

Electronic Supporting Information

## Ring size-reactivity relationship in radical ring-opening copolymerisation of thionolactones with vinyl pivalate

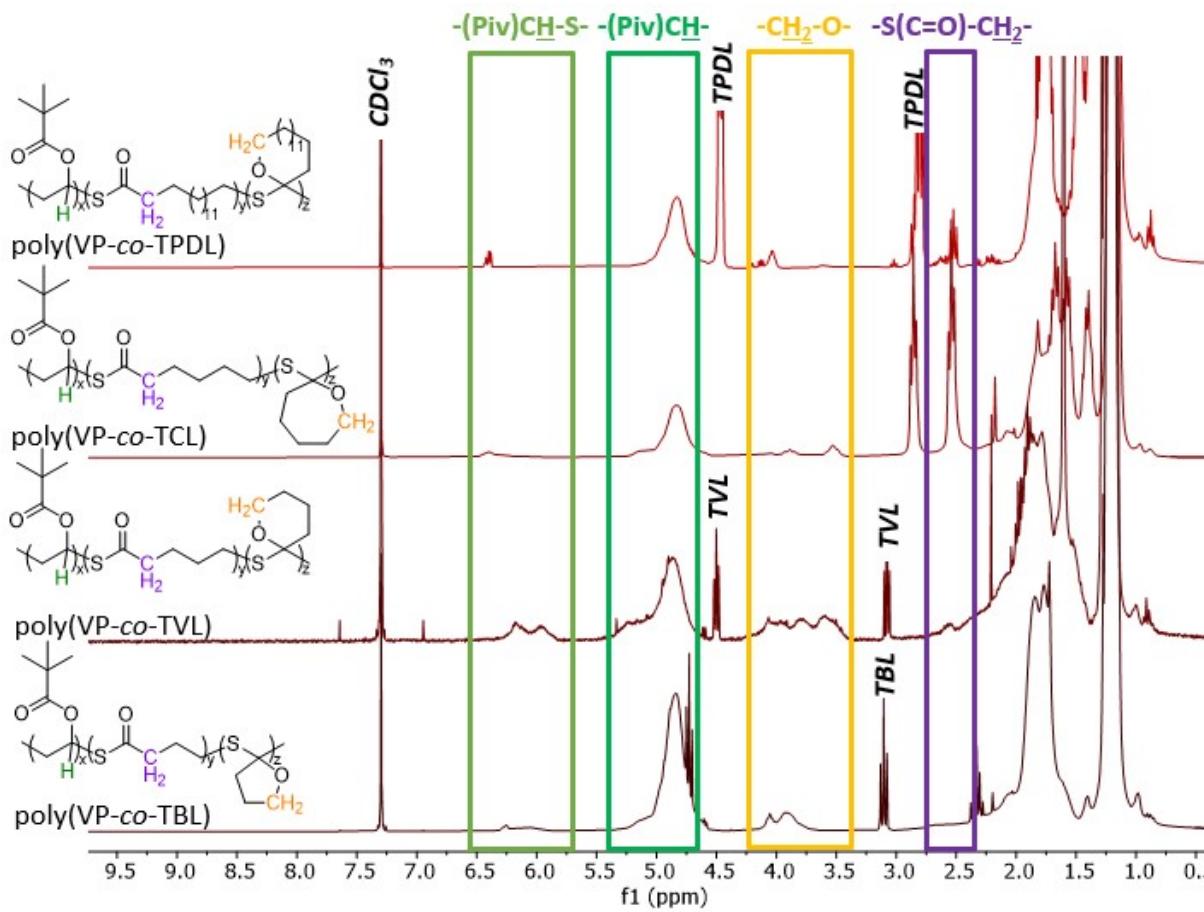
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**Figure S1.** Comparative  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) analysis of poly(VP-*co*-TBL), poly(VP-*co*-TVL), poly(VP-*co*-TCL) and poly(VP-*co*-TPDL) precipitated in MeCN. All copolymers have similar characteristic signals. Full NMR characteristics are shown below:

1) poly(TBL<sub>0.14</sub>-*co*-VP<sub>0.86</sub>) from Fig. 3:  $M_w = 5.7 \text{ kg mol}^{-1}$   $D = 2.2$ ;

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.3-5.8 (m,  $\text{CH}_2\text{-C(Piv)H-S}$ ), 5.3-4.5 (m,  $\text{CH}_2\text{-C(Piv)H-CH}_2$ ), 4.1 – 3.6 (m,  $\text{CH}_2\text{-CH}_2\text{-O}$ ), 2.8-2.5 (m,  $\text{S-(C=O)-CH}_2\text{-CH}_2$ ), 2.25 – 1.2 (m,  $-\text{CH}_2-$  +  $-\text{CH}_3$ ).

2) poly(TVL<sub>0.2</sub>-*co*-VP<sub>0.8</sub>) from Fig. 3:  $M_w = 4.6 \text{ kg mol}^{-1}$   $D = 2.2$ ;

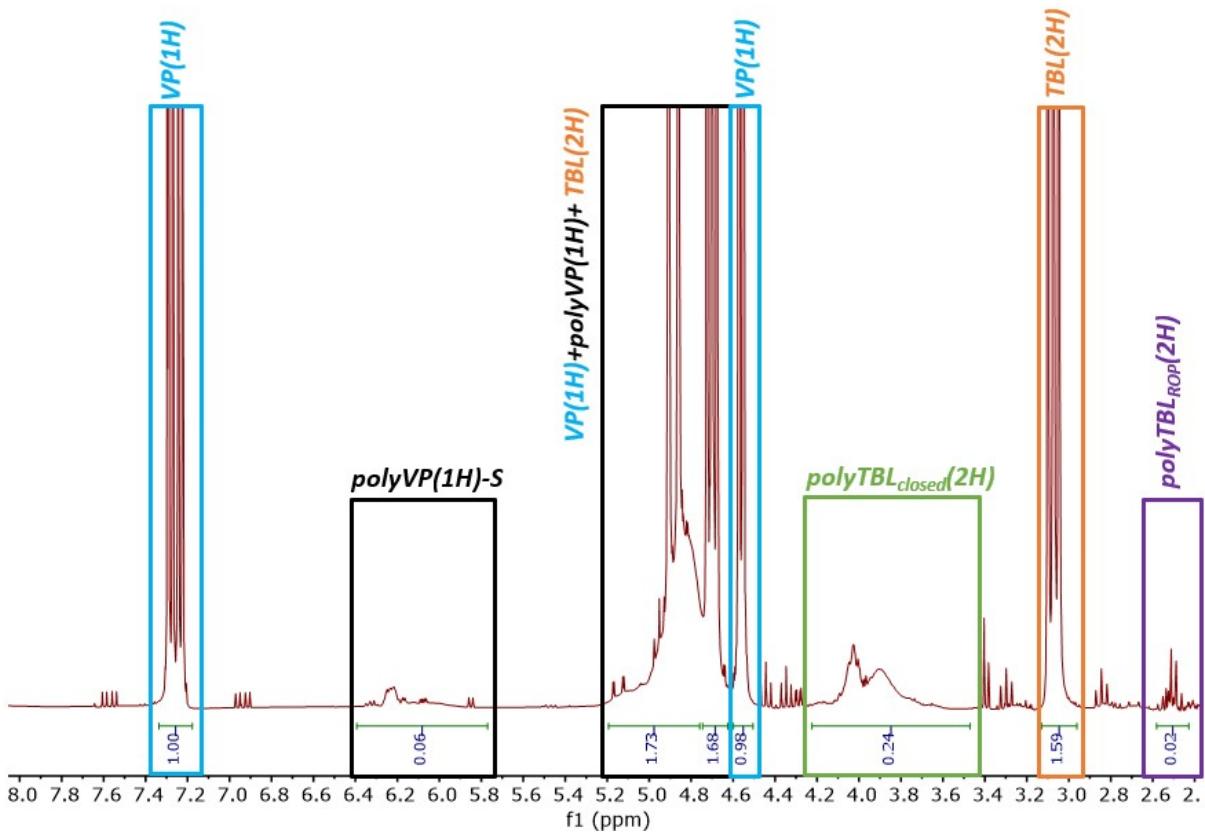
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.4-5.8 (m,  $\text{CH}_2\text{-C(Piv)H-S}$ ), 5.3-4.5 (m,  $\text{CH}_2\text{-C(Piv)H-CH}_2$ ), 4.18 – 3.35 (m,  $\text{CH}_2\text{-CH}_2\text{-O}$ ), 2.4-2.7 (t,  $-\text{S-(C=O)-CH}_2\text{-CH}_2$ ), 2.25 – 1.2 (m,  $-\text{CH}_2-$  +  $-\text{CH}_3$ ).

3) poly(TCL<sub>0.11</sub>-*co*-VP<sub>0.89</sub>) from Table 1 entry 6  $M_w = 96.7 \text{ kg mol}^{-1}$   $D = 7$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.6-5.8 (m,  $\text{CH}_2\text{-C(Piv)H-S}$ ) 5.3-4.5 (m,  $\text{CH}_2\text{-C(Piv)H-CH}_2$ ), 4.2 – 3.4 (m,  $\text{CH}_2\text{-CH}_2\text{-O}$ ), 2.87 (t,  $\text{CH}_2\text{-CH}_2\text{-S}$ ), 2.57 (t,  $\text{S-(C=O)-CH}_2\text{-CH}_2$ ), 2.25 – 1.2 (m,  $-\text{CH}_2-$  +  $-\text{CH}_3$ ).

4) poly(TPDL<sub>0.15</sub>-*co*-VP<sub>0.85</sub>) from Fig. 3:  $M_w = 5.2 \text{ kg mol}^{-1}$   $D = 2.0$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.45-5.8 (m,  $\text{CH}_2\text{-C(Piv)H-S}$ ) 5.3-4.5 (m,  $\text{CH}_2\text{-C(Piv)H-CH}_2$ ), 4.15 – 3.3 (m,  $\text{CH}_2\text{-CH}_2\text{-O}$ ), 2.55 (t,  $-\text{S-(C=O)-CH}_2\text{-CH}_2$ ), 2.25 – 1.2 (m,  $-\text{CH}_2-$  +  $-\text{CH}_3$ ).

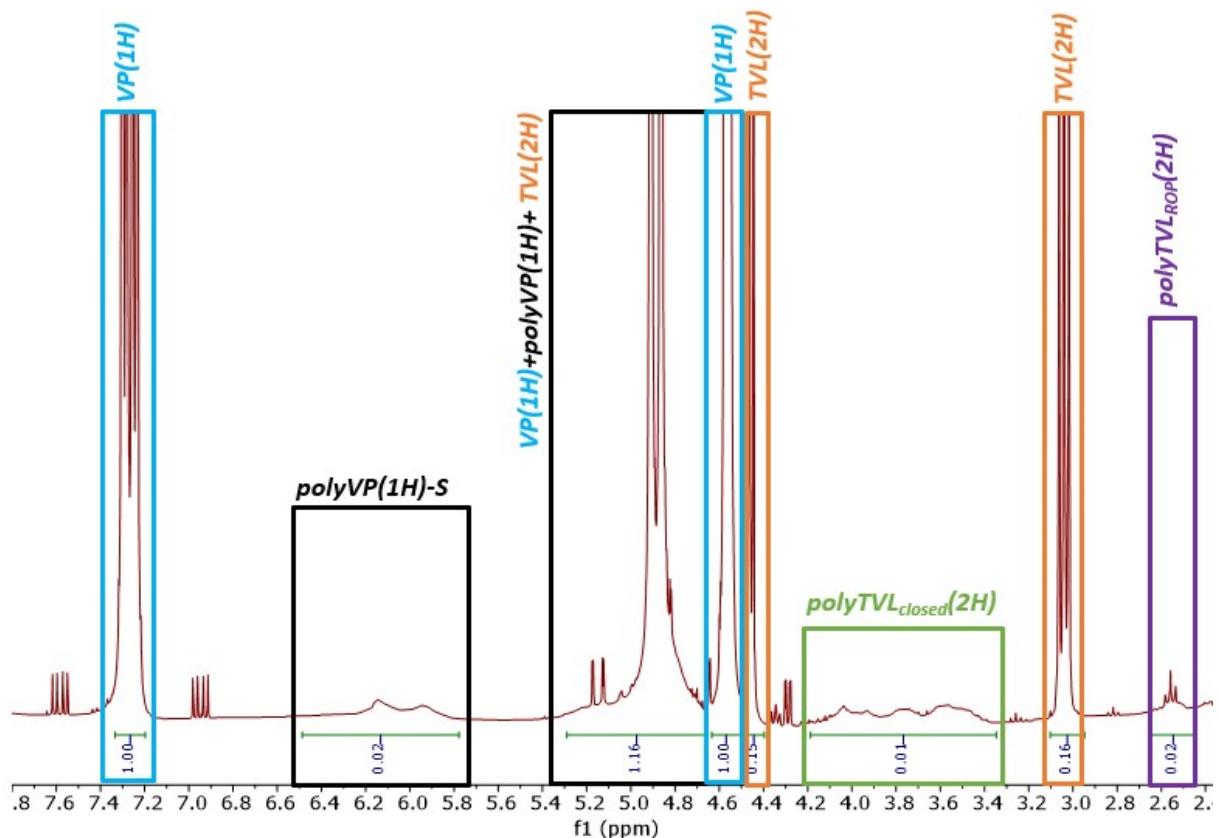


**Figure S2.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of VP/TBL (69/31) crude mixture after polymerization. VP and TBL conversions (X) and fraction of ring-opened TBL were determined from the following equations:

$$X_{\text{VP}} = \frac{\int_{5.8}^{6.4} \text{CH}^{\text{PVP close to } S} + \int_{4.6}^{5.30} (\text{CH}^{\text{PVP}} + \text{VP} + \text{CH}_{\text{2}}^{\text{TBL}}) - \int_{4.55}^{4.63} \text{CH}^{\text{VP}} - \int_{2.95}^{3.15} \text{CH}_{\text{2}}^{\text{TBL}}}{\int_{4.80}^{5.30} \text{CH}^{\text{PVP}} + \text{VP} + \int_{5.8}^{6.4} \text{CH}^{\text{PVP close to } S}} \times 100\%$$

$$X_{\text{TBL}} = \frac{\int_{3.45}^{4.20} \text{CH}_{\text{2}}^{\text{closed PTBL}} + \int_{2.5}^{2.60} \text{CH}_{\text{2}}^{\text{opened PTBL}}}{\int_{2.95}^{3.15} \text{CH}_{\text{2}}^{\text{TBL}} + \int_{3.45}^{4.15} \text{CH}_{\text{2}}^{\text{closed PTBL}} + \int_{2.5}^{2.6} \text{CH}_{\text{2}}^{\text{opened PTBL}}} \times 100\%$$

$$\text{ROP}_{\text{TBL}} = \frac{\int_{3.45}^{4.15} \text{CH}_{\text{2}}^{\text{closed PTBL}} + \int_{2.5}^{2.60} \text{CH}_{\text{2}}^{\text{opened PTBL}}}{\int_{3.45}^{4.15} \text{CH}_{\text{2}}^{\text{closed PTBL}} + \int_{2.5}^{2.6} \text{CH}_{\text{2}}^{\text{opened PTBL}}} \times 100\%$$

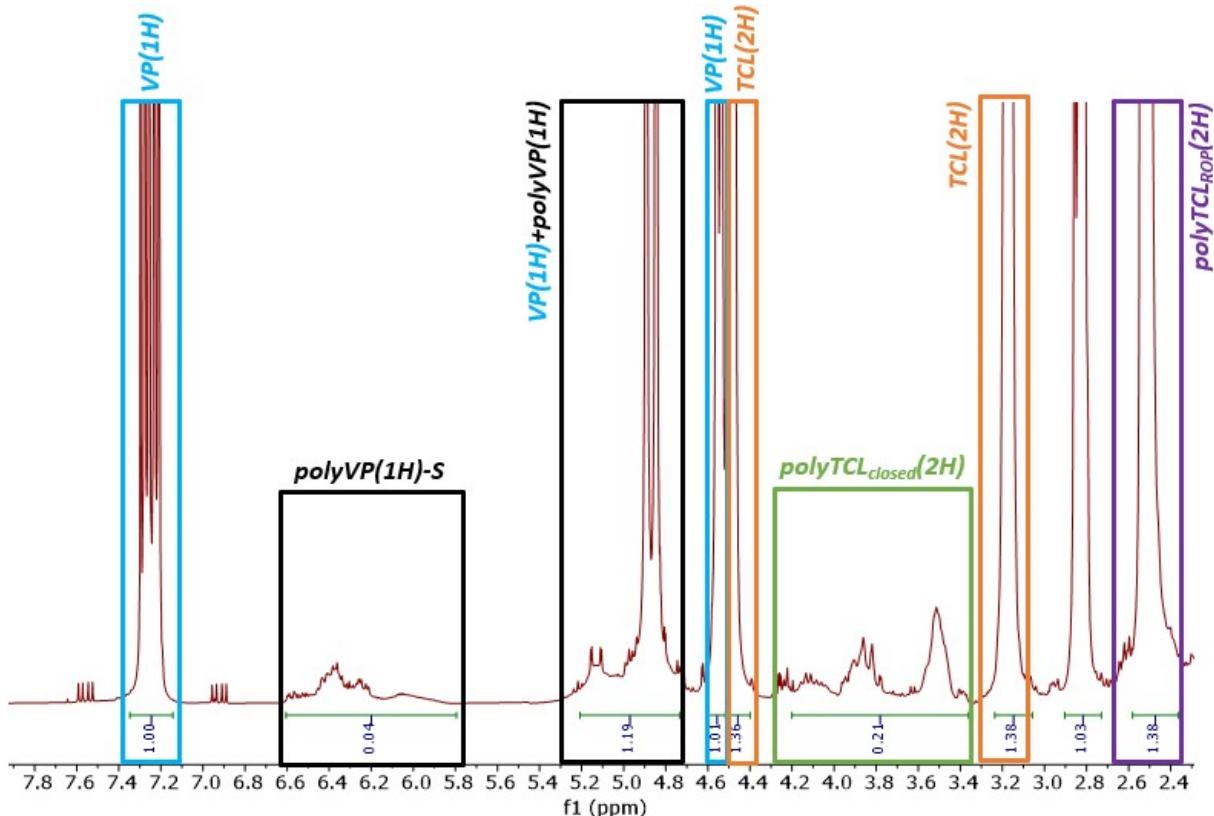


**Figure S3.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of VP/TVL (90/10) crude mixture after polymerization. VP and TVL conversions (X) and fraction of ring-opened TVL were determined from the following equations:

$$X_{\text{VP}} = \frac{\int_{5.8}^{6.4} \text{CH}^{\text{PVP close to } S} + \int_{4.6}^{5.3} \text{CH}^{\text{PVP} + \text{VP}} - \int_{7.4}^{7.2} \text{CH}^{\text{VP}}}{\int_{4.8}^{5.3} \text{CH}^{\text{PVP} + \text{VP}} + \int_{5.8}^{6.4} \text{CH}^{\text{PVP close to } S}} \times 100\%$$

$$X_{\text{TVL}} = \frac{\int_{3.3}^{4.2} \text{CH}_{\frac{1}{2}}^{\text{closed PTVL}} + \int_{2.5}^{2.7} \text{CH}_{\frac{1}{2}}^{\text{opened PTVL}}}{\int_{2.95}^{3.15} \text{CH}_{\frac{1}{2}}^{\text{TVL}} + \int_{3.3}^{4.15} \text{CH}_{\frac{1}{2}}^{\text{closed PTVL}} + \int_{2.5}^{2.6} \text{CH}_{\frac{1}{2}}^{\text{opened PTVL}}} \times 100\%$$

$$ROP_{TVL} = \frac{\int_{3.3}^{4.15} \frac{CH^{\text{opened PTVL}}}{2} + \int_{2.5}^{2.6} \frac{CH^{\text{opened PTVL}}}{2}}{\int_{3.3}^{4.15} \frac{CH^{\text{closed PTVL}}}{2} + \int_{2.5}^{2.6} \frac{CH^{\text{opened PTVL}}}{2}} \times 100\%$$

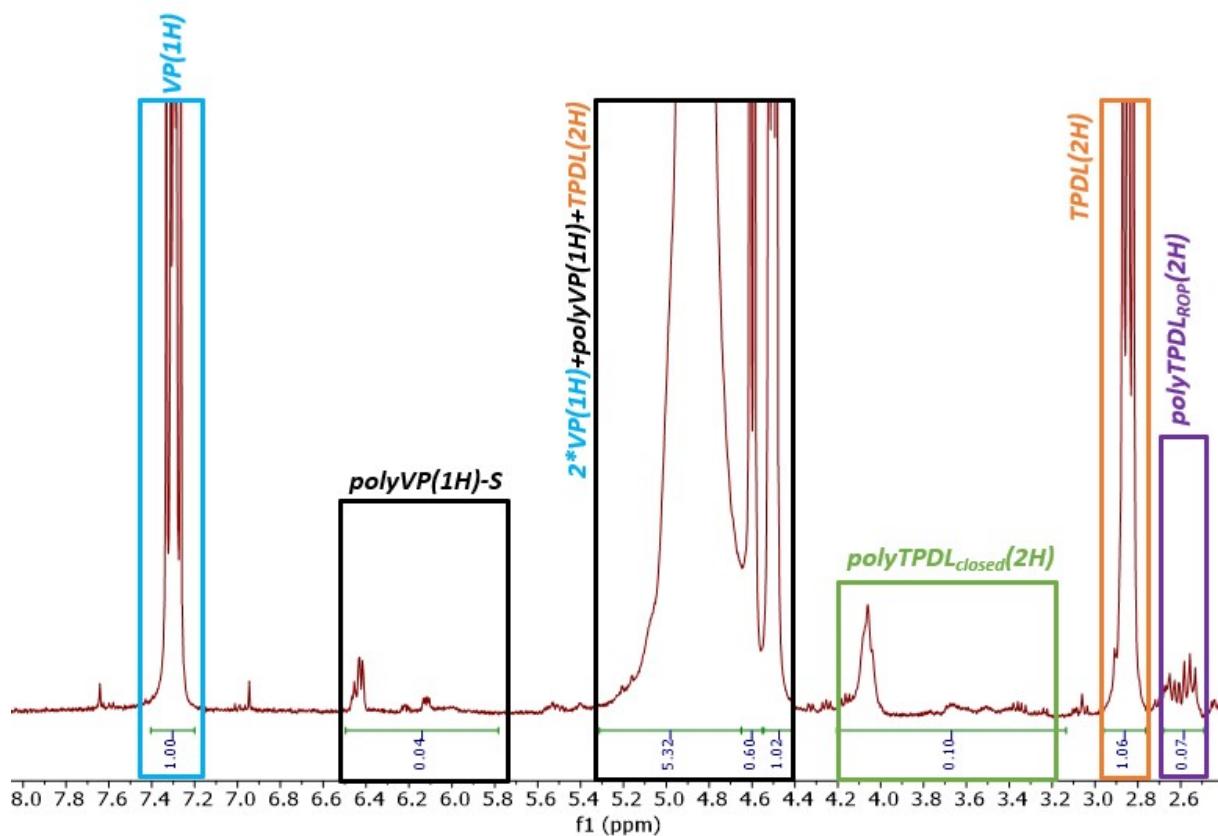


**Figure S4.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of VP/TCL (90/10) crude mixture after polymerization. VP and TCL conversions ( $X$ ) and fraction of ring-opened TCL were determined from the following equations:

$$X_{\text{VP}} = \frac{\int_{5.8}^{6.6} \frac{CH^{\text{PVP close to } S}}{2} + \int_{4.7}^{5.3} \frac{CH^{\text{PVP + VP}}}{2} - \int_{4.55}^{4.63} \frac{CH^{\text{VP}}}{2}}{\int_{4.7}^{5.3} \frac{CH^{\text{PVP + VP}}}{2} + \int_{5.8}^{6.6} \frac{CH^{\text{PVP close to } S}}{2}} \times 100\%$$

$$X_{TVL} = \frac{\int_{3.1}^{3.3} CH^{\text{PTCL}}_2 + \int_{3.4}^{4.2} CH^{\text{closed PTCL}}_2 + \int_{2.4}^{2.7} CH^{\text{opened PTCL}}_2}{\int_{3.1}^{3.3} CH^{\text{PTCL}}_2 + \int_{3.4}^{4.2} CH^{\text{closed PTCL}}_2 + \int_{2.4}^{2.7} CH^{\text{opened PTCL}}_2} \times 100\%$$

$$ROP_{TVL} = \frac{\int_{2.4}^{2.7} CH^{\text{opened PTCL}}_2}{\int_{3.4}^{4.2} CH^{\text{closed PTCL}}_2 + \int_{2.4}^{2.7} CH^{\text{opened PTCL}}_2} \times 100\%$$

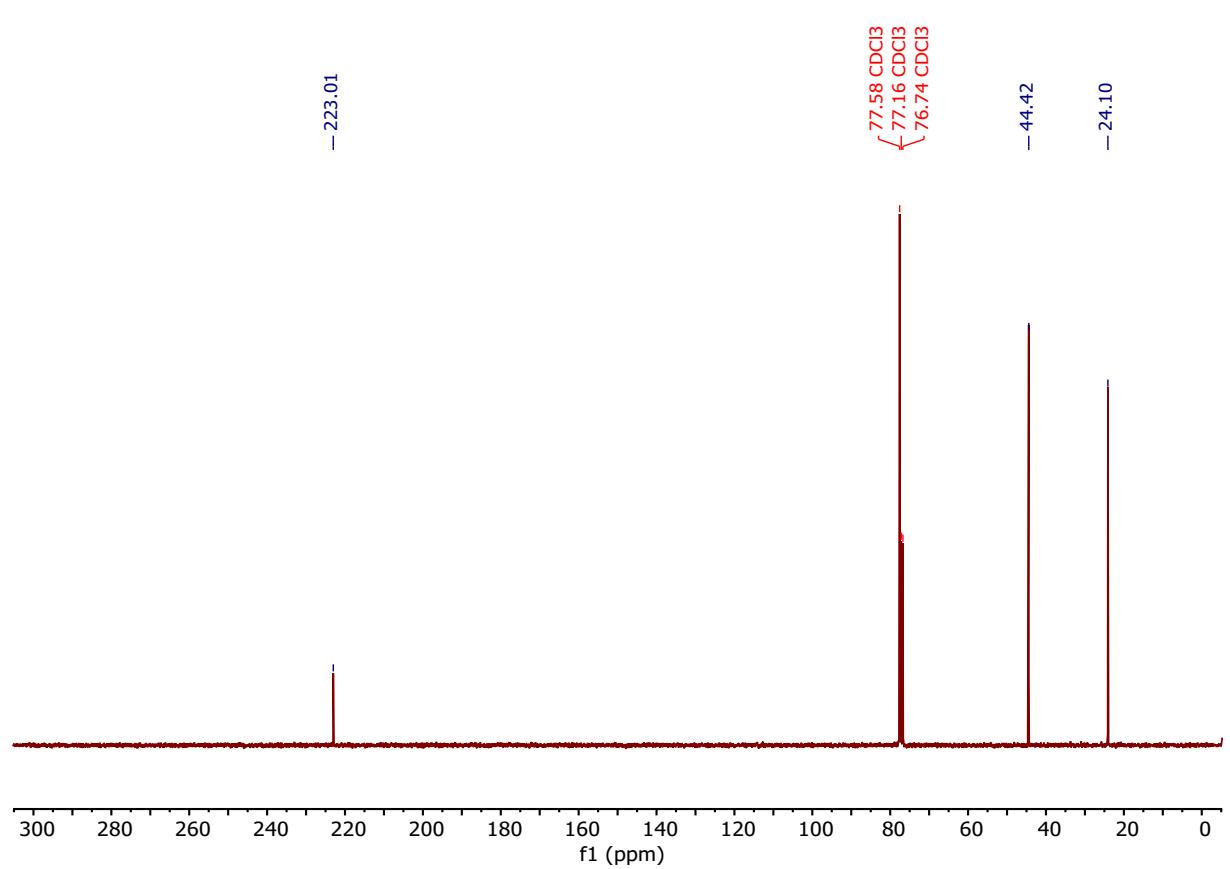
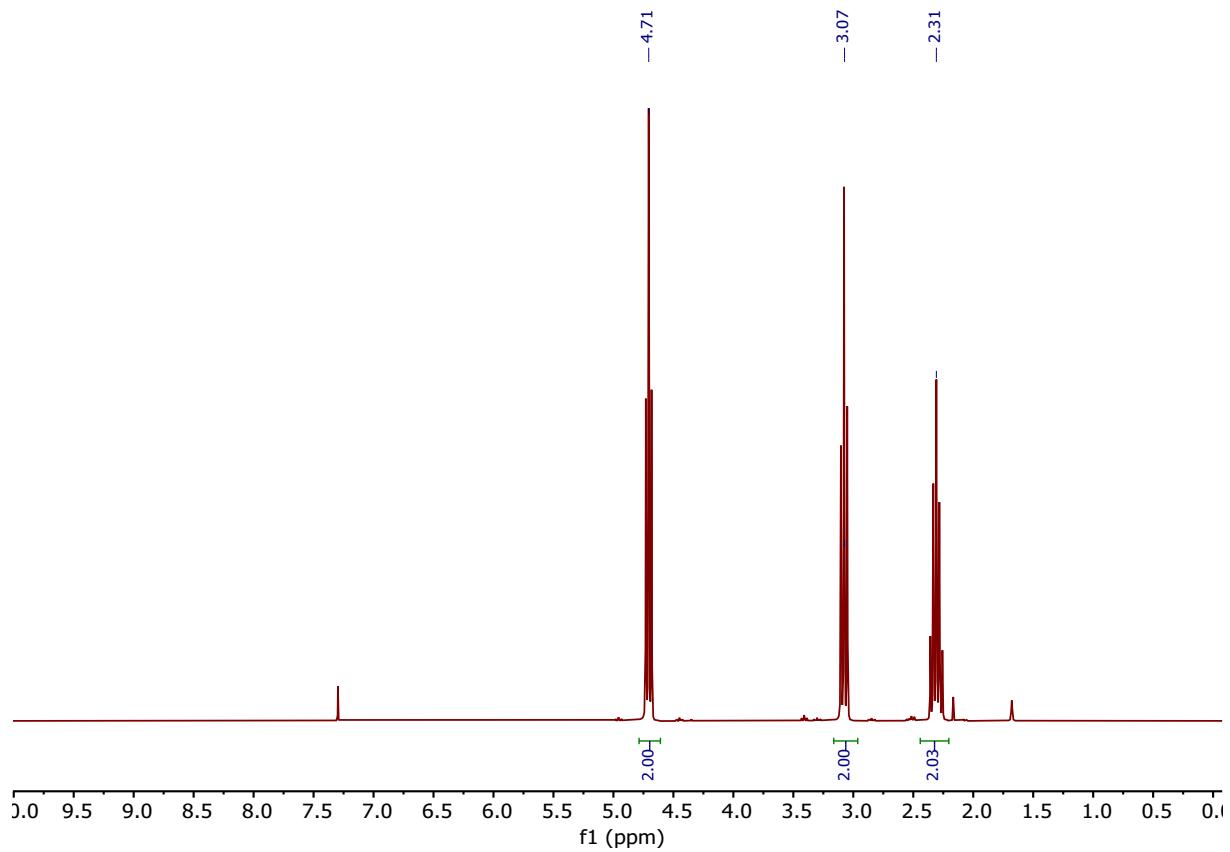


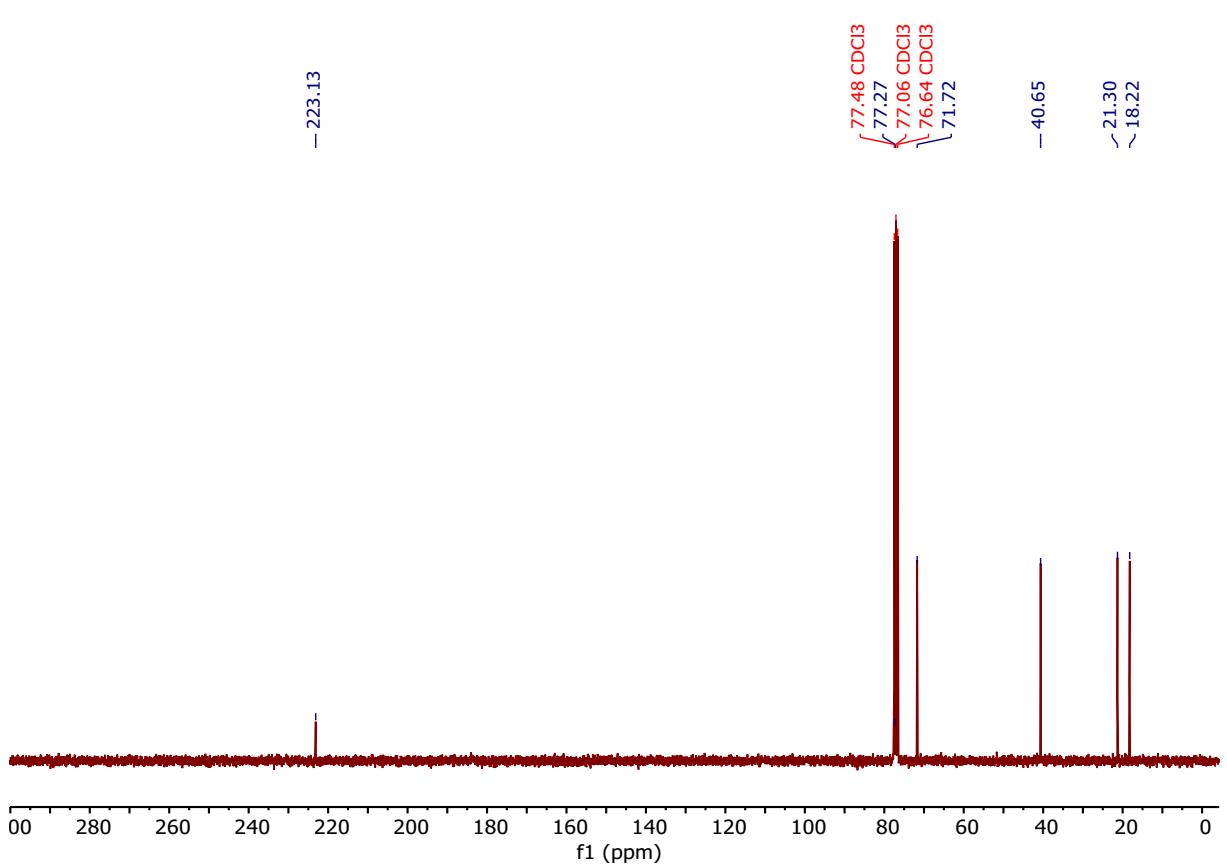
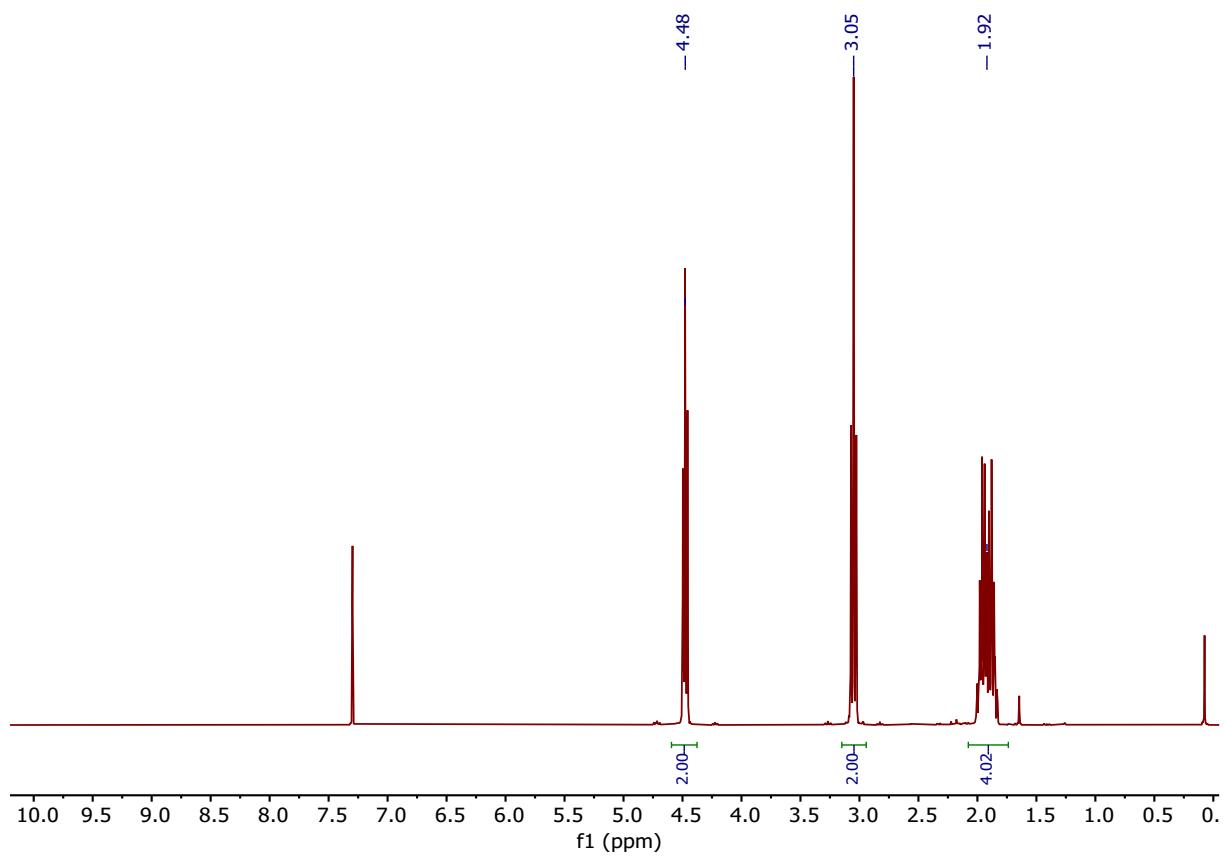
**Figure S5.**  ${}^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of VP/TPDL (90/10) crude mixture after polymerization. VP and TPDL conversions (X) and fraction of ring-opened TPDL were determined from the following equations:

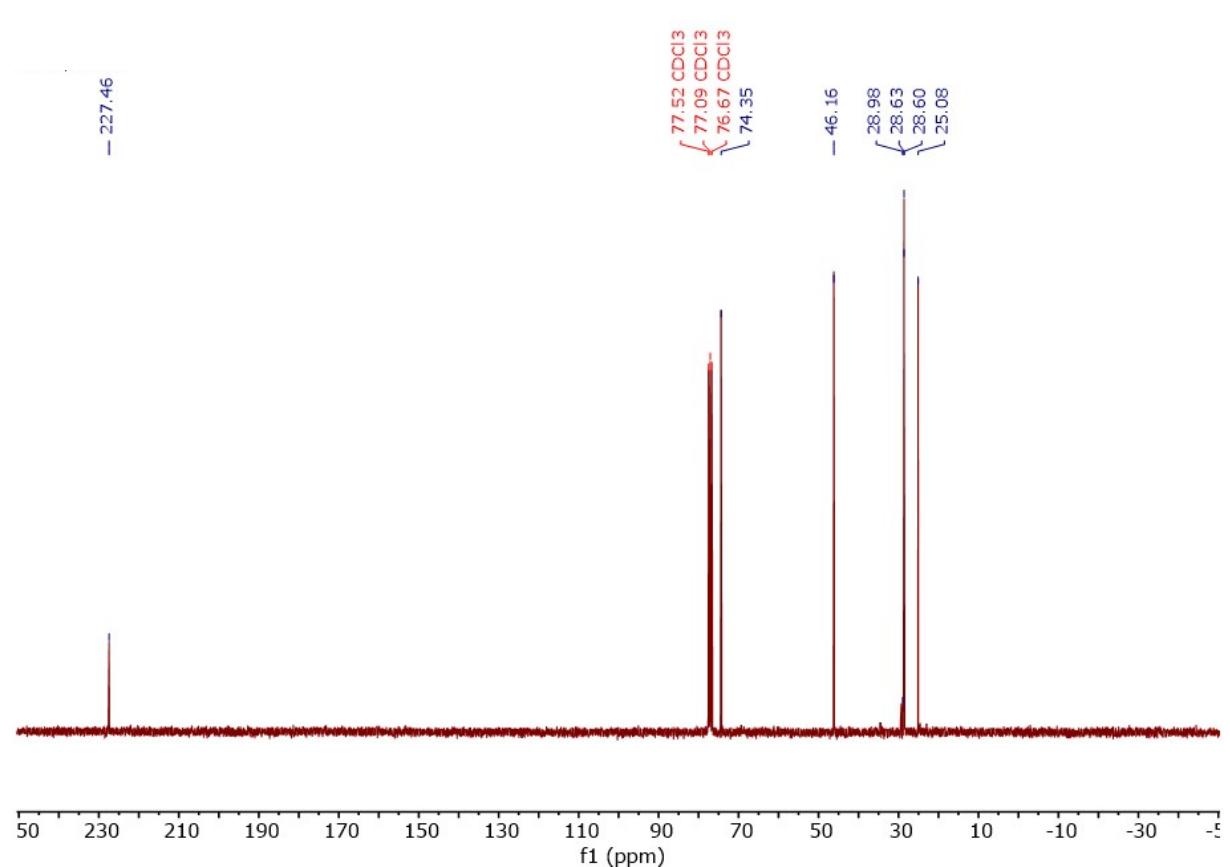
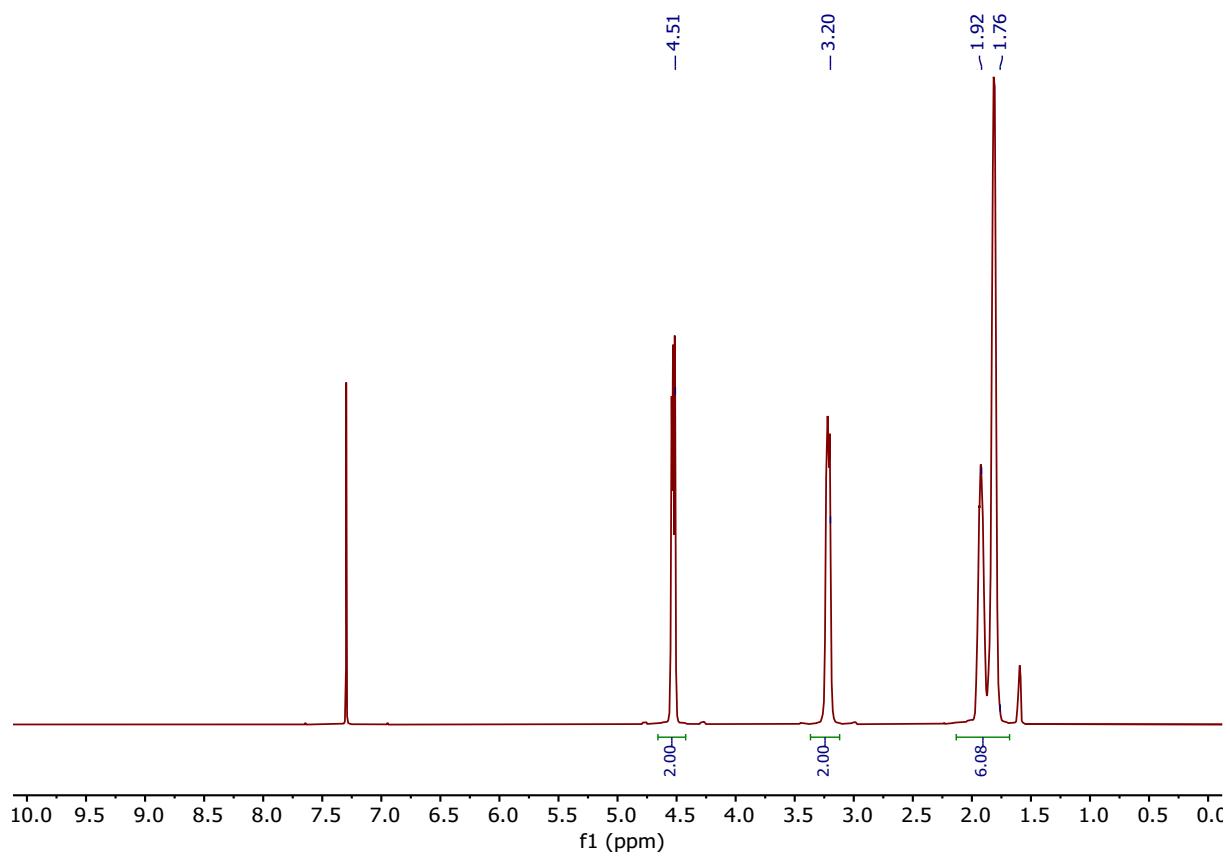
$$X_{VP} = \frac{\int_{5.8}^{6.5} CH^{PVP \text{ close to } S} + \int_{4.4}^{5.3} (CH^{PVP} + 2 * VP + CH^{\frac{TPDL}{2}}) - 2 \times \int_{7.2}^{7.4} CH^{VP} - \int_{2.75}^{3.00} CH^{\frac{TPDL}{2}}}{\int_{5.8}^{6.5} CH^{PVP \text{ close to } S} + \int_{4.4}^{5.3} (CH^{PVP} + 2 * VP + CH^{\frac{TPDL}{2}}) - \int_{7.2}^{7.4} CH^{VP} - \int_{2.75}^{3.00} CH^{\frac{TPDL}{2}}} \times 100\%$$

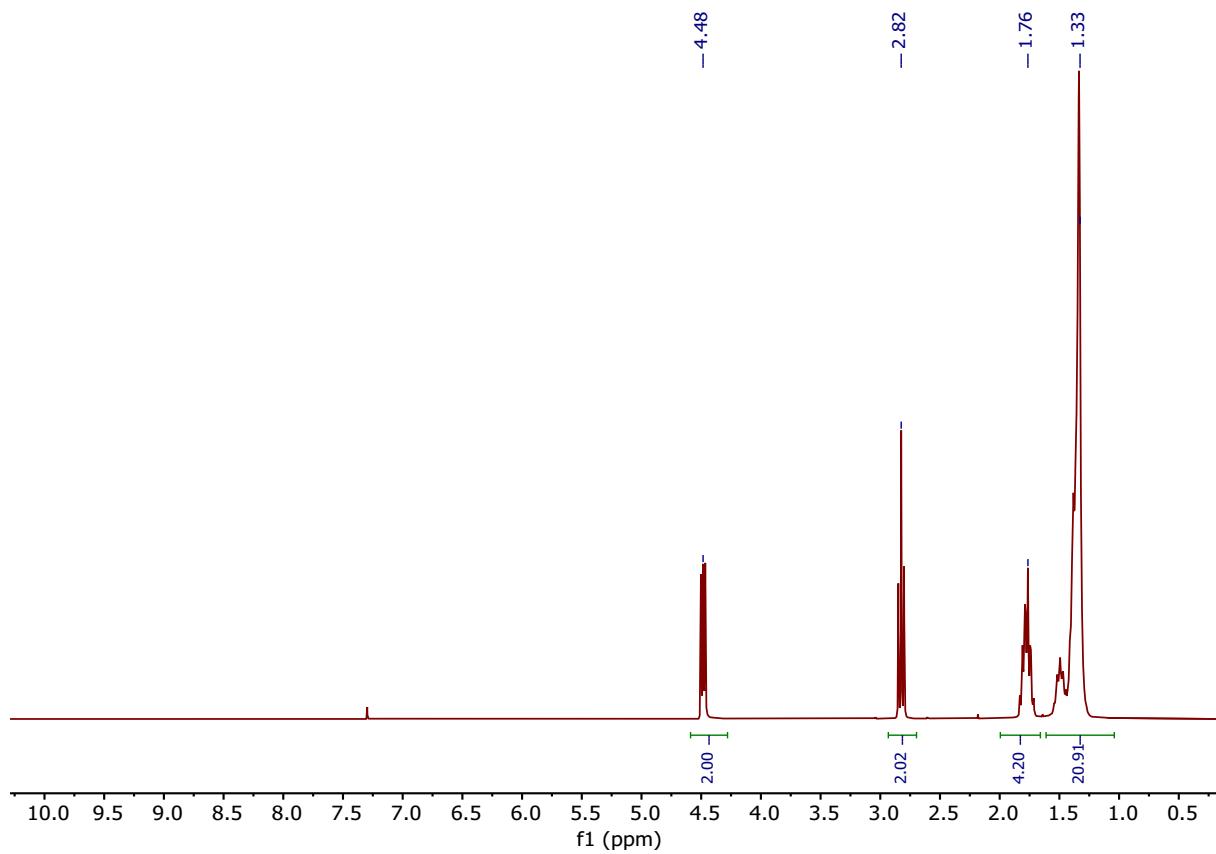
$$X_{TPDL} = \frac{\int_{3.2}^{4.20} CH^{\frac{closed PTPDL}{2}} + \int_{2.5}^{2.7} CH^{\frac{opened PTPDL}{2}}}{\int_{2.75}^{3.00} CH^{\frac{TPDL}{2}} + \int_{3.2}^{4.20} CH^{\frac{closed PTPDL}{2}} + \int_{2.5}^{2.7} CH^{\frac{opened PTPDL}{2}}} \times 100\%$$

$$ROP_{TPDL} = \frac{\int_{2.5}^{2.7} CH^{\frac{opened PTPDL}{2}}}{\int_{3.2}^{4.20} CH^{\frac{closed PTPDL}{2}} + \int_{2.5}^{2.7} CH^{\frac{opened PTPDL}{2}}} \times 100\%$$

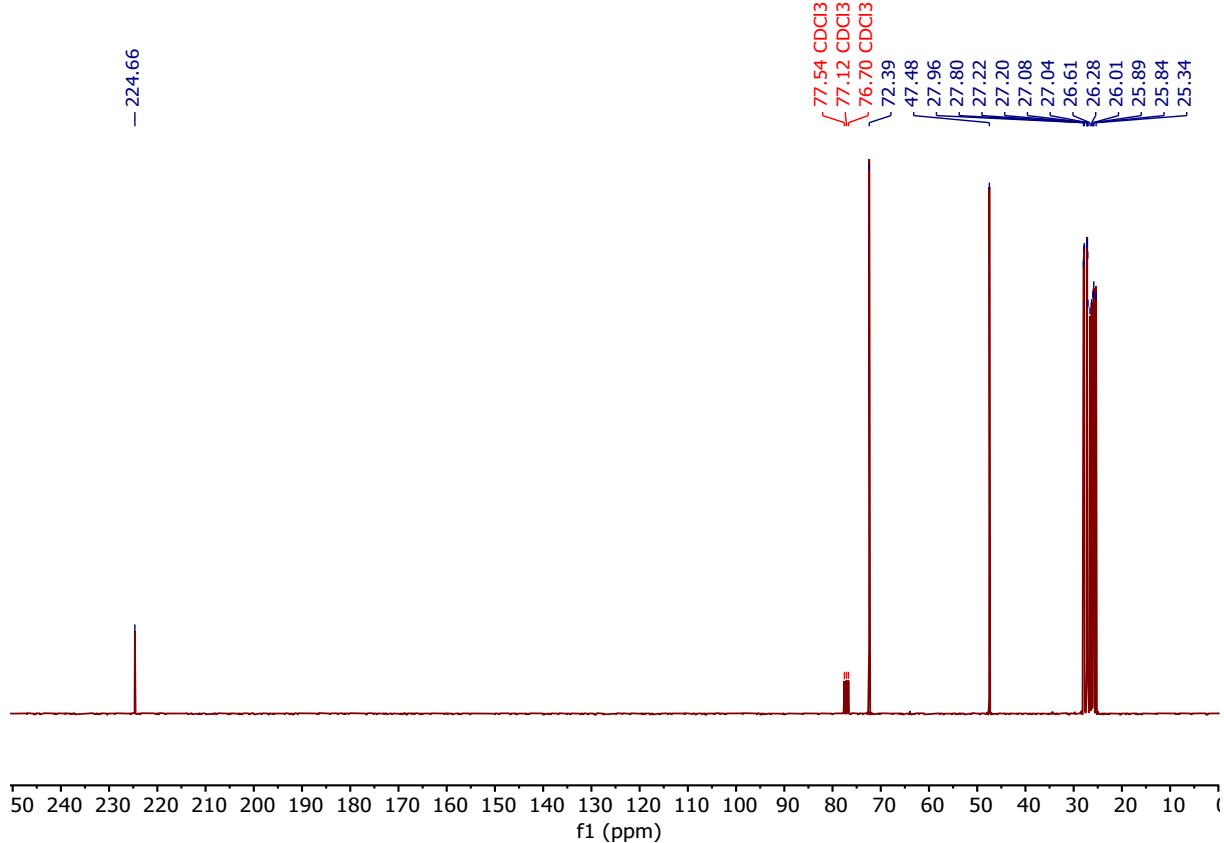




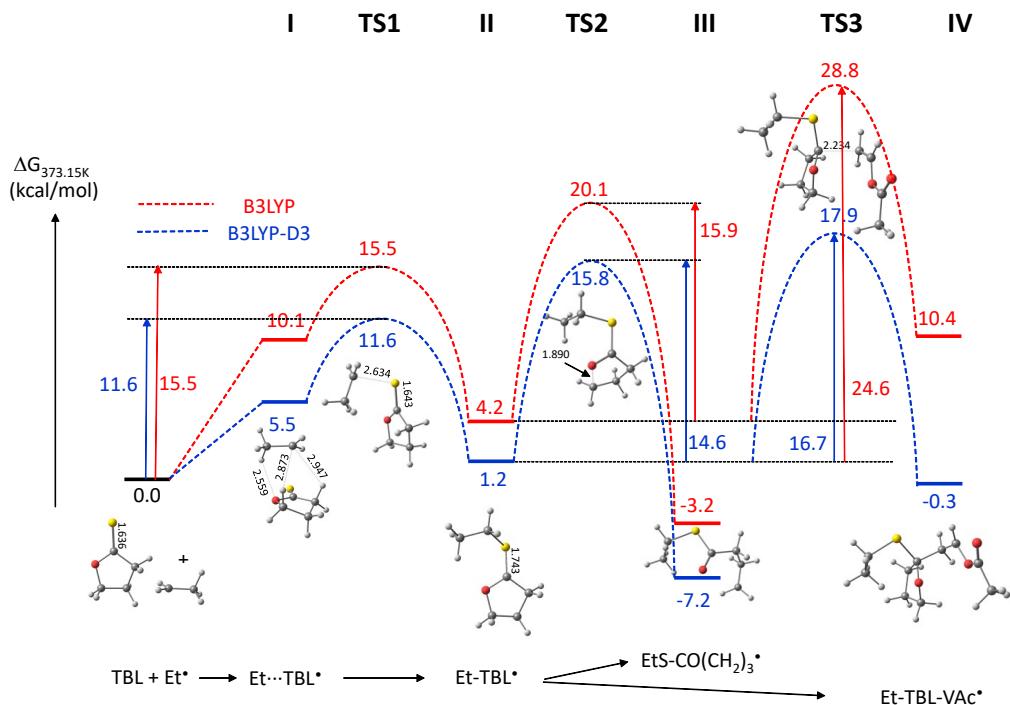




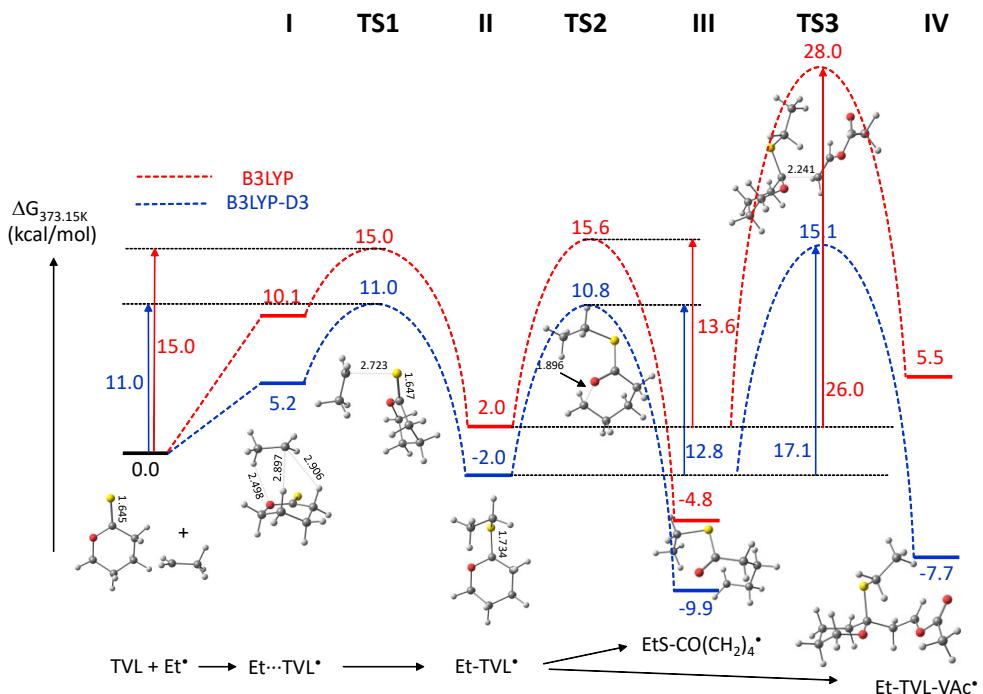
**Figure S12.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of TPDL



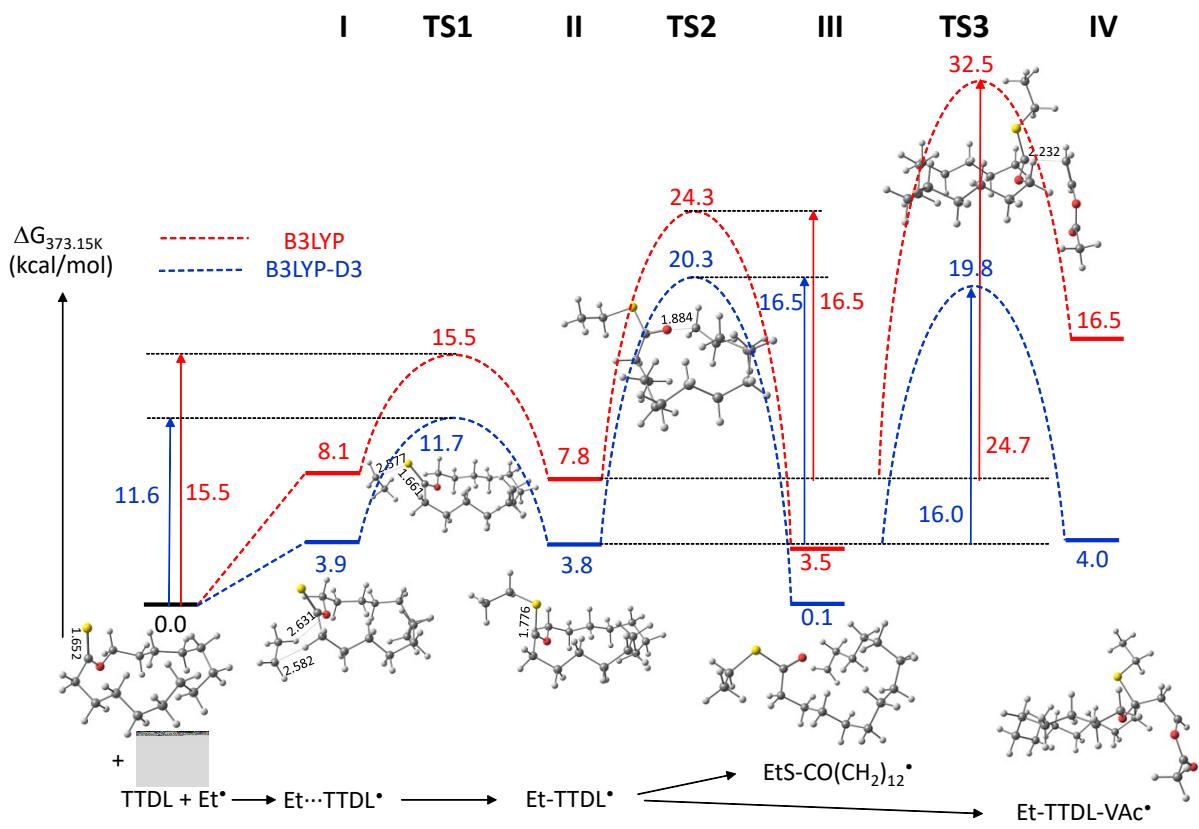
**Figure S13.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) of TPDL



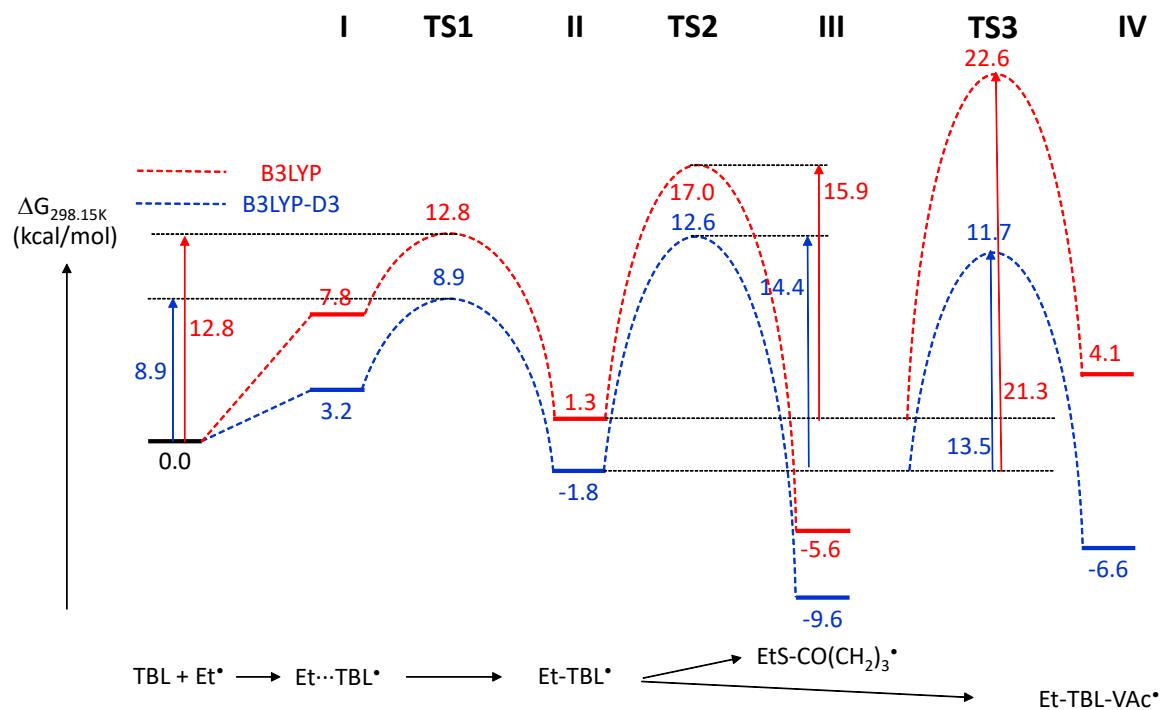
**Figure S14** Gibbs energy profiles at 100 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction, and views of the optimised geometries with key distances (in Å) for the Et<sup>•</sup> addition to TBL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc.



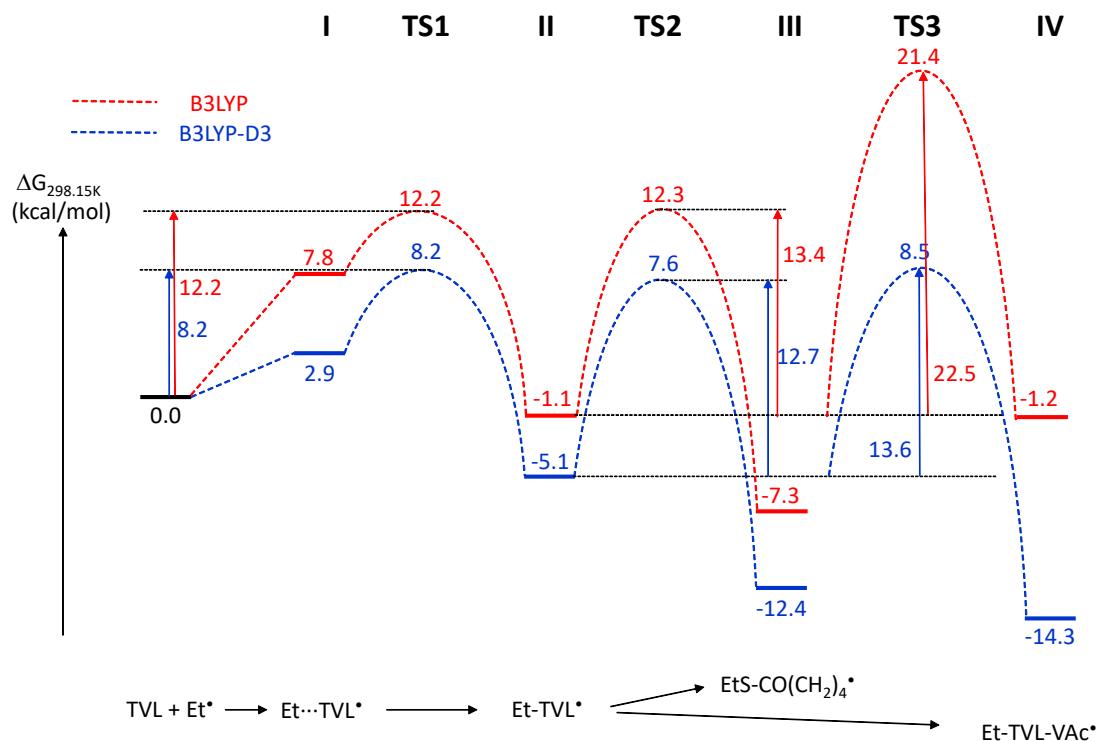
**Figure S15** Gibbs energy profiles at 100 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction, and views of the optimised geometries with key distances (in Å) for the Et<sup>•</sup> addition to TVL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc.



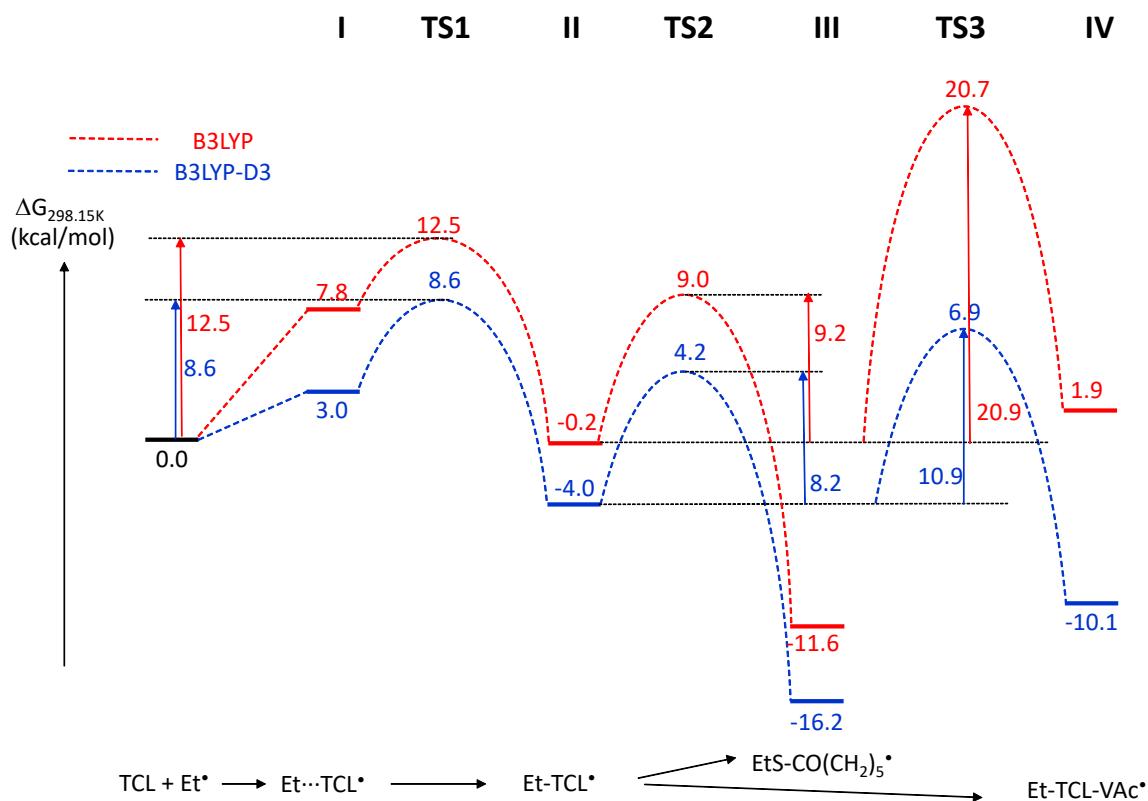
**Figure S16** Gibbs energy profiles at 100 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction, and views of the optimised geometries with key distances (in Å) for the Et<sup>•</sup> addition to TTDL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc. TTDL is a 15 member thionolactone, analogue of 16 member TPDL.



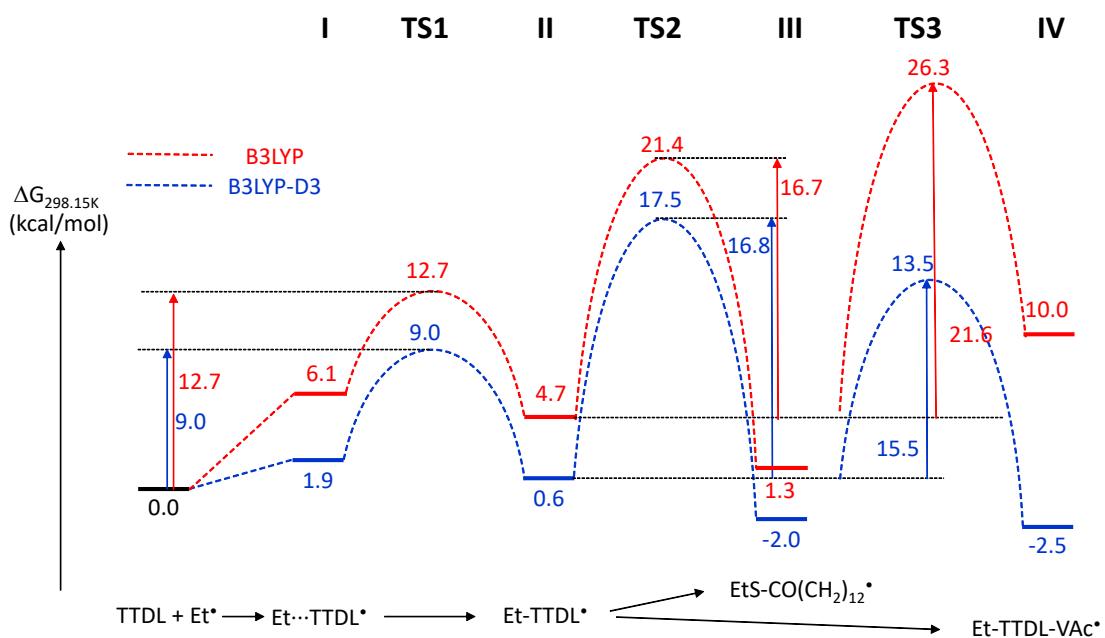
**Figure S17** Gibbs energy profiles at 25 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction for the  $Et^\bullet$  addition to TBL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc.



**Figure S18** Gibbs energy profiles at 25 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction for the  $Et^\bullet$  addition to TVL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc.



**Figure S19** Gibbs energy profiles at 25 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction for the  $Et^{\bullet}$  addition to TCL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc.



**Figure S20** Gibbs energy profiles at 25 °C in the presence (blue profile) and absence (red profile) of a D3 dispersion correction for the  $Et^{\bullet}$  addition to TTDL, for the subsequent ring opening, and for the addition of the ring-closed radical to VAc. TTDL is a 15 member thionolactone, analogue of 16 member TPDL.

**Table S1** Cartesian coordinates (Å), electronic and Gibbs energies at 298 K (hartrees) for all optimized geometries, including the single imaginary frequency (cm<sup>-1</sup>) for the transition states.

<b>A. Reagents</b>			
<b>Ethyl radical</b>			
E = -79.1652073063 E(D3) = -79.1664710303 $G_{298.15,1M}$ = -79.126860 $G_{373.15,1M}$ = -79.134153 $G(D3)_{298.15,1M}$ = -79.128124 $G(D3)_{373.15,1M}$ = -79.135417			
6	-0.694108000	-0.000005000	-0.000993000
1	-1.109451000	0.887036000	-0.493022000
1	-1.109460000	-0.887252000	-0.492634000
1	-1.093141000	0.000232000	1.028646000
6	0.795081000	-0.000002000	-0.022965000
1	1.353088000	0.927515000	0.050376000
1	1.353130000	-0.927491000	0.050379000
<b>VAc</b>			
E = -306.479857151 E(D3) = -306.485813659 $G_{298.15,1M}$ = -306.413372 $G_{373.15,1M}$ = -306.423109 $G(D3)_{298.15,1M}$ = -306.419329 $G(D3)_{373.15,1M}$ = -306.429065			
6	-2.601718000	-0.311547000	-0.000262000
1	-2.694145000	-1.391873000	-0.001056000
1	-3.504496000	0.286659000	-0.000423000
6	-1.415618000	0.285190000	0.000562000
1	-1.251553000	1.356714000	0.001087000
8	-0.259866000	-0.479041000	0.000129000
6	0.947307000	0.171339000	-0.000122000
8	1.066912000	1.372893000	-0.000293000
6	2.068294000	-0.834374000	-0.000004000
1	1.988853000	-1.479846000	-0.879552000
1	1.992149000	-1.475429000	0.883105000
1	3.023237000	-0.310688000	-0.002895000
<b>TBL</b>			
E = -629.449853146 E(D3) = -629.457540225 $G_{298.15,1M}$ = -629.380130 $G_{373.15,1M}$ = -629.389179 $G(D3)_{298.15,1M}$ = -629.387817 $G(D3)_{373.15,1M}$ = -629.396866			
16	-2.080441000	-0.010131000	-0.045289000
8	0.292189000	-1.118952000	-0.025087000
6	-0.446194000	0.002687000	0.032029000
6	1.708135000	-0.824083000	0.116468000
6	0.475674000	1.199998000	0.190840000
6	1.840632000	0.655628000	-0.251962000
1	1.989812000	-1.022383000	1.157402000
1	0.478432000	1.483176000	1.251332000
<b>TVL</b>			
E = -668.762021734 E(D3) = -668.773449999 $G_{298.15,1M}$ = -668.664975 $G_{373.15,1M}$ = -668.674727 $G(D3)_{298.15,1M}$ = -668.676403 $G(D3)_{373.15,1M}$ = -668.686155			
8	-0.065881000	-1.169415000	0.073205000
6	-0.720199000	-0.000705000	0.034887000
6	0.084432000	1.285070000	0.154894000
6	1.540295000	1.182194000	-0.312968000
6	2.163611000	-0.078062000	0.287211000
6	1.362175000	-1.284599000	-0.169214000
1	-0.462142000	2.077136000	-0.359000000
1	0.066646000	1.542912000	1.223502000
1	2.090789000	2.080752000	-0.017452000
1	1.580546000	1.126940000	-1.408438000
1	3.204550000	-0.209024000	-0.027905000
1	2.156717000	-0.017411000	1.382474000
1	1.652137000	-2.201258000	0.348478000
1	1.486035000	-1.443449000	-1.248011000
16	-2.364382000	-0.014042000	-0.028009000
<b>TCL</b>			
E = -708.072353767 E(D3) = -708.088487485 $G_{298.15,1M}$ = -707.947366 $G_{373.15,1M}$ = -707.957751 $G(D3)_{298.15,1M}$ = -707.963499 $G(D3)_{373.15,1M}$ = -707.973885			
16	-2.432213000	-0.053569000	0.383696000
8	-0.200891000	-1.271865000	-0.049182000
6	-0.911256000	-0.144433000	-0.235739000
6	-0.231922000	0.982594000	-0.984043000
6	1.162675000	-1.377832000	-0.522632000
6	0.916464000	1.644117000	-0.162709000
6	2.149323000	-0.583012000	0.347537000
6	1.564746000	0.730663000	0.888640000
1	-0.988380000	1.723311000	-1.239198000
1	1.675192000	2.019403000	-0.859223000
1	1.214047000	-1.068192000	-1.570723000
1	3.044287000	-0.387110000	-0.256482000
1	0.160588000	0.590321000	-1.929720000
1	1.372182000	-2.448272000	-0.484979000
1	0.505883000	2.515883000	0.356513000
1	2.467696000	-1.198351000	1.195614000
1	2.355902000	1.284351000	1.405915000
1	0.814959000	0.488097000	1.650281000

**TPDL**

E = -1022.61070833  
E(D3) = -1022.65977656  
G<sub>298.15,1M</sub> = -1022.268884  
G<sub>373.15,1M</sub> = -1022.284970  
G(D3)<sub>298.15,1M</sub> = -1022.317953  
G(D3)<sub>373.15,1M</sub> = -1022.334038

16	-2.540028000	0.111464000	-1.210035000
6	-2.183832000	0.257375000	0.523799000
6	-2.142656000	1.608044000	1.186805000
6	-0.714225000	2.157933000	1.400683000
6	0.132165000	2.199753000	0.125429000
6	1.518687000	2.812731000	0.359631000
6	2.499488000	2.626779000	-0.809363000
6	2.948079000	1.175829000	-1.063474000
6	3.637156000	0.520305000	0.142765000
6	4.394198000	-0.775427000	-0.187285000
6	3.562232000	-1.950401000	-0.732637000
6	2.503028000	-2.526164000	0.231695000
6	1.109499000	-1.895999000	0.111597000
6	0.069539000	-2.551687000	1.027657000
6	-1.334873000	-2.012292000	0.796619000
8	-1.349258000	-0.625443000	1.156042000
1	-2.078979000	-2.537715000	1.410895000
1	-1.608888000	-2.125242000	-0.257960000
1	0.045535000	-3.636295000	0.854865000
1	0.346436000	-2.405561000	2.079328000
1	1.146658000	-0.826746000	0.335790000
1	0.769820000	-1.976186000	-0.930639000
1	2.401583000	-3.603857000	0.045248000
1	2.860858000	-2.435630000	1.267364000
1	3.077669000	-1.661735000	-1.674683000
1	4.266959000	-2.748913000	-0.995835000
1	5.178418000	-0.540434000	-0.920341000
1	4.917039000	-1.116194000	0.717038000
1	4.354138000	1.235638000	0.569796000
1	2.905382000	0.326279000	0.936100000
1	3.644935000	1.173521000	-1.912915000
1	2.092722000	0.567540000	-1.379494000
1	3.393459000	3.236057000	-0.618499000
1	2.045786000	3.027830000	-1.725770000
1	1.954096000	2.383467000	1.271579000
1	1.403218000	3.885445000	0.563929000
1	-0.391726000	2.763272000	-0.659086000
1	0.233778000	1.177124000	-0.254964000
1	-0.205329000	1.528058000	2.139740000
1	-0.787497000	3.162393000	1.838191000
1	-2.633203000	1.532920000	2.168502000
1	-2.731485000	2.305722000	0.585112000
6	-4.111295000	-0.881734000	-1.200364000
1	-4.333683000	-1.038757000	-2.261062000
1	-3.904810000	-1.860650000	-0.756978000
6	-5.264267000	-0.186991000	-0.484255000
1	-5.498781000	0.771938000	-0.955255000
1	-5.004086000	0.002663000	0.561554000
1	-6.163043000	-0.814156000	-0.505128000

**TBL...Et<sup>•</sup> (I)**

E = -708.616713408  
E(D3) = -708.632910904  
G<sub>298.15,1M</sub> = -708.494635  
G<sub>373.15,1M</sub> = -708.507297  
G(D3)<sub>298.15,1M</sub> = -708.510833  
G(D3)<sub>373.15,1M</sub> = -708.523494

16	-0.667730000	-2.129092000	-0.090190000
8	-0.345556000	0.265827000	-1.092941000
6	-0.769365000	-0.494866000	-0.071074000
6	-0.444454000	1.679702000	-0.765953000
6	-1.295407000	0.399935000	1.036886000
6	-1.503962000	1.749163000	0.335091000
1	0.541008000	2.001744000	-0.412358000
1	-0.512966000	0.465496000	1.802339000
1	-2.185598000	-0.025959000	1.500709000
1	-1.367019000	2.611672000	0.991197000
1	-2.505188000	1.803195000	-0.103399000
1	-0.698055000	2.206581000	-1.687223000
6	2.323230000	0.266175000	1.025567000
1	2.667268000	1.085664000	1.649550000
1	1.801809000	-0.551206000	1.513191000
6	2.823563000	0.099631000	-0.367456000
1	3.027121000	1.063285000	-0.848693000
1	2.108115000	-0.452399000	-0.985042000
1	3.770008000	-0.467656000	-0.392070000

**TBL TS1**

E = -708.610660666  
E(D3) = -708.625924184  
G<sub>298.15,1M</sub> = -708.486542  
G<sub>373.15,1M</sub> = -708.498502  
G(D3)<sub>298.15,1M</sub> = -708.501805  
G(D3)<sub>373.15,1M</sub> = -708.513765  
̄ν<sub>TS</sub> = 193.4728i

16	0.999765000	-1.419227000	-0.232907000
8	-0.885179000	0.195526000	-1.100401000
6	-0.391490000	-0.559200000	-0.082255000
6	-2.055688000	0.929973000	-0.666803000
6	-1.267949000	-0.385210000	1.142540000
6	-2.574444000	0.167756000	0.555611000
1	-1.743164000	1.950885000	-0.412512000
1	-0.792657000	0.343351000	1.813613000
1	-1.373817000	-1.319325000	1.696005000
1	-3.133456000	0.807343000	1.242758000
1	-3.226437000	-0.652489000	0.239445000
1	-2.749512000	0.969697000	-1.509075000
6	2.878847000	0.393119000	0.115417000
1	3.350765000	-0.076165000	0.972502000
1	3.351097000	0.223047000	-0.846179000
6	2.057838000	1.624268000	0.310088000
1	1.489510000	1.583350000	1.245849000
1	1.347167000	1.758513000	-0.512801000
1	2.683022000	2.530983000	0.352526000

**EtTBL<sup>•</sup> (II)****B. TBL system**

E = -708.633100706

$E(D3) = -708.646965248$

$G_{298.15,1M} = -708.504860$

$G_{373.15,1M} = -708.516557$

$G(D3)_{298.15,1M} = -708.518724$

$G(D3)_{373.15,1M} = -708.530421$

16	-1.087207000	1.085537000	-0.432778000
8	0.649171000	-0.966930000	-0.305473000
6	0.378444000	0.322242000	0.122369000
6	2.024828000	-1.260388000	0.005205000
6	1.654724000	1.052087000	0.470325000
6	2.738434000	0.093172000	-0.064855000
1	2.085369000	-1.695567000	1.012879000
1	1.745732000	1.184556000	1.558841000
1	1.709337000	2.051018000	0.025637000
1	3.666068000	0.111422000	0.512744000
1	2.973709000	0.334364000	-1.106201000
1	2.376477000	-1.997282000	-0.720625000
6	-2.389528000	0.149793000	0.501595000
1	-2.128817000	0.198831000	1.562843000
1	-3.299582000	0.740838000	0.351567000
6	-2.579965000	-1.290556000	0.034979000
1	-1.657919000	-1.861996000	0.161756000
1	-2.853987000	-1.324266000	-1.023496000
1	-3.376068000	-1.773171000	0.614578000

$G(D3)_{298.15,1M} = -708.531269$

$G(D3)_{373.15,1M} = -708.543775$

16	-1.052642000	-1.089597000	0.344440000
8	0.141381000	0.579706000	-1.355197000
6	0.302573000	-0.352526000	-0.596039000
6	2.736953000	1.298849000	0.265738000
6	1.658081000	-0.954866000	-0.289272000
6	2.421978000	-0.072635000	0.753666000
1	3.655357000	1.492013000	-0.278792000
1	2.222024000	-0.990451000	-1.226097000
1	1.553095000	-1.972754000	0.101037000
1	3.342358000	-0.609125000	1.011973000
1	1.808792000	-0.030106000	1.663193000
1	1.967052000	2.061339000	0.236864000
6	-2.410920000	0.034588000	-0.178967000
1	-2.307289000	0.162555000	-1.259222000
1	-3.333418000	-0.517233000	0.021229000
6	-2.384464000	1.383519000	0.534945000
1	-1.452302000	1.908112000	0.313380000
1	-2.472880000	1.263679000	1.618417000
1	-3.216785000	2.006292000	0.188126000

### EtTBL+VAc TS3

$E = -1015.09728386$

$E(D3) = -1015.1296616$

$G_{298.15,1M} = -1014.884260$

$G_{373.15,1M} = -1014.900510$

$G(D3)_{298.15,1M} = -1014.916638$

$G(D3)_{373.15,1M} = -1014.932888$

$\tilde{\nu}_{TS} = 460.1613i$

### TBL TS2

$E = -708.606819736$

$E(D3) = -708.646965248$

$G_{298.15,1M} = -708.479986$

$G_{373.15,1M} = -708.491288$

$G(D3)_{298.15,1M} = -708.495794$

$G(D3)_{373.15,1M} = -708.507097$

$\tilde{\nu}_{TS} = 651.4142i$

16	-1.059673000	-1.191853000	0.237807000
8	0.503797000	0.628186000	-1.008812000
6	0.431266000	-0.558375000	-0.536636000
6	1.909384000	1.397150000	-0.006893000
6	1.749590000	-1.079048000	-0.064608000
6	2.310455000	0.160602000	0.737305000
1	2.546553000	1.738818000	-0.816830000
1	2.401416000	-1.266729000	-0.925263000
1	1.698962000	-1.986059000	0.543463000
1	3.397445000	0.074077000	0.831361000
1	1.880282000	0.152209000	1.743037000
1	1.393671000	2.188287000	0.527056000
6	-2.261034000	0.082935000	-0.324222000
1	-2.033461000	0.292797000	-1.372547000
1	-3.239810000	-0.402300000	-0.274483000
6	-2.220689000	1.362410000	0.508290000
1	-1.235299000	1.826166000	0.429199000
1	-2.431593000	1.157723000	1.561947000
1	-2.967612000	2.075129000	0.139222000

16	1.920922000	-1.281990000	-0.671223000
8	0.411127000	0.456478000	0.673843000
6	1.068804000	0.270308000	-0.533013000
6	0.055982000	1.845946000	0.762819000
6	1.712359000	1.589412000	-0.960268000
6	1.232458000	2.589389000	0.116862000
1	-0.882850000	2.009141000	0.218664000
1	1.386319000	1.875213000	-1.966398000
1	2.804263000	1.516904000	-0.995921000
1	0.940404000	3.560742000	-0.290527000
1	2.020221000	2.755464000	0.857984000
1	-0.097927000	2.077744000	1.819320000
6	3.356256000	-1.056829000	0.477693000
1	4.024389000	-1.890849000	0.237507000
1	3.881510000	-0.136782000	0.199574000
6	2.979161000	-1.055760000	1.957476000
1	2.490222000	-1.993746000	2.234556000
1	2.284624000	-0.242579000	2.178211000
1	3.875135000	-0.934096000	2.578166000
6	-0.604713000	-0.070310000	-1.972547000
1	-0.699177000	0.993016000	-2.169206000
1	-0.038029000	-0.646259000	-2.695380000
6	-1.594452000	-0.697833000	-1.273348000
1	-1.700679000	-1.765876000	-1.138280000
8	-2.429555000	0.090132000	-0.499406000
6	-3.302587000	-0.523629000	0.357189000
8	-3.441144000	-1.721053000	0.435746000
6	-4.029579000	0.512059000	1.175740000
1	-4.439665000	1.292802000	0.529826000

### EtTBL open (III)

$E = -708.63832429$

$E(D3) = -708.653603716$

$G_{298.15,1M} = -708.515989$

$G_{373.15,1M} = -708.528496$

1 -3.324451000 0.989180000 1.864307000  
 1 -4.824614000 0.030858000 1.744102000

### EtTBL-VAc<sup>•</sup> (IV)

E = -1015.1303084  
 E(D3) = -1015.16226133  
 $G_{298.15,1M} = -1014.913856$   
 $G_{373.15,1M} = -1014.929863$   
 $G(D3)_{298.15,1M} = -1014.945809$   
 $G(D3)_{373.15,1M} = -1014.961816$

16 1.420127000 -1.320958000 -0.946123000  
 8 0.450422000 0.551559000 0.710983000  
 6 0.912694000 0.431558000 -0.637122000  
 6 0.799354000 1.847477000 1.196136000  
 6 2.069589000 1.473689000 -0.785882000  
 6 2.185961000 2.116105000 0.608288000  
 1 0.068544000 2.597857000 0.855350000  
 1 1.793667000 2.218541000 -1.539486000  
 1 2.997791000 1.008028000 -1.119672000  
 1 2.438629000 3.179480000 0.575365000  
 1 2.944306000 1.603449000 1.208470000  
 1 0.772815000 1.809924000 2.288357000  
 6 2.660406000 -1.593063000 0.385396000  
 1 3.312723000 -2.381150000 -0.003925000  
 1 3.277223000 -0.693307000 0.478320000  
 6 2.057002000 -1.995425000 1.730962000  
 1 1.484718000 -2.922501000 1.636090000  
 1 1.382911000 -1.217481000 2.091668000  
 1 2.851564000 -2.155107000 2.470140000  
 6 -0.256231000 0.742867000 -1.626039000  
 1 -0.475764000 1.813716000 -1.527748000  
 1 0.101905000 0.576373000 -2.648483000  
 6 -1.502432000 -0.023117000 -1.389308000  
 1 -1.641595000 -1.067416000 -1.637584000  
 8 -2.274602000 0.472729000 -0.363315000  
 6 -3.239429000 -0.328215000 0.189157000  
 8 -3.482711000 -1.447653000 -0.194381000  
 6 -3.914513000 0.396544000 1.324330000  
 1 -4.316421000 1.352785000 0.977312000  
 1 -3.180175000 0.613273000 2.106268000  
 1 -4.714151000 -0.224734000 1.725729000

### C. TVL system

#### TVL<sup>•</sup>-Et<sup>•</sup> (I)

E = -747.928603682  
 E(D3) = -747.949100226  
 $G_{298.15,1M} = -747.779394$   
 $G_{373.15,1M} = -747.792793$   
 $G(D3)_{298.15,1M} = -747.799890$   
 $G(D3)_{373.15,1M} = -747.813290$

8 -0.194980000 0.022898000 -1.141366000  
 6 -0.988985000 -0.302332000 -0.114844000  
 6 -1.073482000 0.638697000 1.075045000  
 6 -0.676562000 2.089517000 0.783033000  
 6 0.630680000 2.085298000 -0.008604000  
 6 0.410867000 1.334653000 -1.309541000  
 1 -2.074076000 0.556187000 1.502683000

1 -0.379967000 0.221379000 1.817469000  
 1 -0.573055000 2.641716000 1.722229000  
 1 -1.461830000 2.589386000 0.201248000  
 1 0.971573000 3.099277000 -0.244549000  
 1 1.417887000 1.592208000 0.573848000  
 1 1.345033000 1.132028000 -1.837145000  
 1 -0.252571000 1.897729000 -1.977425000  
 16 -1.757763000 -1.758827000 -0.146548000  
 6 2.082490000 -1.168641000 1.146756000  
 1 2.656125000 -0.766445000 1.976392000  
 1 1.173673000 -1.713839000 1.379399000  
 6 2.672521000 -1.251028000 -0.218501000  
 1 3.294584000 -0.377253000 -0.449781000  
 1 1.893438000 -1.339024000 -0.981538000  
 1 3.328061000 -2.132290000 -0.327189000

### TVL TS1

E = -747.923824155  
 E(D3) = -747.942984624  
 $G_{298.15,1M} = -747.772325$   
 $G_{373.15,1M} = -747.784949$   
 $G(D3)_{298.15,1M} = -747.791486$   
 $G(D3)_{373.15,1M} = -747.804109$   
 $\tilde{\nu}_{TS} = 159.0689i$

8 -0.521939000 0.169486000 -1.132591000  
 6 -0.086356000 -0.604052000 -0.106486000  
 6 -0.838438000 -0.516818000 1.208939000  
 6 -2.347111000 -0.282847000 1.056240000  
 6 -2.576935000 0.866338000 0.073261000  
 6 -1.921828000 0.518080000 -1.253851000  
 1 -0.618764000 -1.409599000 1.796428000  
 1 -0.401708000 0.333846000 1.754158000  
 1 -2.792925000 -0.067905000 2.032701000  
 1 -2.828790000 -1.192983000 0.675854000  
 1 -3.644038000 1.049638000 -0.095076000  
 1 -2.142120000 1.792853000 0.468730000  
 1 -1.937322000 1.352945000 -1.957744000  
 1 -2.434099000 -0.335025000 -1.719524000  
 16 1.334322000 -1.418021000 -0.286539000  
 6 3.174052000 0.563329000 0.039258000  
 1 3.783550000 0.022048000 0.754633000  
 1 3.487389000 0.524260000 -0.997966000  
 6 2.293157000 1.676254000 0.496422000  
 1 1.913157000 1.498763000 1.508007000  
 1 1.435450000 1.801102000 -0.174296000  
 1 2.827335000 2.640804000 0.516740000

### EtTVL<sup>•</sup> (II)

E = -747.95055512  
 E(D3) = -747.96957317  
 $G_{298.15,1M} = -747.793605$   
 $G_{373.15,1M} = -747.805679$   
 $G(D3)_{298.15,1M} = -747.812623$   
 $G(D3)_{373.15,1M} = -747.824697$

8 -0.519338000 0.897429000 -0.716319000  
 6 -0.085783000 -0.384323000 -0.474631000  
 6 -0.760104000 -1.168430000 0.620252000  
 6 -2.286955000 -0.979102000 0.615108000

6	-2.618872000	0.513070000	0.509870000	6	-0.050389000	-0.778822000	0.615551000
6	-1.946357000	1.095516000	-0.727975000	6	-1.450426000	-1.305259000	0.339237000
1	-0.488374000	-2.223393000	0.524672000	6	-2.286459000	-0.435302000	-0.621103000
1	-0.370009000	-0.831612000	1.598522000	6	-2.549154000	0.993711000	-0.098815000
1	-2.726756000	-1.418948000	1.516537000	6	-1.348126000	1.877553000	-0.111661000
1	-2.716014000	-1.506589000	-0.246515000	1	-1.363160000	-2.317028000	-0.074623000
1	-3.700386000	0.679535000	0.446855000	1	-1.944657000	-1.376803000	1.313181000
1	-2.254947000	1.042697000	1.399590000	1	-3.244231000	-0.944377000	-0.781409000
1	-2.082331000	2.177215000	-0.800812000	1	-1.791664000	-0.383380000	-1.598033000
1	-2.355882000	0.630725000	-1.636604000	1	-3.340938000	1.431581000	-0.732241000
16	1.584032000	-0.678897000	-0.921527000	1	-2.970801000	0.939155000	0.912529000
6	2.506286000	-0.168074000	0.615745000	1	-1.089203000	2.501840000	0.735054000
1	2.182851000	-0.809658000	1.441360000	1	-0.736996000	1.950883000	-1.004893000
1	3.550239000	-0.416012000	0.397161000	16	1.069846000	-0.880036000	-0.807596000
6	2.339417000	1.309029000	0.958377000	6	2.540793000	-0.064452000	-0.063805000
1	1.285142000	1.556523000	1.110184000	1	2.655805000	-0.484620000	0.938107000
1	2.711912000	1.942033000	0.148366000	1	3.386752000	-0.386197000	-0.677449000
1	2.888955000	1.554284000	1.875195000	6	2.421508000	1.456259000	-0.006894000
				1	1.561855000	1.743586000	0.602163000
				1	2.301362000	1.884224000	-1.006359000
				1	3.322953000	1.885266000	0.445254000

## TVL TS2

E = -747.926362839

E(D3) = -747.946600521

G<sub>298,15,1M</sub> = -747.772188

G<sub>373,15,1M</sub> = -747.784087

G(D3)<sub>298,15,1M</sub> = -747.792426

G(D3)<sub>373,15,1M</sub> = -747.804325

$\tilde{\nu}_{TS} = 638.0297i$

8	-0.231671000	0.570343000	1.018287000
6	-0.139642000	-0.608555000	0.546862000
6	-1.406741000	-1.384131000	0.286711000
6	-2.324552000	-0.576447000	-0.657265000
6	-2.588150000	0.854791000	-0.142291000
6	-1.336984000	1.676925000	-0.053462000
1	-1.196216000	-2.373623000	-0.130582000
1	-1.919449000	-1.526297000	1.247801000
1	-3.277175000	-1.105195000	-0.770590000
1	-1.864704000	-0.527371000	-1.652792000
1	-3.314543000	1.349260000	-0.806757000
1	-3.058574000	0.805132000	0.848308000
1	-1.351292000	2.569436000	0.563542000
1	-0.736095000	1.760254000	-0.956789000
16	1.332862000	-1.177243000	-0.301645000
6	2.548924000	0.065438000	0.302125000
1	2.318039000	0.244902000	1.355413000
1	3.519715000	-0.434869000	0.242520000
6	2.543228000	1.372108000	-0.486812000
1	1.577187000	1.868961000	-0.381316000
1	2.734723000	1.196277000	-1.549425000
1	3.319460000	2.045502000	-0.104519000

## EtTVL open (III)

E = -747.953040288

E(D3) = -747.973823027

G<sub>298,15,1M</sub> = -747.803454

G<sub>373,15,1M</sub> = -747.816551

G(D3)<sub>298,15,1M</sub> = -747.824237

G(D3)<sub>373,15,1M</sub> = -747.837334

8	0.308614000	-0.353211000	1.691899000
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## EtTVL+VAc TS3

E = -1054.41694139

E(D3) = -1054.45623402

G<sub>298,15,1M</sub> = -1054.171061

G<sub>373,15,1M</sub> = -1054.187286

G(D3)<sub>298,15,1M</sub> = -1054.210354

G(D3)<sub>373,15,1M</sub> = -1054.226579

$\tilde{\nu}_{TS} = 402.8019i$

8	-1.343755000	-0.574720000	0.940711000
6	-1.345227000	-0.220030000	-0.397326000
6	-2.593314000	-0.645034000	-1.141422000
6	-3.860584000	-0.157156000	-0.407087000
6	-3.790738000	-0.565974000	1.071091000
6	-2.480531000	-0.085938000	1.690067000
1	-2.566719000	-0.283493000	-2.174400000
1	-2.604040400	-1.742638000	-1.176851000
1	-4.756980000	-0.570641000	-0.882874000
1	-3.923470000	0.934822000	-0.484253000
1	-4.634770000	-0.152203000	1.635525000
1	-3.842494000	-1.658810000	1.156874000
1	-2.341016000	-0.465694000	2.705404000
1	-2.445891000	1.012720000	1.715767000
16	-0.812904000	1.459439000	-0.767908000
6	0.482673000	1.700920000	0.525386000
1	0.016847000	2.193798000	1.383813000
1	0.798862000	0.707274000	0.845781000
6	1.653338000	2.521298000	-0.012703000
1	1.323209000	3.494243000	-0.390507000
1	2.169731000	1.992040000	-0.816669000
1	2.377533000	2.705085000	0.789135000
6	0.185353000	-1.688843000	-1.118588000
1	-0.296515000	-1.786895000	-2.084633000
1	-0.148048000	-2.342979000	-0.320648000
6	1.452041000	-1.193121000	-1.104580000
1	1.925865000	-0.646691000	-1.909015000
8	2.169519000	-1.243641000	0.082568000
6	3.369478000	-0.595390000	0.148483000
8	3.858573000	0.018742000	-0.772696000

6	3.960571000	-0.741217000	1.526768000	6	-0.063569000	-0.802214000	-0.093855000
1	3.961912000	-1.790198000	1.833697000	6	0.613355000	-0.562295000	1.237970000
1	3.345788000	-0.190228000	2.245957000	6	0.374546000	1.540158000	-0.568260000
1	4.973566000	-0.340666000	1.529246000	6	2.150555000	-0.380665000	1.102002000

### EtTVL-VAc<sup>•</sup> (IV)

E = -1054.45291327				6	1.912424000	1.630791000	-0.517956000
E(D3) = -1054.49258414				6	2.600770000	0.294942000	-0.201860000
G <sub>298.15,1M</sub> = -1054.207033				1	0.389527000	-1.404814000	1.891382000
G <sub>373.15,1M</sub> = -1054.223258				1	2.507999000	0.188745000	1.968005000
G(D3) <sub>298.15,1M</sub> = -1054.246704				1	-0.091503000	1.816594000	0.381442000
G(D3) <sub>373.15,1M</sub> = -1054.262929				1	2.184337000	2.386650000	0.229218000
8	-0.894474000	-0.949022000	0.485630000	1	0.166190000	0.325353000	1.698703000
6	-1.149190000	-0.144123000	-0.645011000	1	-0.036016000	2.197724000	-1.336191000
6	-2.585043000	-0.341948000	-1.174377000	1	2.621427000	-1.367765000	1.155141000
6	-3.645302000	-0.262619000	-0.068731000	1	2.287664000	1.991336000	-1.481544000
6	-3.254754000	-1.185867000	1.091500000	1	3.684103000	0.454179000	-0.167686000
6	-1.841316000	-0.851492000	1.558342000	1	2.419163000	-0.391929000	-1.036166000
1	-2.785341000	0.385184000	-1.968915000	6	-2.646711000	0.914073000	1.182083000
1	-2.618413000	-1.338722000	-1.634114000	1	-2.471083000	-0.096508000	1.536025000
1	-4.625072000	-0.538162000	-0.474095000	1	-2.693070000	1.704137000	1.925649000
1	-3.720948000	0.768412000	0.293687000	6	-3.118278000	1.143588000	-0.211569000
1	-3.952165000	-1.083679000	1.931029000	1	-2.638464000	0.454330000	-0.913567000
1	-3.283148000	-2.233032000	0.764345000	1	-2.924718000	2.169778000	-0.545032000
1	-1.483174000	-1.555874000	2.314073000	1	-4.206844000	0.985845000	-0.302135000
1	-1.814946000	0.160625000	1.985610000				
16	-0.953398000	1.703722000	-0.269570000				
6	0.404199000	1.701868000	0.984877000				
1	-0.046579000	1.938885000	1.953802000				
1	0.779595000	0.678509000	1.045198000				
6	1.516219000	2.694695000	0.654416000				
1	1.123747000	3.710343000	0.544087000				
1	2.035649000	2.418264000	-0.264631000				
1	2.256469000	2.703373000	1.462169000				
6	-0.128597000	-0.607058000	-1.722886000				
1	-0.403478000	-0.117948000	-2.662596000				
1	-0.281413000	-1.688314000	-1.841104000				
6	1.301587000	-0.332848000	-1.459613000				
1	1.799330000	0.599351000	-1.686903000				
8	1.906086000	-1.146841000	-0.529637000				
6	3.099682000	-0.757446000	0.017323000				
8	3.650909000	0.285987000	-0.249878000				
6	3.592262000	-1.808141000	0.977116000				
1	3.772963000	-2.745696000	0.442585000				
1	2.829514000	-2.007258000	1.735296000				
1	4.513131000	-1.464925000	1.446926000				

### D. TCL system

#### TCL---Et<sup>•</sup> (I)

E = -787.238853043				16	1.350664000	-1.202232000	0.802610000
E(D3) = -787.26390166				8	-0.232654000	0.837720000	0.699691000
G <sub>298.15,1M</sub> = -787.061833				6	0.142558000	-0.324117000	0.100941000
G <sub>373.15,1M</sub> = -787.075904				6	-0.563369000	-0.708828000	-1.180028000
G(D3) <sub>298.15,1M</sub> = -787.086882				6	-1.304703000	1.626342000	0.144144000
G(D3) <sub>373.15,1M</sub> = -787.100953				6	-2.059031000	-1.101257000	-0.970985000

16	-0.707306000	-2.244217000	-0.557636000
8	-0.102546000	0.227945000	-0.956551000

#### EtTCL<sup>•</sup> (II)

$E = -787.258477746$   
 $E(D3) = -787.281900396$   
 $G_{298.15,1M} = -787.074535$   
 $G_{373.15,1M} = -787.087484$   
 $G(D3)_{298.15,1M} = -787.097957$   
 $G(D3)_{373.15,1M} = -787.110906$

16	-1.484919000	-1.142600000	-0.195089000
8	0.042586000	0.931325000	0.414577000
6	-0.112342000	-0.424847000	0.651545000
6	1.111977000	-1.277892000	0.841257000
6	1.292341000	1.530929000	0.780994000
6	2.055169000	-1.326640000	-0.391965000
6	2.426398000	1.236763000	-0.236962000
6	2.156968000	0.015761000	-1.132688000
1	0.792981000	-2.288025000	1.113349000
1	3.048925000	-1.655392000	-0.060784000
1	1.571457000	1.218025000	1.793815000
1	3.369129000	1.106210000	0.309625000
1	1.675695000	-0.900587000	1.703805000
1	1.079329000	2.601914000	0.822977000
1	1.690408000	-2.084027000	-1.095251000
1	2.561483000	2.109739000	-0.885024000
1	2.948048000	-0.048606000	-1.888748000
1	1.221081000	0.191508000	-1.673838000
6	-2.846725000	0.023711000	0.258698000
1	-3.757861000	-0.580611000	0.204119000
1	-2.692856000	0.302928000	1.304808000
6	-2.945436000	1.251865000	-0.643727000
1	-3.091466000	0.958864000	-1.687733000
1	-2.032625000	1.846377000	-0.578445000
1	-3.795810000	1.874789000	-0.340791000

## TCL TS2

$E = -787.241167919$   
 $E(D3) = -787.266085715$   
 $G_{298.15,1M} = -787.059930$   
 $G_{373.15,1M} = -787.072568$   
 $G(D3)_{298.15,1M} = -787.084848$   
 $G(D3)_{373.15,1M} = -787.097485$   
 $\tilde{\nu}_{TS} = 602.5327i$

16	1.497490000	-1.112941000	0.580083000
8	-0.010247000	0.362715000	-1.094698000
6	0.043746000	-0.695054000	-0.374926000
6	-1.176571000	-1.565777000	-0.143293000
6	-0.931630000	1.800684000	-0.390138000
6	-2.476948000	-0.812624000	-0.456959000
6	-1.626024000	1.275428000	0.826400000
6	-2.799414000	0.320680000	0.535351000
1	-1.188316000	-1.944169000	0.888152000
1	-2.396510000	-0.403435000	-1.469513000
1	-1.544829000	2.044405000	-1.253846000
1	-1.985025000	2.117436000	1.436308000
1	-1.100657000	-2.455048000	-0.786887000
1	-0.122034000	2.504484000	-0.217631000
1	-3.311356000	-1.522946000	-0.469978000
1	-0.877047000	0.765304000	1.448959000
1	-3.648574000	0.896369000	0.145274000
1	-3.131526000	-0.112247000	1.487548000
6	2.783973000	-0.144225000	-0.313852000
1	3.714813000	-0.695660000	-0.151551000

1	2.536175000	-0.193994000	-1.376958000
6	2.908460000	1.303624000	0.151960000
1	3.115257000	1.359965000	1.224698000
1	1.983402000	1.844928000	-0.052882000
1	3.724801000	1.803526000	-0.382690000

## EtTCL open (III)

16	-1.602436000	-0.944414000	-0.742328000
8	-0.357576000	-0.264316000	1.507725000
6	-0.264852000	-0.879837000	0.467542000
6	0.967505000	-1.686756000	0.084798000
6	1.597108000	2.115241000	0.434992000
6	2.284020000	-0.959929000	0.416065000
6	1.758378000	1.284644000	-0.791701000
6	2.711098000	0.086914000	-0.625036000
1	0.927099000	-1.977634000	-0.970787000
1	2.176946000	-0.495326000	1.401816000
1	2.325613000	2.077995000	1.238175000
1	2.140611000	1.908015000	-1.620866000
1	0.900796000	-2.611015000	0.673512000
1	0.788746000	2.832883000	0.518717000
1	3.078070000	-1.710525000	0.501080000
1	0.775090000	0.941128000	-1.145432000
1	3.702709000	0.466259000	-0.344937000
1	2.835358000	-0.407144000	-1.597903000
6	-2.813069000	0.148513000	0.108825000
1	-3.780697000	-0.088543000	-0.341881000
1	-2.829932000	-0.160218000	1.156791000
6	-2.470022000	1.631020000	-0.017178000
1	-2.434078000	1.943824000	-1.064666000
1	-1.501133000	1.831980000	0.445125000
1	-3.226606000	2.234622000	0.496863000

## EtTCL+VAc TS3

16	-2.592214000	-0.640651000	-0.957178000
8	-0.942177000	0.236393000	0.882968000
6	-0.938489000	-0.166558000	-0.436447000
6	-0.238168000	0.723834000	-1.439579000
6	0.252666000	0.816902000	1.435042000
6	-0.649682000	2.208184000	-1.374315000
6	0.606098000	2.219339000	0.870410000
6	-0.538381000	2.823373000	0.039165000
1	-0.422134000	0.323554000	-2.442730000
1	0.006615000	2.754710000	-2.063045000
1	1.080843000	0.112032000	1.321609000

1	1.517794000	2.162508000	0.265270000
1	0.842226000	0.637574000	-1.286188000
1	0.016950000	0.886656000	2.499750000
1	-1.672273000	2.330447000	-1.746613000
1	0.835129000	2.878268000	1.715403000
1	-0.392975000	3.905562000	-0.049534000
1	-1.479159000	2.676909000	0.579767000
6	-3.242299000	-1.459081000	0.561848000
1	-3.935148000	-2.223722000	0.197968000
1	-2.404560000	-1.970289000	1.042285000
6	-3.932592000	-0.498557000	1.527609000
1	-4.775609000	0.004060000	1.044444000
1	-3.228371000	0.261291000	1.870418000
1	-4.313134000	-1.046394000	2.398108000
6	0.265673000	-2.014667000	-0.461887000
1	0.013149000	-2.232953000	0.571499000
1	-0.361822000	-2.468209000	-1.220485000
6	1.576572000	-1.786123000	-0.783483000
1	1.957669000	-1.662924000	-1.789476000
8	2.492980000	-1.495491000	0.231828000
6	3.366606000	-0.470087000	0.025236000
8	3.324292000	0.267010000	-0.936362000
6	4.365855000	-0.394003000	1.151282000
1	4.985798000	-1.295599000	1.158873000
1	3.846730000	-0.347702000	2.112810000
1	4.993793000	0.485996000	1.017938000

#### EtTCL-VAc<sup>•</sup> (IV)

E = -1093.75580009  
E(D3) = -1093.79824342  
G<sub>298.15,1M</sub> = -1093.484600  
G<sub>373.15,1M</sub> = -1093.501964  
G(D3)<sub>298.15,1M</sub> = -1093.527043  
G(D3)<sub>373.15,1M</sub> = -1093.544408

16	0.932658000	-1.456215000	0.951676000
8	1.709639000	0.215154000	-0.962780000
6	0.514862000	-0.086908000	-0.240507000
6	-0.020583000	1.094552000	0.587667000
6	1.851395000	1.537005000	-1.490487000
6	0.971551000	1.740214000	1.570271000
6	2.350600000	2.572881000	-0.442490000
6	2.368315000	2.015337000	0.987653000
1	-0.909476000	0.755365000	1.128181000
1	0.522786000	2.681700000	1.912533000
1	0.914147000	1.868436000	-1.956357000
1	1.721980000	3.471505000	-0.486252000
1	-0.387281000	1.847597000	-0.120310000
1	2.581372000	1.425382000	-2.296899000
1	1.077654000	1.105085000	2.455142000
1	3.364153000	2.893013000	-0.708429000
1	2.895022000	2.720489000	1.641130000
1	2.945976000	1.086739000	0.991381000
6	2.023745000	-2.532206000	-0.072762000
1	1.834932000	-3.547944000	0.288118000
1	1.678297000	-2.486099000	-1.108862000
6	3.506605000	-2.178867000	0.023816000
1	3.852620000	-2.222400000	1.060780000
1	3.677307000	-1.170606000	-0.356268000
1	4.103600000	-2.884951000	-0.566418000
6	-0.538907000	-0.573619000	-1.287762000

1	-0.664888000	0.234529000	-2.020042000
1	-0.094169000	-1.420940000	-1.819338000
6	-1.866966000	-0.961603000	-0.761224000
1	-2.062567000	-1.855561000	-0.184035000
8	-2.755376000	0.084045000	-0.602465000
6	-3.922966000	-0.137054000	0.084894000
8	-4.216766000	-1.199685000	0.577976000
6	-4.745946000	1.124623000	0.117379000
1	-4.985810000	1.440569000	-0.902304000
1	-4.175718000	1.933181000	0.584339000
1	-5.662669000	0.942102000	0.676571000

#### E. TPDL system

##### TPDL<sup>•</sup>•Et<sup>•</sup> (I)

E = -1101.77792716  
E(D3) = -1101.8349282  
G<sub>298.15,1M</sub> = -1101.386065  
G<sub>373.15,1M</sub> = -1101.406237  
G(D3)<sub>298.15,1M</sub> = -1101.443066  
G(D3)<sub>373.15,1M</sub> = -1101.463238

16	3.273935000	-0.236768000	2.069765000
6	2.291275000	0.240112000	0.829232000
6	2.316498000	1.629458000	0.228013000
6	1.052845000	2.078592000	-0.516464000
6	-0.202088000	2.176030000	0.358429000
6	-1.398072000	2.752226000	-0.410792000
6	-2.740255000	2.674944000	0.334798000
6	-3.308299000	1.256853000	0.526777000
6	-3.567426000	0.511301000	-0.790224000
6	-4.408171000	-0.766829000	-0.645777000
6	-3.816818000	-1.896450000	0.216719000
6	-2.484465000	-2.492995000	-0.285702000
6	-1.228705000	-1.827782000	0.291716000
6	0.075468000	-2.490614000	-0.165548000
6	1.300436000	-1.943630000	0.546871000
8	1.427542000	-0.547056000	0.185843000
1	2.223866000	-2.453689000	0.254343000
1	1.206008000	-2.017842000	1.634784000
1	0.038047000	-3.569510000	0.035687000
1	0.199362000	-2.378143000	-1.250074000
1	-1.197485000	-0.768787000	0.023687000
1	-1.280836000	-1.864122000	1.389287000
1	-2.449877000	-3.559613000	-0.026757000
1	-2.453223000	-2.450916000	-1.383800000
1	-3.693409000	-1.553581000	1.252531000
1	-4.566256000	-2.696255000	0.259088000
1	-5.388335000	-0.493797000	-0.231079000
1	-4.605338000	-1.169335000	-1.648878000
1	-4.091255000	1.189049000	-1.478744000
1	-2.617007000	0.269819000	-1.281312000
1	-4.254355000	1.335839000	1.079803000
1	-2.639964000	0.668120000	1.165886000
1	-3.480845000	3.271059000	-0.215328000
1	-2.632071000	3.154325000	1.317135000
1	-1.485701000	2.239919000	-1.377834000
1	-1.185312000	3.802041000	-0.652752000
1	0.003377000	2.803903000	1.236724000
1	-0.440822000	1.180024000	0.745689000
1	0.860103000	1.392990000	-1.349385000

1	1.262806000	3.058968000	-0.963431000	1	-2.307761000	2.644236000	-0.317431000
1	3.164203000	1.622620000	-0.473670000	6	-5.453235000	-0.252985000	0.012869000
1	2.580295000	2.330866000	1.024045000	1	-5.701916000	0.790924000	0.175771000
6	4.341857000	0.340583000	-2.380963000	1	-6.003465000	-0.747086000	-0.782012000
1	3.811780000	0.887676000	-3.153898000	6	-4.957082000	-1.060989000	1.166540000
1	5.305390000	0.727151000	-2.065605000	1	-4.104500000	-0.577051000	1.659091000
6	3.890403000	-1.014469000	-1.958218000	1	-4.639898000	-2.059878000	0.850664000
1	2.799627000	-1.104118000	-1.989168000	1	-5.734310000	-1.193341000	1.936715000
1	4.221267000	-1.248576000	-0.940120000				
1	4.295775000	-1.805334000	-2.613037000				

## EtTPDL\* (II)

### TPDL TS1

$$E = -1101.77146969$$

$$E(D3) = -1101.82778558$$

$$G_{298.15,1M} = -1101.375464$$

$$G_{373.15,1M} = -1101.394486$$

$$G(D3)_{298.15,1M} = -1101.431780$$

$$G(D3)_{373.15,1M} = -1101.450802$$

$$\tilde{\nu}_{TS} = 213.6363i$$

16	-3.324587000	0.196872000	-1.367858000
6	-2.156115000	0.532381000	-0.236336000
6	-1.992988000	1.891516000	0.411019000
6	-0.595900000	2.214597000	0.959231000
6	0.511165000	2.223578000	-0.100815000
6	1.852699000	2.701495000	0.470176000
6	3.056200000	2.509582000	-0.466888000
6	3.467302000	1.047081000	-0.717364000
6	3.831580000	0.280194000	0.562429000
6	4.538657000	-1.062377000	0.321245000
6	3.760978000	-2.128435000	-0.471135000
6	2.455287000	-2.632106000	0.180800000
6	1.198385000	-1.838067000	-0.197573000
6	-0.090617000	-2.424257000	0.389232000
6	-1.344416000	-1.743420000	-0.135147000
8	-1.324472000	-0.374024000	0.315614000
1	-2.261283000	-2.215957000	0.233570000
1	-1.379778000	-1.759847000	-1.229810000
1	-0.167114000	-3.489794000	0.134114000
1	-0.071139000	-2.363816000	1.484600000
1	1.288228000	-0.797907000	0.124703000
1	1.111752000	-1.812802000	-1.293395000
1	2.293515000	-3.677874000	-0.113313000
1	2.569924000	-2.643964000	1.274219000
1	3.542086000	-1.758706000	-1.481594000
1	4.434839000	-2.982944000	-0.609021000
1	5.483768000	-0.866710000	-0.204120000
1	4.815902000	-1.491309000	1.293996000
1	4.493490000	0.910799000	1.172488000
1	2.935338000	0.117423000	1.172748000
1	4.334696000	1.041893000	-1.391744000
1	2.670358000	0.520509000	-1.255478000
1	3.918134000	3.042367000	-0.042836000
1	2.841961000	2.992843000	-1.429703000
1	2.045209000	2.187668000	1.421060000
1	1.765579000	3.766306000	0.724223000
1	0.220875000	2.871551000	-0.939717000
1	0.608675000	1.214955000	-0.515628000
1	-0.336558000	1.492177000	1.741306000
1	-0.644886000	3.198021000	1.445117000
1	-2.723952000	1.942840000	1.232531000

$$E = -1101.78969062$$

$$E(D3) = -1101.84646429$$

$$G_{298.15,1M} = -1101.388223$$

$$G_{373.15,1M} = -1101.406658$$

$$G(D3)_{298.15,1M} = -1101.444996$$

$$G(D3)_{373.15,1M} = -1101.463432$$

16	-2.540028000	0.111464000	-1.210035000
6	-2.183832000	0.257375000	0.523799000
6	-2.142656000	1.608044000	1.186805000
6	-0.714225000	2.157933000	1.400683000
6	0.132165000	2.199753000	0.125429000
6	1.518687000	2.812731000	0.359631000
6	2.499488000	2.626779000	-0.809363000
6	2.948079000	1.175829000	-1.063474000
6	3.637156000	0.520305000	0.142765000
6	4.394198000	-0.775427000	-0.187285000
6	3.562232000	-1.950401000	-0.732637000
6	2.503028000	-2.526164000	0.231695000
6	1.109499000	-1.895999000	0.111597000
6	0.069539000	-2.551687000	1.027657000
6	-1.334873000	-2.012292000	0.796619000
8	-1.349258000	-0.625443000	1.156042000
1	-2.078979000	-2.537715000	1.410895000
1	-1.608888000	-2.125242000	-0.257960000
1	0.045535000	-3.636295000	0.854865000
1	0.346436000	-2.405561000	2.079328000
1	1.146658000	-0.826746000	0.335790000
1	0.769820000	-1.976186000	-0.930639000
1	2.401583000	-3.603857000	0.045248000
1	2.860858000	-2.435630000	1.267364000
1	3.077669000	-1.661735000	-1.674683000
1	4.266959000	-2.748913000	-0.995835000
1	5.178418000	-0.540434000	-0.920341000
1	4.917039000	-1.116194000	0.717038000
1	4.354138000	1.235638000	0.569796000
1	2.905382000	0.326279000	0.936100000
1	3.644935000	1.173521000	-1.912915000
1	2.092722000	0.567540000	-1.379494000
1	3.393459000	3.236057000	-0.618499000
1	2.045786000	3.027830000	-1.725770000
1	1.954096000	2.383467000	1.271579000
1	1.403218000	3.885445000	0.563929000
1	-0.391726000	2.763272000	-0.659086000
1	0.233778000	1.177124000	-0.254964000
1	-0.205329000	1.528058000	2.139740000
1	-0.787497000	3.162393000	1.838191000
1	-2.633203000	1.532920000	2.168502000
1	-2.731485000	2.305722000	0.585112000
6	-4.111295000	-0.881734000	-1.200364000
1	-4.333683000	-1.038757000	-2.261062000

1	-3.904810000	-1.860650000	-0.756978000
6	-5.264267000	-0.186991000	-0.484255000
1	-5.498781000	0.771938000	-0.955255000
1	-5.004086000	0.002663000	0.561554000
1	-6.163043000	-0.814156000	-0.505128000

1	-5.092592000	1.089671000	-2.189420000
1	-4.052893000	1.936628000	-1.041766000
1	-5.815217000	2.042949000	-0.875857000

### EtTPDL open (III)

#### TPDL TS2

$E = -1101.75751599$   
 $E(D3) = -1101.81412909$   
 $G_{298.15,1M} = -1101.361627$   
 $G_{373.15,1M} = -1101.380467$   
 $G(D3)_{298.15,1M} = -1101.418240$   
 $G(D3)_{373.15,1M} = -1101.437080$   
 $\tilde{\nu}_{TS} = 575.7090i$

16	-3.659954000	-1.070239000	-0.625256000
6	-2.161864000	-0.348165000	0.051509000
6	-2.214879000	0.709953000	1.131400000
6	-0.830132000	1.257934000	1.502522000
6	-0.077103000	1.917531000	0.340782000
6	1.209850000	2.618192000	0.800148000
6	2.199608000	2.923811000	-0.337550000
6	2.927216000	1.694884000	-0.915992000
6	3.814999000	0.975746000	0.109392000
6	4.725511000	-0.117662000	-0.471914000
6	4.013012000	-1.374707000	-1.005220000
6	3.156237000	-2.113176000	0.052567000
6	1.648177000	-1.931542000	-0.157984000
6	0.797695000	-2.427637000	1.022158000
6	-0.660662000	-2.557151000	0.702753000
8	-1.090551000	-0.976238000	-0.227567000
1	-1.365230000	-2.539215000	1.531250000
1	-0.923168000	-3.264345000	-0.079657000
1	1.170546000	-3.415138000	1.346901000
1	0.940574000	-1.757183000	1.879456000
1	1.413847000	-0.877965000	-0.327834000
1	1.346794000	-2.454251000	-1.075467000
1	3.385439000	-3.186405000	0.044819000
1	3.430282000	-1.762846000	1.057655000
1	3.381669000	-1.107396000	-1.862584000
1	4.779863000	-2.050135000	-1.402654000
1	5.335670000	0.316453000	-1.275879000
1	5.430652000	-0.432012000	0.309722000
1	4.446999000	1.724768000	0.606640000
1	3.191849000	0.541200000	0.900469000
1	3.552772000	2.024484000	-1.756800000
1	2.200637000	0.992646000	-1.341387000
1	2.956812000	3.630261000	0.029045000
1	1.665487000	3.441540000	-1.145810000
1	1.707622000	2.001182000	1.559298000
1	0.944712000	3.553050000	1.311384000
1	-0.728767000	2.646987000	-0.161177000
1	0.149486000	1.148919000	-0.402857000
1	-0.215286000	0.442201000	1.900975000
1	-0.957503000	1.981104000	2.319062000
1	-2.696323000	0.286667000	2.029349000
1	-2.860754000	1.536222000	0.811610000
6	-4.992122000	0.140348000	-0.238505000
1	-5.916080000	-0.430318000	-0.373170000
1	-4.937738000	0.410663000	0.819466000
6	-4.986624000	1.375531000	-1.139424000

16	-3.578316000	-0.937483000	-0.973542000
6	-2.090057000	-0.472252000	-0.051908000
6	-2.196921000	0.507527000	1.109360000
6	-0.837149000	0.887711000	1.706130000
6	0.021955000	1.746851000	0.770918000
6	1.365688000	2.140460000	1.397417000
6	2.296593000	2.921903000	0.451602000
6	2.794772000	2.121765000	-0.765126000
6	3.774483000	0.992611000	-0.405415000
6	4.004016000	-0.029608000	-1.534691000
6	2.790035000	-0.890733000	-1.940196000
6	2.434315000	-2.075665000	-1.024233000
6	1.985918000	-1.710766000	0.398460000
6	1.205406000	-2.836579000	1.093251000
6	0.830114000	-2.511460000	2.498780000
8	-1.058335000	-1.015107000	-0.383428000
1	1.506006000	-1.942898000	3.131859000
1	-0.028637000	-2.974605000	2.974047000
1	0.304194000	-3.058448000	0.508048000
1	1.814514000	-3.761115000	1.066720000
1	2.854701000	-1.448539000	1.015356000
1	1.341028000	-0.829084000	0.358331000
1	1.616987000	-2.626676000	-1.508159000
1	3.284373000	-2.771327000	-0.974935000
1	1.899475000	-0.258405000	-2.048419000
1	2.985554000	-1.295081000	-2.941855000
1	4.352367000	0.517285000	-2.422008000
1	4.829276000	-0.697230000	-1.250905000
1	4.738732000	1.442290000	-0.132014000
1	3.427180000	0.473990000	0.490419000
1	3.283519000	2.804203000	-1.472864000
1	1.931413000	1.712714000	-1.300973000
1	3.163782000	3.281594000	1.021936000
1	1.768264000	3.819166000	0.101418000
1	1.870399000	1.232999000	1.751815000
1	1.176760000	2.746890000	2.293584000
1	-0.530603000	2.656853000	0.493470000
1	0.187820000	1.189933000	-0.155971000
1	-0.296148000	-0.028968000	1.969236000
1	-1.016426000	1.430479000	2.643117000
1	-2.832299000	0.031428000	1.868213000
1	-2.738153000	1.401584000	0.779530000
6	-4.942960000	0.142740000	-0.360951000
1	-5.848159000	-0.431562000	-0.580686000
1	-4.880174000	0.224559000	0.726856000
6	-5.000837000	1.513489000	-1.034016000
1	-5.105044000	1.410306000	-2.117412000
1	-4.095605000	2.096691000	-0.842379000
1	-5.857587000	2.083599000	-0.657578000

**EtTPDL+VAc TS3**

E = -1408.25325093  
E(D3) = -1408.32988744  
 $G_{298.15,1M} = -1407.767264$   
 $G_{373.15,1M} = -1407.790378$   
 $G(D3)_{298.15,1M} = -1407.8439$   
 $G(D3)_{373.15,1M} = -1407.867014$   
 $\tilde{\nu}_{TS} = 414.0095i$

16	-0.397648000	2.152106000	-1.196267000
6	-1.199844000	1.034024000	0.016012000
6	-1.140148000	1.433943000	1.478280000
6	0.102259000	0.933800000	2.243359000
6	1.452488000	1.370553000	1.670457000
6	2.632317000	0.898659000	2.528054000
6	4.009138000	1.140001000	1.887325000
6	4.290165000	0.329061000	0.690944000
6	4.239517000	-1.191811000	0.816198000
6	4.823077000	-2.007579000	-0.347930000
6	4.090563000	-1.910658000	-1.698495000
6	2.648332000	-2.463704000	-1.706203000
6	1.556850000	-1.413409000	-1.465016000
6	0.143084000	-2.005341000	-1.470305000
6	-0.949828000	-0.951154000	-1.380216000
8	-0.802350000	-0.267728000	-0.120568000
1	-1.947406000	-1.399417000	-1.408901000
1	-0.863379000	-0.236171000	-2.205264000
1	-0.022128000	-2.579884000	-2.392057000
1	0.032299000	-2.710590000	-0.635974000
1	1.718981000	-0.902883000	-0.511936000
1	1.626856000	-0.638511000	-2.241550000
1	2.449572000	-2.942123000	-2.674524000
1	2.559402000	-3.262685000	-0.956115000
1	4.084691000	-0.870526000	-2.050042000
1	4.687411000	-2.466655000	-2.431908000
1	5.867989000	-1.701227000	-0.496195000
1	4.856842000	-3.065627000	-0.053385000
1	4.804618000	-1.439897000	1.725684000
1	3.209125000	-1.513027000	1.011527000
1	5.288851000	0.601010000	0.240405000
1	3.590927000	0.622732000	-0.182574000
1	4.788145000	0.903813000	2.625131000
1	4.115216000	2.209917000	1.662067000
1	2.513940000	-0.170144000	2.750634000
1	2.596043000	1.409099000	3.499938000
1	1.485839000	2.463433000	1.564955000
1	1.547330000	0.973068000	0.656195000
1	0.068263000	-0.161089000	2.270102000
1	0.014222000	1.274832000	3.283979000
1	-2.028399000	1.018429000	1.969286000
1	-1.215143000	2.524146000	1.553686000
6	-1.489894000	3.632089000	-1.137236000
1	-2.416668000	3.416930000	-1.675414000
1	-1.743123000	3.840910000	-0.093728000
6	-0.769462000	4.827067000	-1.760512000
1	-0.495458000	4.628697000	-2.801341000
1	0.143927000	5.068841000	-1.209608000
1	-1.423118000	5.705351000	-1.746771000
6	-3.387498000	1.005703000	-0.428335000
1	-3.566269000	2.033742000	-0.137762000

1	-3.205181000	0.822732000	-1.481652000
6	-3.956517000	0.036663000	0.345862000
1	-4.324780000	0.170250000	1.354605000
8	-3.918041000	-1.276285000	-0.098888000
6	-4.193254000	-2.277496000	0.791341000
8	-4.516431000	-2.086844000	1.940308000
6	-4.013013000	-3.618120000	0.127089000
1	-2.951985000	-3.773230000	-0.095271000
1	-4.556181000	-3.651574000	-0.820933000
1	-4.364331000	-4.403244000	0.795511000

**EtTPDL-VAc° (IV)**

16	-0.421182000	2.141597000	-1.132969000
6	-1.457317000	0.922791000	-0.092267000
6	-1.370489000	1.259999000	1.412382000
6	-0.150868000	0.722587000	2.175284000
6	1.226099000	1.218546000	1.726829000
6	2.347281000	0.693843000	2.631490000
6	3.762064000	1.038981000	2.140119000
6	4.182039000	0.365240000	0.820963000
6	4.208053000	-1.168441000	0.890689000
6	4.880230000	-1.845022000	-0.313679000
6	4.188490000	-1.670317000	-1.677747000
6	2.776490000	-2.288354000	-1.783380000
6	1.625615000	-1.314576000	-1.498786000
6	0.244656000	-1.969622000	-1.611887000
6	-0.905158000	-0.974299000	-1.547577000
8	-0.868928000	-0.340775000	-0.258378000
1	-1.868727000	-1.478141000	-1.676993000
1	-0.795689000	-0.223756000	-2.339933000
1	0.161676000	-2.509684000	-2.565278000
1	0.120083000	-2.716764000	-0.816717000
1	1.726613000	-0.877878000	-0.502213000
1	1.685176000	-0.474259000	-2.204820000
1	2.634556000	-2.692201000	-2.794792000
1	2.703010000	-3.152039000	-1.106515000
1	4.140952000	-0.605957000	-1.942315000
1	4.836122000	-2.133672000	-2.432240000
1	5.910043000	-1.469838000	-0.394037000
1	4.964706000	-2.921442000	-0.109805000
1	4.748480000	-1.467258000	1.799911000
1	3.190459000	-1.559349000	1.009122000
1	5.186818000	0.721321000	0.554437000
1	3.524156000	0.693227000	0.007495000
1	4.486083000	0.759479000	2.917897000
1	3.842094000	2.128600000	2.025535000
1	2.249481000	-0.395001000	2.736163000
1	2.212225000	1.101616000	3.642685000
1	1.248791000	2.316547000	1.711136000
1	1.396296000	0.904548000	0.695026000
1	-0.166475000	-0.371099000	2.117640000
1	-0.296588000	0.978064000	3.234084000
1	-2.261225000	0.838085000	1.893246000
1	-1.446308000	2.346857000	1.529184000

6	-1.385978000	3.705724000	-1.050276000	6	-3.862155000	0.039032000	0.114604000
1	-2.277281000	3.627655000	-1.680333000	1	-4.397159000	0.271330000	1.026516000
1	-1.713301000	3.870494000	-0.018245000	8	-3.678790000	-1.298439000	-0.150052000
6	-0.510545000	4.871670000	-1.513471000	6	-4.143603000	-2.227448000	0.748114000
1	-0.160677000	4.722334000	-2.539577000	8	-4.725566000	-1.935572000	1.765344000
1	0.365885000	4.985246000	-0.869312000	6	-3.801395000	-3.613614000	0.271329000
1	-1.083087000	5.804768000	-1.485270000	1	-2.713578000	-3.723921000	0.219886000
6	-2.944117000	0.966911000	-0.589897000	1	-4.195405000	-3.775244000	-0.736014000
1	-3.322748000	1.981859000	-0.443077000	1	-4.217322000	-4.346812000	0.961128000
1	-2.949295000	0.773234000	-1.668446000				