

# Substituted glycolides from natural sources: preparation, alcoholysis, and polymerization

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## Supplementary Information

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## S1. NMR spectra of intermediates 1–6 and substituted glycolides

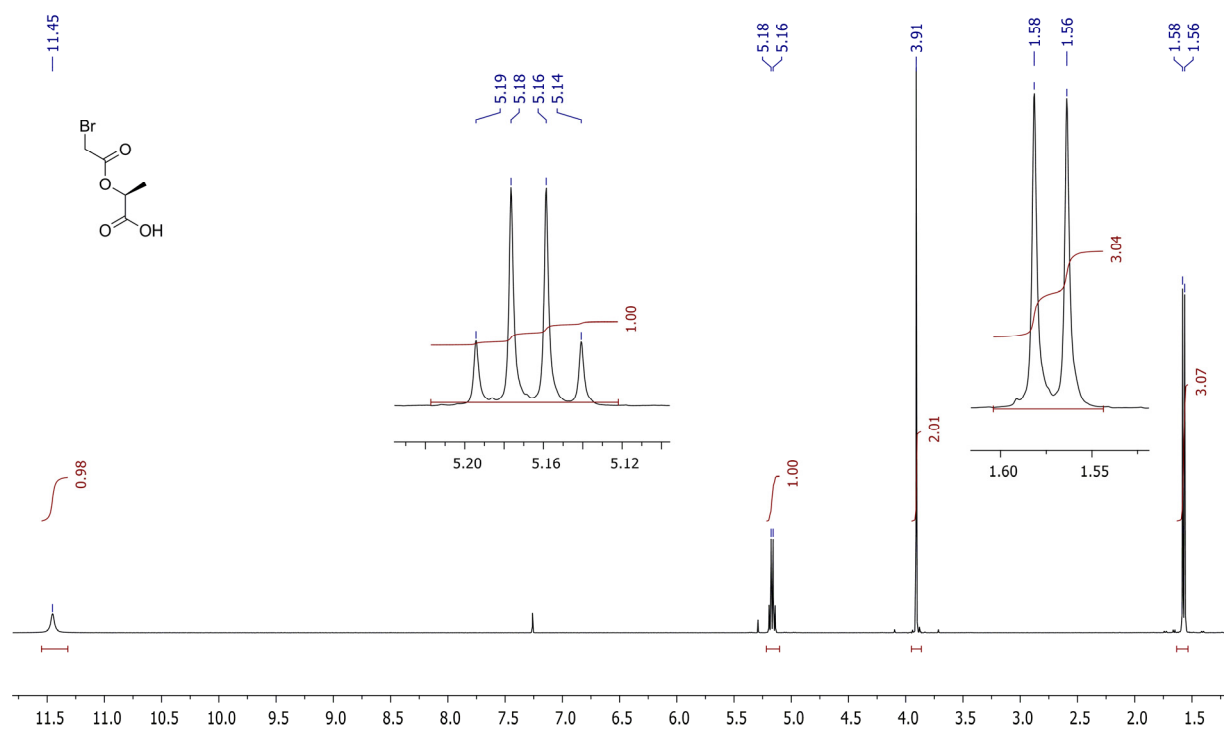


Fig. S1. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of the intermediate 1.

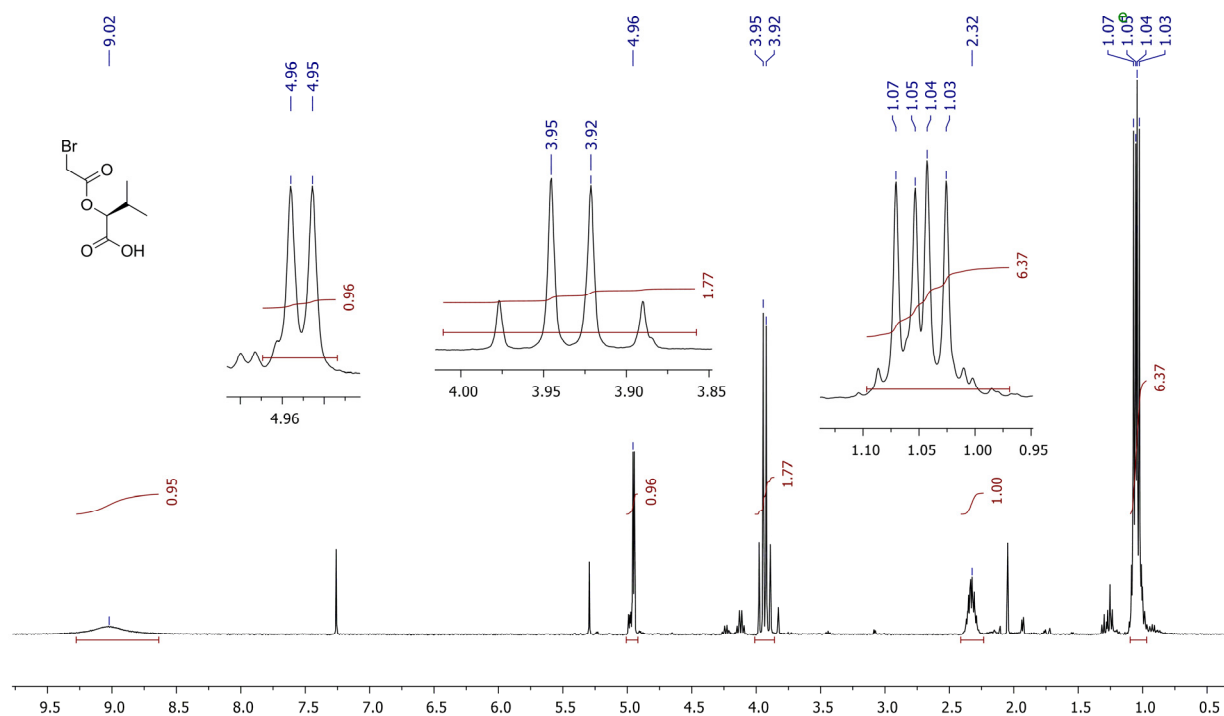
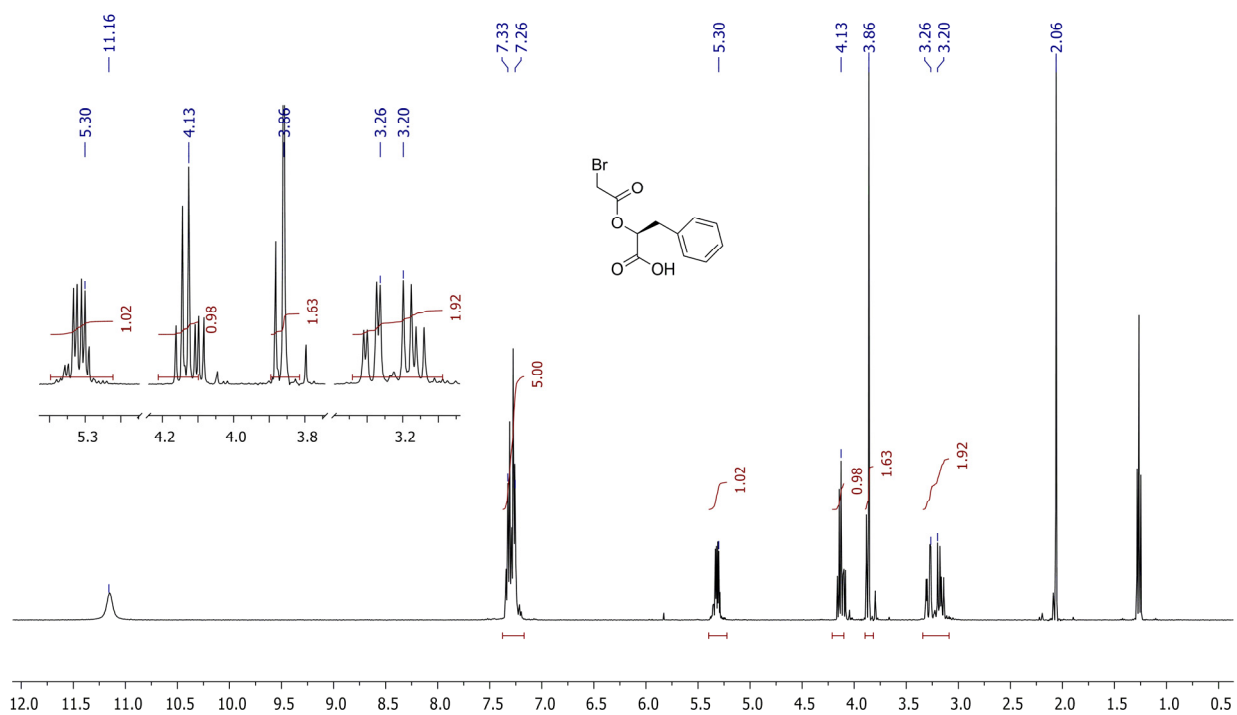
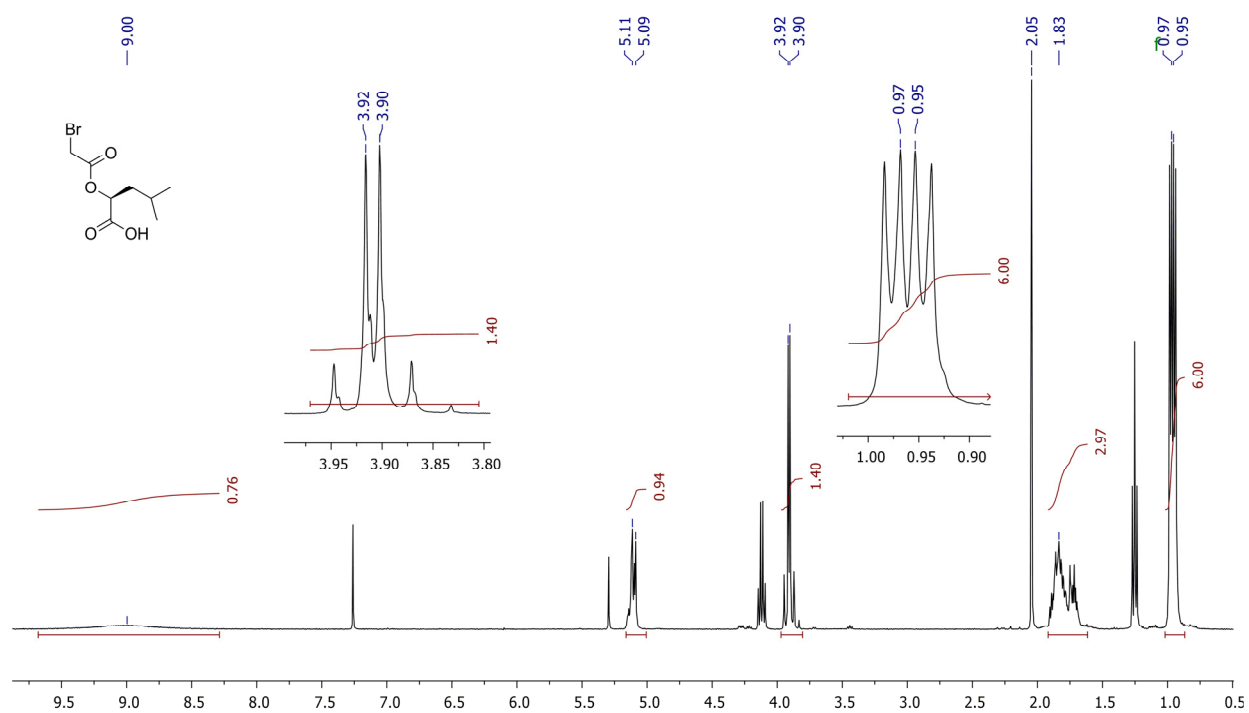


Fig. S2. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of the intermediate 2.



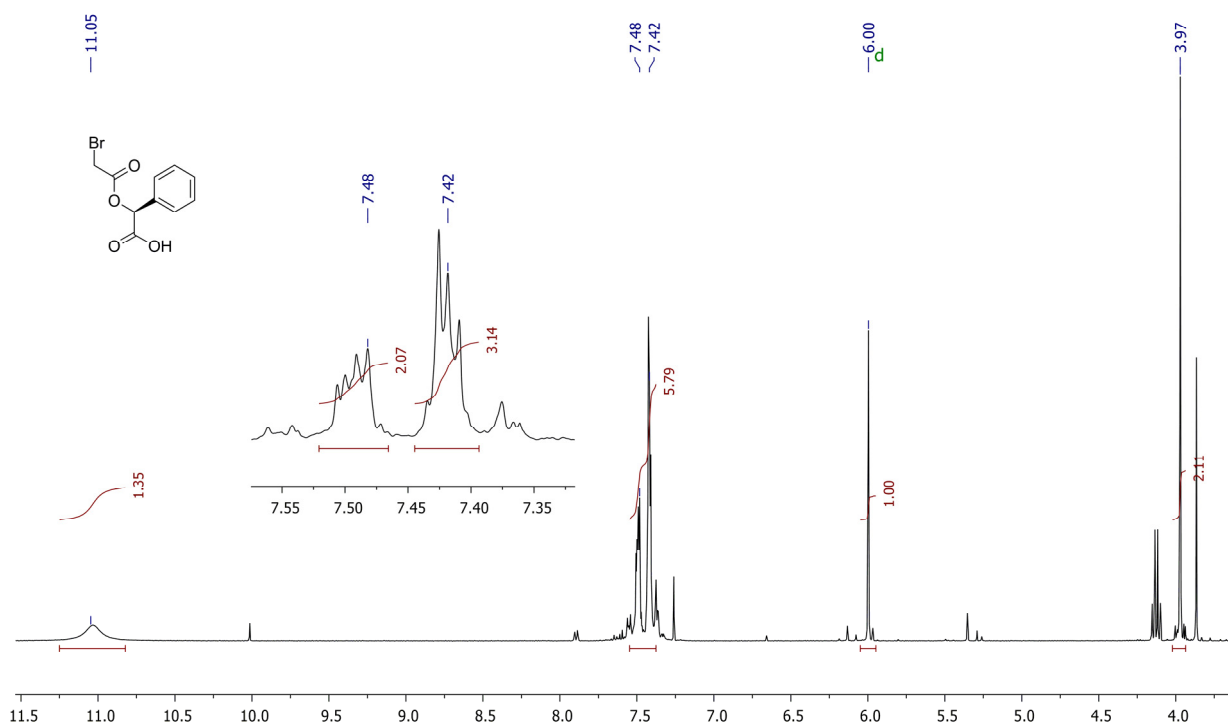


Fig. S5.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the intermediate 5.

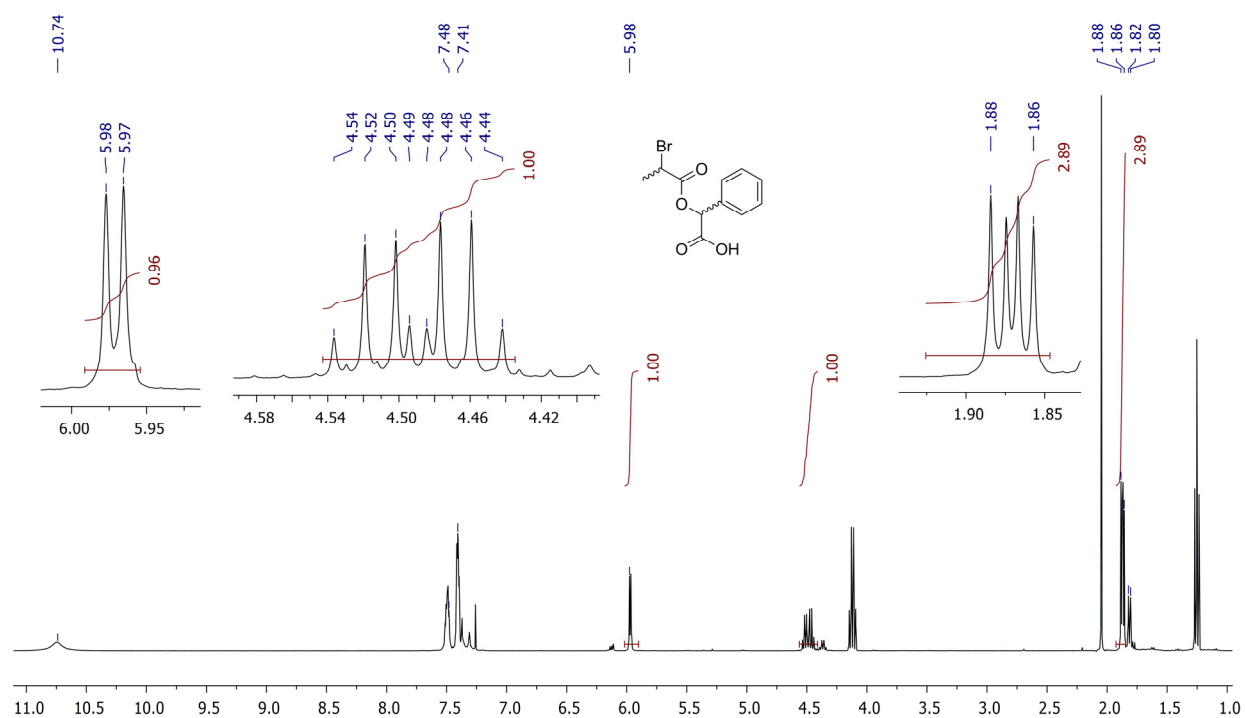


Fig. S6.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the intermediate 6.

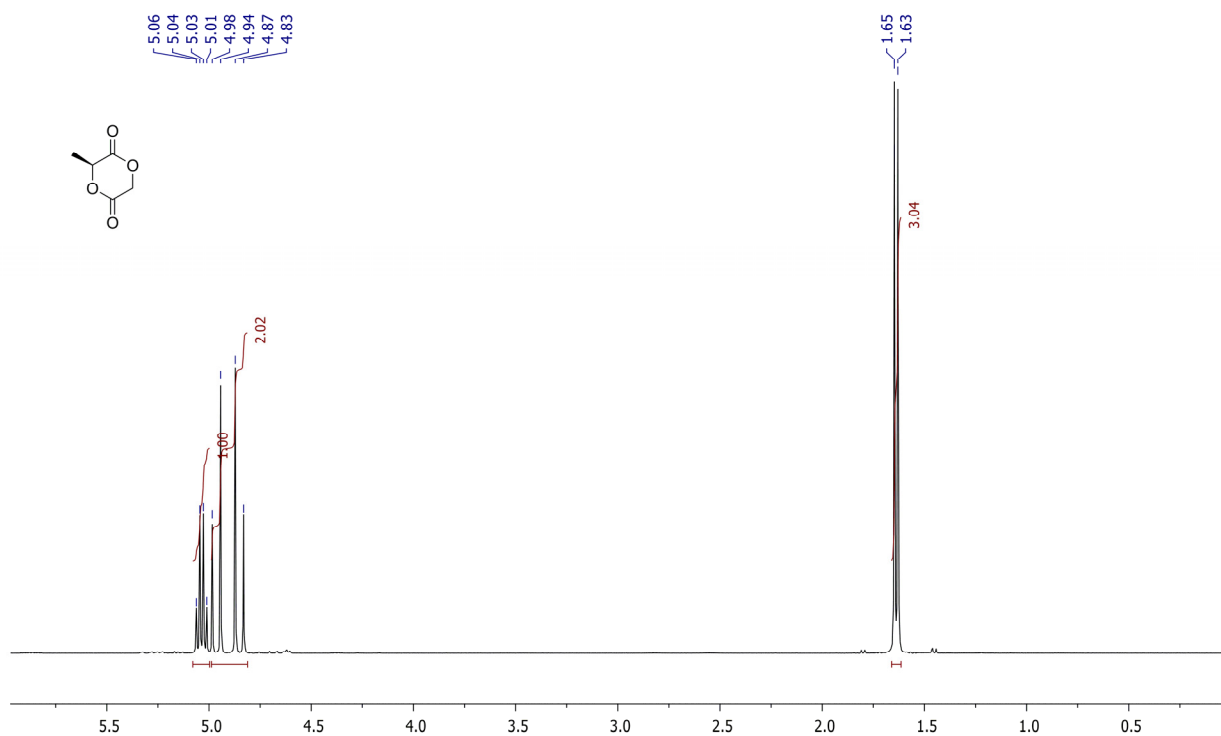


Fig. S7. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of MeGL.

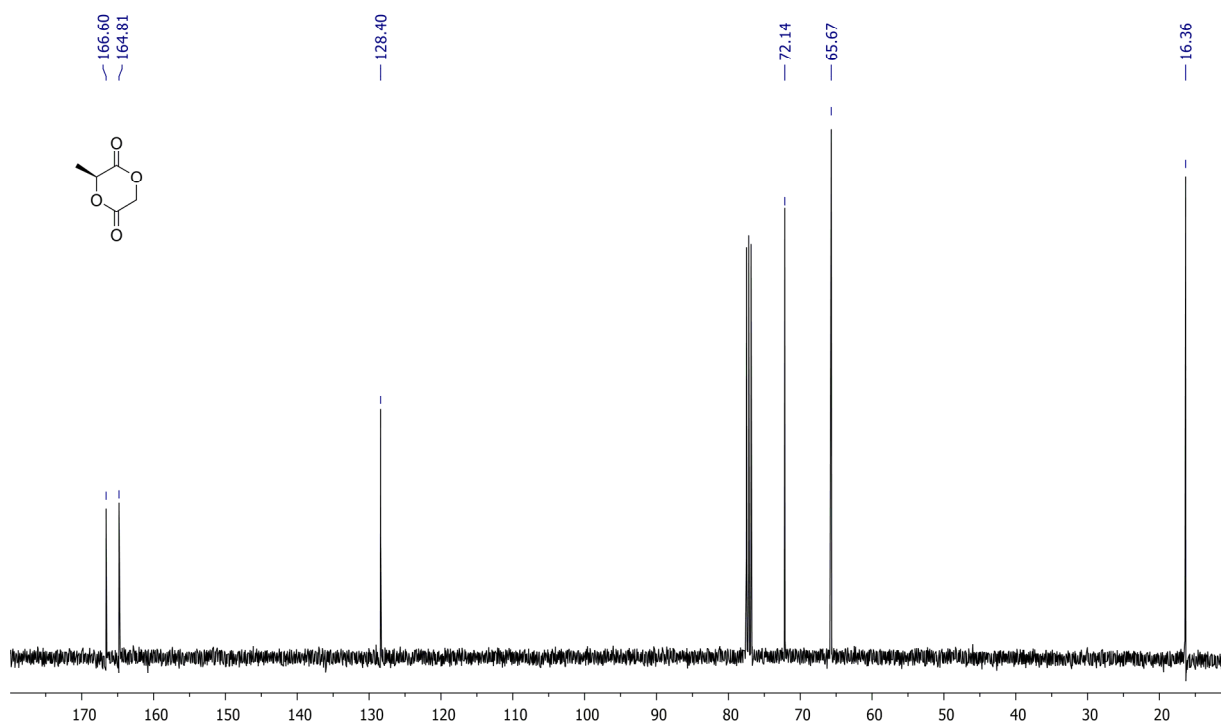


Fig. S8. <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>, 20 °C) of MeGL.

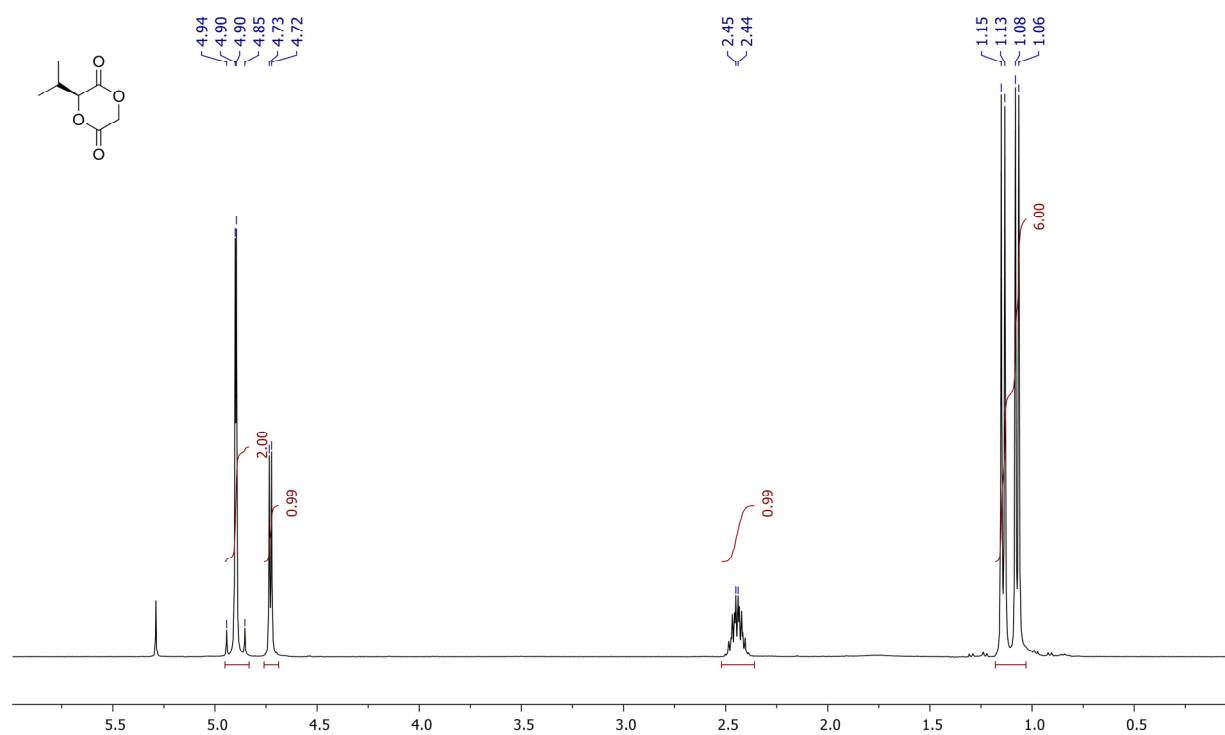


Fig. S9. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of *i*PrGL.

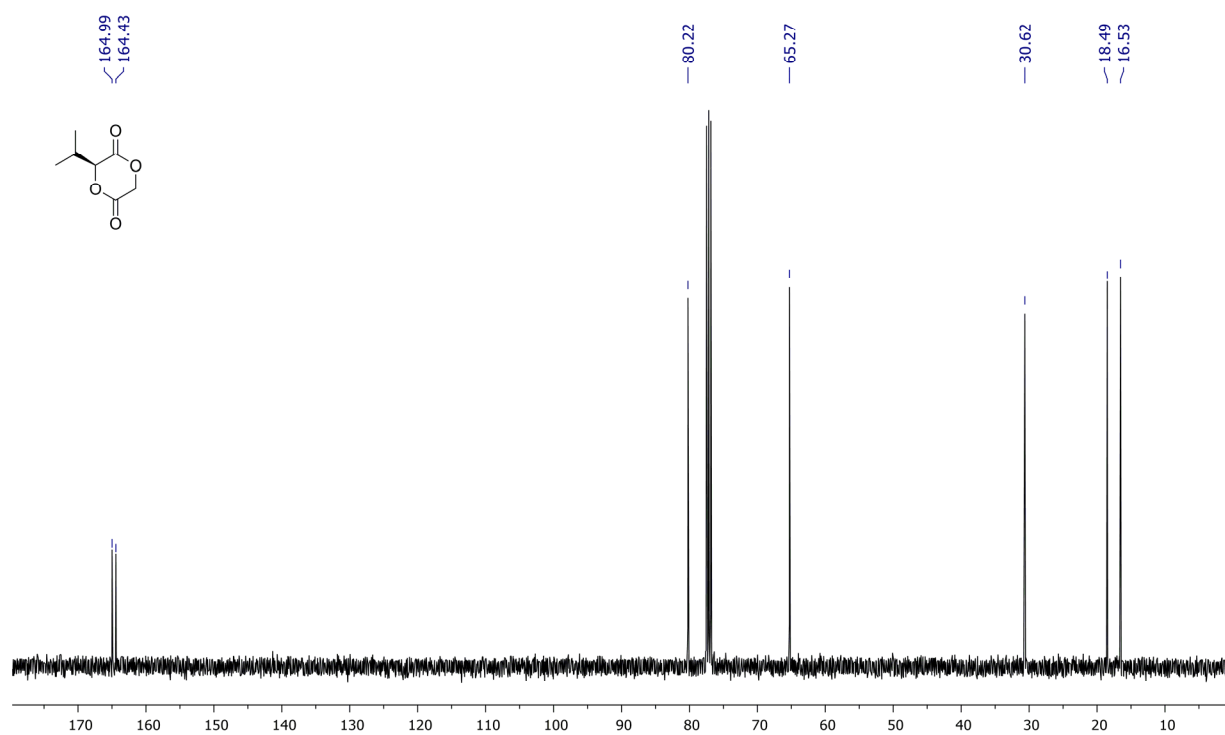


Fig. S10. <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>, 20 °C) of *i*PrGL.

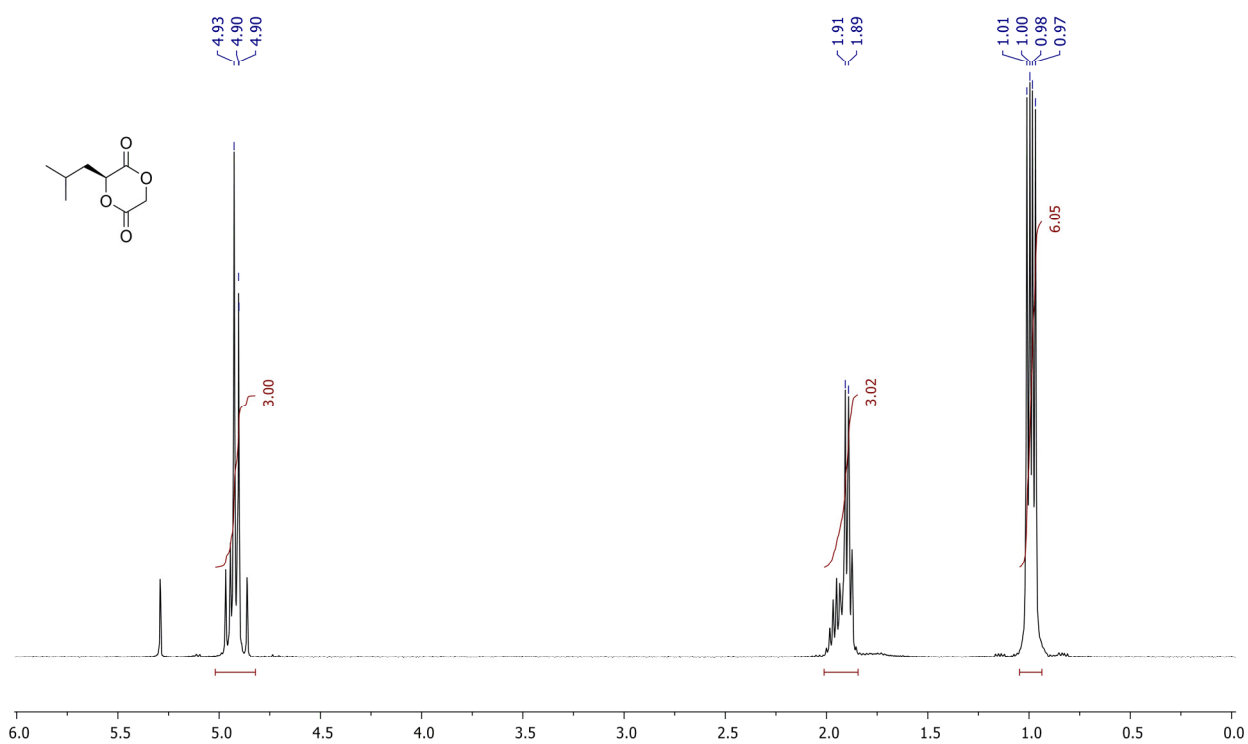


Fig. S11.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of *i*BuGL.

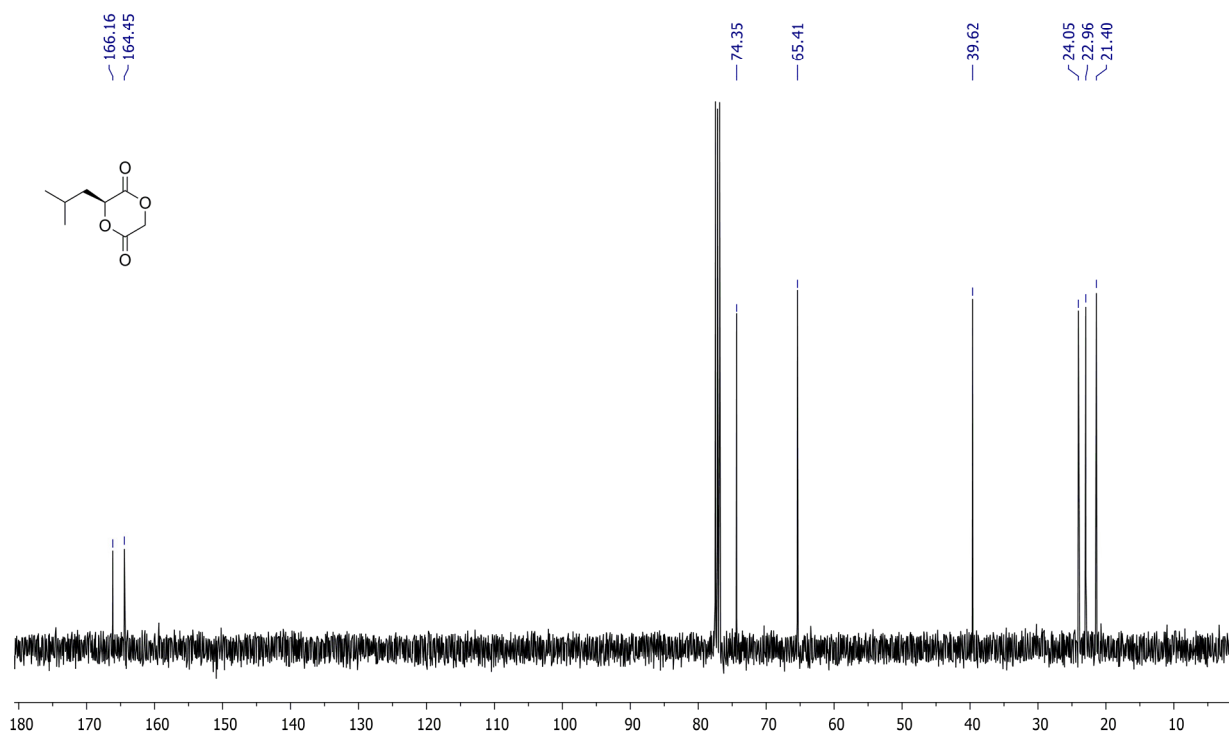
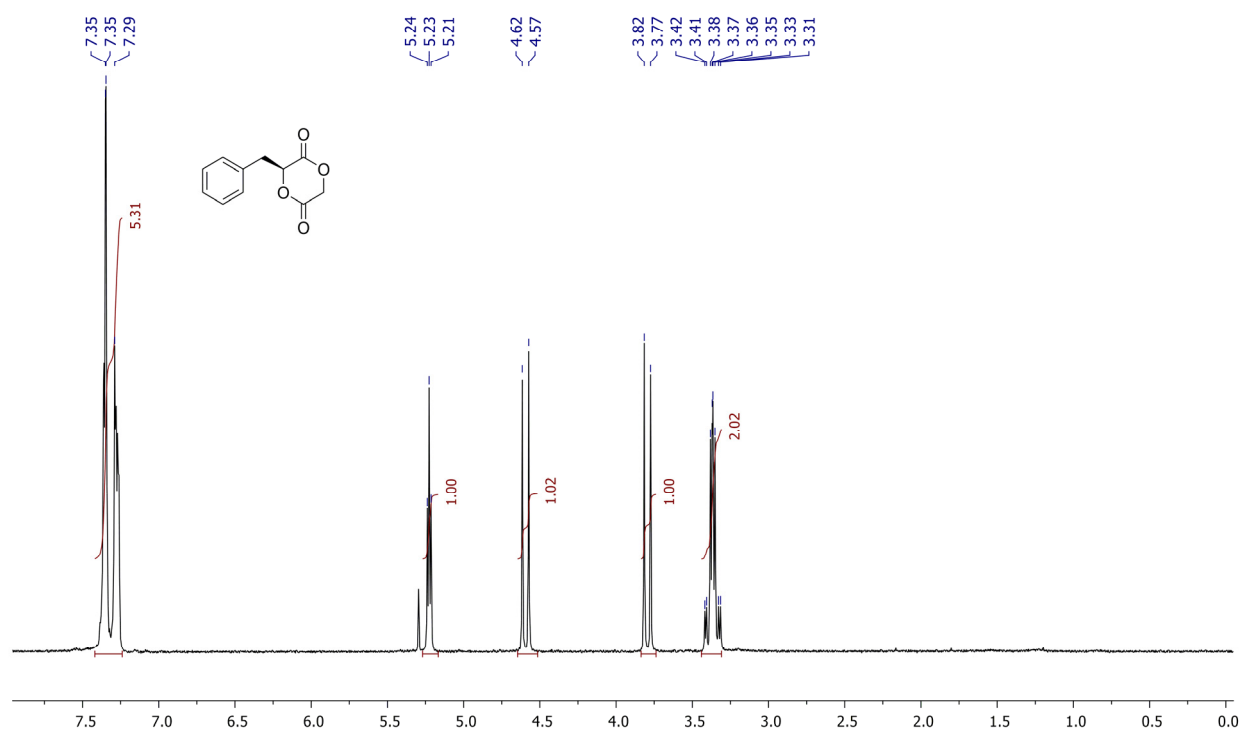
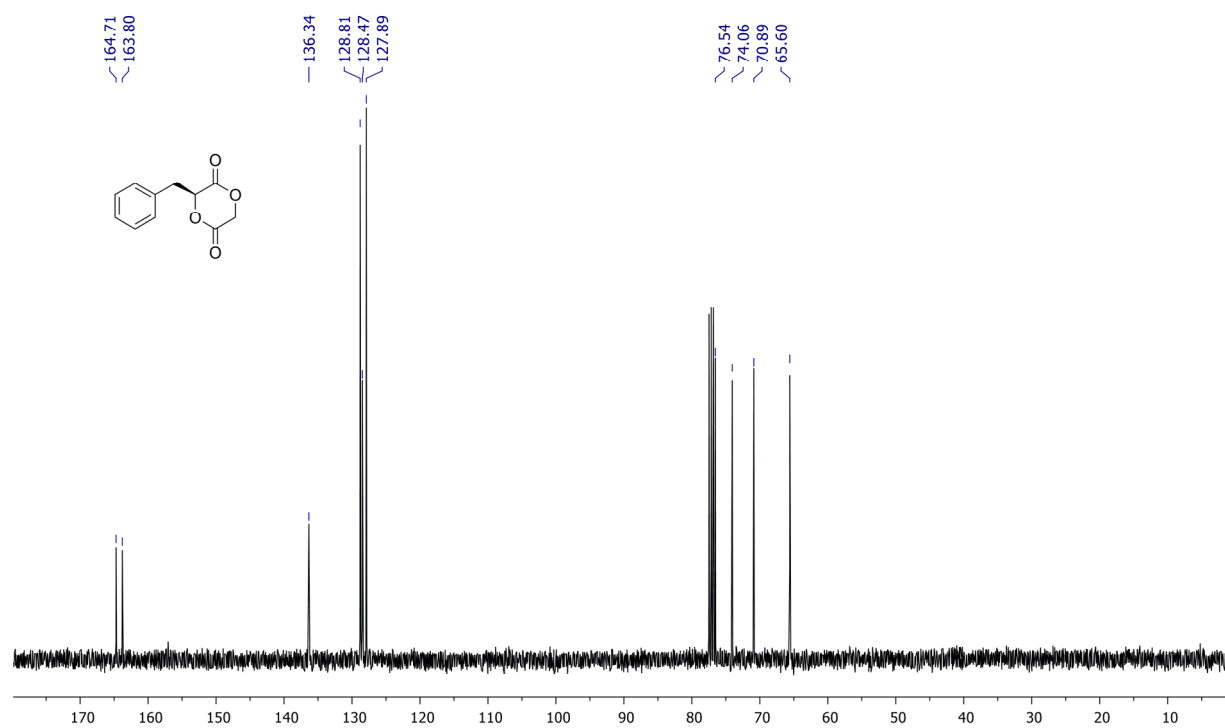


Fig. S12.  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of *i*BuGL.



**Fig. S13.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of BnGL.



**Fig. S14.**  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of BnGL.



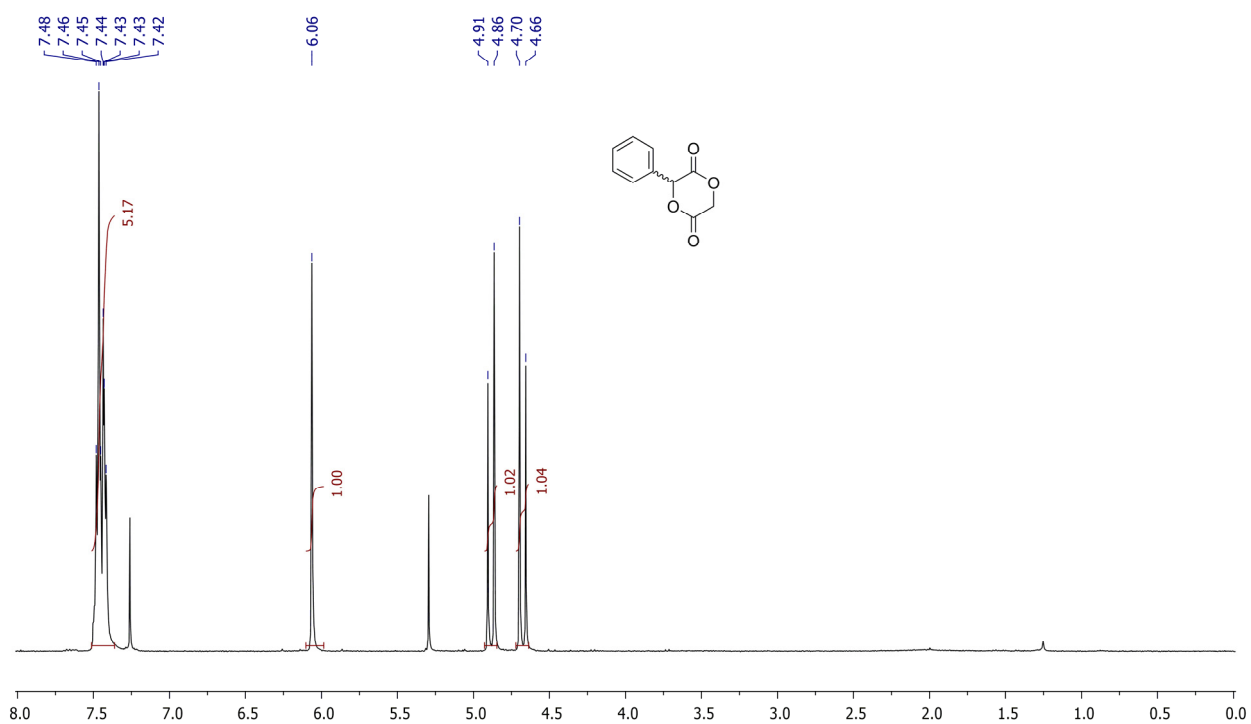


Fig. S15.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of PhGL.

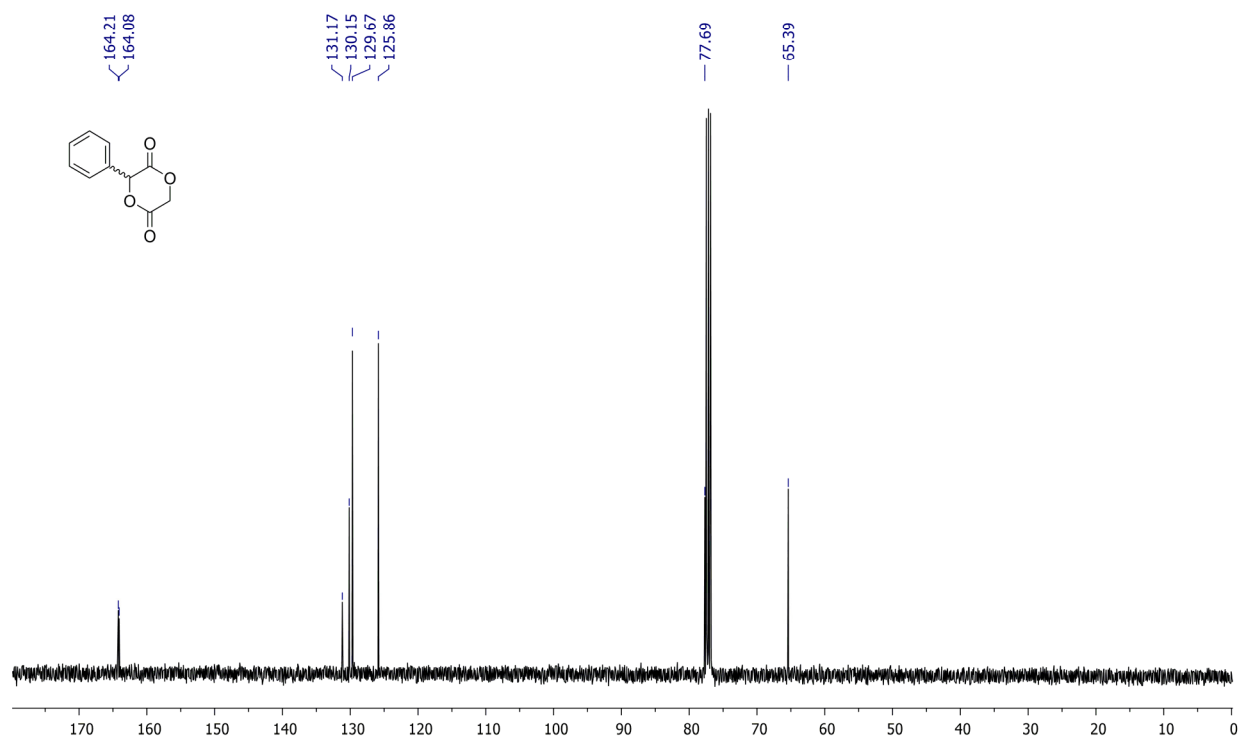
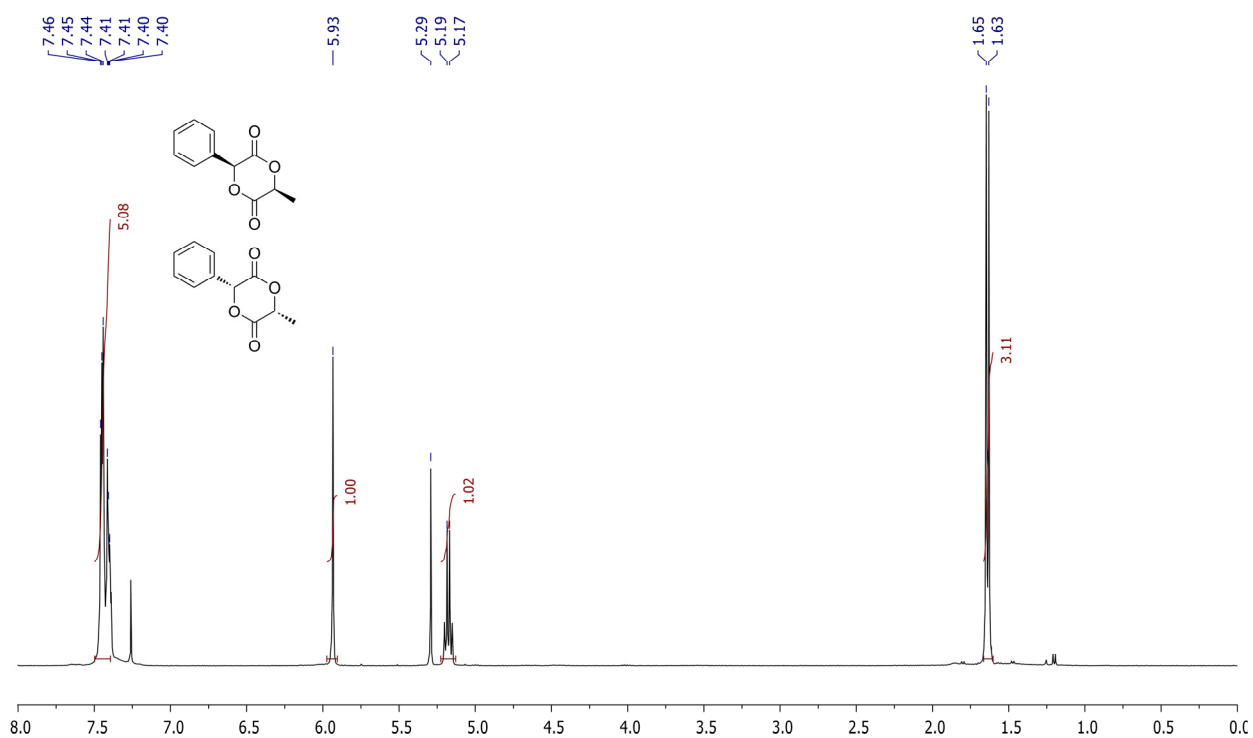
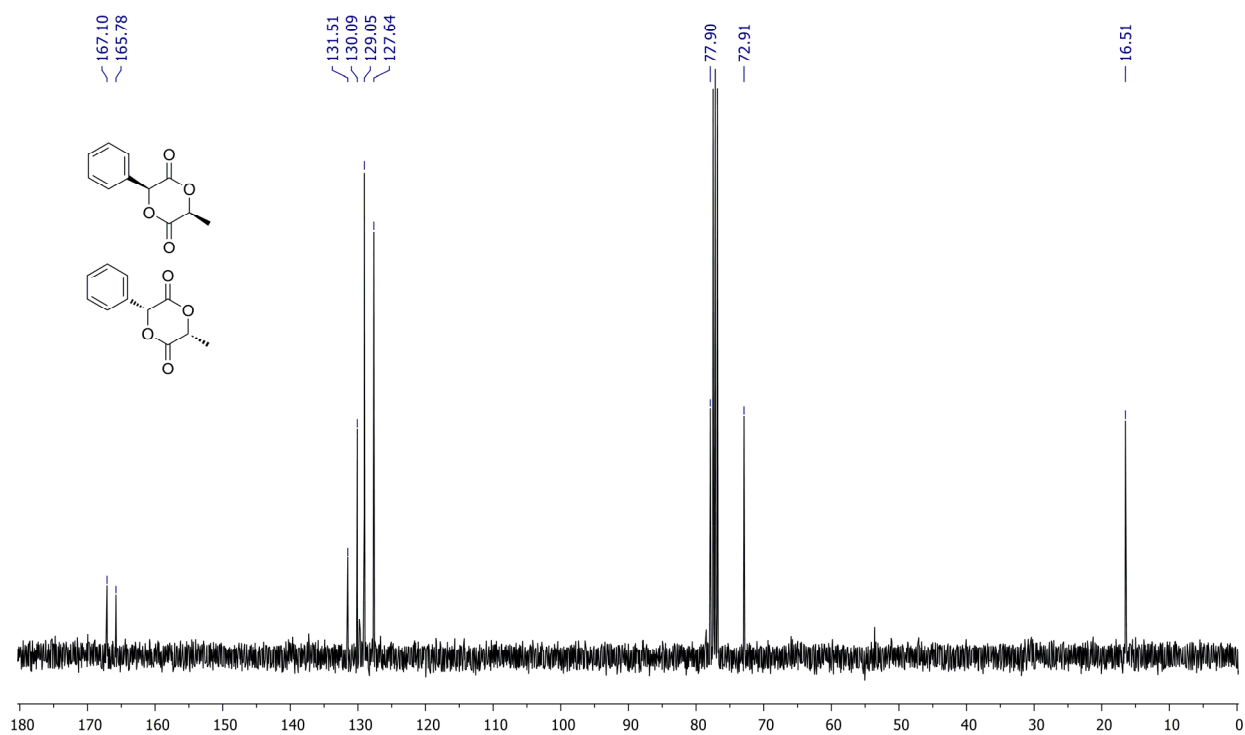


Fig. S16.  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of PhGL.



**Fig. S17.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of MePhGL.



**Fig. S18.**  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of MePhGL.

## S2. DFT modeling of the formation of MePhGL

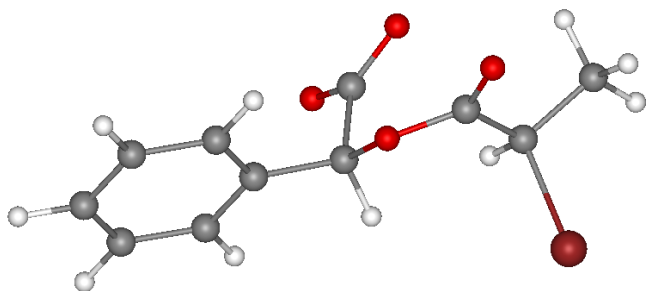
I-1\_SR



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 509017.7 (Joules/Mol)       |
|  | 121.65816 (Kcal/Mol)        |
| Zero-point correction=                       | 0.193875 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.208706                    |
| Thermal correction to Enthalpy=              | 0.209651                    |
| Thermal correction to Gibbs Free Energy=     | 0.148592                    |
| Sum of electronic and zero-point Energies=   | -3300.146157                |
| Sum of electronic and thermal Energies=      | -3300.131325                |
| Sum of electronic and thermal Enthalpies=    | -3300.130381                |
| Sum of electronic and thermal Free Energies= | -3300.191439                |

| cartesian |             |             |             |   |             |             |             |  |  |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|
| 8         | 0.98967302  | 0.49118841  | 0.62914997  | 6 | -2.66492701 | -0.12481159 | 0.08355001  |  |  |
| 6         | -0.39792693 | 0.84378844  | 0.73824996  | 6 | -3.48042679 | -1.21051168 | -0.22614998 |  |  |
| 6         | 1.48517299  | 0.38058841  | -0.60285002 | 1 | -4.53292704 | -1.04411161 | -0.42635000 |  |  |
| 6         | -0.63812697 | 2.25458837  | 0.08535001  | 6 | -2.95782685 | -2.49811172 | -0.27875000 |  |  |
| 1         | -0.52702689 | 1.00668836  | 1.81215000  | 6 | -1.60562706 | -2.69181156 | -0.01374999 |  |  |
| 6         | 3.00157309  | 0.42498839  | -0.59525001 | 1 | -1.18192697 | -3.68901157 | -0.04724999 |  |  |
| 8         | 0.36837307  | 2.83458829  | -0.35374999 | 6 | -0.78962696 | -1.60961163 | 0.29525003  |  |  |
| 8         | 0.84387302  | 0.23948842  | -1.60774994 | 1 | -3.59492683 | -3.34041166 | -0.52174997 |  |  |
| 8         | -1.81082702 | 2.66708827  | 0.15505001  | 1 | -3.06662703 | 0.87768841  | 0.12425000  |  |  |
| 35        | 3.63147306  | -1.31101167 | 0.10995001  | 1 | 0.25997305  | -1.78111160 | 0.50435001  |  |  |
| 1         | 3.33437300  | 0.43178844  | -1.62895000 | 1 | 4.65107298  | 1.60798836  | 0.12555000  |  |  |
| 6         | 3.56567311  | 1.57268834  | 0.21365002  | 1 | 3.13687301  | 2.50118828  | -0.17124999 |  |  |
| 6         | -1.30352700 | -0.30991158 | 0.33615002  | 1 | 3.28417301  | 1.47608840  | 1.26115000  |  |  |

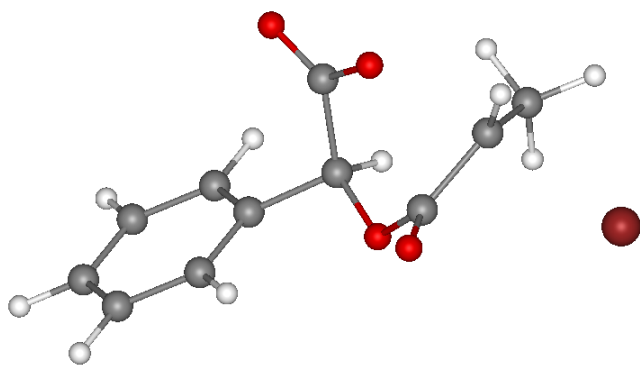
I-1\_SS



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 509344.8 (Joules/Mol)       |
|  | 121.73634 (Kcal/Mol)        |
| Zero-point correction=                       | 0.193999 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.208731                    |
| Thermal correction to Enthalpy=              | 0.209675                    |
| Thermal correction to Gibbs Free Energy=     | 0.149890                    |
| Sum of electronic and zero-point Energies=   | -3300.147737                |
| Sum of electronic and thermal Energies=      | -3300.133005                |
| Sum of electronic and thermal Enthalpies=    | -3300.132061                |
| Sum of electronic and thermal Free Energies= | -3300.191846                |

|   |             |             |             | cartesian                             |
|---|-------------|-------------|-------------|---------------------------------------|
| 8 | 0.77601159  | -0.31306157 | -0.91354614 | 1 -4.08678818 -1.41206157 1.89485383  |
| 6 | 0.06431156  | -0.05796157 | 0.29955384  | 6 -4.06028843 -1.15486157 -0.24084616 |
| 6 | 2.03151155  | 0.12733844  | -1.06464624 | 6 -3.28208852 -0.82056153 -1.34414613 |
| 6 | 0.16131157  | 1.46163845  | 0.70165390  | 1 -3.71738839 -0.82376158 -2.33674598 |
| 1 | 0.49161160  | -0.65206158 | 1.11475384  | 6 -1.94178843 -0.47966158 -1.18204618 |
| 6 | 2.91951156  | 0.23573843  | 0.16975383  | 1 -5.10268831 -1.42126155 -0.36924616 |
| 8 | 0.89631158  | 2.16083837  | -0.02444616 | 1 -1.70718837 -0.80156159 2.18065405  |
| 8 | 2.47541165  | 0.28973845  | -2.16934609 | 1 -1.33538842 -0.22216156 -2.04124618 |
| 8 | -0.48018843 | 1.77153850  | 1.71355379  | 35 3.65501142 -1.59216154 0.42715383  |
| 6 | 4.02991152  | 1.23983848  | -0.01694616 | 1 2.36741161 0.41353843 1.08325386    |
| 6 | -1.36718845 | -0.47506157 | 0.08795385  | 1 4.69111156 1.24813843 0.84865385    |
| 6 | -2.15108848 | -0.81176162 | 1.19215381  | 1 4.60071182 1.01723850 -0.91704613   |
| 6 | -3.48938870 | -1.14866161 | 1.02965379  | 1 3.56131148 2.22103858 -0.12334616   |

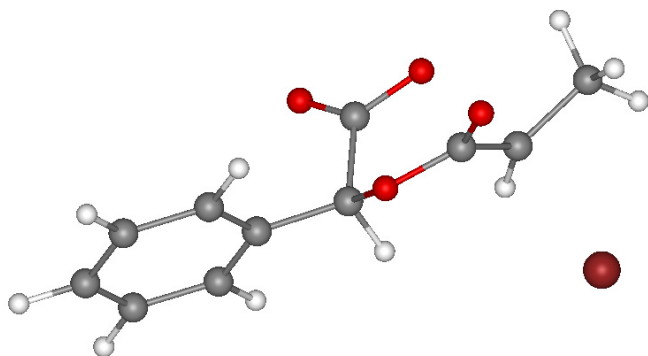
TS-1\_SR



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 507315.8 (Joules/Mol)       |
|  | 121.25139 (Kcal/Mol)        |
| Zero-point correction=                       | 0.193226 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.207569                    |
| Thermal correction to Enthalpy=              | 0.208513                    |
| Thermal correction to Gibbs Free Energy=     | 0.149112                    |
| Sum of electronic and zero-point Energies=   | -3300.112397                |
| Sum of electronic and thermal Energies=      | -3300.098054                |
| Sum of electronic and thermal Enthalpies=    | -3300.097110                |
| Sum of electronic and thermal Free Energies= | -3300.156511                |

|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 8  | 1.05105758  | -0.84487695 | -0.00802693 | 6         | -2.26084232 | 0.34322309  | 0.90977299  |
| 6  | 0.14695764  | 0.24232307  | 0.21367308  | 6         | -3.56834245 | -0.12737693 | 0.87247300  |
| 6  | 2.16695762  | -0.69647694 | -0.76332688 | 1         | -4.34154224 | 0.38392305  | 1.43367302  |
| 6  | 0.33195758  | 1.37392306  | -0.83542693 | 6         | -3.88244224 | -1.25707698 | 0.12127307  |
| 1  | 0.34395760  | 0.68752307  | 1.19377303  | 6         | -2.88274217 | -1.91037691 | -0.59272695 |
| 6  | 2.99015760  | 0.52902305  | -0.48312694 | 1         | -3.12094235 | -2.79137707 | -1.17722690 |
| 8  | 1.44135761  | 1.35292304  | -1.47422695 | 6         | -1.57384229 | -1.43867695 | -0.55792689 |
| 8  | 2.44745755  | -1.52817690 | -1.57502699 | 1         | -4.90024281 | -1.62767696 | 0.09597307  |
| 8  | -0.55334234 | 2.20412302  | -0.95252693 | 1         | -2.01444244 | 1.22222304  | 1.49477303  |
| 35 | 4.96625757  | -0.77927691 | 0.27237308  | 1         | -0.78974235 | -1.94997692 | -1.10312688 |
| 1  | 3.59445763  | 0.85872304  | -1.31172693 | 1         | 3.89925766  | 1.78742301  | 0.97197306  |
| 6  | 2.92145777  | 1.35652304  | 0.77457309  | 1         | 2.21125746  | 2.17552328  | 0.65647304  |
| 6  | -1.25824237 | -0.30997694 | 0.19527307  | 1         | 2.63415766  | 0.74392307  | 1.62837303  |

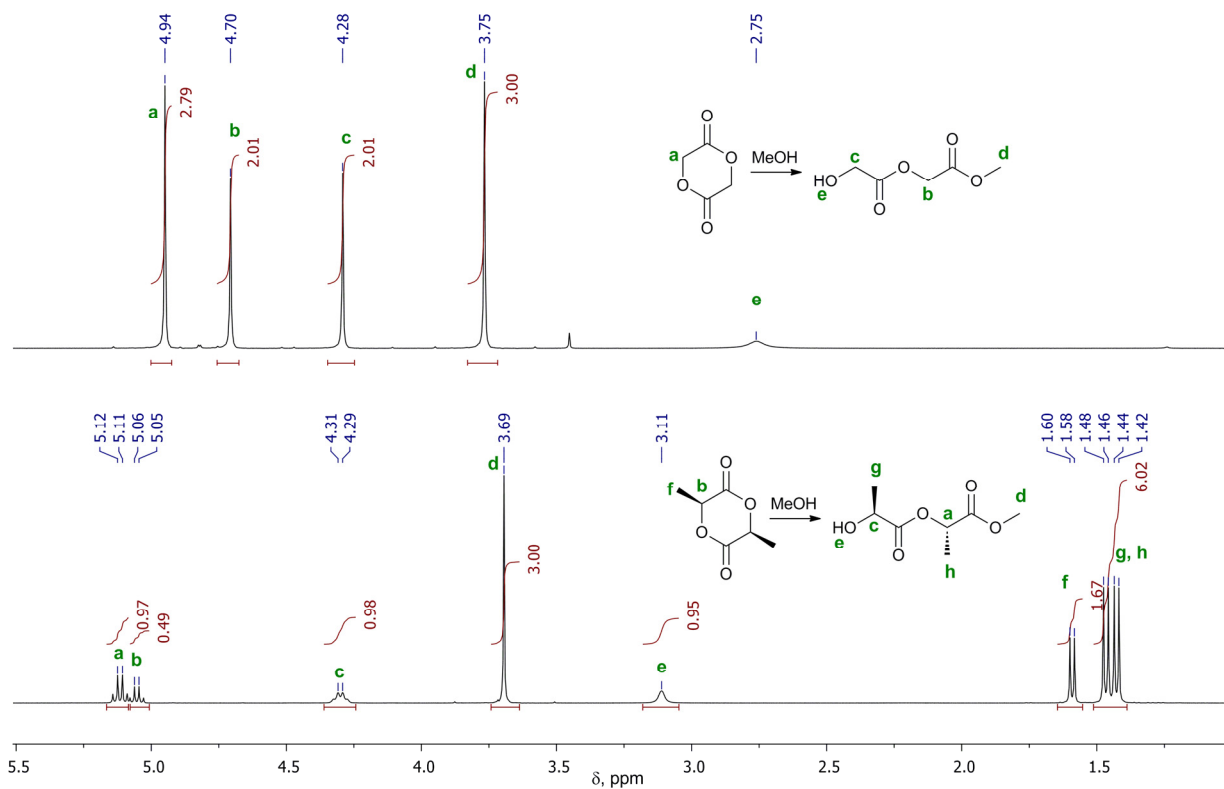
TS-1\_SS



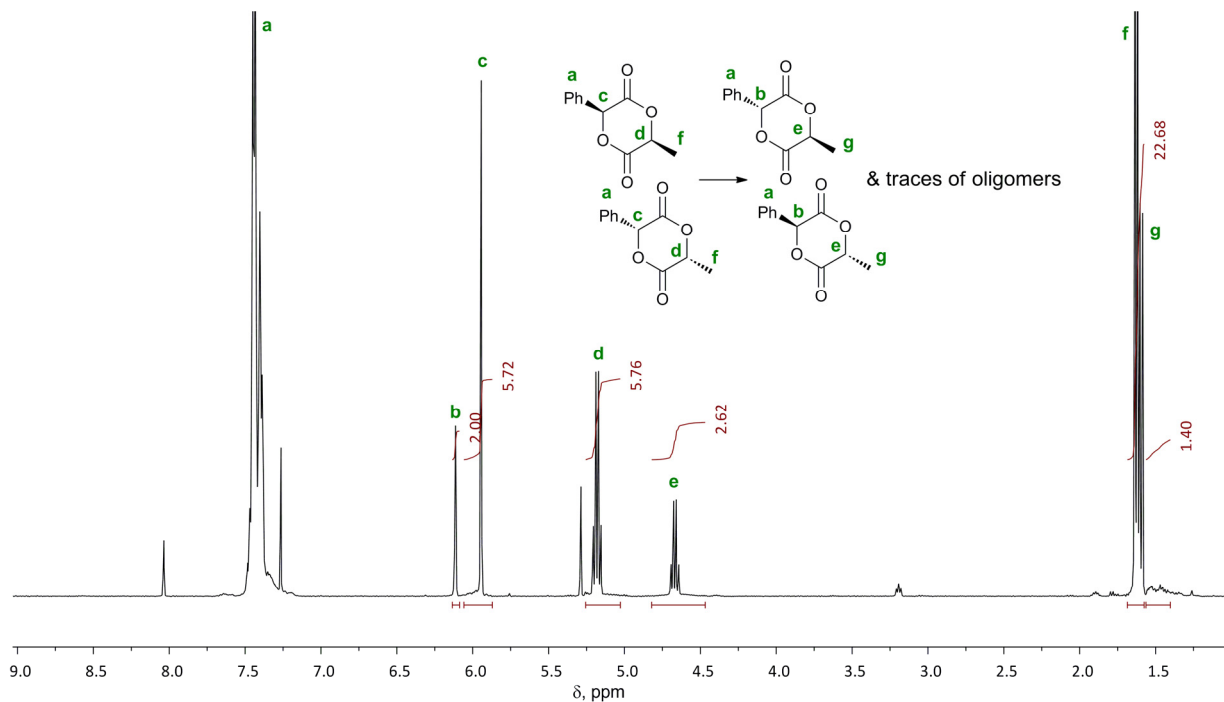
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 506158.4 (Joules/Mol)       |
|  | 120.97475 (Kcal/Mol)        |
| Zero-point correction=                       | 0.192786 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.207346                    |
| Thermal correction to Enthalpy=              | 0.208291                    |
| Thermal correction to Gibbs Free Energy=     | 0.148622                    |
| Sum of electronic and zero-point Energies=   | -3300.123799                |
| Sum of electronic and thermal Energies=      | -3300.109239                |
| Sum of electronic and thermal Enthalpies=    | -3300.108294                |
| Sum of electronic and thermal Free Energies= | -3300.167963                |

|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6  | 3.91567707  | 1.46116531  | -0.04787308 | 6         | -1.94062316 | -0.62703466 | -1.14727306 |
| 8  | 0.79437691  | -0.45503467 | -0.86127305 | 6         | -3.27442312 | -1.00043464 | -1.28227317 |
| 6  | 0.05227691  | -0.06163464 | 0.29732692  | 1         | -3.70782328 | -1.09383464 | -2.27117300 |
| 6  | 2.03117704  | 0.03116536  | -1.05227315 | 6         | -4.04932308 | -1.25443459 | -0.15517309 |
| 6  | 0.17907691  | 1.48056531  | 0.50332695  | 6         | -3.48362303 | -1.13683462 | 1.11152685  |
| 1  | 0.47267690  | -0.55033469 | 1.18452692  | 1         | -4.07892323 | -1.33893466 | 1.99412692  |
| 6  | 2.75437689  | 0.54416537  | 0.15822691  | 6         | -2.15022326 | -0.76803464 | 1.24692690  |
| 8  | 1.29757690  | 1.96306539  | 0.11302692  | 1         | -5.08692312 | -1.54713464 | -0.26237309 |
| 8  | 2.50397682  | 0.05156535  | -2.15407300 | 1         | -1.33602321 | -0.43273467 | -2.02427292 |
| 8  | -0.73912311 | 2.09146523  | 1.02412689  | 1         | -1.70902312 | -0.67703462 | 2.23362708  |
| 35 | 3.95967674  | -1.58573461 | 0.43082690  | 1         | 4.58517694  | 1.42866540  | 0.80832696  |
| 1  | 2.39997673  | 0.33336532  | 1.14962685  | 1         | 4.45417690  | 1.18106532  | -0.95107305 |
| 6  | -1.37262309 | -0.51113462 | 0.11962692  | 1         | 3.52847672  | 2.47406530  | -0.16607308 |

### S3. Alcoholysis and polymerization of substituted glycolides



**Fig. S19.**  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ,  $20^\circ\text{C}$ ) of the reaction mixtures of GL (top) and L-LA (bottom) methanolysis.



**Fig. S20.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ,  $20^\circ\text{C}$ ) reflecting isomerization of MePhGL in the presence of TBD (Table 2, Entry 10).

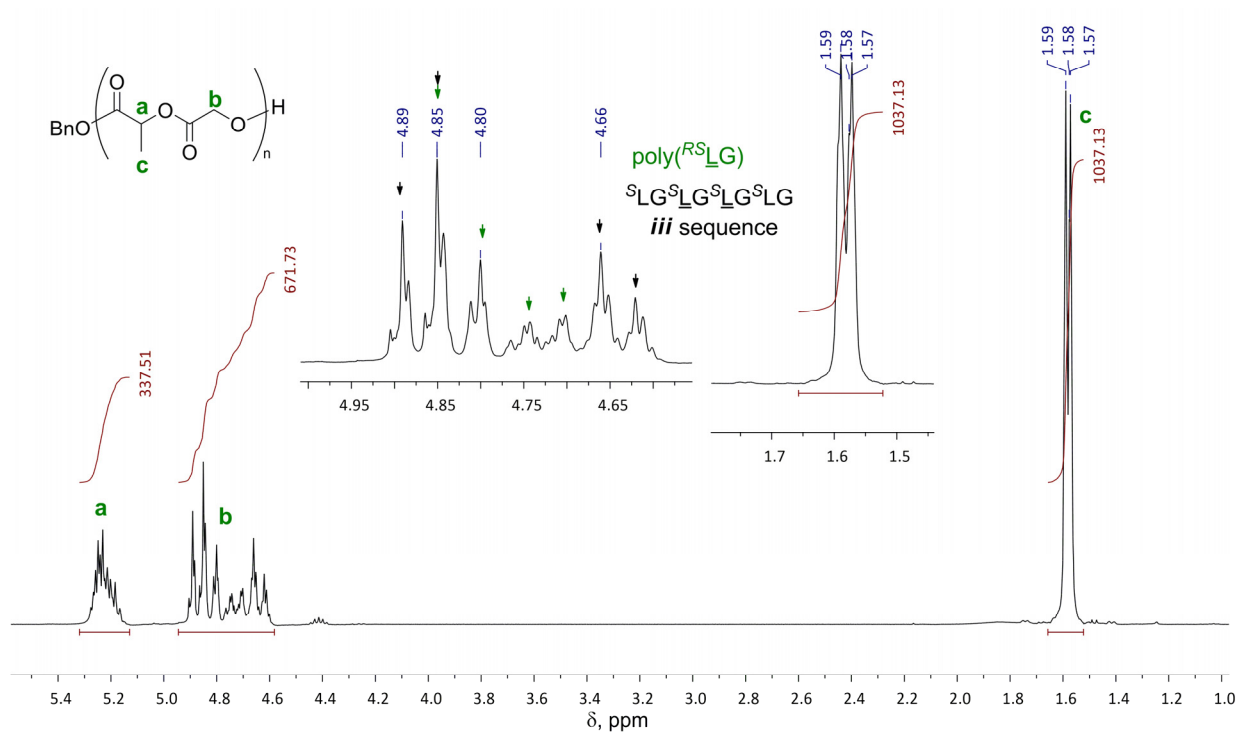


Fig. S21.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20  $^\circ\text{C}$ ) of poly(MeGL) (Table 2, Entry 4).

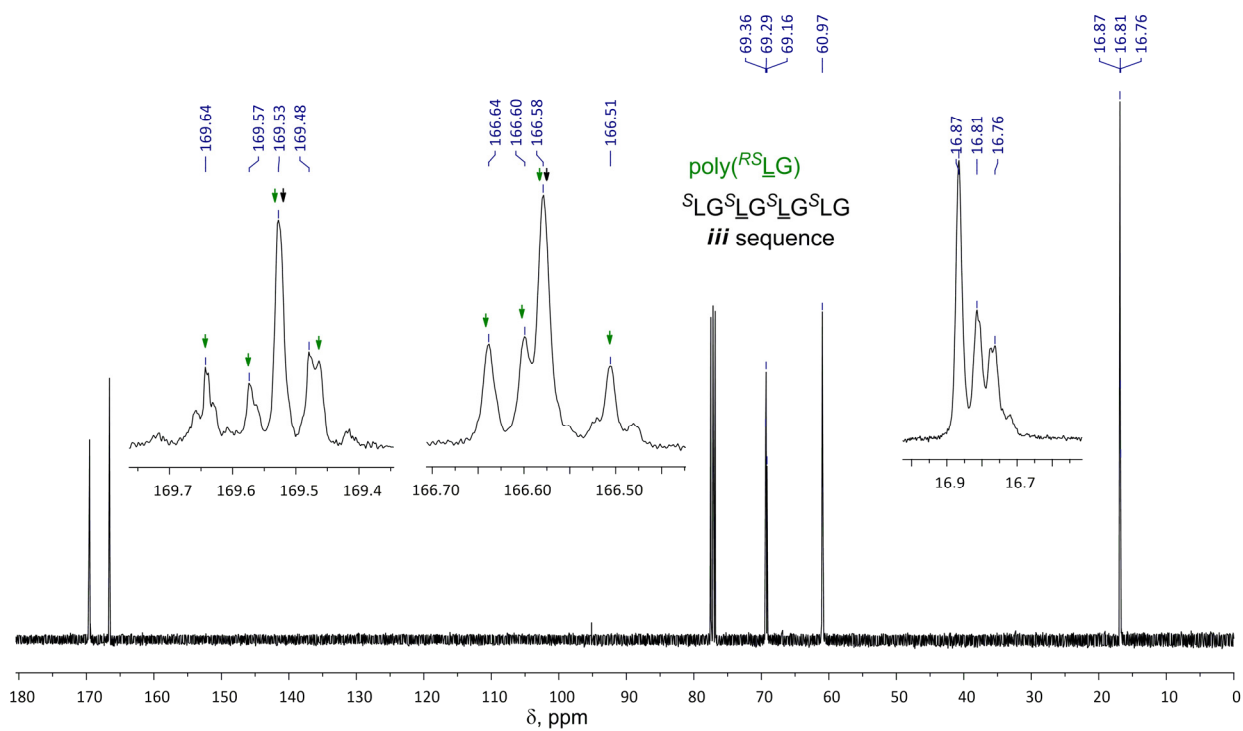
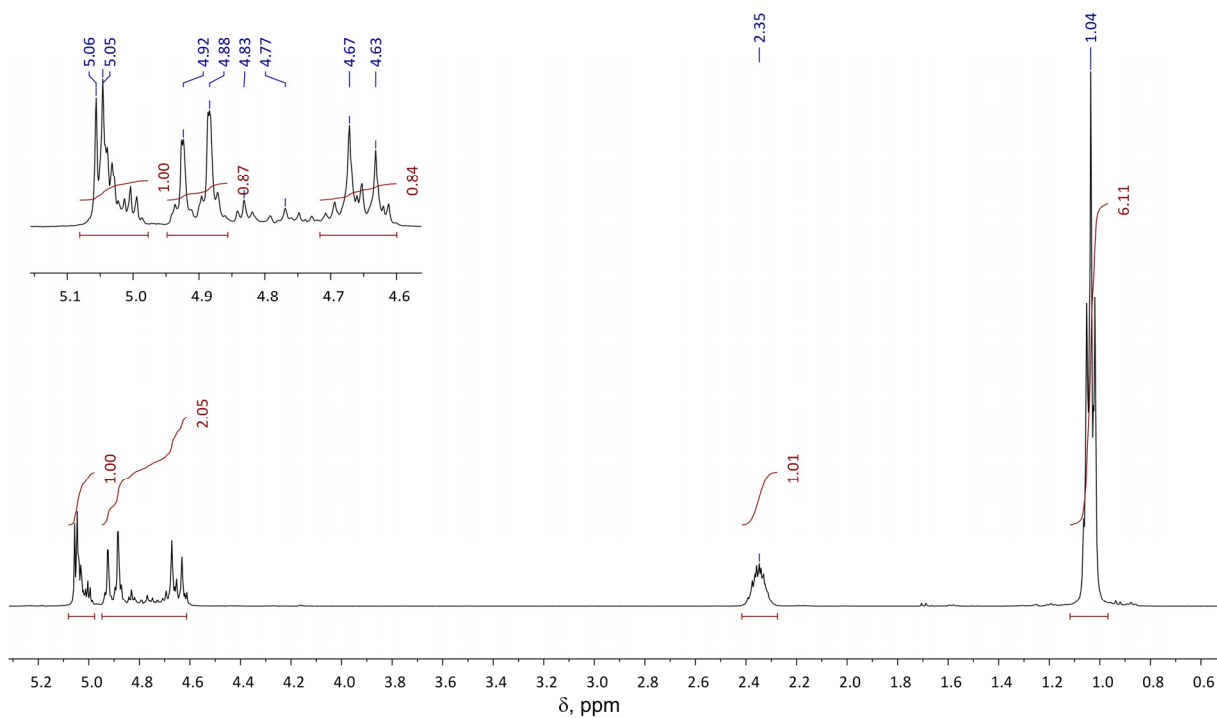
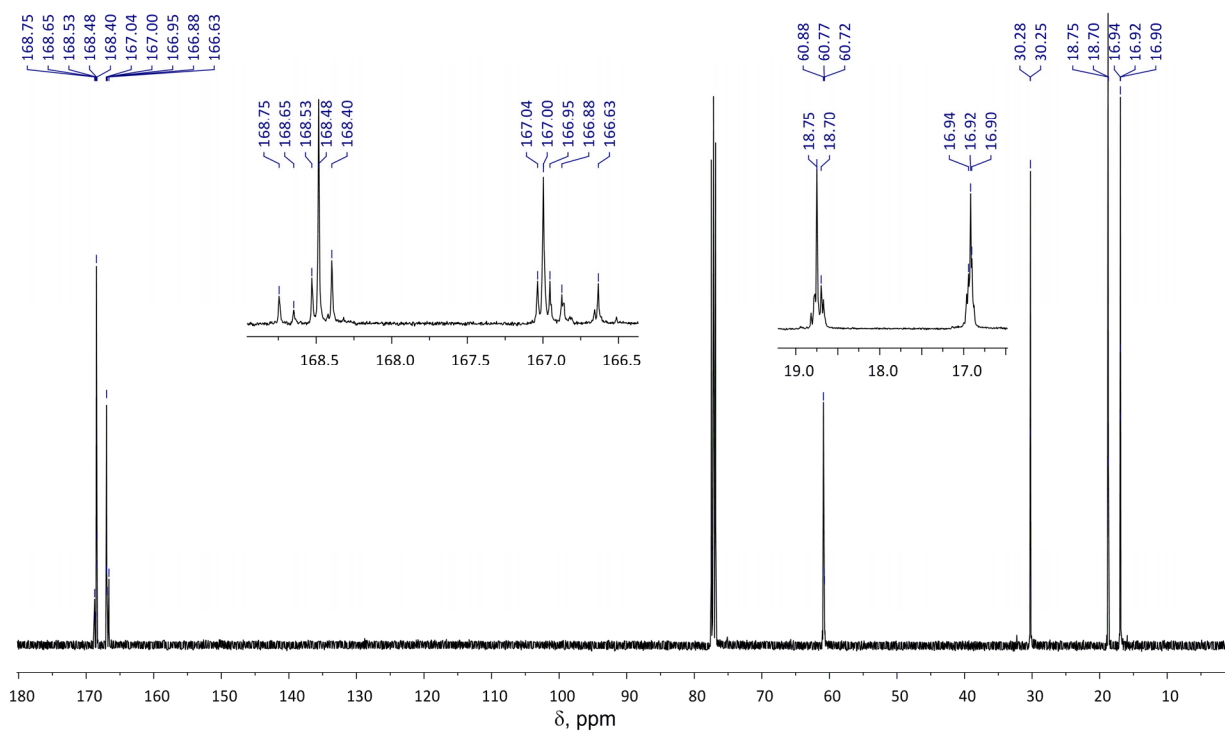


Fig. S22.  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20  $^\circ\text{C}$ ) of poly(MeGL) (Table 2, Entry 4).

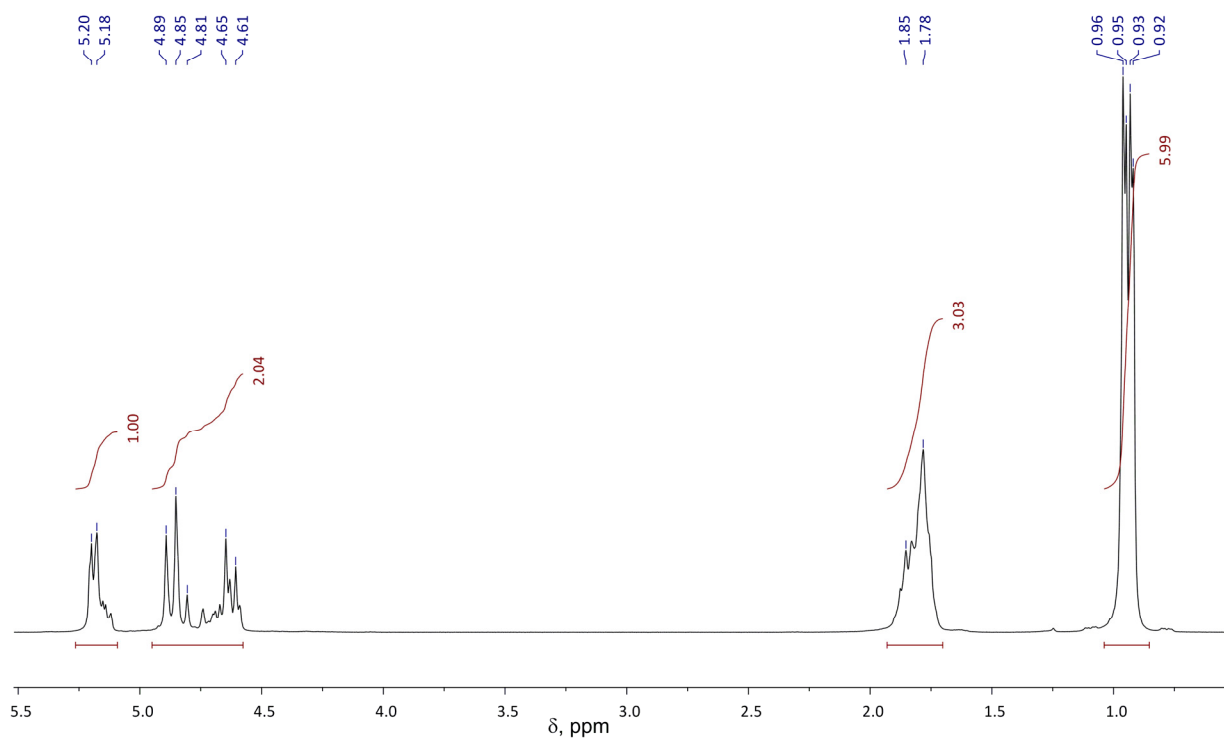




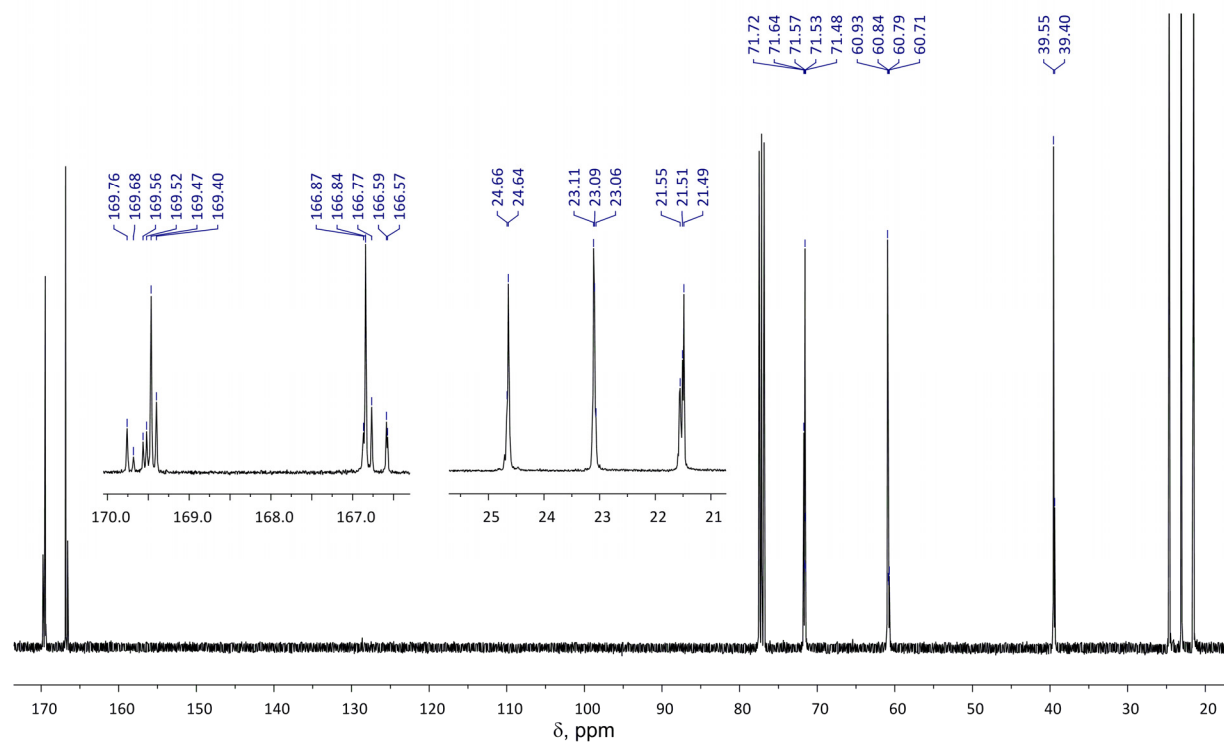
**Fig. S23.** <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of poly(iPrGL) (Table 2, Entry 5).



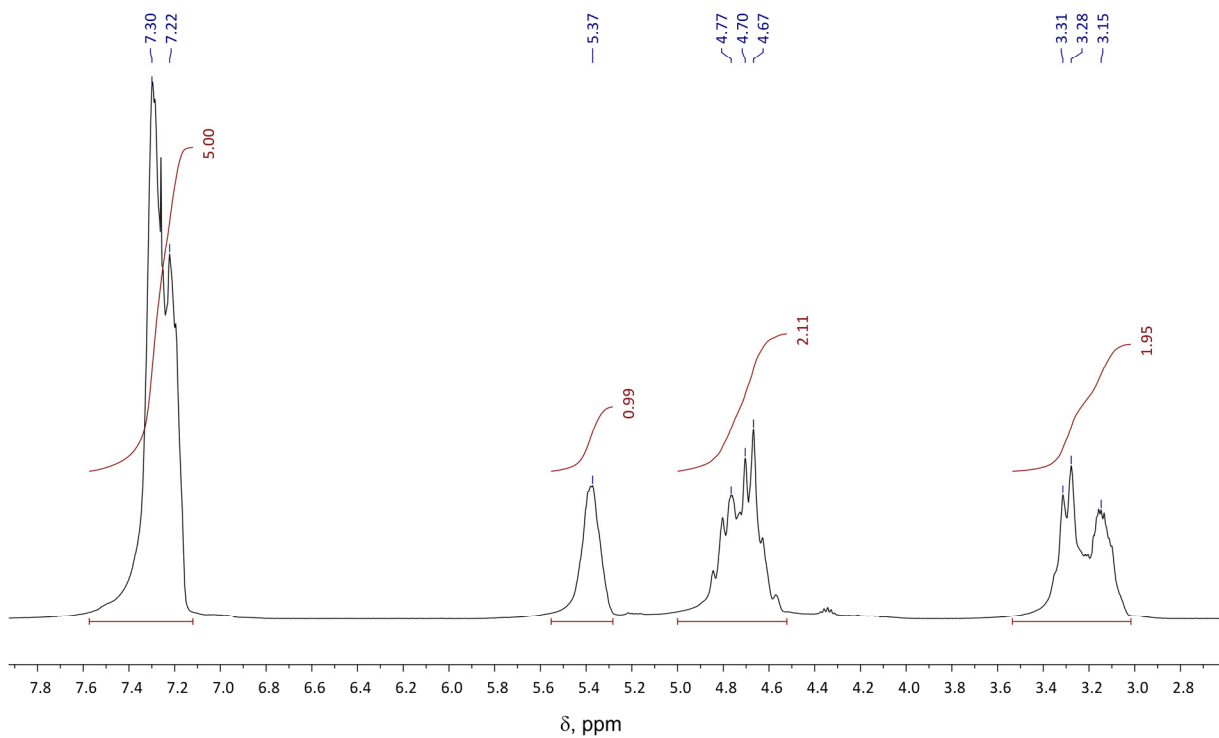
**Fig. S24.** <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>, 20 °C) of poly(iPrGL) (Table 2, Entry 5).



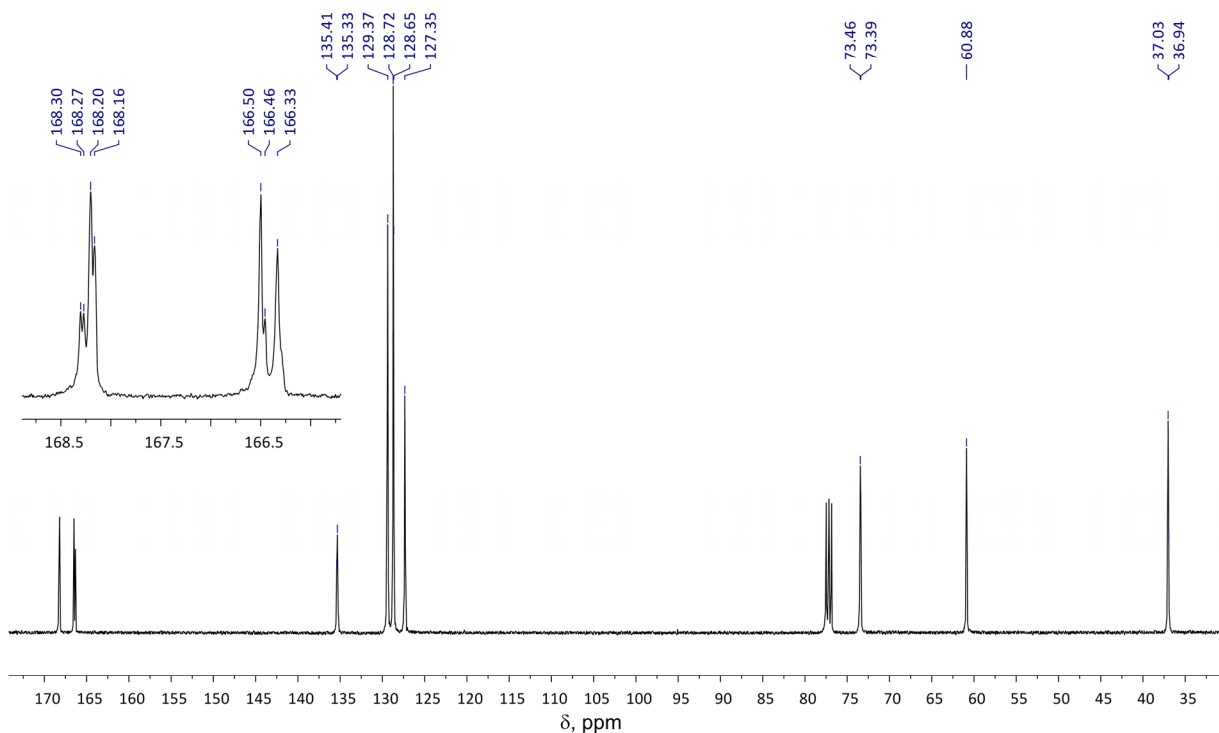
**Fig. S25.** <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of poly(*i*BuGL) (Table 2, Entry 6).



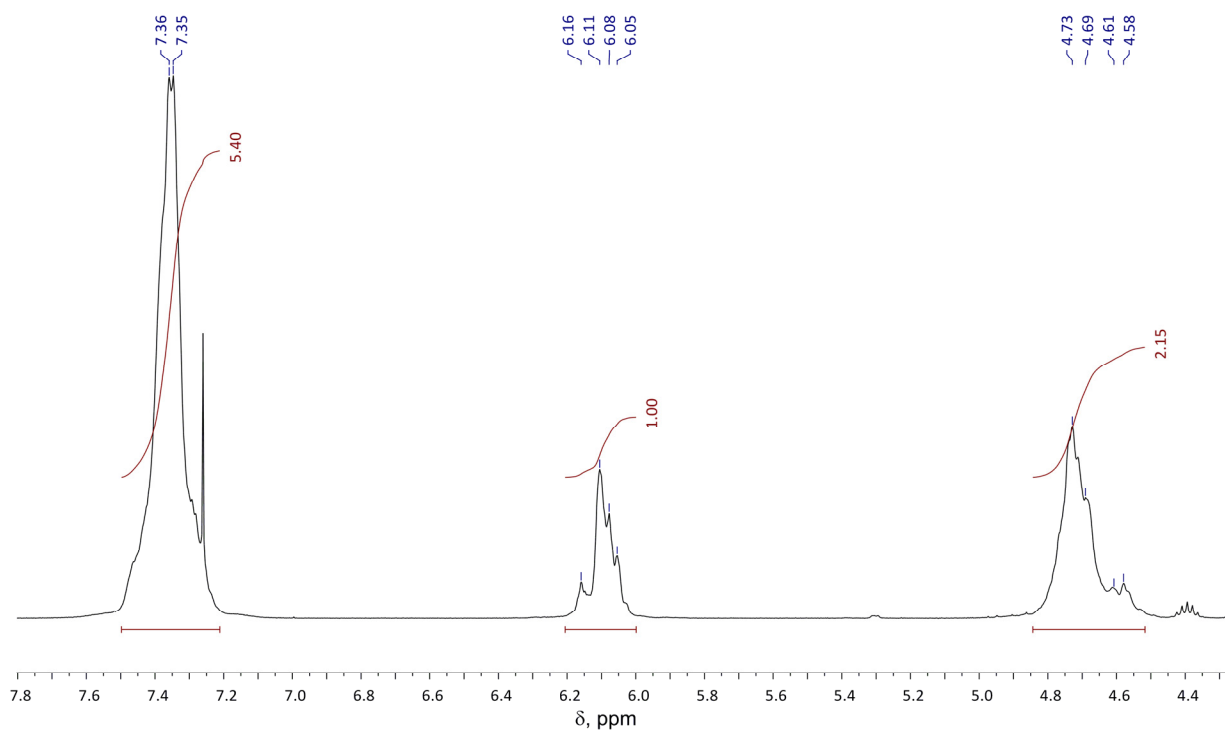
**Fig. S26.** <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>, 20 °C) of poly(*i*BuGL) (Table 2, Entry 6).



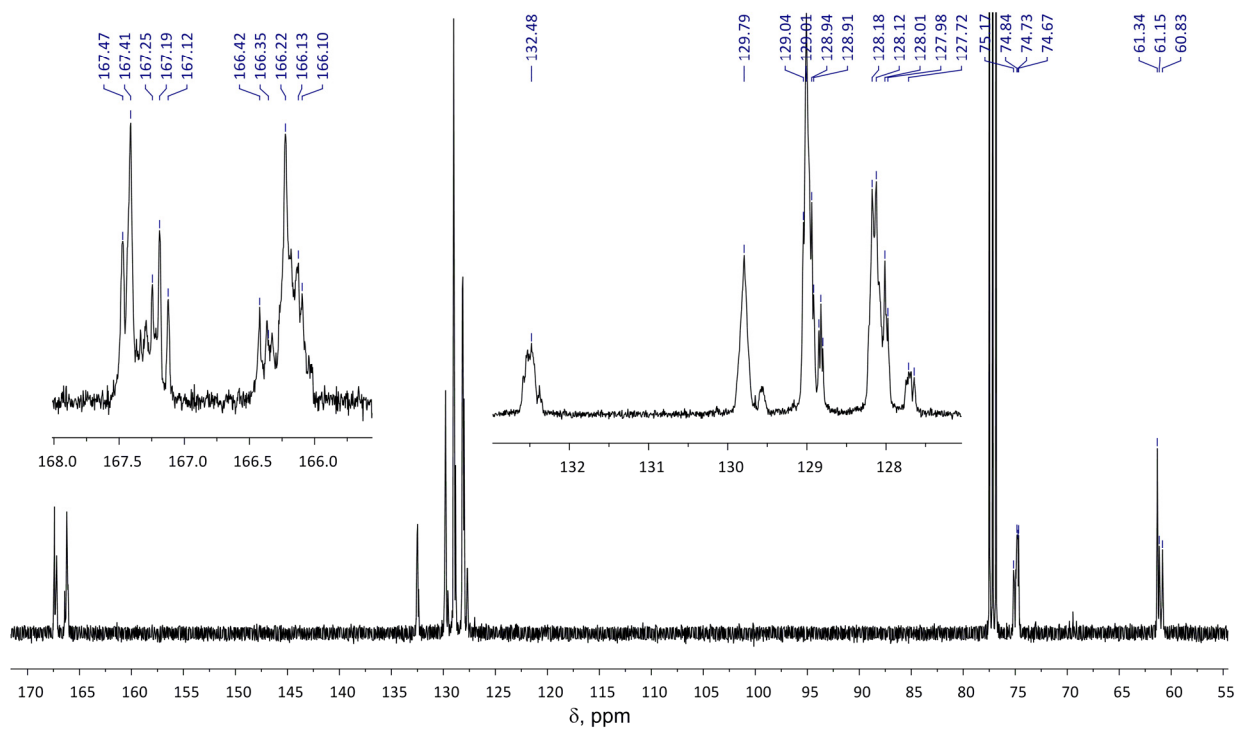
**Fig. S27.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of poly(BnGL) (Table 2, Entry 7).



**Fig. S28.**  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of poly(BnGL) (Table 2, Entry 7).



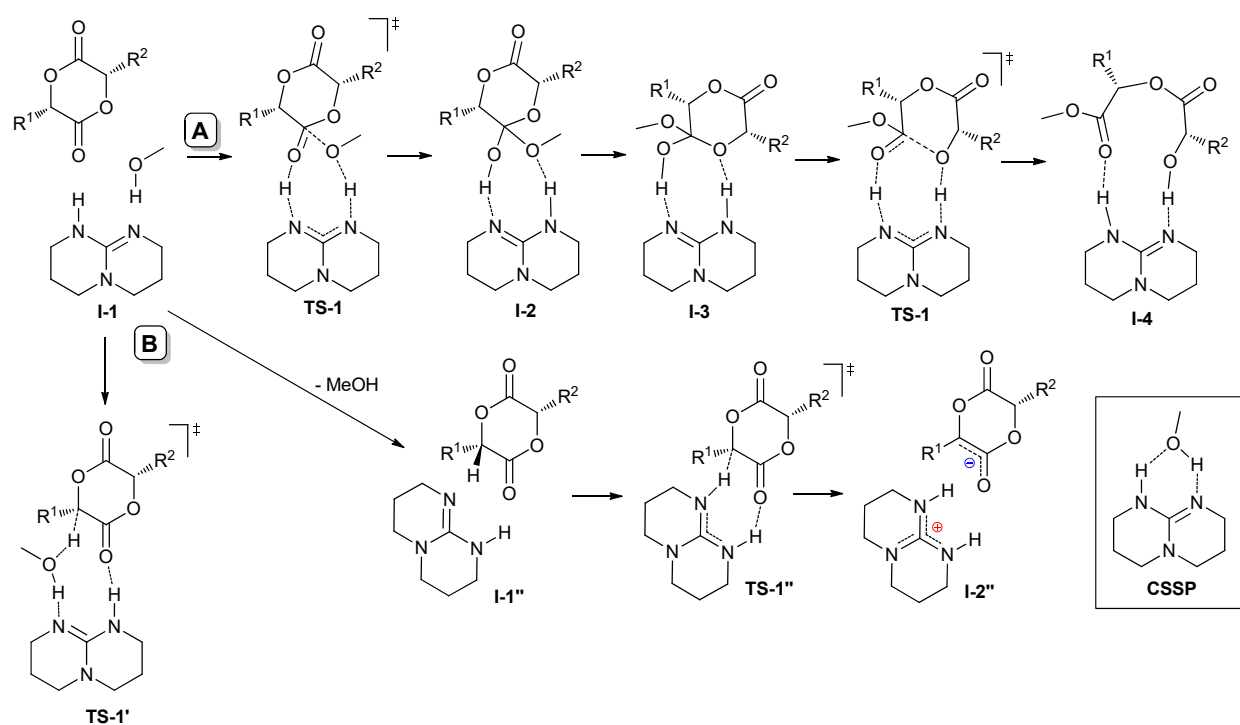
**Fig. S29.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of poly(PhGL) (Table 2, Entry 9).



**Fig. S30.**  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of poly(PhGL) (Table 2, Entry 9).

## S4. DFT modeling of polymerization and enolization of *L*-LA and substituted glycolides

### S4.1. Results of calculations in gas phase



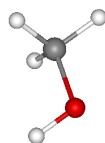
**Table 1.** Results of draft calculations (298 K, gas phase)

|               |   | <i>L</i> -LA  | MeGL                             |                      | MePhGL               |                      |
|---------------|---|---------------|----------------------------------|----------------------|----------------------|----------------------|
|               |   |               | -CH <sub>2</sub> - <sup>a)</sup> | -CHMe- <sup>a)</sup> | -CHPh- <sup>a)</sup> | -CHMe- <sup>a)</sup> |
| <b>I-1</b>    | G | -5.11         | -5.76                            | -3.69                | -5.36                | -6.92                |
|               | H | <b>-17.75</b> | <b>-18.14</b>                    | <b>-16.08</b>        | <b>-18.22</b>        | <b>-20.10</b>        |
| <b>TS-1</b>   | G | 6.69          | 6.64                             | 5.85                 | 5.01                 | 5.09                 |
|               | H | <b>-7.52</b>  | <b>-8.16</b>                     | <b>-8.91</b>         | <b>-10.59</b>        | <b>-10.37</b>        |
| <b>TS-1'</b>  | G | 18.21         | 16.57                            | 18.53                | 13.29                | 18.09                |
|               | H | <b>6.54</b>   | <b>4.53</b>                      | <b>6.33</b>          | <b>0.12</b>          | <b>6.27</b>          |
| <b>I-1''</b>  | G | 0.91          | 1.01                             | 1.04                 | 0.72                 | 2.74                 |
|               | H | <b>-17.75</b> | <b>-17.86</b>                    | <b>-17.75</b>        | <b>-18.52</b>        | <b>-19.69</b>        |
| <b>TS-1''</b> | G | 19.63         | 18.19                            | 19.34                | 13.77                | 18.68                |
|               | H | <b>1.25</b>   | <b>-0.66</b>                     | <b>0.79</b>          | <b>-7.11</b>         | <b>0.28</b>          |
| <b>I-2''</b>  | G | 15.85         | 14.81                            | 18.57                | 6.90                 | 16.21                |
|               | H | <b>-2.09</b>  | <b>-2.34</b>                     | <b>0.10</b>          | <b>-13.98</b>        | <b>-3.41</b>         |

For gas phase calculations  $\Delta G$  between **I-2''** and **I-1''** for MePhGL is 6.18 kcal/mol (endergonic process).

## S4.2. Results of calculations using IEFPCM (THF) correction

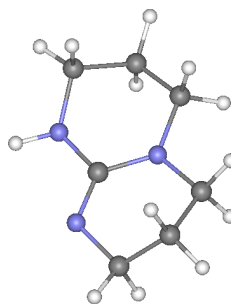
### MeOH



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 136239.8 (Joules/Mol)       |
|  | 32.56208 (Kcal/Mol)         |
| Zero-point correction=                       | 0.051891 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.055160                    |
| Thermal correction to Enthalpy=              | 0.056104                    |
| Thermal correction to Gibbs Free Energy=     | 0.029198                    |
| Sum of electronic and zero-point Energies=   | -115.650785                 |
| Sum of electronic and thermal Energies=      | -115.647517                 |
| Sum of electronic and thermal Enthalpies=    | -115.646573                 |
| Sum of electronic and thermal Free Energies= | -115.673478                 |

|   |             |             |            | cartesian |            |             |             |
|---|-------------|-------------|------------|-----------|------------|-------------|-------------|
| 8 | -0.74750000 | 0.12250000  | 0.00000000 | 1         | 1.02349997 | -0.54519999 | 0.89020002  |
| 6 | 0.66280001  | -0.01940000 | 0.00000000 | 1         | 1.02349997 | -0.54519999 | -0.89020002 |
| 1 | -1.13039994 | -0.75749999 | 0.00000000 | 1         | 1.08669996 | 0.98439997  | 0.00000000  |

### TBD

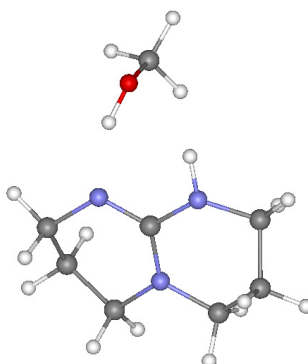


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy              | 543708.4 (Joules/Mol)       |
|  | 129.94942 (Kcal/Mol)        |
| Zero-point correction=                     | 0.207088 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.215774                    |
| Thermal correction to Enthalpy=            | 0.216718                    |
| Thermal correction to Gibbs Free Energy=   | 0.173376                    |
| Sum of electronic and zero-point Energies= | -438.544654                 |
| Sum of electronic and thermal Energies=    | -438.535967                 |

Sum of electronic and thermal Enthalpies= -438.535023  
 Sum of electronic and thermal Free Energies= -438.578365

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | -0.02170000 | 0.63239998  | -0.13300000 | 1         | 2.29830003  | -0.53450000 | 1.51919997  |
| 6 | -0.07030000 | -0.74129999 | -0.08730000 | 1         | 2.52719998  | 0.39500001  | -1.37899995 |
| 7 | 1.15400004  | -1.39380002 | -0.05940000 | 1         | 3.33049989  | 1.16129994  | 0.00280000  |
| 6 | 2.34039998  | -0.71850002 | 0.43590000  | 1         | 1.26409996  | 1.84710002  | 0.99010003  |
| 6 | 2.44779992  | 0.60089999  | -0.30910000 | 1         | 1.12619996  | 2.26130009  | -0.72009999 |
| 6 | 1.20179999  | 1.42190003  | -0.02150000 | 1         | -1.06850004 | 2.26430011  | 0.61000001  |
| 6 | -2.39870000 | 0.56449997  | 0.47970000  | 1         | -1.50199997 | 1.81429994  | -1.04170001 |
| 6 | -2.39919996 | -0.76709998 | -0.26269999 | 1         | -2.25009990 | 0.37599999  | 1.54690003  |
| 7 | -1.13349998 | -1.46739995 | -0.12210000 | 1         | -3.34369993 | 1.09669995  | 0.35510001  |
| 6 | -1.25469995 | 1.41199994  | -0.05140000 | 1         | -2.62050009 | -0.58359998 | -1.32459998 |
| 1 | 1.03590000  | -2.36380005 | 0.19340000  | 1         | -3.19519997 | -1.41359997 | 0.11380000  |
| 1 | 3.20379996  | -1.35329998 | 0.23469999  |           |             |             |             |

### TBD-MeOH

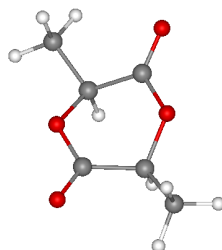


Zero-point vibrational energy 686185.7 (Joules/Mol)  
 164.00231 (Kcal/Mol)  
 Zero-point correction= 0.261354 (Hartree/Particle)  
 Thermal correction to Energy= 0.274311  
 Thermal correction to Enthalpy= 0.275255  
 Thermal correction to Gibbs Free Energy= 0.220911  
 Sum of electronic and zero-point Energies= -554.215028  
 Sum of electronic and thermal Energies= -554.202071  
 Sum of electronic and thermal Enthalpies= -554.201127  
 Sum of electronic and thermal Free Energies= -554.255471

|   |             |             |            | cartesian |            |             |             |
|---|-------------|-------------|------------|-----------|------------|-------------|-------------|
| 7 | 1.28138280  | 0.28218961  | 0.11520346 | 1         | 3.24398255 | -0.37431037 | 0.28050345  |
| 6 | -0.00741722 | -0.01311038 | 0.46460342 | 1         | 2.32838273 | 1.65438962  | -1.03689659 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -0.33241722 | -1.34451044 | 0.57130343  | 1 | 2.28768277  | 2.03138971  | 0.68810344  |
| 6 | 0.49108279  | -2.38101029 | -0.02059655 | 1 | 0.02468278  | 2.32748961  | -1.34399664 |
| 6 | 1.93328273  | -2.09171033 | 0.36170346  | 1 | 0.78318280  | 3.59848952  | -0.37179655 |
| 6 | 2.30728269  | -0.71851039 | -0.16909654 | 1 | -0.11701722 | 2.55418968  | 1.69530344  |
| 6 | 0.47518277  | 2.55118966  | -0.37269652 | 1 | -1.44231725 | 2.86598969  | 0.58140343  |
| 6 | -0.54281723 | 2.26368952  | 0.72410345  | 8 | -3.22671723 | -0.55851036 | 0.62080348  |
| 7 | -0.92841721 | 0.86278963  | 0.73570347  | 6 | -3.46301723 | -0.56251037 | -0.77149653 |
| 6 | 1.68588281  | 1.66088963  | -0.15079655 | 1 | -2.55921745 | -0.82391036 | -1.33839655 |
| 1 | 0.16328278  | -3.34241033 | 0.37490344  | 1 | -3.82161736 | 0.40858960  | -1.13199663 |
| 1 | 0.39278278  | -2.41331029 | -1.11479664 | 1 | -4.22881746 | -1.30931044 | -0.98839658 |
| 1 | 2.02068257  | -2.11341047 | 1.45040345  | 1 | -2.49931741 | 0.09798962  | 0.77460349  |
| 1 | 2.61048269  | -2.83801031 | -0.05569655 | 1 | -1.32611728 | -1.50691044 | 0.68270350  |
| 1 | 2.46598268  | -0.76781040 | -1.25469661 |   |             |             |             |

## LA



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 372576.6 (Joules/Mol)       |
|  | 89.04794 (Kcal/Mol)         |
| Zero-point correction=                       | 0.141907 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.151159                    |
| Thermal correction to Enthalpy=              | 0.152103                    |
| Thermal correction to Gibbs Free Energy=     | 0.107633                    |
| Sum of electronic and zero-point Energies=   | -534.165519                 |
| Sum of electronic and thermal Energies=      | -534.156267                 |
| Sum of electronic and thermal Enthalpies=    | -534.155323                 |
| Sum of electronic and thermal Free Energies= | -534.199793                 |

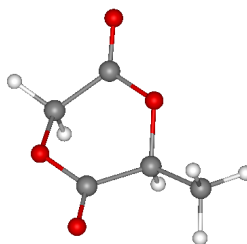
### cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 8 | 1.90189445  | 1.70058334  | 0.55578333  | 1 | -1.11780560 | 0.45048335  | -1.37401664 |
| 6 | 1.02629435  | 0.95848334  | 0.22418335  | 6 | -1.02630556 | -0.95851672 | 0.22398335  |
| 6 | 1.24949443  | -0.45971665 | -0.28571665 | 8 | -1.90190566 | -1.70061672 | 0.55538332  |
| 8 | -0.26030555 | 1.33658326  | 0.28638333  | 1 | -3.38170552 | 0.35978335  | -0.34861666 |
| 8 | 0.26029447  | -1.33671665 | 0.28608334  | 1 | -2.72020555 | 2.00868320  | -0.30561668 |
| 6 | 2.61079454  | -0.99681669 | 0.08218335  | 1 | -2.72780538 | 1.00768328  | 1.16588342  |
| 1 | 1.11799443  | -0.45021665 | -1.37401664 | 1 | 2.72019458  | -2.00861669 | -0.30581665 |



|   |             |            |             |   |            |             |             |
|---|-------------|------------|-------------|---|------------|-------------|-------------|
| 6 | -1.24950564 | 0.45978335 | -0.28571665 | 1 | 2.72769451 | -1.00791669 | 1.16588342  |
| 6 | -2.61080551 | 0.99678332 | 0.08218335  | 1 | 3.38169456 | -0.35971665 | -0.34841669 |

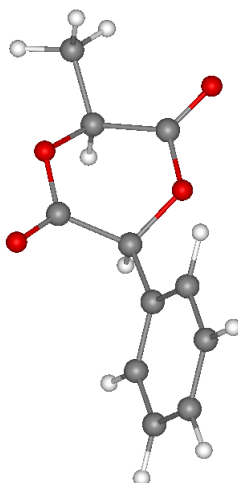
**MeGL**



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 298976.3 (Joules/Mol)       |
|  | 71.45704 (Kcal/Mol)         |
| Zero-point correction=                       | 0.113874 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.121704                    |
| Thermal correction to Enthalpy=              | 0.122648                    |
| Thermal correction to Gibbs Free Energy=     | 0.081208                    |
| Sum of electronic and zero-point Energies=   | -494.882677                 |
| Sum of electronic and thermal Energies=      | -494.874847                 |
| Sum of electronic and thermal Enthalpies=    | -494.873903                 |
| Sum of electronic and thermal Free Energies= | -494.915343                 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 8 | 2.88845992  | 0.45425335  | 0.51920003  | 1         | -0.38653994 | 0.41385332  | -1.32999992 |
| 6 | 1.78856003  | 0.07955334  | 0.24390002  | 6         | -0.82923996 | -0.96344662 | 0.23530002  |
| 6 | 1.46706009  | -1.32194662 | -0.23449998 | 8         | -1.91963995 | -1.33974659 | 0.54440004  |
| 8 | 0.72726011  | 0.89465332  | 0.34460002  | 1         | -2.53193998 | 1.13705337  | -0.30720001 |
| 8 | 0.22606006  | -1.79254663 | 0.29340002  | 1         | -1.31273997 | 2.42785335  | -0.22049998 |
| 1 | 1.44406009  | -1.33774662 | -1.32859993 | 1         | -1.70123994 | 1.46335340  | 1.22390008  |
| 6 | -0.51173991 | 0.44855335  | -0.24139999 | 1         | 2.23725986  | -2.00084662 | 0.11730001  |
| 6 | -1.58563995 | 1.43715334  | 0.14020002  |           |             |             |             |

## MePhGL

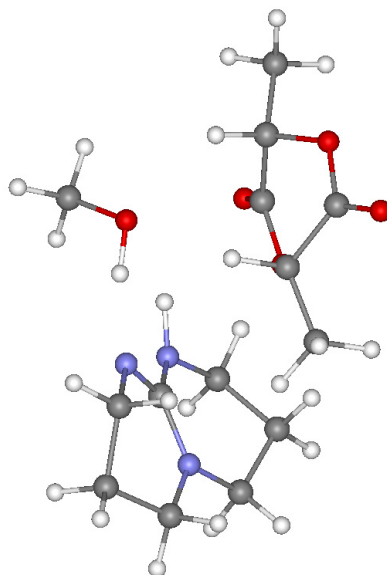


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 511583.3 (Joules/Mol)       |
|  | 122.27135 (Kcal/Mol)        |
| Zero-point correction=                       | 0.194852 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.207317                    |
| Thermal correction to Enthalpy=              | 0.208261                    |
| Thermal correction to Gibbs Free Energy=     | 0.154777                    |
| Sum of electronic and zero-point Energies=   | -725.813917                 |
| Sum of electronic and thermal Energies=      | -725.801452                 |
| Sum of electronic and thermal Enthalpies=    | -725.800508                 |
| Sum of electronic and thermal Free Energies= | -725.853991                 |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 8 | 0.05080002  | -2.07875204 | 0.96250796  | 1 | 4.60890007  | -1.31005192 | 0.08000801  |
| 6 | 0.69950002  | -1.23245192 | 0.42840803  | 1 | 4.27960014  | 0.01174800  | 1.22530794  |
| 6 | 0.11860003  | -0.10805200 | -0.43479198 | 6 | -1.79789996 | 0.90144801  | 0.84290797  |
| 8 | 2.03679991  | -1.20645189 | 0.54420799  | 6 | -2.26990008 | -0.58725202 | -0.99449205 |
| 8 | 0.80510002  | 1.12124801  | -0.15389200 | 6 | -3.16110015 | 1.04084802  | 1.07510805  |
| 6 | -1.35249996 | 0.08784800  | -0.19569199 | 1 | -1.08050001 | 1.43004799  | 1.45870805  |
| 1 | 0.28930002  | -0.37995198 | -1.48339200 | 6 | -3.63330007 | -0.45165199 | -0.75589198 |
| 6 | 2.77329993  | -0.27645200 | -0.27189201 | 1 | -1.92079997 | -1.21895194 | -1.80409205 |
| 6 | 4.21190023  | -0.30115199 | 0.18330801  | 1 | -3.50580001 | 1.67834806  | 1.88010800  |
| 1 | 2.69389987  | -0.59185201 | -1.31879199 | 6 | -4.07999992 | 0.36404800  | 0.27820802  |
| 6 | 2.15059996  | 1.10674810  | -0.14889200 | 1 | -4.34419966 | -0.97755200 | -1.38129199 |
| 8 | 2.77049994  | 2.12184811  | -0.04889199 | 1 | -5.14190006 | 0.47464800  | 0.46190798  |
| 1 | 4.79909992  | 0.38174799  | -0.42869198 |   |             |             |             |

I-1\_LA

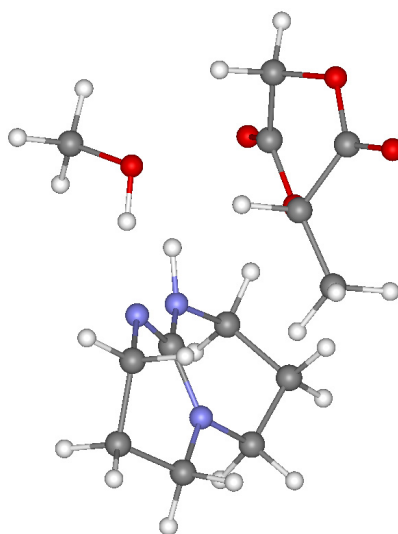


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1062154.1 (Joules/Mol)      |
|  | 253.86093 (Kcal/Mol)        |
| Zero-point correction=                       | 0.404553 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.428278                    |
| Thermal correction to Enthalpy=              | 0.429223                    |
| Thermal correction to Gibbs Free Energy=     | 0.350581                    |
| Sum of electronic and zero-point Energies=   | -1088.401561                |
| Sum of electronic and thermal Energies=      | -1088.377836                |
| Sum of electronic and thermal Enthalpies=    | -1088.376892                |
| Sum of electronic and thermal Free Energies= | -1088.455533                |

|   |             |             |             | cartesian |            |             |             |
|---|-------------|-------------|-------------|-----------|------------|-------------|-------------|
| 7 | -2.63676381 | -0.20978302 | 0.49422973  | 6         | 2.30723596 | 0.61051697  | 0.68352979  |
| 6 | -1.63036394 | 0.45151696  | -0.14757024 | 8         | 1.37083602 | -0.33358303 | 0.85912979  |
| 7 | -0.98206395 | 1.44451702  | 0.54592973  | 6         | 3.51123619 | 0.17721698  | -0.13887024 |
| 6 | -1.10636401 | 1.60931706  | 1.99082971  | 6         | 1.42473602 | -1.48368299 | -0.00467024 |
| 6 | -1.56506395 | 0.31061697  | 2.63182974  | 8         | 1.18313599 | 1.16861701  | -1.74137032 |
| 6 | -2.83726382 | -0.14288303 | 1.93842971  | 6         | 1.16843605 | 2.54621696  | -2.05137014 |
| 6 | -3.44556403 | -0.83888304 | -1.73497033 | 1         | 0.24123602 | 0.81911695  | -1.74977028 |
| 6 | -1.96366382 | -0.83078307 | -2.09187007 | 1         | 0.35513601 | 3.07011700  | -1.53397024 |
| 7 | -1.26056409 | 0.22191697  | -1.37587023 | 1         | 1.05983603 | 2.72231698  | -3.12737012 |
| 6 | -3.57496381 | -1.05758297 | -0.23727025 | 1         | 2.11403608 | 2.98511696  | -1.72437024 |
| 1 | -0.05766398 | 1.62001705  | 0.17522976  | 8         | 3.81963611 | -1.20708299 | 0.13022976  |
| 1 | -0.12986398 | 1.91341698  | 2.36702991  | 6         | 2.81673598 | -2.09568310 | 0.07602976  |
| 1 | -1.82376385 | 2.40591693  | 2.21682978  | 6         | 0.34813601 | -2.44388318 | 0.44022974  |
| 1 | -0.78476399 | -0.44568303 | 2.50912976  | 1         | 1.24873602 | -1.14228296 | -1.03107023 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | -1.75346398 | 0.45131698  | 3.69702983  | 1 | 3.21853614  | 0.27811697  | -1.18747032 |
| 1 | -3.66706395 | 0.53611696  | 2.17362976  | 6 | 4.74423599  | 0.99021691  | 0.17382975  |
| 1 | -3.12566400 | -1.14388299 | 2.27392983  | 8 | 3.03423619  | -3.27168322 | 0.11092976  |
| 1 | -4.58616400 | -0.81958306 | 0.10822976  | 1 | 5.57163572  | 0.65281695  | -0.44927028 |
| 1 | -3.37966394 | -2.10798311 | 0.01402976  | 1 | 5.01403570  | 0.88001692  | 1.22462976  |
| 1 | -3.88286376 | 0.12451697  | -2.01097012 | 1 | 4.54583597  | 2.04151678  | -0.03037025 |
| 1 | -3.98386407 | -1.62428296 | -2.26807022 | 1 | 0.34433603  | -3.31608319 | -0.21247025 |
| 1 | -1.53406405 | -1.81778300 | -1.86107028 | 1 | -0.62256396 | -1.94858301 | 0.38852975  |
| 1 | -1.82536387 | -0.66878307 | -3.16247010 | 1 | 0.53533602  | -2.77278304 | 1.46342969  |
| 8 | 2.18213606  | 1.69211698  | 1.18572974  |   |             |             |             |

### I-1\_MeGL-CH<sub>2</sub>



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 989272.2 (Joules/Mol)       |
|  | 236.44174 (Kcal/Mol)        |
| Zero-point correction=                       | 0.376794 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.399076                    |
| Thermal correction to Enthalpy=              | 0.400021                    |
| Thermal correction to Gibbs Free Energy=     | 0.324073                    |
| Sum of electronic and zero-point Energies=   | -1049.118858                |
| Sum of electronic and thermal Energies=      | -1049.096576                |
| Sum of electronic and thermal Enthalpies=    | -1049.095632                |
| Sum of electronic and thermal Free Energies= | -1049.171579                |

cartesian

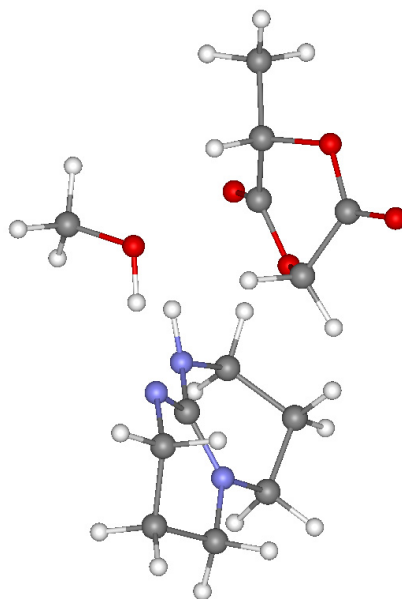
|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -2.29282522 | -0.28992501 | 0.47918865  | 1 | -1.32852519 | -0.90082502 | -3.11601138 |
| 6 | -1.31142521 | 0.40217501  | -0.16831133 | 8 | 2.36667490  | 2.05287504  | 1.12818873  |
| 7 | -0.75002527 | 1.47007501  | 0.48888865  | 6 | 2.59397483  | 0.95397502  | 0.70728868  |
| 6 | -0.91492522 | 1.69647503  | 1.92188871  | 8 | 1.74637473  | -0.05942499 | 0.93458867  |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.33242524 | 0.41027498  | 2.61488867  | 6 | 3.83927488  | 0.58487499  | -0.06701135 |
| 6 | -2.55682516 | -0.13932499 | 1.90598869  | 6 | 1.89417481  | -1.23032498 | 0.10728866  |
| 6 | -2.98852515 | -1.08442497 | -1.73621130 | 8 | 1.46697474  | 1.27767503  | -1.75511134 |
| 6 | -1.49752522 | -1.00492501 | -2.04281139 | 6 | 1.34057474  | 2.63557506  | -2.12231135 |
| 7 | -0.88812530 | 0.13167500  | -1.37081134 | 1 | 0.55867481  | 0.84877497  | -1.76041126 |
| 6 | -3.16062522 | -1.22532499 | -0.23331136 | 1 | 0.50807476  | 3.12307501  | -1.59961128 |
| 1 | 0.16657478  | 1.69577503  | 0.12608866  | 1 | 1.18587482  | 2.75487494  | -3.20041132 |
| 1 | 0.03797477  | 2.06217504  | 2.30438852  | 1 | 2.26107478  | 3.15557504  | -1.84751129 |
| 1 | -1.67182529 | 2.46937513  | 2.09438848  | 8 | 4.26507473  | -0.75572503 | 0.19798866  |
| 1 | -0.51452518 | -0.31372499 | 2.55778861  | 6 | 3.33307481  | -1.72192490 | 0.18498865  |
| 1 | -1.56252515 | 0.59627497  | 3.66488862  | 6 | 0.90757477  | -2.26402497 | 0.59408867  |
| 1 | -3.42052507 | 0.51917499  | 2.06528854  | 1 | 1.67997479  | -0.93802500 | -0.92681134 |
| 1 | -2.81932521 | -1.12792492 | 2.29438853  | 1 | 3.62077498  | 0.71607500  | -1.12911129 |
| 1 | -4.19452524 | -1.02112496 | 0.06338866  | 8 | 3.64817476  | -2.87392497 | 0.24578866  |
| 1 | -2.92172503 | -2.24792504 | 0.08508866  | 1 | 0.97487473  | -3.15502501 | -0.02901134 |
| 1 | -3.47072506 | -0.16642499 | -2.08301139 | 1 | -0.10242519 | -1.85612500 | 0.53328866  |
| 1 | -3.46012521 | -1.92962492 | -2.24021149 | 1 | 1.12817478  | -2.54002500 | 1.62628865  |
| 1 | -1.01772523 | -1.94662499 | -1.73401129 | 1 | 4.65377474  | 1.23587501  | 0.23568866  |

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### I-1\_MeGL-CHMe

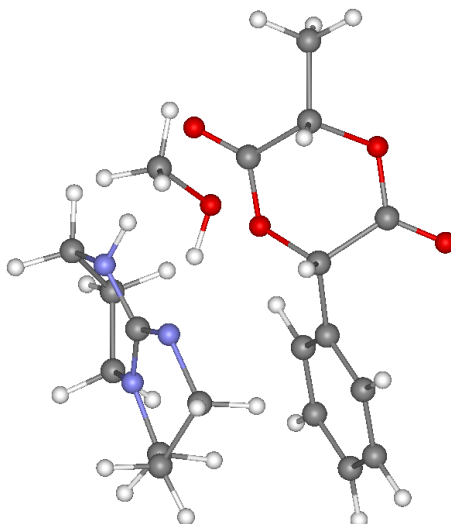


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy              | 987675.7 (Joules/Mol)       |
|  | 236.06017 (Kcal/Mol)        |
| Zero-point correction=                     | 0.376186 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.398674                    |
| Thermal correction to Enthalpy=            | 0.399618                    |
| Thermal correction to Gibbs Free Energy=   | 0.322260                    |
| Sum of electronic and zero-point Energies= | -1049.115917                |

Sum of electronic and thermal Energies= -1049.093429  
 Sum of electronic and thermal Enthalpies= -1049.092485  
 Sum of electronic and thermal Free Energies= -1049.169842

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.66241550 | 0.10449323  | 0.64325452  | 1         | 1.66871572  | 2.41369319  | -2.16454530 |
| 6 | 1.62881565 | -0.14780678 | -0.20954548 | 8         | -2.09428430 | -1.91900682 | 0.29265451  |
| 7 | 1.01901579 | -1.37600684 | -0.12124549 | 6         | -2.27108431 | -0.73840678 | 0.40085453  |
| 6 | 1.17411566 | -2.26320672 | 1.02825451  | 8         | -1.34118438 | 0.03789323  | 0.97825450  |
| 6 | 1.70701551 | -1.49130678 | 2.22305465  | 6         | -3.53708434 | -0.01540677 | -0.03514548 |
| 6 | 2.95611572 | -0.74360681 | 1.79245448  | 6         | -1.49318433 | 1.44759321  | 0.81185448  |
| 6 | 3.36911559 | 1.82229316  | -0.95994544 | 8         | -1.23228431 | 0.06739323  | -1.95394552 |
| 6 | 1.86871552 | 1.97279322  | -1.18614554 | 6         | -1.21098435 | -0.95550680 | -2.92614532 |
| 7 | 1.20321560 | 0.68219322  | -1.11894548 | 1         | -0.28848433 | 0.35229325  | -1.75414550 |
| 6 | 3.58691573 | 1.21349323  | 0.41465449  | 1         | -0.41978431 | -1.68980682 | -2.72904539 |
| 1 | 0.08991566 | -1.36160684 | -0.51914549 | 1         | -1.06388426 | -0.55690676 | -3.93634558 |
| 1 | 0.19611567 | -2.69580674 | 1.24045455  | 1         | -2.16958427 | -1.47960675 | -2.90064526 |
| 1 | 1.86231565 | -3.07920671 | 0.78185451  | 8         | -3.85878444 | 1.03339326  | 0.90485454  |
| 1 | 0.95191568 | -0.77670676 | 2.56245470  | 6         | -2.87988448 | 1.89229321  | 1.22745454  |
| 1 | 1.94141555 | -2.16920686 | 3.04485464  | 1         | -1.30768430 | 1.71589327  | -0.23264547 |
| 1 | 3.76271582 | -1.44860673 | 1.55145454  | 1         | -3.31278443 | 0.43779325  | -1.00474548 |
| 1 | 3.31541562 | -0.09270677 | 2.59475470  | 6         | -4.72848415 | -0.93870676 | -0.11484547 |
| 1 | 4.60731554 | 0.82939321  | 0.51495451  | 8         | -3.11318445 | 2.91099310  | 1.80835450  |
| 1 | 3.44031572 | 1.96849322  | 1.19645452  | 1         | -5.60508442 | -0.37400675 | -0.43014550 |
| 1 | 3.77681541 | 1.16149318  | -1.72974551 | 1         | -4.92098427 | -1.39260674 | 0.85785449  |
| 1 | 3.88591576 | 2.78129315  | -1.02334547 | 1         | -4.52968454 | -1.72790682 | -0.83864552 |
| 1 | 1.46031570 | 2.66419315  | -0.43334550 | 1         | -0.75628436 | 1.92429316  | 1.45135450  |

**I-1\_MePhGL-CHMe**

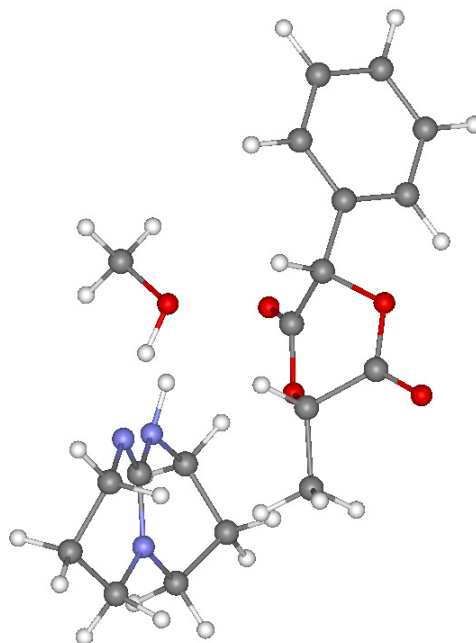


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1201671.3 (Joules/Mol)      |
|  | 287.20633 (Kcal/Mol)        |
| Zero-point correction=                       | 0.457692 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.484500                    |
| Thermal correction to Enthalpy=              | 0.485444                    |
| Thermal correction to Gibbs Free Energy=     | 0.400069                    |
| Sum of electronic and zero-point Energies=   | -1280.052866                |
| Sum of electronic and thermal Energies=      | -1280.026058                |
| Sum of electronic and thermal Enthalpies=    | -1280.025114                |
| Sum of electronic and thermal Free Energies= | -1280.110489                |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -2.03750372 | -1.28880012 | -0.38080370 | 6 | 0.98219639  | 1.50919986  | 0.20169629  |
| 6 | -0.87060356 | -1.58200014 | 0.25859630  | 8 | 2.02659631  | -1.10600007 | 1.68239629  |
| 7 | 0.05909638  | -2.31719995 | -0.43830371 | 6 | 2.63009620  | -2.32019997 | 2.07479620  |
| 6 | -0.10790361 | -2.64980006 | -1.84440362 | 1 | 1.02449632  | -1.19480014 | 1.75549626  |
| 6 | -0.88890362 | -1.55420005 | -2.54950380 | 1 | 2.14499640  | -3.18580008 | 1.60619628  |
| 6 | -2.21260381 | -1.35960007 | -1.83050370 | 1 | 2.60259628  | -2.45980000 | 3.16139627  |
| 6 | -3.00840378 | -0.92940003 | 1.83299637  | 1 | 3.67569637  | -2.30640006 | 1.75839627  |
| 6 | -1.59670365 | -0.57640004 | 2.28349614  | 8 | 3.27689624  | 2.18459988  | -0.18640372 |
| 7 | -0.59030360 | -1.26780009 | 1.49189627  | 6 | 2.03879642  | 2.61669993  | 0.08709627  |
| 6 | -3.12380362 | -0.64140004 | 0.34679630  | 6 | -0.40200359 | 2.04949999  | -0.04840372 |
| 1 | 1.00529635  | -2.14420009 | -0.12810372 | 1 | 1.04909635  | 1.07449996  | 1.20759630  |
| 1 | 0.88599640  | -2.76340008 | -2.27470374 | 1 | 3.46069622  | 0.49739993  | 1.00309634  |
| 1 | -0.63500363 | -3.60590005 | -1.94190371 | 6 | 4.94479609  | 0.52549994  | -0.57410371 |
| 1 | -0.29880363 | -0.63750005 | -2.51180387 | 8 | 1.80799639  | 3.78150010  | 0.21529628  |
| 1 | -1.07430363 | -1.81160009 | -3.59360385 | 1 | 5.65919638  | 1.11639988  | -0.00240372 |
| 1 | -2.90170383 | -2.17820001 | -2.07290387 | 1 | 5.00859642  | 0.79939997  | -1.62780368 |
| 1 | -2.68440366 | -0.42330003 | -2.14860392 | 1 | 5.18669605  | -0.53120005 | -0.46960372 |
| 1 | -4.06730366 | -1.02310014 | -0.05500372 | 6 | -1.06580365 | 2.71810007  | 0.97829622  |
| 1 | -3.09240365 | 0.44079995  | 0.16339628  | 6 | -0.99460363 | 1.95559990  | -1.30440366 |
| 1 | -3.19690371 | -1.99090016 | 2.01759624  | 6 | -2.31950378 | 3.27609992  | 0.75559628  |
| 1 | -3.75370383 | -0.35010004 | 2.38139629  | 1 | -0.59870362 | 2.80730009  | 1.95349634  |
| 1 | -1.46560359 | 0.51079994  | 2.21969628  | 6 | -2.25040364 | 2.51390004  | -1.52650368 |
| 1 | -1.45170355 | -0.85229999 | 3.33089614  | 1 | -0.47000360 | 1.45919991  | -2.11020374 |
| 8 | 2.72449636  | -1.02110016 | -1.42900372 | 1 | -2.82860374 | 3.79250002  | 1.56049633  |
| 6 | 2.49979639  | -0.02780007 | -0.79840374 | 6 | -2.91550374 | 3.17390013  | -0.49830371 |
| 8 | 1.25589645  | 0.47819996  | -0.75260371 | 1 | -2.70500374 | 2.43630004  | -2.50730371 |
| 6 | 3.55139637  | 0.77419996  | -0.05040372 | 1 | -3.89270353 | 3.60859990  | -0.67210376 |

I-1\_MePhGL-CHPh



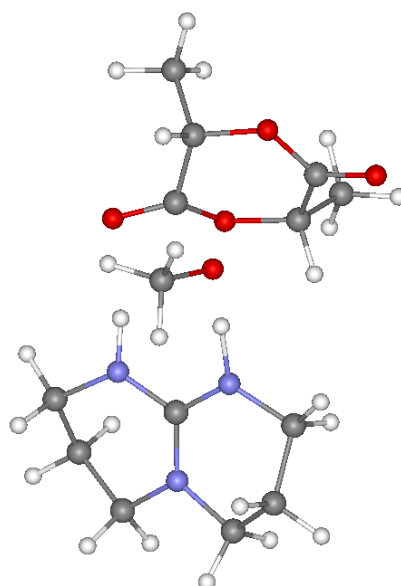
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1201075.3 (Joules/Mol)      |
|  | 287.06387 (Kcal/Mol)        |
| Zero-point correction=                       | 0.457465 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.484300                    |
| Thermal correction to Enthalpy=              | 0.485244                    |
| Thermal correction to Gibbs Free Energy=     | 0.397780                    |
| Sum of electronic and zero-point Energies=   | -1280.050959                |
| Sum of electronic and thermal Energies=      | -1280.024124                |
| Sum of electronic and thermal Enthalpies=    | -1280.023180                |
| Sum of electronic and thermal Free Energies= | -1280.110644                |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 3.49330950 | -0.15242405 | 0.54319263  | 6         | -0.12889048 | 1.85267591  | -0.38780737 |
| 6 | 2.37450957 | -0.71392405 | 0.00129264  | 8         | -0.51189047 | -1.10732412 | -1.62820733 |
| 7 | 1.53340960 | -1.39192414 | 0.84919262  | 6         | -0.81319046 | -2.48402405 | -1.52780735 |
| 6 | 1.59770942 | -1.26322412 | 2.30199265  | 1         | 0.48690951  | -0.98432404 | -1.61770725 |
| 6 | 2.32910943 | 0.01087594  | 2.68839264  | 1         | -0.00659049 | -3.03562403 | -1.02950728 |
| 6 | 3.67210960 | 0.02977594  | 1.97999275  | 1         | -0.97659045 | -2.93562388 | -2.51240730 |
| 6 | 4.42490959 | -0.17512406 | -1.72550726 | 1         | -1.72309041 | -2.60652399 | -0.93260735 |
| 6 | 2.97560954 | 0.03907594  | -2.14690733 | 8         | -2.52959061 | 2.12367606  | -0.34450737 |
| 7 | 2.06450939 | -0.67162406 | -1.26370728 | 6         | -1.35079050 | 2.75917602  | -0.46790737 |
| 6 | 4.58830929 | 0.32177594  | -0.29950738 | 6         | 1.12840962  | 2.61527610  | -0.04650736 |
| 1 | 0.59820950 | -1.46472406 | 0.47259262  | 1         | -0.01789048 | 1.31787586  | -1.33850729 |
| 1 | 0.57240951 | -1.25692415 | 2.67239261  | 1         | -2.17819047 | 0.36837596  | -1.40290725 |
| 1 | 2.11170936 | -2.12922406 | 2.73279262  | 6         | -3.89059043 | 0.16297594  | -0.13510737 |



|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.73460937  | 0.87557596  | 2.38049269  | 8 | -1.30669045 | 3.94557595  | -0.60490739 |
| 1 | 2.47890949  | 0.05567594  | 3.76799273  | 1 | 1.33450961  | 3.34497595  | -0.82880735 |
| 1 | 4.33130932  | -0.75032407 | 2.38189268  | 1 | 1.96490955  | 1.91937590  | 0.03149264  |
| 1 | 4.17230940  | 0.99217594  | 2.12589264  | 1 | 1.00440955  | 3.14247608  | 0.90039265  |
| 1 | 5.52780962  | -0.03572406 | 0.13389264  | 6 | -4.41809034 | -0.83542407 | -0.94730735 |
| 1 | 4.61090946  | 1.41887593  | -0.27590737 | 6 | -4.63139057 | 0.64947593  | 0.94049263  |
| 1 | 4.65510941  | -1.24272406 | -1.77660728 | 6 | -5.89649057 | 0.13747594  | 1.19749272  |
| 1 | 5.11710930  | 0.35587594  | -2.38110733 | 1 | -4.21869040 | 1.43167591  | 1.56749272  |
| 1 | 2.75750947  | 1.11827588  | -2.15040731 | 6 | -5.68279076 | -1.35372412 | -0.68410736 |
| 1 | 2.81400943  | -0.31852406 | -3.16550732 | 1 | -3.84059048 | -1.20462406 | -1.78830731 |
| 8 | -1.60669041 | -0.83452404 | 1.24839270  | 1 | -6.09009075 | -2.13032389 | -1.32000732 |
| 6 | -1.46939039 | 0.14037594  | 0.56769264  | 6 | -6.42239046 | -0.86652404 | 0.38689265  |
| 8 | -0.35069048 | 0.87797594  | 0.64709264  | 1 | -7.40919065 | -1.26522410 | 0.58999264  |
| 6 | -2.51089048 | 0.68387598  | -0.41070735 | 1 | -6.47319031 | 0.51897591  | 2.03139257  |

### TS-1\_LA



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1052431.8 (Joules/Mol)      |
|  | 251.53724 (Kcal/Mol)        |
| Zero-point correction=                       | 0.400850 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.423524                    |
| Thermal correction to Enthalpy=              | 0.424468                    |
| Thermal correction to Gibbs Free Energy=     | 0.347963                    |
| Sum of electronic and zero-point Energies=   | -1088.389929                |
| Sum of electronic and thermal Energies=      | -1088.367255                |
| Sum of electronic and thermal Enthalpies=    | -1088.366311                |
| Sum of electronic and thermal Free Energies= | -1088.442816                |

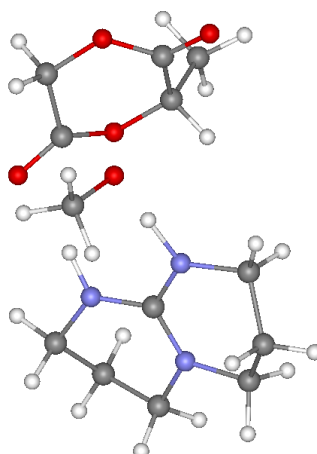
cartesian

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|   |             |             |             |   |            |             |             |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| 7 | -3.06000662 | -0.30007449 | 0.15261912  | 6 | 2.02509356 | 1.10792553  | -0.15038086 |
| 6 | -1.76990640 | -0.00097448 | -0.12728086 | 8 | 1.74649358 | 0.42802551  | 1.00201917  |
| 7 | -1.39320648 | 1.29322553  | -0.15538087 | 6 | 3.45869350 | 0.98442549  | -0.62418085 |
| 6 | -2.32540655 | 2.38802552  | 0.04631913  | 6 | 2.21079350 | -0.91537452 | 1.10601914  |
| 6 | -3.35670662 | 1.96702564  | 1.08061922  | 8 | 1.31479359 | -0.30187449 | -1.35458088 |
| 6 | -4.03520632 | 0.69742548  | 0.59591913  | 6 | 1.07179356 | 0.21302553  | -2.63438106 |
| 6 | -2.65240669 | -2.52207446 | -0.83028084 | 1 | 0.22099352 | -0.60767454 | -0.84228086 |
| 6 | -1.23470652 | -2.32957458 | -0.31128088 | 1 | 1.02509356 | 1.31162560  | -2.61218095 |
| 7 | -0.86620653 | -0.92587453 | -0.38308087 | 1 | 0.10889353 | -0.15117449 | -3.01788092 |
| 6 | -3.58670664 | -1.65737450 | -0.00108087 | 1 | 1.85359347 | -0.09107448 | -3.33968091 |
| 1 | -0.39820647 | 1.50462556  | -0.21768087 | 8 | 3.98859358 | -0.34597448 | -0.51948088 |
| 1 | -1.75340641 | 3.25302553  | 0.38041914  | 6 | 3.34329367 | -1.29207444 | 0.16351913  |
| 1 | -2.82260656 | 2.65472531  | -0.89358085 | 6 | 2.63899374 | -1.15357447 | 2.54631901  |
| 1 | -2.85590649 | 1.78492558  | 2.03441906  | 1 | 1.38189352 | -1.57787442 | 0.84541917  |
| 1 | -4.10610628 | 2.74572539  | 1.22631919  | 1 | 3.47739363 | 1.23002553  | -1.68598080 |
| 1 | -4.71700621 | 0.92192549  | -0.23298088 | 6 | 4.34299374 | 1.93252552  | 0.16971913  |
| 1 | -4.62570620 | 0.24462551  | 1.39721918  | 8 | 3.71019363 | -2.43447447 | 0.09591913  |
| 1 | -4.56780624 | -1.57687449 | -0.47788087 | 1 | 5.37659359 | 1.84062552  | -0.16368087 |
| 1 | -3.73510647 | -2.09587455 | 0.99231911  | 1 | 4.28969336 | 1.69382560  | 1.23421919  |
| 1 | -2.69410658 | -2.21857452 | -1.87968087 | 1 | 4.00549364 | 2.95812535  | 0.02021913  |
| 1 | -2.96420670 | -3.56487465 | -0.76118082 | 1 | 2.90999365 | -2.19977450 | 2.68301892  |
| 1 | -1.16670644 | -2.69687462 | 0.72101915  | 1 | 1.81009352 | -0.90657449 | 3.20981908  |
| 1 | -0.51320648 | -2.89177465 | -0.90678084 | 1 | 3.49409342 | -0.52527452 | 2.80271912  |
| 8 | 1.39499354  | 2.12812543  | -0.38328087 |   |            |             |             |

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### TS-1\_MeGL-CH<sub>2</sub>



Zero-point vibrational energy

978728.8 (Joules/Mol)

233.92180 (Kcal/Mol)

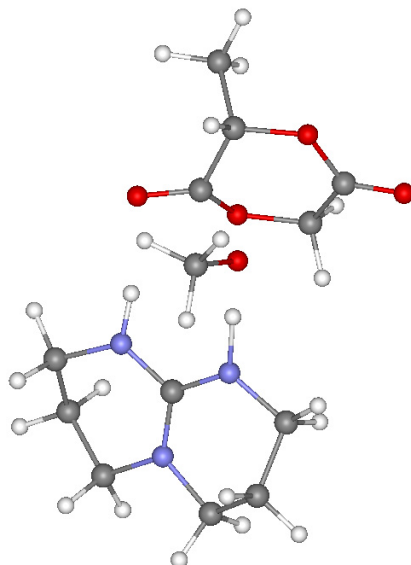
Zero-point correction=

0.372778 (Hartree/Particle)

|  |              |
|--|--------------|
| Thermal correction to Energy=                | 0.394118     |
| Thermal correction to Enthalpy=              | 0.395062     |
| Thermal correction to Gibbs Free Energy=     | 0.320698     |
| Sum of electronic and zero-point Energies=   | -1049.107822 |
| Sum of electronic and thermal Energies=      | -1049.086482 |
| Sum of electronic and thermal Enthalpies=    | -1049.085538 |
| Sum of electronic and thermal Free Energies= | -1049.159902 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | -2.71793175 | 0.37464547  | -0.16062497 | 1         | -0.01103157 | 2.76674533  | 0.97017503  |
| 6 | -1.45853162 | -0.01935453 | 0.13807502  | 8         | 1.52836847  | -2.41735458 | 0.42377502  |
| 7 | -1.17633152 | -1.33655453 | 0.16147503  | 6         | 2.21756840  | -1.45255446 | 0.13467503  |
| 6 | -2.17623138 | -2.36215448 | -0.08042498 | 8         | 1.93726838  | -0.78115451 | -1.01952505 |
| 6 | -3.15933180 | -1.85235453 | -1.12192500 | 6         | 3.66366863  | -1.40285444 | 0.56377500  |
| 6 | -3.75563145 | -0.54755455 | -0.62372500 | 6         | 2.51886845  | 0.50884545  | -1.19462502 |
| 6 | -2.16993141 | 2.55324531  | 0.85067505  | 8         | 1.66366839  | 0.05154547  | 1.32307494  |
| 6 | -0.76043153 | 2.26654530  | 0.35467502  | 6         | 1.44016838  | -0.40535450 | 2.62667489  |
| 7 | -0.49613160 | 0.83884543  | 0.41527504  | 1         | 0.56156844  | 0.44484550  | 0.83887506  |
| 6 | -3.14803171 | 1.76514554  | -0.00382497 | 1         | 1.32986844  | -1.50005448 | 2.64557505  |
| 1 | -0.20203155 | -1.62105453 | 0.24737503  | 1         | 0.51376843  | 0.02394547  | 3.03357506  |
| 1 | -1.65653169 | -3.25575471 | -0.42472497 | 1         | 2.26306844  | -0.12605453 | 3.29527497  |
| 1 | -2.70643139 | -2.61475468 | 0.84497505  | 8         | 4.29966831  | -0.13695452 | 0.39697504  |
| 1 | -2.63283157 | -1.68815446 | -2.06502509 | 6         | 3.68566847  | 0.83814543  | -0.27652496 |
| 1 | -3.95703125 | -2.57605457 | -1.29192507 | 6         | 2.97326851  | 0.62364548  | -2.64282513 |
| 1 | -4.45813131 | -0.73665452 | 0.19647503  | 1         | 1.75076842  | 1.25384557  | -0.97472495 |
| 1 | -4.30663157 | -0.04465453 | -1.42312503 | 1         | 3.72506857  | -1.66285443 | 1.61897492  |
| 1 | -4.14073133 | 1.75164557  | 0.45517504  | 8         | 4.12006855  | 1.95694554  | -0.23732498 |
| 1 | -3.24653149 | 2.22074533  | -0.99562496 | 1         | 3.34296846  | 1.62974548  | -2.83772492 |
| 1 | -2.25213146 | 2.24344540  | 1.89557493  | 1         | 2.12926841  | 0.41474545  | -3.30032492 |
| 1 | -2.40553141 | 3.61634541  | 0.78737503  | 1         | 3.76586819  | -0.09865452 | -2.84792495 |
| 1 | -0.64673162 | 2.63994551  | -0.67132497 | 1         | 4.21036863  | -2.14465451 | -0.02472497 |

TS-1\_MeGL-CHMe

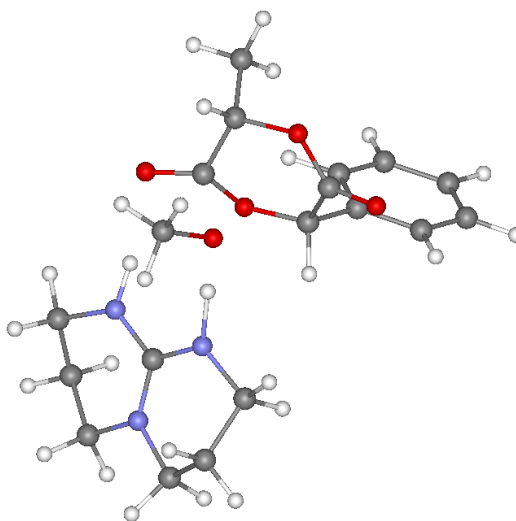


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 979468.0 (Joules/Mol)       |
|  | 234.09848 (Kcal/Mol)        |
| Zero-point correction=                       | 0.373060 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.394199                    |
| Thermal correction to Enthalpy=              | 0.395143                    |
| Thermal correction to Gibbs Free Energy=     | 0.321998                    |
| Sum of electronic and zero-point Energies=   | -1049.108558                |
| Sum of electronic and thermal Energies=      | -1049.087419                |
| Sum of electronic and thermal Enthalpies=    | -1049.086475                |
| Sum of electronic and thermal Free Energies= | -1049.159620                |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.88794065 | 0.25885004  | 0.26326138  | 1         | 0.41654074  | 3.02804995  | -0.47343862 |
| 6 | 1.58374071 | 0.03175002  | -0.02043863 | 8         | -1.66485929 | -1.96394992 | -0.47953862 |
| 7 | 1.16284084 | -1.24024999 | -0.17013863 | 6         | -2.22345924 | -0.97995001 | -0.02173863 |
| 6 | 2.05094075 | -2.38614988 | -0.07183863 | 8         | -1.80355930 | -0.51335001 | 1.19366145  |
| 6 | 3.11974072 | -2.08984995 | 0.96726137  | 6         | -3.68825936 | -0.73145002 | -0.32713866 |
| 6 | 3.83624053 | -0.81194997 | 0.56936133  | 6         | -2.21755934 | 0.79355001  | 1.55346143  |
| 6 | 2.54284072 | 2.58144999  | -0.48313862 | 8         | -1.56145930 | 0.59595001  | -1.03243864 |
| 6 | 1.12924075 | 2.38374996  | 0.04436137  | 6         | -1.46535921 | 0.30875003  | -2.40013862 |
| 7 | 0.70974082 | 1.00805008  | -0.16213864 | 1         | -0.41915923 | 0.78254998  | -0.57983863 |
| 6 | 3.46064067 | 1.60625005  | 0.23416136  | 1         | -1.48415923 | -0.77695000 | -2.57513881 |
| 1 | 0.16214079 | -1.40914989 | -0.25733864 | 1         | -0.52045923 | 0.69274998  | -2.80823874 |
| 1 | 1.44824076 | -3.24915004 | 0.20976137  | 1         | -2.28765917 | 0.76854998  | -2.96013880 |
| 1 | 2.51794076 | -2.60095000 | -1.03993857 | 8         | -4.14245939 | 0.58364999  | 0.02896136  |
| 1 | 2.64834070 | -1.96564984 | 1.94516146  | 6         | -3.40635920 | 1.36985004  | 0.81246138  |

|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.83914065 | -2.90684986 | 1.03086138  | 1 | -1.38995934 | 1.48975003  | 1.40666139  |
| 1 | 4.47484112 | -0.98814994 | -0.30443865 | 1 | -3.81345940 | -0.80634999 | -1.40723860 |
| 1 | 4.47684097 | -0.45934999 | 1.38236141  | 6 | -4.54205894 | -1.76244998 | 0.39346135  |
| 1 | 4.42884111 | 1.54085004  | -0.27043861 | 8 | -3.72365928 | 2.51454997  | 0.98916137  |
| 1 | 3.64394069 | 1.93685007  | 1.26296139  | 1 | -5.59565926 | -1.58574998 | 0.17726137  |
| 1 | 2.55484080 | 2.38555002  | -1.55833864 | 1 | -4.38465929 | -1.69454992 | 1.47216141  |
| 1 | 2.89204073 | 3.60105014  | -0.31513864 | 1 | -4.26775932 | -2.76265001 | 0.05806137  |
| 1 | 1.09454083 | 2.64475012  | 1.11036146  | 1 | -2.48015928 | 0.77775002  | 2.61316133  |

### TS-1\_MePhGL-CHMe



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1191937.5 (Joules/Mol)      |
|  | 284.87989 (Kcal/Mol)        |
| Zero-point correction=                       | 0.453985 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.479863                    |
| Thermal correction to Enthalpy=              | 0.480808                    |
| Thermal correction to Gibbs Free Energy=     | 0.395252                    |
| Sum of electronic and zero-point Energies=   | -1280.041801                |
| Sum of electronic and thermal Energies=      | -1280.015922                |
| Sum of electronic and thermal Enthalpies=    | -1280.014978                |
| Sum of electronic and thermal Free Energies= | -1280.100533                |

cartesian

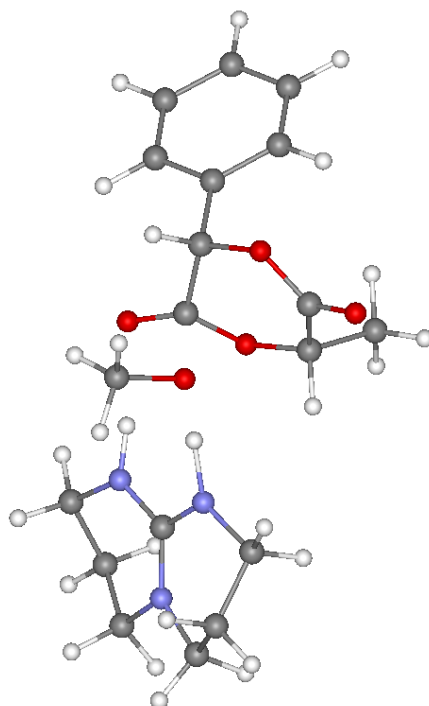
|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -3.41472411 | -0.99409807 | -0.08757591 | 6 | 1.86607599  | -0.08679812 | -0.49857590 |
| 6 | -2.35472393 | -0.15319812 | -0.03747591 | 8 | 0.08377603  | 1.87290192  | -1.08717585 |
| 7 | -2.14032412 | 0.55430186  | 1.09042406  | 6 | -0.62962395 | 3.06900167  | -1.23917592 |
| 6 | -3.02312398 | 0.49590188  | 2.24242401  | 1 | -0.71182400 | 0.93170190  | -1.04697585 |
| 6 | -3.56402397 | -0.91879809 | 2.37162423  | 1 | -0.80022401 | 3.54910183  | -0.26447591 |
| 6 | -4.25522375 | -1.29209805 | 1.07222414  | 1 | -1.61242390 | 2.87580180  | -1.68997586 |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -3.19552398 | -0.95819807 | -2.54117584 | 1 | -0.09132397 | 3.77060175  | -1.88647592 |
| 6 | -1.71092415 | -0.78189808 | -2.25677586 | 8 | 2.83487606  | 2.14580178  | -0.94967592 |
| 7 | -1.52612400 | 0.00610188  | -1.04967594 | 6 | 2.54947591  | 0.93090189  | -1.41407585 |
| 6 | -3.83542418 | -1.62949812 | -1.33777583 | 6 | 2.88427591  | -1.12019813 | -0.03827591 |
| 1 | -1.27962399 | 1.09230185  | 1.16402411  | 1 | 1.11227608  | -0.57029808 | -1.12677586 |
| 1 | -2.44302392 | 0.78220189  | 3.11912417  | 1 | 1.83357596  | 3.63150167  | -0.00657591 |
| 1 | -3.85002398 | 1.20750189  | 2.13692403  | 6 | 3.22857594  | 2.69840169  | 1.36152411  |
| 1 | -2.73602414 | -1.60479808 | 2.56582403  | 8 | 2.90247607  | 0.60690188  | -2.51437593 |
| 1 | -4.27432394 | -0.99139810 | 3.19572401  | 1 | 4.07247591  | 3.31580186  | 1.05412412  |
| 1 | -5.20462370 | -0.75189811 | 0.97522414  | 1 | 3.59337592  | 1.69550192  | 1.59442413  |
| 1 | -4.47972393 | -2.36199832 | 1.04802418  | 1 | 2.77287602  | 3.12930179  | 2.25322413  |
| 1 | -4.92582369 | -1.56209815 | -1.39027584 | 6 | 3.48167586  | -1.96529806 | -0.97547591 |
| 1 | -3.56942415 | -2.69219828 | -1.30397594 | 6 | 3.21597600  | -1.24559808 | 1.30802417  |
| 1 | -3.64752412 | 0.02330188  | -2.70647597 | 6 | 4.41057634  | -2.91389823 | -0.56867588 |
| 1 | -3.36242414 | -1.56799805 | -3.42997599 | 1 | 3.22277594  | -1.86759806 | -2.02287602 |
| 1 | -1.23692393 | -1.76689816 | -2.15357590 | 6 | 4.14727592  | -2.19929814 | 1.71242416  |
| 1 | -1.20722389 | -0.26019812 | -3.07237577 | 1 | 2.73467588  | -0.60949808 | 2.03942418  |
| 8 | 0.23187602  | 2.24410176  | 1.50842416  | 1 | 4.86897612  | -3.56499815 | -1.30347586 |
| 6 | 1.01097608  | 1.80830193  | 0.67852414  | 6 | 4.74817610  | -3.03279829 | 0.77762413  |
| 8 | 1.20287609  | 0.45430186  | 0.63212407  | 1 | 4.39837599  | -2.28959823 | 2.76262403  |
| 6 | 2.20267606  | 2.63640189  | 0.24152410  | 1 | 5.47127628  | -3.77479815 | 1.09462416  |

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### TS-1\_MePhGL-CHPh



Zero-point vibrational energy

1191134.9 (Joules/Mol)

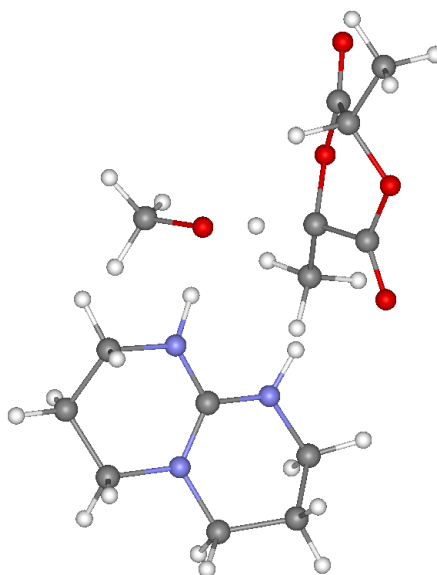
284.68807 (Kcal/Mol)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.453679 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.479611                    |
| Thermal correction to Enthalpy=              | 0.480555                    |
| Thermal correction to Gibbs Free Energy=     | 0.394022                    |
| Sum of electronic and zero-point Energies=   | -1280.042240                |
| Sum of electronic and thermal Energies=      | -1280.016309                |
| Sum of electronic and thermal Enthalpies=    | -1280.015365                |
| Sum of electronic and thermal Free Energies= | -1280.101897                |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -3.85265470 | 0.38530183  | 0.33637035  | 6 | 1.13874531  | -1.53739822 | 1.01697028  |
| 6 | -2.56925488 | 0.27080178  | -0.07772964 | 8 | 0.16364522  | -1.06139815 | -1.45702970 |
| 7 | -1.86175489 | 1.39240181  | -0.32362965 | 6 | -0.04655477 | -0.70879817 | -2.79582977 |
| 6 | -2.42185473 | 2.72760177  | -0.20072964 | 1 | -0.90495479 | -0.96259815 | -0.83712965 |
| 6 | -3.42675471 | 2.73490167  | 0.94027030  | 1 | 0.20364521  | 0.34880179  | -2.96632957 |
| 6 | -4.47185516 | 1.66770172  | 0.66977036  | 1 | -1.10135484 | -0.84809816 | -3.06862974 |
| 6 | -4.17185497 | -1.96519828 | -0.33342963 | 1 | 0.56154525  | -1.32579827 | -3.46722960 |
| 6 | -2.70795488 | -2.11679816 | 0.05327035  | 8 | 2.73914528  | -1.77789819 | -0.86512965 |
| 7 | -1.98315477 | -0.89599818 | -0.25592965 | 6 | 1.95204520  | -2.37229824 | 0.03827035  |
| 6 | -4.74365520 | -0.77409816 | 0.41647035  | 6 | 1.72764528  | -1.66149819 | 2.41497040  |
| 1 | -0.86425483 | 1.29830182  | -0.50392967 | 1 | 0.13344522  | -1.96529818 | 0.98837030  |
| 1 | -1.59895480 | 3.41620183  | -0.01142965 | 1 | 2.65514517  | -0.22899818 | -2.16022968 |
| 1 | -2.91005468 | 3.03290176  | -1.13352966 | 6 | 3.84834528  | 0.33200181  | -0.45632964 |
| 1 | -2.90855479 | 2.52260184  | 1.87857032  | 8 | 1.94994521  | -3.56929827 | 0.12607035  |
| 1 | -3.91205478 | 3.70760179  | 1.02557039  | 1 | 1.75784516  | -2.70909834 | 2.71317029  |
| 1 | -5.12785435 | 1.97470188  | -0.15362965 | 1 | 1.10314524  | -1.10579824 | 3.11457038  |
| 1 | -5.09885502 | 1.50870180  | 1.55137038  | 1 | 2.73684525  | -1.24599826 | 2.44107032  |
| 1 | -5.70815468 | -0.47689819 | -0.00502964 | 6 | 4.73244476  | -0.34449819 | 0.37977037  |
| 1 | -4.90575504 | -1.02439821 | 1.47107029  | 6 | 4.06484509  | 1.68320179  | -0.73492968 |
| 1 | -4.24235439 | -1.79799819 | -1.41122961 | 6 | 5.81544495  | 0.32630181  | 0.94367039  |
| 1 | -4.74445438 | -2.85989833 | -0.08562964 | 1 | 4.59264565  | -1.39999819 | 0.57757032  |
| 1 | -2.63225484 | -2.35269833 | 1.12297034  | 6 | 5.14544487  | 2.34890175  | -0.17172965 |
| 1 | -2.23195481 | -2.93149829 | -0.49532965 | 1 | 3.37474513  | 2.20890188  | -1.38422966 |
| 8 | 1.01624525  | 1.35510182  | -0.92302966 | 1 | 6.49864483  | -0.21069819 | 1.59097028  |
| 6 | 1.36424518  | 0.24750181  | -0.54942966 | 6 | 6.02364540  | 1.67270172  | 0.67217034  |
| 8 | 1.02334523  | -0.15059818 | 0.70697033  | 1 | 6.86734486  | 2.19240189  | 1.11027038  |
| 6 | 2.65414524  | -0.37149817 | -1.07872963 | 1 | 5.30484486  | 3.39750171  | -0.39342964 |

TS-1'\_LA



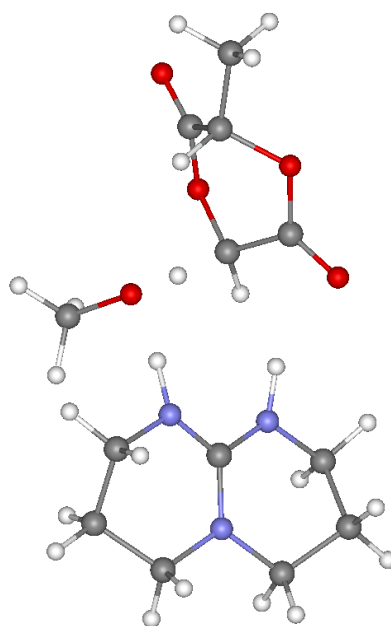
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1044836.7 (Joules/Mol)      |
|  | 249.72197 (Kcal/Mol)        |
| Zero-point correction=                       | 0.397957 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.421588                    |
| Thermal correction to Enthalpy=              | 0.422532                    |
| Thermal correction to Gibbs Free Energy=     | 0.342301                    |
| Sum of electronic and zero-point Energies=   | -1088.372078                |
| Sum of electronic and thermal Energies=      | -1088.348448                |
| Sum of electronic and thermal Enthalpies=    | -1088.347504                |
| Sum of electronic and thermal Free Energies= | -1088.427735                |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 3.25293016 | -0.20018724 | 0.18323831  | 6         | -2.38066983 | -1.39498723 | 0.35683832  |
| 6 | 1.91963017 | -0.08338723 | 0.28913832  | 8         | -3.32476997 | -1.08088720 | 1.27853835  |
| 7 | 1.13863015 | -1.15278733 | 0.06533831  | 6         | -2.43086982 | -0.64368725 | -0.88546169 |
| 6 | 1.67523015 | -2.45868707 | -0.29306170 | 6         | -4.01246977 | 0.16691279  | 1.07193840  |
| 6 | 3.01133013 | -2.64578724 | 0.40713829  | 8         | -1.09766984 | 1.47301269  | -0.15266168 |
| 6 | 3.92453027 | -1.49398732 | 0.02493831  | 6         | -0.94156986 | 2.28671288  | -1.28716159 |
| 6 | 3.36013007 | 2.25261283  | -0.04296169 | 1         | 0.29503015  | 1.19201267  | 0.38213831  |
| 6 | 2.14153004 | 2.25751281  | 0.86733830  | 1         | 0.09963015  | 2.28721285  | -1.64746165 |
| 7 | 1.34253013 | 1.06811273  | 0.60923833  | 1         | -1.22126985 | 3.32651281  | -1.07926166 |
| 6 | 4.13723040 | 0.96961278  | 0.19773832  | 1         | -1.57306981 | 1.93491280  | -2.11586165 |
| 1 | 0.17403015 | -1.12488723 | 0.37673831  | 8         | -3.78746986 | -0.27738723 | -1.26656163 |
| 1 | 0.93943012 | -3.19948721 | 0.01633831  | 6         | -4.60046959 | 0.19021279  | -0.33016169 |
| 1 | 1.80053008 | -2.53138709 | -1.37866163 | 6         | -5.06086969 | 0.30691278  | 2.14733815  |
| 1 | 2.85462999 | -2.65838718 | 1.48823833  | 1         | -3.26976991 | 0.97321278  | 1.12183833  |



|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.47543001  | -3.58758712 | 0.11403832  | 1 | -1.73036981 | 0.46951276  | -0.50486171 |
| 1 | 4.25523043  | -1.59258723 | -1.01466167 | 6 | -1.77236986 | -1.29328728 | -2.07746172 |
| 1 | 4.81433010  | -1.47708726 | 0.65893829  | 8 | -5.70556974 | 0.58771276  | -0.59276170 |
| 1 | 4.88983011  | 0.81821281  | -0.57996172 | 1 | -1.81826985 | -0.62188721 | -2.93626165 |
| 1 | 4.65403032  | 1.00631273  | 1.16263831  | 1 | -2.24786997 | -2.24128723 | -2.34926176 |
| 1 | 3.03283000  | 2.30291295  | -1.08466160 | 1 | -0.72166985 | -1.48438728 | -1.85646164 |
| 1 | 4.00383043  | 3.10911274  | 0.15843831  | 1 | -5.57566977 | 1.25991273  | 2.03313828  |
| 1 | 2.45353007  | 2.28651285  | 1.91653836  | 1 | -4.58786964 | 0.26821280  | 3.12823820  |
| 1 | 1.50523019  | 3.12321281  | 0.68243831  | 1 | -5.79286957 | -0.49738723 | 2.06613827  |
| 8 | -1.49776983 | -2.17568707 | 0.67103833  |   |             |             |             |

### TS-1'\_MeGL-CH<sub>2</sub>



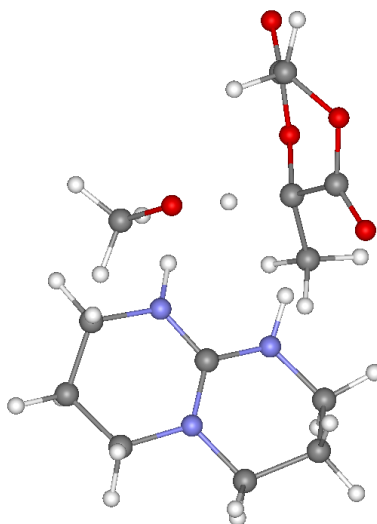
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 972292.9 (Joules/Mol)       |
|  | 232.38357 (Kcal/Mol)        |
| Zero-point correction=                       | 0.370327 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.392111                    |
| Thermal correction to Enthalpy=              | 0.393055                    |
| Thermal correction to Gibbs Free Energy=     | 0.316916                    |
| Sum of electronic and zero-point Energies=   | -1049.091096                |
| Sum of electronic and thermal Energies=      | -1049.069312                |
| Sum of electronic and thermal Enthalpies=    | -1049.068368                |
| Sum of electronic and thermal Free Energies= | -1049.144507                |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -3.12297487 | -0.29235911 | 0.00156592  | 1 | -1.44057488 | 2.96064091  | -0.96653408 |
| 6 | -1.79877496 | -0.18035913 | -0.18473409 | 8 | 1.60832500  | -2.28725910 | -0.66343409 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -0.99407500 | -1.21245909 | 0.12176592  | 6 | 2.45642495  | -1.51545906 | -0.25533408 |
| 6 | -1.50247502 | -2.46435905 | 0.66456592  | 8 | 3.52342510  | -1.23665905 | -1.04013407 |
| 6 | -2.86427498 | -2.74775910 | 0.04956592  | 6 | 2.35672498  | -0.73335916 | 0.96836597  |
| 6 | -3.77537513 | -1.56455910 | 0.32766593  | 6 | 4.17912483  | 0.01844087  | -0.76803404 |
| 6 | -3.24557495 | 2.16944098  | -0.04603408 | 8 | 1.16212499  | 1.41494095  | 0.11006591  |
| 6 | -2.07457495 | 2.07514095  | -1.01333416 | 6 | 0.95452499  | 2.23314095  | 1.23136592  |
| 7 | -1.24747491 | 0.92904085  | -0.66263407 | 1 | -0.19947499 | 1.09684086  | -0.43723410 |
| 6 | -4.01987505 | 0.86374086  | -0.09793408 | 1 | -0.11847502 | 2.38594103  | 1.42896593  |
| 1 | -0.06587499 | -1.23355913 | -0.28463408 | 1 | 1.41162503  | 3.22164083  | 1.10376585  |
| 1 | -0.77267498 | -3.23545909 | 0.42316592  | 1 | 1.38762498  | 1.78244090  | 2.13776588  |
| 1 | -1.58417487 | -2.39755917 | 1.75426590  | 8 | 3.63712502  | -0.36415914 | 1.53276587  |
| 1 | -2.75137496 | -2.89245915 | -1.02743411 | 6 | 4.57162476  | 0.07714087  | 0.70106596  |
| 1 | -3.30407500 | -3.65015912 | 0.47466591  | 6 | 5.36312485  | 0.13554086  | -1.69453406 |
| 1 | -4.06947517 | -1.54555905 | 1.38256586  | 1 | 3.45082498  | 0.82174087  | -0.93643403 |
| 1 | -4.68647528 | -1.62435913 | -0.27273408 | 1 | 1.70792508  | 0.36404085  | 0.53916591  |
| 1 | -4.72937536 | 0.79724085  | 0.73066592  | 8 | 5.63202477  | 0.47994083  | 1.10116589  |
| 1 | -4.58597517 | 0.78784084  | -1.03243411 | 1 | 5.86672497  | 1.08644092  | -1.52553415 |
| 1 | -2.86577487 | 2.34034085  | 0.96456593  | 1 | 5.02522469  | 0.08594087  | -2.72923422 |
| 1 | -3.90737510 | 2.99484086  | -0.30903408 | 1 | 6.07032490  | -0.67255914 | -1.50533414 |
| 1 | -2.44067502 | 1.97904086  | -2.04083419 | 1 | 1.80242491  | -1.25105906 | 1.74406588  |

### TS-1'\_MeGL-CHMe

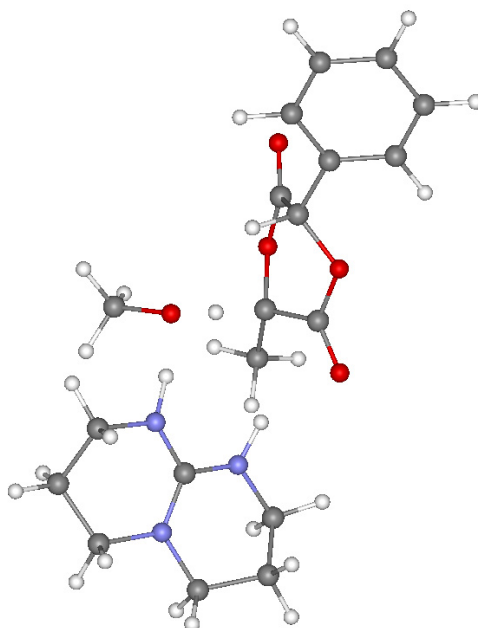


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy              | 971135.8 (Joules/Mol)       |
|  | 232.10702 (Kcal/Mol)        |
| Zero-point correction=                     | 0.369886 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.392036                    |
| Thermal correction to Enthalpy=            | 0.392980                    |
| Thermal correction to Gibbs Free Energy=   | 0.315906                    |
| Sum of electronic and zero-point Energies= | -1049.089473                |

|  |              |
|--|--------------|
| Sum of electronic and thermal Energies=      | -1049.067323 |
| Sum of electronic and thermal Enthalpies=    | -1049.066379 |
| Sum of electronic and thermal Free Energies= | -1049.143453 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.88836145  | -0.20285225 | 0.14913410  | 1         | 1.20996141  | 3.11114788  | 0.89143407  |
| 6 | 1.56806147  | -0.08305224 | 0.35963410  | 8         | -1.83983862 | -2.18065214 | 0.94233406  |
| 7 | 0.76486146  | -1.14195228 | 0.16493410  | 6         | -2.71643877 | -1.37185228 | 0.69003409  |
| 6 | 1.26516140  | -2.43565226 | -0.27956593 | 8         | -3.58293867 | -1.03005219 | 1.67793417  |
| 6 | 2.64706135  | -2.65395212 | 0.31543410  | 6         | -2.82653856 | -0.61195225 | -0.54356593 |
| 6 | 3.53926134  | -1.49435222 | -0.09276590 | 6         | -4.24553871 | 0.22424775  | 1.50603414  |
| 6 | 2.99476147  | 2.25644779  | -0.00986591 | 8         | -1.46043849 | 1.49034774  | 0.16703409  |
| 6 | 1.85156143  | 2.23584795  | 0.99313408  | 6         | -1.38413858 | 2.34754753  | -0.94346589 |
| 7 | 1.02476144  | 1.06114781  | 0.75613409  | 1         | -0.03393859 | 1.19764781  | 0.60353410  |
| 6 | 3.77886152  | 0.96234775  | 0.12473410  | 1         | -0.36233857 | 2.39374781  | -1.35266590 |
| 1 | -0.17003858 | -1.12065220 | 0.55613410  | 1         | -1.68493855 | 3.36984777  | -0.68536592 |
| 1 | 0.54896140  | -3.18505239 | 0.05373409  | 1         | -2.04393864 | 2.00384760  | -1.75356591 |
| 1 | 1.31236148  | -2.46755219 | -1.37326586 | 8         | -4.19323874 | -0.19945225 | -0.83786589 |
| 1 | 2.56816149  | -2.70355225 | 1.40393412  | 6         | -4.91093826 | 0.31554776  | 0.15043409  |
| 1 | 3.08126163  | -3.58765221 | -0.04266590 | 1         | -3.51553869 | 1.03744781  | 1.58583415  |
| 1 | 3.79776144  | -1.56215227 | -1.15496588 | 1         | -2.09373856 | 0.48694777  | -0.18586589 |
| 1 | 4.46976137  | -1.50015223 | 0.47983408  | 6         | -2.26143861 | -1.26715219 | -1.77856588 |
| 1 | 4.46216154  | 0.83164775  | -0.71816593 | 8         | -5.99323845 | 0.80674773  | -0.03506590 |
| 1 | 4.37536144  | 0.96554780  | 1.04293406  | 1         | -2.33093858 | -0.58235228 | -2.62516594 |
| 1 | 2.58656120  | 2.34544754  | -1.01976585 | 1         | -2.78613853 | -2.19335222 | -2.03436589 |
| 1 | 3.65936136  | 3.10194778  | 0.16893409  | 1         | -1.20793855 | -1.49915218 | -1.61916590 |
| 1 | 2.24456120  | 2.22454786  | 2.01523399  | 1         | -4.99473858 | 0.30454776  | 2.28723407  |

TS-1'\_PhMeGL-CHMe



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1185163.3 (Joules/Mol)      |
|  | 283.26083 (Kcal/Mol)        |
| Zero-point correction=                       | 0.451405 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.478075                    |
| Thermal correction to Enthalpy=              | 0.479019                    |
| Thermal correction to Gibbs Free Energy=     | 0.390747                    |
| Sum of electronic and zero-point Energies=   | -1280.021362                |
| Sum of electronic and thermal Energies=      | -1279.994692                |
| Sum of electronic and thermal Enthalpies=    | -1279.993748                |
| Sum of electronic and thermal Free Energies= | -1280.082020                |

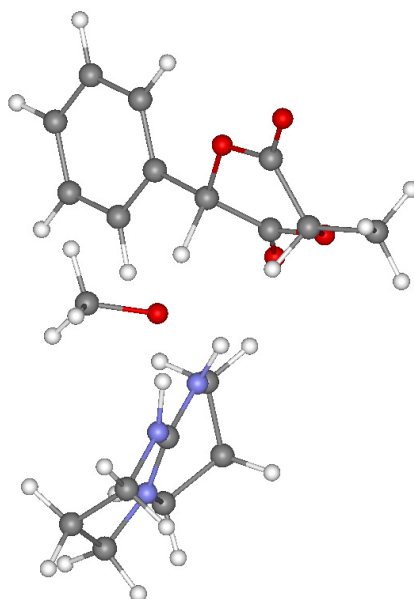
| cartesian |            |             |             |   |             |             |             |
|-----------|------------|-------------|-------------|---|-------------|-------------|-------------|
| 7         | 4.09383869 | 0.12250556  | 0.64881665  | 6 | -3.16916132 | -0.14629446 | -0.14088336 |
| 6         | 2.76483846 | 0.10580555  | 0.46241665  | 8 | -0.17176142 | 1.14680564  | -0.96848339 |
| 7         | 2.11783862 | -1.06899440 | 0.39091665  | 6 | 0.17313856  | 1.69790554  | -2.21378326 |
| 6         | 2.80023861 | -2.35129452 | 0.49671665  | 1 | 1.08623862  | 1.16790557  | -0.10848335 |
| 6         | 3.96443844 | -2.20519447 | 1.46361673  | 1 | 1.26503861  | 1.79100561  | -2.32878327 |
| 6         | 4.86373854 | -1.08209443 | 0.97611666  | 1 | -0.26136145 | 2.69560552  | -2.34858322 |
| 6         | 4.09453869 | 2.43970537  | -0.19608335 | 1 | -0.18766144 | 1.06690562  | -3.03938341 |
| 6         | 2.71083856 | 2.52560544  | 0.43071666  | 8 | -2.35756159 | -1.13369441 | -2.16318321 |
| 7         | 2.06233859 | 1.22540557  | 0.34391665  | 6 | -3.39806151 | -0.53339446 | -1.60328329 |
| 6         | 4.88153839 | 1.35250556  | 0.51561666  | 6 | -4.45136166 | 0.16820554  | 0.57761663  |
| 1         | 1.10963857 | -1.07529449 | 0.49241665  | 1 | -2.50646138 | 0.72920555  | -0.15418336 |
| 1         | 2.06483865 | -3.07549453 | 0.84361660  | 1 | -0.60986143 | 0.00170554  | -1.18358326 |
| 1         | 3.15973854 | -2.67189455 | -0.48688334 | 6 | -0.15906143 | -2.08779454 | -2.20088339 |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.58013868  | -1.97419441 | 2.45981669  | 8 | -4.41066170 | -0.32099444 | -2.21308327 |
| 1 | 4.53973866  | -3.12929463 | 1.521111673 | 1 | -0.00676143 | -1.64639437 | -3.18698335 |
| 1 | 5.42213869  | -1.39269435 | 0.08641665  | 1 | -0.51976144 | -3.11329460 | -2.32878327 |
| 1 | 5.58813858  | -0.80359447 | 1.74551666  | 1 | 0.80543852  | -2.12049437 | -1.69348335 |
| 1 | 5.78683853  | 1.09910560  | -0.04138336 | 6 | -4.99586153 | 1.44570553  | 0.46811667  |
| 1 | 5.18323851  | 1.68400562  | 1.51471674  | 6 | -5.11626148 | -0.80509448 | 1.31801665  |
| 1 | 3.99413872  | 2.19740558  | -1.25718331 | 6 | -6.31786156 | -0.49869448 | 1.94861674  |
| 1 | 4.62533855  | 3.38790536  | -0.10808335 | 1 | -4.68676138 | -1.79499435 | 1.40791667  |
| 1 | 2.78703856  | 2.84390545  | 1.47571671  | 6 | -6.19946146 | 1.74880564  | 1.09361672  |
| 1 | 2.07633853  | 3.24160552  | -0.09178335 | 1 | -4.47656155 | 2.20400548  | -0.10818335 |
| 8 | -0.53456146 | -2.22879457 | 0.67641664  | 1 | -6.82876158 | -1.25889444 | 2.52751660  |
| 6 | -1.34186149 | -1.65049446 | -0.02848335 | 6 | -6.86216164 | 0.77670550  | 1.83741665  |
| 8 | -2.49686146 | -1.21289444 | 0.53991663  | 1 | -6.61686134 | 2.74460554  | 1.00461674  |
| 6 | -1.12046146 | -1.24149442 | -1.40438330 | 1 | -7.79756165 | 1.01320565  | 2.33031678  |

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### TS-1'\_PhMeGL-CHPh



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1183991.3 (Joules/Mol)      |
|  | 282.98070 (Kcal/Mol)        |
| Zero-point correction=                       | 0.450958 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.476672                    |
| Thermal correction to Enthalpy=              | 0.477616                    |
| Thermal correction to Gibbs Free Energy=     | 0.393738                    |
| Sum of electronic and zero-point Energies=   | -1280.028836                |
| Sum of electronic and thermal Energies=      | -1280.003122                |
| Sum of electronic and thermal Enthalpies=    | -1280.002178                |
| Sum of electronic and thermal Free Energies= | -1280.086056                |

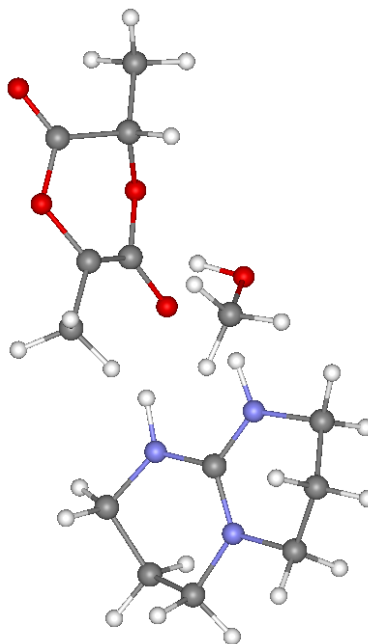
cartesian

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -3.58970499 | -0.20671290 | 0.31023890  | 6 | 3.19579482  | -2.36481285 | 0.65473884  |
| 6 | -2.26640511 | -0.42901292 | 0.24433887  | 8 | 0.74319482  | -1.04591286 | -1.31026113 |
| 7 | -1.45110524 | 0.17428710  | 1.12423897  | 6 | 0.70749480  | -0.45871291 | -2.58446097 |
| 6 | -1.92290533 | 1.12158716  | 2.12173891  | 1 | -0.65960526 | -1.18511283 | -0.85276115 |
| 6 | -3.29190516 | 0.66778713  | 2.60283899  | 1 | -0.24700519 | 0.06288709  | -2.76206112 |
| 6 | -4.21670532 | 0.54308712  | 1.40333891  | 1 | 0.83339477  | -1.20261288 | -3.38206100 |
| 6 | -3.75560522 | -1.04891288 | -2.00046110 | 1 | 1.50769472  | 0.28748709  | -2.69976115 |
| 6 | -2.57210517 | -1.92951286 | -1.62916112 | 8 | 3.93339491  | -0.26231292 | -0.21546112 |
| 7 | -1.73370516 | -1.22941291 | -0.66766113 | 6 | 4.27509499  | -1.53201294 | -0.01516113 |
| 6 | -4.50530529 | -0.68501288 | -0.73006111 | 6 | 3.72669482  | -3.64961290 | 1.23943889  |
| 1 | -0.48540524 | -0.12531291 | 1.17953897  | 1 | 2.41629481  | -2.55051279 | -0.09456113 |
| 1 | -1.18960524 | 1.13438714  | 2.92653894  | 1 | 1.69919479  | -0.46411291 | -0.64366114 |
| 1 | -1.97920525 | 2.12888718  | 1.69473886  | 6 | 2.44639492  | 1.61568713  | -0.10866113 |
| 1 | -3.19430518 | -0.29811293 | 3.10373902  | 8 | 5.35389471  | -1.94791293 | -0.33896112 |
| 1 | -3.71210527 | 1.38248706  | 3.31063890  | 1 | 4.15759468  | -4.25991297 | 0.44683886  |
| 1 | -4.49990511 | 1.53368711  | 1.03103888  | 1 | 2.91479492  | -4.19861317 | 1.71543896  |
| 1 | -5.13320494 | 0.01368709  | 1.67503893  | 1 | 4.50109482  | -3.43631291 | 1.97683895  |
| 1 | -5.22750521 | 0.11298709  | -0.91936117 | 6 | 3.55959487  | 2.44848704  | -0.23626111 |
| 1 | -5.05490494 | -1.55031288 | -0.34416115 | 6 | 1.16839480  | 2.17558718  | -0.21086113 |
| 1 | -3.39130521 | -0.14361291 | -2.49266100 | 6 | 3.39649487  | 3.81428719  | -0.44816113 |
| 1 | -4.42990494 | -1.56531286 | -2.68406105 | 1 | 4.55269480  | 2.02278709  | -0.17376111 |
| 1 | -2.92470503 | -2.87851286 | -1.21076107 | 6 | 1.00959480  | 3.54088712  | -0.41216111 |
| 1 | -1.95270526 | -2.15741301 | -2.49706101 | 1 | 0.29919478  | 1.53038716  | -0.15236111 |
| 8 | 1.26769483  | 0.11838710  | 2.09723878  | 1 | 4.27089453  | 4.44768667  | -0.54436111 |
| 6 | 2.12199473  | -0.37891293 | 1.39503896  | 6 | 2.12359476  | 4.36798668  | -0.53126115 |
| 8 | 2.60939479  | -1.59701288 | 1.72393894  | 1 | 1.99929476  | 5.43178701  | -0.69526112 |
| 6 | 2.58379483  | 0.14568709  | 0.10003888  | 1 | 0.01219478  | 3.95868707  | -0.48986113 |

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I-2'\_LA

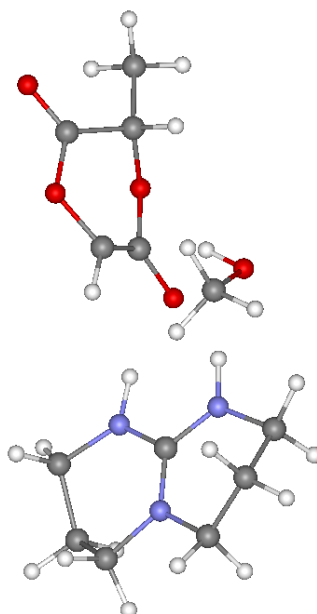


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1062564.3 (Joules/Mol)      |
|  | 253.95897 (Kcal/Mol)        |
| Zero-point correction=                       | 0.404709 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.428628                    |
| Thermal correction to Enthalpy=              | 0.429572                    |
| Thermal correction to Gibbs Free Energy=     | 0.349809                    |
| Sum of electronic and zero-point Energies=   | -1088.378097                |
| Sum of electronic and thermal Energies=      | -1088.354179                |
| Sum of electronic and thermal Enthalpies=    | -1088.353234                |
| Sum of electronic and thermal Free Energies= | -1088.432997                |

|   |            |             |             |   | cartesian   |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | 3.26280618 | -0.26092553 | 0.08120427  | 6 | -2.23679376 | -0.76642549 | 0.52390426  |
| 6 | 1.96110642 | -0.40072554 | 0.37050426  | 8 | -3.36829376 | -0.81532550 | 1.32810426  |
| 7 | 1.35550630 | -1.58552551 | 0.26700425  | 6 | -2.44579363 | -0.56042552 | -0.80919576 |
| 6 | 2.03500628 | -2.77342558 | -0.22509573 | 6 | -4.45459366 | -0.03612552 | 0.84490424  |
| 6 | 3.49280620 | -2.71192551 | 0.20190427  | 8 | -1.22579372 | 2.18637443  | 0.08260426  |
| 6 | 4.10000610 | -1.40722561 | -0.28509575 | 6 | -0.67159373 | 2.66187453  | -1.13029575 |
| 6 | 2.93310618 | 2.18607450  | 0.01110426  | 1 | 0.24550626  | 0.47447449  | 0.96170425  |
| 6 | 1.82260621 | 1.95207453  | 1.02210426  | 1 | 0.11380628  | 1.99437451  | -1.50619566 |
| 7 | 1.23350632 | 0.64887452  | 0.76330423  | 1 | -0.22929372 | 3.64067435  | -0.93609577 |
| 6 | 3.93260622 | 1.04387438  | 0.09770426  | 1 | -1.43229377 | 2.77917433  | -1.90879571 |
| 1 | 0.35840628 | -1.59082556 | 0.53100425  | 8 | -3.75649381 | -0.70332551 | -1.34829569 |
| 1 | 1.53580630 | -3.64332557 | 0.19910426  | 6 | -4.80889368 | -0.47532552 | -0.56819576 |
| 1 | 1.95880640 | -2.83422565 | -1.31609571 | 6 | -5.61629391 | -0.18072551 | 1.79940426  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.55290604  | -2.76522565 | 1.29150426  | 1 | -4.13059378 | 1.01387441  | 0.77470422  |
| 1 | 4.05090618  | -3.54982567 | -0.21579574 | 1 | -1.73679364 | 1.38627446  | -0.12239574 |
| 1 | 4.22870636  | -1.42012560 | -1.37269568 | 6 | -1.39289367 | -0.58152550 | -1.86369574 |
| 1 | 5.08110619  | -1.24722552 | 0.16730426  | 8 | -5.93119383 | -0.60982549 | -0.98349577 |
| 1 | 4.61620617  | 1.06597447  | -0.75389576 | 1 | -1.57129371 | 0.18287449  | -2.62579584 |
| 1 | 4.53070641  | 1.11977446  | 1.01190424  | 1 | -1.33459377 | -1.55112553 | -2.37309575 |
| 1 | 2.50520611  | 2.23237443  | -0.99349576 | 1 | -0.42189372 | -0.38382554 | -1.40549564 |
| 1 | 3.44450617  | 3.12807441  | 0.20970426  | 1 | -6.45669365 | 0.42307448  | 1.45920432  |
| 1 | 2.22110629  | 1.99677444  | 2.04140425  | 1 | -5.31389380 | 0.14787449  | 2.79340410  |
| 1 | 1.02440631  | 2.68627453  | 0.93270427  | 1 | -5.93309402 | -1.22352552 | 1.84660435  |
| 8 | -1.12809372 | -0.87302548 | 1.12920427  |   |             |             |             |

### I-2'\_MeGL-CH<sub>2</sub>



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 986816.7 (Joules/Mol)       |
|  | 235.85486 (Kcal/Mol)        |
| Zero-point correction=                       | 0.375859 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.398550                    |
| Thermal correction to Enthalpy=              | 0.399494                    |
| Thermal correction to Gibbs Free Energy=     | 0.320320                    |
| Sum of electronic and zero-point Energies=   | -1049.096760                |
| Sum of electronic and thermal Energies=      | -1049.074068                |
| Sum of electronic and thermal Enthalpies=    | -1049.073124                |
| Sum of electronic and thermal Free Energies= | -1049.152299                |

cartesian

|   |             |             |            |   |             |            |             |
|---|-------------|-------------|------------|---|-------------|------------|-------------|
| 7 | -3.06959486 | -0.41510230 | 0.16462499 | 1 | -1.23239505 | 2.72129774 | -0.93367499 |
|---|-------------|-------------|------------|---|-------------|------------|-------------|

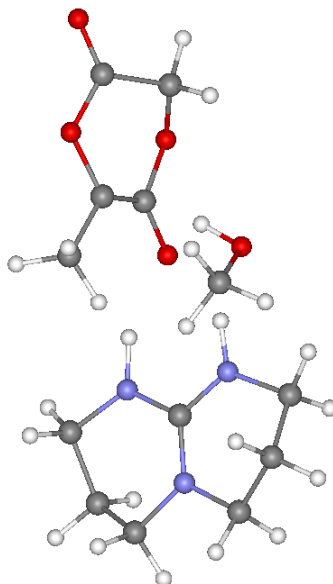


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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.81359518 | -0.43780231 | -0.30187500 | 8 | 1.22240496  | -0.66850227 | -1.43737507 |
| 7 | -1.09519506 | -1.56190228 | -0.29227501 | 6 | 2.19660497  | -0.59660232 | -0.63697499 |
| 6 | -1.59509504 | -2.80880237 | 0.26542500  | 8 | 3.45030499  | -0.81640232 | -1.18027508 |
| 6 | -3.09649515 | -2.87730241 | 0.03672500  | 6 | 2.16330481  | -0.28130233 | 0.69362503  |
| 6 | -3.74699497 | -1.63370228 | 0.61932504  | 6 | 4.49890518  | -0.11120231 | -0.52257496 |
| 6 | -2.95749521 | 2.05049777  | 0.21492499  | 8 | 1.11400485  | 2.44879770  | -0.28107500 |
| 6 | -1.97189510 | 1.92269778  | -0.93527496 | 6 | 0.61460495  | 2.79429770  | 0.99752504  |
| 7 | -1.24639511 | 0.67119771  | -0.78567499 | 1 | -0.27639508 | 0.59339768  | -1.09247506 |
| 6 | -3.85299492 | 0.82259768  | 0.24212500  | 1 | -0.03649509 | 2.01039767  | 1.40422499  |
| 1 | -0.15939510 | -1.48300231 | -0.71897501 | 1 | 0.02950493  | 3.70959759  | 0.89312500  |
| 1 | -1.08099508 | -3.62770224 | -0.23547500 | 1 | 1.42080498  | 2.98079777  | 1.71442497  |
| 1 | -1.36719513 | -2.86750221 | 1.33482492  | 8 | 3.29880476  | -0.49590230 | 1.51762497  |
| 1 | -3.29689503 | -2.93250227 | -1.03577507 | 6 | 4.50430489  | -0.45520234 | 0.96062499  |
| 1 | -3.51799488 | -3.76310229 | 0.51162499  | 6 | 5.80610514  | -0.45630229 | -1.19517505 |
| 1 | -3.72989511 | -1.66190231 | 1.71402490  | 1 | 4.29090500  | 0.96729767  | -0.59217501 |
| 1 | -4.78909492 | -1.56080234 | 0.30092499  | 1 | 1.66590488  | 1.66099775  | -0.14817502 |
| 1 | -4.42539501 | 0.78429770  | 1.17142498  | 8 | 5.49670506  | -0.66950232 | 1.60822499  |
| 1 | -4.56379509 | 0.84179771  | -0.59077495 | 1 | 6.62420511  | 0.07929769  | -0.71517497 |
| 1 | -2.41089487 | 2.13229775  | 1.15742493  | 1 | 5.76020527  | -0.17950231 | -2.24817491 |
| 1 | -3.57249498 | 2.94279766  | 0.09722500  | 1 | 5.99530506  | -1.52740228 | -1.11297500 |
| 1 | -2.50219488 | 1.94389772  | -1.89327502 | 1 | 1.25440490  | -0.18930233 | 1.26562500  |

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### I-2'\_MeGL-CHMe

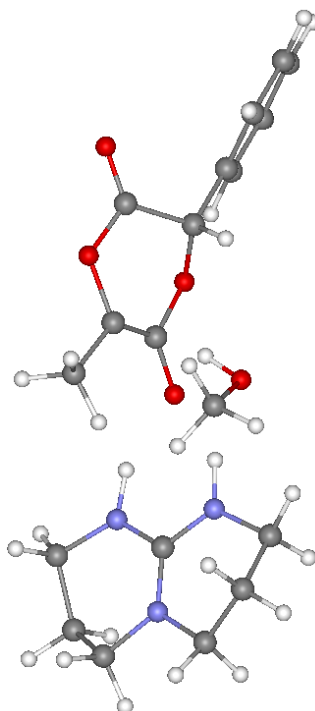


|                               |                             |
|-------------------------------|-----------------------------|
| Zero-point vibrational energy | 989180.1 (Joules/Mol)       |
|                               | 236.41972 (Kcal/Mol)        |
| Zero-point correction=        | 0.376759 (Hartree/Particle) |
| Thermal correction to Energy= | 0.399237                    |

|  |              |
|--|--------------|
| Thermal correction to Enthalpy=              | 0.400182     |
| Thermal correction to Gibbs Free Energy=     | 0.323529     |
| Sum of electronic and zero-point Energies=   | -1049.095534 |
| Sum of electronic and thermal Energies=      | -1049.073056 |
| Sum of electronic and thermal Enthalpies=    | -1049.072111 |
| Sum of electronic and thermal Free Energies= | -1049.148764 |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.86789751 | -0.24485457 | 0.07908179  | 1         | 0.63639760  | 2.67524552  | 1.03458178  |
| 6 | 1.58289766 | -0.39835453 | 0.42908180  | 8         | -1.45740247 | -0.88665456 | 1.35338175  |
| 7 | 0.98469758 | -1.58935463 | 0.34798181  | 6         | -2.60850239 | -0.78085452 | 0.83548176  |
| 6 | 1.65179753 | -2.76555443 | -0.18701822 | 8         | -3.67050242 | -0.77915454 | 1.73318172  |
| 6 | 3.12629747 | -2.69505453 | 0.17658179  | 6         | -2.92060256 | -0.62055457 | -0.48411819 |
| 6 | 3.70179749 | -1.38105464 | -0.32461822 | 6         | -4.77860260 | -0.02095456 | 1.29248178  |
| 6 | 2.51149750 | 2.19874549  | 0.03568179  | 8         | -1.61950243 | 2.14514542  | 0.21888179  |
| 6 | 1.44759750 | 1.95194542  | 1.09238183  | 6         | -1.09650242 | 2.57524562  | -1.02421820 |
| 7 | 0.86479759 | 0.64074546  | 0.86198175  | 1         | -0.11220244 | 0.45454544  | 1.10228181  |
| 6 | 3.52529764 | 1.06654537  | 0.07658179  | 1         | -0.34240246 | 1.87834537  | -1.41031826 |
| 1 | 0.00339758 | -1.60775459 | 0.66108179  | 1         | -0.62210244 | 3.54614544  | -0.86971819 |
| 1 | 1.17929757 | -3.64455438 | 0.24878180  | 1         | -1.88060248 | 2.69474554  | -1.77881825 |
| 1 | 1.52819753 | -2.81515455 | -1.27411819 | 8         | -4.27100277 | -0.76065457 | -0.91981828 |
| 1 | 3.23379755 | -2.75745440 | 1.26188171  | 6         | -5.25380230 | -0.47025454 | -0.07281820 |
| 1 | 3.67259741 | -3.52445459 | -0.27271822 | 1         | -4.51060247 | 1.04294538  | 1.22428179  |
| 1 | 3.79079771 | -1.38615465 | -1.41621828 | 1         | -2.14800239 | 1.34644544  | 0.05738179  |
| 1 | 4.69729757 | -1.21415460 | 0.09268180  | 6         | -1.94830239 | -0.69025457 | -1.61121821 |
| 1 | 4.17489767 | 1.09914541  | -0.80081820 | 8         | -6.40880251 | -0.55615455 | -0.39961824 |
| 1 | 4.15819740 | 1.14374542  | 0.96708179  | 1         | -2.18430233 | 0.04084544  | -2.39011812 |
| 1 | 2.04169750 | 2.24284554  | -0.95001829 | 1         | -1.92510247 | -1.68075466 | -2.08171821 |
| 1 | 3.02109766 | 3.14544559  | 0.21508178  | 1         | -0.94680244 | -0.47385454 | -1.23411822 |
| 1 | 1.88779759 | 2.00464559  | 2.09398174  | 1         | -5.58440256 | -0.14945456 | 2.01028180  |

I-2'\_PhMeGL-CHMe



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1201611.5 (Joules/Mol)      |
|  | 287.19204 (Kcal/Mol)        |
| Zero-point correction=                       | 0.457670 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.484860                    |
| Thermal correction to Enthalpy=              | 0.485804                    |
| Thermal correction to Gibbs Free Energy=     | 0.396147                    |
| Sum of electronic and zero-point Energies=   | -1280.028420                |
| Sum of electronic and thermal Energies=      | -1280.001230                |
| Sum of electronic and thermal Enthalpies=    | -1280.000286                |
| Sum of electronic and thermal Free Energies= | -1280.089943                |

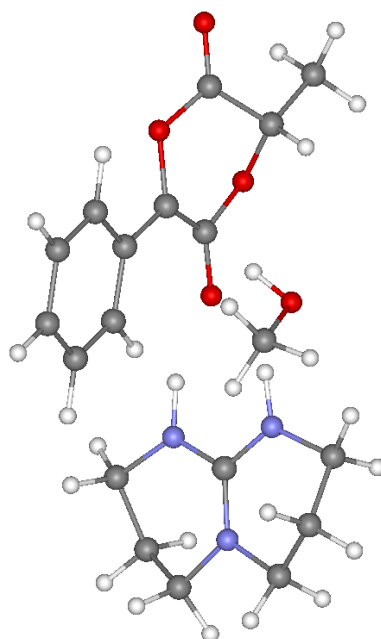
|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 4.21378469 | -0.27481294 | 0.44683516  | 6         | -3.49441504 | -0.00091294 | -0.26256481 |
| 6 | 2.88338494 | -0.43611294 | 0.45803517  | 8         | -0.19401515 | 2.21788692  | -0.12246482 |
| 7 | 2.32498503 | -1.58241296 | 0.06203518  | 6         | 0.60828489  | 2.83698702  | -1.11096489 |
| 6 | 3.10058498 | -2.68871307 | -0.47636482 | 1         | 1.07438493  | 0.36148703  | 0.83783519  |
| 6 | 4.45178461 | -2.71831298 | 0.21973519  | 1         | 1.45888495  | 2.20548701  | -1.39626491 |
| 6 | 5.12148476 | -1.36271298 | 0.07033518  | 1         | 0.99508482  | 3.76798701  | -0.69256479 |
| 6 | 3.87248492 | 2.15928698  | 0.69703519  | 1         | 0.03468484  | 3.07928705  | -2.01126480 |
| 6 | 2.58528495 | 1.79398704  | 1.41883516  | 8         | -2.39981508 | -0.44741297 | -2.34466481 |
| 7 | 2.07918501 | 0.55208707  | 0.85843521  | 6         | -3.58541512 | -0.27901295 | -1.76596487 |
| 6 | 4.84958458 | 0.99898708  | 0.80103523  | 6         | -4.81821537 | -0.15901294 | 0.43703517  |
| 1 | 1.29778481 | -1.61441290 | 0.13023518  | 1         | -3.14981508 | 1.04198706  | -0.17236482 |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 2.54348493  | -3.60671306 | -0.29526484 | 1 | -0.64071512 | 1.46108699  | -0.53406483 |
| 1 | 3.22948480  | -2.57541299 | -1.55826485 | 6 | 0.01938486  | -0.29291296 | -2.38616467 |
| 1 | 4.30688477  | -2.94501305 | 1.27853513  | 8 | -4.60181522 | -0.33011293 | -2.40526485 |
| 1 | 5.09088469  | -3.48781300 | -0.21336481 | 1 | -0.03991514 | 0.54258704  | -3.08976483 |
| 1 | 5.45628452  | -1.20461297 | -0.96046478 | 1 | 0.20838487  | -1.20401299 | -2.96636462 |
| 1 | 5.99558449  | -1.29361296 | 0.72143519  | 1 | 0.87808484  | -0.12621294 | -1.73296487 |
| 1 | 5.68848467  | 1.14108706  | 0.11623518  | 6 | -5.82281542 | 0.78158706  | 0.21143518  |
| 1 | 5.25308466  | 0.92008710  | 1.81593513  | 6 | -5.05401516 | -1.22331297 | 1.30123520  |
| 1 | 3.65388513  | 2.36898708  | -0.35286483 | 6 | -6.28741550 | -1.34441292 | 1.93643510  |
| 1 | 4.32198477  | 3.04918694  | 1.13773513  | 1 | -4.26891518 | -1.94671297 | 1.47833514  |
| 1 | 2.76998496  | 1.68168700  | 2.49263525  | 6 | -7.05311537 | 0.65828705  | 0.84383518  |
| 1 | 1.81018496  | 2.54538703  | 1.28073514  | 1 | -5.63951540 | 1.61018705  | -0.46406484 |
| 8 | -0.29411516 | -0.94851297 | 0.54883522  | 1 | -6.46361542 | -2.17371297 | 2.61153531  |
| 6 | -1.26131511 | -0.74641293 | -0.24216482 | 6 | -7.28841543 | -0.40701294 | 1.70973516  |
| 8 | -2.53061509 | -0.85541296 | 0.32183516  | 1 | -7.82741547 | 1.39468706  | 0.66453522  |
| 6 | -1.21541524 | -0.39171296 | -1.55776489 | 1 | -8.24691486 | -0.50281292 | 2.20583534  |

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### I-2'\_PhMeGL-CHPh



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy              | 1201777.8 (Joules/Mol)      |
|  | 287.23178 (Kcal/Mol)        |
| Zero-point correction=                     | 0.457733 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.484888                    |
| Thermal correction to Enthalpy=            | 0.485832                    |
| Thermal correction to Gibbs Free Energy=   | 0.398269                    |
| Sum of electronic and zero-point Energies= | -1280.044851                |
| Sum of electronic and thermal Energies=    | -1280.017695                |

Sum of electronic and thermal Enthalpies= -1280.016751  
Sum of electronic and thermal Free Energies= -1280.104314

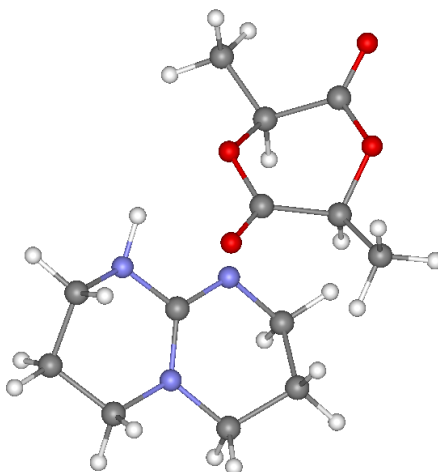
cartesian

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -3.56667638 | -0.56184262 | 0.09438702  | 6 | 4.08002377  | -1.99944270 | -0.24441297 |
| 6 | -2.25477624 | -0.77994263 | 0.26038700  | 8 | 1.06752384  | 0.09605737  | -2.06631303 |
| 7 | -1.73197627 | -0.89484262 | 1.48558700  | 6 | 0.52152383  | 1.37755728  | -2.34131312 |
| 6 | -2.51807618 | -0.71144259 | 2.69698691  | 1 | -0.44417617 | -0.98684263 | -0.61411297 |
| 6 | -3.92417598 | -1.22844267 | 2.44308686  | 1 | -0.36547616 | 1.57035732  | -1.72671306 |
| 6 | -4.49867582 | -0.52404261 | 1.22618699  | 1 | 0.23712382  | 1.39995730  | -3.39511299 |
| 6 | -3.11357617 | 0.06865737  | -2.25211310 | 1 | 1.24552381  | 2.17615747  | -2.15351295 |
| 6 | -1.94657612 | -0.90054262 | -2.15921307 | 8 | 4.19042397  | 0.17215736  | 0.75798702  |
| 7 | -1.44397616 | -0.88454264 | -0.79421300 | 6 | 4.91052389  | -0.85354263 | 0.30648702  |
| 6 | -4.16267586 | -0.32554266 | -1.22611308 | 6 | 4.85872412  | -3.29114246 | -0.32061297 |
| 1 | -0.73197615 | -1.09954274 | 1.53088701  | 1 | 3.72982383  | -1.69004273 | -1.24041307 |
| 1 | -2.02897620 | -1.26454270 | 3.49708700  | 1 | 1.61852384  | 0.16895737  | -1.27691305 |
| 1 | -2.54287624 | 0.34635735  | 2.97928691  | 6 | 2.17232394  | 1.46035731  | 0.71578705  |
| 1 | -3.88747621 | -2.30584264 | 2.26718688  | 8 | 6.11142397  | -0.83354264 | 0.35568702  |
| 1 | -4.56427574 | -1.04064262 | 3.30498695  | 1 | 5.72912407  | -3.16254258 | -0.96251291 |
| 1 | -4.73147583 | 0.52115738  | 1.45588696  | 1 | 4.22282410  | -4.07704258 | -0.72711295 |
| 1 | -5.42087603 | -1.00994265 | 0.90018702  | 1 | 5.19762421  | -3.58164263 | 0.67458701  |
| 1 | -4.90457582 | 0.46715733  | -1.10681307 | 6 | 2.97552371  | 2.60325742  | 0.52728701  |
| 1 | -4.68857574 | -1.23384273 | -1.53851306 | 6 | 0.79002380  | 1.66295731  | 0.89878702  |
| 1 | -2.75917625 | 1.08365726  | -2.05621314 | 6 | 2.41902375  | 3.87415743  | 0.50308704  |
| 1 | -3.55737615 | 0.04565736  | -3.24751306 | 1 | 4.04262400  | 2.48065734  | 0.39658701  |
| 1 | -2.26867628 | -1.91074264 | -2.43291306 | 6 | 0.24602382  | 2.94055748  | 0.87408704  |
| 1 | -1.11967623 | -0.61794263 | -2.80681300 | 1 | 0.14562383  | 0.81215739  | 1.05508697  |
| 8 | 0.90142381  | -1.31664264 | 0.79088706  | 1 | 3.06612372  | 4.73085737  | 0.35078701  |
| 6 | 2.13202381  | -1.08434272 | 0.71418703  | 6 | 1.04832387  | 4.05875731  | 0.67168701  |
| 8 | 2.94862390  | -2.19694257 | 0.59588701  | 1 | 0.61902380  | 5.05295753  | 0.65208703  |
| 6 | 2.77252388  | 0.13825737  | 0.68948704  | 1 | -0.82317626 | 3.05915737  | 1.01688695  |

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I-1''\_LA

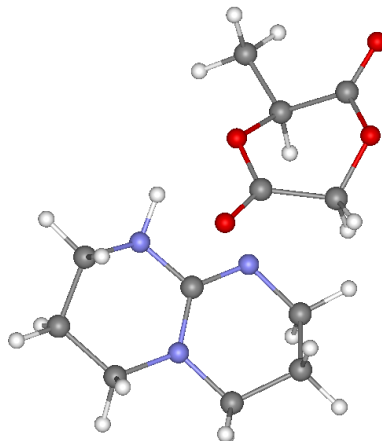


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 920284.4 (Joules/Mol)       |
|  | 219.95325 (Kcal/Mol)        |
| Zero-point correction=                       | 0.350518 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.370128                    |
| Thermal correction to Enthalpy=              | 0.371072                    |
| Thermal correction to Gibbs Free Energy=     | 0.301573                    |
| Sum of electronic and zero-point Energies=   | -972.728432                 |
| Sum of electronic and thermal Energies=      | -972.708822                 |
| Sum of electronic and thermal Enthalpies=    | -972.707878                 |
| Sum of electronic and thermal Free Energies= | -972.777377                 |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.37836599 | 0.28618291  | 0.30386829  | 1         | 0.91866606  | 1.47648287  | 2.74036837  |
| 6 | 1.20936608 | -0.35901707 | 0.60876828  | 1         | -0.59123397 | 1.93438280  | 1.97326815  |
| 7 | 1.11616611 | -1.68401706 | 0.22886831  | 8         | -4.96983385 | -0.23591709 | 0.61296833  |
| 6 | 1.93256593 | -2.19371700 | -0.86193168 | 6         | -3.83873391 | -0.11441709 | 0.24376830  |
| 6 | 3.37116599 | -1.80961716 | -0.56303173 | 8         | -3.49593401 | 0.86148286  | -0.61423171 |
| 6 | 3.45946598 | -0.29571709 | -0.48963171 | 6         | -2.69053411 | -1.01501703 | 0.66736829  |
| 6 | 1.17836595 | 2.37318301  | 0.80236828  | 6         | -2.09073400 | 1.07368290  | -0.85533172 |
| 6 | 0.39386606 | 1.49998283  | 1.77456820  | 8         | -1.87623405 | -1.30451715 | -0.48903170 |
| 7 | 0.21106607 | 0.15318289  | 1.25876820  | 6         | -1.41893387 | -0.25191709 | -1.18663180 |
| 6 | 2.52636600 | 1.71808290  | 0.55646831  | 6         | -1.96323395 | 2.07848310  | -1.97443175 |
| 1 | 0.15496606 | -1.99641716 | 0.25046828  | 1         | -1.63113403 | 1.44538283  | 0.06576829  |
| 1 | 1.81436586 | -3.27711701 | -0.89533168 | 1         | -2.04963398 | -0.47541708 | 1.37576818  |
| 1 | 1.61596608 | -1.78211713 | -1.82883179 | 6         | -3.16253400 | -2.32671690 | 1.24316823  |
| 1 | 3.66606593 | -2.25371695 | 0.39076829  | 8         | -0.57673395 | -0.38931710 | -2.02663159 |
| 1 | 4.04686642 | -2.17411709 | -1.33793175 | 1         | -2.30203390 | -2.92471695 | 1.54316819  |
| 1 | 3.42186594 | 0.12798291  | -1.50223172 | 1         | -3.74983406 | -2.87641692 | 0.50716829  |

|   |            |            |             |   |             |             |             |
|---|------------|------------|-------------|---|-------------|-------------|-------------|
| 1 | 4.40856600 | 0.01548291 | -0.04183171 | 1 | -3.78443408 | -2.13441706 | 2.11646843  |
| 1 | 3.01586604 | 2.16188312 | -0.31593171 | 1 | -0.91003394 | 2.26668310  | -2.17903161 |
| 1 | 3.18946600 | 1.87018287 | 1.41656828  | 1 | -2.44703412 | 3.01068306  | -1.68523180 |
| 1 | 0.62876600 | 2.44438291 | -0.14213170 | 1 | -2.43133402 | 1.69288290  | -2.88053155 |
| 1 | 1.32196593 | 3.38368297 | 1.18916821  |   |             |             |             |

### I-1''\_MeGL-CH<sub>2</sub>

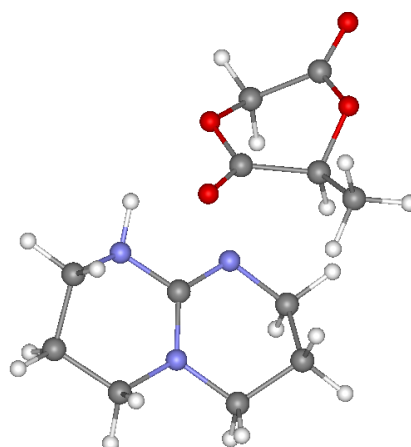


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 848326.1 (Joules/Mol)       |
|  | 202.75481 (Kcal/Mol)        |
| Zero-point correction=                       | 0.323110 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.341093                    |
| Thermal correction to Enthalpy=              | 0.342037                    |
| Thermal correction to Gibbs Free Energy=     | 0.276178                    |
| Sum of electronic and zero-point Energies=   | -933.444958                 |
| Sum of electronic and thermal Energies=      | -933.426976                 |
| Sum of electronic and thermal Enthalpies=    | -933.426031                 |
| Sum of electronic and thermal Free Energies= | -933.491891                 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 2.23350787  | 0.39805263  | 0.09884738  | 1         | 0.60700792  | 2.44575262  | -0.91805261 |
| 6 | 1.02670789  | -0.09464738 | 0.51824737  | 1         | 1.32380795  | 3.66295266  | 0.15164736  |
| 7 | 0.86690789  | -1.46644735 | 0.46404737  | 1         | 0.81500798  | 2.21875262  | 2.12174749  |
| 6 | 1.66730785  | -2.25714731 | -0.45845264 | 1         | -0.66359204 | 2.54905272  | 1.23974741  |
| 6 | 3.12100792  | -1.89434731 | -0.21365263 | 8         | -5.13019228 | 0.15785262  | 0.23934737  |
| 6 | 3.29860783  | -0.41164735 | -0.49125263 | 6         | -3.98409200 | 0.20595263  | -0.09695262 |
| 6 | 1.13590789  | 2.59485269  | 0.02894738  | 8         | -3.59549212 | 1.02255261  | -1.09205258 |
| 6 | 0.29760796  | 2.03015256  | 1.17024732  | 6         | -2.86569214 | -0.61734742 | 0.52074736  |
| 7 | 0.04700795  | 0.60845262  | 0.99554741  | 6         | -2.18959212 | 1.15725267  | -1.31465268 |
| 6 | 2.45290780  | 1.83915269  | -0.00715262 | 8         | -2.00839210 | -1.11044729 | -0.53345263 |
| 1 | -0.11109206 | -1.71474731 | 0.52214736  | 6         | -1.49359202 | -0.18714738 | -1.36245263 |

|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.48440790 | -3.31114745 | -0.24805263 | 1 | -1.73699212 | 1.75895262  | -0.52245259 |
| 1 | 1.39260793 | -2.05864739 | -1.50225258 | 1 | -2.24539208 | 0.03215263  | 1.15094733  |
| 1 | 3.37250781 | -2.11984730 | 0.82544738  | 6 | -3.37929201 | -1.80604732 | 1.29414737  |
| 1 | 3.78610802 | -2.46584725 | -0.86255264 | 8 | -0.58969206 | -0.44624737 | -2.10225248 |
| 1 | 3.31260800 | -0.23604737 | -1.57525265 | 1 | -2.54149222 | -2.34684730 | 1.73404741  |
| 1 | 4.25270796 | -0.05384737 | -0.09165262 | 1 | -3.94019222 | -2.47294736 | 0.63874739  |
| 1 | 2.97890782 | 2.02765274  | -0.94815266 | 1 | -4.03709221 | -1.46214736 | 2.09114742  |
| 1 | 3.10800791 | 2.17015266  | 0.80764735  | 1 | -2.06929207 | 1.65385270  | -2.27265263 |

### I-1''\_MeGL-CHMe



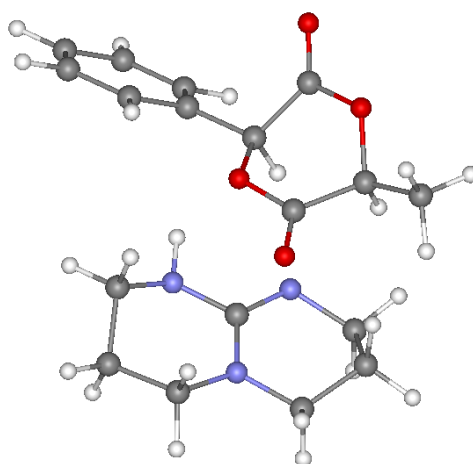
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 847332.9 (Joules/Mol)       |
|  | 202.51743 (Kcal/Mol)        |
| Zero-point correction=                       | 0.322732 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.340833                    |
| Thermal correction to Enthalpy=              | 0.341777                    |
| Thermal correction to Gibbs Free Energy=     | 0.275073                    |
| Sum of electronic and zero-point Energies=   | -933.445241                 |
| Sum of electronic and thermal Energies=      | -933.427140                 |
| Sum of electronic and thermal Enthalpies=    | -933.426196                 |
| Sum of electronic and thermal Free Energies= | -933.492900                 |

| cartesian |             |             |             |   |             |             |             |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7         | 2.12528944  | 0.37216052  | 0.25893161  | 1 | 0.19798946  | 2.16766047  | -0.73726845 |
| 6         | 1.01828945  | -0.24163947 | 0.78213155  | 1 | 0.82658947  | 3.50366068  | 0.23903161  |
| 7         | 1.03448939  | -1.62253940 | 0.81173158  | 1 | 0.59688950  | 2.11206055  | 2.29053164  |
| 6         | 1.87078953  | -2.36143947 | -0.12096839 | 1 | -0.95391059 | 2.20746064  | 1.47593153  |
| 6         | 3.27898955  | -1.80633938 | 0.00413161  | 8 | -5.11601067 | -0.38593948 | 1.25553155  |
| 6         | 3.24998951  | -0.33093947 | -0.35626841 | 6 | -4.03911066 | -0.41313946 | 0.73733163  |
| 6         | 0.76168942  | 2.41626048  | 0.16793162  | 8 | -3.82221055 | 0.18186054  | -0.44736841 |
| 6         | 0.06168944  | 1.81036067  | 1.37883162  | 6 | -2.82911062 | -1.10483944 | 1.32483160  |
| 7         | -0.01311055 | 0.36126056  | 1.28643155  | 6 | -2.44841051 | 0.34636053  | -0.85416842 |



|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 2.15658951 | 1.82226062  | 0.07823161  | 8 | -2.05121040 | -1.74053943 | 0.30503160  |
| 1 | 0.10668945 | -1.99183941 | 0.97033155  | 6 | -1.71441054 | -0.98423946 | -0.75386834 |
| 1 | 1.83808947 | -3.41533947 | 0.15623161  | 1 | -1.95941055 | 1.03156054  | -0.15546839 |
| 1 | 1.50758946 | -2.26583934 | -1.15226841 | 1 | -2.18671060 | -0.38683945 | 1.84693158  |
| 1 | 3.62208939 | -1.94043946 | 1.03253162  | 8 | -0.92021054 | -1.37833941 | -1.55766845 |
| 1 | 3.96968937 | -2.32633948 | -0.66136837 | 6 | -2.44631052 | 0.90016055  | -2.25766826 |
| 1 | 3.18178940 | -0.21663946 | -1.44636846 | 1 | -1.41981053 | 1.04806054  | -2.59046841 |
| 1 | 4.17188931 | 0.16396055  | -0.03496839 | 1 | -2.97231054 | 1.85396051  | -2.27386832 |
| 1 | 2.59978938 | 2.02626061  | -0.90146840 | 1 | -2.93731046 | 0.20356053  | -2.93776822 |
| 1 | 2.81318951 | 2.26966047  | 0.83423162  | 1 | -3.16051054 | -1.88533938 | 2.00243163  |

### I-1''\_MePhGL-CHMe

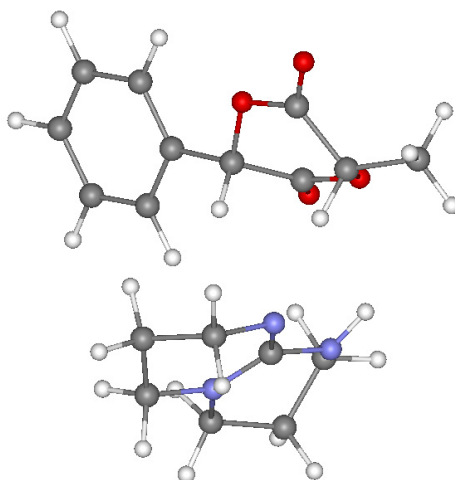


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1061231.7 (Joules/Mol)      |
|  | 253.64046 (Kcal/Mol)        |
| Zero-point correction=                       | 0.404202 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.426840                    |
| Thermal correction to Enthalpy=              | 0.427784                    |
| Thermal correction to Gibbs Free Energy=     | 0.350805                    |
| Sum of electronic and zero-point Energies=   | -1164.378440                |
| Sum of electronic and thermal Energies=      | -1164.355803                |
| Sum of electronic and thermal Enthalpies=    | -1164.354858                |
| Sum of electronic and thermal Free Energies= | -1164.431837                |

| cartesian |             |             |             |   |             |            |             |
|-----------|-------------|-------------|-------------|---|-------------|------------|-------------|
| 7         | -2.30753112 | -1.33347297 | -0.16352084 | 6 | 1.85716879  | 2.57202697 | -0.01332084 |
| 6         | -1.14653122 | -0.98257291 | -0.79722083 | 8 | 0.81256878  | 3.35012698 | 0.32107916  |
| 7         | -0.03533125 | -1.74557292 | -0.49952087 | 6 | 1.50406873  | 1.09152699 | -0.10832084 |
| 6         | 0.09396876  | -2.42207313 | 0.78037918  | 6 | -0.50153124 | 2.75922704 | 0.33377916  |
| 6         | -1.18593121 | -3.20907307 | 1.00447917  | 8 | 0.65426874  | 0.74962699 | 0.99747920  |
| 6         | -2.35793114 | -2.24297309 | 0.98067915  | 6 | -0.47623125 | 1.45922709 | 1.12957907  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -3.24993110 | 0.78322709  | -1.01572084 | 6 | -1.44813120 | 3.77892685  | 0.92217916  |
| 6 | -2.23813128 | 0.59692705  | -2.14112091 | 1 | -0.77913117 | 2.50282693  | -0.69592083 |
| 7 | -1.01493120 | -0.04577297 | -1.68502092 | 1 | 0.92116880  | 0.94062698  | -1.03042090 |
| 6 | -3.53253126 | -0.56197298 | -0.36802086 | 6 | 2.70206881  | 0.18462703  | -0.10692085 |
| 1 | 0.80776870  | -1.37837291 | -0.91612083 | 8 | -1.35803115 | 1.08202708  | 1.84537911  |
| 1 | 0.96236873  | -3.07997298 | 0.73037916  | 1 | -2.46163130 | 3.38092685  | 0.94137919  |
| 1 | 0.25046876  | -1.70807290 | 1.59967911  | 1 | -1.42933118 | 4.68312740  | 0.31517914  |
| 1 | -1.29303122 | -3.95307326 | 0.21147916  | 1 | -1.14783120 | 4.02152729  | 1.94197917  |
| 1 | -1.16443121 | -3.72657299 | 1.96487916  | 6 | 3.38176870  | -0.02237298 | -1.30612087 |
| 1 | -2.36903119 | -1.64477289 | 1.90137911  | 6 | 3.13716888  | -0.44477299 | 1.05647910  |
| 1 | -3.30373120 | -2.78987312 | 0.92847919  | 6 | 4.49556875  | -0.85297298 | -1.34202087 |
| 1 | -4.00243139 | -0.41677299 | 0.60937917  | 1 | 3.03536868  | 0.46362704  | -2.21222091 |
| 1 | -4.22503138 | -1.14837289 | -0.98322088 | 6 | 4.24836874  | -1.28157294 | 1.01507914  |
| 1 | -2.84103131 | 1.45892704  | -0.26232085 | 1 | 2.60456872  | -0.28707296 | 1.98597908  |
| 1 | -4.18123102 | 1.21692705  | -1.38492084 | 1 | 5.01866865  | -1.01107299 | -2.27722096 |
| 1 | -2.69973111 | 0.00552703  | -2.94442081 | 6 | 4.92916870  | -1.48547292 | -0.18072084 |
| 1 | -1.97843122 | 1.56332707  | -2.58292079 | 1 | 5.79366875  | -2.13787317 | -0.20832086 |
| 8 | 2.93636870  | 3.04132700  | -0.21182084 | 1 | 4.58216858  | -1.77367294 | 1.92067909  |

### I-1''\_MePhGL-CHPh



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1059782.8 (Joules/Mol)      |
|  | 253.29417 (Kcal/Mol)        |
| Zero-point correction=                       | 0.403650 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.426386                    |
| Thermal correction to Enthalpy=              | 0.427331                    |
| Thermal correction to Gibbs Free Energy=     | 0.350399                    |
| Sum of electronic and zero-point Energies=   | -1164.377955                |
| Sum of electronic and thermal Energies=      | -1164.355218                |
| Sum of electronic and thermal Enthalpies=    | -1164.354274                |
| Sum of electronic and thermal Free Energies= | -1164.431205                |

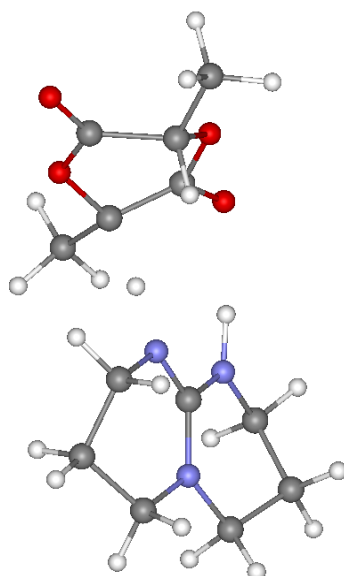
## cartesian

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -2.41627312 | -0.47474378 | -0.55328751 | 6 | 3.63222694  | -1.02174366 | -0.26618752 |
| 6 | -1.42677307 | -1.32004368 | -0.12368751 | 8 | 3.17762685  | 0.24595623  | -0.20468751 |
| 7 | -1.51787305 | -1.75344372 | 1.18301249  | 6 | 2.63022685  | -2.07744384 | 0.17991248  |
| 6 | -2.27267313 | -0.98354375 | 2.15871239  | 6 | 1.77862692  | 0.41335624  | 0.05591249  |
| 6 | -3.65777302 | -0.76384377 | 1.57521248  | 8 | 1.94382691  | -1.60434365 | 1.35751247  |
| 6 | -3.51727295 | 0.01355623  | 0.27671248  | 6 | 1.40512693  | -0.37814376 | 1.31171250  |
| 6 | -1.02227306 | -0.04194377 | -2.53558731 | 6 | 1.43702698  | 1.87285626  | 0.15651248  |
| 6 | -0.45807302 | -1.43204367 | -2.25948763 | 1 | 1.20982695  | -0.04274376 | -0.76048750 |
| 7 | -0.43937302 | -1.75744367 | -0.84038752 | 1 | 1.87112701  | -2.21044374 | -0.59978753 |
| 6 | -2.40337300 | 0.06185624  | -1.91188753 | 6 | 3.29372692  | -3.38754392 | 0.52541250  |
| 1 | -0.65167308 | -2.17024374 | 1.49521244  | 8 | 0.71022695  | 0.02045624  | 2.19881248  |
| 1 | -2.31837296 | -1.55924368 | 3.08291245  | 1 | 2.53742695  | -4.10284376 | 0.84621251  |
| 1 | -1.78947306 | -0.02244376 | 2.37821245  | 1 | 4.02372694  | -3.24604392 | 1.32271254  |
| 1 | -4.12077284 | -1.73544371 | 1.38871253  | 1 | 3.80482697  | -3.77684379 | -0.35408750 |
| 1 | -4.29287291 | -0.20364377 | 2.26281261  | 6 | 0.08812696  | 2.22935629  | 0.21571249  |
| 1 | -3.34437299 | 1.07625628  | 0.49541250  | 6 | 2.41742706  | 2.85735607  | 0.18521249  |
| 1 | -4.43777323 | -0.04924377 | -0.31218752 | 6 | 2.04872704  | 4.19815636  | 0.26881248  |
| 1 | -2.72197294 | 1.10825634  | -1.85848749 | 1 | 3.46162701  | 2.57705617  | 0.13651249  |
| 1 | -3.14177299 | -0.47424376 | -2.52068758 | 6 | -0.27477306 | 3.56655622  | 0.29981250  |
| 1 | -0.36567307 | 0.71995622  | -2.10478735 | 1 | -0.67467308 | 1.45545626  | 0.20051250  |
| 1 | -1.08957303 | 0.15185623  | -3.60758734 | 1 | 2.81552696  | 4.96325636  | 0.28941250  |
| 1 | -1.04867303 | -2.17644382 | -2.81108761 | 6 | 0.70702696  | 4.55485630  | 0.32511249  |
| 1 | 0.56422698  | -1.50654376 | -2.64528751 | 1 | 0.42442697  | 5.59885645  | 0.38831249  |
| 8 | 4.74412680  | -1.25104368 | -0.63668752 | 1 | -1.32267308 | 3.83845615  | 0.34531248  |

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## TS-1''\_LA



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 905085.8 (Joules/Mol)       |
|  | 216.32070 (Kcal/Mol)        |
| Zero-point correction=                       | 0.344729 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.364345                    |
| Thermal correction to Enthalpy=              | 0.365290                    |
| Thermal correction to Gibbs Free Energy=     | 0.295084                    |
| Sum of electronic and zero-point Energies=   | -972.706153                 |
| Sum of electronic and thermal Energies=      | -972.686536                 |
| Sum of electronic and thermal Enthalpies=    | -972.685592                 |
| Sum of electronic and thermal Free Energies= | -972.755798                 |

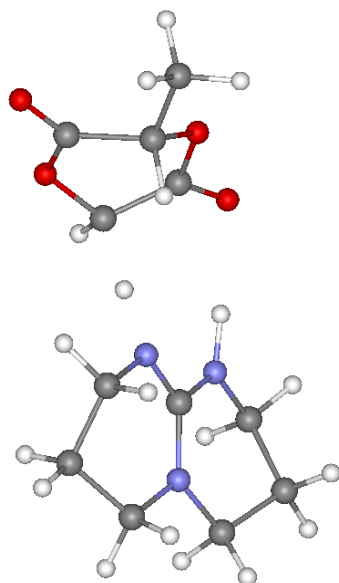
cartesian

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|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | 2.57033181 | 0.54944146  | 0.19483900  | 1 | 0.27443179  | 2.37034154  | 1.33263898  |
| 6 | 1.35613179 | -0.03905857 | 0.10513900  | 1 | -0.66946816 | 2.47864151  | -0.15426099 |
| 7 | 1.29753184 | -1.38455856 | -0.01646100 | 8 | -4.76156807 | 1.38584137  | -0.44396102 |
| 6 | 2.48083186 | -2.21685839 | -0.15896100 | 6 | -3.83106828 | 0.63284147  | -0.31976098 |
| 6 | 3.58253169 | -1.63985860 | 0.71463901  | 8 | -3.02536821 | 0.35214144  | -1.33296096 |
| 6 | 3.82413173 | -0.19855857 | 0.30223900  | 6 | -3.47166824 | -0.06575857 | 0.98253894  |
| 6 | 1.47593176 | 2.66264153  | -0.43326098 | 6 | -1.87896824 | -0.50685859 | -1.10446095 |
| 6 | 0.25683179 | 2.08724141  | 0.27323902  | 8 | -3.09996819 | -1.42545867 | 0.72203898  |
| 7 | 0.22603181 | 0.64024144  | 0.13313900  | 6 | -2.12626815 | -1.61035860 | -0.21386099 |
| 6 | 2.71733189 | 2.00544143  | 0.14483900  | 6 | -1.24966824 | -0.81535858 | -2.43786097 |
| 1 | 0.38163182 | -1.82345855 | -0.01686100 | 1 | -0.81236815 | 0.12784143  | -0.38076097 |
| 1 | 2.21693182 | -3.22755837 | 0.14893900  | 1 | -2.59626818 | 0.45364147  | 1.39643896  |
| 1 | 2.80833173 | -2.25475860 | -1.20436096 | 6 | -4.61236811 | -0.07375856 | 1.97123897  |
| 1 | 3.27173185 | -1.68435860 | 1.76103902  | 8 | -1.44706821 | -2.62425852 | -0.14656100 |
| 1 | 4.50613213 | -2.20855856 | 0.60343897  | 1 | -4.30546808 | -0.59105855 | 2.87973905  |
| 1 | 4.34513187 | -0.15795857 | -0.66156101 | 1 | -5.47566795 | -0.58215857 | 1.54053903  |
| 1 | 4.44913197 | 0.31364143  | 1.03863895  | 1 | -4.89596796 | 0.94894141  | 2.21603918  |
| 1 | 3.59413171 | 2.22444153  | -0.47026098 | 1 | -0.41926819 | -1.50685859 | -2.29386091 |
| 1 | 2.91733170 | 2.38024139  | 1.15513897  | 1 | -0.85646820 | 0.09904143  | -2.88866091 |
| 1 | 1.40613174 | 2.44984150  | -1.50336099 | 1 | -1.96256816 | -1.26845860 | -3.13376093 |
| 1 | 1.53883183 | 3.74344158  | -0.30066097 |   |             |             |             |

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TS-1''\_MeGL-CH<sub>2</sub>



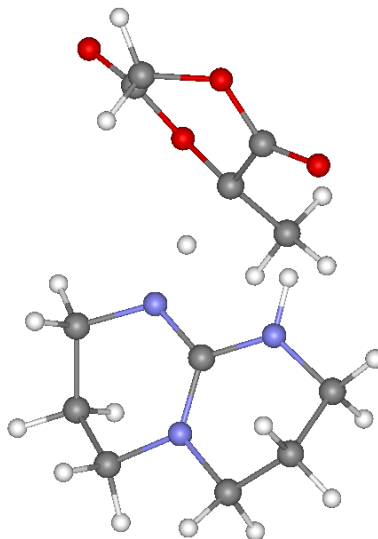
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 832143.6 (Joules/Mol)       |
|  | 198.88709 (Kcal/Mol)        |
| Zero-point correction=                       | 0.316947 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.334917                    |
| Thermal correction to Enthalpy=              | 0.335861                    |
| Thermal correction to Gibbs Free Energy=     | 0.268990                    |
| Sum of electronic and zero-point Energies=   | -933.424944                 |
| Sum of electronic and thermal Energies=      | -933.406974                 |
| Sum of electronic and thermal Enthalpies=    | -933.406030                 |
| Sum of electronic and thermal Free Energies= | -933.472902                 |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | -2.50679731 | 0.49080265  | -0.02253158 | 1 | -1.29429746 | 2.51510262  | 1.48616838  |
| 6 | -1.29869747 | -0.10539739 | 0.09996842  | 1 | -1.42249751 | 3.69890261  | 0.17516842  |
| 7 | -1.25539756 | -1.43449736 | 0.34446841  | 1 | -0.19459745 | 2.17170262  | -1.34273160 |
| 6 | -2.44779730 | -2.23719740 | 0.55996841  | 1 | 0.76470256  | 2.39220262  | 0.12116842  |
| 6 | -3.55009723 | -1.72029734 | -0.35013157 | 8 | 4.83970261  | 1.25170267  | 0.86716843  |
| 6 | -3.77049756 | -0.24749738 | -0.05483158 | 6 | 3.90660262  | 0.51650262  | 0.67536843  |
| 6 | -1.37379754 | 2.63310266  | 0.40236843  | 8 | 3.04140258  | 0.23050262  | 1.63666844  |
| 6 | -0.17079750 | 1.97860265  | -0.26353160 | 6 | 3.61280251  | -0.14759739 | -0.66303158 |
| 7 | -0.15789750 | 0.54810262  | -0.00213158 | 6 | 1.90530252  | -0.59999740 | 1.31346834  |
| 6 | -2.63239741 | 1.94720268  | -0.10033159 | 8 | 3.20270252  | -1.50919735 | -0.46273157 |
| 1 | -0.34799746 | -1.88979733 | 0.32666841  | 6 | 2.17470264  | -1.69139743 | 0.40836841  |
| 1 | -2.19879746 | -3.27309728 | 0.33376843  | 1 | 0.85100251  | 0.05670261  | 0.60856843  |
| 1 | -2.76799750 | -2.18629742 | 1.60686839  | 1 | 2.77200270  | 0.39580262  | -1.11523163 |
| 1 | -3.24869728 | -1.85419738 | -1.39173162 | 6 | 4.80950260  | -0.15109739 | -1.58283162 |

|   |             |             |             |   |            |             |             |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -4.47939777 | -2.26639748 | -0.18553159 | 8 | 1.47700250 | -2.68399739 | 0.28986841  |
| 1 | -4.27879763 | -0.12299739 | 0.90846837  | 1 | 4.54900217 | -0.64219737 | -2.51973152 |
| 1 | -4.39929771 | 0.21070261  | -0.82313156 | 1 | 5.63850260 | -0.68289739 | -1.11443162 |
| 1 | -3.49769735 | 2.23320270  | 0.50356841  | 1 | 5.12160254 | 0.87220263  | -1.78583157 |
| 1 | -2.84079742 | 2.23380256  | -1.13763165 | 1 | 1.46850252 | -0.93079740 | 2.24996829  |

### TS-1''\_MeGL-CHMe

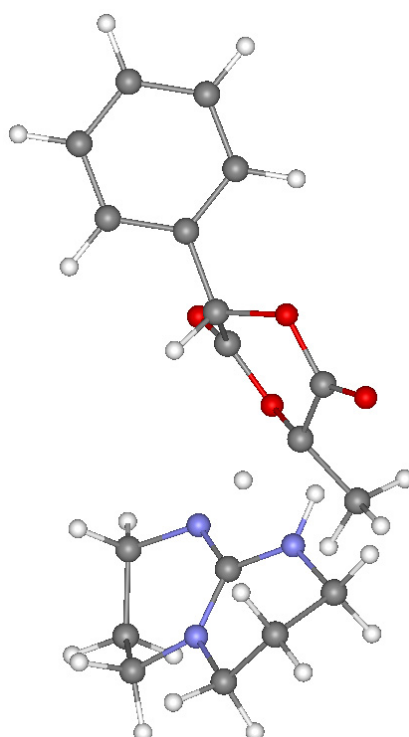


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 832249.4 (Joules/Mol)       |
|  | 198.91238 (Kcal/Mol)        |
| Zero-point correction=                       | 0.316987 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.335095                    |
| Thermal correction to Enthalpy=              | 0.336039                    |
| Thermal correction to Gibbs Free Energy=     | 0.269383                    |
| Sum of electronic and zero-point Energies=   | -933.423292                 |
| Sum of electronic and thermal Energies=      | -933.405184                 |
| Sum of electronic and thermal Enthalpies=    | -933.404240                 |
| Sum of electronic and thermal Free Energies= | -933.470897                 |

| cartesian |             |             |             |   |             |             |             |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7         | 2.19782901  | 0.54607630  | 0.19706053  | 1 | 0.83762908  | 2.44557643  | -1.36053944 |
| 6         | 0.98282909  | -0.04492372 | 0.24376053  | 1 | 1.10962915  | 3.73767638  | -0.18023947 |
| 7         | 0.91422915  | -1.39092374 | 0.13366053  | 1 | 0.04892910  | 2.35597634  | 1.58906054  |
| 6         | 2.07252908  | -2.21602368 | -0.16583946 | 1 | -1.06317091 | 2.46967626  | 0.22356054  |
| 6         | 3.27042913  | -1.64552379 | 0.57536054  | 8 | -5.10957050 | 1.44097626  | 0.10506053  |
| 6         | 3.45762897  | -0.19942372 | 0.15306053  | 6 | -4.21027088 | 0.64417624  | 0.16176054  |
| 6         | 1.03362906  | 2.65677643  | -0.30593947 | 8 | -3.46357083 | 0.35437629  | -0.89253944 |
| 6         | -0.09307092 | 2.07737637  | 0.53796053  | 6 | -3.82867098 | -0.09792371 | 1.42386055  |
| 7         | -0.13977090 | 0.63077629  | 0.39736053  | 6 | -2.31317091 | -0.51432371 | -0.71633947 |

|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 2.33652902 | 2.00207639  | 0.11956052  | 8 | -3.45137095 | -1.44492376 | 1.16376054  |
| 1 | 0.00382912 | -1.83062375 | 0.22936052  | 6 | -2.51877093 | -1.61962378 | 0.18396053  |
| 1 | 1.85152912 | -3.23222351 | 0.15726054  | 6 | -1.75157094 | -0.82542372 | -2.07903957 |
| 1 | 2.26952910 | -2.23752356 | -1.24403942 | 1 | -1.21127093 | 0.12167628  | -0.04893947 |
| 1 | 3.08852911 | -1.70392370 | 1.65086055  | 1 | -2.99897099 | 0.43397626  | 1.90486050  |
| 1 | 4.17492867 | -2.20972371 | 0.34606054  | 8 | -1.83397090 | -2.63072371 | 0.21916053  |
| 1 | 3.86252904 | -0.14812371 | -0.86443949 | 1 | -0.93357086 | -1.53862369 | -1.97873938 |
| 1 | 4.16292953 | 0.30887628  | 0.81616056  | 1 | -1.35717082 | 0.08317629  | -2.54063964 |
| 1 | 3.13062906 | 2.21547627  | -0.60103947 | 1 | -2.50727081 | -1.25422370 | -2.74443960 |
| 1 | 2.66072917 | 2.38237643  | 1.09476054  | 1 | -4.68177128 | -0.12232371 | 2.09546041  |

### TS-1''\_PhMeGL-CHMe

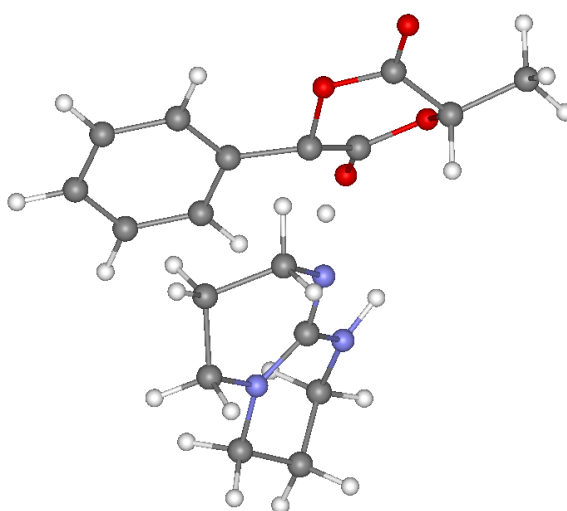


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1044501.3 (Joules/Mol)      |
|  | 249.64179 (Kcal/Mol)        |
| Zero-point correction=                       | 0.397830 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.420724                    |
| Thermal correction to Enthalpy=              | 0.421668                    |
| Thermal correction to Gibbs Free Energy=     | 0.341972                    |
| Sum of electronic and zero-point Energies=   | -1164.355598                |
| Sum of electronic and thermal Energies=      | -1164.332704                |
| Sum of electronic and thermal Enthalpies=    | -1164.331760                |
| Sum of electronic and thermal Free Energies= | -1164.411456                |

cartesian

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | 3.48398733  | 0.64321876  | 0.52562714  | 6 | -2.55921268 | 0.39611876  | -1.63047290 |
| 6 | 2.32018757  | 0.00751873  | 0.26142710  | 8 | -1.49791253 | 0.00881873  | -2.32207298 |
| 7 | 2.28028727  | -1.33928132 | 0.37722713  | 6 | -2.58991241 | -0.12788127 | -0.19297290 |
| 6 | 3.46008730  | -2.14218140 | 0.65302712  | 6 | -0.46161252 | -0.76468128 | -1.66657293 |
| 6 | 4.32918739  | -1.38808131 | 1.64612710  | 8 | -2.15421247 | -1.48568130 | -0.15167290 |
| 6 | 4.66988754  | -0.02948127 | 1.05962706  | 6 | -0.94931257 | -1.75168133 | -0.74017286 |
| 6 | 2.59098768  | 2.56861877  | -0.71947289 | 6 | 0.51998746  | -1.22038126 | -2.71447301 |
| 6 | 1.23378742  | 2.09011865  | -0.22367290 | 1 | 0.35308748  | 0.00851873  | -0.78397286 |
| 7 | 1.22088742  | 0.64091873  | -0.10027289 | 1 | -1.87631249 | 0.48531872  | 0.37572712  |
| 6 | 3.65408754  | 2.07001877  | 0.24352710  | 6 | -3.95901251 | -0.02518127 | 0.42312711  |
| 1 | 1.39348745  | -1.80498123 | 0.21452712  | 8 | -0.32081252 | -2.71878123 | -0.34267288 |
| 1 | 3.12668753  | -3.09588122 | 1.05982709  | 1 | 1.28958750  | -1.83418131 | -2.24557304 |
| 1 | 4.02148771  | -2.34258127 | -0.26687288 | 1 | 1.00648749  | -0.35578126 | -3.17207289 |
| 1 | 3.78128767  | -1.26768136 | 2.58352709  | 1 | 0.03788745  | -1.80718136 | -3.50237298 |
| 1 | 5.24958754  | -1.93508124 | 1.85202706  | 6 | -4.38291264 | 1.19641876  | 0.94122714  |
| 1 | 5.40858746  | -0.13498127 | 0.25662708  | 6 | -4.81511259 | -1.12218118 | 0.45052713  |
| 1 | 5.10108757  | 0.62391871  | 1.82292712  | 6 | -5.65651226 | 1.32181883  | 1.48302710  |
| 1 | 4.65328741  | 2.20121861  | -0.18047290 | 1 | -3.71521235 | 2.05111861  | 0.91952711  |
| 1 | 3.61558771  | 2.62841868  | 1.18572700  | 6 | -6.08861256 | -0.99608129 | 0.99732715  |
| 1 | 2.77298737  | 2.16121864  | -1.71757293 | 1 | -4.47931242 | -2.07218122 | 0.05442710  |
| 1 | 2.63218737  | 3.65691876  | -0.77887291 | 1 | -5.98001242 | 2.27461863  | 1.88482702  |
| 1 | 1.00498748  | 2.55971861  | 0.74052709  | 6 | -6.51221228 | 0.22421873  | 1.51262701  |
| 1 | 0.43868744  | 2.36821866  | -0.92017287 | 1 | -6.74951220 | -1.85448122 | 1.01942706  |
| 8 | -3.39871264 | 1.10881877  | -2.10997295 | 1 | -7.50391245 | 0.32071874  | 1.93832707  |

### TS-1''\_PhMeGL-CHPh



Zero-point vibrational energy

1047258.3 (Joules/Mol)

250.30075 (Kcal/Mol)

Zero-point correction=

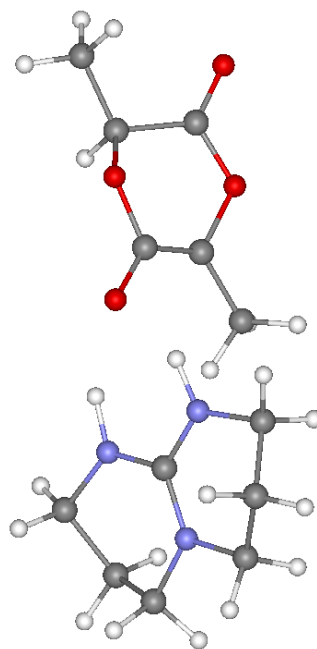
0.398880 (Hartree/Particle)



|  |              |
|--|--------------|
| Thermal correction to Energy=                | 0.421295     |
| Thermal correction to Enthalpy=              | 0.422239     |
| Thermal correction to Gibbs Free Energy=     | 0.346443     |
| Sum of electronic and zero-point Energies=   | -1164.363386 |
| Sum of electronic and thermal Energies=      | -1164.340970 |
| Sum of electronic and thermal Enthalpies=    | -1164.340026 |
| Sum of electronic and thermal Free Energies= | -1164.415822 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | -2.33112907 | -0.75858748 | -0.81312501 | 6         | 3.80107093  | 0.19741252  | -0.67072505 |
| 6 | -1.06712902 | -1.08458745 | -0.47142500 | 8         | 2.86317086  | 1.03871250  | -0.24262503 |
| 7 | -0.88222909 | -1.91248751 | 0.59027499  | 6         | 3.65057087  | -1.21708751 | -0.13942501 |
| 6 | -1.94922900 | -2.22658753 | 1.52527499  | 6         | 1.76267099  | 0.51821256  | 0.53147495  |
| 6 | -3.20372915 | -2.49988747 | 0.71217495  | 8         | 3.28657103  | -1.16108739 | 1.24697495  |
| 6 | -3.51822901 | -1.27408743 | -0.12732503 | 6         | 2.17607093  | -0.43578747 | 1.56287503  |
| 6 | -1.38382900 | 1.15071249  | -2.02902508 | 6         | 0.81757092  | 1.61261261  | 0.86337495  |
| 6 | -0.15542910 | 0.27091253  | -2.21982479 | 1         | 0.95147097  | -0.23218748 | -0.29442501 |
| 7 | 0.00777093  | -0.66048753 | -1.10762501 | 1         | 2.83087087  | -1.69168746 | -0.69472504 |
| 6 | -2.59302902 | 0.25291252  | -1.83952498 | 6         | 4.92307091  | -2.01988769 | -0.25872502 |
| 1 | 0.07447091  | -2.06418753 | 0.87137496  | 8         | 1.58277094  | -0.70738745 | 2.58067513  |
| 1 | -1.64932895 | -3.10118747 | 2.10047483  | 1         | 4.76547050  | -3.01918769 | 0.14567497  |
| 1 | -2.12252903 | -1.39928746 | 2.22547483  | 1         | 5.72657061  | -1.52938747 | 0.29167497  |
| 1 | -3.02992916 | -3.36558747 | 0.06907497  | 1         | 5.21217060  | -2.09488750 | -1.30602503 |
| 1 | -4.04962921 | -2.71828747 | 1.36437500  | 6         | -0.33572909 | 1.34621251  | 1.61677504  |
| 1 | -3.92832923 | -0.47648749 | 0.50367498  | 6         | 0.96767092  | 2.88761234  | 0.30577499  |
| 1 | -4.26442909 | -1.50888741 | -0.89092505 | 6         | -0.00562909 | 3.86391234  | 0.49577498  |
| 1 | -3.45752907 | 0.83341253  | -1.50752497 | 1         | 1.84657097  | 3.11061239  | -0.28432503 |
| 1 | -2.86442900 | -0.24578747 | -2.77672482 | 6         | -1.30232906 | 2.32701254  | 1.80387497  |
| 1 | -1.24792910 | 1.77641261  | -1.14162505 | 1         | -0.46552911 | 0.36861253  | 2.06137514  |
| 1 | -1.53892910 | 1.80071259  | -2.89122486 | 1         | 0.13297093  | 4.84421253  | 0.05387498  |
| 1 | -0.22862908 | -0.27908748 | -3.16472483 | 6         | -1.14852905 | 3.59091234  | 1.23987496  |
| 1 | 0.75187087  | 0.87991250  | -2.26562500 | 1         | -2.18332911 | 2.09801245  | 2.39317513  |
| 8 | 4.68157053  | 0.56291252  | -1.40002501 | 1         | -1.90632915 | 4.35211277  | 1.38187492  |

I-2''\_LA

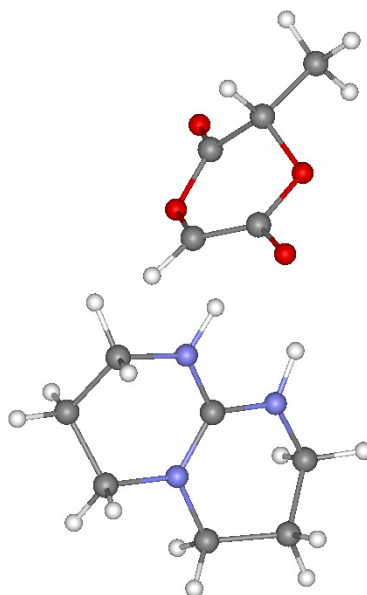


|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 918879.9 (Joules/Mol)       |
|  | 219.61757 (Kcal/Mol)        |
| Zero-point correction=                       | 0.349983 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.369932                    |
| Thermal correction to Enthalpy=              | 0.370877                    |
| Thermal correction to Gibbs Free Energy=     | 0.298710                    |
| Sum of electronic and zero-point Energies=   | -972.712586                 |
| Sum of electronic and thermal Energies=      | -972.692636                 |
| Sum of electronic and thermal Enthalpies=    | -972.691692                 |
| Sum of electronic and thermal Free Energies= | -972.763859                 |

|   |            |             |             | cartesian |             |             |             |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | 3.10414386 | -0.12292189 | -0.06429024 | 1         | 2.46254396  | 2.66077805  | 1.35900974  |
| 6 | 1.82104397 | -0.02642189 | 0.31130975  | 1         | 1.28194380  | 3.20517802  | 0.15940975  |
| 7 | 1.07154393 | -1.11332190 | 0.49960974  | 8         | -5.89485598 | -0.60702187 | -1.16549027 |
| 6 | 1.56484389 | -2.45822191 | 0.24980976  | 6         | -4.82365608 | -0.25532189 | -0.73939019 |
| 6 | 3.04824400 | -2.50022197 | 0.58030981  | 8         | -3.70575595 | -0.48682189 | -1.41899025 |
| 6 | 3.76794386 | -1.42162192 | -0.21209025 | 6         | -4.61305618 | 0.47847810  | 0.57660979  |
| 6 | 3.04274392 | 2.26287818  | -0.68409020 | 6         | -2.45185614 | -0.10212189 | -0.86369020 |
| 6 | 1.98994398 | 2.41427803  | 0.40220976  | 8         | -3.47645617 | -0.05342189 | 1.23850977  |
| 7 | 1.24984384 | 1.16737819  | 0.50560975  | 6         | -2.30825615 | 0.01147811  | 0.47810975  |
| 6 | 3.91634417 | 1.05987811  | -0.36729026 | 6         | -1.37405610 | -0.03672189 | -1.88649023 |
| 1 | 0.09774387 | -0.91692185 | 0.78650975  | 1         | 0.26084387  | 1.13547814  | 0.78040975  |
| 1 | 0.99974388 | -3.14402175 | 0.87940979  | 1         | -4.41355610 | 1.52957809  | 0.31840974  |
| 1 | 1.39764380 | -2.73912191 | -0.79559022 | 6         | -5.80785608 | 0.36297810  | 1.49430978  |

|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.18514395 | -2.32682180 | 1.65020978  | 8 | -1.23375607 | 0.16417810  | 1.15240979  |
| 1 | 3.46984386 | -3.47442198 | 0.33260974  | 1 | -5.60915613 | 0.90167814  | 2.42060971  |
| 1 | 3.80874395 | -1.68132186 | -1.27539027 | 1 | -6.00115585 | -0.68572187 | 1.72450984  |
| 1 | 4.79304409 | -1.30222189 | 0.14520974  | 1 | -6.69165611 | 0.78247815  | 1.01520979  |
| 1 | 4.54684401 | 0.80707812  | -1.22239017 | 1 | -0.47345611 | 0.38147810  | -1.43509018 |
| 1 | 4.57134390 | 1.26917815  | 0.48510975  | 1 | -1.66355610 | 0.60547811  | -2.72439027 |
| 1 | 2.54934406 | 2.12037802  | -1.64849019 | 1 | -1.12385607 | -1.02172184 | -2.29919028 |
| 1 | 3.66454411 | 3.15617824  | -0.74309021 |   |             |             |             |

### I-2''\_MeGL-CH<sub>2</sub>



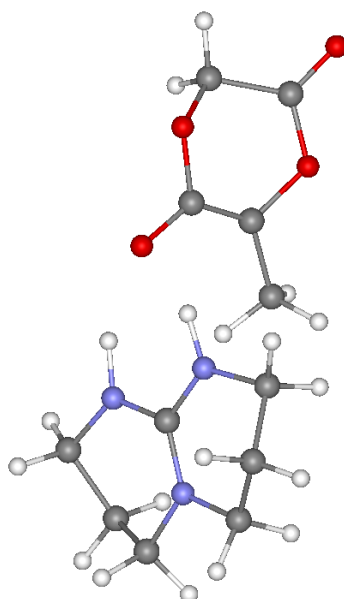
|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 846048.8 (Joules/Mol)       |
|  | 202.21051 (Kcal/Mol)        |
| Zero-point correction=                       | 0.322243 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.340494                    |
| Thermal correction to Enthalpy=              | 0.341438                    |
| Thermal correction to Gibbs Free Energy=     | 0.273146                    |
| Sum of electronic and zero-point Energies=   | -933.431564                 |
| Sum of electronic and thermal Energies=      | -933.413313                 |
| Sum of electronic and thermal Enthalpies=    | -933.412368                 |
| Sum of electronic and thermal Free Energies= | -933.480661                 |

#### cartesian

|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| 7 | -2.78135538 | -0.00783159 | 0.33173946  | 1 | -1.75775552 | 2.38726830 | 1.28423953  |
| 6 | -1.64535546 | -0.07893159 | -0.37366053 | 1 | -3.01575541 | 3.37336826 | 0.52153951  |
| 7 | -0.99685538 | -1.23703158 | -0.52406055 | 1 | -2.41755533 | 2.49646831 | -1.69876051 |
| 6 | -1.39855540 | -2.44583178 | 0.17703944  | 1 | -0.93045545 | 3.06166840 | -0.92586052 |
| 6 | -2.91635537 | -2.46953177 | 0.26023945  | 8 | 5.05064440  | 0.15916841 | 1.95833945  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -3.40345550 | -1.19443154 | 0.92823946  | 6 | 4.19604492  | 0.28176841  | 1.11723948  |
| 6 | -2.47395539 | 2.42966843  | 0.45973945  | 8 | 2.93784451  | 0.54546839  | 1.45253944  |
| 6 | -1.73165536 | 2.32606840  | -0.86286050 | 6 | 4.43534470  | 0.16626841  | -0.38206056 |
| 7 | -1.13095546 | 1.00436842  | -0.96286052 | 6 | 1.95674455  | 0.62386841  | 0.43203944  |
| 6 | -3.45305538 | 1.27276850  | 0.57253951  | 8 | 3.37604451  | -0.56653160 | -0.98416054 |
| 1 | -0.09205538 | -1.16223156 | -1.00826049 | 6 | 2.11994457  | -0.01403159 | -0.75486052 |
| 1 | -1.02165544 | -3.29993176 | -0.38366055 | 1 | 1.05944467  | 1.12126839  | 0.75653946  |
| 1 | -0.95825541 | -2.47323179 | 1.17963946  | 1 | -0.21505541 | 0.85276836  | -1.40356052 |
| 1 | -3.33115530 | -2.54373169 | -0.74766052 | 1 | 4.42364454  | 1.19256842  | -0.77826053 |
| 1 | -3.25505543 | -3.33103156 | 0.83563948  | 6 | 5.74074459  | -0.52393162 | -0.70086050 |
| 1 | -3.18135548 | -1.20683157 | 2.00043941  | 8 | 1.26984453  | -0.18103158 | -1.68676054 |
| 1 | -4.48395538 | -1.08733153 | 0.80943948  | 1 | 5.87644482  | -0.56863165 | -1.78126049 |
| 1 | -3.87995529 | 1.22686839  | 1.57643950  | 1 | 5.73304462  | -1.53803158 | -0.29866055 |
| 1 | -4.27565527 | 1.38746846  | -0.14116055 | 1 | 6.57144451  | 0.02096841  | -0.25436056 |

### I-2" \_MeGL-CHMe



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 846037.5 (Joules/Mol)       |
|  | 202.20782 (Kcal/Mol)        |
| Zero-point correction=                       | 0.322239 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.340540                    |
| Thermal correction to Enthalpy=              | 0.341484                    |
| Thermal correction to Gibbs Free Energy=     | 0.273710                    |
| Sum of electronic and zero-point Energies=   | -933.429919                 |
| Sum of electronic and thermal Energies=      | -933.411618                 |
| Sum of electronic and thermal Enthalpies=    | -933.410674                 |
| Sum of electronic and thermal Free Energies= | -933.478448                 |

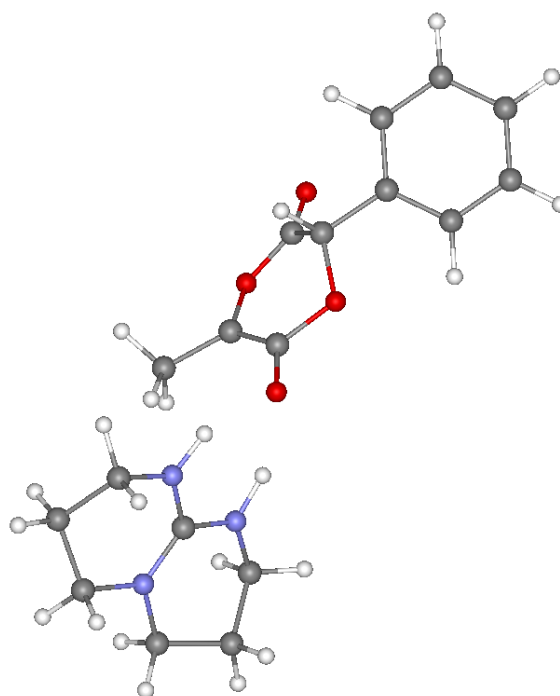
cartesian

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 7 | 2.52516580  | -0.26954216 | -0.08583684 | 1 | 2.05736566  | 2.03335786  | -1.58143687 |
| 6 | 1.32726574  | -0.01764215 | 0.45806319  | 1 | 3.39856577  | 2.92195773  | -0.84063685 |
| 7 | 0.46926576  | -1.00144219 | 0.72806317  | 1 | 2.42606568  | 2.58745790  | 1.40226316  |
| 6 | 0.72676581  | -2.38284230 | 0.35706317  | 1 | 1.16606569  | 3.25085783  | 0.35436317  |
| 6 | 2.21806574  | -2.64774227 | 0.49426317  | 8 | -6.19963408 | -0.60014212 | -0.86033684 |
| 6 | 2.98586583  | -1.63794219 | -0.34313682 | 6 | -5.15613413 | -0.19984215 | -0.41133684 |
| 6 | 2.68546581  | 2.11155772  | -0.69033682 | 8 | -4.01623392 | -0.33924216 | -1.08023691 |
| 6 | 1.80846572  | 2.38735771  | 0.52076316  | 6 | -5.00803423 | 0.50335789  | 0.92126316  |
| 7 | 0.95326585  | 1.23325777  | 0.75156319  | 6 | -2.80623436 | 0.15795784  | -0.51303685 |
| 6 | 3.43796587  | 0.80885786  | -0.47563684 | 8 | -3.83553433 | 0.09485784  | 1.59056306  |
| 1 | -0.43483418 | -0.68214214 | 1.11546314  | 6 | -2.67843437 | 0.28155783  | 0.83046317  |
| 1 | 0.14826578  | -3.02204227 | 1.02226317  | 6 | -1.74493408 | 0.35695785  | -1.53683686 |
| 1 | 0.39576584  | -2.57234216 | -0.67013681 | 1 | -0.01303422 | 1.32735777  | 1.08056319  |
| 1 | 2.50476575  | -2.55394220 | 1.54426312  | 1 | -4.98743439 | 1.58525777  | 0.73056316  |
| 1 | 2.46316576  | -3.65554214 | 0.15936317  | 1 | -5.86283445 | 0.25805783  | 1.54646313  |
| 1 | 2.87346578  | -1.85244215 | -1.41123688 | 8 | -1.62613416 | 0.52975786  | 1.50986314  |
| 1 | 4.05106592  | -1.67074215 | -0.10373683 | 1 | -0.90123421 | 0.88275790  | -1.08803689 |
| 1 | 3.93246555  | 0.49485782  | -1.39723694 | 1 | -2.11563420 | 0.96075785  | -2.37123680 |
| 1 | 4.20606565  | 0.92515785  | 0.29636317  | 1 | -1.37433422 | -0.58774215 | -1.95343685 |

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### I-2''\_PhMeGL-CHMe



Zero-point vibrational energy

1058640.4 (Joules/Mol)

253.02114 (Kcal/Mol)

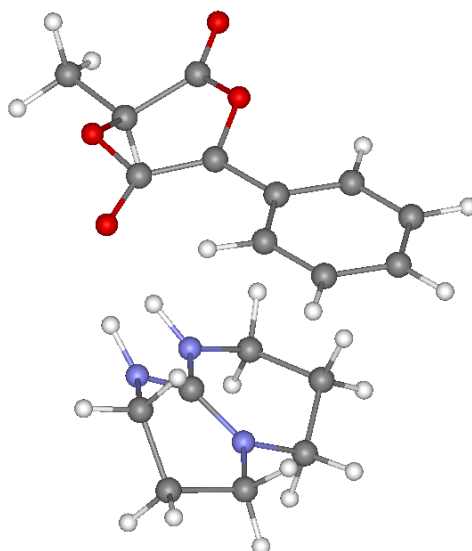
Zero-point correction=

0.403215 (Hartree/Particle)

|  |              |
|--|--------------|
| Thermal correction to Energy=                | 0.426268     |
| Thermal correction to Enthalpy=              | 0.427212     |
| Thermal correction to Gibbs Free Energy=     | 0.346617     |
| Sum of electronic and zero-point Energies=   | -1164.362979 |
| Sum of electronic and thermal Energies=      | -1164.339926 |
| Sum of electronic and thermal Enthalpies=    | -1164.338982 |
| Sum of electronic and thermal Free Energies= | -1164.419576 |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | -4.24110842 | -0.19636245 | -0.14457293 | 6         | 3.39699149  | 0.50163752  | 1.72052717  |
| 6 | -2.92050838 | -0.17846246 | -0.36987293 | 8         | 2.15959144  | 0.56463754  | 2.20012712  |
| 7 | -2.13070846 | -1.15746248 | 0.07362708  | 6         | 3.46219158  | 0.52043754  | 0.19042708  |
| 6 | -2.62730837 | -2.25466228 | 0.88802707  | 6         | 1.04839158  | 0.60993749  | 1.31232715  |
| 6 | -4.04580879 | -2.58116245 | 0.44812709  | 8         | 2.43569160  | -0.29006246 | -0.34047294 |
| 6 | -4.89480877 | -1.32346249 | 0.52802706  | 6         | 1.15169156  | 0.08773755  | 0.06802708  |
| 6 | -4.31640863 | 2.19593763  | -0.72677290 | 6         | -0.18520844 | 1.11833751  | 1.96942711  |
| 6 | -3.11960840 | 1.91913748  | -1.62227297 | 1         | -1.33190846 | 0.76553750  | -1.13687301 |
| 7 | -2.35200834 | 0.82603753  | -1.04637289 | 1         | 3.28329158  | 1.56783748  | -0.10047293 |
| 6 | -5.11090851 | 0.91363752  | -0.54487294 | 6         | 4.80099154  | 0.06763755  | -0.33087292 |
| 1 | -1.13030839 | -1.03616250 | -0.15317293 | 8         | 0.23339155  | -0.12316246 | -0.79137290 |
| 1 | -1.96240830 | -3.10506248 | 0.74472708  | 1         | -0.96470851 | 1.25103748  | 1.21792698  |
| 1 | -2.61000848 | -1.98286247 | 1.94892716  | 1         | -0.00660843 | 2.08613753  | 2.44852710  |
| 1 | -4.02910852 | -2.95346236 | -0.57877290 | 1         | -0.56480843 | 0.43483755  | 2.73842716  |
| 1 | -4.47820854 | -3.35106230 | 1.08722711  | 6         | 4.94489145  | -1.16216254 | -0.96577293 |
| 1 | -5.08830881 | -1.05036247 | 1.57092714  | 6         | 5.91329145  | 0.89213753  | -0.16667292 |
| 1 | -5.85800886 | -1.47756243 | 0.03682708  | 6         | 6.19409132  | -1.56376243 | -1.43227291 |
| 1 | -5.86050844 | 1.03523755  | 0.23992708  | 1         | 4.07699156  | -1.79496253 | -1.09677291 |
| 1 | -5.63190842 | 0.64283752  | -1.46927285 | 6         | 7.15899134  | 0.49013755  | -0.63147295 |
| 1 | -3.96550822 | 2.55503774  | 0.24382707  | 1         | 5.80129147  | 1.85003746  | 0.32972708  |
| 1 | -4.95690870 | 2.96043754  | -1.16647291 | 1         | 8.01749134  | 1.13813746  | -0.50037295 |
| 1 | -3.45030856 | 1.66313756  | -2.63427281 | 6         | 7.30219126  | -0.74146247 | -1.26667285 |
| 1 | -2.46640849 | 2.78793764  | -1.68777299 | 1         | 6.29889154  | -2.52236247 | -1.92687297 |
| 8 | 4.34699154  | 0.45623755  | 2.45682716  | 1         | 8.27299118  | -1.05576253 | -1.63107300 |

I-2''\_PhMeGL-CHPh



|  |                             |
|--|-----------------------------|
| Zero-point vibrational energy                | 1062102.9 (Joules/Mol)      |
|  | 253.84868 (Kcal/Mol)        |
| Zero-point correction=                       | 0.404534 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.427057                    |
| Thermal correction to Enthalpy=              | 0.428001                    |
| Thermal correction to Gibbs Free Energy=     | 0.352465                    |
| Sum of electronic and zero-point Energies=   | -1164.380648                |
| Sum of electronic and thermal Energies=      | -1164.358125                |
| Sum of electronic and thermal Enthalpies=    | -1164.357180                |
| Sum of electronic and thermal Free Energies= | -1164.432717                |

|   |             |             |             | cartesian |             |             |             |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 7 | -2.60605431 | -0.39645615 | -0.75822091 | 6         | 4.44114590  | 0.32864386  | -0.05372089 |
| 6 | -1.52875412 | -1.04825616 | -0.31872088 | 8         | 3.44734573  | 1.00914383  | 0.51077908  |
| 7 | -1.58285415 | -1.83175611 | 0.77117914  | 6         | 4.12714577  | -1.13425612 | -0.31582087 |
| 6 | -2.75035429 | -1.83215618 | 1.64247906  | 6         | 2.20864582  | 0.37424386  | 0.80187911  |
| 6 | -3.99205422 | -1.74065614 | 0.77207911  | 8         | 3.37924576  | -1.65685618 | 0.77307910  |
| 6 | -3.90775418 | -0.49255615 | -0.08962090 | 6         | 2.18254590  | -0.98865616 | 1.01147914  |
| 6 | -1.11305416 | 1.08774388  | -2.01922083 | 6         | 1.11324584  | 1.31414390  | 0.92927909  |
| 6 | -0.10605416 | -0.04855615 | -2.07002091 | 1         | 0.41734582  | -1.38145614 | -0.47062087 |
| 7 | -0.36675420 | -0.97645617 | -0.97272092 | 1         | 3.50474572  | -1.16575611 | -1.22312093 |
| 6 | -2.51635432 | 0.51854384  | -1.90082085 | 6         | 5.37644577  | -1.96535611 | -0.49162090 |
| 1 | -0.66905415 | -2.05745602 | 1.16467905  | 8         | 1.21274579  | -1.71185613 | 1.34577906  |
| 1 | -2.73845434 | -2.75565600 | 2.21907926  | 1         | 5.10274601  | -2.99925613 | -0.70072091 |
| 1 | -2.70995426 | -0.98895621 | 2.34207916  | 1         | 5.97644615  | -1.93075621 | 0.41877908  |
| 1 | -4.05305386 | -2.62835598 | 0.13817911  | 1         | 5.97084618  | -1.57415617 | -1.31622100 |
| 1 | -4.88925409 | -1.69675612 | 1.38917911  | 6         | -0.09265420 | 0.98184383  | 1.57947910  |

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|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| 1 | -4.05875397 | 0.41024384  | 0.51237911  | 6 | 1.23024583  | 2.61984396 | 0.41177911  |
| 1 | -4.67185402 | -0.51075613 | -0.86952084 | 6 | 0.18324584  | 3.52774405 | 0.50887913  |
| 1 | -3.23825431 | 1.31744385  | -1.72232091 | 1 | 2.15524578  | 2.91614389 | -0.06592089 |
| 1 | -2.81255436 | -0.01085614 | -2.81252074 | 6 | -1.13685417 | 1.89344382 | 1.66127908  |
| 1 | -0.90395415 | 1.71984386  | -1.15402091 | 1 | -0.18705419 | 0.00544386 | 2.03337908  |
| 1 | -1.03905416 | 1.69524384  | -2.92142081 | 1 | 0.30694583  | 4.52334356 | 0.09677911  |
| 1 | -0.16575417 | -0.57985616 | -3.02412081 | 6 | -1.01585412 | 3.17374396 | 1.12267911  |
| 1 | 0.90954578  | 0.32934386  | -1.94232094 | 1 | -2.04895425 | 1.60924387 | 2.17657924  |
| 8 | 5.48584604  | 0.86444384  | -0.31592089 | 1 | -1.83035409 | 3.88404393 | 1.19607902  |

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