-1.397163000	-0.437256000
H	2.647082000	-2.379465000	0.017135000

H	2.476951000	-1.457037000	-1.471089000
C	4.330210000	-1.015738000	-0.373944000
H	5.013774000	-1.857468000	-0.570297000
C	4.534488000	0.192872000	-1.313154000
H	4.103832000	0.004471000	-2.308685000
H	5.603034000	0.406235000	-1.467452000
C	3.818341000	1.344897000	-0.548123000
H	4.502123000	2.179084000	-0.328913000
H	2.963665000	1.772601000	-1.088999000
C	3.329050000	0.675269000	0.759959000
C	4.461532000	-0.377167000	1.040837000
C	4.176670000	-1.355715000	2.195146000
H	4.997126000	-2.087666000	2.279100000
H	3.244891000	-1.925959000	2.085266000
H	4.120294000	-0.815492000	3.154158000
C	5.838127000	0.246352000	1.326767000
H	5.849776000	0.708071000	2.327460000
H	6.134095000	1.022142000	0.608794000
H	6.619152000	-0.532366000	1.314798000
C	2.985998000	1.656294000	1.866175000
H	2.180411000	2.329641000	1.537043000
H	3.855752000	2.276393000	2.138581000
H	2.637756000	1.135524000	2.773859000
N	-1.947934000	-0.043684000	2.886537000
N	-1.947320000	-0.624580000	1.654727000
N	-0.121012000	-2.413812000	-0.659326000
N	-0.263671000	-1.952458000	0.614203000
N	1.044571000	0.484414000	-0.256026000
H	0.962014000	0.275208000	-1.624668000
Zn	-0.514595000	-1.304215000	-2.314405000
C	1.084129000	0.135805000	-2.994143000
H	2.014542000	0.712350000	-2.870689000
H	1.402949000	-0.762549000	-3.559780000
H	0.431207000	0.733352000	-3.651131000
C	-1.843165000	-1.663328000	-3.749598000
H	-1.840236000	-0.857020000	-4.502327000
H	-1.628569000	-2.610992000	-4.275292000
H	-2.863955000	-1.735029000	-3.338485000

**[6c-ZnMe]**

ZVPE at 353.15 K: -3450.068995

Gibbs Energy at 353.15 K: -3450.167451

C	3.650556000	-0.069495000	1.024727000
C	4.861597000	0.562541000	0.807581000
H	5.647630000	0.735190000	1.540060000
C	4.851181000	0.939997000	-0.565023000
C	5.920014000	1.656389000	-1.332238000
H	5.582115000	1.855563000	-2.359174000
H	6.846392000	1.059927000	-1.380633000
H	6.176438000	2.617165000	-0.856585000
C	3.033573000	-0.647704000	2.256022000
H	2.166691000	-0.046384000	2.579117000
H	3.762941000	-0.664693000	3.076973000
H	2.672716000	-1.673771000	2.081304000
C	2.012085000	-2.525129000	-1.918532000
C	1.784032000	-3.890307000	-1.761748000
H	1.989793000	-4.668088000	-2.493494000
C	1.212609000	-4.046141000	-0.482577000
C	2.541047000	-1.757721000	-3.081746000
H	1.828959000	-0.967637000	-3.370016000
H	2.697677000	-2.429901000	-3.935947000
H	3.481820000	-1.246169000	-2.834164000
C	0.725451000	-5.286811000	0.196516000
H	1.560548000	-5.973521000	0.409774000
H	0.007708000	-5.829298000	-0.438813000
H	0.233671000	-5.035975000	1.146853000
C	1.679714000	-0.549571000	-0.406069000
C	0.535993000	0.154421000	-0.065694000
C	0.729846000	1.670701000	0.160106000
H	1.810583000	1.826430000	0.060586000
C	0.399022000	2.186225000	1.558979000
C	-0.397954000	1.510694000	2.493588000
H	-0.838396000	0.553324000	2.230930000
C	-0.629384000	2.047247000	3.766624000
H	-1.255078000	1.495689000	4.473408000
C	-0.069532000	3.272847000	4.130486000
H	-0.251952000	3.692350000	5.123147000
C	0.733875000	3.957061000	3.209759000
H	1.186111000	4.914661000	3.481114000
C	0.965992000	3.416069000	1.944979000
H	1.596722000	3.957152000	1.233878000
C	0.145560000	2.505904000	-0.985869000
C	0.685549000	2.332437000	-2.271354000
H	1.514894000	1.632693000	-2.406297000
C	0.178069000	3.045056000	-3.359777000
H	0.607628000	2.893907000	-4.353735000
C	-0.873701000	3.951083000	-3.180614000
H	-1.275420000	4.505956000	-4.032311000
C	-1.397896000	4.149268000	-1.899717000
H	-2.212843000	4.861164000	-1.744508000
C	-0.887676000	3.435398000	-0.810037000
H	-1.307922000	3.596483000	0.184490000
C	-1.891710000	0.179301000	-0.269914000
H	-1.894182000	1.191913000	0.159143000
C	-2.117659000	0.280066000	-1.819775000
H	-2.009752000	1.312015000	-2.175794000

H	-1.369383000	-0.325002000	-2.352601000
C	-3.548324000	-0.256818000	-2.022518000
H	-4.022635000	0.076454000	-2.958981000
C	-3.496995000	-1.788781000	-1.856426000
H	-2.692496000	-2.233498000	-2.461906000
H	-4.437814000	-2.265742000	-2.170029000
C	-3.250006000	-1.954391000	-0.330344000
H	-4.047999000	-2.528499000	0.163347000
H	-2.320940000	-2.505570000	-0.130694000
C	-3.211563000	-0.499709000	0.215804000
C	-4.268287000	0.204861000	-0.722243000
C	-4.360672000	1.734130000	-0.574134000
H	-5.100393000	2.132205000	-1.287895000
H	-3.418909000	2.263851000	-0.760671000
H	-4.703134000	2.006784000	0.437408000
C	-5.700987000	-0.334392000	-0.566388000
H	-6.147726000	0.023017000	0.375411000
H	-5.773534000	-1.429687000	-0.565533000
H	-6.332817000	0.037454000	-1.389687000
C	-3.467727000	-0.382303000	1.711024000
H	-2.711031000	-0.928084000	2.293251000
H	-4.448566000	-0.806467000	1.978782000
H	-3.444937000	0.668818000	2.038490000
N	3.717167000	0.566979000	-1.148963000
N	2.989049000	-0.051487000	-0.177906000
N	1.121688000	-2.850195000	0.113593000
N	1.612903000	-1.927980000	-0.763308000
N	-0.648656000	-0.495540000	0.095938000
Zn	-0.441480000	-2.082846000	1.275736000
C	-1.078569000	-3.021561000	2.903559000
H	-1.258128000	-2.325738000	3.741527000
H	-0.347759000	-3.772433000	3.250689000
H	-2.030679000	-3.546206000	2.710124000

## ZnMe<sub>2</sub>

ZVPE at 353.15 K: -1858.891031

Gibbs Energy at 353.15 K: -1858.929368

C	1.974781000	-0.000596000	0.000137000
Zn	0.000000000	0.000417000	-0.000102000
H	2.382593000	0.313039000	-0.977302000
H	2.381285000	-1.004461000	0.217216000
H	2.382464000	0.688799000	0.760818000
C	-1.974800000	-0.000560000	0.000132000
H	-2.381517000	-0.697844000	-0.753843000
H	-2.381571000	-0.305620000	0.980723000
H	-2.383140000	1.000502000	-0.226152000

## CH<sub>4</sub>

ZVPE at 353.15 K: -40.44373 Ha

Gibbs Energy at 353.15 K: -40.465042 Ha

C	0.000000000	0.000000000	0.000000000
H	0.634983000	0.634983000	0.634983000
H	-0.634983000	-0.634983000	0.634983000
H	0.634983000	-0.634983000	-0.634983000
H	-0.634983000	0.634983000	-0.634983000

## 1.2. References

- (1) M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, G.A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A.V. Marenich, J. Bloino, B.G. Janesko, R. Gomperts, B. Mennucci, H.P. Hratchian, J.V. Ortiz, A.F. Izmaylov, J.L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V.G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. Montgomery, J.A., J.E. Peralta, F. Ogliaro, M.J. Bearpark, J.J. Heyd, E.N. Brothers, K.N. Kudin, V.N. Staroverov, T.A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A.P. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, J.M. Millam, M. Klene, C. Adamo, R. Cammi, J.W. Ochterski, R.L. Martin, K. Morokuma, O. Farkas, J.B. Foresman, D.J. Fox, Gaussian 16, Revision B.01, (2016).
- (2) a) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098; b) J. P. Perdew, *Phys. Rev. B* **1986**, *33*, 8822.
- (3) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.
- (4) K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *242*, 652.
- (5) a) S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.* **1981**, *55*, 117; b) J. L. Pascual-Ahuir, E. Silla, I. Tuñón, *J. Comput. Chem.* **1994**, *15*, 1127; c) V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995.
- (6) Grimme, S. *Chem. — Eur. J.* **2012**, *18*, 9955–9964.
- (7) Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. *F1000 Research* **2020**, *9*, 291