

Supplementary Information

Comparison of three different elements in the same period (In, Sn, and Sb) as catalysts in the ring-opening polymerization of L-lactide: from amorphous to semicrystalline polyester

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Tables

Table S1. Optimized cartesian coordinates (xyz) for all species in **9** the energy profile of Figure 9. Coordinates are given in Å.

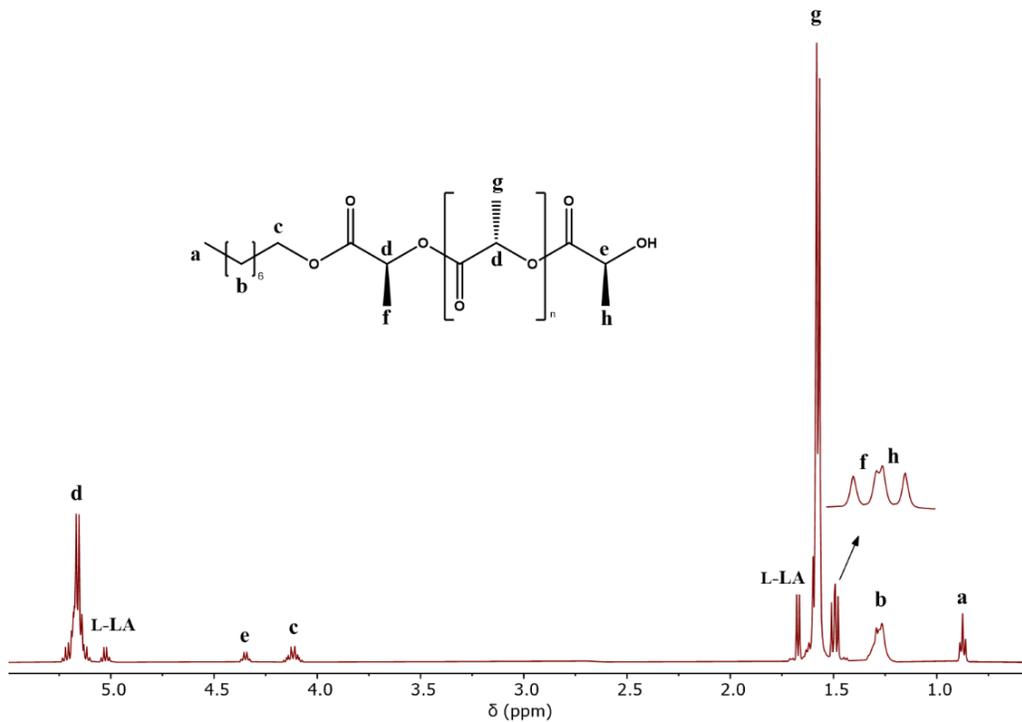


Figure S1. ^1H NMR spectrum of the oligomers obtained from ROP of L-lactide catalyzed by tin(III) acetate (Entry 10, Table 4) in presence of 1-octanol as initiator.

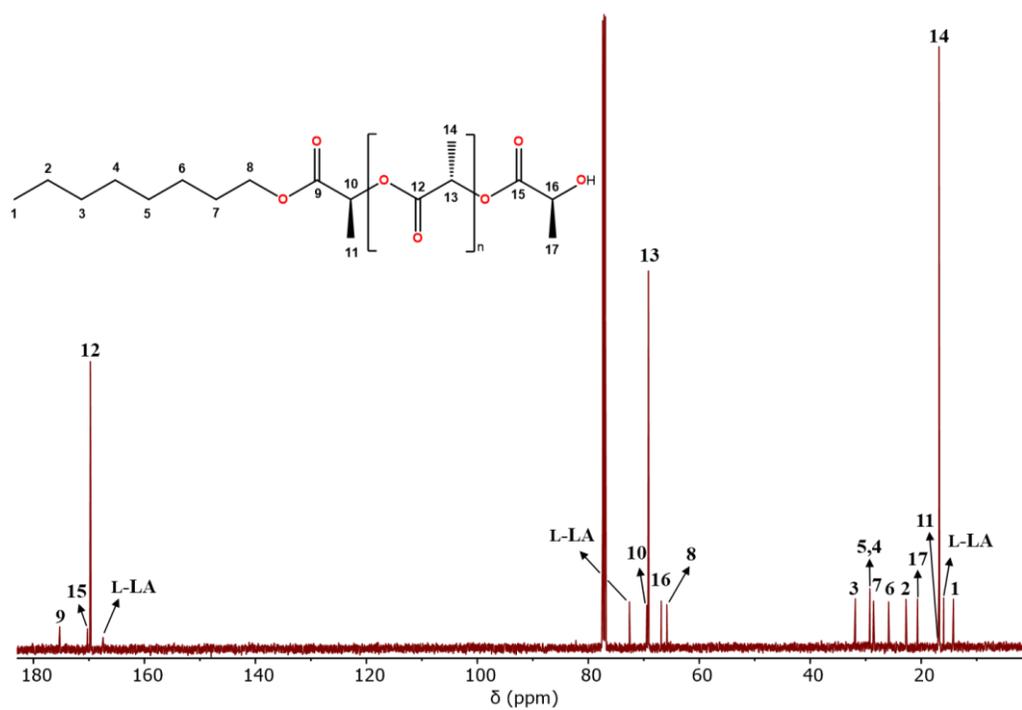


Figure S2. ^{13}C NMR spectrum of the oligomers obtained from ROP of L-lactide catalyzed by tin (III) acetate (Entry 10, Table 4) in presence of 1-octanol as initiator.

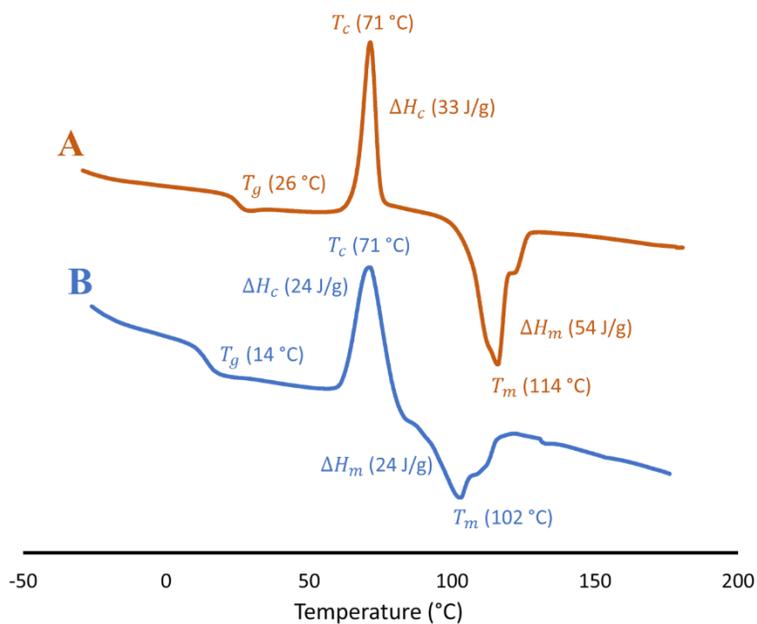


Figure S3. Thermograms (DSC) of oligomers obtained from ROP of L-LA initiated by $\text{Sn}(\text{OAc})_2$ and 1-octanol: A) Purified oligomers and B) Reaction crude.

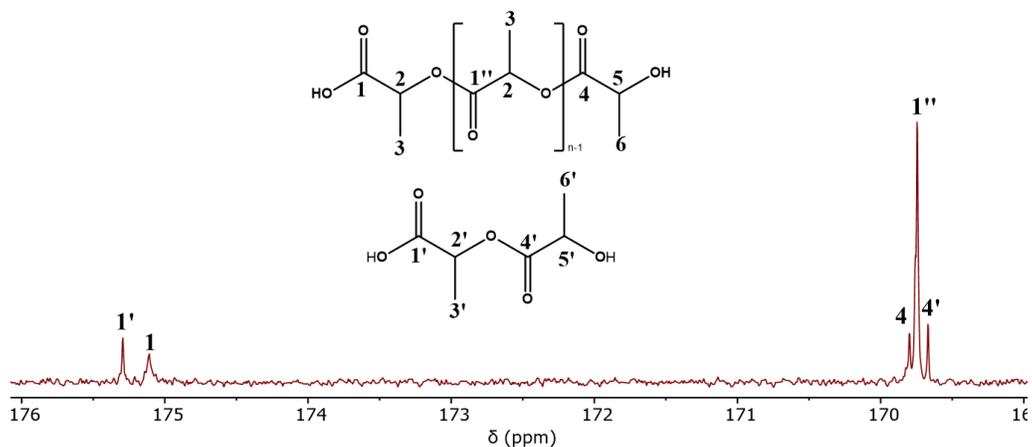


Figure S4. ^{13}C NMR spectrum of the carbonyl region of the oligomers obtained from the ROP of L-LA catalyzed by antimony(III) acetate (Entry 8, Table 3) in presence of water (H_2O) as initiator.

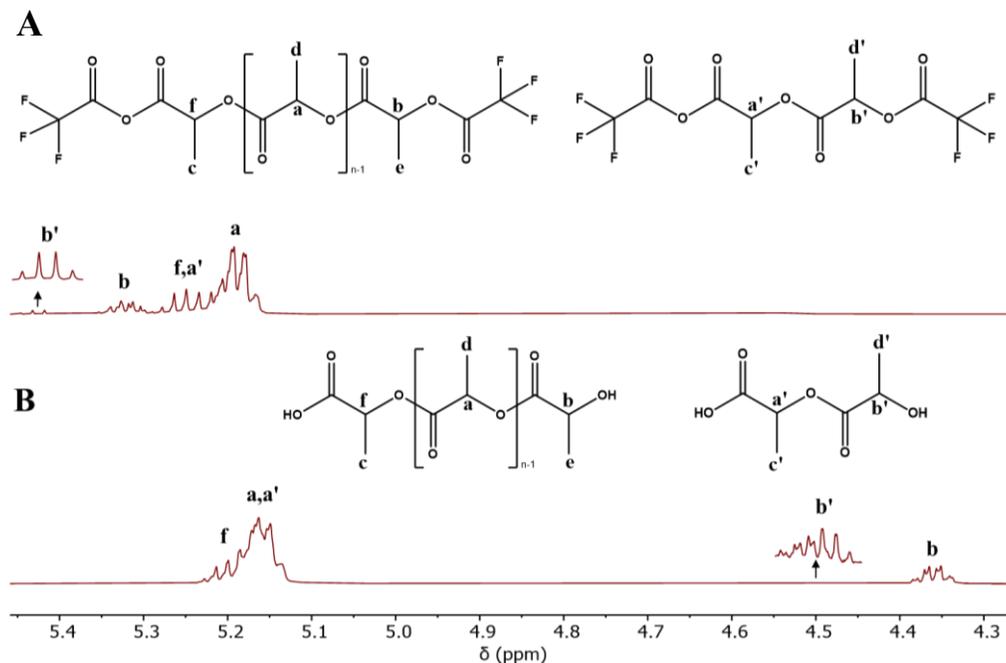


Figure S5. ^1H NMR spectrum of methine region of oligomers obtained from ROP L-LA catalyzed by antimony(III) acetate (Entry 8, Table 3) in presence of water (H_2O) as initiator: A) After the derivatization reaction and B) before the derivatization reaction.

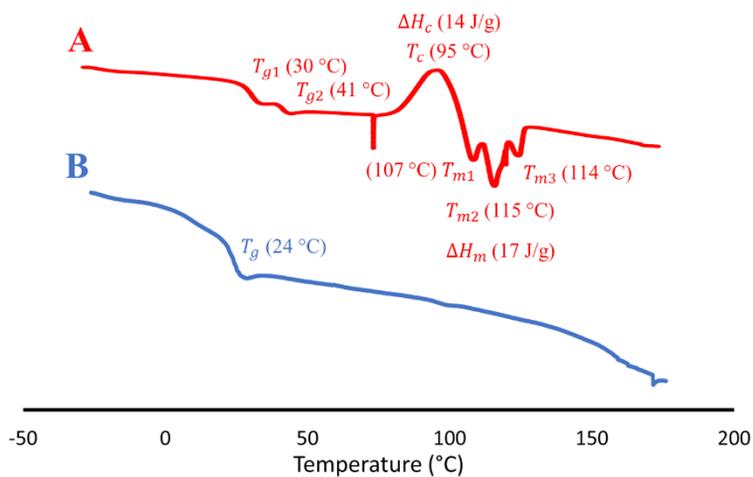


Figure S6. Thermograms (DSC) of oligomers obtained from ROP of L-LA using water (H_2O) as initiator and tin(II) acetate (A, Entry 6, Table 3) and antimony(III) acetate (B, Entry 8, Table 3) as catalysts.

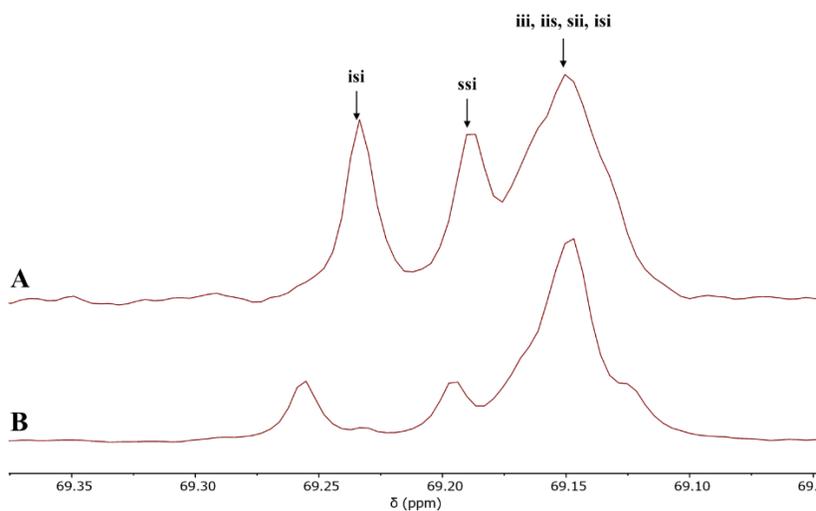


Figure S7. ^{13}C NMR spectrum of methine $[-\text{OOC}-\text{CH}(\text{CH}_3)-\text{O}-]$ region of the oligomers obtained from ROP of L-LA catalyzed by indium(II) (A) acetate and antimony(III) acetate (B) in presence of water (H_2O) as initiator (Solvent: CDCl_3 , i = isotactic tetrad, s = syndiotactic tetrad).

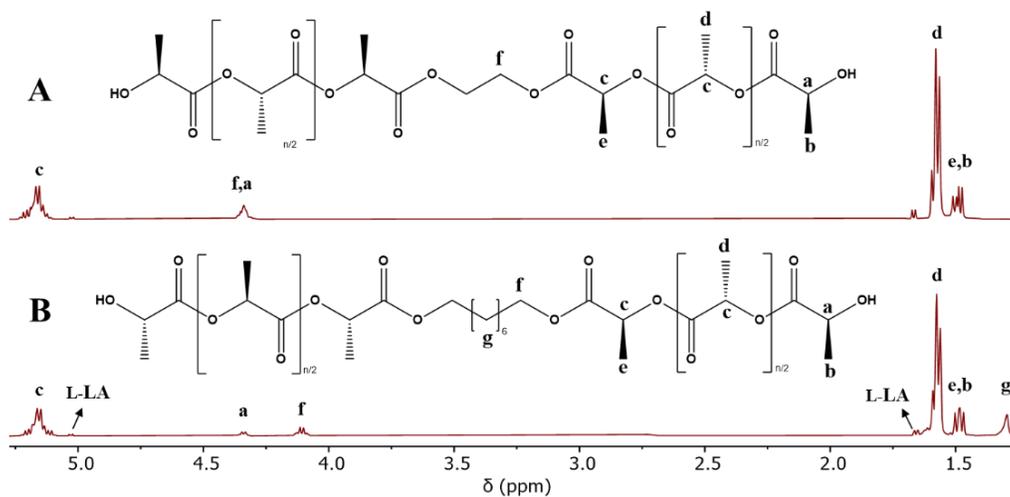


Figure S8. ^1H NMR spectrum of the oligomers obtained from ROP of L-lactide catalyzed by tin(II) acetate in presence of ethylene glycol (A, Entry 13, Table 4) and 1,8-octanediol (B, Entry 14, Table 4) as initiators.

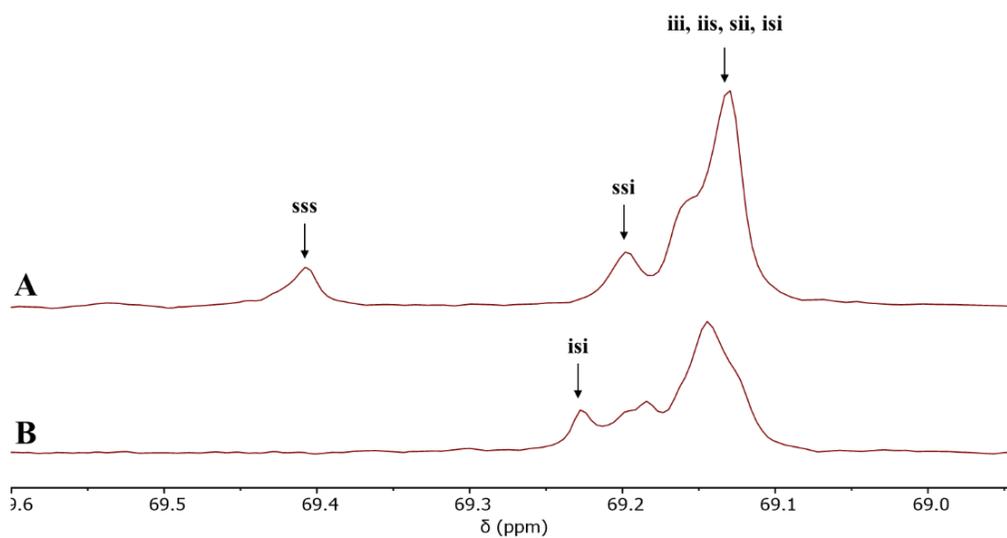


Figure S9. ^{13}C NMR spectrum of methine $[-\text{OOC}-\text{CH}(\text{CH}_3)-\text{O}-]$ region of the oligomers obtained from ROP of L-LA catalyzed by tin(II) acetate in presence of 1,8-octanediol (A) and ethylene glycol (B) as initiators (Solvent: CDCl_3 , i = isotactic tetrad, s = syndiotactic tetrad).

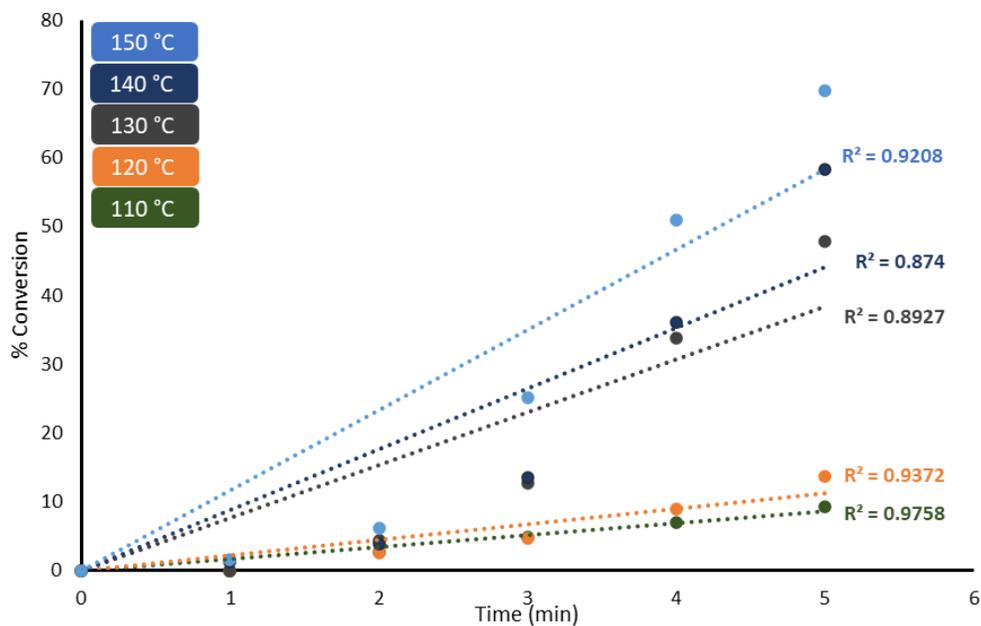


Figure S10. Thermal effect in the ROP of L-lactide initiated by tin(II) acetate and 1-octanol.

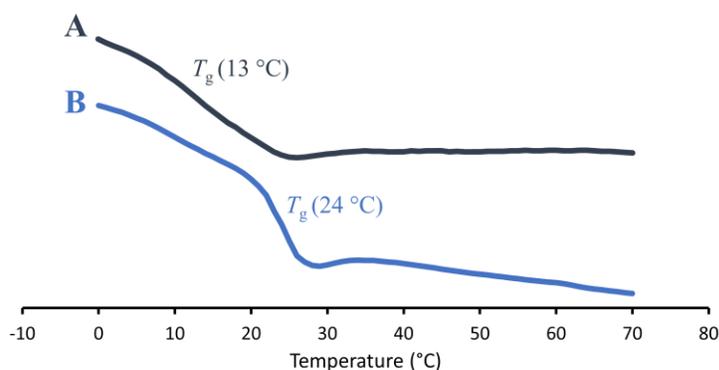


Figure S11. Thermograms (DSC) of oligomers obtained from ROP of L-LA using water (H₂O) as initiator and antimony(III) acetate (B, Entry 8, Table 3) as catalyst, respectively: after the reaction time finishes (B) and one year later (A).

Table S1. Optimized cartesian coordinates (xyz) for all species in the energy profile of Figure 9. Coordinates are given in Å.

Add E(scf)= -900.931340804				TS ₁ E(scf)= -900.913850235 v _{min} = -726.4915			
50	0.707313000	0.083547000	-1.072647000	50	0.207299000	-0.181284000	-1.032709000
8	1.716436000	1.421843000	0.519895000	8	-1.750995000	-1.076018000	-0.024134000
8	0.166398000	-1.179090000	0.637000000	8	1.716568000	1.527489000	-0.095116000
6	0.665748000	2.091699000	0.702244000	6	-2.895869000	-0.416677000	0.181225000
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8	2.236428000	-1.600616000	0.050855000	8	-0.460723000	1.630534000	0.074993000
6	0.625734000	3.182954000	1.736098000	6	-3.286563000	-0.318932000	1.640162000
8	-0.369490000	1.823271000	0.028789000	8	-3.529795000	0.054214000	-0.724113000
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1	-3.199950000	-2.285435000	-2.039912000	1	-2.589548000	1.123999000	3.197241000
1	-1.785247000	-2.907598000	-1.134319000	1	-1.340928000	2.126800000	2.392801000
50	1.277620000	-1.083936000	-0.777169000	50	1.514675000	0.568377000	0.836665000
8	3.021206000	1.395926000	0.911827000	8	1.964282000	-1.720655000	1.089780000
6	2.819675000	1.620556000	-0.290443000	6	2.499184000	-1.769926000	-0.039398000
6	3.151921000	2.968054000	-0.878839000	6	3.014737000	-3.063716000	-0.602932000
8	2.320470000	0.767315000	-1.111276000	8	2.587720000	-0.705107000	-0.735598000
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1	3.675255000	2.843020000	-1.839539000	1	2.292275000	-3.426559000	-1.354200000
1	3.758146000	3.558901000	-0.178149000	1	3.113411000	-3.818091000	0.189795000
8	-0.773721000	-1.686195000	1.014004000	8	-0.894336000	2.060145000	-0.220685000
6	-0.214039000	-1.544864000	2.308486000	6	-0.562923000	2.516233000	-1.515872000
1	0.179415000	-2.545597000	2.545904000	1	-0.193561000	3.542374000	-1.363199000
1	-0.994282000	-1.284696000	3.041847000	1	-1.460416000	2.553536000	-2.155863000
6	0.897679000	-0.514470000	2.388226000	6	0.496595000	1.693652000	-2.224425000
1	0.488935000	0.497849000	2.244209000	1	0.124783000	0.672365000	-2.403913000
1	1.358133000	-0.574678000	3.390196000	1	0.712664000	2.174266000	-3.196663000
8	1.895494000	-0.775606000	1.408367000	8	1.678923000	1.657354000	-1.435621000
1	2.479886000	0.081626000	1.312664000	1	2.258670000	0.949843000	-1.769407000
	Int₆				Int₇		
	E(scf)= -1205.87700229				E(scf)= -1205.87489056		
8	1.199612000	0.286800000	1.143650000	8	-2.116750000	0.287326000	-0.277153000
6	1.047066000	0.447806000	-0.236270000	6	-0.906895000	-0.092696000	0.314326000
6	2.435649000	0.746134000	-0.825505000	6	-1.222688000	-0.981349000	1.530183000
8	0.464311000	-0.600819000	-0.837488000	8	-0.045683000	-0.675019000	-0.531214000
8	3.311085000	-0.341781000	-0.521564000	8	-2.036820000	-2.086338000	1.129220000
6	2.005754000	-0.811148000	1.521640000	6	-2.911818000	-0.773601000	-0.770106000
6	3.097764000	-1.169604000	0.507589000	6	-2.798490000	-2.072560000	0.032247000
8	3.786517000	-2.137213000	0.658950000	8	-3.405231000	-3.051490000	-0.296838000
6	1.162893000	-2.025633000	1.892698000	6	-2.674001000	-1.025080000	-2.255820000
1	2.560124000	-0.474123000	2.415439000	1	-3.955304000	-0.444646000	-0.625606000
1	0.591140000	-2.375363000	1.019178000	1	-1.649997000	-1.391641000	-2.422799000
1	0.461848000	-1.736362000	2.692845000	1	-2.812599000	-0.080674000	-2.807014000
1	1.810717000	-2.838547000	2.254836000	1	-3.392315000	-1.771486000	-2.628089000
6	2.434676000	0.928180000	-2.326711000	6	0.012007000	-1.548205000	2.194689000
1	2.834927000	1.647227000	-0.327946000	1	-1.811205000	-0.382656000	2.246846000
1	2.043148000	0.019156000	-2.809138000	1	0.542231000	-2.192800000	1.476184000
1	3.460370000	1.109961000	-2.685283000	1	-0.274928000	-2.146728000	3.074330000
1	1.802831000	1.788218000	-2.602379000	1	0.686229000	-0.735068000	2.506149000
50	-1.499750000	-0.139941000	-1.349778000	50	1.516361000	0.637478000	-0.977125000

8	-2.090936000	-2.077746000	-0.265558000	8	2.628909000	0.116858000	0.898964000
6	-2.344808000	-1.434070000	0.786780000	6	3.140213000	-0.924837000	0.380043000
6	-2.779223000	-2.149404000	2.032214000	6	4.005895000	-1.820567000	1.216231000
8	-2.202146000	-0.172292000	0.793789000	8	2.885245000	-1.203092000	-0.820571000
1	-3.394227000	-1.491479000	2.662984000	1	4.627563000	-2.464407000	0.578451000
1	-1.873849000	-2.429907000	2.597347000	1	3.346259000	-2.457794000	1.830508000
1	-3.320959000	-3.070707000	1.773891000	1	4.626879000	-1.220199000	1.897734000
8	0.170622000	1.552371000	-0.421013000	8	-0.284666000	1.117242000	0.738865000
6	0.248531000	2.694948000	0.419203000	6	-1.036002000	2.169413000	1.320120000
1	0.096383000	3.578680000	-0.221165000	1	-0.437042000	2.580063000	2.148401000
1	1.245363000	2.765922000	0.880143000	1	-1.984512000	1.787736000	1.727532000
6	-0.812772000	2.656295000	1.505401000	6	-1.319481000	3.257364000	0.297704000
1	-1.810084000	2.534611000	1.035529000	1	-0.357997000	3.573624000	-0.161433000
1	-0.639151000	1.773735000	2.146830000	1	-1.958004000	2.835064000	-0.500980000
8	-0.705172000	3.869752000	2.205410000	8	-1.941914000	4.309801000	0.984388000
1	-1.325368000	3.862417000	2.944139000	1	-2.210478000	4.988084000	0.353070000

TS₃

E(scf)= -1205.86857227

v_{min}= -46.1064

8	-1.124477000	0.749118000	-0.795911000
6	-0.760807000	0.542959000	0.553350000
6	-1.957837000	0.910207000	1.458286000
8	-0.434902000	-0.747672000	0.770166000
8	-3.039440000	0.027248000	1.160813000
6	-2.441562000	0.395628000	-1.176971000
6	-3.240884000	-0.353068000	-0.101300000
8	-4.066007000	-1.177518000	-0.373829000
6	-2.390840000	-0.382832000	-2.477940000
1	-3.005782000	1.337368000	-1.339834000
1	-1.901355000	-1.359091000	-2.321603000
1	-1.817945000	0.189908000	-3.224733000
1	-3.406000000	-0.567973000	-2.858924000
6	-1.652537000	0.781745000	2.933250000
1	-2.278275000	1.940863000	1.222062000
1	-1.318691000	-0.243777000	3.152888000
1	-2.556790000	1.003703000	3.522523000
1	-0.854996000	1.485766000	3.216233000
50	0.902817000	-1.900580000	-0.252506000
8	2.257195000	-0.217567000	-0.886999000
6	2.886036000	-0.266333000	0.213329000
6	3.927791000	0.758418000	0.540119000
8	2.595767000	-1.169025000	1.048162000
1	4.697527000	0.329497000	1.198336000
1	3.422279000	1.573769000	1.086513000
1	4.373421000	1.169683000	-0.376762000
8	0.339701000	1.354695000	0.809951000
6	0.323207000	2.697388000	0.375630000
1	0.826257000	3.292627000	1.155954000
1	-0.703288000	3.087505000	0.268954000
6	1.056881000	2.887661000	-0.943144000
1	2.077900000	2.469023000	-0.856353000
1	0.532279000	2.321691000	-1.733797000
8	1.071613000	4.272710000	-1.192629000
1	1.480328000	4.431883000	-2.051621000

TS₄

E(scf)= -1205.85609641

v_{min}= -169.0548

8	-0.717362000	0.070176000	-0.886511000
6	-0.381928000	0.878607000	0.961703000

Int₈

E(scf)= -1205.87172199

8	-0.859021000	-0.336038000	0.629112000
6	-0.686551000	-0.459500000	-0.809879000
6	-2.067212000	-0.654244000	-1.471115000
8	-0.085703000	0.653083000	-1.235941000
8	-2.968710000	0.354283000	-1.008713000
6	-2.172013000	-0.322696000	1.168937000
6	-3.100458000	0.539322000	0.306996000
8	-3.892278000	1.318246000	0.753414000
6	-2.098436000	0.163831000	2.599942000
1	-2.577911000	-1.354490000	1.156545000
1	-1.735957000	1.204585000	2.637785000
1	-1.415632000	-0.480397000	3.176403000
1	-3.097435000	0.137879000	3.059767000
6	-1.990806000	-0.553301000	-2.977358000
1	-2.472679000	-1.640124000	-1.181106000
1	-1.603862000	0.437048000	-3.259865000
1	-2.990613000	-0.698386000	-3.416582000
1	-1.306850000	-1.324333000	-3.363940000
50	0.818438000	1.698422000	0.314350000
8	2.217117000	0.005312000	0.768689000
6	3.004195000	0.333871000	-0.172914000
6	4.148367000	-0.563778000	-0.536405000
8	2.783138000	1.392177000	-0.818651000
1	4.946873000	0.006403000	-1.032285000
1	3.762948000	-1.317541000	-1.245128000
1	4.527966000	-1.086199000	0.353805000
8	0.135131000	-1.553187000	-1.061310000
6	-0.087937000	-2.763439000	-0.375682000
1	-0.038250000	-3.583121000	-1.112248000
1	-1.085076000	-2.803834000	0.096717000
6	0.968844000	-2.983703000	0.693671000
1	1.969837000	-2.920354000	0.221433000
1	0.905757000	-2.170963000	1.439666000
8	0.722819000	-4.250686000	1.252935000
1	1.361072000	-4.410965000	1.958096000

Int₉

E(scf)= -1205.85775399

8	0.762696000	-0.065375000	1.036213000
6	0.234802000	1.045874000	-1.041430000

6	-1.702306000	1.638605000	0.995614000	6	1.480819000	1.894268000	-0.820419000
8	-0.259347000	-0.202623000	1.571019000	8	0.281336000	-0.016975000	-1.646983000
8	-2.791548000	0.747341000	0.887687000	8	2.634078000	1.092169000	-0.863100000
6	-2.014044000	0.190542000	-1.378876000	6	2.088503000	0.171318000	1.379185000
6	-3.047759000	0.058714000	-0.248215000	6	3.000936000	0.252102000	0.139058000
8	-4.036026000	-0.612780000	-0.309277000	8	4.008927000	-0.377939000	0.005466000
6	-2.309507000	-0.795465000	-2.501079000	6	2.640728000	-0.842933000	2.373958000
1	-2.138653000	1.217372000	-1.790667000	1	2.144283000	1.174106000	1.859985000
1	-2.296625000	-1.833518000	-2.126630000	1	2.704993000	-1.845733000	1.917593000
1	-1.543107000	-0.684828000	-3.285264000	1	1.965290000	-0.885412000	3.243787000
1	-3.304199000	-0.615440000	-2.937680000	1	3.652491000	-0.569179000	2.712881000
6	-1.840955000	2.362055000	2.327959000	6	1.604286000	2.924483000	-1.939302000
1	-1.732037000	2.370221000	0.172394000	1	1.405369000	2.411773000	0.148234000
1	-1.804040000	1.632243000	3.151938000	1	1.685290000	2.412874000	-2.911519000
1	-2.808142000	2.887629000	2.359268000	1	2.513814000	3.524111000	-1.779675000
1	-1.028490000	3.095465000	2.457711000	1	0.729875000	3.595477000	-1.954833000
50	0.148432000	-1.771667000	0.006855000	50	0.055573000	-1.761501000	-0.040143000
8	2.000597000	-0.810815000	-0.700267000	8	-1.870714000	-1.020946000	0.620715000
6	2.737113000	-1.139648000	0.296900000	6	-2.622596000	-1.363052000	-0.373649000
6	4.149813000	-0.625559000	0.340792000	6	-4.079073000	-0.984406000	-0.294621000
8	2.264958000	-1.831067000	1.215638000	8	-2.148565000	-1.944182000	-1.352651000
1	4.769053000	-1.258337000	0.992520000	1	-4.672937000	-1.605391000	-0.980408000
1	4.124456000	0.393559000	0.764579000	1	-4.178036000	0.071009000	-0.602658000
1	4.576065000	-0.567840000	-0.671899000	1	-4.450348000	-1.077130000	0.737383000
8	0.723726000	1.555187000	0.706056000	8	-0.933737000	1.533472000	-0.695916000
6	0.766321000	2.577003000	-0.280492000	6	-1.087493000	2.437064000	0.397544000
1	0.451592000	3.542875000	0.152064000	1	-0.809964000	3.461924000	0.096376000
1	0.111420000	2.304360000	-1.121417000	1	-0.460087000	2.094169000	1.234147000
6	2.198762000	2.659758000	-0.769605000	6	-2.546404000	2.392115000	0.804822000
1	2.867511000	2.836392000	0.097961000	1	-3.176531000	2.598907000	-0.084736000
1	2.461039000	1.682184000	-1.216568000	1	-2.768588000	1.368554000	1.160856000
8	2.244397000	3.714341000	-1.694102000	8	-2.705680000	3.364305000	1.803008000
1	3.104360000	3.715252000	-2.131208000	1	-3.577354000	3.267786000	2.204847000

Int₁₀

E(scf)= -1205.88683317

8	2.436636000	-0.896519000	1.289944000
6	-3.267340000	-0.003463000	0.528161000
6	-2.122629000	-0.864965000	0.006338000
8	-3.253798000	0.638268000	1.537507000
8	-1.102521000	-0.808136000	0.997153000
6	1.163003000	-0.668771000	1.745189000
6	0.155925000	-0.848836000	0.616737000
8	0.493421000	-1.000398000	-0.547150000
6	0.976988000	0.727874000	2.359306000
1	0.887886000	-1.422061000	2.513862000
1	1.143191000	1.497819000	1.587627000
1	1.728000000	0.857067000	3.154664000
1	-0.033493000	0.852327000	2.782688000
6	-2.526556000	-2.307586000	-0.264466000
1	-1.743561000	-0.405193000	-0.921320000
1	-2.882550000	-2.788929000	0.661157000
1	-1.659976000	-2.866738000	-0.651363000
1	-3.329741000	-2.336924000	-1.015989000
50	2.945530000	-0.731784000	-0.690221000
8	2.204132000	1.390148000	-0.780033000
6	3.306888000	1.894867000	-0.386226000
6	3.395676000	3.382840000	-0.181649000
8	4.282064000	1.152344000	-0.138030000
1	4.432650000	3.726443000	-0.307860000

1	3.082488000	3.603843000	0.853870000
1	2.717896000	3.911286000	-0.867828000
8	-4.294271000	-0.056093000	-0.323338000
6	-5.451250000	0.702112000	0.014310000
1	-5.188768000	1.766583000	0.125529000
1	-5.864314000	0.351823000	0.974339000
6	-6.457048000	0.508872000	-1.102506000
1	-6.011826000	0.864047000	-2.054066000
1	-6.667560000	-0.574265000	-1.214624000
8	-7.599021000	1.238158000	-0.745949000
1	-8.261920000	1.152238000	-1.441624000