

# Cyclic ethylene phosphates with $(\text{CH}_2)_n\text{COOR}$ and $\text{CH}_2\text{CONMe}_2$ substituents: Synthesis and mechanistic insights of diverse reactivity in aryloxy-Mg catalyzed (co)polymerization

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## Supplementary Information

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## S1. NMR spectra of 1–7

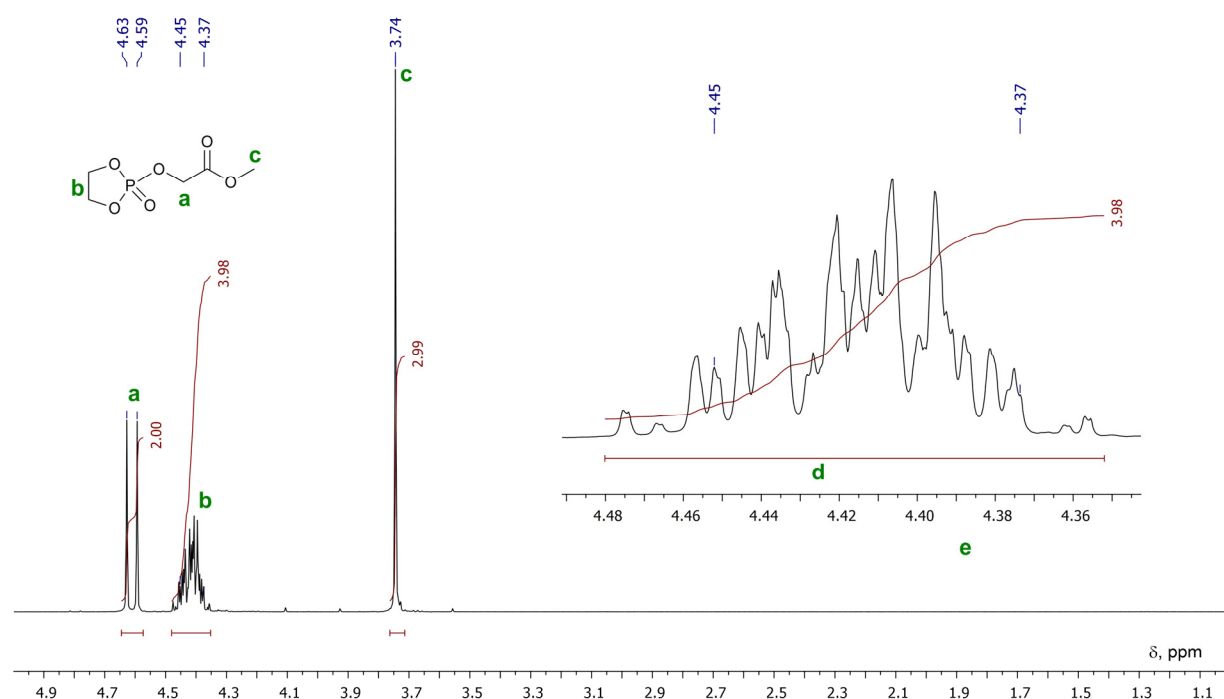


Fig. S1.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of **1**.

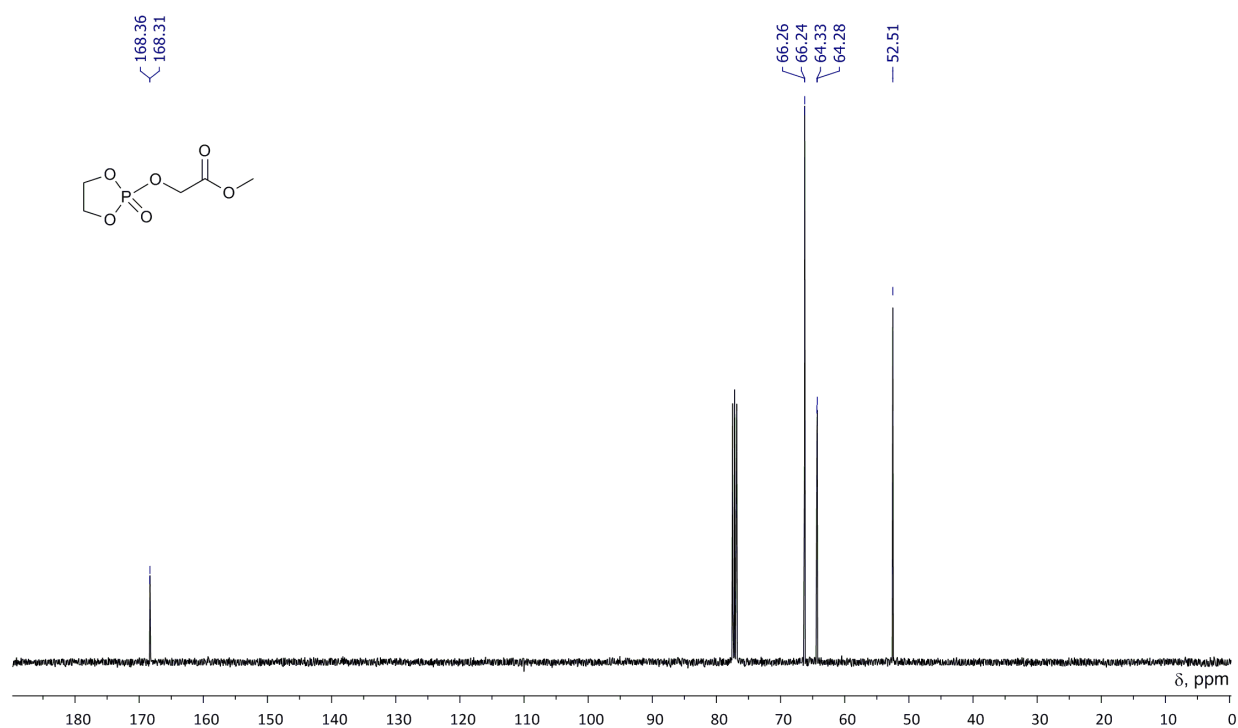
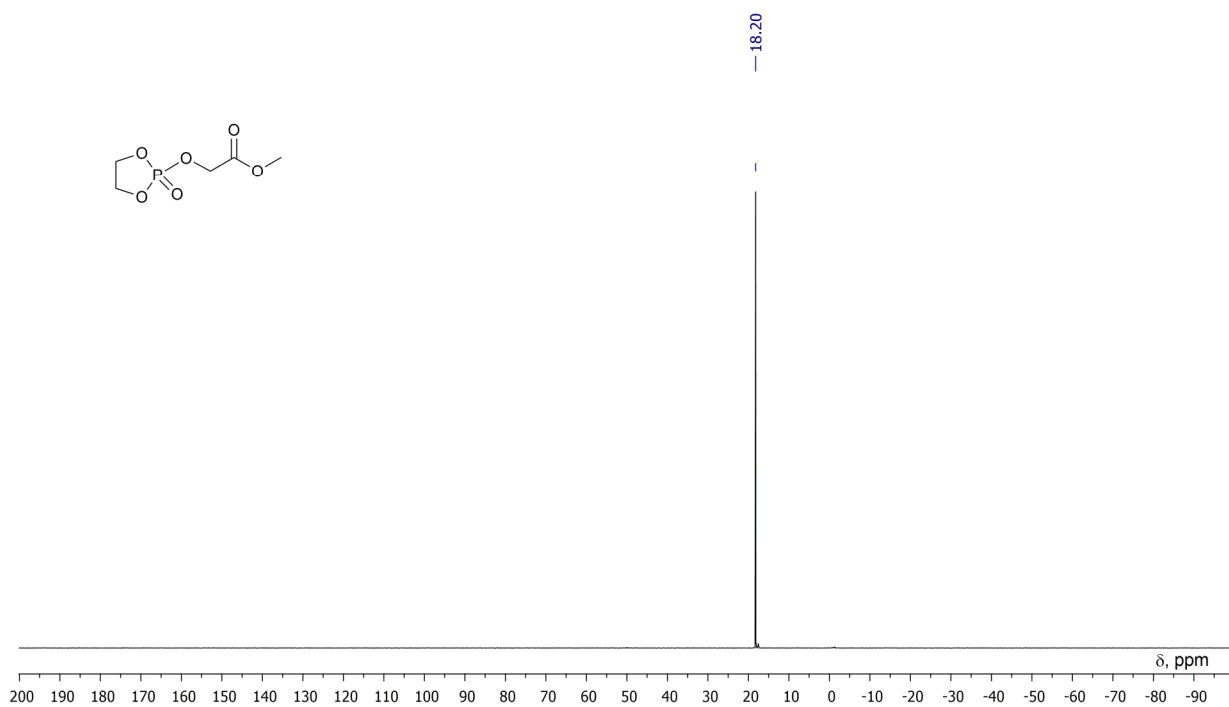
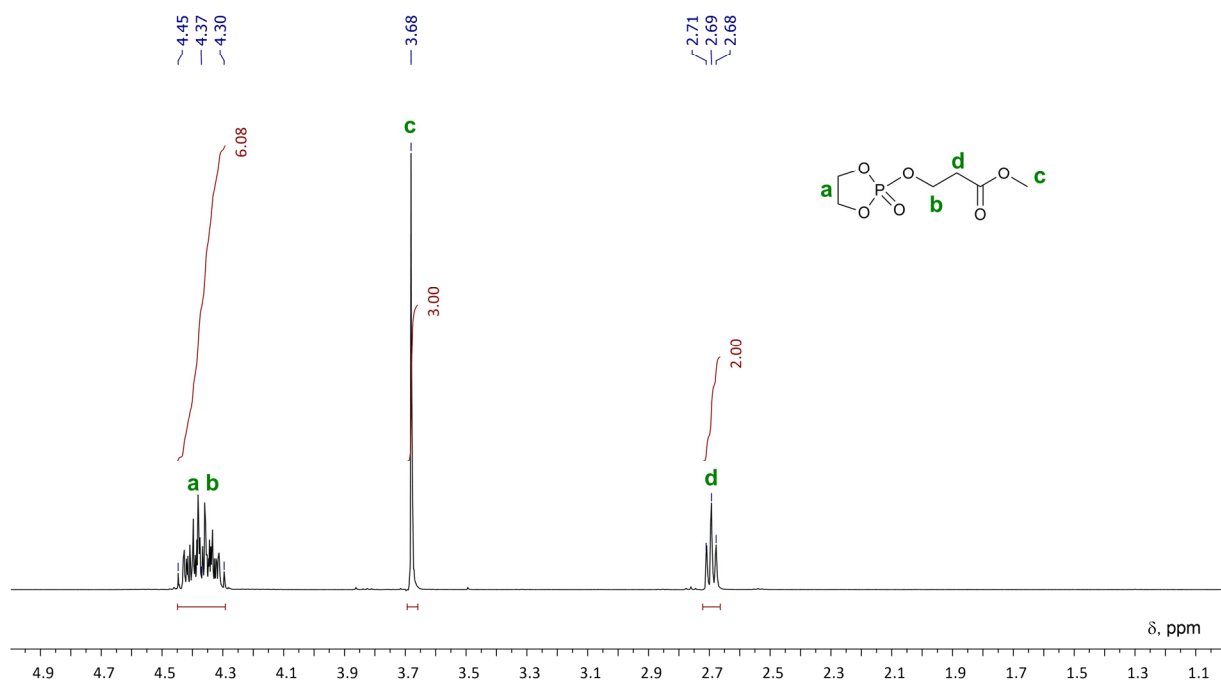


Fig. S2.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of **1**.



**Fig. S3.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of **1**.



**Fig. S4.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of **2**.

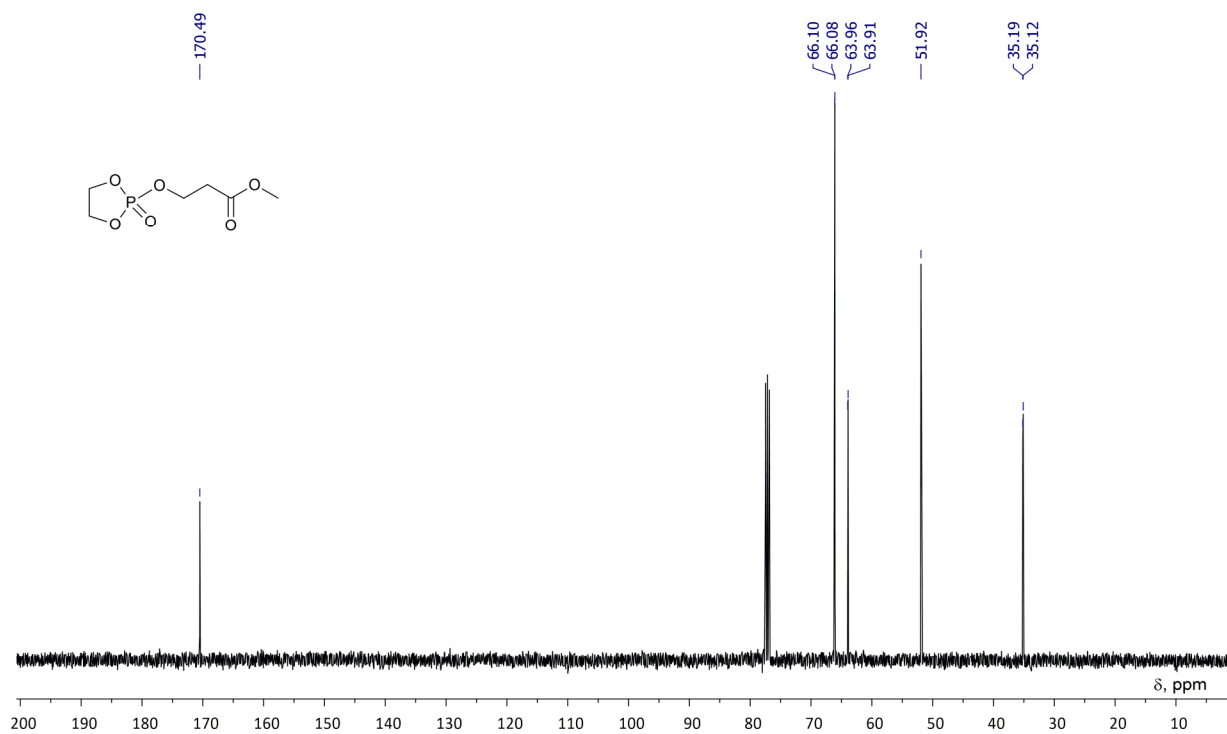


Fig. S5.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of 2.

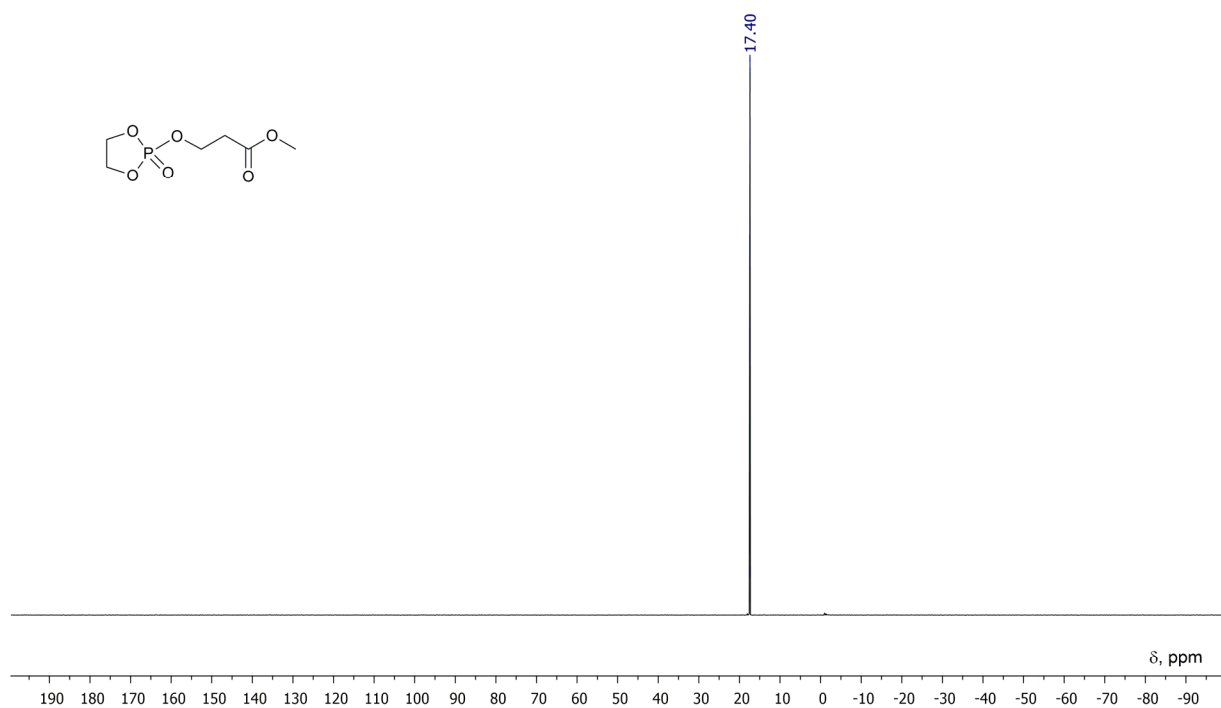


Fig. S6.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of 2.

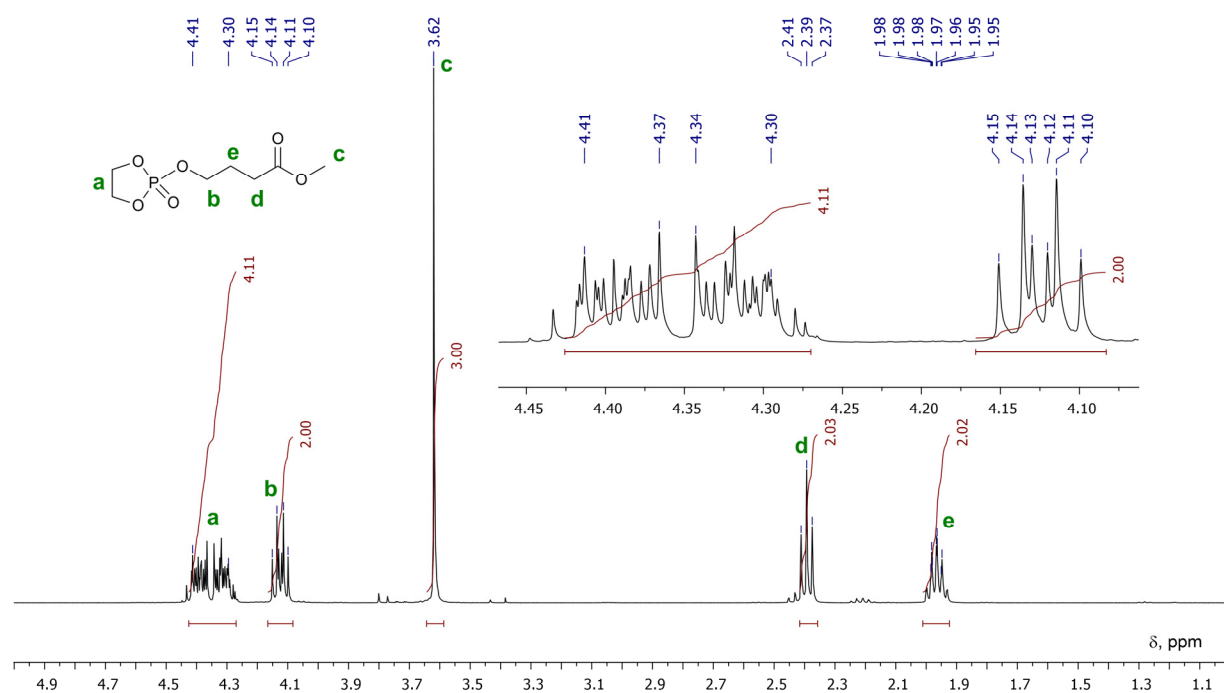


Fig. S7.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of **3**.

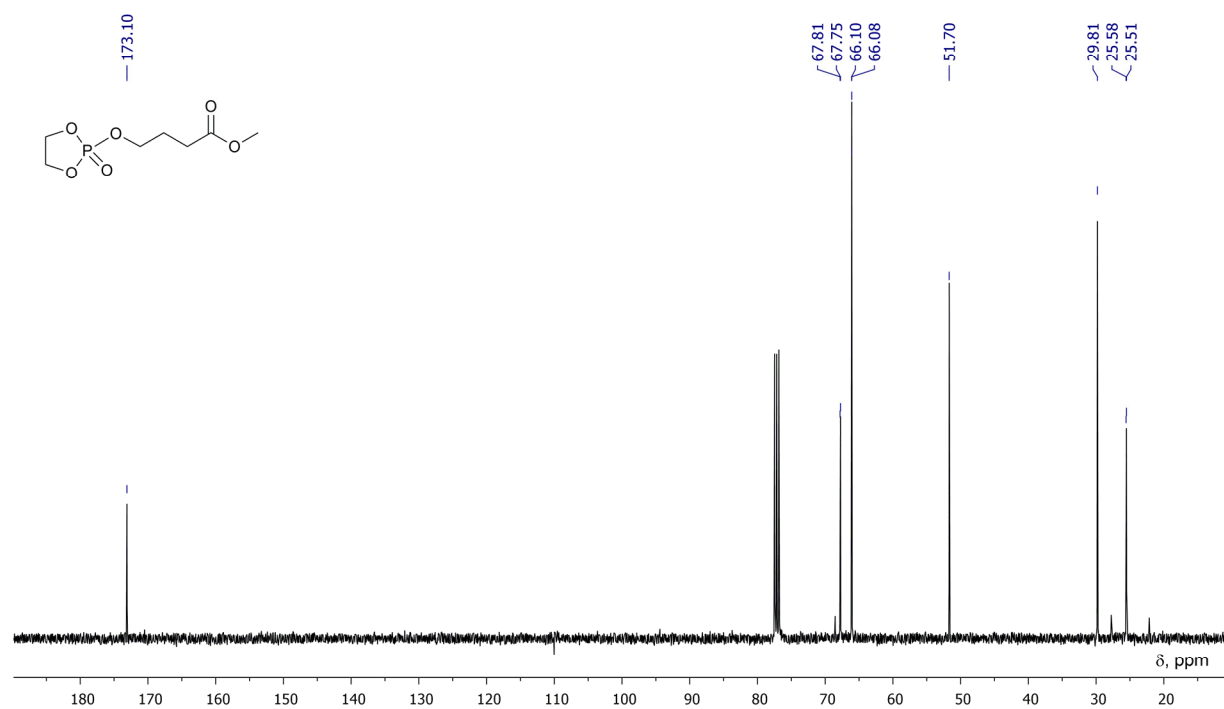
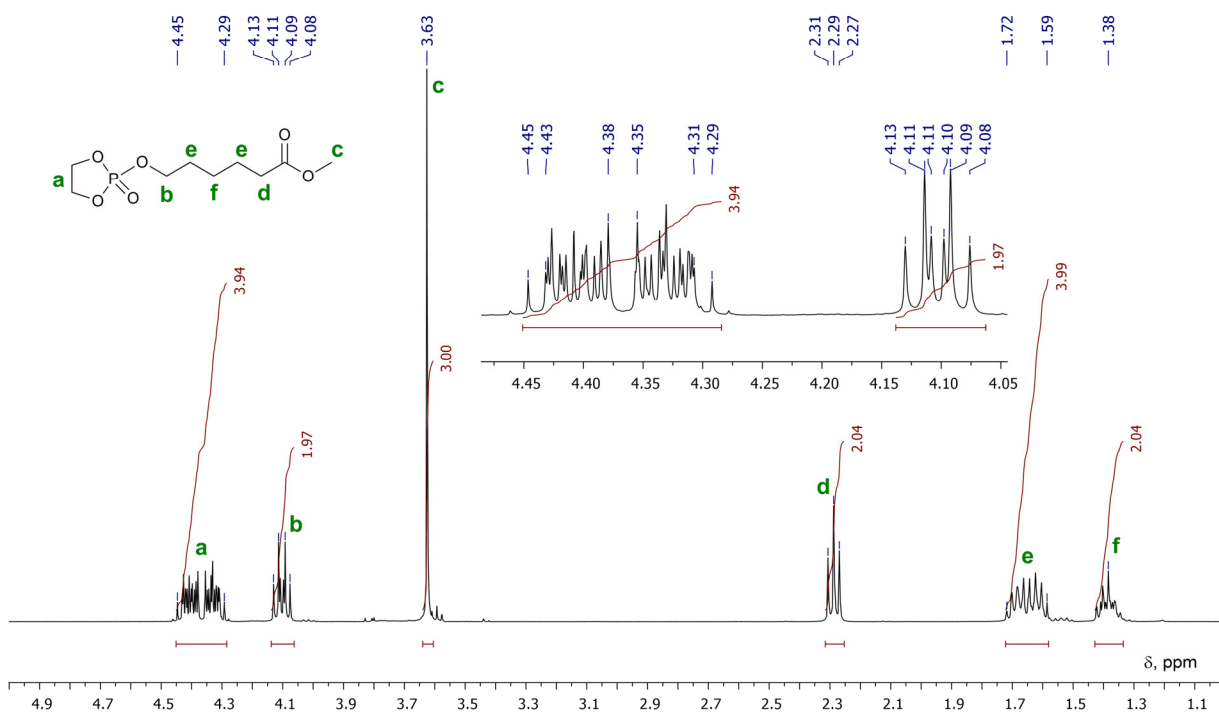


Fig. S8.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of **3**.



**Fig. S9.**  $^{31}\text{P}$  { $^1\text{H}$ } NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of **3**.



**Fig. S10.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of **4**.

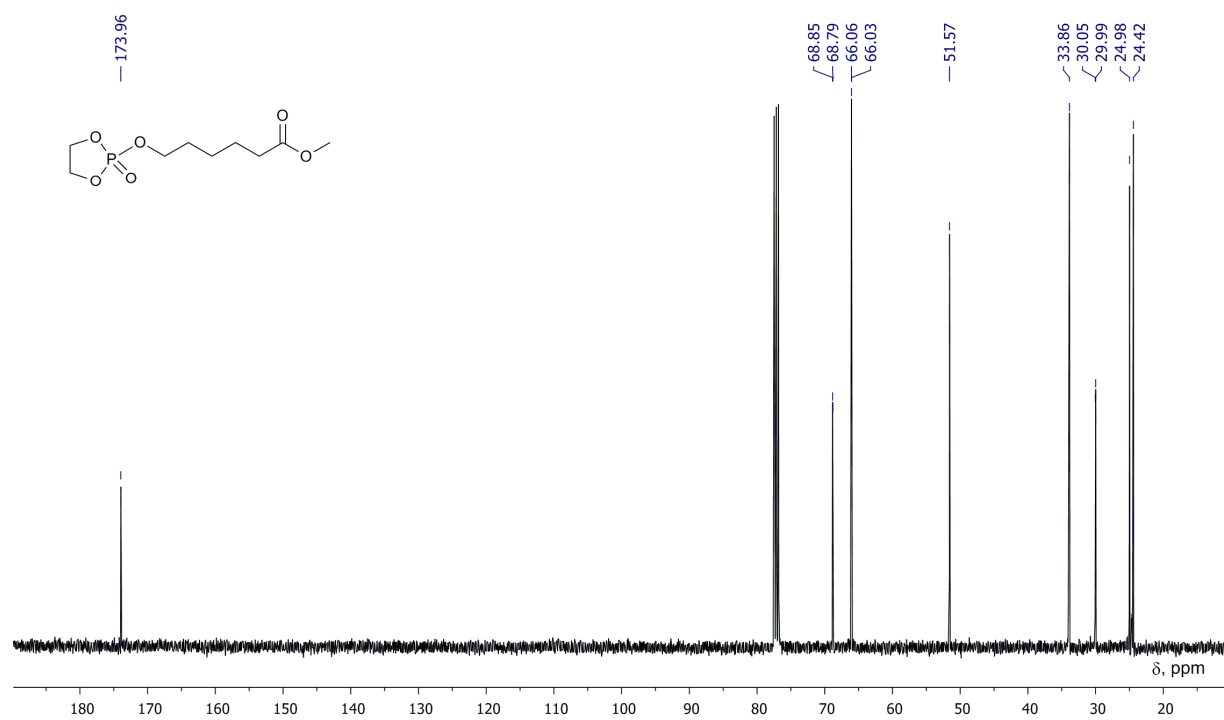


Fig. S11.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of 4.



Fig. S12.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of 4.

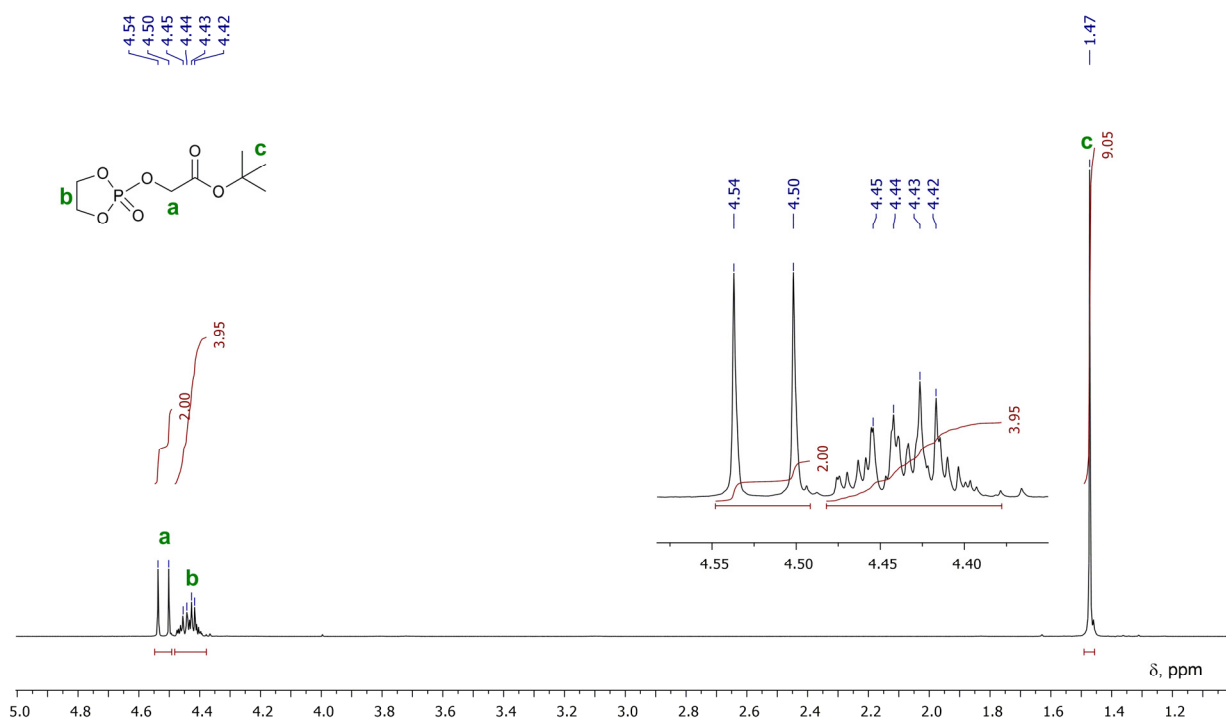


Fig. S13. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of 5.

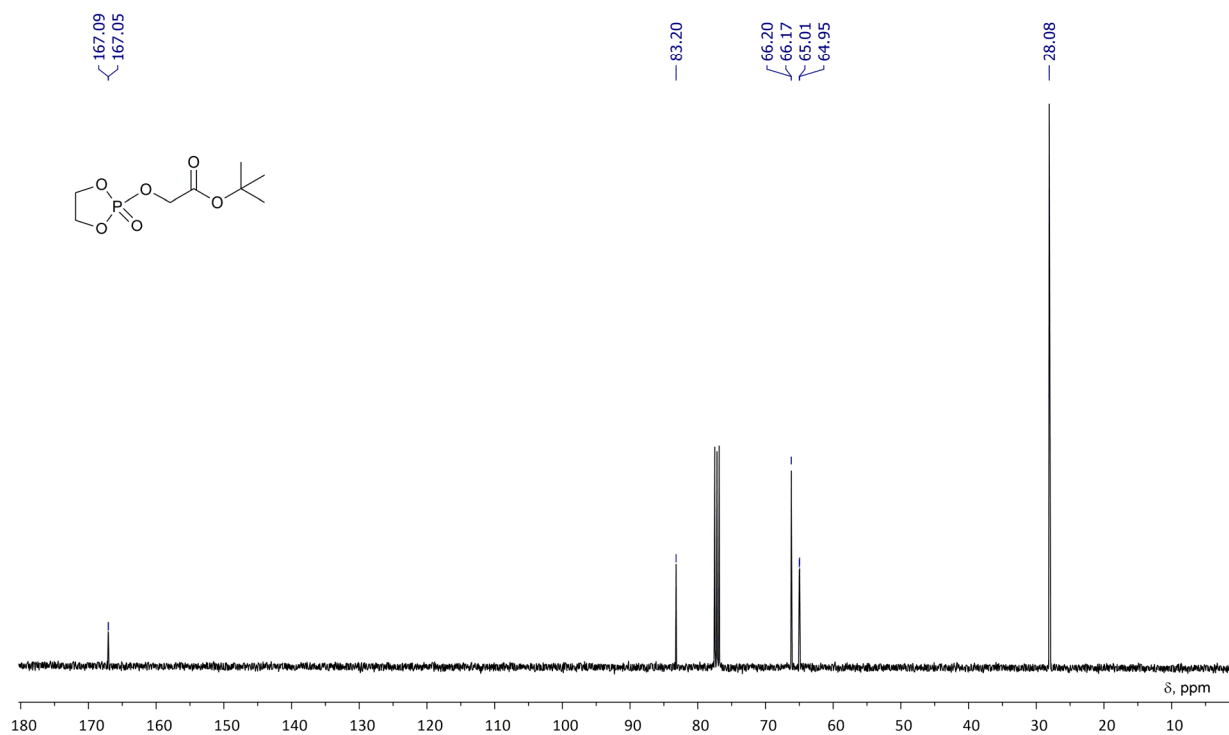


Fig. S14. <sup>13</sup>C {<sup>1</sup>H} NMR spectrum (101 MHz, CDCl<sub>3</sub>, 20 °C) of 5.



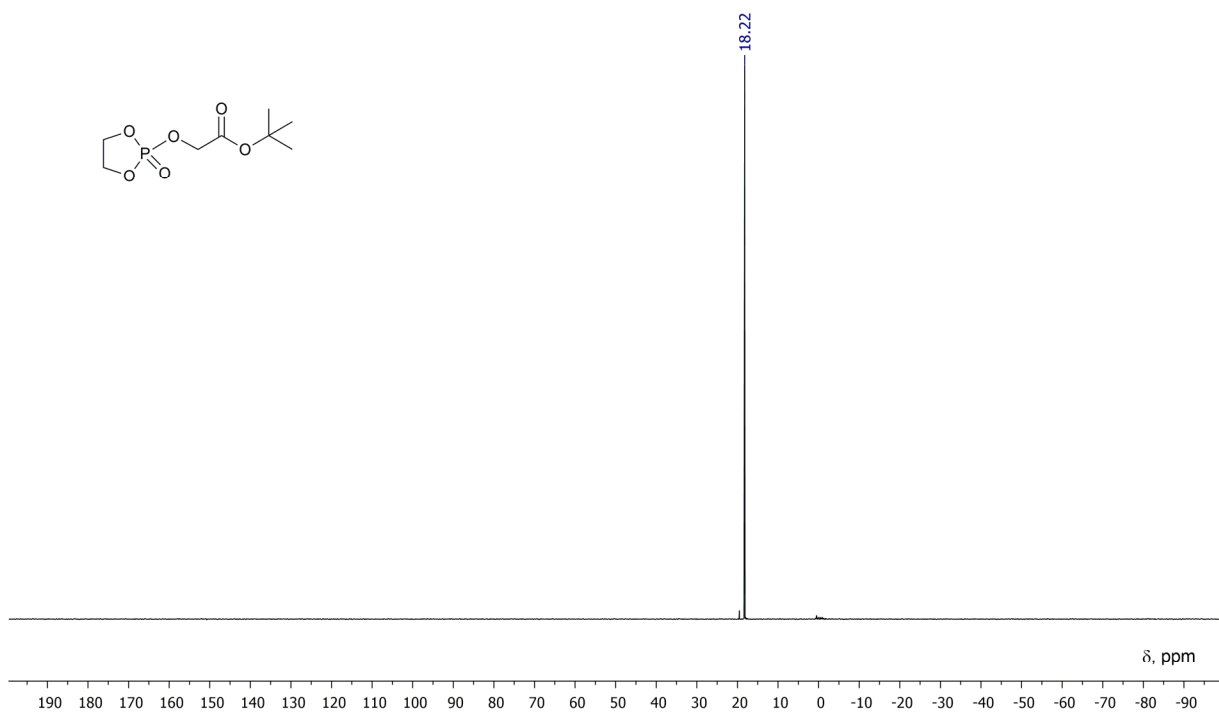


Fig. S15.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of 5.

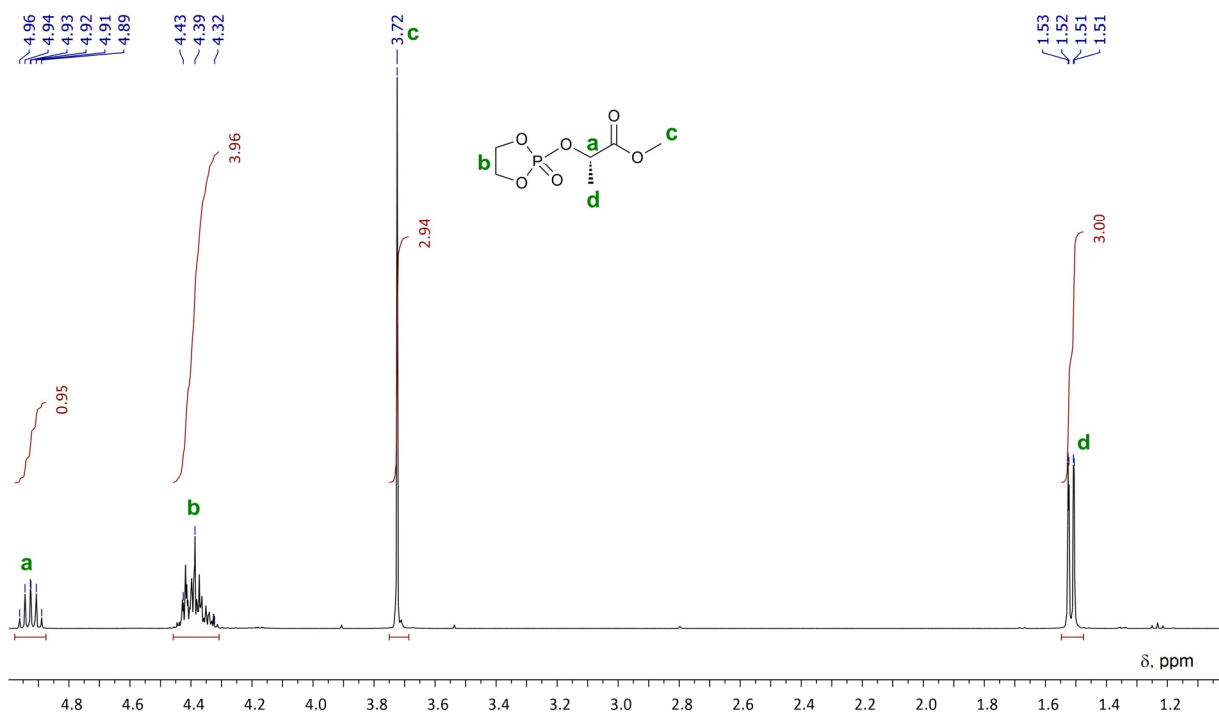


Fig. S16.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of 6.

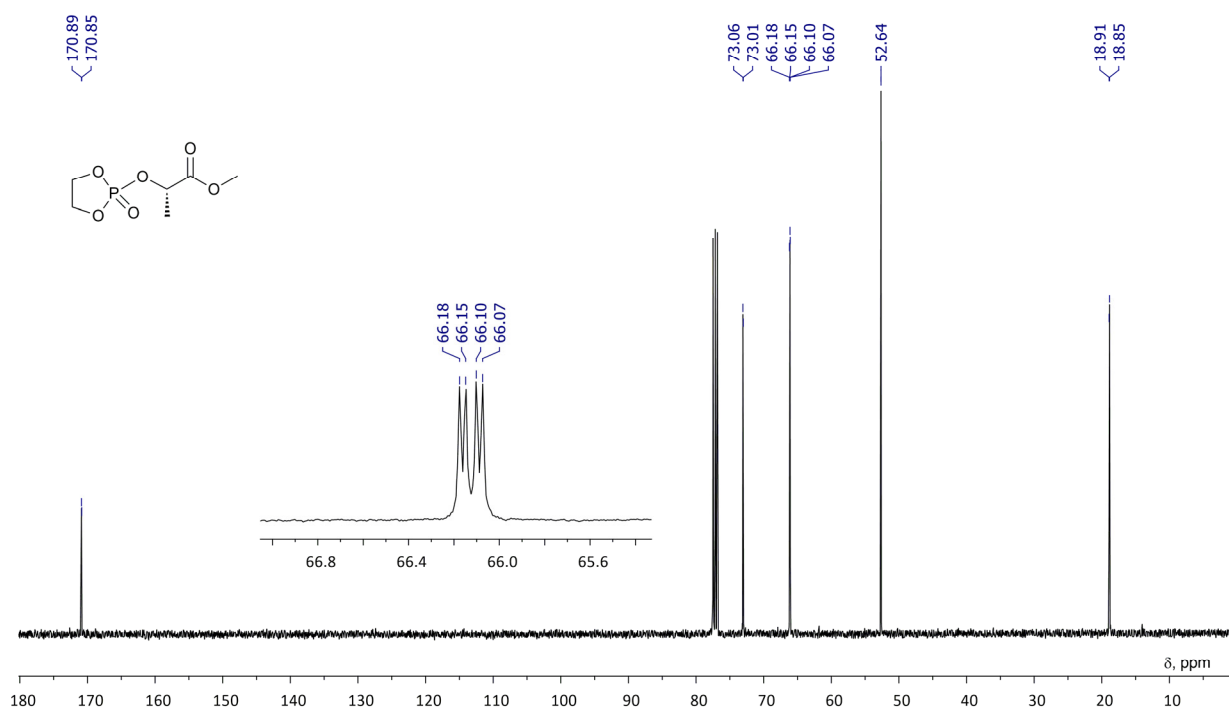


Fig. S17.  $^{13}\text{C}$  { $^1\text{H}$ } NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of 6.

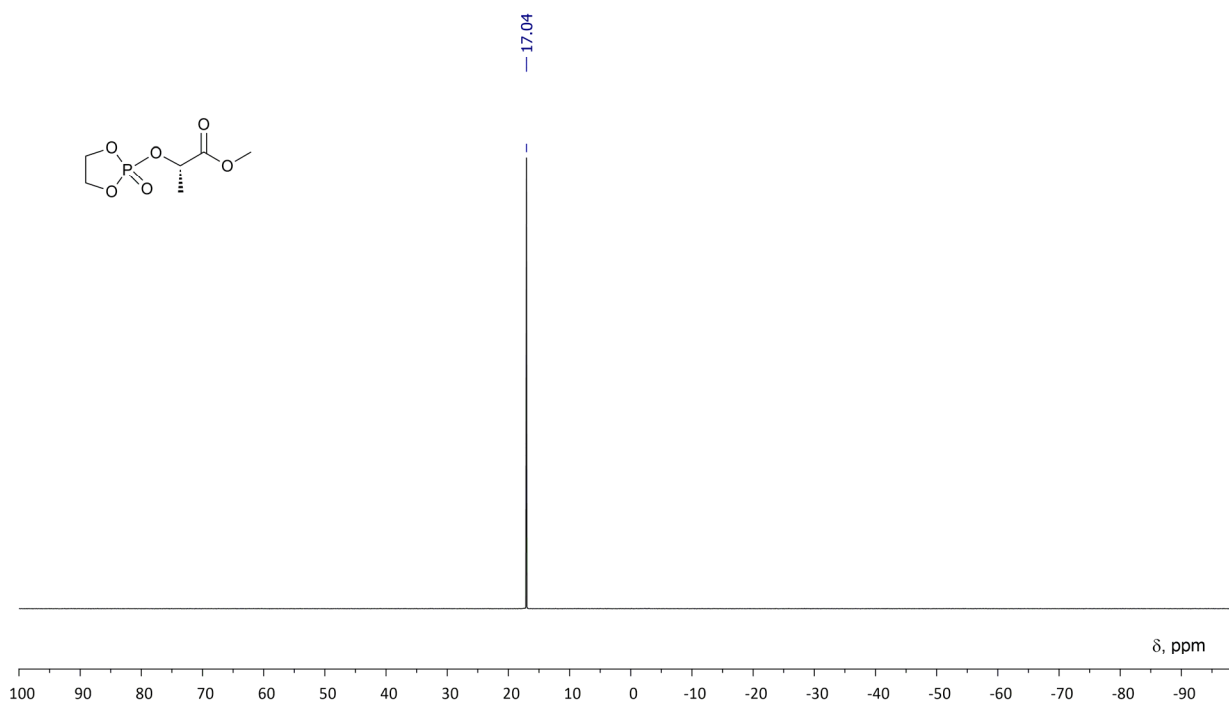


Fig. S18.  $^{31}\text{P}$  { $^1\text{H}$ } NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of 6.

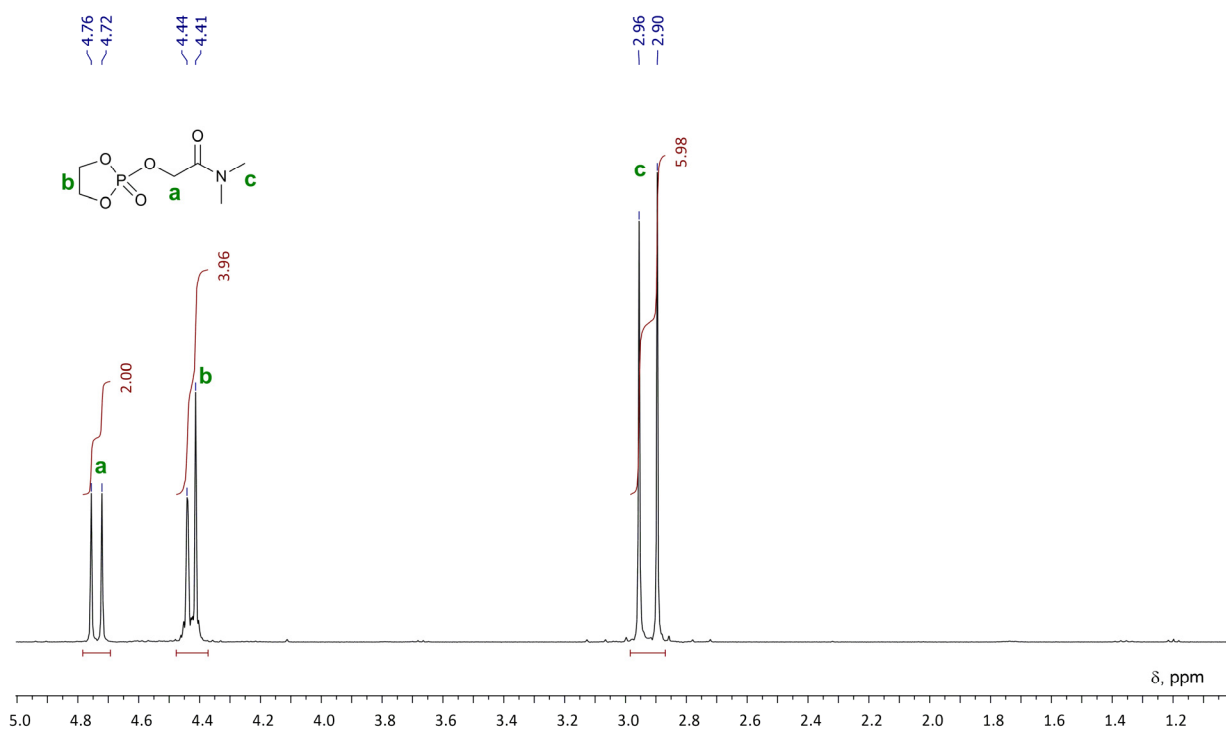


Fig. S19.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of 7.

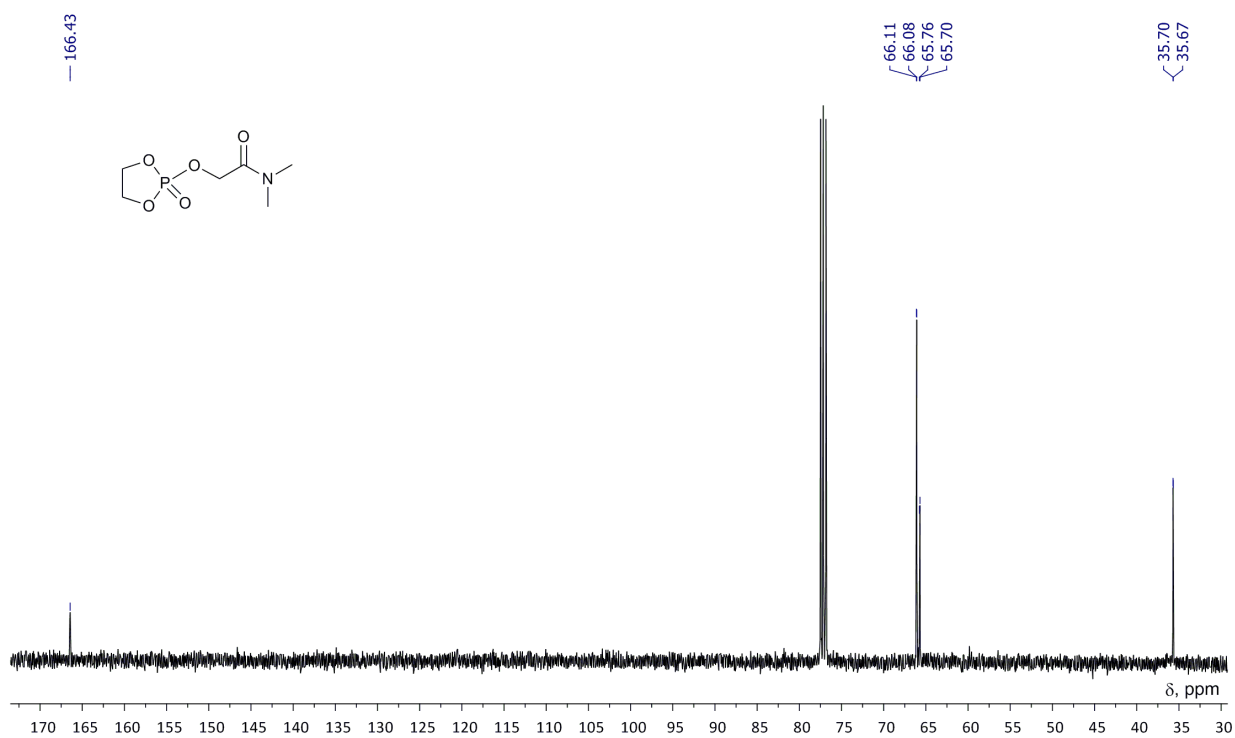
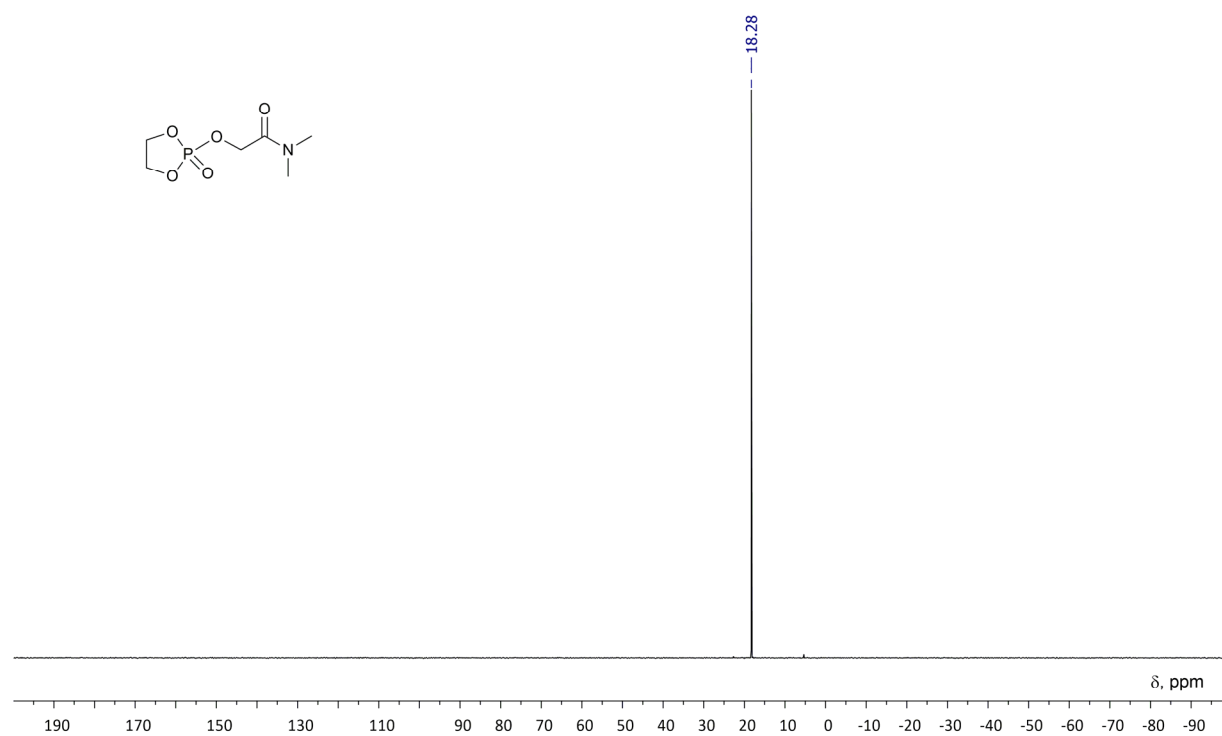


Fig. S20.  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ , 20 °C) of 7.



**Fig. S21.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of 7.

## S2. Synthesis and spectra of the homopolymers of 1–6

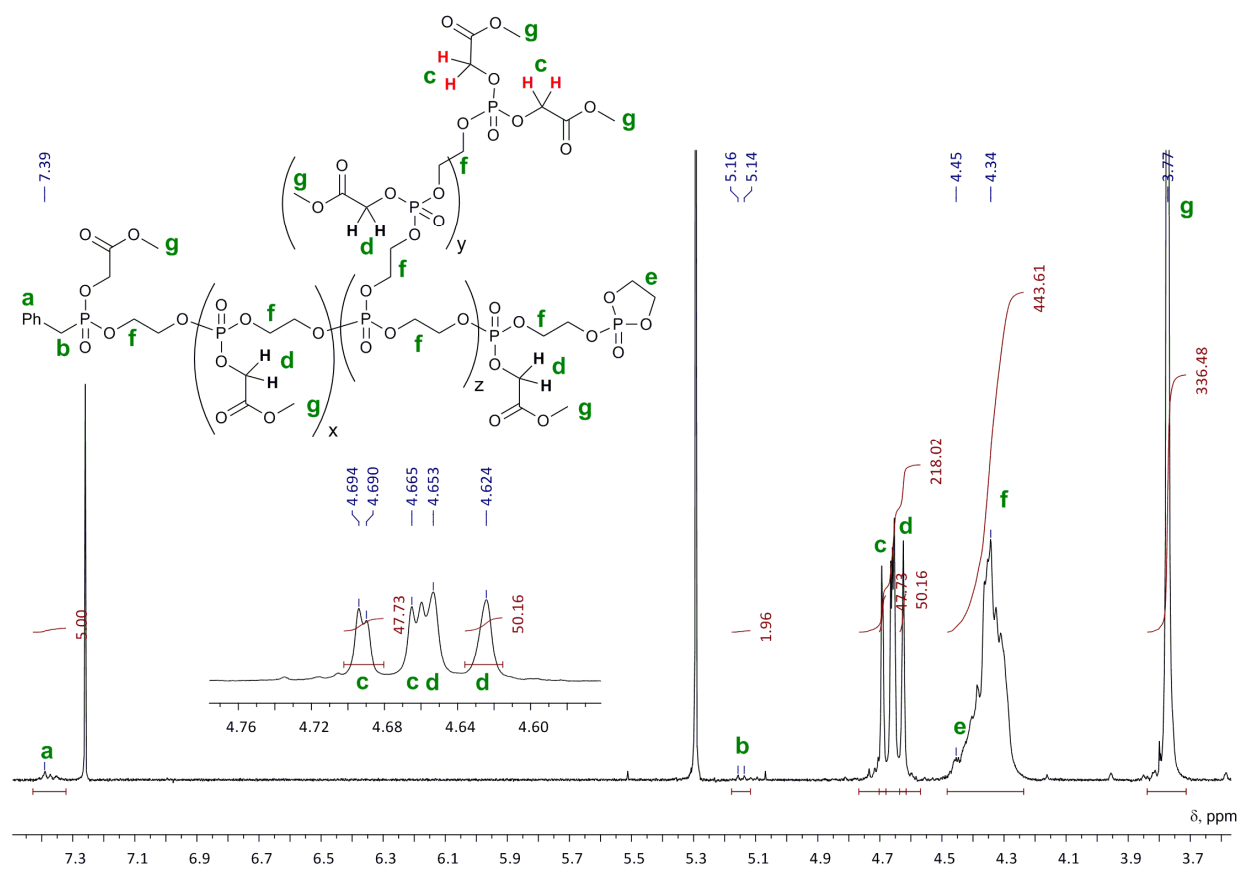


Fig. S22.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 1.

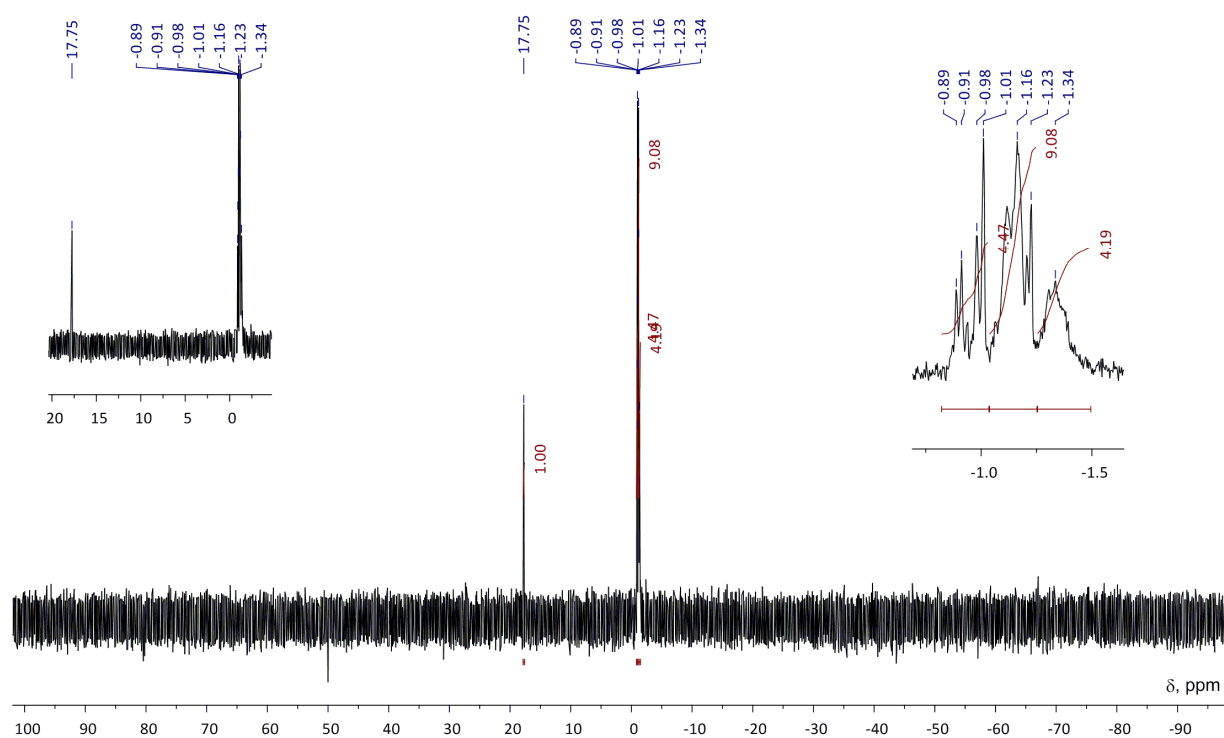
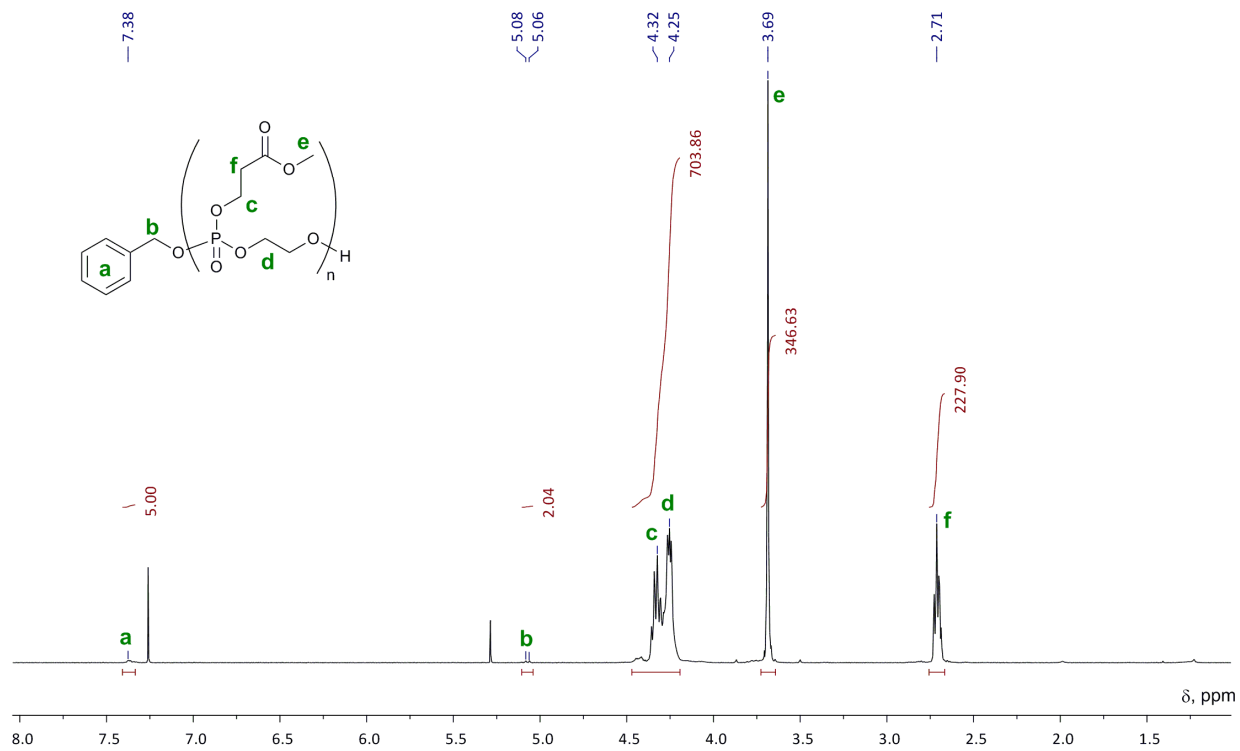
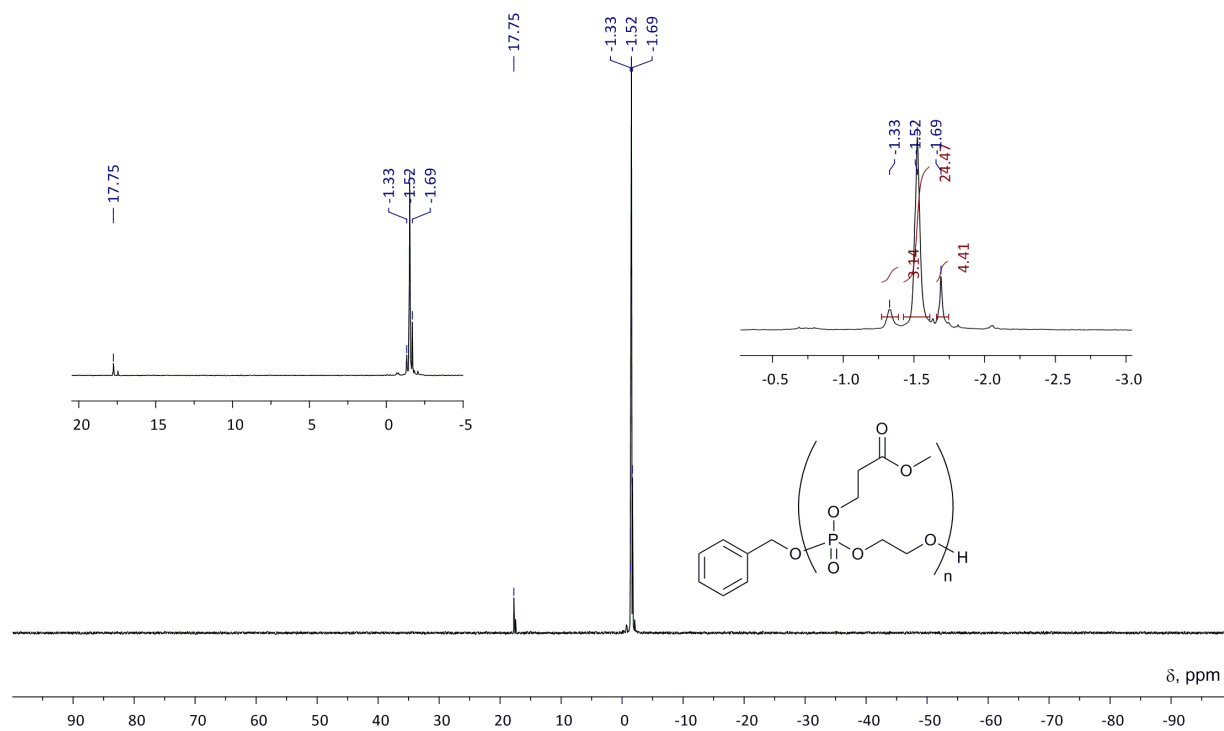


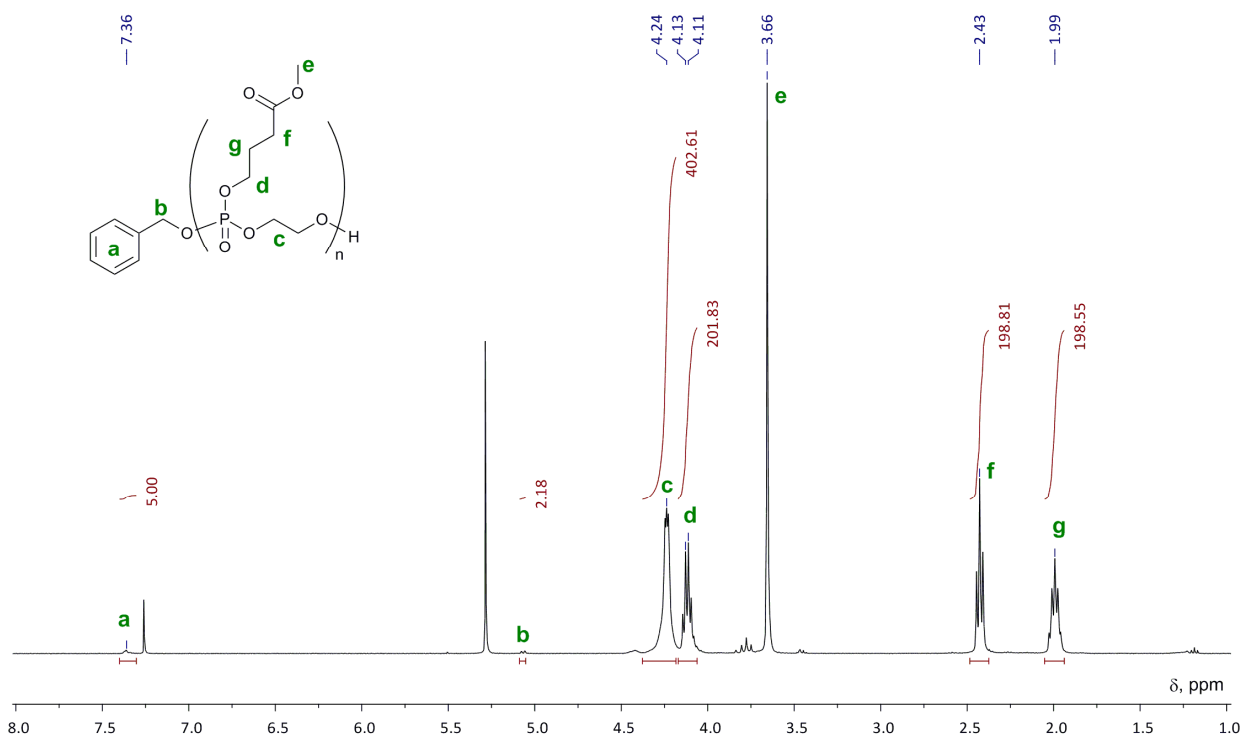
Fig. S23.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 1.



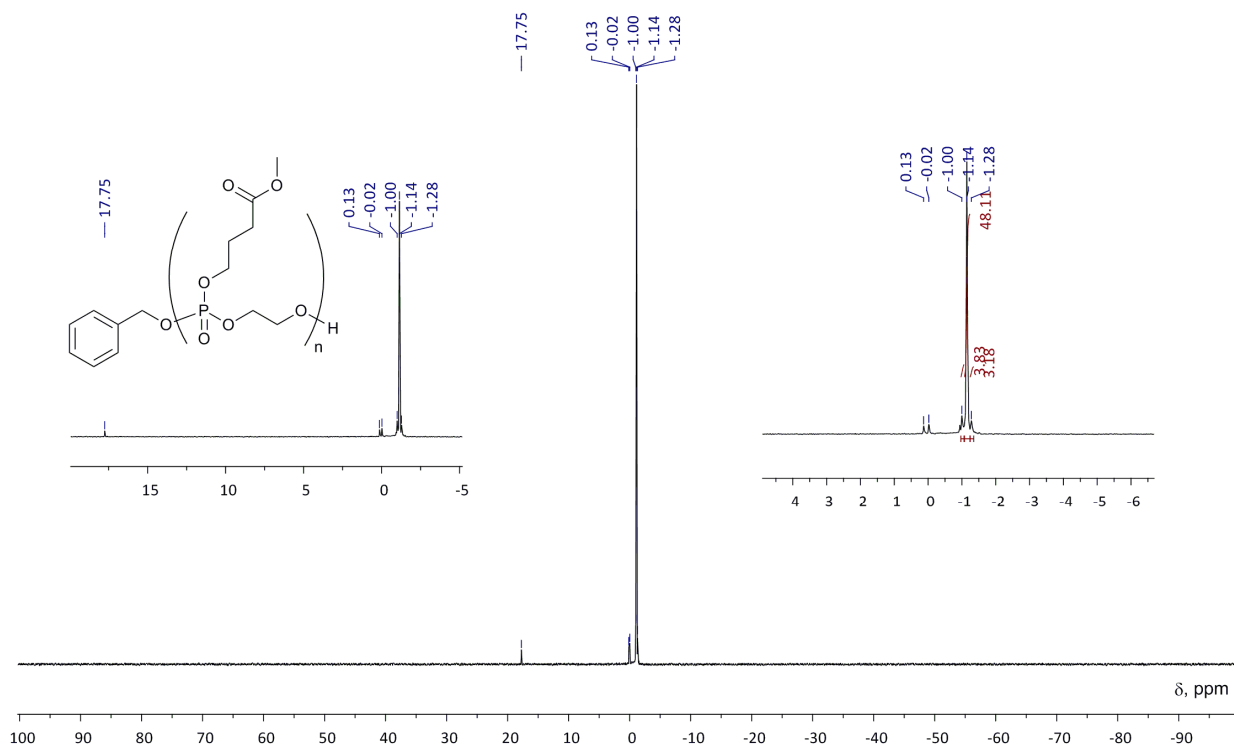
**Fig. S24.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **2**.



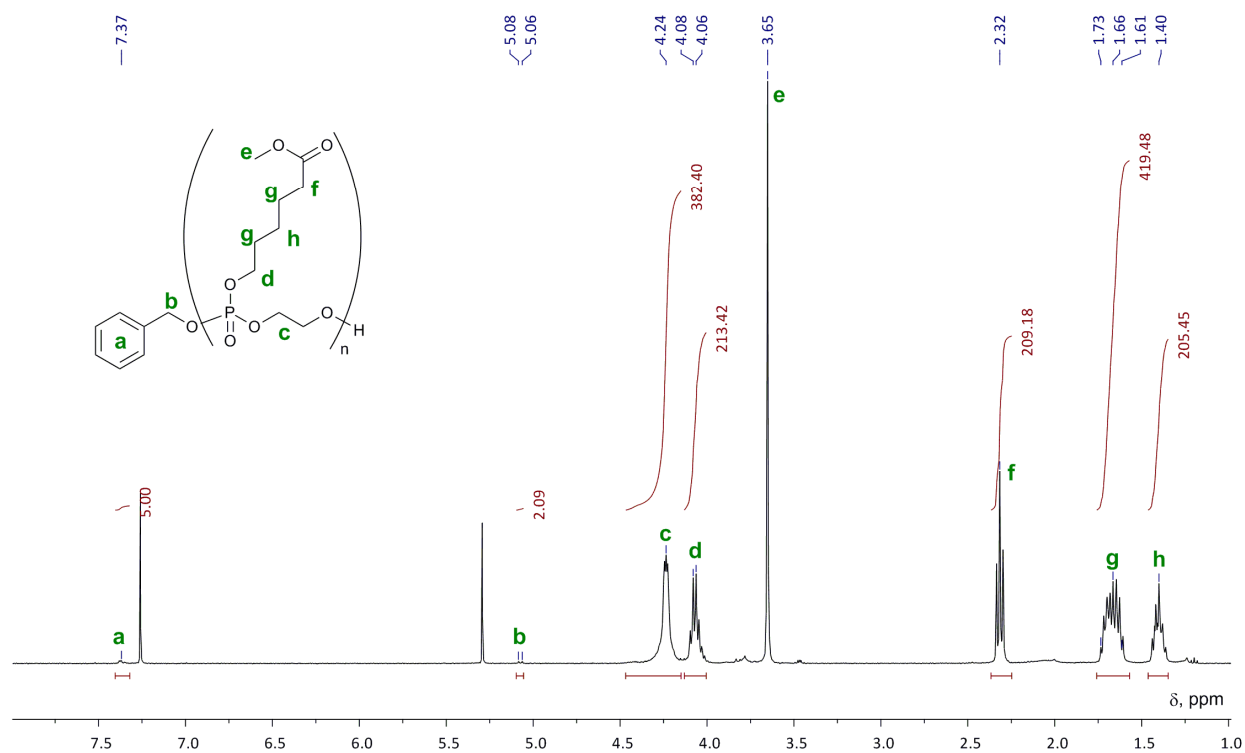
**Fig. S25.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **2**.



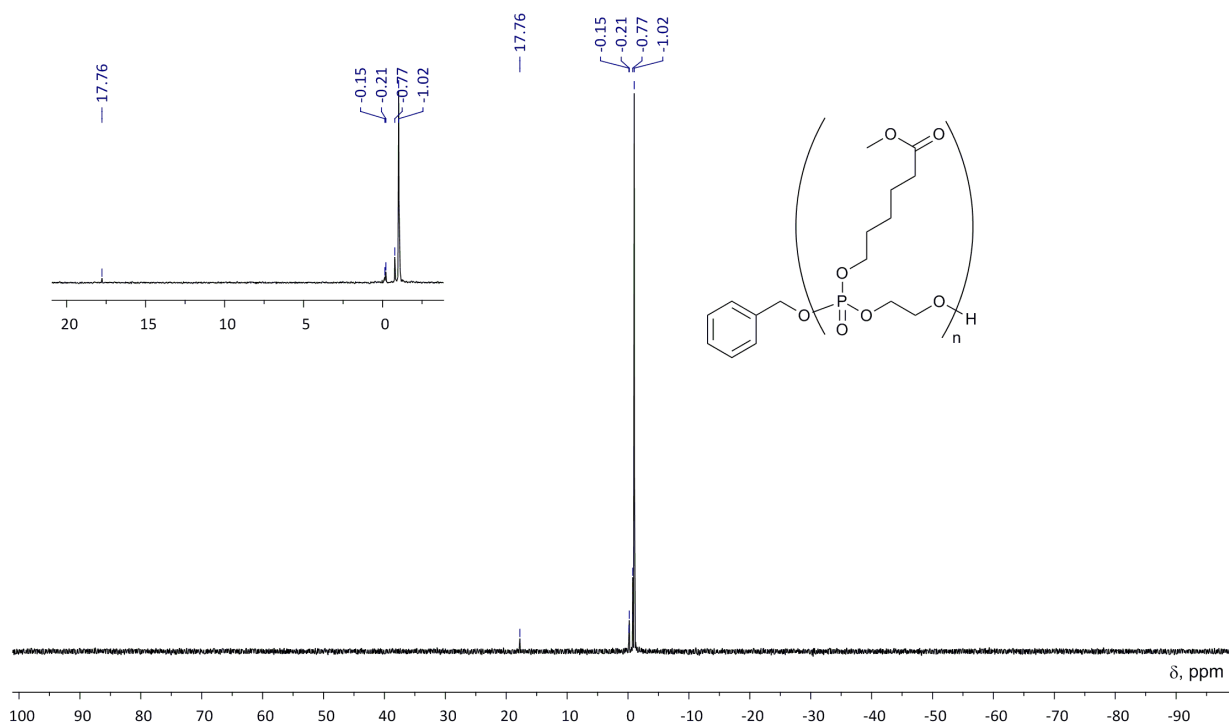
**Fig. S26.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **3**.



**Fig. S27.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **3**.

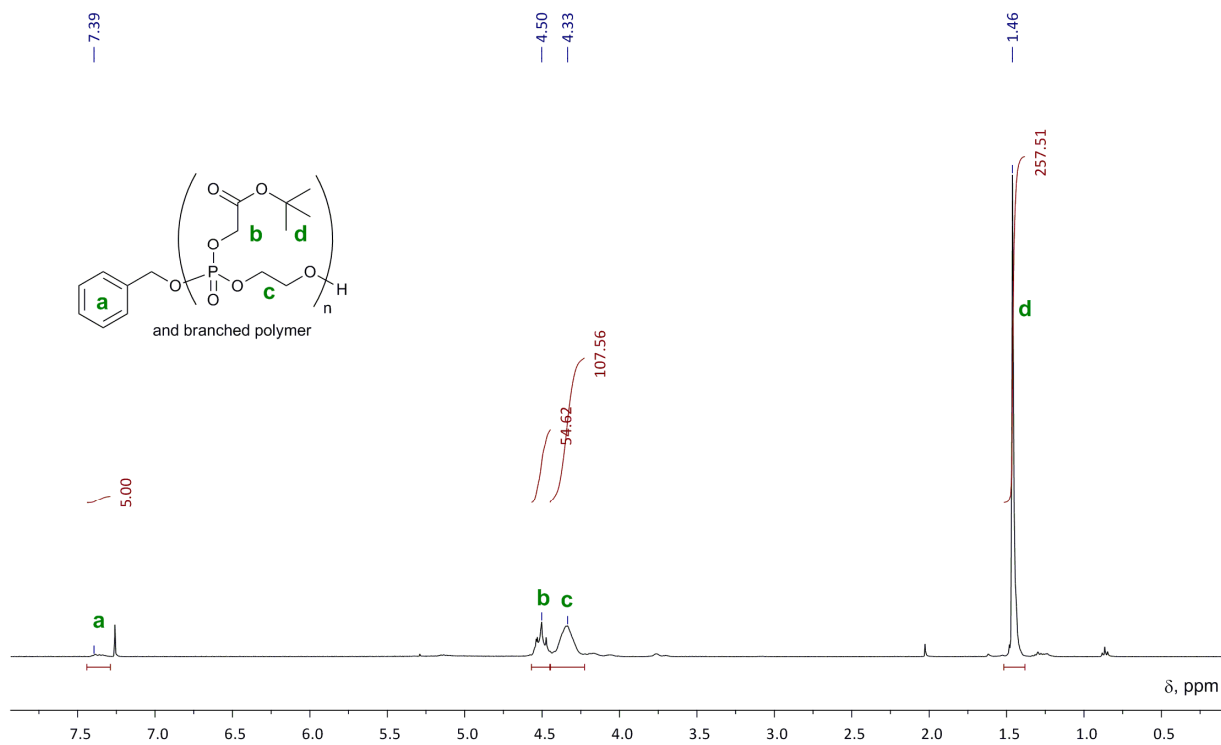


**Fig. S28.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 4.

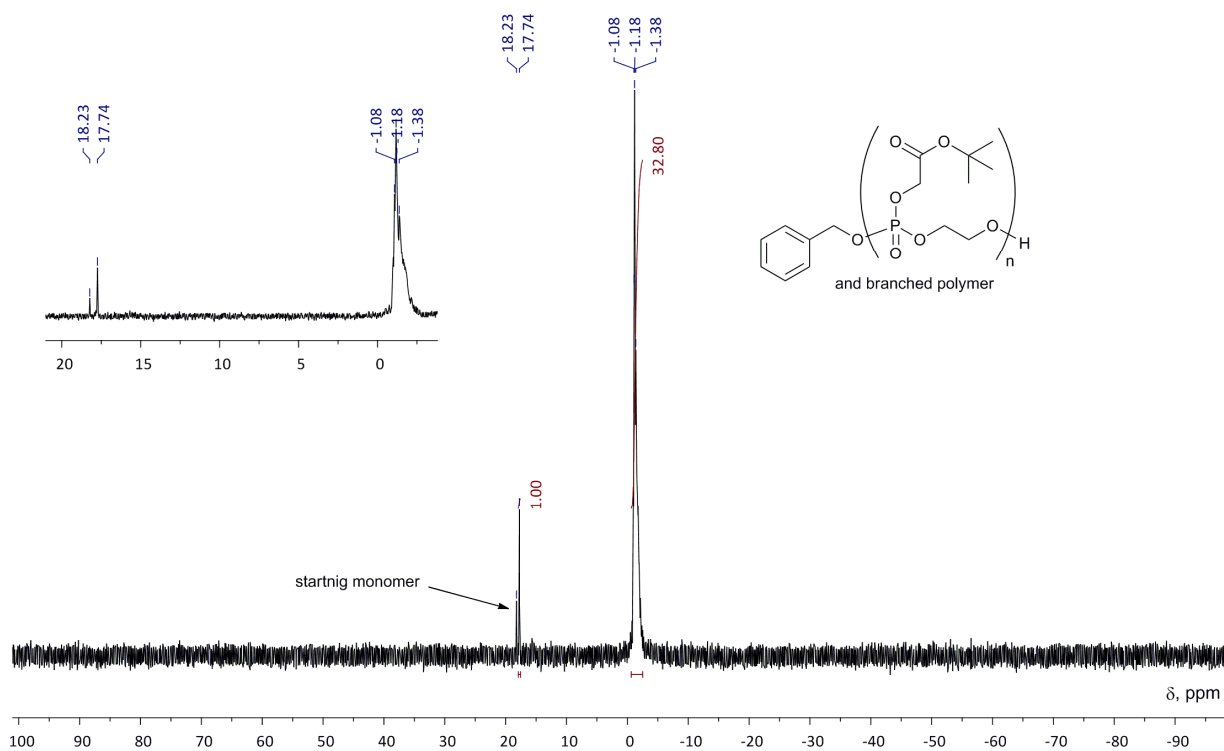


**Fig. S29.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 4.

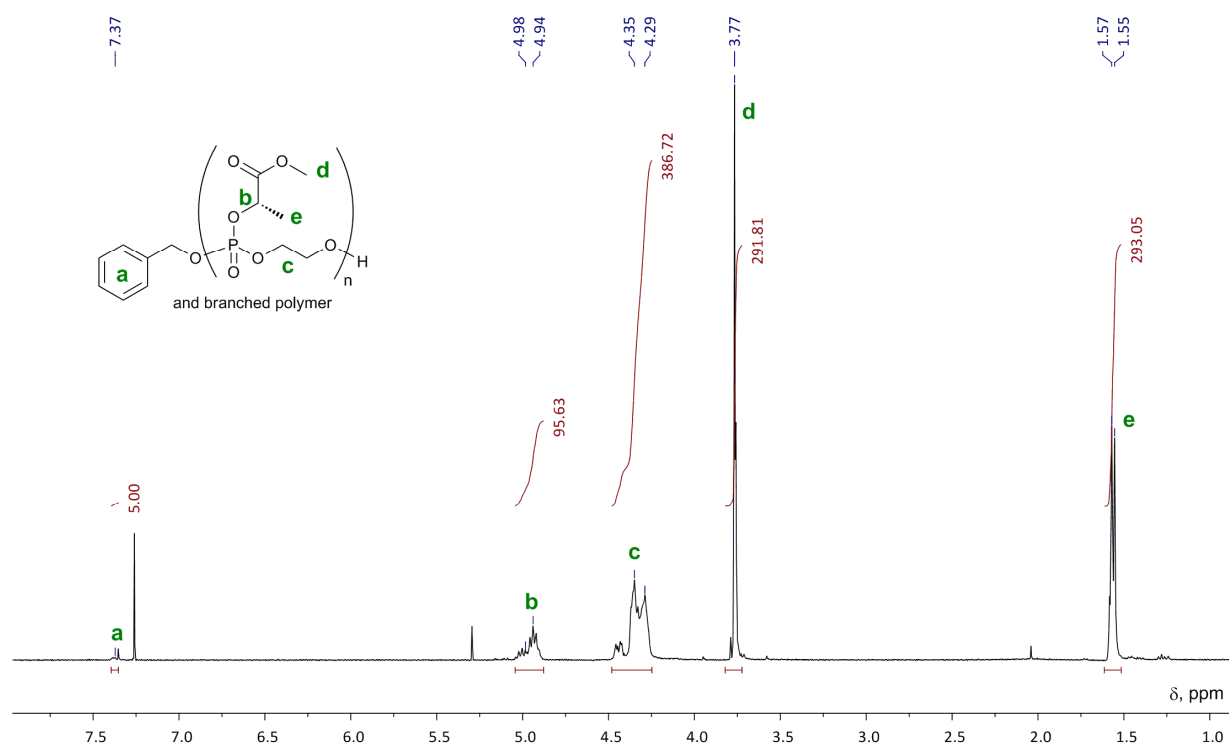




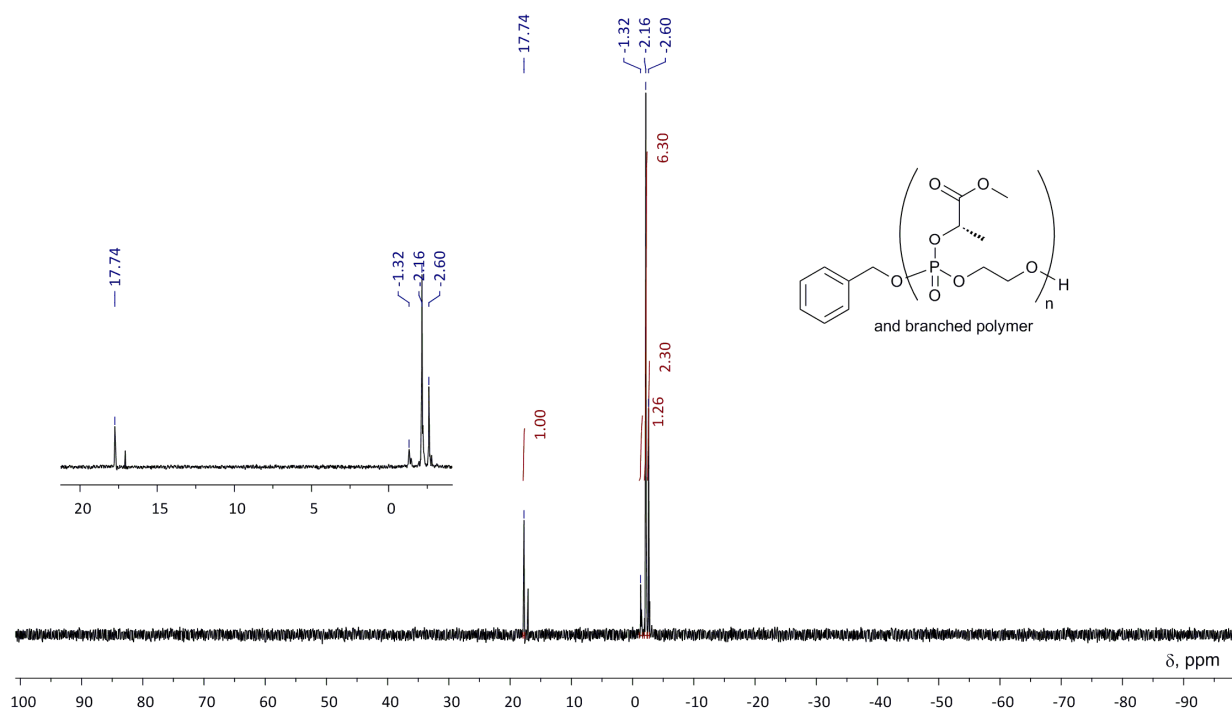
**Fig. S30.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 5.



**Fig. S31.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of 5.

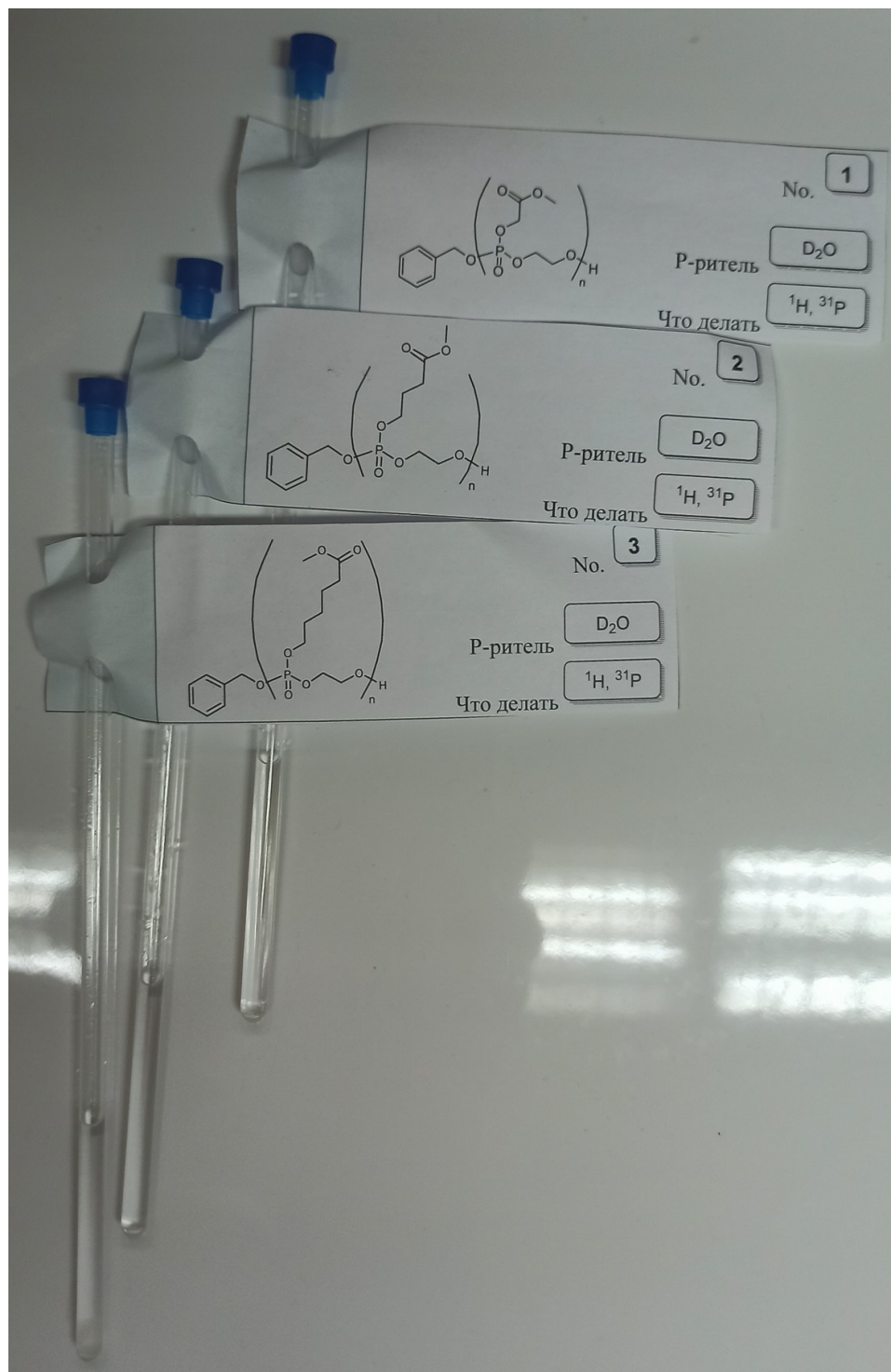


**Fig. S32.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **6**.

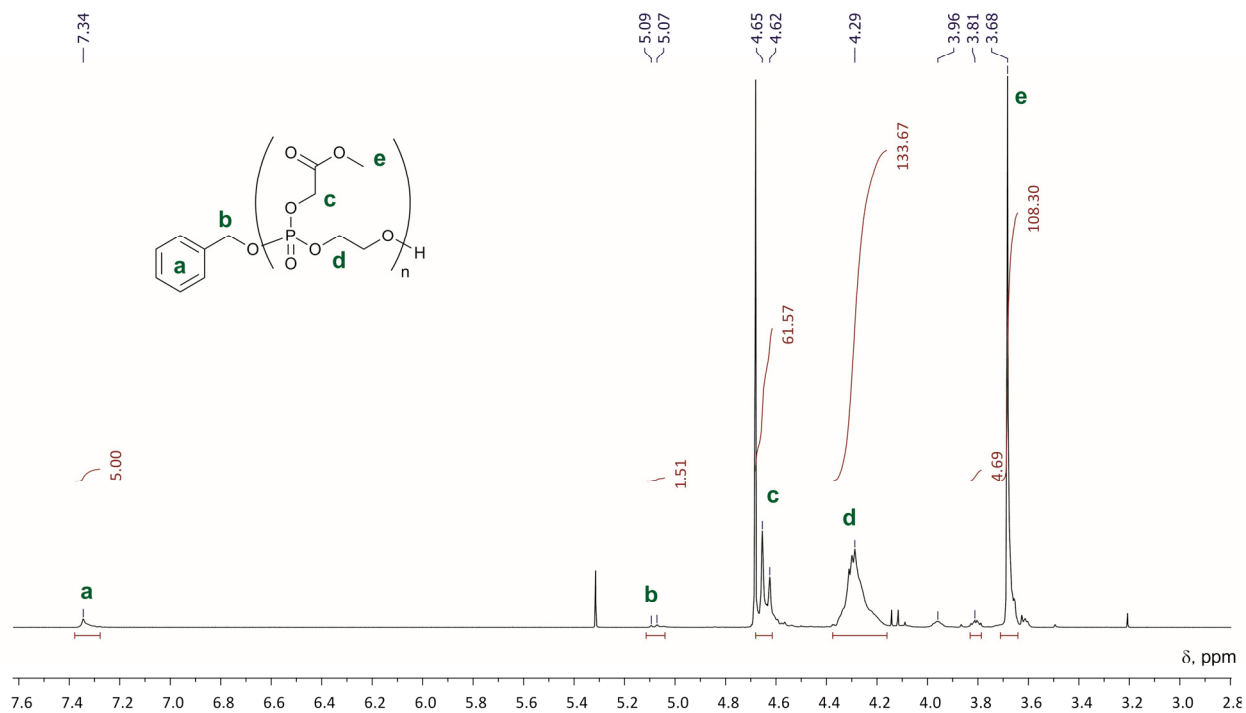


**Fig. S33.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the homopolymer of **6**.

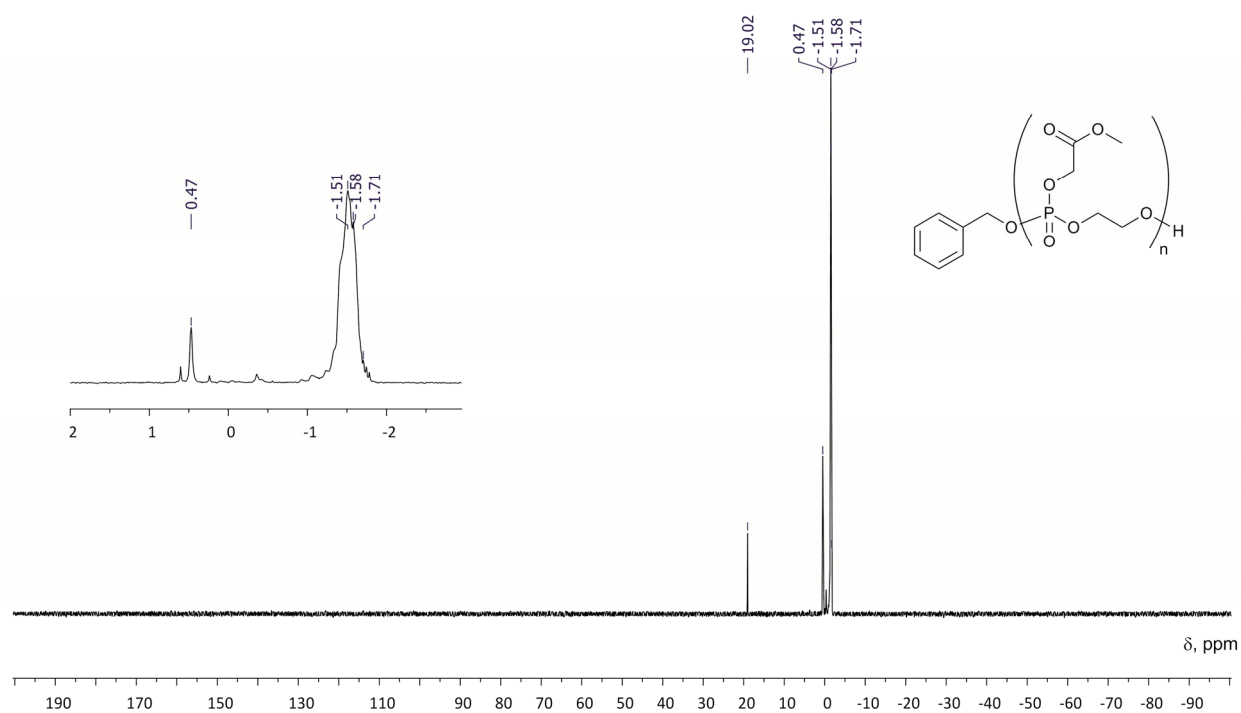
To confirm water solubility of the polymers under study, we prepared solutions of the homopolymers of **1**, **3**, **4**, and **1**/EtEP copolymer in D<sub>2</sub>O (Fig. S34) and registered <sup>1</sup>H and <sup>31</sup>P NMR spectra (Figs. S35–S40). The weight of the each sample was 25 mg, and we observed fast and full dissolution in D<sub>2</sub>O for homopolymers of **1** and **3**. It is notable that homopolymer of **4** has also proven to be soluble.



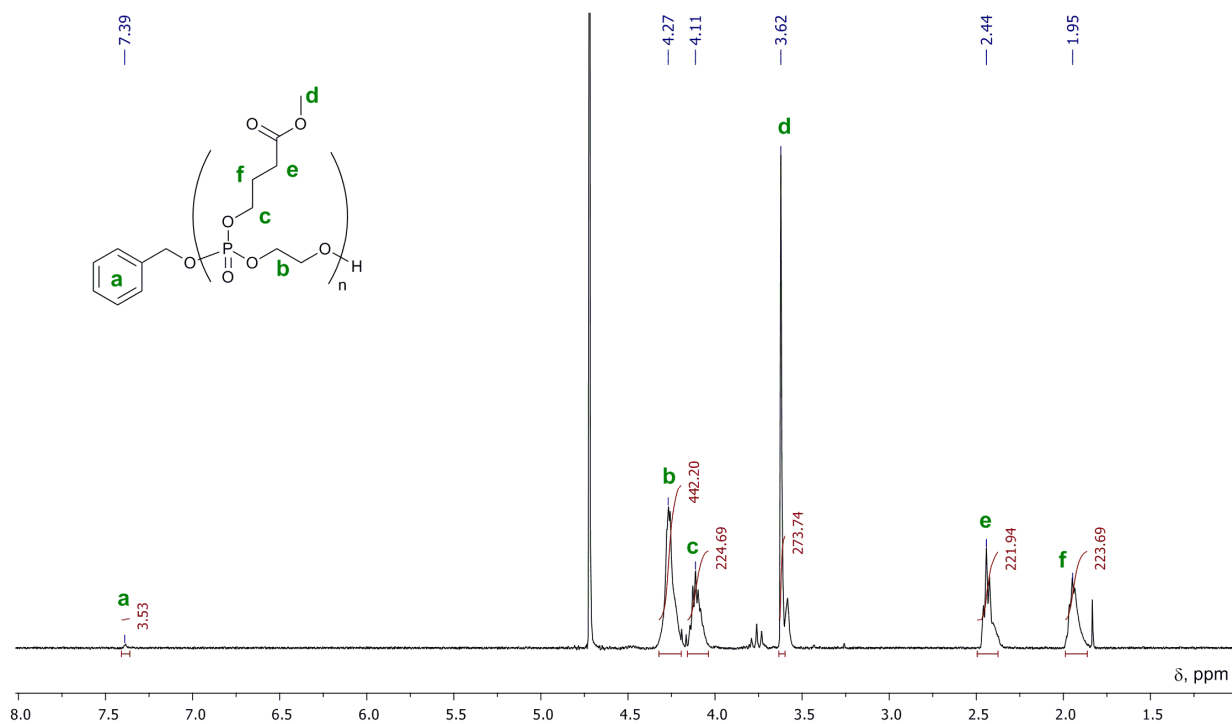
**Fig. S34.** Outward appearance of the NMR samples of the homopolymers of **1**, **3** and **4** prepared in D<sub>2</sub>O.



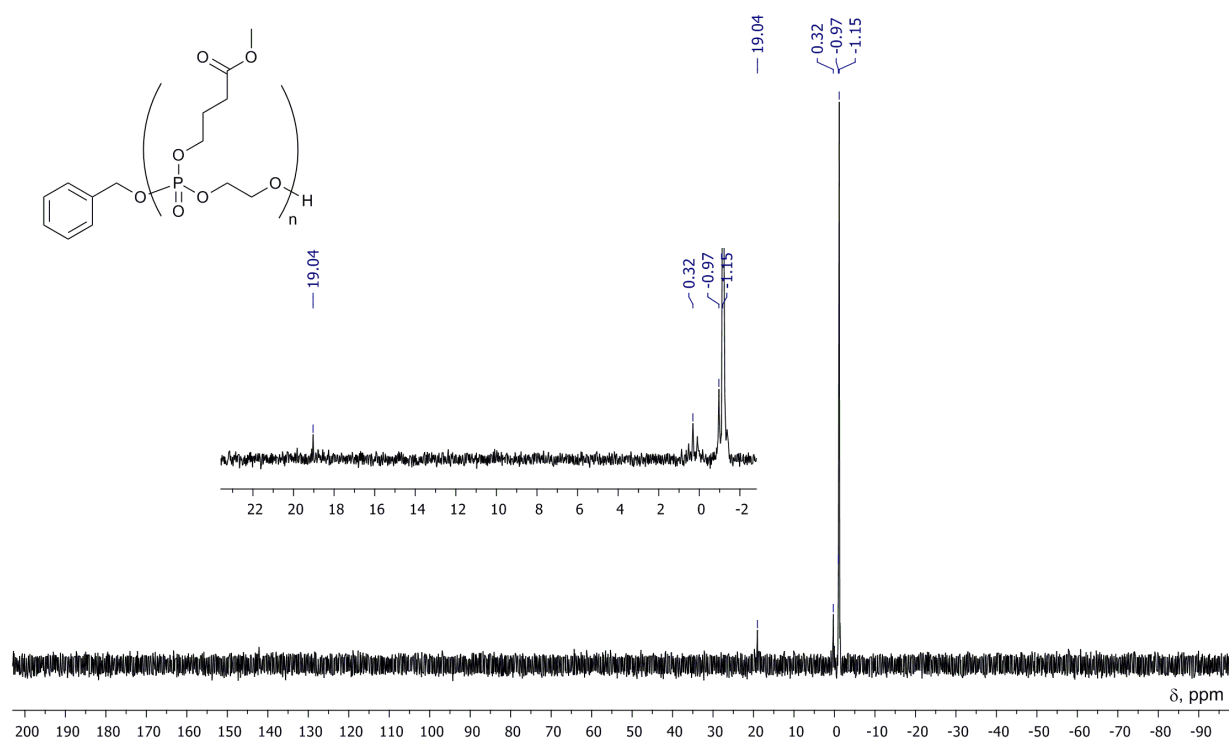
**Fig. S35.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **1**.



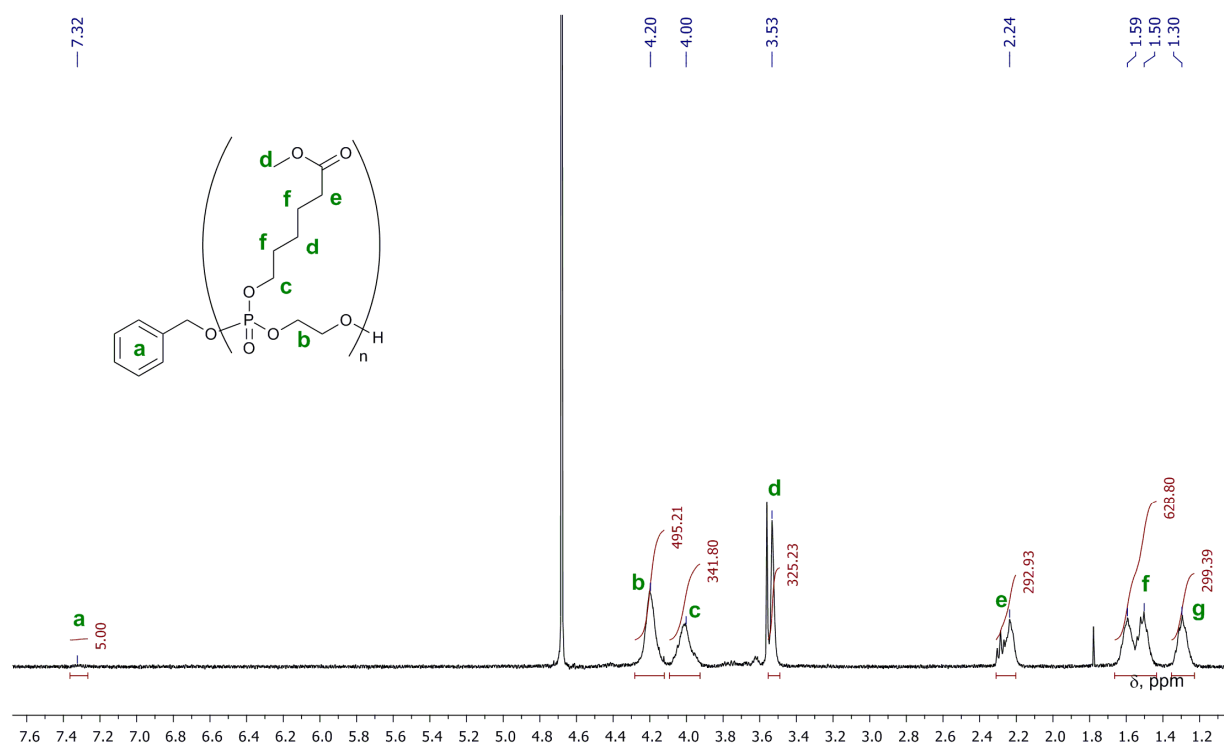
**Fig. S36.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **1**.



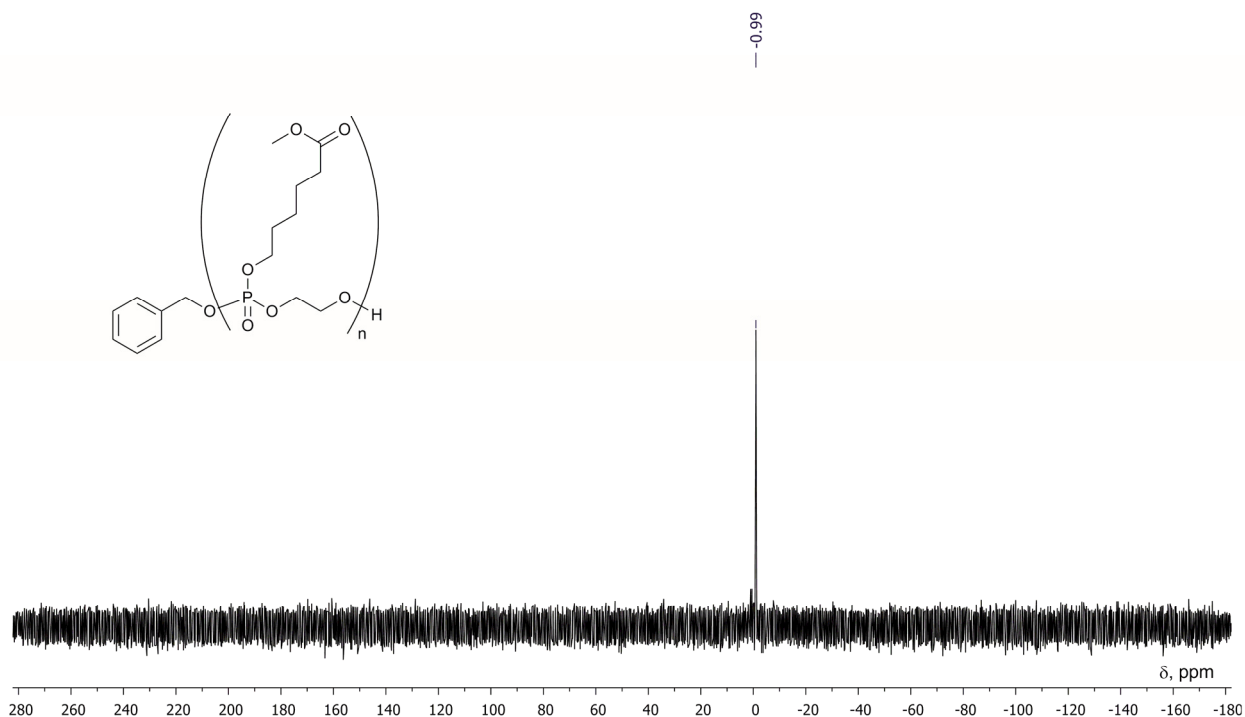
**Fig. S37.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **3**.



**Fig. S38.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **3**.



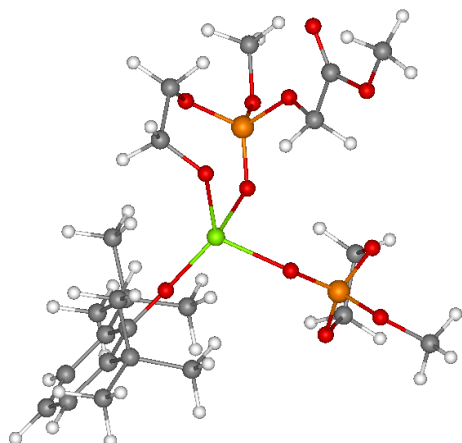
**Fig. S39.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **4**.



**Fig. S40.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{D}_2\text{O}$ , 20 °C) of the homopolymer of **4**.

### S3. DFT calculation data

A-1



Zero-point vibrational energy	1679093.2 (Joules/Mol)
	401.31291 (Kcal/Mol)
Zero-point correction=	0.639533 (Hartree/Particle)
Thermal correction to Energy=	0.684810
Thermal correction to Enthalpy=	0.685755
Thermal correction to Gibbs Free Energy=	0.555194
Sum of electronic and zero-point Energies=	-2684.988444
Sum of electronic and thermal Energies=	-2684.943166
Sum of electronic and thermal Enthalpies=	-2684.942222
Sum of electronic and thermal Free Energies=	-2685.072783

cartesian

12	-0.22704700	-0.02950510	-0.50233841	1	1.39985299	0.08279490	1.95946157
8	-2.80774713	-2.34320521	2.26236153	1	-4.75414705	-3.04960513	1.97906148
8	1.62105298	-0.19870511	-0.34013844	8	-0.81374699	1.90599489	-0.19543841
6	-3.79054713	-3.39120507	2.36416149	15	-1.04694700	2.84049487	0.93216157
1	-3.87404704	-3.62010527	3.42606163	8	0.14875302	2.95529485	1.99416149
1	-3.45514703	-4.27520514	1.81786156	8	-2.22384691	2.47069478	1.96546149
6	2.94025302	-0.33320510	-0.36523843	6	-0.28154701	2.57679486	3.32326150
6	3.70395279	0.18029490	-1.46303844	6	-1.63234699	1.87149489	3.14866161
6	5.09235287	0.01699490	-1.44503844	1	-0.36104700	3.48959494	3.91996145
1	5.68965292	0.39709491	-2.26713848	1	0.47885302	1.91899490	3.74336147
6	5.74965286	-0.62280512	-0.39963841	1	-1.52144706	0.79979491	2.97196150
6	5.00295305	-1.11770511	0.66416156	1	-2.31314707	2.05479479	3.97986150
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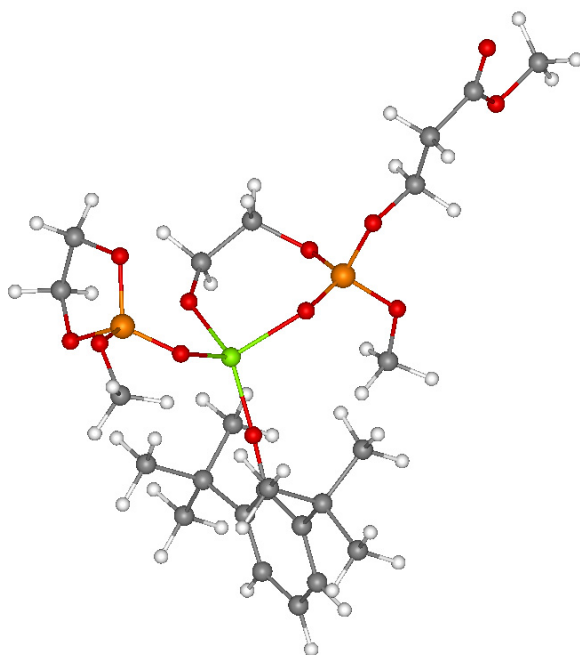
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6	3.61155319	-0.99310511	0.71466160	6	-1.58294702	5.40289497	1.21036148
6	3.03355289	0.90239489	-2.64643860	1	-2.43274713	5.22679520	1.87376153
6	2.83375287	-1.56540513	1.91426146	1	-0.67664701	5.60729504	1.78486156
6	2.30515289	2.16999483	-2.15573859	1	-1.79664707	6.24149513	0.54996157
1	1.57975292	1.94769490	-1.37313855	8	-1.36054695	-0.69530511	1.09196150
1	1.78025293	2.65989494	-2.98553848	15	-2.44394708	-1.70780516	0.85176158
1	3.02645302	2.88469481	-1.74323845	8	-2.11454701	-2.98270512	-0.02653844
6	2.05905294	-0.04490510	-3.37583852	8	-1.42154706	-0.87720507	-1.73013854
1	1.29035294	-0.44580507	-2.71403837	6	-2.34724689	-3.05930519	-1.46723855
1	2.60465288	-0.89600509	-3.79833841	6	-1.35844696	-2.17530513	-2.21253848
1	1.55745292	0.47779492	-4.19973850	1	-3.38234711	-2.75820518	-1.65313852
6	4.05015278	1.36899483	-3.70443845	1	-2.22794700	-4.11850500	-1.70703852
1	4.59785318	0.53239489	-4.15123844	1	-0.35264701	-2.62080526	-2.11603856
1	4.77795315	2.07949495	-3.29783845	1	-1.62444699	-2.23620510	-3.28353858
1	3.51595306	1.87839484	-4.51463842	8	-3.84514713	-1.12220514	0.36086157
6	3.75605297	-2.21490526	2.96066141	6	-4.01954699	0.01129490	-0.49433845
1	4.47175312	-1.50270510	3.38576150	1	-4.08404684	0.91839492	0.11066157
1	4.31615305	-3.06110525	2.54916143	1	-3.17924714	0.08549490	-1.19813848
1	3.14745307	-2.59980512	3.78736162	6	-5.28934717	-0.18560511	-1.29253852
6	1.86125302	-2.66600513	1.44526148	8	-5.65904713	0.98959488	-1.83503854
1	1.17115295	-2.29970527	0.68546158	1	6.83125305	-0.73470509	-0.41423842
1	1.27285302	-3.04830527	2.28846145	8	-5.86904716	-1.23480511	-1.45923853
1	2.42075300	-3.50400519	1.01506150	6	-6.79864693	0.93159491	-2.70923853
6	2.07285309	-0.43770510	2.64146161	1	-6.94394684	1.95029485	-3.06533837
1	2.78275299	0.29349491	3.04596162	1	-7.67934704	0.58519489	-2.16473842
1	1.48735297	-0.84780508	3.47496152	1	-6.60294724	0.25769490	-3.54563856

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A-2



Zero-point vibrational energy	1753790.0 (Joules/Mol)
	419.16586 (Kcal/Mol)
Zero-point correction=	0.667983 (Hartree/Particle)
Thermal correction to Energy=	0.714959
Thermal correction to Enthalpy=	0.715904
Thermal correction to Gibbs Free Energy=	0.580230
Sum of electronic and zero-point Energies=	-2724.271281
Sum of electronic and thermal Energies=	-2724.224305
Sum of electronic and thermal Enthalpies=	-2724.223361
Sum of electronic and thermal Free Energies=	-2724.359034

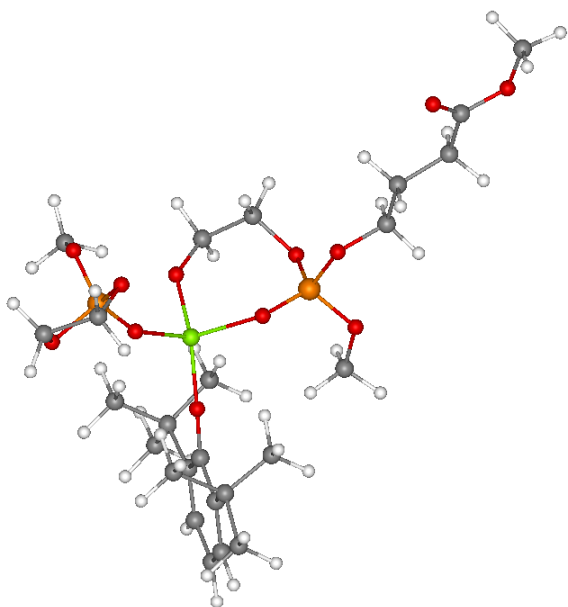
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12	-0.52412820	0.92076194	-0.00711852	6	2.38287187	1.59066188	2.01928163
8	-1.67032814	-0.55893815	-0.15071853	6	0.96057177	1.83476186	2.51178145
6	-2.50692821	-1.58713818	-0.14871852	8	2.59597182	-1.79973805	0.11638148
6	-3.17502809	-1.97993815	1.05808139	6	1.54127169	-2.58823800	0.72688150
6	-3.99442840	-3.11293793	1.03158140	1	1.53517175	-2.41743803	1.80478144
1	-4.49782848	-3.43603802	1.93668139	1	0.57327175	-2.33673811	0.29048148
6	-4.19762850	-3.85273790	-0.12801853	1	1.78847170	-3.62613797	0.51058149
6	-3.58692813	-3.43823791	-1.30661857	8	8.52527237	0.62126189	-1.36391854
1	-3.77582812	-4.01223803	-2.20761847	6	7.57747173	0.08076189	-0.83701849
6	-2.75282812	-2.31743813	-1.35871851	6	6.13627148	0.43726191	-1.12721860
6	-3.03032827	-1.17633808	2.36468148	8	3.80877185	0.21126190	-0.70491850
6	-2.14062810	-1.88663805	-2.70561838	6	5.10477161	-0.27123812	-0.26841852
6	-3.51352811	0.27266189	2.15228152	1	5.14017153	-1.35373819	-0.40161851

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1	-2.97372818	0.76916194	1.34578145	1	5.23787165	-0.04283810	0.79218149
1	-3.37752819	0.86136186	3.06768155	1	-4.83722830	-4.73223782	-0.11691853
1	-4.57872820	0.28126189	1.89638150	1	2.62997174	2.27616191	1.20248139
6	-1.57252812	-1.19493818	2.86378145	1	3.10697174	1.71506190	2.82958150
1	-0.88962823	-0.75863814	2.13428164	1	1.03277183	2.77736187	3.09638166
1	-1.25252819	-2.22423792	3.06348157	1	0.73087180	1.04666185	3.25358152
1	-1.47852826	-0.62423813	3.79598165	1	6.04397154	1.52176189	-1.02171850
6	-3.88492799	-1.75423825	3.50758147	1	5.95617151	0.21926190	-2.18451834
1	-3.58582807	-2.77273798	3.77828145	8	7.69077158	-0.91203809	0.07038148
1	-4.95242834	-1.76223814	3.26368165	6	9.03767204	-1.31013811	0.38248149
1	-3.75922799	-1.13073814	4.40018177	1	8.94237232	-2.10683799	1.11868143
6	-2.59182811	-2.78503799	-3.87121844	1	9.59657192	-0.46833810	0.79558146
1	-3.67872810	-2.77703810	-4.00581837	1	9.54347229	-1.67293823	-0.51421857
1	-2.26762819	-3.82393789	-3.74671841	8	-1.19292831	2.44196200	-1.17621851
1	-2.14482808	-2.41583800	-4.80151844	15	-1.45422816	3.88406205	-0.89291847
6	-0.60272825	-1.96543825	-2.66201854	8	-0.17572823	4.77056217	-0.52891850
1	-0.18372822	-1.31553817	-1.89471853	8	-2.34902811	4.20936203	0.39368147
1	-0.17542821	-1.66723812	-3.62791848	6	-0.36502820	5.44796181	0.73598146
1	-0.28022820	-2.99333811	-2.45851851	6	-1.48562813	4.69276190	1.45668149
6	-2.59452820	-0.45483813	-3.05721855	8	-2.13772821	4.59986210	-2.12331843
1	-3.68242812	-0.42373809	-3.18801832	6	-2.87322807	3.85766196	-3.12671852
1	-2.13052821	-0.12883809	-3.99731851	1	-2.39022827	2.90076208	-3.32461834
1	-2.32812810	0.25546190	-2.27411842	1	-3.89652801	3.70256209	-2.78031850
8	1.29807186	0.32186189	-0.68101847	1	-2.86832809	4.48206186	-4.01871872
15	2.48087192	-0.22273812	0.04668148	1	0.57887179	5.40266180	1.27868140
8	2.58537173	0.20846190	1.56978142	1	-2.08882809	5.33876181	2.09468150
8	0.01527177	1.93016183	1.51898146	1	-1.10292816	3.82136202	1.99388134
1	-0.62792820	6.48706198	0.52058148				

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## A-3



Zero-point vibrational energy	1829695.5 (Joules/Mol)
	437.30772 (Kcal/Mol)
Zero-point correction=	0.696894 (Hartree/Particle)
Thermal correction to Energy=	0.744999
Thermal correction to Enthalpy=	0.745944
Thermal correction to Gibbs Free Energy=	0.607229
Sum of electronic and zero-point Energies=	-2763.545351
Sum of electronic and thermal Energies=	-2763.497246
Sum of electronic and thermal Enthalpies=	-2763.496302
Sum of electronic and thermal Free Energies=	-2763.635016

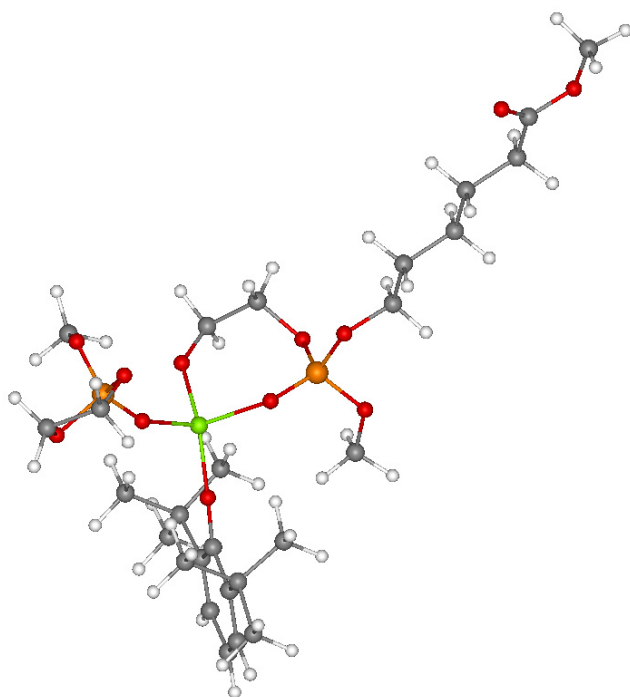
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12	-0.85988963	0.65098554	0.64889050	8	1.85591042	-2.29511452	-0.43650952
8	-2.20198965	-0.43561444	-0.09020953	6	0.66211033	-3.09771442	-0.24610952
6	-3.17278981	-1.24181449	-0.49390954	1	0.59731036	-3.41461444	0.79629046
6	-3.93048978	-2.00351453	0.45649046	1	-0.22808963	-2.53581452	-0.53380954
6	-4.89618969	-2.89641452	-0.01810953	1	0.78241038	-3.96261454	-0.89640951
1	-5.47128963	-3.49251437	0.68279046	8	8.26760960	1.02198553	-0.83390951
6	-5.15798950	-3.05121446	-1.37500954	6	8.27970982	-0.15081444	-0.52470952
6	-4.45668936	-2.27231455	-2.28920960	6	7.06131029	-0.99841452	-0.23260954
1	-4.69228935	-2.38631439	-3.34210944	8	3.36461020	-0.31741443	-0.29460952
6	-3.47608972	-1.35851443	-1.89110959	6	5.75571060	-0.23241445	-0.41430953
6	-3.72148967	-1.84171438	1.97409046	6	4.56161070	-1.10581446	-0.08150953
6	-2.77078962	-0.48801443	-2.94920945	1	5.66861057	0.12378554	-1.44440949
6	-3.99818969	-0.38261446	2.39209056	1	5.74951029	0.65498555	0.22459047

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1	-3.37688971	0.32378554	1.84049046	1	4.51011038	-1.98631454	-0.72900951
1	-3.80558991	-0.24441448	3.46289039	1	4.58991051	-1.44081450	0.96109045
1	-5.04588938	-0.12731445	2.19799042	1	-5.91188955	-3.75741434	-1.71500957
6	-2.29738975	-2.26541448	2.38139057	1	2.42011023	0.85608554	2.30269051
1	-1.53748965	-1.66951454	1.87599051	1	2.68011022	-0.41961446	3.52469039
1	-2.13038969	-3.31981444	2.13209057	1	0.78941035	0.82518554	4.21319008
1	-2.15518975	-2.14571452	3.46229053	1	0.21361037	-0.75321448	3.67149043
6	-4.68238926	-2.71801448	2.79819036	1	7.10641050	-1.88091445	-0.88120955
1	-4.53078938	-3.78761435	2.61629057	1	7.16561031	-1.37981451	0.79029047
1	-5.73328972	-2.48081446	2.60189056	8	9.40931034	-0.87711453	-0.39050952
1	-4.50228930	-2.54171443	3.86499047	6	10.63150978	-0.16331446	-0.63850951
6	-3.30218983	-0.74801445	-4.37050962	1	11.42901039	-0.88881445	-0.48380953
1	-4.37348938	-0.53751445	-4.45930958	1	10.73400974	0.67308557	0.05599047
1	-3.12428975	-1.77741456	-4.70050955	1	10.65211010	0.21618554	-1.66220951
1	-2.78088975	-0.08841446	-5.07390976	8	-1.23818958	2.58448553	0.17439047
6	-1.25878966	-0.78121448	-2.98840952	15	-1.06238961	4.05458546	0.25559047
1	-0.77848959	-0.57701445	-2.03220963	8	-2.36088967	4.83998537	-0.28290954
1	-0.76768959	-0.16421446	-3.75200963	8	0.02871037	4.73118544	-0.70460951
1	-1.08198965	-1.83191442	-3.24720955	6	-1.95688951	5.94458532	-1.11570954
6	-3.02078962	1.00508559	-2.65450954	6	-0.62358963	5.51358557	-1.72850955
1	-4.09178972	1.22998559	-2.71420956	8	-0.66588962	4.60138559	1.67759049
1	-2.50328970	1.62968552	-3.39500952	6	-1.05128956	3.90948558	2.90479040
1	-2.67268968	1.28708553	-1.66070950	1	-0.78128958	2.84858561	2.84549046
8	0.88881040	0.11938554	-0.25360954	1	-0.49228963	4.41148567	3.69329047
15	1.94581044	-0.83961451	0.18259047	1	-2.12298965	4.04178572	3.06879044
8	1.99851036	-1.12401450	1.74199045	1	-1.85138953	6.83848572	-0.49380952
8	-0.23668963	0.84378552	2.42989039	1	-2.73578978	6.10008574	-1.86220956
6	2.00361037	-0.05341446	2.74719048	1	0.02731037	6.35488558	-1.96680951
6	0.61111033	0.21208555	3.30529046	1	-0.76188958	4.88398552	-2.61130953

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## A-4



Zero-point vibrational energy	1979972.3 (Joules/Mol)
	473.22474 (Kcal/Mol)
Zero-point correction=	0.754132 (Hartree/Particle)
Thermal correction to Energy=	0.804989
Thermal correction to Enthalpy=	0.805933
Thermal correction to Gibbs Free Energy=	0.660049
Sum of electronic and zero-point Energies=	-2842.093980
Sum of electronic and thermal Energies=	-2842.043123
Sum of electronic and thermal Enthalpies=	-2842.042178
Sum of electronic and thermal Free Energies=	-2842.188063

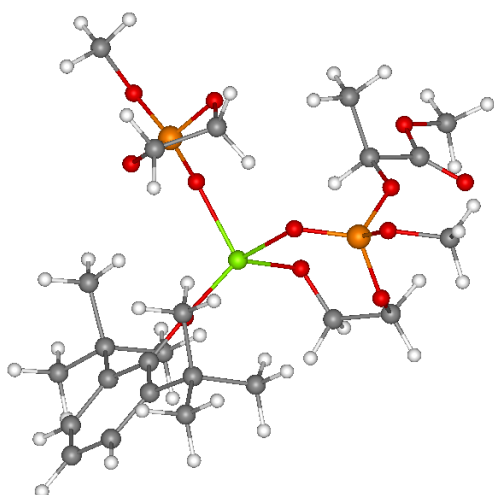
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8	-2.97712445	-0.46876878	-0.11941332	1	0.10537551	-3.92566872	-0.84841335
6	-3.91692448	-1.29986882	-0.54501331	6	7.52517557	0.04103121	-0.34811333
6	-4.67322445	-2.08466887	0.38768667	6	6.31317520	-0.83646882	-0.03221333
6	-5.60482454	-3.00156879	-0.10851333	8	2.58847570	-0.22516876	-0.17371333
1	-6.17792463	-3.61466885	0.57918668	6	4.98637533	-0.10636878	-0.24991333
6	-5.83452463	-3.15946889	-1.47091329	6	3.79757571	-0.98936880	0.07428667
6	-5.13522482	-2.35986876	-2.36871338	1	4.90527534	0.22723122	-1.29031336
1	-5.34582472	-2.47766876	-3.42651343	1	4.94387531	0.79243124	0.37568668
6	-4.18772459	-1.42146873	-1.94841337	1	3.77377558	-1.88046885	-0.55971330
6	-4.49842453	-1.92256880	1.90968668	1	3.81117558	-1.30596876	1.12258673

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6	-3.48292446	-0.53076881	-2.98991346	1	-6.56202459	-3.88466883	-1.82801330
6	-4.82022476	-0.47266877	2.32658648	1	1.54527545	0.93033123	2.38458657
1	-4.20802450	0.25093120	1.78748667	1	1.80197549	-0.33506876	3.61808658
1	-4.64962482	-0.33276880	3.40088654	1	-0.13052449	0.87263119	4.25528669
1	-5.87082481	-0.24446881	2.11518645	1	-0.66052449	-0.71906877	3.70518661
6	-3.07192445	-2.31146884	2.34298658	1	6.34167528	-1.73916888	-0.65731335
1	-2.31792450	-1.69246876	1.85678673	1	6.37507534	-1.18386877	1.00808668
1	-2.87212443	-3.35936880	2.09068656	6	8.84467506	-0.69096881	-0.12911332
1	-2.95432448	-2.19566870	3.42728662	6	10.05617523	0.16443121	-0.42161334
6	-5.45252466	-2.82586884	2.71228647	8	11.19707584	-0.52966881	-0.21441332
1	-5.27122450	-3.89076900	2.52948666	8	-2.09802437	2.57343125	0.16138667
1	-6.50512457	-2.61386871	2.49668646	15	-1.98632443	4.04923153	0.24798667
1	-5.29712486	-2.64936876	3.78288651	8	-3.31482434	4.78033113	-0.29431331
6	-3.97632432	-0.80286884	-4.42261314	8	-0.92052454	4.77393103	-0.70571333
1	-5.05062485	-0.62096876	-4.53441334	6	-2.95342445	5.90523100	-1.11941338
1	-3.76412439	-1.82686877	-4.74931335	6	-1.60152447	5.53243113	-1.72911334
1	-3.45772433	-0.12886879	-5.11431313	8	-1.61872447	4.60903120	1.67278671
6	-1.96302450	-0.78336883	-2.99601340	6	-2.00052428	3.90893126	2.89678645
1	-1.50912452	-0.56286877	-2.03051353	1	-1.70832455	2.85363126	2.84058666
1	-1.47272456	-0.15576878	-3.75141335	1	-1.45902455	4.42243099	3.69018650
1	-1.75242448	-1.82976890	-3.24661350	1	-3.07612443	4.01973152	3.05098653
6	-3.77902436	0.95473123	-2.69961333	1	-2.88692451	6.79933119	-0.49251330
1	-4.85402441	1.15073121	-2.78331351	1	-3.73542428	6.03273106	-1.86821330
1	-3.26192451	1.59383118	-3.42791343	1	-0.98542452	6.40083122	-1.96241331
1	-3.46142435	1.24503124	-1.69801331	1	-1.71092451	4.90053129	-2.61431336
8	0.10407551	0.16143122	-0.20491332	1	7.47297525	0.39063120	-1.38481331
15	1.16827548	-0.77636874	0.26108667	1	7.50507545	0.94303119	0.27288666
8	1.17817545	-1.05966878	1.82218671	8	10.03607559	1.32003117	-0.79191333
8	-1.11242449	0.86443120	2.44718647	6	12.41087532	0.19623122	-0.46291333
6	1.13717544	0.01383123	2.82258654	1	8.93447495	-1.04976881	0.90328670
6	-0.27362448	0.25293121	3.34548664	1	8.91177559	-1.58806884	-0.75601333
8	1.12497544	-2.23316884	-0.36021331	1	13.21827507	-0.50306880	-0.24881333
6	-0.05402449	-3.06346869	-0.20291331	1	12.47697544	1.06863117	0.19088668
1	-0.14112449	-3.38166881	0.83748668	1	12.45537567	0.52513123	-1.50331330

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## A-6



Zero-point vibrational energy	1753681.6 (Joules/Mol)
	419.13996 (Kcal/Mol)
Zero-point correction=	0.667942 (Hartree/Particle)
Thermal correction to Energy=	0.714457
Thermal correction to Enthalpy=	0.715401
Thermal correction to Gibbs Free Energy=	0.584008
Sum of electronic and zero-point Energies=	-2724.265289
Sum of electronic and thermal Energies=	-2724.218774
Sum of electronic and thermal Enthalpies=	-2724.217830
Sum of electronic and thermal Free Energies=	-2724.349223

				cartesian			
12	-0.16953211	0.01937656	-0.44324943	8	-0.49793211	2.03847647	-0.47444943
8	-2.76753211	-1.56732345	2.75835061	15	-0.43713212	3.17867637	0.47295058
8	1.66136789	-0.32162344	-0.29544941	8	0.85166788	3.21587658	1.42635059
6	-3.75593209	-2.55802345	3.09585047	8	-1.56073213	3.23727655	1.62385058
1	-3.79513216	-2.58242345	4.18445063	6	0.47816792	3.13907647	2.82345057
1	-3.45593214	-3.53552341	2.71225047	6	-0.98793209	2.69287658	2.84305048
6	2.94796777	-0.63942349	-0.35314941	1	0.61816788	4.13157654	3.26025057
6	3.71256804	-0.37242344	-1.53544939	1	1.13956785	2.41917658	3.30475044
6	5.06686831	-0.71982348	-1.54864943	1	-1.09223211	1.60577655	2.81475067
1	5.66306829	-0.52782345	-2.43464947	1	-1.54653215	3.11177635	3.67975044
6	5.69116831	-1.31132340	-0.45574942	8	-0.53993213	4.52497625	-0.34084940
6	4.94456816	-1.56802344	0.68895054	6	-0.42763209	5.80497646	0.31395060
1	5.44546795	-2.03132343	1.53265059	1	-1.21043205	5.91607666	1.06765056
6	3.58596778	-1.25052345	0.77545059	1	0.56256795	5.91067648	0.76275057
6	3.08176780	0.28437656	-2.77754951	1	-0.55883211	6.54957628	-0.46914938

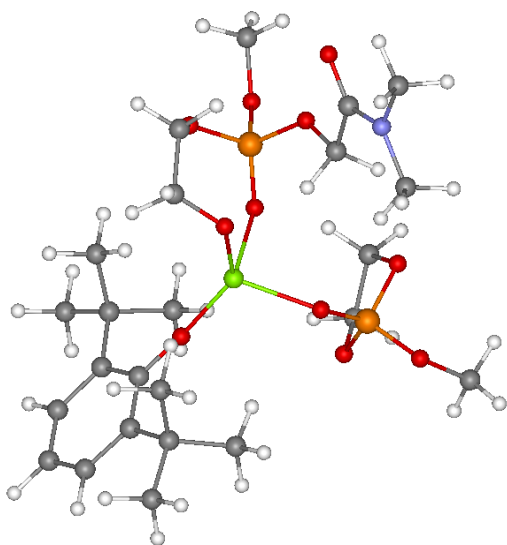
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6	2.80766797	-1.56832337	2.06555057	8	-1.33413219	-0.21512344	1.24615061
6	2.55576777	1.69087660	-2.42734933	15	-2.43233204	-1.24252343	1.23815060
1	1.84596777	1.66607654	-1.60054946	8	-2.10803199	-2.67362356	0.64495057
1	2.06016779	2.14537644	-3.29454947	8	-1.43763208	-0.97872341	-1.47214949
1	3.38616776	2.34237647	-2.13214946	6	-2.34513211	-3.06512356	-0.74184942
6	1.95196795	-0.59922349	-3.34394956	6	-1.37563217	-2.35072351	-1.67284942
1	1.16866791	-0.79962349	-2.61214948	1	-3.38683224	-2.83322358	-0.97814941
1	2.35326791	-1.56622338	-3.66704941	1	-2.20553207	-4.14882374	-0.74664944
1	1.48666787	-0.11942343	-4.21394920	1	-0.36463210	-2.76252341	-1.50524938
6	4.09336805	0.47227657	-3.92254949	1	-1.65973210	-2.63532352	-2.70244932
1	4.50166798	-0.48032346	-4.27684927	8	-3.84253216	-0.76362348	0.67435056
1	4.92866802	1.12077653	-3.63734937	6	-4.08823204	0.11007656	-0.44534943
1	3.58876777	0.94577658	-4.77244949	6	-4.45413208	1.49637663	0.06245058
6	3.69476771	-2.20062351	3.15245056	1	-3.19503212	0.12557656	-1.08324945
1	4.51496792	-1.54142344	3.45705056	6	-5.19263172	-0.53992343	-1.27064943
1	4.12256813	-3.15712357	2.83415055	8	-5.56213188	0.28197658	-2.26944947
1	3.08606791	-2.39832354	4.04255056	1	6.74646807	-1.57072341	-0.49644938
6	1.68306780	-2.58102345	1.77305055	8	-5.65753174	-1.64362335	-1.08964944
1	1.00776792	-2.22122359	0.99695057	6	-6.55393171	-0.24652344	-3.16534948
1	1.09336782	-2.77892351	2.67665052	1	-6.72303200	0.53457654	-3.90504932
1	2.10976791	-3.53072357	1.43215060	1	-7.47583199	-0.47062346	-2.62484956
6	2.22816777	-0.27432343	2.67245054	1	-6.18643188	-1.15562344	-3.64524937
1	3.04076791	0.41027656	2.94345045	1	-4.65923166	2.15887642	-0.78074944
1	1.65166783	-0.50122344	3.57875061	1	-3.62243223	1.90837657	0.63685054
1	1.57776785	0.23157656	1.95845056	1	-5.33933210	1.45417655	0.70365053
1	-4.73143196	-2.27592349	2.69295049				

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A-7



Zero-point vibrational energy	1785903.7 (Joules/Mol)
	426.84124 (Kcal/Mol)
Zero-point correction=	0.680215 (Hartree/Particle)
Thermal correction to Energy=	0.727147
Thermal correction to Enthalpy=	0.728091
Thermal correction to Gibbs Free Energy=	0.593991
Sum of electronic and zero-point Energies=	-2704.379681
Sum of electronic and thermal Energies=	-2704.332749
Sum of electronic and thermal Enthalpies=	-2704.331805
Sum of electronic and thermal Free Energies=	-2704.465905

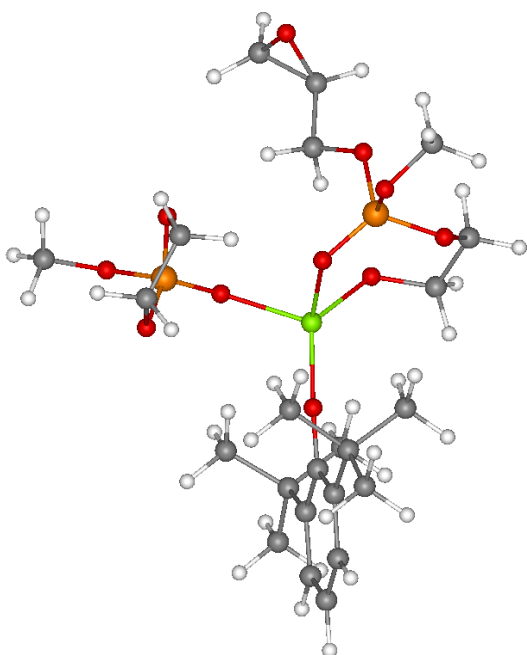
cartesian							
12	0.01382458	-0.03816095	0.32584149	8	0.60342455	1.83943915	-0.26915848
8	2.53142452	-2.66056108	-2.23035860	15	0.67262459	2.58733892	-1.54935849
8	-1.84447527	-0.18066095	0.28924149	8	-0.60847545	2.44513893	-2.50245857
6	3.59142470	-3.63816094	-2.24545860	8	1.79042459	2.13003898	-2.61135864
1	3.64542460	-4.00236082	-3.27085853	6	-0.25137544	1.88233912	-3.78825855
1	3.34992456	-4.46126080	-1.56975853	6	1.15362453	1.29463911	-3.61585855
6	-3.14917541	-0.35736093	0.45214152	1	-0.27927542	2.69043899	-4.52425861
6	-3.86657548	0.39683908	1.43664157	1	-0.99297541	1.12293911	-4.03485870
6	-5.24187565	0.18403906	1.57094157	1	1.12812459	0.26943907	-3.24115849
1	-5.80347538	0.74363905	2.31164145	1	1.75482464	1.36153913	-4.52225876
6	-5.93017578	-0.73106098	0.78174150	8	0.93882459	4.10993910	-1.23025846
6	-5.22867584	-1.45936096	-0.17295849	6	0.96712458	5.09973907	-2.27845860
1	-5.77927542	-2.17006111	-0.78045851	1	1.75952458	4.87193918	-2.99505854
6	-3.85287547	-1.30156088	-0.36385849	1	-0.00437543	5.14873934	-2.77505851

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6	-3.16097546	1.42853916	2.33654141	1	1.17562461	6.04733944	-1.78465843
6	-3.12707543	-2.14066100	-1.43195844	8	1.05452454	-0.93576097	-1.21055853
6	-2.53427529	2.54393888	1.47564149	15	2.21562457	-1.84236085	-0.90695846
1	-1.84607530	2.14293909	0.73154151	8	1.99132466	-2.98196101	0.16804151
1	-1.98857546	3.25733900	2.10634136	8	1.25492454	-0.67476094	1.63224149
1	-3.31807542	3.09423900	0.94274151	6	2.26702452	-2.84526110	1.59564149
6	-2.09307528	0.74223906	3.21214151	6	1.25882459	-1.91466093	2.25424147
1	-1.35387540	0.19873905	2.62284136	1	3.29422474	-2.48566103	1.70364153
1	-2.56557536	0.02183906	3.88904142	1	2.20232463	-3.86486101	1.98314154
1	-1.56217551	1.48233914	3.82414150	1	0.27072456	-2.40696096	2.23274136
6	-4.13137579	2.12343907	3.30844140	1	1.54762459	-1.84416091	3.31894135
1	-4.60427570	1.41713905	3.99924135	8	3.60452461	-1.12036085	-0.62555850
1	-4.92007542	2.67513895	2.78574133	6	3.82782459	0.00563906	0.22984152
1	-3.57437539	2.84733891	3.91464138	1	3.92822456	0.88793904	-0.40885848
6	-4.08127546	-3.07236099	-2.20005870	1	2.97392464	0.12413906	0.90964150
1	-4.86037540	-2.51966095	-2.73635864	6	5.10622454	-0.25156093	1.02894151
1	-4.56667566	-3.80116105	-1.54235852	7	5.52712440	0.78363901	1.81584156
1	-3.50907540	-3.63766098	-2.94485855	1	-7.00037575	-0.87556094	0.90994155
6	-2.07097530	-3.04756093	-0.76995850	8	5.68752432	-1.33096087	0.96824157
1	-1.35597539	-2.47296095	-0.18135850	6	6.76912451	0.65093905	2.55844140
1	-1.51467538	-3.61366105	-1.52725852	1	6.58652449	0.77003902	3.63264132
1	-2.55747533	-3.76426101	-0.09915850	1	7.49012423	1.41373909	2.24024129
6	-2.47547531	-1.21896088	-2.48365855	1	7.18592453	-0.33776093	2.37274146
1	-3.24807549	-0.64546096	-3.00955868	6	4.85872459	2.06993890	1.90794146
1	-1.92317533	-1.81216085	-3.22395849	1	4.88192415	2.41313887	2.94684148
1	-1.78757548	-0.51536095	-2.01425862	1	3.81122470	2.00313902	1.61714149
1	4.53892422	-3.17726111	-1.95855844	1	5.35292435	2.82933903	1.28714156

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## A-Gly



Zero-point vibrational energy	1668387.6 (Joules/Mol)
	398.75421 (Kcal/Mol)
Zero-point correction=	0.635455 (Hartree/Particle)
Thermal correction to Energy=	0.678924
Thermal correction to Enthalpy=	0.679868
Thermal correction to Gibbs Free Energy=	0.554896
Sum of electronic and zero-point Energies=	-2609.735344
Sum of electronic and thermal Energies=	-2609.691876
Sum of electronic and thermal Enthalpies=	-2609.690932
Sum of electronic and thermal Free Energies=	-2609.815904

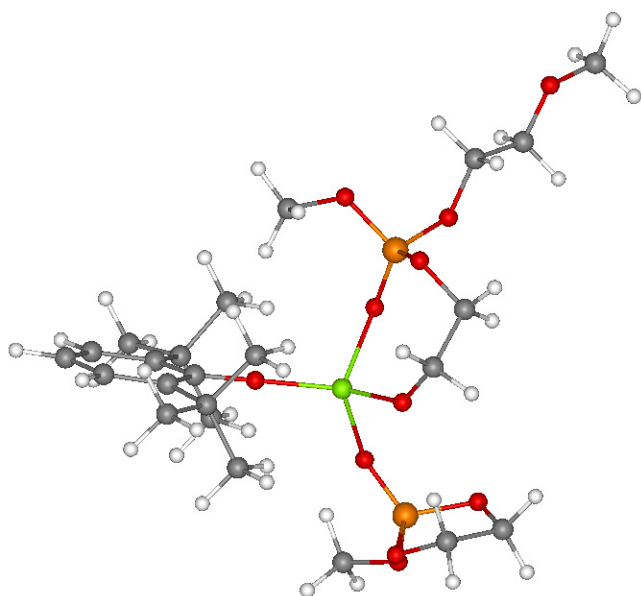
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12	-0.28035176	-0.02741566	-0.71308964	1	0.94254827	-0.01431566	1.96831048
8	-3.11595154	-2.51931572	1.60171044	1	-4.99365187	-3.26901579	1.08191037
8	1.53054821	-0.13221566	-0.28278965	8	-0.95515174	1.88648438	-0.45098963
6	-4.06795168	-3.59691572	1.56121039	15	-1.33885169	2.77628422	0.67251039
1	-4.26405191	-3.86341572	2.59931040	8	-0.32415175	2.80888438	1.91261041
1	-3.64675188	-4.45461559	1.03181040	8	-2.67195177	2.39088440	1.48621047
6	2.83984804	-0.24001566	-0.10298963	6	-0.97065175	2.39018416	3.13881040
6	3.75334835	0.35778433	-1.03098953	6	-2.28705168	1.72538424	2.71941042
6	5.12534809	0.22748435	-0.79538965	1	-1.12895179	3.28108430	3.75251031
1	5.83504820	0.67218435	-1.48498952	1	-0.29935175	1.69858432	3.64731050
6	5.62654829	-0.46161568	0.30381036	1	-2.16385174	0.66088432	2.51011038
6	4.73514795	-1.04471564	1.19781041	1	-3.08955193	1.88658428	3.43881035

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1	5.14154816	-1.58331561	2.04771042	8	-1.54415178	4.23658466	0.11211037
6	3.35044813	-0.95701569	1.02761042	6	-1.83915174	5.34188461	0.99011034
6	3.26014805	1.12908435	-2.26998949	1	-2.78175163	5.16938448	1.51491046
6	2.40954828	-1.63371563	2.04131031	1	-1.02055168	5.48858452	1.69831038
6	2.42164803	2.35068417	-1.84378958	1	-1.92865181	6.21488476	0.34601036
1	1.57994819	2.06768417	-1.21178961	8	-1.62285173	-0.77361566	0.67321038
1	2.03154802	2.87598419	-2.72468948	15	-2.57225180	-1.86191559	0.25751036
1	3.04074812	3.05548429	-1.27698958	8	-2.01765180	-3.11841583	-0.53028965
6	2.44614840	0.20168434	-3.19478965	8	-1.19485176	-0.94651562	-2.11698961
1	1.58564830	-0.23911566	-2.69028950	6	-1.95915174	-3.19901562	-1.98688960
1	3.07444811	-0.62061566	-3.55458951	6	-0.92265177	-2.23541570	-2.54378963
1	2.08054829	0.75438434	-4.06928968	1	-2.95715189	-2.96751571	-2.37098956
6	4.42044830	1.67608428	-3.12138963	1	-1.71915174	-4.24481535	-2.19318962
1	5.06264830	0.87868434	-3.51038957	1	0.07854825	-2.59161568	-2.24128962
1	5.04584789	2.38288426	-2.56558967	1	-0.96605176	-2.33131576	-3.64468956
1	4.00984812	2.21358418	-3.98398948	8	-3.88065195	-1.38251567	-0.51638961
6	3.17254829	-2.33821583	3.17691040	6	-4.00575161	-0.06841566	-1.12558961
1	3.78454828	-1.64171576	3.76031041	1	-3.90005159	0.69428432	-0.35058963
1	3.82124805	-3.13901567	2.80651045	1	-3.21125174	0.03108434	-1.87188959
1	2.45194817	-2.79631567	3.86441040	6	-5.36015177	0.00988434	-1.75548959
6	1.56494820	-2.71771574	1.34271038	1	6.69954824	-0.54571563	0.46001035
1	0.98944819	-2.30811572	0.51271039	6	-6.03975201	1.30348444	-1.89978957
1	0.86644828	-3.18191576	2.04991031	8	-6.46015167	0.36338434	-0.90858966
1	2.21564817	-3.50341582	0.94301039	1	-5.59095192	-0.77621567	-2.47458959
6	1.50114822	-0.58281565	2.71261048	1	-5.56915188	2.20618439	-1.51128960
1	2.10784817	0.12048434	3.29541039	1	-6.73115206	1.45158434	-2.72788954
1	0.78984821	-1.07101560	3.39151049				

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A-OCH<sub>2</sub>CH<sub>2</sub>OMe



Zero-point vibrational energy	1726680.0 (Joules/Mol)
	412.68643 (Kcal/Mol)
Zero-point correction=	0.657658 (Hartree/Particle)
Thermal correction to Energy=	0.702761
Thermal correction to Enthalpy=	0.703705
Thermal correction to Gibbs Free Energy=	0.573874
Sum of electronic and zero-point Energies=	-2610.951908
Sum of electronic and thermal Energies=	-2610.906805
Sum of electronic and thermal Enthalpies=	-2610.905861
Sum of electronic and thermal Free Energies=	-2611.035692

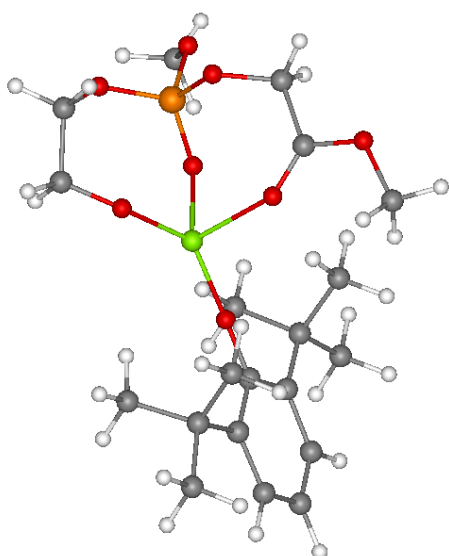
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12	-0.16406567	0.89105189	0.05162273	8	0.46793437	1.84665191	1.57802272
8	-1.47716570	-0.44544807	-0.10097727	6	2.72383428	1.13475192	2.18052268
6	-2.41836572	-1.37854815	-0.10667726	6	1.34463441	1.61815190	2.61222267
6	-3.13436556	-1.69864810	1.09402275	8	2.51753426	-2.23844814	0.24502274
6	-4.06256580	-2.74414802	1.06142282	6	1.33813441	-2.88304806	0.79372275
1	-4.60426569	-3.01214814	1.96242261	1	1.33173430	-2.76494813	1.87852263
6	-4.32706594	-3.46424818	-0.09827727	1	0.43093437	-2.46534824	0.35392272
6	-3.67046571	-3.11284804	-1.27277732	1	1.42953432	-3.93504810	0.52892274
1	-3.90786576	-3.66564822	-2.17557740	6	8.70423412	-0.85854816	-1.10207725
6	-2.73046565	-2.07894802	-1.31937718	8	7.55543423	-1.18294811	-0.34347728
6	-2.92656565	-0.90704811	2.39972258	6	6.38313389	-0.58634806	-0.85267729
6	-2.07956576	-1.70314813	-2.66477728	8	4.04403400	-0.40964809	-0.47077727
6	-3.25506568	0.58275187	2.17512274	6	5.24073410	-1.04524815	0.03362273

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1	-2.65026569	1.01855195	1.37962270	1	5.12703419	-2.13064814	-0.01227727
1	-3.07906556	1.15825188	3.09222269	1	5.41293430	-0.74334812	1.07042265
1	-4.30836582	0.69975191	1.89732265	1	-5.04906607	-4.27734804	-0.09097727
6	-1.48586559	-1.07214808	2.92102265	1	3.11793447	1.76595187	1.37762284
1	-0.75016564	-0.71164811	2.20132256	1	3.42413425	1.13635194	3.02062273
1	-1.27606559	-2.12784815	3.12922263	1	1.54723430	2.54745197	3.18692279
1	-1.34786570	-0.51024806	3.85302258	1	0.96013433	0.89255190	3.35312271
6	-3.85276556	-1.38924813	3.53142262	1	6.45403433	0.51205188	-0.83457726
1	-3.66176558	-2.43074822	3.81172276	1	6.19553423	-0.89554811	-1.89177728
1	-4.91156578	-1.29134810	3.26972270	8	-0.62906563	2.46285176	-1.14687729
1	-3.67906570	-0.77604818	4.42312288	15	-0.75166565	3.92765188	-0.88787729
6	-2.62456560	-2.54164815	-3.83527732	8	0.60553432	4.69345188	-0.53537726
1	-3.70596576	-2.42344809	-3.96377730	8	-1.61216569	4.35755205	0.39142272
1	-2.40586567	-3.60894823	-3.72097731	6	0.48293436	5.39985180	0.72202271
1	-2.14696574	-2.21144819	-4.76497746	6	-0.70406562	4.76285172	1.45062280
6	-0.55766565	-1.93924809	-2.62907743	8	-1.36216569	4.68565178	-2.13167739
1	-0.07026567	-1.34654808	-1.85577726	6	-2.17266560	4.00065184	-3.11787724
1	-0.10566565	-1.67294812	-3.59317732	1	-1.77476561	3.00515199	-3.31417727
1	-0.34156567	-2.99754810	-2.44107723	1	-3.20046568	3.93455195	-2.75677729
6	-2.38536572	-0.22964808	-3.00317740	1	-2.12776566	4.61615181	-4.01507711
1	-3.46556568	-0.08354810	-3.11797738	1	0.31963432	6.45665169	0.49472272
1	-1.90276575	0.05065191	-3.94867730	1	1.41883433	5.27085209	1.26522279
1	-2.03416562	0.44365191	-2.22077727	1	-1.24066567	5.46965170	2.08382273
8	1.57973433	0.05405191	-0.58337724	1	-0.40756565	3.86175179	1.99402261
15	2.62973428	-0.66154814	0.19952273	1	9.55063438	-1.36214817	-0.63227725
8	2.70093441	-0.26184812	1.73322272	1	8.88933372	0.22525190	-1.10787725
				1	8.61103439	-1.20604813	-2.14087725

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A'-1



Zero-point vibrational energy	1373124.8 (Joules/Mol)
	328.18470 (Kcal/Mol)
Zero-point correction=	0.522996 (Hartree/Particle)
Thermal correction to Energy=	0.557968
Thermal correction to Enthalpy=	0.558912
Thermal correction to Gibbs Free Energy=	0.454209
Sum of electronic and zero-point Energies=	-1924.413992
Sum of electronic and thermal Energies=	-1924.379020
Sum of electronic and thermal Enthalpies=	-1924.378076
Sum of electronic and thermal Free Energies=	-1924.482779

				cartesian			
12	-0.96345717	-0.75817937	0.29601595	6	0.51444286	2.66092062	-0.85818410
8	0.77694279	-0.12297940	0.32641596	1	1.09264278	2.81292057	-1.77698398
6	2.06794286	0.18082060	0.28441596	1	-0.23585719	3.45962048	-0.79468405
6	3.05714273	-0.85277939	0.22531596	1	-0.00275719	1.70382059	-0.93438399
6	4.40514278	-0.48357940	0.18041596	8	-2.42965722	0.63252062	0.69491601
1	5.17284298	-1.24927938	0.13751595	15	-3.85665727	0.19162059	0.54841590
6	4.80784273	0.84752065	0.19091596	8	-4.46845722	-0.82867938	1.56281602
6	3.84134293	1.84582055	0.24971595	8	-1.96135712	-2.23347950	0.86911595
1	4.17404270	2.87862062	0.26021594	6	-4.22495699	-2.28017950	1.63381600
6	2.47514272	1.55342054	0.29791597	6	-2.76975727	-2.61237955	1.91051602
6	2.66964269	-2.34367943	0.21541595	8	-4.83615732	1.44182062	0.63021600
6	1.44604278	2.69712067	0.37071595	6	-4.60855722	2.47642064	1.61321592
6	1.82124281	-2.66947937	-1.03158402	1	-4.91845703	2.12212062	2.59871578
1	0.94644278	-2.02307940	-1.11398399	1	-3.55615735	2.76572061	1.62431598

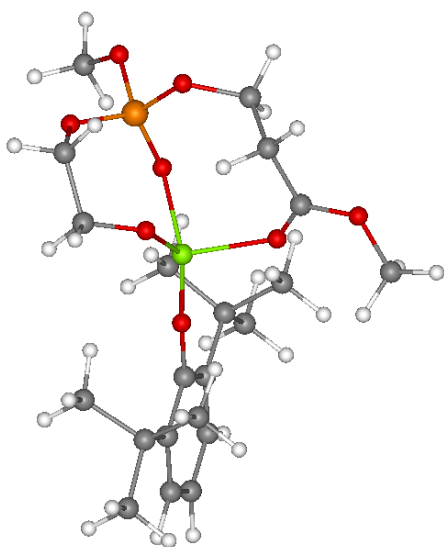
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1	1.47854280	-3.71087933	-1.00648403	1	-5.22995710	3.31802058	1.31021595
1	2.41734266	-2.52937937	-1.94078398	8	-1.49035716	-0.67497939	-1.76058400
6	1.91434264	-2.71467948	1.50791597	6	-2.35625720	-0.24047941	-2.50238419
1	1.01164293	-2.11927938	1.64611602	6	-3.74885726	0.20332059	-2.08358407
1	2.55684280	-2.55127954	2.38001585	8	-4.19635725	-0.42707941	-0.89368403
1	1.62244272	-3.77157950	1.49331594	1	5.86404276	1.10422051	0.15701595
6	3.89784288	-3.26947951	0.15131596	1	-4.54705715	-2.70417953	0.67971599
1	4.55274296	-3.14907932	1.02061594	1	-4.89175701	-2.60727954	2.43451595
1	4.49284267	-3.10797954	-0.75388408	1	-2.74985719	-3.70747948	2.07701588
1	3.56144285	-4.31247950	0.13891596	1	-2.49395728	-2.15327954	2.87931585
6	2.10944271	4.08572054	0.37281597	1	-3.74125719	1.29532051	-1.99088407
1	2.69364285	4.26882076	-0.53548408	1	-4.45745707	-0.05937940	-2.86998415
1	2.76434278	4.23132038	1.23831594	8	-2.18205714	-0.06267940	-3.80078411
1	1.33154273	4.85672045	0.42061594	6	-0.85995722	-0.36067939	-4.31688404
6	0.62684280	2.59792066	1.67351604	1	-0.90975714	-0.11887940	-5.37598372
1	0.10354280	1.64482057	1.74941599	1	-0.63645720	-1.41717947	-4.16728401
1	-0.11515719	3.40532064	1.72161603	1	-0.11505717	0.25182059	-3.80848408
1	1.28554273	2.69322062	2.54361582				

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A'-2



Zero-point vibrational energy	1450333.1 (Joules/Mol)
	346.63792 (Kcal/Mol)
Zero-point correction=	0.552403 (Hartree/Particle)
Thermal correction to Energy=	0.588281
Thermal correction to Enthalpy=	0.589225
Thermal correction to Gibbs Free Energy=	0.482931
Sum of electronic and zero-point Energies=	-1963.695889
Sum of electronic and thermal Energies=	-1963.660011
Sum of electronic and thermal Enthalpies=	-1963.659066
Sum of electronic and thermal Free Energies=	-1963.765361

cartesian

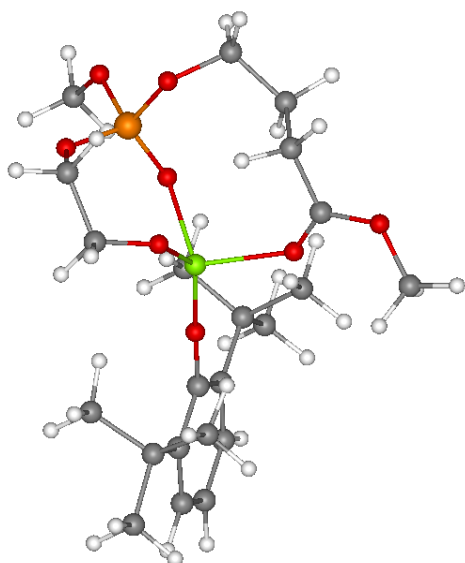
12	-0.89796960	-0.36690754	0.11096220	1	1.78823042	1.81019247	-2.90123796
8	0.88973039	0.11439248	0.19776221	1	0.44763041	2.89729238	-2.49183774
6	2.20633030	0.28139246	0.20786220	1	0.48513043	1.24129248	-1.85193789
6	3.06343031	-0.73900753	0.73086220	8	-2.23696971	1.16019249	0.30156219
6	4.44433022	-0.51990753	0.72446221	15	-3.63826966	0.94269246	0.80336219
1	5.11293030	-1.27920747	1.11606216	8	-3.84136963	0.27599245	2.21656203
6	5.00323057	0.65259248	0.22796220	8	-2.08956957	-1.62170744	0.91906220
6	4.16423035	1.63919258	-0.27923781	6	-3.84826970	-1.16390753	2.47686219
1	4.61753035	2.54749250	-0.66233778	6	-2.48756957	-1.79400742	2.23206210
6	2.77443027	1.49069250	-0.30573779	8	-4.39286947	2.33309245	0.95376217
6	2.49793029	-2.05660748	1.29206216	6	-3.74416971	3.42799234	1.63476217
6	1.89193034	2.61539245	-0.87823778	1	-3.67766976	3.21599245	2.70456219
6	1.75313044	-2.83330750	0.18696220	1	-2.75036955	3.60049248	1.21686220
1	0.96983045	-2.23320770	-0.27843779	1	-4.37756968	4.29849243	1.46986210

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1	1.29313040	-3.74240756	0.59276217	8	-1.30076957	-0.95440751	-1.85993791
1	2.45363045	-3.12820768	-0.60243779	6	-2.27486968	-1.50770748	-2.37193775
6	1.57203031	-1.77590752	2.49296212	6	-3.65006971	-1.51210749	-1.77103782
1	0.76773041	-1.08560753	2.23546219	8	-4.58116961	0.12969248	-0.18943779
1	2.14313030	-1.32510746	3.31196213	6	-4.21236944	-0.09270752	-1.56713784
1	1.12453032	-2.70670748	2.86196208	1	-3.50226974	0.67439246	-1.88293791
6	3.60053015	-2.99870753	1.80996215	1	-5.13566971	0.03919248	-2.13153791
1	4.17543030	-2.55220771	2.62806225	1	6.08113050	0.79639244	0.23656221
1	4.29873037	-3.29580760	1.02016211	1	-4.61026955	-1.60730743	1.82996213
1	3.13933039	-3.91430759	2.19806218	1	-4.16316938	-1.24350750	3.51986217
6	2.71883035	3.81879234	-1.36463785	1	-2.59776974	-2.86280751	2.49716210
1	3.41363025	3.54849243	-2.16703796	1	-1.77506971	-1.37220752	2.96376204
1	3.29193044	4.28309250	-0.55483782	1	-4.31796932	-2.12760758	-2.37483788
1	2.04253030	4.58329248	-1.76403785	1	-3.51886964	-1.96840751	-0.78003782
6	0.93153042	3.14979243	0.20396221	8	-2.18246961	-2.16270757	-3.51783776
1	0.28053039	2.36549234	0.59016222	6	-0.86496961	-2.23430753	-4.11283779
1	0.30353040	3.95109248	-0.20653780	1	-0.99976963	-2.80200768	-5.03103781
1	1.50063038	3.56409240	1.04376209	1	-0.17796960	-2.74390769	-3.43653774
6	1.10063028	2.10639238	-2.10073781	1	-0.49496961	-1.23060751	-4.32443810

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A'-3



Zero-point vibrational energy	1526129.7 (Joules/Mol)
	364.75375 (Kcal/Mol)
Zero-point correction=	0.581272 (Hartree/Particle)
Thermal correction to Energy=	0.618427
Thermal correction to Enthalpy=	0.619371
Thermal correction to Gibbs Free Energy=	0.510255
Sum of electronic and zero-point Energies=	-2002.973691
Sum of electronic and thermal Energies=	-2002.936537
Sum of electronic and thermal Enthalpies=	-2002.935593
Sum of electronic and thermal Free Energies=	-2003.044708

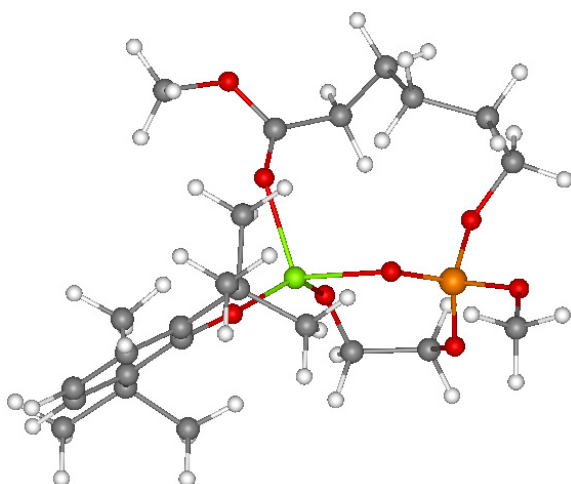
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12	-0.72765243	-0.52761161	0.13493633	1	0.59484756	1.10668850	-1.88326371
8	1.03774750	0.05708843	0.19683632	8	-2.05645227	0.99748844	0.47563630
6	2.34554768	0.27718842	0.20473632	15	-3.36065221	0.85098839	1.21063626
6	3.24354768	-0.68881160	0.76283634	8	-3.36705232	0.03778842	2.55563641
6	4.61434746	-0.41471156	0.74903637	8	-1.85645247	-1.83331156	0.93403637
1	5.31234741	-1.13301158	1.16623628	6	-3.46985221	-1.42201149	2.66163635
6	5.12724733	0.76188838	0.21403632	6	-2.17895246	-2.10811162	2.24713635
6	4.24954748	1.69758844	-0.32336369	8	-3.92025232	2.28258848	1.61923623
1	4.66634750	2.61128855	-0.73396367	6	-3.02265239	3.29968858	2.11573648
6	2.86704779	1.49258852	-0.34486368	1	-2.72815228	3.06368852	3.14073634
6	2.73144770	-2.00701165	1.37103629	1	-2.14255238	3.37818837	1.47523630
6	1.94114745	2.56418848	-0.94906360	1	-3.58795238	4.23058844	2.09883642
6	2.02924776	-2.85711145	0.29263633	8	-1.06295240	-1.09851158	-1.85266376
1	1.22944760	-2.31011152	-0.20876369	6	-2.06745243	-1.51581156	-2.43216348

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1	1.59954751	-3.76571155	0.73133636	6	-3.46225238	-1.28891158	-1.93216372
1	2.75064778	-3.15741158	-0.47556368	8	-4.55365276	0.20998842	0.37703630
6	1.78804767	-1.71941149	2.55663633	6	-3.82525229	0.20748842	-1.99016368
1	0.95914757	-1.07051158	2.27063632	6	-4.88915253	0.59968841	-0.97536367
1	2.33624768	-1.21621156	3.36073637	1	-4.20655251	0.46708843	-2.98456359
1	1.37604761	-2.65311146	2.95813632	1	-2.93555236	0.81848842	-1.82206368
6	3.86974788	-2.88031149	1.93043625	1	-5.07095242	1.67828846	-1.00196373
1	4.42334747	-2.37741160	2.73033643	1	-5.83455276	0.08798843	-1.16786373
1	4.58244753	-3.18101144	1.15503633	1	6.19844723	0.94858843	0.21743631
1	3.44484758	-3.79731154	2.35493636	1	-4.30735254	-1.73791158	2.03443646
6	2.71754766	3.78798842	-1.46696377	1	-3.71295238	-1.59311152	3.71293640
1	3.42234778	3.52668858	-2.26376367	1	-2.35105228	-3.18911147	2.41673636
1	3.27184772	4.29558849	-0.67026365	1	-1.39095247	-1.81101155	2.96253633
1	2.00994778	4.51378870	-1.88456368	1	-4.17025232	-1.89661157	-2.49946356
6	0.95734751	3.08608842	0.11833632	1	-3.44505239	-1.63091159	-0.88976365
1	0.34504756	2.28228855	0.52753633	8	-1.98715246	-2.19281149	-3.56636357
1	0.29334757	3.84508848	-0.31626368	6	-0.65485239	-2.44371152	-4.07106400
1	1.50724757	3.55158854	0.94403636	1	-0.80165243	-2.99911165	-4.99506378
6	1.17284751	1.98998845	-2.15686369	1	-0.08735242	-3.03191161	-3.34916353
1	1.87284744	1.70088851	-2.94916368	1	-0.14165242	-1.50011158	-4.25966406
1	0.48844758	2.74268842	-2.56986356				

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A'-4



Zero-point vibrational energy	1676979.9 (Joules/Mol)
	400.80782 (Kcal/Mol)
Zero-point correction=	0.638728 (Hartree/Particle)
Thermal correction to Energy=	0.678630
Thermal correction to Enthalpy=	0.679574
Thermal correction to Gibbs Free Energy=	0.564063
Sum of electronic and zero-point Energies=	-2081.513759
Sum of electronic and thermal Energies=	-2081.473857
Sum of electronic and thermal Enthalpies=	-2081.472913
Sum of electronic and thermal Free Energies=	-2081.588424

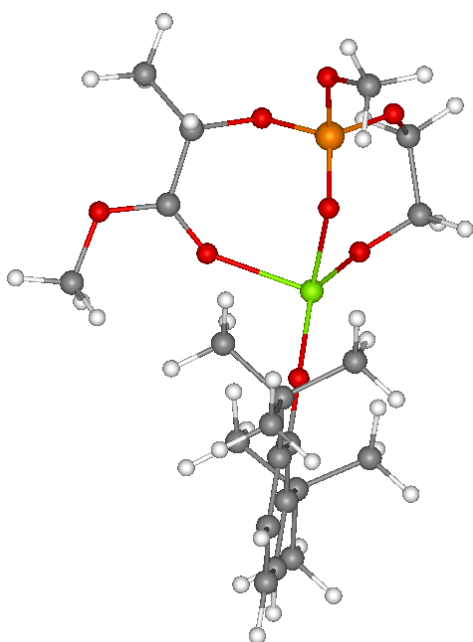
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12	0.33661333	-0.45732933	-0.49791196	8	2.76581335	0.57827067	-2.89971185
8	-1.41428661	0.14947067	-0.29491198	8	1.30331337	-1.56432927	-1.69771194
6	-2.70638657	0.40117067	-0.14021197	6	2.78991342	-0.79662931	-3.40561199
6	-3.69188666	-0.43892932	-0.75371194	6	1.50331342	-1.52842927	-3.06061196
6	-5.04308701	-0.13412932	-0.56441200	8	3.66461349	2.41207075	-1.45801198
1	-5.80528688	-0.75602931	-1.02231193	6	2.87441325	3.61237073	-1.60271204
6	-5.45598698	0.95297068	0.19848803	1	2.50931334	3.69207072	-2.62901187
6	-4.49488688	1.76517069	0.79118800	1	2.03841329	3.60427070	-0.90141201
1	-4.83368683	2.61037087	1.38128805	1	3.54591346	4.44177055	-1.38341200
6	-3.12578654	1.52357066	0.64498806	8	0.74231339	-1.51072931	1.24798799
6	-3.29348660	-1.65642929	-1.60721195	6	1.57951331	-2.28472924	1.71278799
6	-2.10508657	2.45927072	1.31818795	6	3.02511334	-2.34332919	1.31238794
6	-2.52728653	-2.68322921	-0.74781191	8	4.08751345	0.02917068	-0.83541203
1	-1.66718662	-2.23682928	-0.24701196	6	4.69101334	0.86817068	1.45108795
1	-2.17058659	-3.51782918	-1.36361206	6	5.14961290	0.38167068	0.08538803

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1	-3.18678665	-3.08952928	0.02778803	1	5.60371304	0.92157066	2.06038809
6	-2.45088673	-1.21092927	-2.81921196	1	4.32341290	1.89667070	1.36728799
1	-1.56398666	-0.65412933	-2.51541185	1	5.78261328	1.13357067	-0.39371198
1	-3.04348660	-0.56062931	-3.47211194	1	5.72311306	-0.54392934	0.16668802
1	-2.12858653	-2.08022928	-3.40521193	1	-6.51448679	1.16637063	0.32738802
6	-4.51268673	-2.40152931	-2.18081188	1	3.65831327	-1.29432929	-2.96581197
1	-5.11208677	-1.76712930	-2.84261179	1	2.93461347	-0.68322933	-4.48271179
1	-5.16718674	-2.79532909	-1.39591205	1	1.60841334	-2.54182911	-3.49551177
1	-4.16588688	-3.25522923	-2.77441192	1	0.67731333	-1.04472935	-3.61371183
6	-2.78018665	3.59977078	2.10088801	1	3.35051346	-3.38592911	1.36498797
1	-3.41898656	3.22907090	2.90988803	1	3.09341335	-1.99882936	0.27798802
1	-3.38348675	4.24577045	1.45408797	8	1.26701331	-3.13182926	2.68488812
1	-2.00788665	4.22837067	2.55888820	6	-0.10228667	-3.10542917	3.14778805
6	-1.20818663	3.12737083	0.25618804	1	-0.15358666	-3.86472917	3.92558813
1	-0.66888666	2.38997078	-0.33841199	1	-0.77998662	-3.34272909	2.32718801
1	-0.47608665	3.78777075	0.73978806	1	-0.34498665	-2.12042928	3.54838800
1	-1.81518674	3.73657084	-0.42311198	6	3.62831330	0.03017068	2.17478824
6	-1.24928665	1.67797065	2.33628821	1	3.53631330	0.44117066	3.18578815
1	-1.88278675	1.28277063	3.13878822	6	3.89401340	-1.48602927	2.26068807
1	-0.49838665	2.33607078	2.79238820	1	2.66091347	0.21467067	1.70028806
1	-0.73558664	0.83647066	1.87058794	1	3.73371339	-1.83802927	3.28498816
8	1.70771337	1.06327069	-0.55061197	1	4.94331312	-1.70932937	2.03748822
15	2.95331335	0.98767066	-1.38991201				

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A'-6



Zero-point vibrational energy	1446305.8 (Joules/Mol)
	345.67539 (Kcal/Mol)
Zero-point correction=	0.550869 (Hartree/Particle)
Thermal correction to Energy=	0.587326
Thermal correction to Enthalpy=	0.588270
Thermal correction to Gibbs Free Energy=	0.480783
Sum of electronic and zero-point Energies=	-1963.692811
Sum of electronic and thermal Energies=	-1963.656354
Sum of electronic and thermal Enthalpies=	-1963.655410
Sum of electronic and thermal Free Energies=	-1963.762897

				cartesian			
12	-0.71301520	-0.75301516	0.51856208	1	1.21418476	2.85438466	-1.64003789
8	1.02888489	-0.12901516	0.40536207	1	-0.04171517	3.48358464	-0.55623788
6	2.31538486	0.17288485	0.28816211	1	0.17148483	1.73108482	-0.74863791
6	3.29488468	-0.86161512	0.14306210	8	-2.14981508	0.64988488	0.97856212
6	4.63838482	-0.49471518	0.01786210	15	-3.57851529	0.19728482	0.89726210
1	5.39868498	-1.26081514	-0.09083790	8	-4.13551521	-0.79411513	1.97176206
6	5.04648495	0.83478487	0.03026210	8	-1.64261508	-2.21751523	1.21646214
6	4.08988476	1.83378482	0.17476210	6	-3.87631512	-2.24061537	2.07396221
1	4.42648458	2.86518478	0.18696210	6	-2.40901518	-2.55711532	2.30206203
6	2.72858477	1.54378486	0.30596209	8	-4.56321526	1.44468486	0.98496211
6	2.90268469	-2.35091519	0.13136210	6	-4.29631519	2.51118469	1.92246211
6	1.71258473	2.68858480	0.47506207	1	-4.56441545	2.18988466	2.93116212

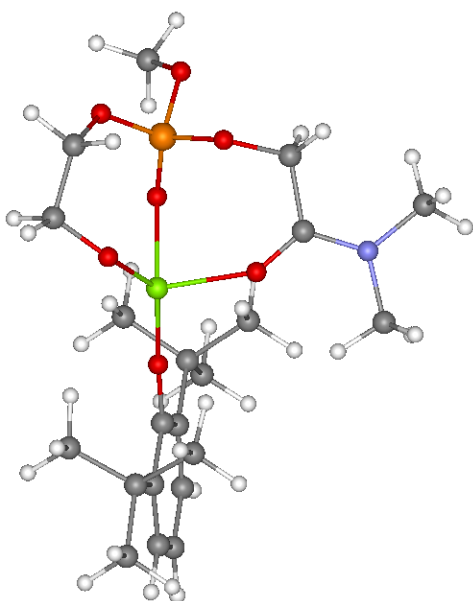
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6	1.97388482	-2.65391517	-1.06263793	1	-3.24461532	2.80028462	1.88076210
1	1.09768486	-2.00421524	-1.07843792	1	-4.93041515	3.34298468	1.61816216
1	1.63018489	-3.69491529	-1.03203785	8	-1.39151514	-0.67861515	-1.49563789
1	2.51128483	-2.50181532	-2.00593781	6	-2.26171517	-0.20391515	-2.20813799
6	2.23568487	-2.74631524	1.46436214	6	-3.67621517	0.16158482	-1.75343788
1	1.33678484	-2.16531515	1.67216206	8	-3.97371531	-0.46971518	-0.50453788
1	2.93218470	-2.58881521	2.29516220	1	6.09918499	1.08928490	-0.06713790
1	1.95428467	-3.80611515	1.45346212	1	-4.23251534	-2.69501519	1.14616215
6	4.12148476	-3.27801538	-0.03013790	1	-4.50741529	-2.54961514	2.91006207
1	4.83158493	-3.17831516	0.79776210	1	-2.37811518	-3.64521527	2.50876212
1	4.65898466	-3.10131526	-0.96793795	1	-2.09631515	-2.06141520	3.24136209
1	3.78068495	-4.31971502	-0.04173790	1	-3.68721533	1.25288486	-1.63513792
6	2.38138485	4.07458496	0.46276212	6	-4.75441504	-0.25271517	-2.74413800
1	2.90448475	4.27508497	-0.47853786	8	-2.06651521	0.09278484	-3.48173785
1	3.09358478	4.19908476	1.28536212	6	-0.72811520	-0.13341516	-3.99263787
1	1.61228466	4.84698486	0.57926214	1	-0.75981516	0.20648482	-5.02533817
6	0.98488480	2.56198478	1.82876205	1	-0.48781517	-1.19551516	-3.93843794
1	0.46158487	1.61008489	1.91896212	1	-0.00591516	0.44008484	-3.41143799
1	0.25308484	3.37128472	1.94856215	1	-5.72661543	0.05758484	-2.35693789
1	1.70338488	2.63218474	2.65276217	1	-4.75931501	-1.33751512	-2.87313795
6	0.69878489	2.68388486	-0.68743789	1	-4.58721542	0.22078484	-3.71223783

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A'-7



Zero-point vibrational energy	1478975.8 (Joules/Mol)
	353.48369 (Kcal/Mol)
Zero-point correction=	0.563312 (Hartree/Particle)
Thermal correction to Energy=	0.600169
Thermal correction to Enthalpy=	0.601113
Thermal correction to Gibbs Free Energy=	0.492516
Sum of electronic and zero-point Energies=	-1943.810514
Sum of electronic and thermal Energies=	-1943.773657
Sum of electronic and thermal Enthalpies=	-1943.772713
Sum of electronic and thermal Free Energies=	-1943.881310

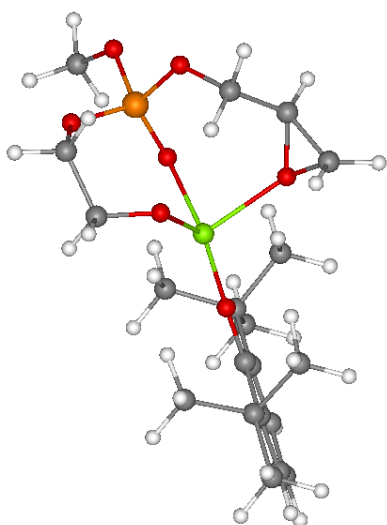
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12	0.76383877	0.93729556	0.37077022	1	-2.93286133	3.17369556	1.63597023
8	-0.98466128	0.32219553	0.52017021	1	-1.96036124	4.12609577	0.49827021
6	-2.26396132	-0.01990448	0.47627020	1	-1.32796121	2.61249542	1.15777016
6	-2.66246128	-1.33800447	0.87177020	8	2.23613882	-0.23350447	1.24127018
6	-4.01706123	-1.67650449	0.80657023	15	3.63953876	0.23119551	0.98917019
1	-4.34046125	-2.66930461	1.10187030	8	4.19523859	1.48579550	1.74077022
6	-4.98326111	-0.77390444	0.37487021	8	1.67143869	2.55359554	0.65447021
6	-4.59096098	0.50679553	-0.00002978	6	3.87793875	2.90189552	1.49237025
1	-5.35816097	1.20039546	-0.32812980	6	2.39463878	3.19799542	1.62367022
6	-3.25486135	0.91719556	0.03787022	8	4.67963886	-0.91690457	1.36717021
6	-1.63496137	-2.37240458	1.36807024	6	4.48633909	-1.69070446	2.57067013
6	-2.88196135	2.35249543	-0.37952977	1	4.75103903	-1.08910453	3.44317031
6	-0.91796130	-1.85350454	2.63107014	1	3.45173860	-2.03120446	2.64287019

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1	-0.40946126	-0.90700448	2.44767022	1	5.16113901	-2.54230452	2.49147010
1	-0.17546129	-2.58380461	2.97767019	8	1.40973878	0.32229552	-1.49862981
1	-1.64056134	-1.69810450	3.43977022	6	2.26843882	-0.33830449	-2.09932971
6	-0.61276132	-2.68940449	0.25727022	6	3.69813871	-0.45750448	-1.55892980
1	-0.09916127	-1.78830457	-0.07952978	8	3.98083878	0.50419551	-0.55522978
1	-1.11806130	-3.13730454	-0.60652977	1	-6.03086090	-1.06330454	0.33647022
1	0.13813874	-3.40390444	0.61887020	1	4.23213863	3.13389540	0.48497021
6	-2.28866124	-3.71120453	1.75407016	1	4.48203897	3.42869544	2.23457026
1	-2.79716134	-4.18570423	0.90777022	1	2.31183863	4.30039549	1.54527020
1	-3.01026130	-3.59980440	2.57037020	1	2.08653879	2.94399548	2.65687013
1	-1.51266122	-4.40500450	2.09817028	1	3.86733866	-1.47490454	-1.18672979
6	-4.11096096	3.18019557	-0.79752976	1	4.42163897	-0.26670450	-2.35412979
1	-4.83046103	3.29359555	0.02027022	7	1.99173880	-0.98750448	-3.24552989
1	-4.63216114	2.74649549	-1.65782976	6	2.97823858	-1.73840451	-4.01132965
1	-3.78496146	4.18589592	-1.08672976	6	0.65813875	-0.88670456	-3.83452988
6	-1.94336128	2.32979560	-1.60372984	1	0.22013873	-1.88440442	-3.93022990
1	-1.05406117	1.72349548	-1.42722976	1	0.72463870	-0.42710450	-4.82592964
1	-1.61946130	3.34469557	-1.86392975	1	0.02463874	-0.27750447	-3.19462967
1	-2.46386123	1.90669549	-2.47092986	1	2.46903872	-2.55560446	-4.52642965
6	-2.23066139	3.10629559	0.79777020	1	3.73703861	-2.18570447	-3.36902976
				1	3.46783876	-1.10930455	-4.76392937

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## A'-Gly



Zero-point vibrational energy	1361910.3 (Joules/Mol)
	325.50438 (Kcal/Mol)
Zero-point correction=	0.518724 (Hartree/Particle)
Thermal correction to Energy=	0.551901
Thermal correction to Enthalpy=	0.552846
Thermal correction to Gibbs Free Energy=	0.452894
Sum of electronic and zero-point Energies=	-1849.161111
Sum of electronic and thermal Energies=	-1849.127934
Sum of electronic and thermal Enthalpies=	-1849.126990
Sum of electronic and thermal Free Energies=	-1849.226941

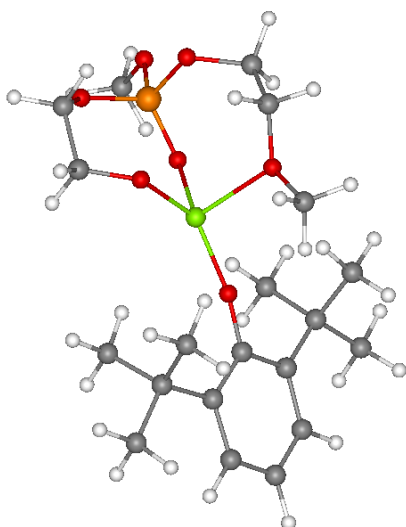
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12	-0.96379507	-0.41144353	-0.07743064	1	1.28040481	3.06185651	1.93696928
8	0.82520491	0.01585647	0.02946937	6	0.82620496	2.65675640	-1.50103068
6	2.13010478	0.26365647	0.06766936	1	1.49490499	2.68705654	-2.36843061
6	3.06220484	-0.81164354	0.21446937	1	0.10850489	3.48095655	-1.59803069
6	4.42720509	-0.51004356	0.24836938	1	0.27540493	1.71645641	-1.54033065
1	5.15400505	-1.30784357	0.35796934	8	-2.44429517	0.96575648	0.02316937
6	4.89740467	0.79455644	0.14686938	15	-3.86889505	0.54275644	0.25736937
6	3.98400497	1.83375645	0.00646937	8	-4.18179512	-0.11644352	1.66316938
1	4.36800480	2.84545636	-0.06973063	8	-2.08169508	-1.78704357	0.63366938
6	2.60500479	1.60895646	-0.03793063	6	-4.01579523	-1.52194357	2.01206923
6	2.59560490	-2.27414346	0.34156936	6	-2.56499505	-1.96564353	1.91966927
6	1.63770485	2.79675651	-0.19683063	8	-4.84919500	1.78915644	0.23526938
6	1.83000493	-2.70874357	-0.92493063	6	-4.53449535	2.94415641	1.03976929
1	0.98490494	-2.04944348	-1.13033068	1	-4.64249516	2.70405650	2.10016942

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1	1.45400500	-3.73364353	-0.81603062	1	-3.52099514	3.29055643	0.82696939
1	2.49100494	-2.67894363	-1.79813063	1	-5.25799513	3.70775652	0.75816941
6	1.72180486	-2.45394349	1.59936929	8	-1.52199507	-0.65264356	-2.13353062
1	0.84040493	-1.81194353	1.58336937	8	-4.54279518	-0.31964353	-0.90263063
1	2.29820490	-2.20764351	2.49776936	6	-2.86819506	-0.84394354	-2.63033056
1	1.38370490	-3.49374366	1.68756938	6	-3.89679503	-1.36094356	-1.66633070
6	3.77360487	-3.25464344	0.49036935	1	-4.70879507	-1.81994355	-2.23613071
1	4.36260509	-3.05914354	1.39256930	1	-3.44179511	-2.08344364	-0.98393059
1	4.44760466	-3.23094344	-0.37273064	1	5.96490479	0.99935645	0.17756937
1	3.38410497	-4.27594376	0.57156938	1	-4.65179491	-2.10594344	1.33896935
6	2.37440491	4.14555645	-0.28513065	1	-4.40909481	-1.59594357	3.02856922
1	3.04760480	4.19635630	-1.14753067	1	-2.54479504	-3.02724361	2.22736931
1	2.95480490	4.36155653	0.61826938	1	-1.98779511	-1.41434360	2.68376923
1	1.63880491	4.95015621	-0.39903066	6	-1.76989508	-1.72944355	-3.05253077
6	0.69950491	2.89325643	1.02356935	1	-3.17519522	-0.04074352	-3.29703069
1	0.11630493	1.98255646	1.16206932	1	-1.31039500	-1.58734357	-4.02673054
1	0.00270492	3.73275638	0.90576941	1	-1.68709517	-2.72134352	-2.61503077

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**A'-OCH<sub>2</sub>CH<sub>2</sub>OMe**



Zero-point vibrational energy	1423729.2 (Joules/Mol)
	340.27943 (Kcal/Mol)
Zero-point correction=	0.542270 (Hartree/Particle)
Thermal correction to Energy=	0.576320
Thermal correction to Enthalpy=	0.577264
Thermal correction to Gibbs Free Energy=	0.476644
Sum of electronic and zero-point Energies=	-1850.374625
Sum of electronic and thermal Energies=	-1850.340574
Sum of electronic and thermal Enthalpies=	-1850.339630
Sum of electronic and thermal Free Energies=	-1850.440251

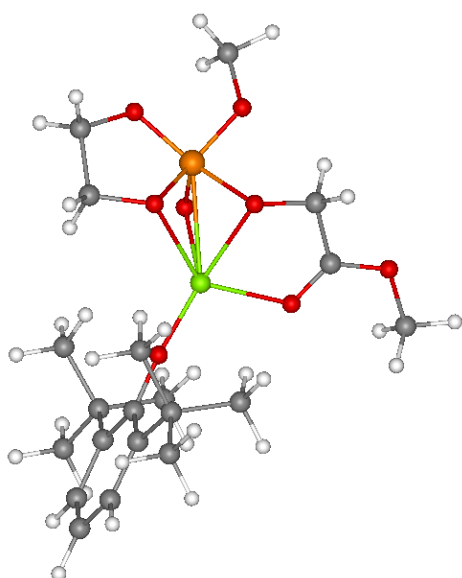
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12	0.99697030	0.39106560	-0.21161562	6	-1.18152976	-2.81903434	-1.18441558
8	-0.80522972	-0.01983440	-0.05151563	1	-1.91142988	-2.80653429	-2.00201583
6	-2.10992980	-0.11783440	0.18778437	1	-0.62342972	-3.76203442	-1.24661565
6	-2.90682983	1.05796552	0.36678436	1	-0.48152971	-1.99793446	-1.33721554
6	-4.28462982	0.90686560	0.55438435	8	2.34307027	-0.72963440	0.79438436
1	-4.91182995	1.78296554	0.68058431	15	3.79907012	-0.35343438	0.71538436
6	-4.89232969	-0.34293440	0.58858442	8	4.27077055	0.99946564	1.36318445
6	-4.10462999	-1.48123443	0.45638436	8	2.12597036	1.89336550	-0.38431564
1	-4.59392977	-2.44803429	0.50748438	6	4.19267035	2.32246566	0.73538435
6	-2.72132969	-1.41003442	0.26678437	6	2.75797033	2.75476575	0.48588437
6	-2.28632975	2.46856570	0.37668437	8	4.68417025	-1.44083440	1.46448445
6	-1.89452982	-2.70763421	0.17758438	6	4.29347038	-1.90613449	2.77338433
6	-1.64512968	2.79836559	-0.98571563	1	4.45617008	-1.11863446	3.51298428
1	-0.85562974	2.09466577	-1.24971557	1	3.24677014	-2.21703434	2.76968431

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1	-1.20592976	3.80296564	-0.97331560	1	4.93727016	-2.75693440	2.99238420
1	-2.40162969	2.76716566	-1.77781558	8	1.49467039	-0.32913437	-2.17671561
6	-1.25282979	2.58596563	1.51628435	6	2.83577013	-0.28973439	-2.68301582
1	-0.48712969	1.81026554	1.46018445	6	3.78787017	-1.10513449	-1.82981563
1	-1.74762988	2.48276567	2.48808432	8	4.38827038	-0.34423438	-0.75991559
1	-0.75392967	3.56186557	1.48858440	1	-5.96692991	-0.42973438	0.73018432
6	-3.33242989	3.56846571	0.63438439	1	4.75297022	2.26846576	-0.20161563
1	-3.83822966	3.44276571	1.59718442	1	4.71136999	2.97676563	1.43978441
1	-4.09272957	3.60946560	-0.15271564	1	2.82297015	3.78316569	0.08118437
1	-2.83142972	4.54296541	0.65348434	1	2.25067019	2.84456563	1.46458435
6	-2.76702976	-3.96793437	0.31678438	1	3.28767014	-1.99673450	-1.44221556
1	-3.50962973	-4.05043459	-0.48421565	1	4.63127041	-1.41983449	-2.44741583
1	-3.29042983	-4.00743437	1.27788436	1	2.82537031	-0.73403436	-3.68641567
1	-2.12702966	-4.85573435	0.25868437	1	3.17477012	0.75006562	-2.74991584
6	-0.86432976	-2.75663424	1.32448435	6	0.54277027	0.11816560	-3.15801573
1	-0.18132973	-1.90723443	1.29468441	1	0.58187032	-0.53793436	-4.03421593
1	-0.26962972	-3.67723441	1.26518440	1	0.75347030	1.15226555	-3.45081568
1	-1.37412977	-2.74703431	2.29428434	1	-0.44152969	0.05326560	-2.69481564

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A'B'-1



Zero-point vibrational energy	1374931.1 (Joules/Mol)
	328.61643 (Kcal/Mol)
Zero-point correction=	0.523684 (Hartree/Particle)
Thermal correction to Energy=	0.557328
Thermal correction to Enthalpy=	0.558273
Thermal correction to Gibbs Free Energy=	0.457373
Sum of electronic and zero-point Energies=	-1924.397948
Sum of electronic and thermal Energies=	-1924.364304
Sum of electronic and thermal Enthalpies=	-1924.363359
Sum of electronic and thermal Free Energies=	-1924.464259

cartesian

12	1.02779222	0.18301116	-0.15659687	6	-1.27130783	-0.25248885	-2.98439670
8	-0.77910781	-0.07308884	0.04020312	1	-1.97550786	0.47511119	-3.40259671
6	-2.10680771	-0.14668885	0.04520312	1	-0.68210781	-0.66868883	-3.81059670
6	-2.84750795	0.40761113	1.13570309	1	-0.59790790	0.29511118	-2.32299685
6	-4.24100780	0.29551119	1.11770308	8	2.56729221	-0.89908886	-0.94799691
1	-4.82570791	0.70521116	1.93450308	15	3.37049198	-0.82198888	0.36290312
6	-4.91740751	-0.33058882	0.07620312	8	3.95079231	-2.33448863	0.75460309
6	-4.18900776	-0.85698885	-0.98499691	8	2.10849214	-1.03168881	1.53160310
1	-4.73380756	-1.33728886	-1.79089689	6	3.12079191	-3.15118885	1.56470311
6	-2.79370785	-0.78208888	-1.03629696	6	1.79139209	-2.41128874	1.69780314
6	-2.14780807	1.11951113	2.30880332	8	4.89209223	-0.26658887	0.15950312
6	-2.03520775	-1.36838889	-2.24219680	6	5.96639204	-1.09138882	-0.31559688
6	-1.37760782	2.35591125	1.80080307	1	6.32589245	-1.74698889	0.47850314

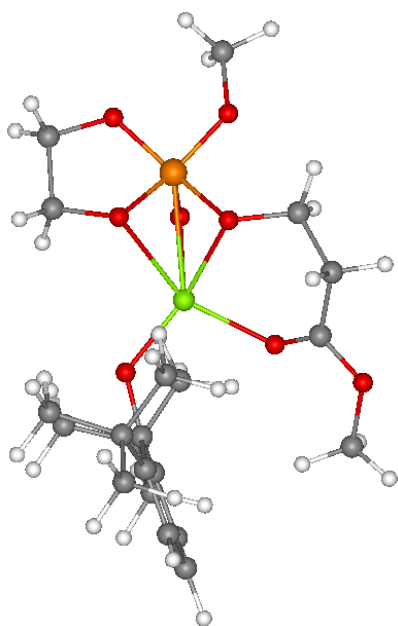
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1	-0.65890789	2.09371138	1.02250314	1	5.65479231	-1.68988883	-1.17459691
1	-0.83840787	2.84001136	2.62490320	1	6.75589228	-0.39938885	-0.61629689
1	-2.07080793	3.08841133	1.37280309	8	1.36919212	2.03701115	-1.05499685
6	-1.19670784	0.15171115	3.04160333	6	2.45309210	2.57621121	-0.82499689
1	-0.43420786	-0.25288886	2.37590313	6	3.47259235	1.99721110	0.12880312
1	-1.76080787	-0.69028884	3.45820332	8	2.92329216	0.88191116	0.78000307
1	-0.69200790	0.66351116	3.87060332	1	-6.00210762	-0.40478885	0.09010312
6	-3.14440775	1.63141119	3.36420321	1	3.61359215	-3.28338885	2.53380322
1	-3.71710777	0.81721115	3.82040310	1	2.99739218	-4.12568903	1.08620310
1	-3.85020781	2.36081123	2.95270324	1	1.33309221	-2.53668880	2.67990327
1	-2.59160805	2.13061118	4.16800308	1	1.08239222	-2.72388864	0.92400306
6	-2.97930765	-2.00768876	-3.27609682	1	4.37829208	1.75841117	-0.43499687
1	-3.68810797	-1.28628886	-3.69629669	1	3.73579216	2.76391125	0.86670309
1	-3.54710770	-2.84388876	-2.85469675	8	2.82589197	3.70981121	-1.38329685
1	-2.38590765	-2.40308881	-4.10819721	6	1.89379215	4.30861092	-2.31489682
6	-1.07300782	-2.48548865	-1.78959692	1	2.38019228	5.21961117	-2.65639687
1	-0.35070789	-2.13008881	-1.05399692	1	0.95469213	4.53411102	-1.80859685
1	-0.51780784	-2.88788867	-2.64529681	1	1.71179211	3.62841129	-3.14759684
1	-1.63640797	-3.30728865	-1.33409691				

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A'B'-2



Zero-point vibrational energy	1452586.6 (Joules/Mol)
	347.17652 (Kcal/Mol)
Zero-point correction=	0.553261 (Hartree/Particle)
Thermal correction to Energy=	0.587579
Thermal correction to Enthalpy=	0.588523
Thermal correction to Gibbs Free Energy=	0.487465
Sum of electronic and zero-point Energies=	-1963.675558
Sum of electronic and thermal Energies=	-1963.641241
Sum of electronic and thermal Enthalpies=	-1963.640297
Sum of electronic and thermal Free Energies=	-1963.741355

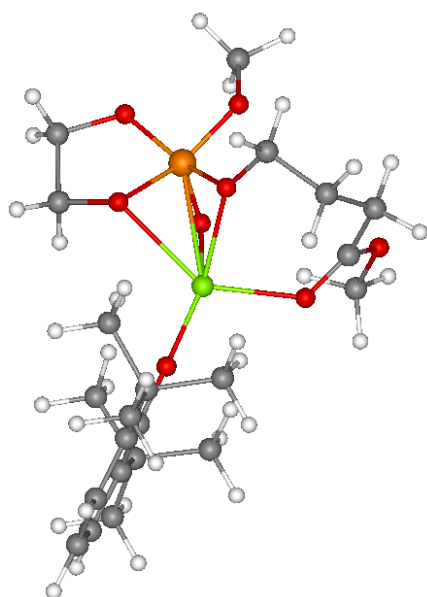
				cartesian			
12	-1.01719987	-0.07539691	0.35268635	1	0.70200014	-0.87539691	2.85088634
8	0.49140015	-0.85649693	-0.46711361	1	0.39960012	-2.57939696	3.20358634
6	1.77500010	-0.54369694	-0.27521360	1	-0.26569986	-1.89749682	1.74708641
6	2.43480015	0.35420310	-1.17241359	8	-2.70179987	-0.90649694	1.11088634
6	3.73660016	0.76310307	-0.86131364	15	-3.59049988	-0.21569692	0.05488637
1	4.25410032	1.46220315	-1.51021361	8	-4.66279984	-1.35799682	-0.53281361
6	4.40920019	0.28920308	0.26168638	8	-2.64979982	-0.39639693	-1.37871361
6	3.79570031	-0.66839695	1.06538641	6	-4.23399973	-2.11169696	-1.65301359
1	4.35770035	-1.06839693	1.90288639	6	-2.78099990	-1.71089685	-1.91101360
6	2.49840021	-1.12539685	0.81238639	8	-4.82119942	0.65910310	0.67088640
6	1.76550007	0.82580304	-2.47931361	6	-6.06939983	0.09090308	1.08958638
6	1.90130019	-2.27549696	1.64878643	1	-6.68259954	-0.17249693	0.22678638

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6	0.52790010	1.70650315	-2.21371365	1	-5.91299963	-0.79329693	1.71138644
1	-0.30289987	1.13530314	-1.79581356	1	-6.56189966	0.87010306	1.67548645
1	0.16300014	2.14330316	-3.15141368	8	-0.17419986	1.43530309	1.46358633
1	0.77490008	2.53510308	-1.53921366	6	-0.38369986	2.65100312	1.43698645
6	1.35350013	-0.39949691	-3.32141352	6	-1.67529988	3.28060317	0.99418640
1	0.67060006	-1.04469693	-2.76681352	8	-2.65859985	1.32320309	0.02398637
1	2.23580003	-0.98719698	-3.59741354	6	-2.85789990	2.31910324	1.02138638
1	0.86030006	-0.07659692	-4.24691343	1	-2.96029997	1.86600316	2.01508641
6	2.72170019	1.66620314	-3.34431362	1	-3.77469993	2.87450314	0.80868638
1	3.63410020	1.11840308	-3.60131359	1	5.41790056	0.62980306	0.48378634
1	3.00929999	2.60560322	-2.85881352	1	-4.88099957	-1.86289692	-2.50131369
1	2.22210002	1.92720318	-4.28381348	1	-4.32709980	-3.17819691	-1.43121362
6	2.88810015	-2.77479696	2.71998644	1	-2.53529978	-1.67199683	-2.97341371
1	3.11240005	-2.00749683	3.46978641	1	-2.08349991	-2.38529682	-1.40271366
1	3.83220029	-3.11869693	2.28568649	1	-1.87139988	4.15380335	1.62358642
1	2.44520020	-3.62649679	3.24768639	1	-1.52349985	3.65600324	-0.02471363
6	1.59340012	-3.46859694	0.72018641	8	0.53930008	3.52000308	1.79918635
1	0.90490007	-3.17609692	-0.07531363	6	1.83510017	2.97350311	2.16298628
1	1.13990009	-4.28929710	1.29018641	1	2.46360016	3.84320307	2.34238648
1	2.51310015	-3.84439683	0.25938636	1	2.23050022	2.36020303	1.35218644
6	0.61240005	-1.86799681	2.39698648	1	1.73780012	2.37230325	3.06758642

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A'B'-3



Zero-point vibrational energy	1527408.8 (Joules/Mol)
	365.05947 (Kcal/Mol)
Zero-point correction=	0.581759 (Hartree/Particle)
Thermal correction to Energy=	0.617599
Thermal correction to Enthalpy=	0.618543
Thermal correction to Gibbs Free Energy=	0.513088
Sum of electronic and zero-point Energies=	-2002.946228
Sum of electronic and thermal Energies=	-2002.910389
Sum of electronic and thermal Enthalpies=	-2002.909444
Sum of electronic and thermal Free Energies=	-2003.014900

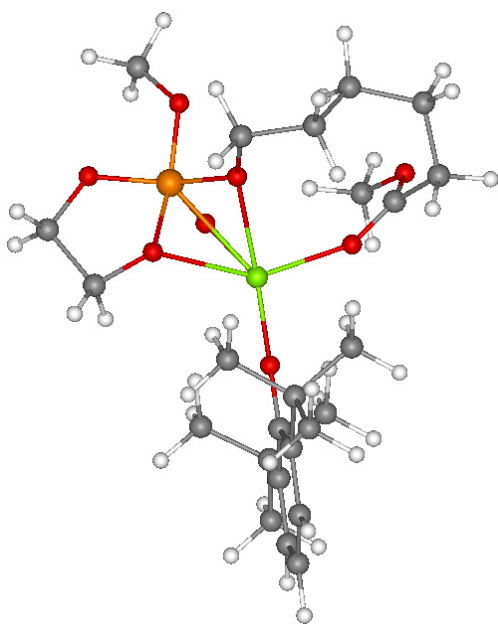
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12	-0.71408838	0.04018985	-0.11973041	1	0.99141157	1.57348979	-1.81953037
8	1.12121165	0.02798985	-0.03703041	8	-2.23898840	1.37538981	0.17746958
6	2.44551182	0.03098985	0.06226959	15	-2.97578859	0.40788984	1.12806964
6	3.14281178	-1.17851019	0.37296960	8	-3.61258841	1.15738976	2.46566963
6	4.53531170	-1.13321018	0.48916960	8	-1.57668841	-0.03131014	2.11456966
1	5.08641148	-2.03641009	0.72856957	6	-2.73058844	1.38748980	3.55936956
6	5.25341129	0.04328986	0.30386958	6	-1.33848834	0.97518986	3.08336973
6	4.56881142	1.21028984	-0.01763041	8	-4.49088860	0.12998985	0.55006957
1	5.14571142	2.11648989	-0.16953042	6	-5.57988834	1.03438985	0.75306958
6	3.17731142	1.24148977	-0.15023042	1	-5.96128845	0.96568984	1.77356958
6	2.39651155	-2.51181030	0.56636959	1	-5.28238869	2.06558990	0.54386955
6	2.47001171	2.55748987	-0.52453041	1	-6.35538864	0.73078984	0.04576959
6	1.64011157	-2.88811016	-0.72443044	8	-1.24488831	-0.38171014	-2.08513045

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1	0.95411158	-2.09991026	-1.03943038	6	-2.37408829	-0.55931014	-2.54963040
1	1.07181168	-3.81621027	-0.57983041	6	-3.13868856	-1.85671020	-2.48723030
1	2.34671164	-3.05231023	-1.54533041	8	-2.48918819	-1.07061017	0.34616959
6	1.42871165	-2.42691016	1.76406968	6	-2.76528835	-2.77601027	-1.32403040
1	0.69781160	-1.62461019	1.65746963	6	-3.20118856	-2.26771021	0.04366959
1	1.98651159	-2.24101019	2.68866968	1	-1.68698835	-2.96441031	-1.32523036
1	0.88561165	-3.37271023	1.88636959	1	-3.25018835	-3.74551010	-1.48673034
6	3.35161161	-3.68141031	0.86546957	1	-4.27388859	-2.06111026	0.06356959
1	3.90951157	-3.53381014	1.79616964	1	-2.97038841	-3.01531029	0.81146955
1	4.06991148	-3.84981012	0.05606959	1	6.33631134	0.04898985	0.40176958
1	2.76821184	-4.60231018	0.98006958	1	-3.07358837	0.77678984	4.40066957
6	3.45891142	3.71858978	-0.72923040	1	-2.77868843	2.44418979	3.83316970
1	4.17261171	3.51628971	-1.53493035	1	-0.73078835	0.55388987	3.88676953
1	4.02251148	3.94988990	0.18076958	1	-0.80878842	1.82198977	2.63216972
1	2.90251160	4.62158966	-1.00503039	1	-4.20588827	-1.62021017	-2.48943043
6	1.51151156	2.99478984	0.60126960	1	-2.93538857	-2.36541009	-3.43863034
1	0.76121163	2.23218989	0.81396961	8	-3.02038860	0.37638986	-3.21903038
1	0.99021161	3.92068982	0.32886958	6	-2.38738823	1.67688978	-3.29433036
1	2.06981182	3.17888975	1.52576959	1	-3.05438852	2.27868986	-3.90863037
6	1.70721161	2.39618969	-1.85603034	1	-1.40478837	1.59008980	-3.75963044
1	2.40781164	2.18668985	-2.67193031	1	-2.30158854	2.08938980	-2.28803039
1	1.16781163	3.31978989	-2.10243034				

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A'B'-4



Zero-point vibrational energy	1678774.5 (Joules/Mol)
	401.23673 (Kcal/Mol)
Zero-point correction=	0.639411 (Hartree/Particle)
Thermal correction to Energy=	0.677816
Thermal correction to Enthalpy=	0.678760
Thermal correction to Gibbs Free Energy=	0.567355
Sum of electronic and zero-point Energies=	-2081.492991
Sum of electronic and thermal Energies=	-2081.454586
Sum of electronic and thermal Enthalpies=	-2081.453642
Sum of electronic and thermal Free Energies=	-2081.565047

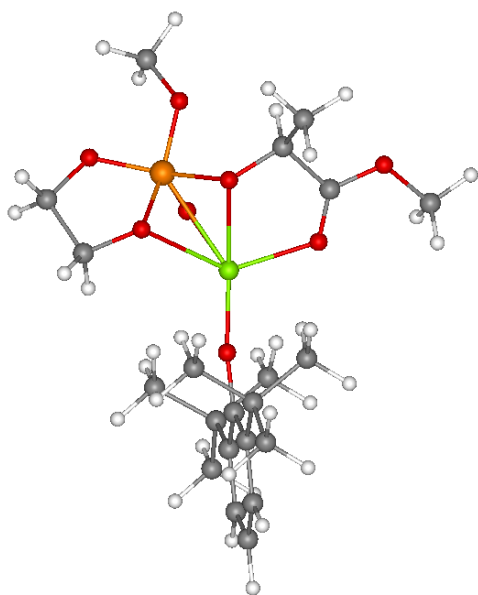
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12	0.48483098	-0.35617739	-0.14183199	8	2.92443085	-3.13397741	1.34396803
8	-1.35066903	-0.19667739	-0.01443199	8	1.11513102	-1.61237741	1.65826809
6	-2.66896915	-0.07897738	0.07596801	6	1.89853096	-3.75727749	2.10936785
6	-3.24736905	0.76932263	1.07356811	6	0.63553095	-2.92027736	1.91296804
6	-4.64066935	0.84662259	1.15806806	8	4.18793106	-1.42117739	0.35796800
1	-5.10166931	1.47752261	1.91066802	6	5.11283112	-2.47687745	0.08696801
6	-5.47276926	0.13602261	0.29986802	1	5.36703110	-3.02117729	0.99896801
6	-4.90316916	-0.66717738	-0.68233198	1	4.71453094	-3.17667747	-0.65303200
1	-5.56726933	-1.20497739	-1.35073197	1	6.00613070	-1.99377739	-0.31613198
6	-3.51846910	-0.79447740	-0.82713199	8	0.97263098	1.13722265	-1.47583199
6	-2.37346911	1.59422266	2.03676796	6	1.75713098	1.89582253	-2.04233193
6	-2.94246912	-1.68207741	-1.94713187	6	2.03433084	3.30042267	-1.58143198

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6	-1.48306894	2.57212257	1.24156809	8	2.42693090	0.03372262	0.80176800
1	-0.87476897	2.05402255	0.49816802	6	3.09033084	2.27702260	1.24446809
1	-0.82066905	3.12622261	1.91946805	6	3.07533097	0.85262263	1.78156805
1	-2.10246921	3.30092263	0.70696801	1	2.05083084	2.58202267	1.08026803
6	-1.51396894	0.66842258	2.92036796	1	3.48233080	2.94312263	2.02236795
1	-0.87166905	0.01052262	2.33396792	1	4.09413099	0.47942263	1.92816806
1	-2.15726900	0.03452262	3.54066801	1	2.52783084	0.78902262	2.72906804
1	-0.87976897	1.26022255	3.59316802	1	-6.55356932	0.21292262	0.39076802
6	-3.21036911	2.45802259	2.99756789	1	2.22303081	-3.76897740	3.15486789
1	-3.84956932	1.85332263	3.64956784	1	1.77383101	-4.78367710	1.75616813
1	-3.84296894	3.17702270	2.46616793	1	0.00563097	-2.90317750	2.80506802
1	-2.53736901	3.03172255	3.64506793	1	0.04753098	-3.28547740	1.06336808
6	-4.04226923	-2.33647728	-2.80213213	1	1.89143097	3.97812247	-2.42933202
1	-4.67796898	-1.59627736	-3.29953194	1	1.28153098	3.54152250	-0.82993197
1	-4.68336916	-3.00217748	-2.21453214	8	2.44453096	1.54092264	-3.11423206
1	-3.57436919	-2.94317746	-3.58563209	6	2.27703094	0.17572261	-3.57453203
6	-2.10936904	-2.83627748	-1.35493195	1	3.01203084	0.05532262	-4.36823177
1	-1.27236903	-2.46777749	-0.76103199	1	1.26683104	0.04572262	-3.96643209
1	-1.70666897	-3.47177744	-2.15313196	1	2.45453095	-0.52627736	-2.75783205
1	-2.73206902	-3.46147728	-0.70543200	6	3.91713095	2.39432263	-0.04513199
6	-2.08626914	-0.83547741	-2.91113210	1	3.90733099	1.42342257	-0.55223197
1	-2.70776916	-0.08437738	-3.41103196	1	4.96633101	2.57952261	0.21286801
1	-1.63706899	-1.47217739	-3.68423200	6	3.46683097	3.47532272	-1.03253198
1	-1.28876901	-0.30607736	-2.38753200	1	4.16383123	3.48782253	-1.87673187
8	1.84063101	-1.78887737	-0.71533197	1	3.51913095	4.46812296	-0.57033199
15	2.58493090	-1.67587745	0.62856799				

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**A'B'-6**



Zero-point vibrational energy	1449165.3 (Joules/Mol)
	346.35883 (Kcal/Mol)
Zero-point correction=	0.551958 (Hartree/Particle)
Thermal correction to Energy=	0.587007
Thermal correction to Enthalpy=	0.587951
Thermal correction to Gibbs Free Energy=	0.484445
Sum of electronic and zero-point Energies=	-1963.676640
Sum of electronic and thermal Energies=	-1963.641591
Sum of electronic and thermal Enthalpies=	-1963.640647
Sum of electronic and thermal Free Energies=	-1963.744153

cartesian

12	0.83858973	-0.06812578	-0.23665461	1	-2.15381026	-0.39712578	-3.45145464
8	-0.97391033	-0.17052579	0.04484539	1	-0.94691026	-1.69482577	-3.54205465
6	-2.30331016	-0.15082580	0.05864539	1	-0.78931034	-0.39942580	-2.34155464
6	-2.99321008	0.69047421	0.98674542	8	2.28818989	-1.37462580	-0.83885461
6	-4.39121056	0.67677420	0.98534542	15	3.13328981	-1.09562576	0.41674539
1	-4.93761063	1.30427420	1.68144536	8	3.65458989	-2.54122567	1.06624544
6	-5.12031031	-0.12382579	0.11264539	8	1.90498972	-1.01972580	1.63524544
6	-4.44071054	-0.93442577	-0.79005462	6	2.82218981	-3.14232588	2.04434538
1	-5.02571058	-1.55052578	-1.46465456	6	1.53218973	-2.32562566	2.06764531
6	-3.04421020	-0.97322577	-0.84725457	8	4.67458963	-0.66472578	0.08884539
6	-2.23321009	1.60107422	1.97014546	6	5.69658947	-1.61522579	-0.24575461
6	-2.34181023	-1.88642573	-1.87025464	1	6.04138947	-2.13842583	0.64694542
6	-1.39041030	2.63537431	1.19604540	1	5.33758974	-2.33902574	-0.98095459
1	-0.70331025	2.15517426	0.49774539	1	6.51198959	-1.02922583	-0.67525458

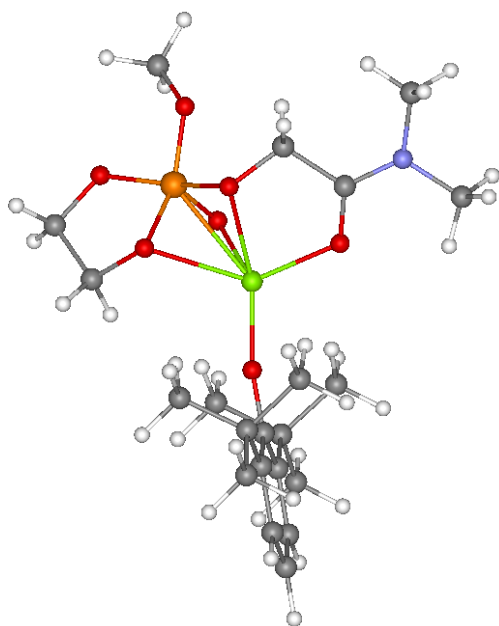
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1	-0.80871034	3.25567412	1.88964546	8	1.24838972	1.56737423	-1.45835459
1	-2.04051018	3.29787421	0.61384541	6	2.36228967	2.08467412	-1.34905457
6	-1.33901024	0.76347423	2.90724540	6	3.38418984	1.64867425	-0.31165460
1	-0.61221027	0.16717421	2.35494542	8	2.77488995	0.67527425	0.51134539
1	-1.95251024	0.07807422	3.50254536	1	-6.20731020	-0.11542579	0.13534538
1	-0.79391026	1.41577423	3.60094547	1	3.34438992	-3.10682583	3.00644541
6	-3.18131018	2.40517426	2.87724543	1	2.63898993	-4.18432570	1.77074540
1	-3.80490994	1.75727427	3.50214529	1	1.10248971	-2.24072576	3.06704545
1	-3.83871007	3.07027411	2.30704546	1	0.78458977	-2.74332571	1.38534546
1	-2.58761024	3.03397417	3.55054545	1	4.22418976	1.22107422	-0.86795461
6	-3.33971024	-2.68472576	-2.72795463	6	3.88088989	2.81367421	0.54104543
1	-3.99571013	-2.03412580	-3.31565452	8	2.77238989	3.05897427	-2.13685465
1	-3.96540999	-3.34952569	-2.12325454	6	1.84658968	3.49467421	-3.16015458
1	-2.78501010	-3.31262589	-3.43465471	1	2.36488986	4.28977442	-3.69165468
6	-1.46001029	-2.92642570	-1.14985454	1	0.93038976	3.86617422	-2.69995451
1	-0.70811033	-2.45182586	-0.51835459	1	1.61438966	2.66557431	-3.82945466
1	-0.94301033	-3.56502581	-1.87615454	1	4.62578964	2.43237424	1.24194539
1	-2.07611012	-3.56812572	-0.51045460	1	3.05808973	3.24867415	1.11414540
6	-1.50301027	-1.04582584	-2.85495448	1	4.33778954	3.58907413	-0.07805461

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A'B'-7



Zero-point vibrational energy	1482382.3 (Joules/Mol)
	354.29787 (Kcal/Mol)
Zero-point correction=	0.564610 (Hartree/Particle)
Thermal correction to Energy=	0.599892
Thermal correction to Enthalpy=	0.600836
Thermal correction to Gibbs Free Energy=	0.496490
Sum of electronic and zero-point Energies=	-1943.797120
Sum of electronic and thermal Energies=	-1943.761838
Sum of electronic and thermal Enthalpies=	-1943.760893
Sum of electronic and thermal Free Energies=	-1943.865240

cartesian

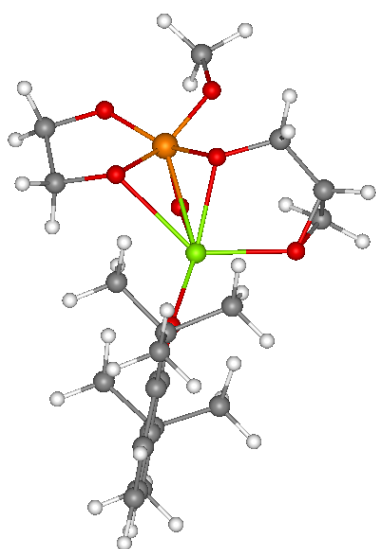
12	0.77800894	-0.11856119	-0.07688961	1	-0.85999107	-0.64376122	-3.80238962
8	-1.05319107	-0.25646120	0.07531039	1	-0.73889101	0.23143880	-2.26538968
6	-2.37879086	-0.18216118	0.02761039	8	2.16320896	-1.35266113	-0.93588960
6	-3.10189104	0.38143885	1.12611043	15	2.96030903	-1.47946119	0.37311038
6	-4.49719095	0.42903882	1.05091047	8	3.34680891	-3.08166122	0.64041042
1	-5.06799078	0.84993881	1.87211037	8	1.68460894	-1.62216115	1.53321040
6	-5.19329071	-0.05046119	-0.05358960	6	2.41420889	-3.84906125	1.38331044
6	-4.48209095	-0.59076118	-1.11958957	6	1.19090891	-2.95696115	1.58661044
1	-5.04129076	-0.95786119	-1.97368956	8	4.54660892	-1.11416125	0.19681039
6	-3.08619118	-0.67096120	-1.11608958	6	5.49230909	-2.02946115	-0.37278962
6	-2.37839079	0.93093884	2.37021041	1	5.76430893	-2.80016112	0.34961039
6	-2.34719086	-1.26966119	-2.32818961	1	5.09550905	-2.49726129	-1.27688956

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6	-1.46199107	2.10773873	1.97671044	1	6.36880922	-1.42826116	-0.62558961
1	-0.74839103	1.82703876	1.20061040	8	1.34120893	1.73473883	-0.69598961
1	-0.90379107	2.47113872	2.84891033	6	2.49580908	2.15653872	-0.45818964
1	-2.05879116	2.93983889	1.58661044	6	3.44100904	1.31223881	0.39471039
6	-1.56649101	-0.18436119	3.05971050	8	2.74020910	0.22083880	0.92961043
1	-0.83329105	-0.62756121	2.38601041	1	-6.27929068	-0.00286119	-0.08368961
1	-2.23519087	-0.98216116	3.40251040	1	2.88070917	-4.12476110	2.33531046
1	-1.03699100	0.21093880	3.93571043	1	2.16780901	-4.75636148	0.82601041
6	-3.35609102	1.47533882	3.42641044	1	0.71760899	-3.10386109	2.55861044
1	-4.03389072	0.70073885	3.80051041	1	0.44920897	-3.10936117	0.79571044
1	-3.95889091	2.30683875	3.04581046	1	4.29010916	0.98873878	-0.21368963
1	-2.78579092	1.85153878	4.28341055	1	3.82920885	1.91483879	1.22491038
6	-3.31279087	-1.74266112	-3.42988968	7	2.91460896	3.33823872	-0.93648958
1	-3.92209101	-0.92436117	-3.82778955	6	2.00880909	4.18383837	-1.70678961
1	-3.98429108	-2.53426123	-3.08078957	1	1.90770900	5.15803862	-1.21778953
1	-2.73219109	-2.15206122	-4.26438951	1	1.03370905	3.70603871	-1.76748955
6	-1.52789104	-2.50676107	-1.90858960	1	2.40490913	4.33313847	-2.71628952
1	-0.79179108	-2.26396108	-1.14198959	6	4.23750877	3.88923860	-0.68228960
1	-0.99609101	-2.92776108	-2.77028966	1	4.63220930	4.31243849	-1.61018956
1	-2.18999100	-3.28116107	-1.50538957	1	4.93270922	3.12333894	-0.34408963
6	-1.43819106	-0.20706119	-2.97928953	1	4.19160891	4.68463850	0.07021040
1	-2.04169083	0.61243880	-3.38498950				

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## A'B'-Gly



Zero-point vibrational energy	1365205.7 (Joules/Mol)
	326.29200 (Kcal/Mol)
Zero-point correction=	0.519979 (Hartree/Particle)
Thermal correction to Energy=	0.551601
Thermal correction to Enthalpy=	0.552545
Thermal correction to Gibbs Free Energy=	0.456729
Sum of electronic and zero-point Energies=	-1849.135868
Sum of electronic and thermal Energies=	-1849.104246
Sum of electronic and thermal Enthalpies=	-1849.103302
Sum of electronic and thermal Free Energies=	-1849.199118

cartesian

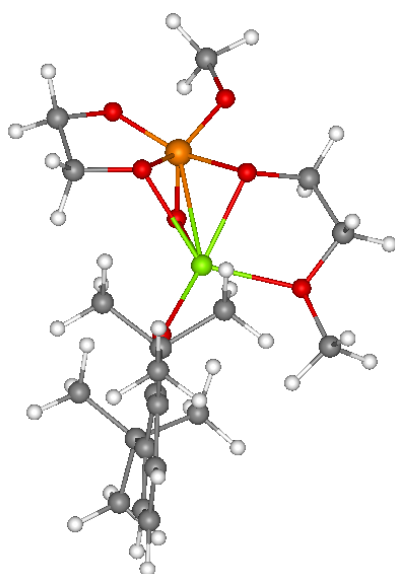
12	-0.96098697	-0.02574674	-0.41186935	1	1.60441291	2.94285321	1.88393068
8	0.83271301	-0.02074674	-0.05416935	6	1.32471299	2.59275317	-1.57936931
6	2.15721297	0.03525326	0.05623065	1	2.04921293	2.55905318	-2.40026951
6	2.90501285	-1.16734672	0.24803065	1	0.71341300	3.49505329	-1.70276928
6	4.29471302	-1.07234681	0.36903065	1	0.67881298	1.71955323	-1.68786931
1	4.88651323	-1.96964681	0.51613063	8	-2.55928707	1.20285320	-0.09476935
6	4.95791340	0.14865325	0.30743065	15	-3.39858699	0.05075327	0.49923062
6	4.22061300	1.31265318	0.11833065	8	-4.25548697	0.56295329	1.82833076
1	4.75571299	2.25535321	0.07223065	8	-2.21588707	-0.64104670	1.56493068
6	2.82851291	1.29505324	-0.01116935	6	-3.58548713	0.50105327	3.08053064
6	2.21411300	-2.54184675	0.32313064	6	-2.14228702	0.10835326	2.77053046
6	2.05591297	2.61105323	-0.22116934	8	-4.78658676	-0.15214674	-0.34406936
6	1.48481297	-2.84894681	-1.00126934	6	-5.96438694	0.63515329	-0.12616935
1	0.76591301	-2.06934667	-1.25996935	1	-6.46968699	0.32775325	0.79043067

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1	0.95251298	-3.80614686	-0.93436939	1	-5.72348690	1.69955325	-0.07246935
1	2.20221305	-2.91744685	-1.82626927	1	-6.60828686	0.44735324	-0.98826939
6	1.22941291	-2.58624673	1.50993073	6	-2.44738698	0.43425325	-3.06926942
1	0.47061297	-1.80594683	1.44313073	8	-2.71138716	-1.27194679	-0.48946935
1	1.76871300	-2.44824672	2.45373058	6	-2.45198703	-1.02104676	-2.89656949
1	0.72161293	-3.55794668	1.55153072	6	-3.14078712	-1.74944675	-1.75186932
6	3.21501303	-3.68974686	0.54313064	8	-1.27528703	-0.25154674	-2.52986932
1	3.76361299	-3.58484674	1.48503065	1	-2.28178692	-1.62604678	-3.78586936
1	3.94181275	-3.76984668	-0.27226937	1	-4.22488689	-1.68144679	-1.85866928
1	2.67001295	-4.63944674	0.58803064	1	-2.85218716	-2.80504680	-1.78876925
6	2.98491287	3.83845329	-0.24976934	1	6.04001331	0.19275326	0.40463063
1	3.71341300	3.78885317	-1.06566930	1	-4.09018707	-0.24914674	3.69783068
1	3.52931285	3.96705317	0.69163066	1	-3.65058708	1.47655320	3.56793070
1	2.38351297	4.74155331	-0.40446937	1	-1.70338702	-0.52714670	3.54143047
6	1.06401300	2.84775329	0.93583065	1	-1.51268709	0.99325329	2.62463069
1	0.35461298	2.02585316	1.04153073	1	-2.94948697	1.06935322	-2.34516931
1	0.49611297	3.77195334	0.77433062	1	-2.26918697	0.84715331	-4.05876923

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A'B'-OCH<sub>2</sub>CH<sub>2</sub>OMe



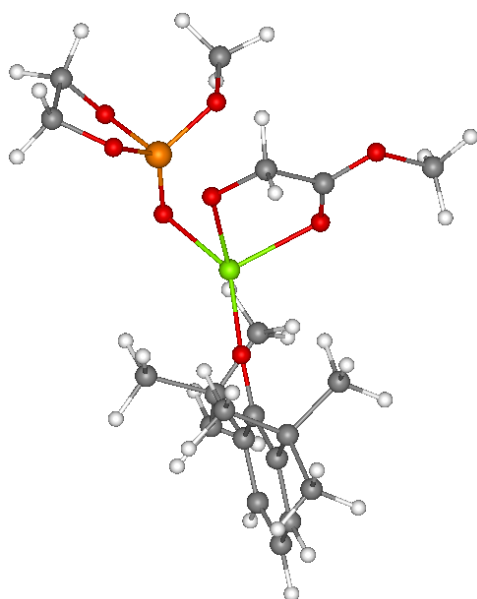
Zero-point vibrational energy	1425382.2 (Joules/Mol)
	340.67452 (Kcal/Mol)
Zero-point correction=	0.542899 (Hartree/Particle)
Thermal correction to Energy=	0.575707
Thermal correction to Enthalpy=	0.576651
Thermal correction to Gibbs Free Energy=	0.479047
Sum of electronic and zero-point Energies=	-1850.353119
Sum of electronic and thermal Energies=	-1850.320311
Sum of electronic and thermal Enthalpies=	-1850.319367
Sum of electronic and thermal Free Energies=	-1850.416971

cartesian											
12	-1.08059883	0.03073438	-0.39347658	6	0.93850124	2.89373446	-0.97317660				
8	0.64190125	0.02183438	0.27892342	1	1.55100131	2.92323446	-1.88127661				
6	1.97090137	0.10083438	0.25932342	1	0.38160127	3.83563447	-0.90947652				
6	2.75570107	-1.09446561	0.32212344	1	0.20380127	2.09533453	-1.09437656				
6	4.14540148	-0.98216563	0.21532343	8	-2.62579870	1.26363432	0.10052343				
1	4.76310158	-1.87356567	0.24252343	15	-3.56159878	0.06233438	0.34852344				
6	4.77750158	0.24943438	0.08212343	8	-4.38549852	0.35573438	1.77412343				
6	4.01030159	1.40913439	0.09452343	8	-2.53449869	-1.03896558	1.18802345				
1	4.52490139	2.36173439	0.02862343	6	-3.80279875	-0.15356562	2.96012330				
6	2.61540127	1.37703431	0.19692343	6	-2.42669868	-0.68686563	2.56572342				
6	2.11150122	-2.47736549	0.54482341	8	-4.95509863	0.06913438	-0.49807659				
6	1.82260120	2.69813442	0.27342343	6	-6.12759876	0.79113436	-0.09547657				
6	1.20740128	-2.87436557	-0.63857663	1	-6.62269878	0.29013440	0.73742342				

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1	0.38980126	-2.16546559	-0.78007662	1	-5.88409853	1.81773436	0.18712343
1	0.76480126	-3.86366558	-0.47047657	1	-6.77979851	0.79533434	-0.97117662
1	1.78670132	-2.91736555	-1.56767654	8	-0.82979876	-0.16536561	-2.48877668
6	1.29980123	-2.47176552	1.85652339	6	-1.92019880	-0.82746565	-3.15227652
1	0.52730125	-1.70226562	1.84272337	6	-3.16929865	-0.53506565	-2.34707665
1	1.95900118	-2.27586555	2.70922351	8	-2.89569855	-0.92606562	-1.00507665
1	0.82130122	-3.44626546	2.01492357	1	5.85980129	0.30643439	-0.00397657
6	3.16130114	-3.59516549	0.67852342	1	-4.44959879	-0.94816566	3.34872341
1	3.84640121	-3.41866541	1.51402342	1	-3.73009872	0.64583439	3.70202351
1	3.75490141	-3.72216558	-0.23327658	1	-2.14289880	-1.58106565	3.12262344
1	2.65200138	-4.54636574	0.86952341	1	-1.65359879	0.07943439	2.68802333
6	2.74900103	3.92723441	0.33472344	1	-3.39699888	0.53473437	-2.40447664
1	3.35600138	4.04063463	-0.56987655	1	-4.01929855	-1.09746563	-2.74597669
1	3.42060137	3.89243436	1.19862342	1	-2.01839876	-0.43836561	-4.17287636
1	2.13900137	4.83233452	0.43062344	1	-1.70819879	-1.90306568	-3.19197655
6	0.96390128	2.73693442	1.55442345	6	0.41210127	-0.23296562	-3.20227671
1	0.25520128	1.90963435	1.59442341	1	0.65500128	-1.27336562	-3.43977666
1	0.39930123	3.67543459	1.60682344	1	1.18280125	0.17993438	-2.55307651
1	1.60470116	2.67713451	2.44082332	1	0.33860123	0.35463437	-4.12347651

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**B'-1**

Zero-point vibrational energy	1377002.1 (Joules/Mol)
	329.11140 (Kcal/Mol)
Zero-point correction=	0.524472 (Hartree/Particle)
Thermal correction to Energy=	0.558367
Thermal correction to Enthalpy=	0.559311
Thermal correction to Gibbs Free Energy=	0.457739
Sum of electronic and zero-point Energies=	-1924.409084
Sum of electronic and thermal Energies=	-1924.375190
Sum of electronic and thermal Enthalpies=	-1924.374246
Sum of electronic and thermal Free Energies=	-1924.475818

				cartesian			
12	0.70360672	-0.17978416	-0.15135394	6	-0.63379335	-1.83308423	-1.98345387
8	-1.08219337	-0.04338417	0.33484608	1	-0.85269332	-2.10598397	-3.02115393
6	-2.35779333	-0.38358417	0.16634606	1	0.41180670	-2.12788415	-1.81265390
6	-3.38449335	0.47021583	0.67294604	1	-0.73749340	-0.74328417	-1.95575392
6	-4.71579313	0.09641583	0.46964604	8	2.23470664	-1.39858413	0.07194606
1	-5.51549292	0.72861582	0.84154606	15	3.41970658	-0.54478419	0.53574604
6	-5.06229305	-1.07398415	-0.20065394	8	4.57510710	-1.77208424	0.52284604
6	-4.05599308	-1.90548420	-0.68075395	8	3.77420664	-0.14788416	2.08474588
1	-4.34059334	-2.82018399	-1.19155395	6	5.51670694	-1.63048422	1.56864607
6	-2.70449328	-1.59008420	-0.51575392	6	4.71510696	-1.02808416	2.71214604
6	-3.04079342	1.77071583	1.42084610	8	4.13460684	0.40401581	-0.58515394
6	-1.60779333	-2.55058408	-1.00085390	6	5.06090689	-0.12638417	-1.54525387
6	-2.27749324	2.73301601	0.48744607	1	6.00450706	-0.40818417	-1.07395387

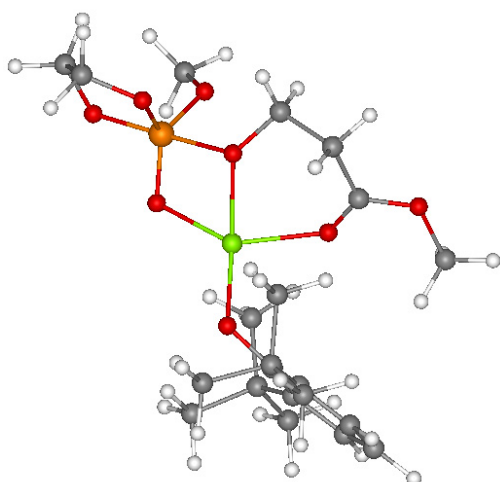
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1	-1.35339332	2.27801585	0.12714607	1	4.64100695	-0.99248415	-2.06065392
1	-2.02959323	3.66191602	1.01704609	1	5.23570681	0.68101579	-2.25885391
1	-2.89179325	2.99381590	-0.38185394	8	1.11840665	1.34501576	-1.59135389
6	-2.19529343	1.46521580	2.67464590	6	1.84440660	2.23861599	-1.14605391
1	-1.27359331	0.94181579	2.41824603	6	2.41920662	2.16891599	0.25624606
1	-2.76089334	0.83891582	3.37334609	8	2.22060680	0.88021582	0.75154603
1	-1.93569326	2.39631605	3.19434595	1	-6.10779333	-1.33728421	-0.34155393
6	-4.29719305	2.51731586	1.90084612	1	6.34010696	-0.96458417	1.27044606
1	-4.90389299	1.91101587	2.58194590	1	5.92570686	-2.61418414	1.81084609
1	-4.93279314	2.84111595	1.06924605	1	5.31520700	-0.43248418	3.40254593
1	-3.99489331	3.41681600	2.44884610	1	4.16230679	-1.79288423	3.26644588
6	-2.17299342	-3.76168418	-1.76325393	1	3.46720672	2.47901583	0.24464606
1	-2.78859329	-3.45798397	-2.61655402	1	1.86240661	2.88881588	0.87324607
1	-2.77329326	-4.41158438	-1.11865389	8	2.14460683	3.33021593	-1.82145393
1	-1.34369338	-4.36418438	-2.15195394	6	1.54540670	3.46681595	-3.12995410
6	-0.85879338	-3.11958408	0.22634606	1	1.91930664	4.41191578	-3.51795411
1	-0.48529330	-2.33688402	0.89104605	1	0.45830670	3.48621583	-3.04165411
1	-0.01089332	-3.74268413	-0.07985394	1	1.84950662	2.63691592	-3.76895404
1	-1.54079330	-3.73668408	0.82014602				

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**B'-2**



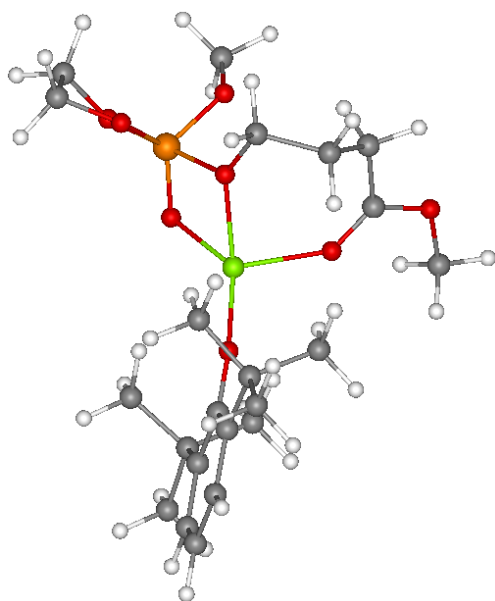
Zero-point vibrational energy	1452958.4 (Joules/Mol)
	347.26540 (Kcal/Mol)
Zero-point correction=	0.553403 (Hartree/Particle)
Thermal correction to Energy=	0.588418
Thermal correction to Enthalpy=	0.589362
Thermal correction to Gibbs Free Energy=	0.486069
Sum of electronic and zero-point Energies=	-1963.687071
Sum of electronic and thermal Energies=	-1963.652055
Sum of electronic and thermal Enthalpies=	-1963.651111
Sum of electronic and thermal Free Energies=	-1963.754404

				cartesian			
12	-0.83017445	0.26886827	0.06439395	1	0.34182557	2.09386826	-1.47700608
8	0.76012552	0.37686825	1.07709396	1	0.03312561	3.75826812	-1.00720608
6	2.01592565	0.38246825	0.63049394	1	-0.40427440	2.51466823	0.11899395
6	2.85052562	-0.76403171	0.81499398	8	-2.49157453	1.05206823	0.80009395
6	4.11412573	-0.76683170	0.21489395	15	-3.67107439	0.21426825	0.27989393
1	4.76012564	-1.63263178	0.31989396	8	-4.88337421	1.11096823	1.05009389
6	4.58612537	0.32156825	-0.51460606	8	-4.25047445	-1.18903172	0.92479396
6	3.80772543	1.47376823	-0.59440601	6	-5.98147440	0.30976826	1.43039393
1	4.21642542	2.33196831	-1.11780608	6	-5.35807467	-1.02393174	1.81539392
6	2.53872561	1.54806828	-0.01160605	8	-4.18287420	0.49266824	-1.24810612
6	2.39922547	-1.94823182	1.69139385	6	-4.97697449	1.63796818	-1.58220613
6	1.76482558	2.88186812	0.01369395	1	-6.00507450	1.52876818	-1.22900605
6	1.18892562	-2.67633176	1.07639396	1	-4.55007458	2.55306816	-1.16640615
1	0.31472561	-2.02323174	1.03869390	1	-4.97117424	1.69096828	-2.67280602
1	0.91962552	-3.55263186	1.67889392	8	-0.02117440	-0.43553174	-1.74380612

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1	1.42102551	-3.02563167	0.06299395	6	-0.20727441	-1.53683174	-2.26800609
6	2.03442550	-1.44123173	3.10239410	6	-1.30627441	-2.49433184	-1.89120615
1	1.24182558	-0.69263172	3.06099391	8	-2.40147448	-0.89813173	-0.47110605
1	2.90922546	-0.98983169	3.58289409	6	-2.62337446	-1.81113172	-1.52490604
1	1.69762564	-2.27503181	3.73119402	1	-3.03807449	-1.28623176	-2.39310598
6	3.50862551	-3.00103188	1.86019385	1	-3.34157443	-2.57853174	-1.21380615
1	4.41312551	-2.57603168	2.30729413	1	5.56882572	0.28846827	-0.97920603
1	3.78392553	-3.47623181	0.91189396	1	-6.69177437	0.18576826	0.59859395
1	3.15482545	-3.79343176	2.52909398	1	-6.49757433	0.78936827	2.26589394
6	2.51422548	3.99136806	-0.74530602	1	-6.02877426	-1.87513173	1.67889392
1	2.62382555	3.76516819	-1.81230605	1	-4.98057461	-1.01223171	2.84289408
1	3.50902557	4.17546844	-0.32840604	1	-1.45387447	-3.20883179	-2.70490599
1	1.95312548	4.92866850	-0.66340601	1	-0.93687439	-3.06013179	-1.02760601
6	1.61752558	3.34206820	1.47929394	8	0.59782565	-1.99593174	-3.21040606
1	1.09892559	2.58666825	2.07369399	6	1.74912548	-1.17253172	-3.52650595
1	1.04742551	4.27806854	1.53339386	1	2.32552552	-1.75903177	-4.23900604
1	2.60182548	3.51826835	1.92539394	1	2.32662559	-0.96813172	-2.62380600
6	0.35522559	2.78316832	-0.62410605	1	1.41952562	-0.23463175	-3.97540593

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**B'-3**

Zero-point vibrational energy	1529068.8 (Joules/Mol)
	365.45621 (Kcal/Mol)
Zero-point correction=	0.582392 (Hartree/Particle)
Thermal correction to Energy=	0.618734
Thermal correction to Enthalpy=	0.619678
Thermal correction to Gibbs Free Energy=	0.513501
Sum of electronic and zero-point Energies=	-2002.965691
Sum of electronic and thermal Energies=	-2002.929349
Sum of electronic and thermal Enthalpies=	-2002.928405
Sum of electronic and thermal Free Energies=	-2003.034582

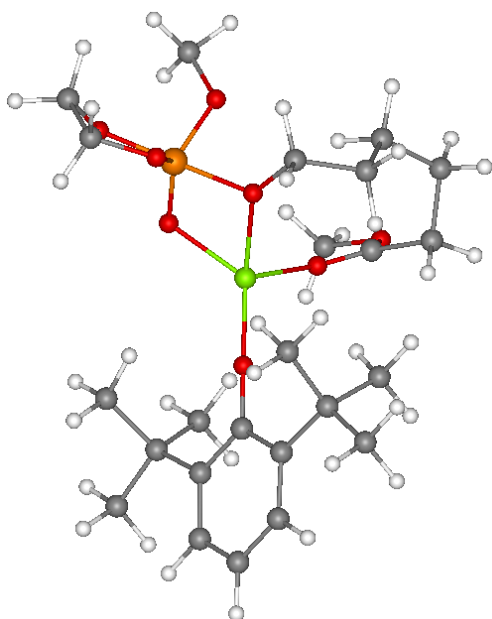
				cartesian			
12	0.58643484	-0.11292316	-0.30444786	1	-1.23426509	-0.50922316	-2.34104800
8	-1.23156512	-0.15332316	-0.01184786	8	1.92913485	-1.55312324	-0.39344785
6	-2.52976513	-0.36932313	0.17375213	15	3.13093495	-1.08812320	0.44775215
6	-3.24106503	0.38897681	1.15605223	8	4.03223467	-2.51332331	0.26965216
6	-4.60526514	0.14077684	1.33235216	8	3.27503490	-1.16692317	2.08985209
1	-5.16446495	0.70077688	2.07455206	6	4.78393507	-2.83102322	1.42095220
6	-5.28406525	-0.81202316	0.58045214	6	3.92873478	-2.34022331	2.58015203
6	-4.58676529	-1.53872323	-0.37854785	8	4.23063469	-0.10522316	-0.27824786
1	-5.13206530	-2.27612329	-0.95804787	6	5.26693487	-0.61682314	-1.12514782
6	-3.22106504	-1.34672320	-0.60904789	1	6.03843498	-1.13492322	-0.55064785
6	-2.53896523	1.46667683	2.00305200	1	4.86573505	-1.29492319	-1.88084781
6	-2.49696517	-2.18592310	-1.67844784	1	5.70873499	0.25697684	-1.61024785
6	-1.98016500	2.57477689	1.08705223	8	0.94083488	1.41157675	-1.64814782

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1	-1.30556512	2.16557670	0.33245215	6	1.71963489	2.35627675	-1.78744781
1	-1.44266510	3.32827687	1.67785215	6	2.66723490	2.90317678	-0.75404787
1	-2.79646516	3.08217669	0.56105214	8	2.17933488	0.43487686	0.79235214
6	-1.41346514	0.84317684	2.85315204	6	2.18943477	2.83797669	0.70725214
1	-0.66786516	0.33857685	2.23755217	6	2.65893483	1.59447682	1.45315218
1	-1.82476521	0.10167684	3.54635215	1	1.09803486	2.91267681	0.75915211
1	-0.90836513	1.61497676	3.44815207	1	2.57873487	3.71487689	1.23665214
6	-3.49796510	2.15587687	2.98945212	1	3.75283480	1.56747675	1.48625219
1	-3.92326498	1.45247674	3.71315217	1	2.28833485	1.60647678	2.48455215
1	-4.32226515	2.66607690	2.48025203	1	-6.34566498	-0.98562312	0.73915213
1	-2.94706511	2.91417670	3.55795217	1	5.76153469	-2.32452321	1.41205215
6	-3.44726515	-3.14892316	-2.41294789	1	4.94903469	-3.91112328	1.44905221
1	-4.25216532	-2.62152314	-2.93614793	1	4.50843477	-2.05872321	3.46185207
1	-3.89826488	-3.88162327	-1.73564780	1	3.16603494	-3.07412314	2.85935211
1	-2.88006520	-3.70902324	-3.16504788	1	3.58713484	2.31507683	-0.86654788
6	-1.41216516	-3.06562328	-1.02474785	1	2.90873480	3.92597699	-1.05234778
1	-0.68856514	-2.48782325	-0.44954786	8	1.80683494	3.00027680	-2.94334793
1	-0.86146510	-3.63302326	-1.78464782	6	0.97393489	2.51477671	-4.01964760
1	-1.87426519	-3.78252316	-0.33734787	1	1.17983484	3.17657685	-4.85834789
6	-1.89096522	-1.27172315	-2.76414800	1	-0.07696515	2.56537676	-3.73284793
1	-2.68676519	-0.74762315	-3.30524802	1	1.23903489	1.48527682	-4.26444769
1	-1.32006514	-1.86272323	-3.49114799				

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**B'-4**



Zero-point vibrational energy	1679467.5 (Joules/Mol)
	401.40236 (Kcal/Mol)
Zero-point correction=	0.639675 (Hartree/Particle)
Thermal correction to Energy=	0.677853
Thermal correction to Enthalpy=	0.678797
Thermal correction to Gibbs Free Energy=	0.569063
Sum of electronic and zero-point Energies=	-2081.511203
Sum of electronic and thermal Energies=	-2081.473025
Sum of electronic and thermal Enthalpies=	-2081.472081
Sum of electronic and thermal Free Energies=	-2081.581815

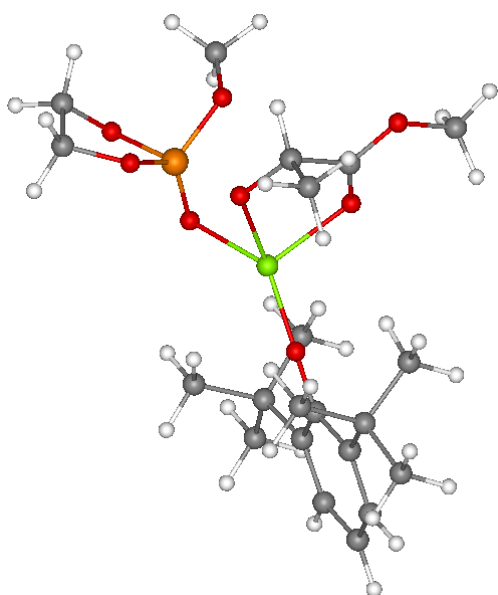
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12	-0.43762124	-0.21140400	0.30398795	8	-3.54402113	-3.07480407	0.09328796	8	-2.73282123	-2.05460405	-1.90801203
8	1.38467872	-0.34780401	0.03758796	6	-4.09272099	-3.74370408	-1.02061200	6	-3.16212130	-3.39140415	-2.17241192
6	2.69557881	-0.44600397	-0.15401204	8	-4.09702110	-0.66310400	0.06228796	6	-5.17522097	-1.13000405	0.87868798
6	3.32927871	0.27629602	-1.21411204	1	-5.80732107	-1.84360409	0.34388795	6	4.85547876	-1.36810398	0.47308797
6	4.71027899	0.13979600	-1.38471198	1	-5.76402092	-0.24210399	1.12108803	6	3.47927880	-1.28210402	0.70348799
1	5.21147919	0.67689604	-2.18311191	8	-0.77582127	1.34369600	1.60048795	6	2.52817869	1.19609594	-2.15261197
6	5.47807884	-0.67140400	-0.55711198	6	-1.08862126	2.48459601	1.94138801	6	2.84157872	-2.08450389	1.85378802
6	4.85547876	-1.36810398	0.47308797	6	-1.13992119	3.66969585	1.02188802				
1	5.47047901	-1.99570405	1.10918796								

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6	1.87657881	2.33229589	-1.33931196	8	-2.03022122	-0.05310400	-0.92011201
1	1.25187874	1.93509603	-0.53611207	6	-2.33072114	2.23669600	-1.59291196
1	1.26567876	2.97219586	-1.98991203	6	-2.56362128	0.77489603	-1.95351195
1	2.64657879	2.95919585	-0.87621200	1	-1.25202119	2.37889600	-1.45611203
6	1.46187878	0.39079601	-2.92261195	1	-2.60722113	2.86299586	-2.45071197
1	0.79107881	-0.14880399	-2.25301194	1	-3.63432121	0.57169604	-2.05501199
1	1.94167876	-0.35020399	-3.57071209	1	-2.07612109	0.52249604	-2.90141201
1	0.86227870	1.05469596	-3.55831194	1	6.55057907	-0.76020396	-0.71321201
6	3.41227865	1.87369585	-3.21451211	1	-5.11842108	-3.40030408	-1.22671199
1	3.90027881	1.14549601	-3.87051201	1	-4.11672115	-4.81690359	-0.81421208
1	4.18587923	2.50789595	-2.76891208	1	-3.65322113	-3.40100408	-3.14801192
1	2.78907871	2.51549602	-3.84821200	1	-2.28302121	-4.04350376	-2.19631195
6	3.88137889	-2.89890409	2.64468789	1	-0.86482126	4.56259632	1.58928800
1	4.64257908	-2.26320410	3.11008811	1	-0.38952124	3.51299596	0.24538796
1	4.38727903	-3.64140415	2.01868796	8	-1.43812120	2.76359606	3.18768787
1	3.37517881	-3.44410396	3.44948792	6	-1.44562125	1.66209590	4.12368822
6	1.81887865	-3.09890413	1.30328798	1	-1.76992118	2.09419584	5.06808805
1	1.02107871	-2.62260413	0.73358798	1	-0.44322121	1.24209595	4.21418810
1	1.35677874	-3.66030407	2.12418795	1	-2.14032125	0.89019603	3.78998804
1	2.31807876	-3.81680393	0.64308798	6	-3.11052132	2.66409588	-0.34301203
6	2.17417884	-1.13410401	2.86958790	1	-3.18062115	1.80679595	0.33468795
1	2.92257881	-0.47690398	3.32708788	1	-4.14372110	2.89439607	-0.62901199
1	1.69067872	-1.70750403	3.67038798	6	-2.54172134	3.87369609	0.40348795
1	1.42297876	-0.50060397	2.39568806	1	-3.23332119	4.16409636	1.20228803
8	-1.65992129	-1.70300400	0.69628799	1	-2.46762133	4.73609638	-0.26931202
15	-2.80902123	-1.60120404	-0.32151204				

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**B'-6**



Zero-point vibrational energy	1449594.9 (Joules/Mol)
	346.46150 (Kcal/Mol)
Zero-point correction=	0.552122 (Hartree/Particle)
Thermal correction to Energy=	0.587745
Thermal correction to Enthalpy=	0.588689
Thermal correction to Gibbs Free Energy=	0.483525
Sum of electronic and zero-point Energies=	-1963.689164
Sum of electronic and thermal Energies=	-1963.653541
Sum of electronic and thermal Enthalpies=	-1963.652597
Sum of electronic and thermal Free Energies=	-1963.757760

				cartesian			
12	0.64381051	-0.24189395	-0.14412272	1	-0.33878946	-2.95729399	-2.32212257
8	-1.16858959	-0.18459395	0.18627727	1	-0.72068948	-1.27229404	-1.89452279
6	-2.47228956	-0.45109394	0.14187728	8	2.08031058	-1.56919384	0.06697727
6	-3.40318966	0.52280605	0.61927730	15	3.35731053	-0.81999397	0.46967727
6	-4.76758909	0.22560605	0.55767727	8	4.38261080	-2.15849400	0.47367728
1	-5.49408913	0.94850606	0.91367728	8	3.80191040	-0.40699396	1.99347723
6	-5.23738909	-0.98149395	0.05047727	6	5.37471056	-2.06839395	1.47717726
6	-4.32448912	-1.92549396	-0.40652272	6	4.67871046	-1.35029387	2.62287736
1	-4.70748949	-2.86399388	-0.79342270	8	4.13351059	0.00740605	-0.70612270
6	-2.94538951	-1.69749403	-0.37492272	6	4.93611050	-0.66509396	-1.68922281
6	-2.93008947	1.87240601	1.18947721	1	5.87581062	-1.01769400	-1.25942278
6	-1.97198963	-2.78159380	-0.87012273	1	4.39891052	-1.50859404	-2.12712264
6	-2.18428946	2.67500615	0.10397728	1	5.14331055	0.08190605	-2.45802259

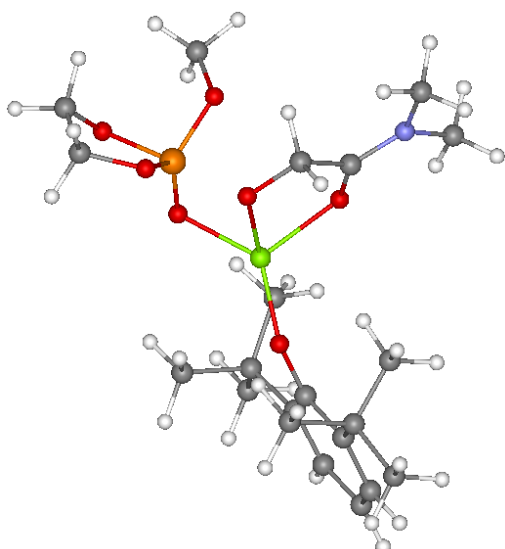
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1	-1.33258939	2.11620617	-0.28702274	8	1.09271049	1.20650601	-1.63262284
1	-1.82668948	3.63010621	0.51077724	6	1.90981054	2.05450606	-1.25942278
1	-2.85368967	2.89690614	-0.73472273	6	2.54761052	2.00470614	0.12407728
6	-2.02308965	1.65120602	2.41727734	8	2.25951052	0.73940605	0.65807730
1	-1.14968944	1.04590607	2.17157745	1	-6.30478954	-1.18559384	0.01507727
1	-2.57558966	1.13600612	3.21077728	1	6.24451065	-1.49529386	1.12287724
1	-1.68088961	2.61370611	2.81877732	1	5.69891071	-3.07679391	1.74487722
6	-4.10148954	2.75170612	1.66187727	1	5.35841084	-0.79039395	3.26807737
1	-4.67948914	2.27550602	2.46087742	1	4.07721043	-2.03769398	3.22577739
1	-4.78628922	3.00760603	0.84617728	1	3.62441039	2.15150619	0.00127727
1	-3.70708966	3.69270611	2.06217742	6	1.97911048	3.10570621	1.02177727
6	-2.69538951	-4.04349422	-1.37562275	8	2.26821041	3.07970619	-2.00672269
1	-3.36038947	-3.83259392	-2.21972275	6	1.63301063	3.19040608	-3.30092263
1	-3.28158951	-4.52619410	-0.58692271	1	2.04811049	4.09210587	-3.74642277
1	-1.95118952	-4.77119398	-1.71892273	1	0.55271053	3.27780604	-3.18012261
6	-1.06428957	-3.24809384	0.28767729	1	1.86681056	2.31460619	-3.90752268
1	-0.53858948	-2.42609382	0.77517730	1	2.44821048	3.02110600	2.00407720
1	-0.31578952	-3.96669388	-0.06502272	1	0.89911050	2.99310613	1.14597726
1	-1.67038965	-3.73739386	1.05747724	1	2.18961048	4.09600592	0.60867727
6	-1.14868951	-2.26319385	-2.06982255	1	-1.79098964	-2.15569401	-2.95062256

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**B'-7**



Zero-point vibrational energy	1482862.3 (Joules/Mol)
	354.41260 (Kcal/Mol)
Zero-point correction=	0.564792 (Hartree/Particle)
Thermal correction to Energy=	0.600588
Thermal correction to Enthalpy=	0.601532
Thermal correction to Gibbs Free Energy=	0.495743
Sum of electronic and zero-point Energies=	-1943.809593
Sum of electronic and thermal Energies=	-1943.773798
Sum of electronic and thermal Enthalpies=	-1943.772854
Sum of electronic and thermal Free Energies=	-1943.878643

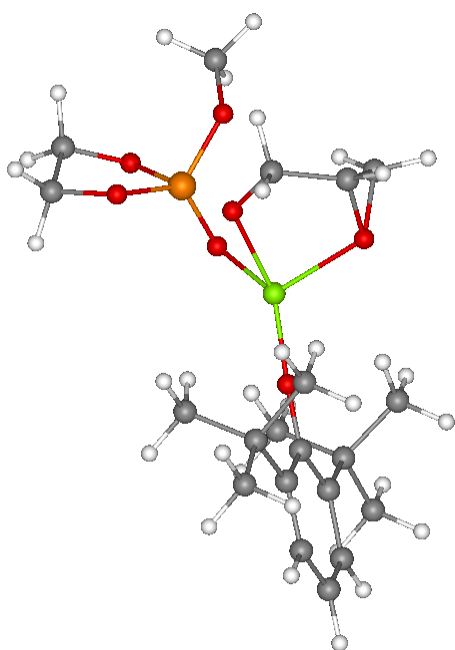
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12	-0.53131509	-0.43060154	0.10478656	1	0.94368494	-2.03060150	3.18898654
8	1.22988486	-0.46410155	-0.48291343	1	-0.09181505	-2.12910151	1.79248655
6	2.52978492	-0.55020154	-0.22021344	1	0.99508488	-0.71200156	2.05058670
6	3.44738483	0.33079845	-0.87051344	8	-1.96681511	-1.78080153	-0.07221344
6	4.80508471	0.22269846	-0.55501342	15	-3.22651505	-1.06310153	-0.57201344
1	5.52328491	0.88199842	-1.03161347	8	-4.24611473	-2.40960145	-0.52051342
6	5.28028488	-0.71310157	0.35978657	8	-3.63491511	-0.75210154	-2.13101339
6	4.38198471	-1.58150160	0.97198659	6	-5.22061491	-2.37670159	-1.54311347
1	4.76908493	-2.31400156	1.67328656	6	-4.50251532	-1.72980154	-2.71741343
6	3.01228499	-1.52980161	0.70058656	8	-4.05951500	-0.16330154	0.51078659
6	2.96418500	1.36749840	-1.90051353	6	-4.83201504	-0.78520155	1.54778647
6	2.04158497	-2.53540158	1.34058654	1	-5.75241518	-1.21840155	1.15088654
6	2.01878500	2.38649845	-1.23161352	1	-4.25731516	-1.56240153	2.05598664
1	1.15228486	1.88899851	-0.79301345	1	-5.07541513	0.01229845	2.25298667

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1	1.66468489	3.12009835	-1.96751344	8	-0.96071506	1.14329839	1.37728655
1	2.53948498	2.93019843	-0.43501344	6	-1.74051511	2.02119851	0.93588656
6	2.24448490	0.66509843	-3.07031345	6	-2.43371511	1.76599848	-0.40901342
1	1.38728487	0.08789846	-2.72221327	8	-2.13051510	0.47229844	-0.82871342
1	2.93028498	-0.01810154	-3.58341336	1	6.34218502	-0.76970154	0.58668655
1	1.89618492	1.40499842	-3.80231333	1	-6.09481525	-1.78120160	-1.23891354
6	4.12628508	2.17199850	-2.50781345	1	-5.54441500	-3.39830160	-1.75661349
1	4.84158468	1.53019845	-3.03341341	1	-5.16941500	-1.20900154	-3.40751338
1	4.67218494	2.75019836	-1.75421345	1	-3.89281511	-2.45360160	-3.26741338
1	3.72938490	2.88409853	-3.24021339	1	-3.51251507	1.91799855	-0.31771344
6	2.74418497	-3.46520162	2.34568667	1	-2.04511499	2.48419833	-1.14561343
1	3.20618486	-2.90910149	3.16878653	7	-1.94551504	3.16789842	1.60218656
1	3.51508498	-4.07850122	1.86828649	6	-1.25381505	3.42649841	2.85918665
1	2.00788498	-4.15080118	2.78078651	1	-0.59531504	4.29499865	2.75308657
6	1.45088494	-3.44430161	0.23958655	1	-0.66041505	2.55589843	3.12918663
1	0.94108486	-2.86890149	-0.53541344	1	-1.98451507	3.63199854	3.64828658
1	0.73498487	-4.15720129	0.66608655	6	-2.79991508	4.24209881	1.12158656
1	2.25178480	-4.01380157	-0.24351345	1	-2.20961499	5.15379858	0.98058659
6	0.90628493	-1.80090153	2.11868668	1	-3.58911514	4.44899845	1.85208654
				1	-3.26701498	3.98769832	0.17308655

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## B'-Gly



Zero-point vibrational energy	1364274.4 (Joules/Mol)
	326.06940 (Kcal/Mol)
Zero-point correction=	0.519625 (Hartree/Particle)
Thermal correction to Energy=	0.552150
Thermal correction to Enthalpy=	0.553094
Thermal correction to Gibbs Free Energy=	0.453725
Sum of electronic and zero-point Energies=	-1849.147854
Sum of electronic and thermal Energies=	-1849.115329
Sum of electronic and thermal Enthalpies=	-1849.114385
Sum of electronic and thermal Free Energies=	-1849.213753

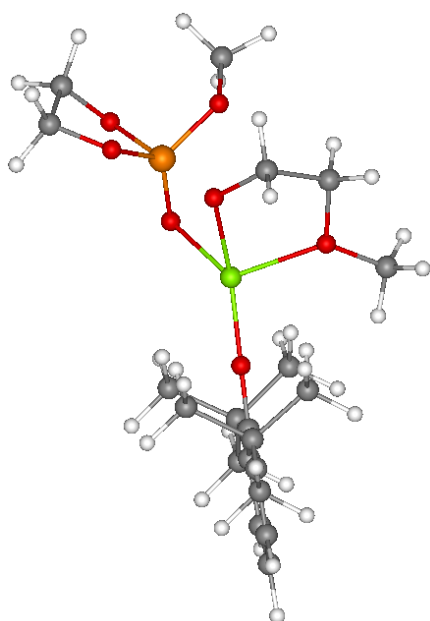
				cartesian			
12	-0.72574496	0.23609674	-0.42285809	1	1.83085501	2.79739690	2.25764179
8	1.05705500	0.08409675	-0.05045807	6	1.78105509	2.80559683	-1.23365808
6	2.36695504	0.05279675	0.17564192	1	2.55655503	2.80259681	-2.00745821
6	3.03375506	-1.20400321	0.30764192	1	1.23685503	3.75569677	-1.30385804
6	4.41245508	-1.20260322	0.53854197	1	1.09275496	1.99149680	-1.47095799
1	4.94355488	-2.14300323	0.64124197	8	-2.19164491	1.12119675	0.56674194
6	5.14045477	-0.02210325	0.64424193	15	-3.41404486	0.18819675	0.52054197
6	4.48035479	1.19579673	0.51974195	8	-4.38984489	1.06309676	1.58124197
1	5.06365490	2.10609698	0.60884196	8	-3.55094481	-1.17330325	1.42534196
6	3.10355520	1.27199674	0.28754193	6	-5.07564497	0.24429674	2.50844193
6	2.26735520	-2.53630304	0.20474193	6	-4.16544485	-0.95940328	2.70154190
6	2.41475511	2.64439678	0.16394192	8	-4.41584492	0.29129675	-0.76465803

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6	1.62575495	-2.68090320	-1.19065809	6	-5.59684515	1.10719669	-0.77915806
1	0.96275496	-1.84480321	-1.41995800	1	-6.35414505	0.72139674	-0.09335807
1	1.05065501	-3.61340308	-1.25425804	1	-5.36874533	2.14269686	-0.52225804
1	2.39925504	-2.70750308	-1.96585810	1	-5.97664499	1.04919672	-1.80145800
6	1.19475496	-2.62780309	1.30974197	6	-2.22984505	0.64969677	-3.11375809
1	0.48965505	-1.79660320	1.26684201	8	-2.36194491	-0.93540323	-0.58015805
1	1.66555512	-2.61010313	2.29864192	6	-2.04434490	-0.79390323	-2.95185828
1	0.63005507	-3.56420302	1.22144198	6	-2.65814495	-1.57570326	-1.79455805
6	3.18595505	-3.75720310	0.38934192	8	-0.98514497	0.13489676	-2.56365824
1	3.66835523	-3.76700306	1.37244201	1	-1.77324498	-1.36910331	-3.83515811
1	3.96585536	-3.81080317	-0.37775809	1	-3.73694491	-1.67350328	-1.95025802
1	2.58885503	-4.67300320	0.31074193	1	-2.22024488	-2.58090305	-1.77285802
6	3.40375519	3.81289697	0.32454193	1	6.21235466	-0.05100325	0.82464194
1	4.18405485	3.80459690	-0.44375807	1	-6.05594492	-0.06070325	2.11314178
1	3.88685489	3.81259680	1.30724192	1	-5.22814512	0.80799675	3.43214178
1	2.86125517	4.76029682	0.22894192	1	-4.69954491	-1.87300324	2.96854186
6	1.35455501	2.81779695	1.27144194	1	-3.38174486	-0.76090324	3.43924189
1	0.60305500	2.02749681	1.25854194	1	-2.85104489	1.18209672	-2.39965820
1	0.84025502	3.78089690	1.16604197	1	-2.10374498	1.10429680	-4.09295797

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### B'-OCH<sub>2</sub>CH<sub>2</sub>OMe



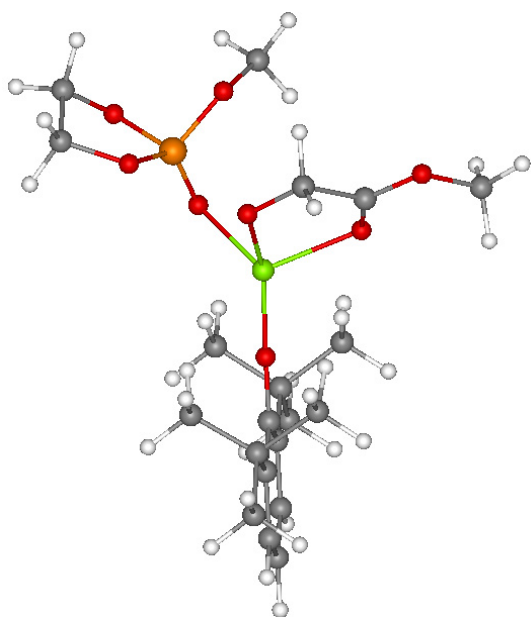
Zero-point vibrational energy	1426045.1 (Joules/Mol)
	340.83297 (Kcal/Mol)
Zero-point correction=	0.543152 (Hartree/Particle)
Thermal correction to Energy=	0.576634
Thermal correction to Enthalpy=	0.577579
Thermal correction to Gibbs Free Energy=	0.477823
Sum of electronic and zero-point Energies=	-1850.362497
Sum of electronic and thermal Energies=	-1850.329014
Sum of electronic and thermal Enthalpies=	-1850.328070
Sum of electronic and thermal Free Energies=	-1850.427826

				cartesian			
12	-0.79088593	-0.10473744	-0.12888744	6	1.30631399	2.65126252	-1.42548740
8	1.01951396	0.04136256	0.13561258	1	2.01371408	2.55316257	-2.25668740
6	2.32891417	0.20336255	0.30861256	1	0.69971395	3.54816270	-1.59898734
6	3.14891410	-0.92313743	0.62941253	1	0.64231396	1.78516257	-1.45148742
6	4.52761412	-0.72673744	0.75411254	8	-2.23748589	1.07056248	0.51531255
1	5.17341423	-1.56583750	0.99011254	15	-3.52758598	0.23146255	0.52161258
6	5.11191416	0.52386260	0.58741260	8	-4.54768610	1.44976246	1.09871256
6	4.30131435	1.61916256	0.30991256	8	-3.98648596	-0.78813744	1.72641265
1	4.77341413	2.58976269	0.20251256	6	-5.52778578	0.95746255	1.98941267
6	2.91451406	1.50086248	0.17371257	6	-4.83588600	-0.18903744	2.71041250
6	2.54931402	-2.32503748	0.85121256	8	-4.30498600	0.01416256	-0.90128744
6	2.05761409	2.75606275	-0.08318742	6	-5.20658588	0.99176258	-1.43968737

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6	1.88031399	-2.84153748	-0.43838745	1	-6.13908577	1.02956247	-0.87258744
1	1.08691406	-2.17583728	-0.78018743	1	-4.75328588	1.98456252	-1.45568740
1	1.44971395	-3.83763742	-0.27448744	1	-5.41818571	0.66386259	-2.45988750
1	2.61871409	-2.92343736	-1.24408734	8	-0.92148602	-1.00153744	-2.06008744
6	1.53661406	-2.29763746	2.01461267	6	-2.17368603	-1.65953743	-2.33648753
1	0.73831403	-1.57253754	1.84721267	6	-2.70698595	-2.17733741	-1.00278735
1	2.03731418	-2.02283740	2.94901252	8	-2.45968580	-1.22623754	0.01401257
1	1.08191395	-3.28623748	2.15351248	1	6.18791389	0.64626259	0.68531257
6	3.61731410	-3.36573744	1.23211265	1	-6.41488600	0.60006255	1.44471264
1	4.13951397	-3.10323739	2.15801239	1	-5.82788610	1.76176250	2.66531253
1	4.36371422	-3.50443745	0.44271258	1	-5.52178574	-0.95853740	3.07021260
1	3.13301420	-4.33533764	1.39481258	1	-4.21558619	0.16986255	3.53791261
6	2.90801406	4.03656244	-0.17008743	1	-3.77258587	-2.40613747	-1.09198737
1	3.62571406	4.00576258	-0.99718744	1	-2.17648602	-3.09433746	-0.72138745
1	3.45801401	4.23086262	0.75641257	6	-0.12648596	-0.73463744	-3.21848750
1	2.24891424	4.89496231	-0.34158742	1	-0.65358597	-0.05493744	-3.89758754
6	1.06521404	2.96796274	1.07841253	1	0.10491404	-1.67123747	-3.73628759
1	0.40851405	2.11006260	1.22591257	1	0.79751396	-0.27373743	-2.87088752
1	0.43591401	3.84626269	0.89251256	1	-2.85728598	-0.93533742	-2.79068756
1	1.60961401	3.13376260	2.01421261	1	-1.99778605	-2.48683739	-3.03488755

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**B'C'-1**

Zero-point vibrational energy	1372397.8 (Joules/Mol)
	328.01095 (Kcal/Mol)
Zero-point correction=	0.522719 (Hartree/Particle)
Thermal correction to Energy=	0.556735
Thermal correction to Enthalpy=	0.557679
Thermal correction to Gibbs Free Energy=	0.455597
Sum of electronic and zero-point Energies=	-1924.409711
Sum of electronic and thermal Energies=	-1924.375694
Sum of electronic and thermal Enthalpies=	-1924.374750
Sum of electronic and thermal Free Energies=	-1924.476832

cartesian							
12	0.82243013	0.21479364	-0.12075715	6	-1.63546991	-1.23530638	-2.71975732
8	-0.97516984	-0.13730636	0.04094285	1	-2.40556979	-0.68200636	-3.26885724
6	-2.28496981	-0.28250638	0.20414284	1	-1.08826995	-1.85670638	-3.44015718
6	-2.98296976	0.50989366	1.16874290	1	-0.94516987	-0.50370634	-2.29705715
6	-4.36237001	0.32819363	1.30754292	8	2.14543009	-1.30870640	-0.04595716
1	-4.91396999	0.91739362	2.03264284	15	3.49273014	-0.96010637	0.52854282
6	-5.06526995	-0.59450632	0.54044282	8	4.25232983	-2.40400624	0.67424285
6	-4.37736988	-1.36280644	-0.39325714	8	3.74933028	-0.46850637	2.03274274
1	-4.94096994	-2.07950640	-0.98125714	6	5.13962984	-2.37140632	1.79584289
6	-2.99876976	-1.23640645	-0.58705717	6	4.43812990	-1.47430646	2.81064272
6	-2.24956989	1.54289365	2.04484272	8	4.48713017	-0.12250637	-0.40745717
6	-2.28126979	-2.11470628	-1.62925708	6	4.67523003	-0.58010638	-1.76255715

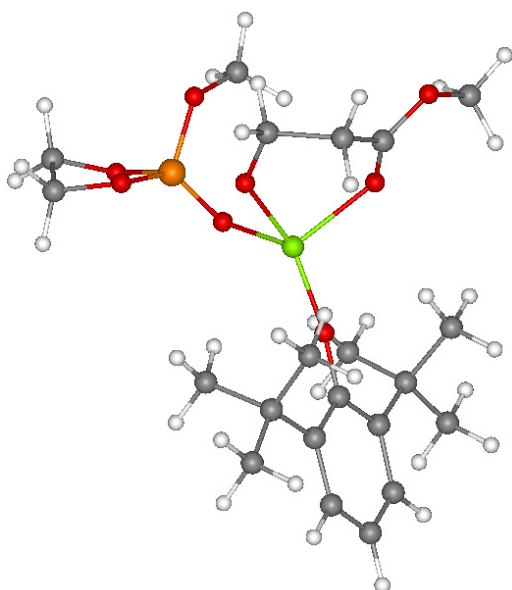
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6	-1.60986972	2.63609362	1.16394293	1	5.07372999	-1.59780645	-1.77065706
1	-0.94206983	2.21479368	0.41024286	1	3.73313022	-0.54530632	-2.31485724
1	-1.04026985	3.34429359	1.77864289	1	5.39492989	0.10439364	-2.21065712
1	-2.38676977	3.19619370	0.63194281	8	1.20893013	1.58489358	-1.70365715
6	-1.18806982	0.84869367	2.92264271	6	2.03873014	2.42649364	-1.33625710
1	-0.47896987	0.26899362	2.33034277	6	2.73813009	2.31529379	0.00814285
1	-1.67146993	0.15799363	3.62214279	8	2.32123017	1.18929362	0.67334282
1	-0.62466985	1.58629358	3.50704288	1	-6.13817024	-0.71510637	0.66994286
6	-3.19856977	2.27189374	3.01304269	1	6.10902977	-1.95930636	1.49324286
1	-3.68266988	1.58309364	3.71344280	1	5.27232981	-3.39290619	2.15484285
1	-3.97816968	2.83349371	2.48764277	1	5.12662983	-0.95350635	3.47684288
1	-2.62356973	2.99079370	3.60814285	1	3.69273019	-2.01980639	3.39514279
6	-3.24696994	-3.06840634	-2.35485721	1	3.82273006	2.32359362	-0.19345716
1	-4.02647018	-2.53220630	-2.90705729	1	2.52413011	3.24989367	0.55674285
1	-3.73176980	-3.76850629	-1.66605711	8	2.36643004	3.47229362	-2.07545733
1	-2.68416977	-3.66490626	-3.08195734	6	1.67773008	3.61459374	-3.33685732
6	-1.22186995	-3.00300622	-0.94565719	1	2.06983018	4.52999353	-3.77575731
1	-0.48456991	-2.41660619	-0.39745718	1	0.60253012	3.69409370	-3.17055726
1	-0.69306988	-3.61150622	-1.69025707	1	1.88613009	2.75769377	-3.97935700
1	-1.70206976	-3.68430638	-0.23455717				

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**B'C'-2**



Zero-point vibrational energy	1447756.6 (Joules/Mol)
	346.02213 (Kcal/Mol)
Zero-point correction=	0.551421 (Hartree/Particle)
Thermal correction to Energy=	0.586838
Thermal correction to Enthalpy=	0.587782
Thermal correction to Gibbs Free Energy=	0.480854
Sum of electronic and zero-point Energies=	-1963.683868
Sum of electronic and thermal Energies=	-1963.648451
Sum of electronic and thermal Enthalpies=	-1963.647507
Sum of electronic and thermal Free Energies=	-1963.754436

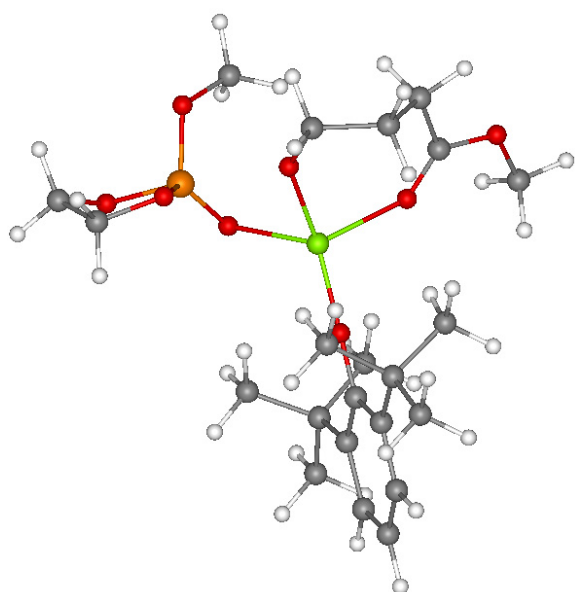
				cartesian			
12	-0.75844860	0.22521216	-0.14429852	1	2.93195128	3.08261228	0.42860147
8	1.06795144	-0.00788785	0.01610148	1	1.66925156	3.48401213	1.60720146
6	2.34395123	-0.34258783	0.16540149	1	1.34435141	2.31661224	0.30810148
6	2.90385127	-1.41488779	-0.59869850	8	-1.94824851	-0.38918784	1.37490153
6	4.25465155	-1.72798789	-0.41909853	15	-3.28694868	-0.94738781	0.97350150
1	4.70295143	-2.53478789	-0.98949850	8	-3.88804865	-1.58188784	2.35850143
6	5.06005144	-1.03358781	0.47700149	8	-3.51574874	-2.24868774	0.06420148
6	4.50755119	0.00571215	1.21820152	6	-4.71204853	-2.71078777	2.05420136
1	5.15025139	0.53551215	1.91350150	6	-4.05044842	-3.34788775	0.83650148
6	3.16615129	0.37731215	1.08940148	8	-4.41364861	0.09841215	0.53050148
6	2.05565143	-2.21668792	-1.60299850	6	-4.50154877	1.33781219	1.25690150
6	2.60275126	1.53811216	1.92990148	1	-4.70194864	1.15141213	2.31560135
6	1.51045144	-1.28718781	-2.70669866	1	-3.57724857	1.91011214	1.14890146

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1	0.89465141	-0.48728785	-2.29199862	1	-5.33354855	1.88541222	0.81430149
1	0.90665150	-1.85458779	-3.42569852	8	-1.10824859	2.20681214	-0.75839847
1	2.33765125	-0.81768787	-3.25039864	6	-1.71794856	2.47011209	-1.80309844
6	0.90595150	-2.94478774	-0.87609851	6	-2.08174849	1.46001220	-2.84299850
1	0.30625144	-2.26518774	-0.26889852	8	-2.28414869	-0.31758785	-1.18389845
1	1.30965149	-3.71018791	-0.20419851	6	-2.92034864	0.29711217	-2.23979855
1	0.24165145	-3.43838787	-1.59579849	1	-3.90324855	0.69891214	-1.93759847
6	2.87065125	-3.30608773	-2.32329869	1	-3.10964870	-0.40058783	-3.07249856
1	3.28775144	-4.04078817	-1.62669849	1	6.10755157	-1.29988790	0.59710151
1	3.69175148	-2.88618779	-2.91409850	1	-5.73294878	-2.37908792	1.83360147
1	2.21485138	-3.84848785	-3.01389861	1	-4.72084856	-3.36968780	2.92370129
6	3.66495132	2.16621208	2.85030150	1	-4.75014877	-3.88458776	0.19480148
1	4.50445127	2.58851218	2.28760147	1	-3.22074866	-4.00218773	1.11570156
1	4.06215143	1.44911218	3.57670140	1	-2.60814857	1.94711220	-3.66729856
1	3.20895123	2.98571205	3.41780138	1	-1.14694858	1.03661215	-3.22729850
6	1.47075140	1.03671217	2.85000134	8	-2.11584854	3.70811224	-2.07209873
1	0.66315150	0.56321216	2.29060149	6	-1.76344860	4.72231197	-1.10809851
1	1.04975152	1.86721218	3.43120146	1	-2.13474870	5.65551186	-1.52719855
1	1.85655153	0.29471216	3.55770135	1	-0.68114853	4.75791168	-0.97749853
6	2.09985137	2.66951227	1.01010144	1	-2.23914862	4.51501179	-0.14819852

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**B'C'-3**



Zero-point vibrational energy	1523520.6 (Joules/Mol)
	364.13015 (Kcal/Mol)
Zero-point correction=	0.580278 (Hartree/Particle)
Thermal correction to Energy=	0.616032
Thermal correction to Enthalpy=	0.616976
Thermal correction to Gibbs Free Energy=	0.512173
Sum of electronic and zero-point Energies=	-2002.955909
Sum of electronic and thermal Energies=	-2002.920155
Sum of electronic and thermal Enthalpies=	-2002.919211
Sum of electronic and thermal Free Energies=	-2003.024014

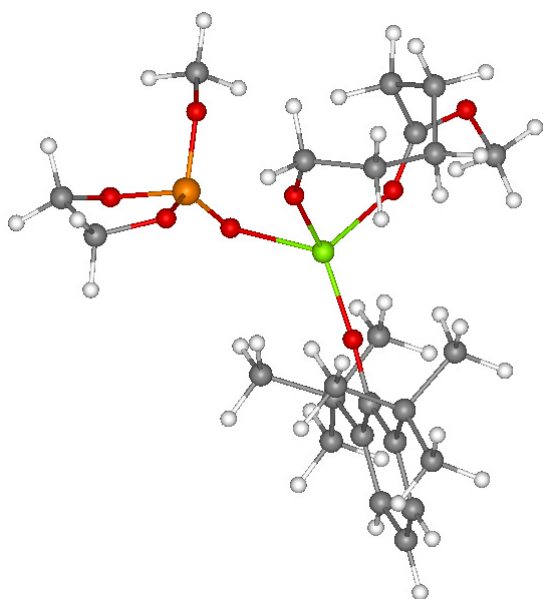
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12	-0.85492766	0.22751009	0.31696665	1	1.00707221	0.00721011	2.41466665
8	0.92967230	-0.23078987	0.07656666	8	-2.05622768	-1.29788995	0.92776668
6	2.20127225	-0.56978989	-0.09563334	15	-3.25192785	-1.55768991	0.05036666
6	2.90537214	-0.14828989	-1.26963329	8	-3.64492774	-3.12058997	0.32266667
6	4.24137259	-0.52988988	-1.42373335	8	-3.18372774	-1.68348992	-1.55543327
1	4.79157257	-0.22568989	-2.30803347	6	-4.16502762	-3.71918988	-0.86503339
6	4.90457249	-1.29568994	-0.47143331	6	-3.40202785	-3.04048991	-1.99823320
6	4.21837234	-1.69398987	0.67076671	8	-4.60782766	-0.79958987	0.40586665
1	4.75147247	-2.28868985	1.40496671	6	-4.67072773	0.12651011	1.50116670
6	2.88007236	-1.35508990	0.89156663	1	-4.43742752	-0.37428990	2.44416666
6	2.22797227	0.71771014	-2.34763336	1	-3.97392774	0.94631010	1.32176673
6	2.17007232	-1.84018993	2.16906667	1	-5.69742727	0.49251011	1.52236664
6	1.80427217	2.06991005	-1.74013329	8	-0.76202768	2.07591009	1.27726674

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1	1.15237236	1.93181014	-0.87593329	6	-1.31242776	3.17061019	1.14356673
1	1.28307223	2.68411016	-2.48603344	6	-2.38382769	3.53161001	0.14716667
1	2.68607235	2.62631011	-1.40313327	8	-2.47302771	0.65821016	-0.60503340
6	1.01567221	-0.01498988	-2.95723343	6	-2.21132779	2.96861005	-1.27753329
1	0.27867234	-0.29148987	-2.20263338	6	-2.90712786	1.62151003	-1.50433326
1	1.34107232	-0.93568987	-3.45393348	1	-1.14652777	2.87501001	-1.51813328
1	0.52177233	0.61511016	-3.70763350	1	-2.62102771	3.70341015	-1.98143327
6	3.16837215	1.04381013	-3.52193332	1	-3.99852777	1.77231014	-1.40843332
1	3.50357223	0.14261010	-4.04623318	1	-2.72972775	1.31651008	-2.54933333
1	4.05267239	1.60641003	-3.20413351	1	5.94447231	-1.57828987	-0.61713338
1	2.63277221	1.66391003	-4.25003338	1	-5.24322748	-3.53418994	-0.93263328
6	3.10527229	-2.63628983	3.09716654	1	-3.98042774	-4.79338980	-0.81533337
1	3.96257234	-2.04348993	3.43456650	1	-3.96522784	-2.99278998	-2.93113351
1	3.48217225	-3.54878998	2.62316656	1	-2.42792773	-3.50518990	-2.17293334
1	2.54767227	-2.94228983	3.98966646	1	-3.32572770	3.16341019	0.57466662
6	1.00977230	-2.78638983	1.80146670	1	-2.45542765	4.62151051	0.14066666
1	0.28187233	-2.31288981	1.14356673	8	-0.99702770	4.18761015	1.93716669
1	0.48217231	-3.12028980	2.70356655	6	0.00277230	3.93160987	2.94806647
1	1.39817238	-3.67448997	1.29026663	1	0.12537232	4.87741041	3.47196651
6	1.66167235	-0.64228988	2.99726653	1	0.93787235	3.62051010	2.48116660
1	2.50547218	-0.03428988	3.34346652	1	-0.34182769	3.15301013	3.63026667
1	1.11197233	-0.99168986	3.88036656				

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**B'C'-4**



Zero-point vibrational energy	1676609.4 (Joules/Mol)
	400.71926 (Kcal/Mol)
Zero-point correction=	0.638587 (Hartree/Particle)
Thermal correction to Energy=	0.677549
Thermal correction to Enthalpy=	0.678494
Thermal correction to Gibbs Free Energy=	0.565495
Sum of electronic and zero-point Energies=	-2081.498850
Sum of electronic and thermal Energies=	-2081.459887
Sum of electronic and thermal Enthalpies=	-2081.458943
Sum of electronic and thermal Free Energies=	-2081.571942

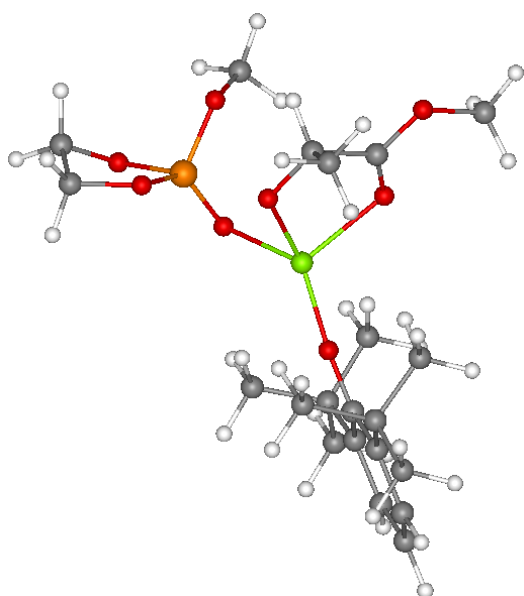
				cartesian			
12	-0.56237185	-0.03342406	0.21116936	8	-3.26137185	-3.47352409	0.37056938
8	1.28052807	-0.24812406	0.07806937	8	-2.84357190	-2.17582393	-1.62363064
6	2.57772803	-0.48162407	-0.08443063	6	-3.88637185	-4.11212397	-0.74453068
6	3.24032807	-0.07472406	-1.28773069	6	-3.16777182	-3.54302406	-1.96393061
6	4.60862827	-0.32892406	-1.41973066	8	-4.17987156	-1.11542404	0.30376935
1	5.12812805	-0.02852407	-2.32353067	6	-4.60947180	-1.07832408	1.67746937
6	5.34202814	-0.96172404	-0.42243063	1	-4.81567192	-2.08752394	2.04416943
6	4.69332790	-1.35742414	0.74216938	1	-3.85107183	-0.60572410	2.30696940
1	5.27872801	-1.85292411	1.50956929	1	-5.52357197	-0.48502406	1.68956935
6	3.32722807	-1.13952410	0.94456935	8	-0.84747183	1.46657586	1.63446939
6	2.48392820	0.63697588	-2.42423058	6	-1.69197190	2.34517598	1.83106935
6	2.66352820	-1.62222409	2.24776936	6	-2.96697187	2.51497602	1.05896938
6	1.91462803	1.97617590	-1.91583061	8	-2.08157182	0.20567593	-0.91153061

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1	1.28182817	1.83317602	-1.03823066	6	-2.23427176	2.25067592	-2.26773071
1	1.32652807	2.47207594	-2.69813061	6	-2.84877181	0.91787589	-1.82823062
1	2.72932816	2.64997602	-1.62763071	1	-1.36527193	2.04797602	-2.90473056
6	1.36322808	-0.26582408	-2.97763062	1	-2.97317195	2.75767612	-2.90493059
1	0.64552820	-0.55212402	-2.20883060	1	-3.85347199	1.11117589	-1.40723062
1	1.78992820	-1.18562412	-3.39313078	1	-3.02127194	0.31517592	-2.73453069
1	0.81682819	0.24457595	-3.78063059	1	6.40592813	-1.14602411	-0.55173063
6	3.39282823	0.97647595	-3.61943078	1	-4.95677185	-3.87632394	-0.76033068
1	3.82572794	0.08077595	-4.07753038	1	-3.75157189	-5.18982410	-0.64023066
1	4.20952797	1.65197587	-3.34363055	1	-3.78957176	-3.51862407	-2.85963058
1	2.79862809	1.48167586	-4.38983059	1	-2.23237181	-4.06902409	-2.17163062
6	3.66512823	-2.28892398	3.20766926	1	-3.23137188	1.53977585	0.64926934
1	4.46332836	-1.60572410	3.51766944	1	-3.74257183	2.85457611	1.75226939
1	4.12562799	-3.18232393	2.77266932	8	-1.51487184	3.26267600	2.77226925
1	3.13582802	-2.60542393	4.11386967	6	-0.28027183	3.19217610	3.52016926
6	1.58952808	-2.68262386	1.93276930	1	-0.32547182	4.02237606	4.22216940
1	0.82652813	-2.30982399	1.25056934	1	0.57292819	3.29617596	2.84876943
1	1.09062815	-3.01232386	2.85296941	1	-0.21397182	2.23987603	4.04756927
1	2.05232811	-3.56042409	1.46796930	6	-1.78487182	3.21157598	-1.15843070
6	2.05192804	-0.43362406	3.01666927	1	-1.47797191	4.14807606	-1.63973069
1	2.84002805	0.26307595	3.32576942	1	-0.87107182	2.82887602	-0.68983066
1	1.53962815	-0.78672409	3.92106938	6	-2.81697178	3.55457592	-0.07593064
1	1.33892810	0.12047595	2.40616941	1	-3.80667186	3.68297601	-0.52963066
8	-1.62867188	-1.65762413	0.80646932	1	-2.56217194	4.51837587	0.37946936
15	-2.84437180	-1.93782413	-0.03393064				

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**B'C'-6**



Zero-point vibrational energy	1446277.4 (Joules/Mol)
	345.66861 (Kcal/Mol)
Zero-point correction=	0.550858 (Hartree/Particle)
Thermal correction to Energy=	0.586395
Thermal correction to Enthalpy=	0.587339
Thermal correction to Gibbs Free Energy=	0.481885
Sum of electronic and zero-point Energies=	-1963.687541
Sum of electronic and thermal Energies=	-1963.652004
Sum of electronic and thermal Enthalpies=	-1963.651060
Sum of electronic and thermal Free Energies=	-1963.756514

				cartesian			
12	0.70672292	0.03033036	-0.13941064	1	-2.12837696	-1.61616969	-3.14271069
8	-1.09777713	-0.24546963	0.09828934	1	-0.78087711	-2.73816967	-2.87191081
6	-2.41477704	-0.41126963	0.15278935	1	-0.80037713	-1.14716959	-2.08701062
6	-3.22727704	0.54133034	0.84448934	8	2.00902295	-1.50696969	-0.05991066
6	-4.61057711	0.34043038	0.87518936	15	3.36142302	-1.15286958	0.50288934
1	-5.24747705	1.04973042	1.39308929	8	4.10552311	-2.60806966	0.65658933
6	-5.21087694	-0.75186962	0.25828934	8	3.64202309	-0.65746963	2.00428939
6	-4.41237688	-1.67796969	-0.40421066	6	5.00642300	-2.57726955	1.76548934
1	-4.89727688	-2.52736974	-0.87371063	6	4.32562304	-1.66676962	2.78158927
6	-3.02257705	-1.54396963	-0.47501066	8	4.36742306	-0.35066962	-0.45471066
6	-2.61277699	1.76763034	1.54468930	6	4.56702280	-0.85736966	-1.79001069
6	-2.18277693	-2.61116958	-1.20161068	1	4.95672321	-1.87796962	-1.75811076
6	-1.91887724	2.67803025	0.51098931	1	3.63142300	-0.83456963	-2.35421062

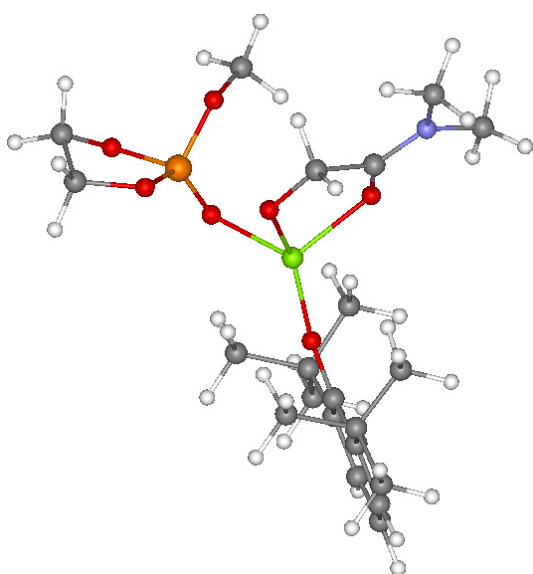
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1	-1.15837717	2.13993025	-0.05761066	1	5.29702282	-0.19446965	-2.25401068
1	-1.44547713	3.53453040	1.00788927	8	1.11882293	1.37493038	-1.72461069
1	-2.65027690	3.06683040	-0.20621067	6	1.98022282	2.19523025	-1.38041067
6	-1.61917722	1.32683039	2.63908935	6	2.67932296	2.10713029	-0.02451066
1	-0.81277716	0.71273035	2.23718929	8	2.24112296	0.97503042	0.63028938
1	-2.13547707	0.73663038	3.40408921	1	-6.28977680	-0.88246965	0.29728934
1	-1.17417717	2.20083046	3.13088918	1	5.97662306	-2.17636967	1.44978929
6	-3.67207718	2.63713026	2.24498940	1	5.13392305	-3.59746957	2.13048935
1	-4.20857716	2.08813047	3.02628922	1	5.02592278	-1.15036964	3.43908930
1	-4.40777683	3.04343033	1.54278934	1	3.57922292	-2.20066953	3.37558937
1	-3.17757702	3.48853040	2.72648931	1	3.75692296	2.04623032	-0.25491065
6	-3.04897690	-3.73986959	-1.78901076	6	2.43832302	3.38773036	0.78868937
1	-3.76467705	-3.37256956	-2.53251076	8	2.35272288	3.19313025	-2.16341066
1	-3.60347700	-4.28126955	-1.01531076	6	1.67712283	3.30593038	-3.43471074
1	-2.40037704	-4.46636963	-2.29191065	1	2.10692286	4.18523026	-3.91071081
6	-1.20457709	-3.28136969	-0.21551067	1	0.60502291	3.43393040	-3.27991080
1	-0.53617716	-2.56136966	0.25648934	1	1.85562289	2.41393042	-4.03721094
1	-0.58987713	-4.02916956	-0.73161066	1	2.95762300	3.28083038	1.74358928
1	-1.76077712	-3.79076958	0.57908934	1	1.37232292	3.51563025	0.99548936
6	-1.42327714	-1.98966968	-2.39191079	1	2.81462288	4.27693033	0.27428934

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**B'C'-7**



Zero-point vibrational energy	1479589.4 (Joules/Mol)
	353.63035 (Kcal/Mol)
Zero-point correction=	0.563546 (Hartree/Particle)
Thermal correction to Energy=	0.599237
Thermal correction to Enthalpy=	0.600181
Thermal correction to Gibbs Free Energy=	0.494675
Sum of electronic and zero-point Energies=	-1943.808869
Sum of electronic and thermal Energies=	-1943.773178
Sum of electronic and thermal Enthalpies=	-1943.772234
Sum of electronic and thermal Free Energies=	-1943.877741

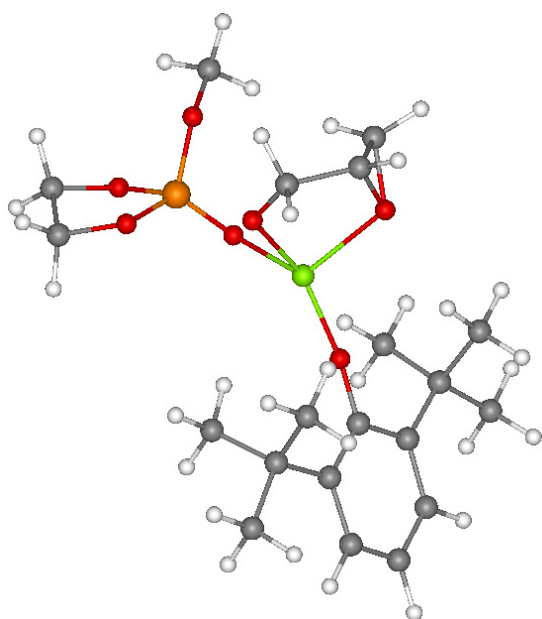
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12	-0.63407445	-0.11472839	-0.00396718	1	1.06972551	-2.07302833	3.35393286
8	1.18252552	-0.40762839	-0.15326717	1	0.95462561	-0.74122840	2.18543291
6	2.50782561	-0.45712841	-0.18406719	8	-1.85207450	-1.73292840	0.11023282
6	3.23722577	0.36277163	-1.10246718	15	-3.22037435	-1.55842841	-0.48626718
6	4.63322544	0.28497159	-1.10266709	8	-3.90087438	-3.04452848	-0.39196718
1	5.20802546	0.89717168	-1.78976715	8	-3.52457428	-1.31692839	-2.04186726
6	5.32502556	-0.56222838	-0.24356717	6	-4.80387449	-3.22992849	-1.48546708
6	4.60792542	-1.36182845	0.64063281	6	-4.16347456	-2.46722841	-2.64096713
1	5.16312551	-2.02092838	1.29993284	8	-4.24987459	-0.63052839	0.31623280
6	3.21142578	-1.33852839	0.69683284	6	-4.30227423	-0.77662838	1.75043285
6	2.51802564	1.31307161	-2.07846713	1	-4.55357456	-1.80512846	2.02273297
6	2.46262574	-2.25632834	1.68153286	1	-3.34807444	-0.49222839	2.19923282
6	1.73102558	2.38597155	-1.29846716	1	-5.08907461	-0.10292839	2.08953285

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1	1.03232551	1.94147158	-0.58816719	8	-1.16837442	1.39017153	1.31303287
1	1.16842556	3.02857161	-1.98746717	6	-2.00877428	2.18427157	0.81673282
1	2.41822577	3.02017164	-0.72726721	6	-2.63787436	1.81767154	-0.53976715
6	1.58432555	0.52027160	-3.01646709	8	-2.14477444	0.62547159	-0.99826717
1	0.84562552	-0.06242839	-2.46526718	1	6.41152525	-0.60202837	-0.26546717
1	2.16722560	-0.17772840	-3.62736702	1	-5.78887463	-2.82372832	-1.22876716
1	1.05142558	1.19887161	-3.69396710	1	-4.88847446	-4.30002832	-1.67996716
6	3.49962568	2.07367158	-2.98796701	1	-4.88667440	-2.09522843	-3.36756706
1	4.09282541	1.39787161	-3.61296701	1	-3.39497423	-3.05762839	-3.14656711
1	4.18682528	2.70887160	-2.41876721	1	-3.73447442	1.78567159	-0.40446720
1	2.93332577	2.72777152	-3.66126704	1	-2.43477440	2.65167165	-1.23766708
6	3.41962576	-3.12412834	2.51743293	7	-2.33817434	3.32207155	1.45323288
1	4.09452534	-2.52202845	3.13543296	6	-1.67447448	3.69967151	2.69443297
1	4.02522564	-3.79062843	1.89433289	1	-1.13787436	4.64517164	2.55993295
1	2.83312559	-3.75562835	3.19473290	1	-0.96717441	2.92157149	2.97353292
6	1.54642558	-3.23012853	0.91163284	1	-2.41387439	3.82637167	3.49243283
1	0.82102561	-2.70652843	0.28893280	6	-3.26177430	4.30067158	0.90223283
1	0.99792552	-3.87482834	1.60993290	1	-2.72077441	5.17327166	0.51763284
1	2.14482570	-3.87482834	0.25823280	1	-3.94557428	4.63647175	1.68783283
6	1.64612556	-1.41912842	2.68753290	1	-3.85537434	3.87377167	0.09643281
1	2.31242561	-0.80782837	3.30633283				

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## B'C'-Gly



Zero-point vibrational energy	1360084.5 (Joules/Mol)
	325.06799 (Kcal/Mol)
Zero-point correction=	0.518029 (Hartree/Particle)
Thermal correction to Energy=	0.550620
Thermal correction to Enthalpy=	0.551564
Thermal correction to Gibbs Free Energy=	0.451858
Sum of electronic and zero-point Energies=	-1849.142450
Sum of electronic and thermal Energies=	-1849.109859
Sum of electronic and thermal Enthalpies=	-1849.108915
Sum of electronic and thermal Free Energies=	-1849.208621

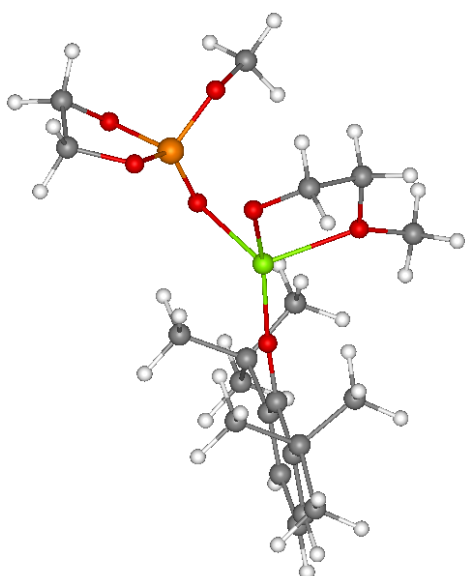
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12	0.76693857	-0.37748387	-0.57172257	1	-1.91136146	-1.84398389	2.95517731
8	-1.01256144	-0.18558387	-0.14012258	6	-2.29886150	-2.92928386	-0.33882257
6	-2.25936151	0.17481613	0.14197743	1	-3.14276147	-2.98508382	-1.03542256
6	-2.69796133	1.51471603	-0.09972258	1	-1.96376133	-3.95458388	-0.13472258
6	-4.02146149	1.84751606	0.20447743	1	-1.49156141	-2.39368391	-0.83932257
1	-4.37986135	2.85661602	0.02857742	8	2.07163858	-0.47598389	0.99977744
6	-4.91146135	0.91901612	0.73307747	15	3.43033862	0.12931612	0.78567743
6	-4.47426128	-0.38038388	0.97017747	8	4.08023834	0.29061612	2.27717733
1	-5.18226147	-1.08988392	1.38557744	8	3.65123868	1.64501607	0.31567740
6	-3.16606140	-0.78558385	0.69007742	6	4.89553881	1.46801603	2.32417727
6	-1.74746132	2.57881618	-0.67742258	6	4.20873833	2.44951606	1.37967741
6	-2.72786140	-2.23518395	0.96997744	8	4.50153875	-0.76758385	0.00457743

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6	-1.26066136	2.16251612	-2.08102274	6	4.94673872	-1.99228394	0.62357742
1	-0.79926145	1.17341614	-2.08312273	1	5.50933838	-1.77738392	1.53497744
1	-0.53276139	2.88441610	-2.47042274	1	4.10053825	-2.64218402	0.86317742
1	-2.10616136	2.12251616	-2.77622271	1	5.59143877	-2.47808385	-0.10822257
6	-0.55966139	2.81061602	0.28027740	8	0.92823857	-1.88608396	-2.12652278
1	-0.04706141	1.88221610	0.53817743	6	2.00063848	-1.50338387	-3.05112267
1	-0.91506135	3.24891615	1.21947742	6	2.61043859	-0.12888387	-2.76282263
1	0.16983859	3.49891615	-0.16382258	8	2.34183860	0.27431610	-1.46992254
6	-2.42826152	3.94851613	-0.85162258	1	-5.93566132	1.20521605	0.95997745
1	-2.78936148	4.35571623	0.09877742	1	5.91163874	1.22911608	1.99077749
1	-3.26996136	3.90701604	-1.55092251	1	4.92193842	1.82051611	3.35607743
1	-1.70226145	4.66241598	-1.25762260	1	4.89683867	3.16121602	0.92257744
6	-3.86556149	-3.08518386	1.56327748	1	3.38873863	2.98281598	1.86747742
1	-4.72206163	-3.16368389	0.88507742	1	3.69383860	-0.20008387	-2.96212268
1	-4.21976137	-2.69358397	2.52287722	1	2.20053864	0.58001614	-3.50252271
1	-3.49876142	-4.10238409	1.74257743	6	2.17563868	-2.62528396	-2.12762260
6	-1.57886136	-2.26248384	1.99877739	1	1.74333858	-1.74138391	-4.08212280
1	-0.71846139	-1.68068397	1.66607749	1	2.78363848	-2.47198391	-1.23982251
1	-1.25226140	-3.29478383	2.17937732	1	2.06933856	-3.65028381	-2.47432256

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**B'C'-OCH<sub>2</sub>CH<sub>2</sub>OMe**



Zero-point vibrational energy	1420557.9 (Joules/Mol)
	339.52150 (Kcal/Mol)
Zero-point correction=	0.541062 (Hartree/Particle)
Thermal correction to Energy=	0.574822
Thermal correction to Enthalpy=	0.575766
Thermal correction to Gibbs Free Energy=	0.474428
Sum of electronic and zero-point Energies=	-1850.356508
Sum of electronic and thermal Energies=	-1850.322748
Sum of electronic and thermal Enthalpies=	-1850.321804
Sum of electronic and thermal Free Energies=	-1850.423142

cartesian

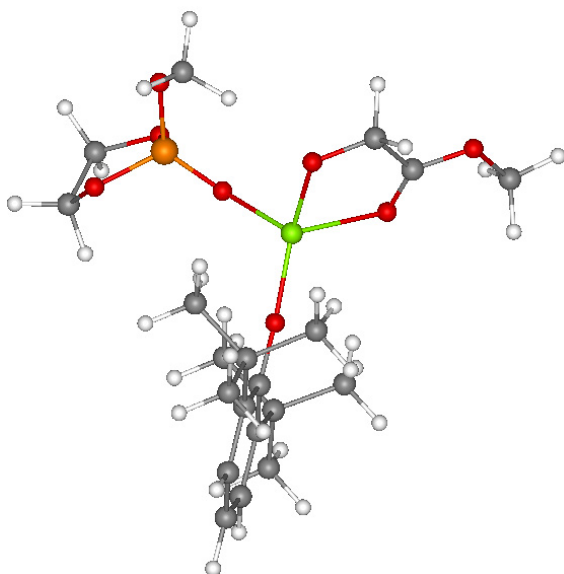
12	-0.82712018	-0.52483433	-0.12570775	6	1.00867987	2.44736576	-1.69270778
8	0.90737987	0.03986563	0.16659226	1	1.73237991	2.30936575	-2.50420761
6	2.19807982	0.31486562	0.32029223	1	0.33547986	3.26646566	-1.97400773
6	3.10417986	-0.69573432	0.77389228	1	0.41657984	1.53506565	-1.60800779
6	4.46047974	-0.37283438	0.88329220	8	-2.24922013	0.90076566	0.21809226
1	5.16868019	-1.12333441	1.21829224	15	-3.63132024	0.43446562	0.57169223
6	4.94517994	0.89376563	0.57639229	8	-4.42172050	1.75716555	1.11119223
6	4.05268002	1.87866557	0.16669226	8	-3.96072006	-0.51353437	1.81729221
1	4.44627953	2.86606574	-0.05050775	6	-5.37582016	1.36716557	2.10669231
6	2.68287992	1.63126564	0.03669225	6	-4.72092056	0.19056562	2.82619238
6	2.62107992	-2.11073422	1.14579225	8	-4.53742027	-0.09903437	-0.63090777
6	1.73197985	2.77336574	-0.37100774	6	-4.61641979	0.70786566	-1.82190776
6	2.04117990	-2.82663417	-0.09020776	1	-5.04331970	1.68806565	-1.59320784

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1	1.22017980	-2.26903439	-0.54280770	1	-3.62812018	0.83106565	-2.27150774
1	1.67097974	-3.82383418	0.17849225	1	-5.27171993	0.16926563	-2.50570774
1	2.81587982	-2.94953418	-0.85540771	8	-0.86182016	-1.46053445	-2.04130769
6	1.58017981	-2.04613423	2.28219223	6	-2.06102014	-2.25113440	-2.19040775
1	0.72517991	-1.41943443	2.02459240	6	-2.45422006	-2.73823428	-0.78950775
1	2.03267980	-1.62543440	3.18669224	8	-2.28452015	-1.73943436	0.15759225
1	1.20927989	-3.04933429	2.52439237	1	6.00607967	1.11456561	0.66679227
6	3.76417994	-3.00333428	1.66379225	1	-6.31542015	1.07596564	1.62449217
1	4.23427963	-2.59273434	2.56359243	1	-5.54901981	2.22116566	2.76269245
1	4.54298019	-3.16363430	0.91059220	1	-5.44072056	-0.51463437	3.24289227
1	3.36007977	-3.98753428	1.92709219	1	-4.02742004	0.52026564	3.60399222
6	2.47757983	4.09996557	-0.60370779	1	-3.49962020	-3.08643436	-0.84280777
1	3.20967984	4.03046560	-1.41570783	1	-1.83832014	-3.62233424	-0.54780769
1	2.99407983	4.44776535	0.29699224	6	-0.18802014	-1.16703439	-3.26250768
1	1.75377989	4.87436533	-0.88220775	1	-0.83442014	-0.58783436	-3.93340755
6	0.70807981	3.03286576	0.75269222	1	0.11467987	-2.09573436	-3.75840759
1	0.11257985	2.14686561	0.97289228	1	0.69797981	-0.58453435	-3.01020765
1	0.02337986	3.84156561	0.46869224	1	-2.83642006	-1.61153436	-2.63210773
1	1.22407985	3.33346581	1.67119217	1	-1.85622013	-3.08573437	-2.87350774

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C'-1



Zero-point vibrational energy	1371280.9 (Joules/Mol)
	327.74401 (Kcal/Mol)
Zero-point correction=	0.522293 (Hartree/Particle)
Thermal correction to Energy=	0.557681
Thermal correction to Enthalpy=	0.558625
Thermal correction to Gibbs Free Energy=	0.449985
Sum of electronic and zero-point Energies=	-1924.419011
Sum of electronic and thermal Energies=	-1924.383623
Sum of electronic and thermal Enthalpies=	-1924.382679
Sum of electronic and thermal Free Energies=	-1924.491319

				cartesian			
12	0.95337784	1.01977611	0.08110947	6	-1.32762218	-0.05912380	-3.01749063
8	-0.71702218	0.22107621	-0.06109053	1	-2.25912213	0.42477620	-3.33179045
6	-1.92722225	-0.31012380	0.05020947	1	-0.72492218	-0.24612379	-3.91569042
6	-2.71762228	-0.08152380	1.22180951	1	-0.78722215	0.63847619	-2.37739062
6	-3.98712230	-0.66262376	1.29520953	8	2.34727788	-0.44542378	0.02750947
1	-4.60402250	-0.50162381	2.17340946	15	3.40797782	-1.37242389	0.49570948
6	-4.49892235	-1.45082390	0.26990947	8	4.22387791	-2.08102393	-0.68489051
6	-3.72612214	-1.66752386	-0.86639053	8	2.88317776	-2.69522381	1.24540949
1	-4.14192247	-2.28242373	-1.65799057	6	4.26897764	-3.51142383	-0.48329049
6	-2.44862223	-1.11832380	-1.01039052	6	3.05157781	-3.84122396	0.38350949
6	-2.20002222	0.78617620	2.38330936	8	4.49147749	-0.70972377	1.42270947
6	-1.63442206	-1.38402390	-2.29009056	6	4.17917776	0.37517622	2.34850955
6	-1.93882227	2.22787619	1.90020943	1	3.47707772	1.08797610	1.90290952

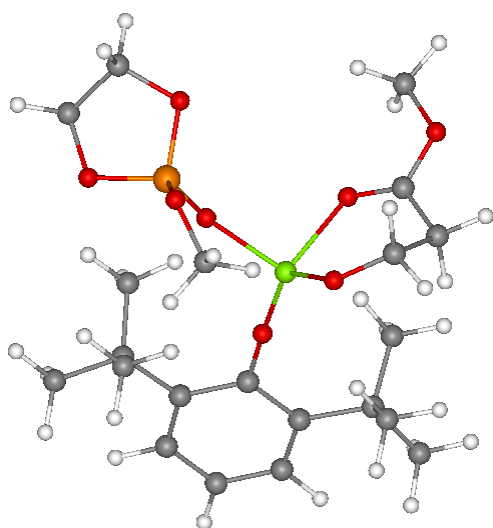
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1	-1.24262214	2.26267624	1.06140947	1	3.76917791	-0.05642380	3.26370955
1	-1.52522218	2.83937621	2.71090937	1	5.13517761	0.85247624	2.55820942
1	-2.87642217	2.68757606	1.56880951	8	1.30017781	2.42647624	-1.46339047
6	-0.92792213	0.16177621	2.99430943	6	1.79807782	3.44617605	-0.96959054
1	-0.16442218	-0.03862379	2.24060941	8	1.84797788	2.35377622	1.15050948
1	-1.16842222	-0.79602379	3.46890950	6	2.13547778	3.52767611	0.51130944
1	-0.49672219	0.82257622	3.75540948	1	3.20327783	3.81847620	0.56440949
6	-3.21562219	0.89777619	3.53460956	1	1.57957780	4.40187597	0.90250945
1	-3.45372224	-0.07652380	3.97470951	1	-5.49052238	-1.88932383	0.35420948
1	-4.15122223	1.37007618	3.21660948	1	5.20967770	-3.75822377	0.01590947
1	-2.79072213	1.52017617	4.33030939	1	4.23017788	-3.98482370	-1.46429050
6	-2.39052224	-2.27192378	-3.29389048	1	3.20817780	-4.71362400	1.01790941
1	-3.32582211	-1.81252384	-3.63109064	1	2.14337778	-3.96832395	-0.21109053
1	-2.62202215	-3.26062393	-2.88269043	8	2.06367779	4.52537632	-1.68829048
1	-1.76542211	-2.42582393	-4.18119049	6	1.72557783	4.46607637	-3.08979058
6	-0.32572219	-2.12532377	-1.94619048	1	2.00427771	5.43747616	-3.49389052
1	0.27597779	-1.56382382	-1.23099053	1	0.65607780	4.28847599	-3.21219063
1	0.27017778	-2.28872395	-2.85399055	1	2.28677773	3.66857624	-3.57949042
1	-0.55302215	-3.10482383	-1.50819051				

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C'-2



Zero-point vibrational energy	1448068.8 (Joules/Mol)
	346.09676 (Kcal/Mol)
Zero-point correction=	0.551540 (Hartree/Particle)
Thermal correction to Energy=	0.587921
Thermal correction to Enthalpy=	0.588865
Thermal correction to Gibbs Free Energy=	0.478806
Sum of electronic and zero-point Energies=	-1963.690797
Sum of electronic and thermal Energies=	-1963.654416
Sum of electronic and thermal Enthalpies=	-1963.653472
Sum of electronic and thermal Free Energies=	-1963.763532

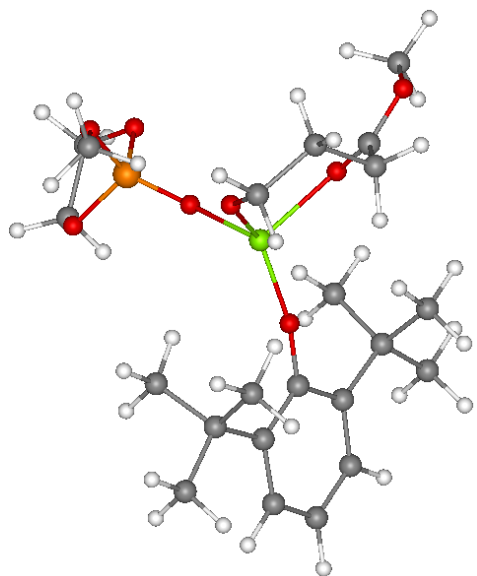
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12	-0.61008501	0.77039701	-0.38861513	1	0.45031503	-2.81880283	2.39058471
8	0.95701504	-0.18490300	-0.07701513	1	-1.02378500	-3.16400290	1.46448493
6	2.10331488	-0.84400296	0.03688487	1	-0.29088497	-1.54880309	1.40808487
6	3.35081482	-0.14150298	-0.00761513	8	-2.25998497	-0.38250297	-0.09561513
6	4.53591537	-0.87140298	0.12498486	15	-3.66198516	-0.80000299	-0.34241512
1	5.49111509	-0.35800299	0.09378487	8	-4.72848463	-0.12240299	0.65168488
6	4.54001522	-2.25120282	0.29678488	8	-3.99128509	-2.33830285	-0.00321513
6	3.32631493	-2.92860293	0.33578485	6	-5.61078501	-1.12110305	1.20528495
1	3.34581494	-4.00530338	0.46798486	6	-4.80938482	-2.42370296	1.18028498
6	2.10191488	-2.26630282	0.20918487	8	-4.19038486	-0.55760300	-1.80181503
6	3.41241503	1.38509691	-0.19901514	6	-3.32038498	-0.27120298	-2.94061518
6	0.79001498	-3.07080293	0.25488487	1	-2.60798502	0.52199697	-2.69011521
6	2.69431496	2.09709716	0.96508485	1	-2.80948520	-1.18930304	-3.23641515
1	1.66391504	1.75779700	1.07558489	1	-3.99698520	0.04889701	-3.73161530

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1	2.69611502	3.18449712	0.81108487	8	-0.97068501	2.29609704	0.99308485
1	3.21101499	1.89399695	1.90998495	6	-1.07528496	3.47579718	0.63158488
6	2.79451489	1.78059697	-1.55541503	6	-0.67058498	3.98369718	-0.71131516
1	1.75631511	1.46049690	-1.65411508	8	-1.16188502	1.85999691	-1.85011506
1	3.35751486	1.32119691	-2.37541509	6	-1.39698493	3.21269703	-1.85741508
1	2.83561492	2.86929703	-1.69391513	1	-2.47648501	3.45309711	-1.78311503
6	4.85551500	1.92089701	-0.20991513	1	-1.04368496	3.68829703	-2.78941512
1	5.44681501	1.50489700	-1.03251505	1	5.47801495	-2.79210281	0.39738485
1	5.38161516	1.71939695	0.72938484	1	-6.50748491	-1.17770302	0.58198488
1	4.83351517	3.00859714	-0.34341514	1	-5.87738466	-0.80690300	2.21448469
6	1.02881503	-4.58010340	0.44058487	1	-5.44018507	-3.30770302	1.08648491
1	1.53871500	-4.80750322	1.38278496	1	-4.15698481	-2.52150297	2.05228472
1	1.61141503	-5.01220322	-0.38001513	1	-0.85928500	5.05839682	-0.77371514
1	0.06181502	-5.09640312	0.45988485	1	0.40421501	3.80489707	-0.82121515
6	0.02441502	-2.91520286	-1.07471502	8	-1.59478498	4.39449692	1.43938494
1	-0.16548499	-1.86750305	-1.30911505	6	-2.01338506	3.93979716	2.74158478
1	-0.93698502	-3.44270301	-1.03061509	1	-2.38518500	4.82829666	3.24868488
1	0.60811508	-3.34070301	-1.89851511	1	-1.16778493	3.51129699	3.28188491
6	-0.07288498	-2.61570287	1.44938493	1	-2.80198503	3.19169712	2.64478469

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C'-3



Zero-point vibrational energy	1522570.6 (Joules/Mol)
	363.90311 (Kcal/Mol)
Zero-point correction=	0.579917 (Hartree/Particle)
Thermal correction to Energy=	0.617900
Thermal correction to Enthalpy=	0.618844
Thermal correction to Gibbs Free Energy=	0.502738
Sum of electronic and zero-point Energies=	-2002.962762
Sum of electronic and thermal Energies=	-2002.924779
Sum of electronic and thermal Enthalpies=	-2002.923834
Sum of electronic and thermal Free Energies=	-2003.039941

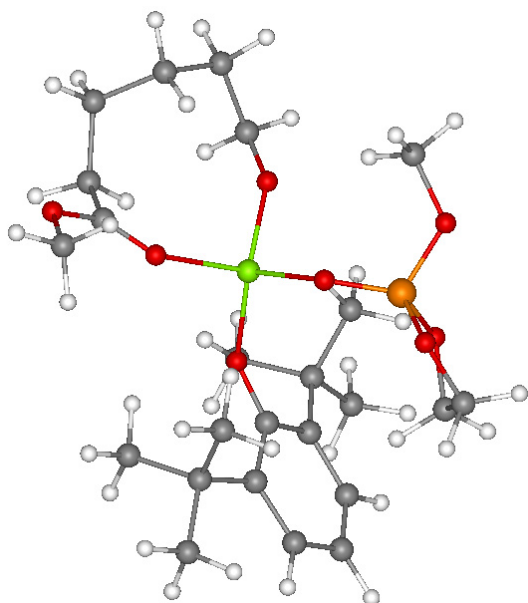
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8	-0.95807791	0.14976227	0.05984639	8	2.00592208	-0.96113771	-0.37625360
6	-2.18627787	-0.31873772	-0.11105361	15	3.06322193	-1.99633765	-0.47535360
6	-2.84767795	-1.03503776	0.93874639	8	3.78922200	-2.05373788	-1.90305364
6	-4.14167786	-1.51283765	0.71034640	8	2.53322196	-3.51613760	-0.42355362
1	-4.66117811	-2.05753779	1.49184644	6	3.83222198	-3.41163778	-2.39285374
6	-4.80187798	-1.31243765	-0.49725360	6	2.65162206	-4.12183809	-1.72715366
6	-4.15787792	-0.60903770	-1.50995362	8	4.22542191	-1.86983764	0.57534641
1	-4.68987799	-0.45643774	-2.44355345	6	3.99972200	-1.43733776	1.95374644
6	-2.86557794	-0.10003772	-1.35355365	1	3.30482197	-0.58963770	1.99284637
6	-2.16737795	-1.28513765	2.29714632	1	3.62092209	-2.28723764	2.52524662
6	-2.20447803	0.68586230	-2.50045347	1	4.98432207	-1.15123773	2.32104635
6	-1.80847788	0.05086228	2.97914648	8	1.45352209	2.16206241	-0.63955361
1	-1.14787793	0.66126227	2.36344624	6	1.73702204	3.26656222	-0.17215361

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1	-1.30867791	-0.13013773	3.93834639	6	1.34702206	3.78306222	1.18364644
1	-2.71777797	0.63066232	3.17324638	8	1.80642200	0.90226233	2.00434637
6	-0.91427791	-2.16473770	2.11094618	6	2.26812196	3.28006220	2.32304621
1	-0.22827795	-1.75073767	1.37034643	6	1.83362210	1.93426228	2.92194653
1	-1.20097792	-3.16313767	1.76254642	1	2.26162195	4.04056215	3.11384630
1	-0.37247798	-2.27603769	3.05824661	1	3.30112195	3.20996237	1.96224630
6	-3.07907796	-2.03773785	3.28364658	1	2.53482199	1.71116233	3.74844646
1	-3.36167789	-3.03043771	2.91724634	1	0.84812200	2.08806229	3.40454626
1	-3.99427795	-1.47973776	3.50844622	1	-5.80887794	-1.69533765	-0.64575362
1	-2.54367805	-2.18093777	4.22934628	1	4.79162216	-3.85183764	-2.10775375
6	-3.11997795	0.81466228	-3.73085356	1	3.74602199	-3.37463760	-3.47885370
1	-4.04857779	1.34876227	-3.50285339	1	2.82572198	-5.18843794	-1.58485365
1	-3.37967801	-0.15923773	-4.16005325	1	1.71672201	-3.96563768	-2.27215338
1	-2.59887791	1.38446236	-4.50905371	1	1.37052202	4.87396193	1.13504636
6	-0.92647791	-0.03233773	-2.97925377	1	0.31482202	3.47246242	1.37664640
1	-0.21477798	-0.17693773	-2.16615343	8	2.45302200	4.14076185	-0.87275362
1	-0.43507800	0.54436231	-3.77355337	6	2.89492202	3.70956230	-2.17555380
1	-1.17807794	-1.01873767	-3.38605356	1	3.45712209	4.54966211	-2.57925367
6	-1.88247800	2.12226224	-2.04055357	1	2.03592205	3.47866225	-2.80695343
1	-2.80577803	2.65246224	-1.78115356	1	3.52982211	2.82656240	-2.08575344
1	-1.38727796	2.68136239	-2.84545374				

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## C'-4



Zero-point vibrational energy	1675466.7 (Joules/Mol)
	400.44614 (Kcal/Mol)
Zero-point correction=	0.638152 (Hartree/Particle)
Thermal correction to Energy=	0.678321
Thermal correction to Enthalpy=	0.679265
Thermal correction to Gibbs Free Energy=	0.562395
Sum of electronic and zero-point Energies=	-2081.506397
Sum of electronic and thermal Energies=	-2081.466227
Sum of electronic and thermal Enthalpies=	-2081.465283
Sum of electronic and thermal Free Energies=	-2081.582154

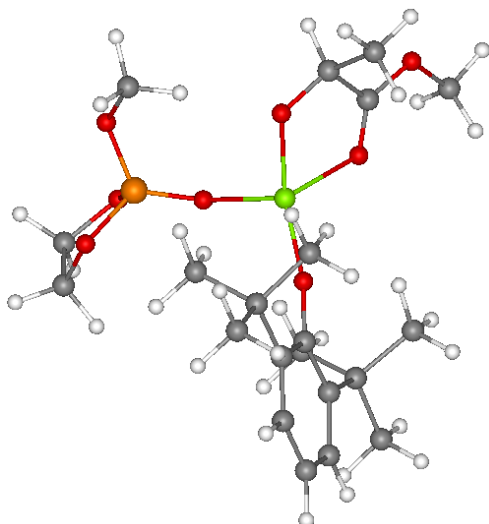
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12	0.94455230	0.32965460	0.11657868	8	-1.57894766	2.50255466	3.14487863
8	-0.50354767	-0.74524540	-0.47152132	8	-1.90934765	2.71715450	0.75417864
6	-1.82184768	-0.86094540	-0.54562134	6	-2.99434757	2.53295445	2.83897853
6	-2.54714775	-0.25854540	-1.62822127	6	-3.11154771	2.17435455	1.35447872
6	-3.94474769	-0.26484540	-1.57622123	8	0.00415234	4.01315451	1.79857874
1	-4.51494741	0.21635459	-2.36402130	6	1.40455234	4.16035461	1.41947877
6	-4.64774752	-0.88784546	-0.54832131	1	1.69465232	3.41545463	0.67317867
6	-3.93754768	-1.59164548	0.41987869	1	1.48655236	5.16815472	1.01427865
1	-4.49974728	-2.13834548	1.17017865	1	2.01555228	4.06355476	2.31837869
6	-2.53824759	-1.62564540	0.43727869	8	2.25045228	-1.02714539	1.01687872
6	-1.83134770	0.33625460	-2.85922146	6	3.30155230	-1.53484535	0.62227869
6	-1.81164765	-2.51184535	1.47027874	6	3.87695241	-1.39304543	-0.75752133
6	-0.87384766	-0.71274543	-3.46142149	8	2.11715221	1.51815462	-0.72882134

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1	-0.13864766	-1.04764533	-2.72842145	6	4.43495274	1.92635465	-1.33252132
1	-0.34254766	-0.28964537	-4.32292128	6	2.98975229	1.67545462	-1.79122126
1	-1.43384767	-1.58864546	-3.80742121	1	5.09025240	1.96255469	-2.21532130
6	-1.05714762	1.62395453	-2.51952147	1	4.47885275	2.92255449	-0.87292129
1	-0.19864766	1.44735456	-1.86962116	1	2.69475222	2.53145456	-2.42592144
1	-1.70894766	2.35735464	-2.03442144	1	2.98425221	0.80485457	-2.47792149
1	-0.66464770	2.07785463	-3.43802142	1	-5.73514748	-0.87344545	-0.53472131
6	-2.82684779	0.71235460	-3.97312117	1	-3.36184764	3.53985453	3.05327868
1	-3.49084759	1.53385448	-3.68162131	1	-3.48884773	1.80735469	3.48487854
1	-3.44444776	-0.13774541	-4.28212118	1	-3.96164775	2.65155458	0.86867869
1	-2.26814771	1.04975462	-4.85322142	1	-3.14064765	1.09645462	1.17667866
6	-2.78604770	-3.42844558	2.23287868	1	4.12345266	-2.39824557	-1.11662126
1	-3.36814761	-4.06334543	1.55687869	1	3.10325241	-0.97894543	-1.40292132
1	-3.48344779	-2.86904550	2.86617851	8	4.04815245	-2.28104544	1.42707872
1	-2.21374774	-4.08864546	2.89467859	6	3.56985235	-2.44854546	2.77747869
6	-1.08704770	-1.66174531	2.52957869	1	4.30565262	-3.08564544	3.26437855
1	-0.34484768	-0.99794537	2.08957863	1	2.58795238	-2.92334557	2.77187872
1	-0.57584769	-2.30814552	3.25477862	1	3.50525236	-1.48044538	3.27657866
1	-1.80124772	-1.04334545	3.08567858	6	4.99325275	0.92775458	-0.31212133
6	-0.80884767	-3.44084549	0.75517869	1	4.36585236	0.96595460	0.58677870
1	-1.33444762	-4.10514545	0.06027868	1	5.98445272	1.28185463	-0.00242132
1	-0.28614765	-4.06924534	1.48817873	6	5.15275240	-0.52574539	-0.78252131
1	-0.07224766	-2.87074542	0.18867868	1	5.90655279	-1.02744532	-0.16572131
8	0.24675234	1.47625470	1.62967873	1	5.53695250	-0.54374540	-1.80932128
15	-0.70754766	2.60875463	1.80387878				

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C'-6



Zero-point vibrational energy	1445407.7 (Joules/Mol)
	345.46072 (Kcal/Mol)
Zero-point correction=	0.550527 (Hartree/Particle)
Thermal correction to Energy=	0.587345
Thermal correction to Enthalpy=	0.588289
Thermal correction to Gibbs Free Energy=	0.477538
Sum of electronic and zero-point Energies=	-1963.697205
Sum of electronic and thermal Energies=	-1963.660387
Sum of electronic and thermal Enthalpies=	-1963.659442
Sum of electronic and thermal Free Energies=	-1963.770193

cartesian

12	1.05648315	-0.60828030	-0.16570458	1	-2.53181672	-2.44498038	2.32309556
8	-0.77891690	-0.36518031	-0.02400457	1	-1.19201684	-2.08588052	3.42799544
6	-2.04201674	0.03871967	-0.01960457	1	-0.96061689	-1.96218026	1.67199540
6	-2.69141674	0.40411967	-1.24240458	8	1.99138308	1.10091960	0.39279544
6	-4.01891708	0.83951968	-1.18910456	15	2.73898315	2.37461948	0.24139541
1	-4.53001690	1.12381971	-2.10300446	8	3.30708313	2.96521950	1.61659539
6	-4.72311687	0.91981971	0.00769543	8	1.85758305	3.64171958	-0.21110457
6	-4.09171724	0.54561967	1.18929541	6	2.94268322	4.35631943	1.75969541
1	-4.65841722	0.60231966	2.11269546	6	1.68568325	4.53891945	0.90659541
6	-2.76681685	0.10081967	1.21389544	8	3.97458315	2.29481959	-0.72830462
6	-1.96441674	0.31781965	-2.59740448	6	3.99578309	1.43771970	-1.90970457
6	-2.12001681	-0.31768036	2.54749560	1	3.49618316	0.48201966	-1.71760464
6	-1.50531697	-1.12888026	-2.87170458	1	3.51548314	1.97051966	-2.73260450
1	-0.84511691	-1.50638032	-2.09090447	1	5.05108309	1.28441966	-2.13070440
1	-0.97231680	-1.18858027	-3.82830453	8	1.80958319	-2.18528032	1.01159549

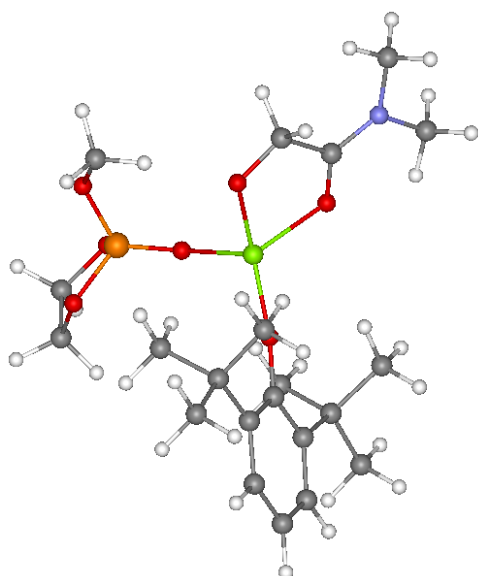
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1	-2.37381673	-1.79468036	-2.92550445	6	2.59138322	-2.86248040	0.33109543
6	-0.76871687	1.29121971	-2.62840438	8	2.28008318	-1.33668029	-1.46290457
1	-0.09341687	1.13391960	-1.78550458	6	2.89548326	-2.51588035	-1.12770462
1	-1.11881685	2.32771945	-2.57130456	1	4.00098324	-2.44078040	-1.17350459
1	-0.19711685	1.17411971	-3.55710459	6	2.48138309	-3.68898034	-2.03440452
6	-2.87121677	0.71241969	-3.77760458	1	-5.75551701	1.26141965	0.01809543
1	-3.22511673	1.74651968	-3.70540452	1	3.77538323	4.96821976	1.40279543
1	-3.74291682	0.05531967	-3.86500454	1	2.76658320	4.54461956	2.81869555
1	-2.30391669	0.62701964	-4.71160460	1	1.58688307	5.54911947	0.50939542
6	-3.09631681	-0.21098034	3.73269558	1	0.77638316	4.25821972	1.44429541
1	-3.97161698	-0.85698032	3.60639548	8	3.21478319	-3.92028046	0.82609540
1	-3.44571686	0.81461966	3.89409542	6	2.92448330	-4.25598049	2.19889545
1	-2.58621669	-0.52878034	4.64939547	1	3.51418328	-5.14658022	2.40809560
6	-0.92671686	0.60191965	2.87809563	1	1.85958314	-4.45958042	2.32019544
1	-0.18541688	0.60721970	2.07819557	1	3.21658325	-3.43588042	2.85699558
1	-0.43531686	0.27851969	3.80459547	1	2.71938324	-3.41628051	-3.06520438
1	-1.27191687	1.63271964	3.02199554	1	1.40108323	-3.85248041	-1.97250450
6	-1.66751671	-1.79098034	2.48379540	1	3.00308323	-4.61708021	-1.78090465

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C'-7



Zero-point vibrational energy	1477772.0 (Joules/Mol)
	353.19599 (Kcal/Mol)
Zero-point correction=	0.562854 (Hartree/Particle)
Thermal correction to Energy=	0.600026
Thermal correction to Enthalpy=	0.600971
Thermal correction to Gibbs Free Energy=	0.488800
Sum of electronic and zero-point Energies=	-1943.817729
Sum of electronic and thermal Energies=	-1943.780557
Sum of electronic and thermal Enthalpies=	-1943.779613
Sum of electronic and thermal Free Energies=	-1943.891783

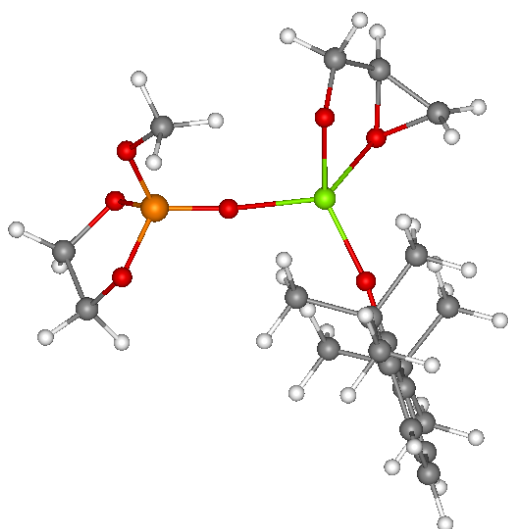
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12	1.05690014	-0.22129110	-0.23166573	1	-0.69249988	-2.12499118	3.38373423
8	-0.79279995	-0.36809108	-0.07796572	1	-0.51939988	-1.96439123	1.62453437
6	-2.11659980	-0.33499113	-0.06846572	8	1.57060003	1.63930893	0.40833429
6	-2.84709978	-0.15869111	-1.28806567	15	1.90230012	3.08010888	0.27993429
6	-4.24340010	-0.12069109	-1.23136568	8	2.27370024	3.79200888	1.66533434
1	-4.81629992	0.01300889	-2.14326572	8	0.68400013	4.03740883	-0.15476573
6	-4.93870020	-0.25349107	-0.03376572	6	1.50170004	5.00120926	1.83763433
6	-4.22370005	-0.43519112	1.14573431	6	0.24750012	4.81180906	0.98163426
1	-4.78130007	-0.54549110	2.07023430	8	3.10390019	3.38810897	-0.68826574
6	-2.82679987	-0.48219112	1.16693437	6	3.36390018	2.60150886	-1.88976562
6	-2.12739968	-0.02129111	-2.64256573	1	3.12280011	1.54400885	-1.73656571
6	-2.08269978	-0.69369113	2.49843431	1	2.77340031	3.01800895	-2.70806575
6	-1.29459989	-1.28559113	-2.93936563	1	4.42609978	2.73210883	-2.09226561

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1	-0.55859983	-1.48599112	-2.16056561	8	2.14460015	-1.67389119	0.73293430
1	-0.76119983	-1.17989111	-3.89186573	6	3.04010010	-2.15499115	-0.00676572
1	-1.95130002	-2.15969110	-3.01236558	8	2.35500026	-0.51789105	-1.63136566
6	-1.23689997	1.23820889	-2.65136576	6	3.22760010	-1.54319108	-1.40976560
1	-0.53689992	1.24640894	-1.81446564	1	4.28870010	-1.22479117	-1.47996569
1	-1.85299981	2.14050889	-2.56816554	1	3.11540031	-2.36999106	-2.14046574
1	-0.66299987	1.30060887	-3.58396578	1	-6.02570009	-0.22229108	-0.02076572
6	-3.10869980	0.13570890	-3.81786561	1	2.10740018	5.84600925	1.49943435
1	-3.72989988	1.03310895	-3.72526574	1	1.27790010	5.10220909	2.89963436
1	-3.76949978	-0.73139107	-3.92306566	1	-0.15539989	5.75290918	0.60753429
1	-2.54069972	0.22780889	-4.75086594	1	-0.53189993	4.25440884	1.50773430
6	-3.04279971	-0.84899116	3.69083428	7	3.80460024	-3.17639112	0.42233428
1	-3.70249987	-1.71639109	3.58123446	6	3.59690022	-3.75859094	1.74093437
1	-3.66519976	0.03960890	3.84303427	1	3.35130024	-4.82219076	1.64703429
1	-2.45839977	-0.99779117	4.60633421	1	2.77720022	-3.24169111	2.23523426
6	-1.18979990	0.52440894	2.81173444	1	4.50680017	-3.66089106	2.34333444
1	-0.48409989	0.72730887	2.00553417	6	4.84480000	-3.79239106	-0.38346571
1	-0.62289989	0.35990891	3.73703432	1	4.59480000	-4.83899069	-0.59116572
1	-1.80910003	1.41880882	2.95093441	1	5.79860020	-3.76569104	0.15493429
6	-1.23959994	-1.98429108	2.44253445	1	4.97219992	-3.27409124	-1.33106565
1	-1.89029992	-2.85409117	2.29803443				

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## C'-Gly



Zero-point vibrational energy	1360311.6 (Joules/Mol)
	325.12228 (Kcal/Mol)
Zero-point correction=	0.518115 (Hartree/Particle)
Thermal correction to Energy=	0.551763
Thermal correction to Enthalpy=	0.552707
Thermal correction to Gibbs Free Energy=	0.448582
Sum of electronic and zero-point Energies=	-1849.155567
Sum of electronic and thermal Energies=	-1849.121920
Sum of electronic and thermal Enthalpies=	-1849.120975
Sum of electronic and thermal Free Energies=	-1849.225101

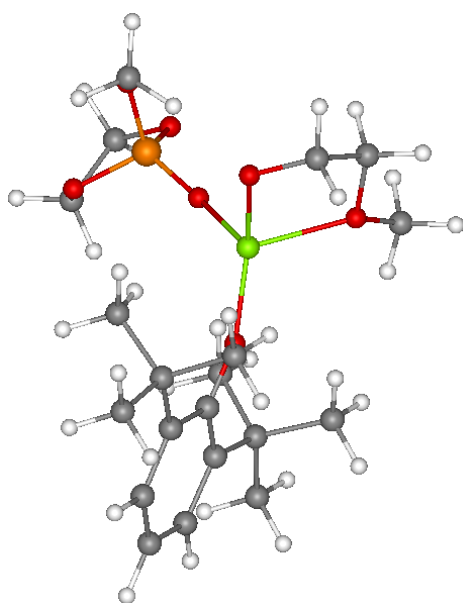
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8	-2.37494993	-0.31237260	0.30758381	6	0.27404997	0.84182745	-2.68811631		
15	-3.51495004	-0.92117256	-0.42511621	1	-0.31775001	0.52172744	-1.82851624		
8	-4.41774988	-1.89557254	0.46688381	1	0.33124998	-0.01147257	-3.37291622		
8	-3.10634995	-1.96667254	-1.57671618	1	-0.26075000	1.65352750	-3.19601631		
6	-4.62055016	-3.15667272	-0.20991619	6	2.43974996	1.59772742	-3.58631611		
6	-3.42545009	-3.30947256	-1.15301621	1	2.50574994	0.72272748	-4.24161625		
8	-4.51205015	0.11362743	-1.06301618	1	3.45365000	1.96962750	-3.40481615		
6	-4.07625008	1.39382744	-1.61431623	1	1.90074992	2.37732744	-4.13671637		
1	-3.34905005	1.88172746	-0.95571619	6	2.91415000	-2.80317259	2.55838370		
1	-3.65234995	1.22222745	-2.60561609	1	3.93245006	-2.44267273	2.73888373		
1	-4.98375034	1.98972738	-1.69581616	1	2.97315001	-3.70517278	1.93968379		
1	-5.56945038	-3.10837269	-0.75051618	1	2.49745011	-3.09987259	3.52778387		
1	-4.66235018	-3.93637276	0.55058378	6	0.61415005	-2.34827256	1.78258383		
1	-3.66054988	-3.89217257	-2.04361629	1	-0.09415001	-1.65207255	1.33168375		

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1	-2.55314994	-3.73297262	-0.64841622	1	0.22354999	-2.65517259	2.76118374
12	-0.91825002	1.03972745	0.66658378	1	0.66455007	-3.23807263	1.14418375
8	0.75444996	0.32332742	0.31008381	6	1.97904992	-0.54797256	2.93188381
6	1.85864997	-0.22637257	-0.18021619	1	2.98804998	-0.14997257	3.08708382
6	2.38024998	0.19632743	-1.44451618	1	1.59375000	-0.88177258	3.90368390
6	3.54835010	-0.40767258	-1.91981626	1	1.34794998	0.26402742	2.57068372
1	3.96485019	-0.10217257	-2.87401628	8	-1.06834996	1.65862739	2.71278381
6	4.21084976	-1.39917254	-1.20421624	8	-1.75405002	2.73302722	0.32398379
6	3.69935012	-1.80287254	0.02468381	6	-1.77055001	2.94622731	2.72858381
1	4.23144960	-2.57477260	0.57098377	6	-2.40584993	3.31622744	1.38978374
6	2.53695011	-1.24407256	0.56398380	1	-3.47265005	3.01962733	1.45418382
6	1.69024992	1.29372740	-2.27631617	1	-2.40365005	4.42152739	1.33278382
6	2.01585007	-1.72167253	1.93218374	1	5.11844969	-1.85037255	-1.59841621
6	1.64115000	2.62022734	-1.49121618	6	-0.31735000	2.89292741	2.89718390
1	1.09105003	2.52812743	-0.55451620	1	-2.37465000	3.06542730	3.62728381
1	1.15904999	3.40372729	-2.08781624	1	0.12504998	2.97872734	3.88608384
1	2.65755010	2.95192742	-1.25211620	1	0.31995001	3.15752745	2.05608368

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### C'-OCH<sub>2</sub>CH<sub>2</sub>OMe



Zero-point vibrational energy 1421264.8 (Joules/Mol)

339.69044 (Kcal/Mol)

Zero-point correction= 0.541331 (Hartree/Particle)

Thermal correction to Energy= 0.575964

Thermal correction to Enthalpy= 0.576908

Thermal correction to Gibbs Free Energy= 0.470850

Sum of electronic and zero-point Energies= -1850.365455

Sum of electronic and thermal Energies= -1850.330822

Sum of electronic and thermal Enthalpies= -1850.329878

Sum of electronic and thermal Free Energies= -1850.435936

cartesian

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12	-0.80729079	-1.08950472	-0.50309372	6	1.66920912	1.70179534	-2.53529382
8	0.80810928	-0.16630471	-0.32079375	1	2.67180920	1.53859532	-2.94549370
6	1.95310915	0.24839529	0.21110627	1	1.10400927	2.30429530	-3.25899363
6	2.67190909	-0.56980473	1.14090633	1	1.19050920	0.72729528	-2.42839384
6	3.87000918	-0.08450472	1.67370629	8	-2.26899076	0.18949528	0.09830626
1	4.43030930	-0.69000471	2.37870622	15	-3.38809085	0.70859528	0.92480630
6	4.38070917	1.16199529	1.32810628	8	-4.28769064	1.80479527	0.17790626
6	3.68230891	1.94929528	0.41830623	8	-2.95169091	1.59449530	2.19520617
1	4.09720945	2.91649508	0.15380627	6	-4.44489050	2.98009515	1.00310624
6	2.48000908	1.52789533	-0.15639375	6	-3.23299098	2.98649526	1.93700624
6	2.15020919	-1.95670474	1.55450630	8	-4.39059067	-0.38400471	1.44340622
6	1.75750911	2.42539525	-1.17679369	6	-3.99309087	-1.76120472	1.73260629
6	2.03560901	-2.87720490	0.32010627	1	-3.28469086	-2.13680482	0.98520625

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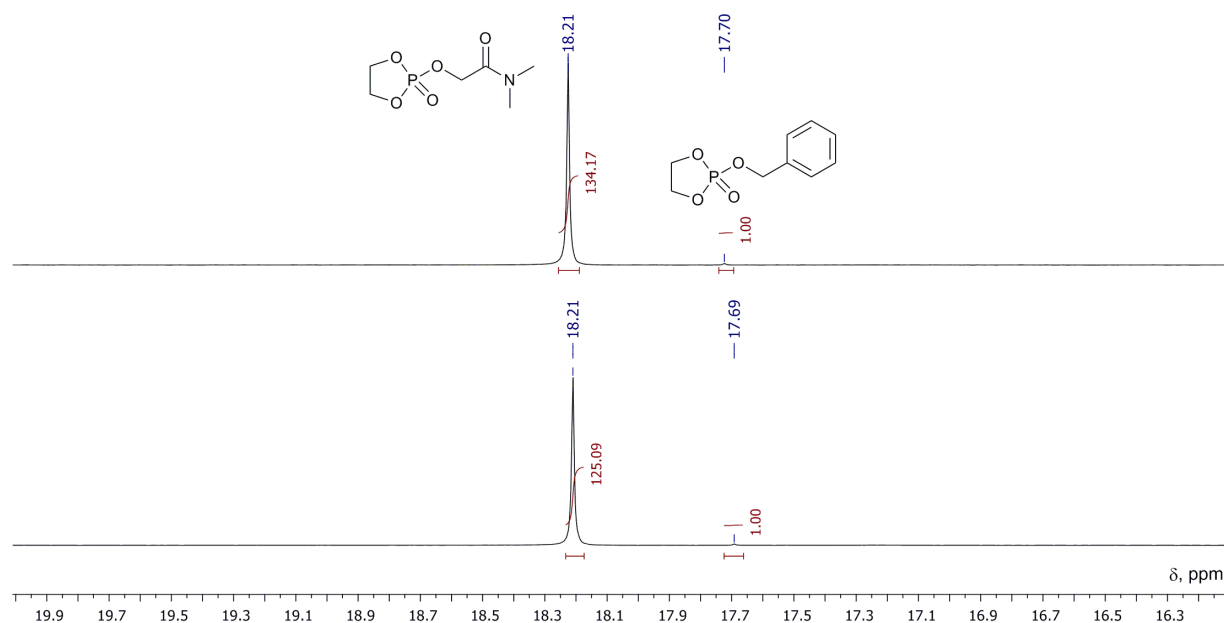
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1	1.45390928	-2.42930484	-0.48689371	1	-3.56199098	-1.79270470	2.73500633
1	1.57170928	-3.83310485	0.58840626	1	-4.92049074	-2.33150482	1.70850623
1	3.03360915	-3.08170485	-0.08299375	8	-1.26499081	-1.47710466	-2.55669379
6	0.80200922	-1.81580472	2.29490638	6	-2.11669087	-2.64550471	-2.60329366
1	0.10870919	-1.14640474	1.78010631	8	-1.65029073	-2.78750491	-0.24919374
1	0.96460927	-1.37920475	3.28650618	6	-1.72739077	-3.52980471	-1.41779375
1	0.31340918	-2.78800488	2.41960621	1	-2.48229098	-4.33500481	-1.35529375
6	3.09420919	-2.67980480	2.53230619	1	-0.76869082	-4.02620459	-1.66179371
1	3.22440910	-2.12840486	3.46940637	1	5.31510925	1.51379526	1.75900626
1	4.08300924	-2.85660481	2.09610629	1	-5.38699055	2.89249516	1.55080628
1	2.66940904	-3.65800476	2.78580618	1	-4.47499084	3.84699512	0.34300625
6	2.49630904	3.75129509	-1.42699373	1	-3.43779087	3.46719527	2.89360619
1	3.50280905	3.59679508	-1.82959378	1	-2.35509086	3.44009519	1.46970630
1	2.57900906	4.35819530	-0.51859373	1	-3.15879083	-2.30800486	-2.51769376
1	1.93900931	4.34089565	-2.16419363	1	-1.97479081	-3.14890480	-3.56899381
6	0.34860918	2.79459524	-0.66849375	6	-1.49339080	-0.56850469	-3.63049364
1	-0.25439081	1.90539527	-0.48349375	1	-2.53239083	-0.21700472	-3.62459373
1	-0.16839080	3.42679524	-1.40289378	1	-1.27739084	-1.05500472	-4.58819389
1	0.42400917	3.35839510	0.26900625	1	-0.81919080	0.27679527	-3.49519372

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#### S4. Reaction of **7** with **Mg1**

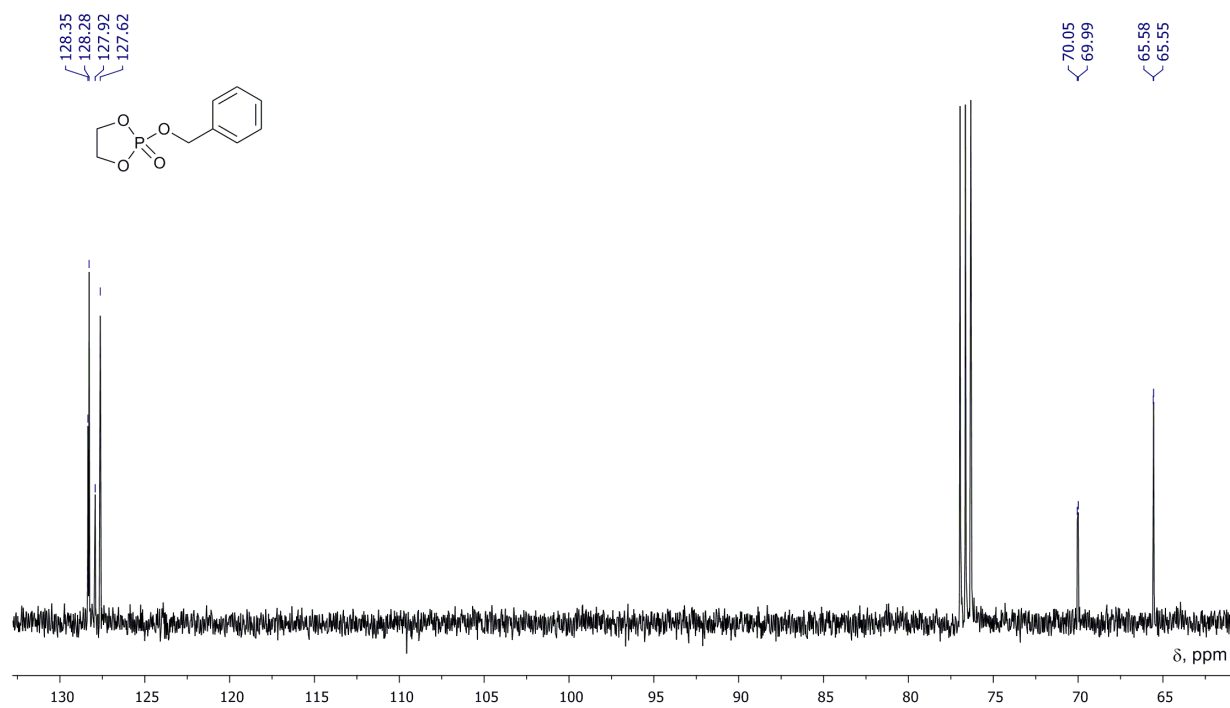
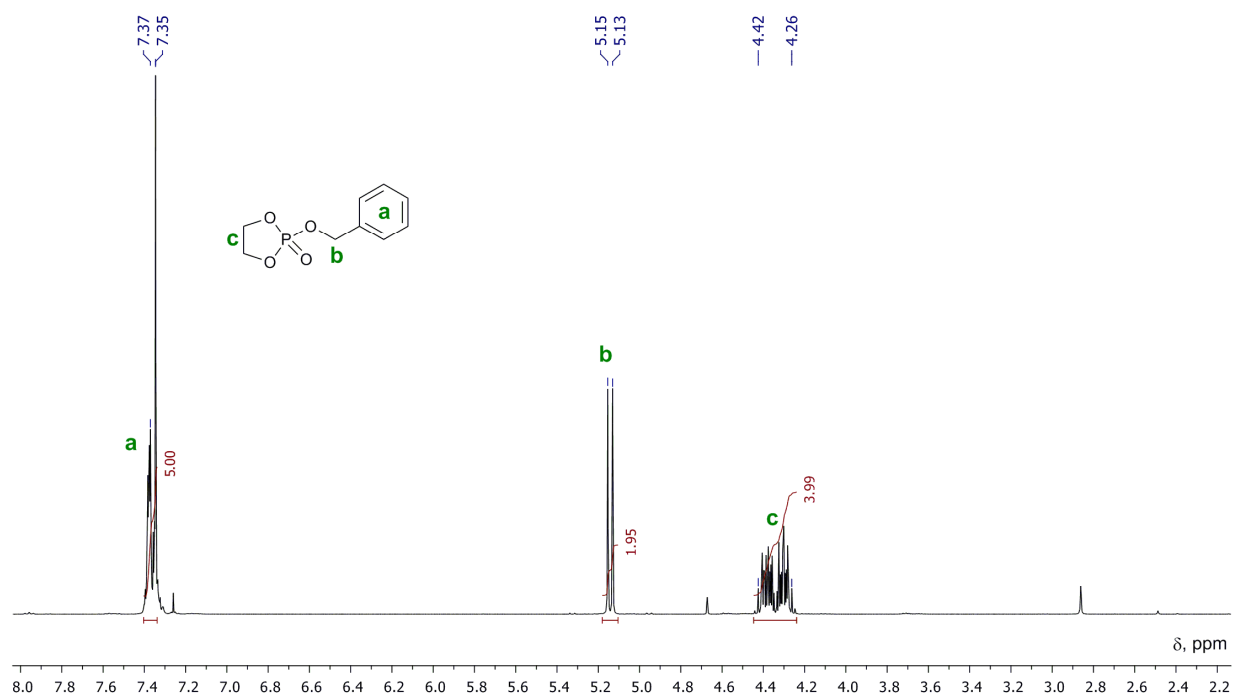
In the manuscript, we illustrated low reactivity of **7** in ROP by  $^{31}\text{P}$  NMR spectra of the reaction mixtures obtained when  $\sim 1:1$  and  $10:1$  **7**/[**Mg**] ratios were used. At  $100:1$  ratio, **7** remained inactive (Fig. S41)



**Fig. S41.** Fragments of  $^{31}\text{P}$  NMR spectra (162 MHz,  $\text{CDCl}_3$ ,  $20^\circ\text{C}$ ) of the reaction mixtures of **7** and **Mg1** after 5 (top), and 60 min (bottom), initial **7**/[**Mg**] ratio = 100.

The signal at 17.7 ppm should be evidently attributed to **BnOEP**, however, explicit interpretation of these results required oncoming synthesis of **BnOEP** to use this compound as an internal standard. Polymerization-grade **BnOEP** was prepared by the reaction of **CIEP** with **BnOH** using the method proposed by Iwasaki et al.<sup>56</sup> Polymerization-grade **BnOEP** was obtained without further purification (Figs. S42–S44).

To confirm the identity of the product of the reaction of **7** with **Mg1** and **BnOEP**, we conducted this reaction at [**7**]/[**Mg**] ratio of 30:1 (in  $\text{CH}_2\text{Cl}_2$ , 1 h at  $20^\circ\text{C}$ ), and then added **BnOEP** in [**BnOEP**]/[**Mg**] ratio of 3:1. NMR spectra of the reaction probe are presented in Figs. S38, S39. As can be seen,  $^1\text{H}$  NMR spectrum (Fig. S45) contains characteristic signals of all the expected reaction products. The ratio of the integral intensities of the signals in  $^{31}\text{P}$  NMR spectrum (Fig. S46) corresponds to the expected [**7**]/**BnOEP** ratio of  $\sim 7:1$  (one eq. of **BnOEP** formed, three eqs. of **BnOEP** added).





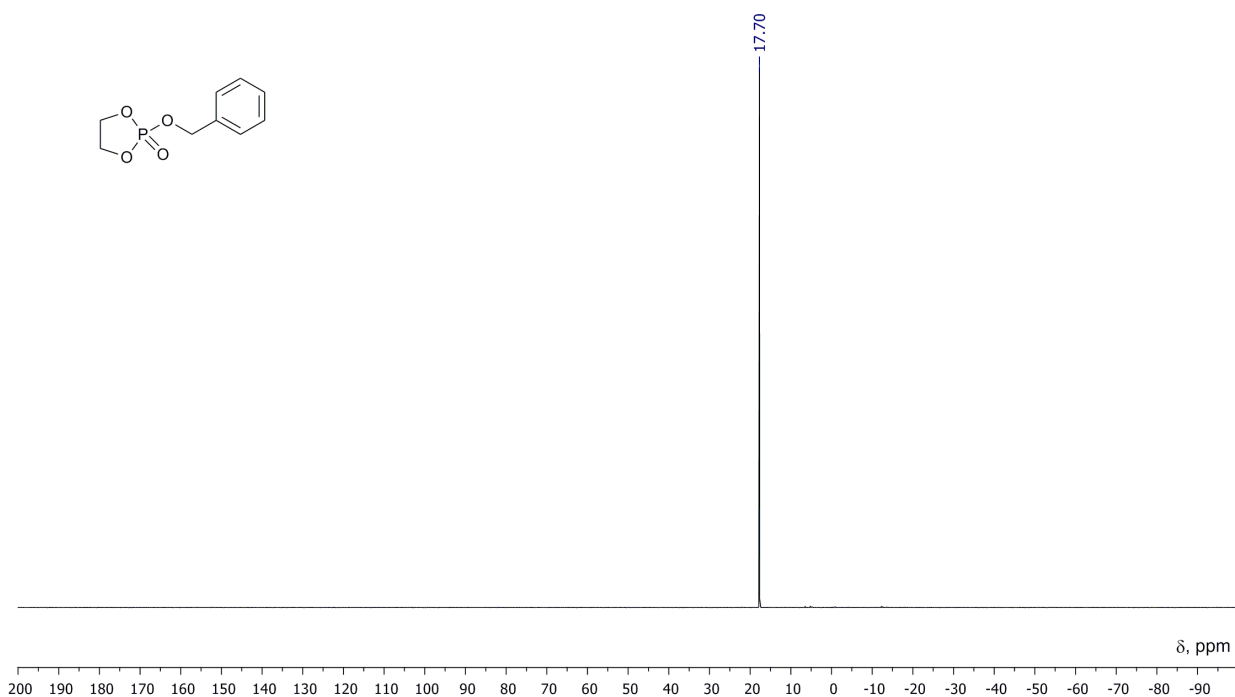


Fig. S44.  $^{31}\text{P}$  { $^1\text{H}$ } NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of BnOEP.

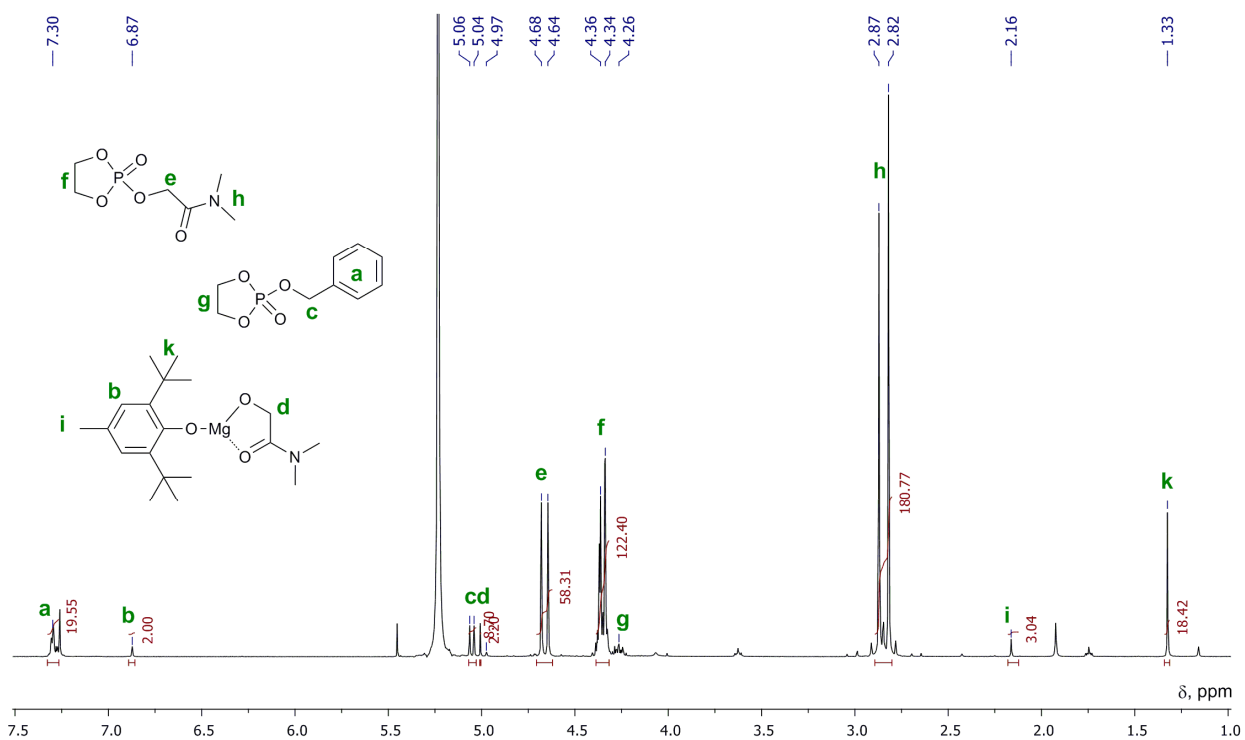
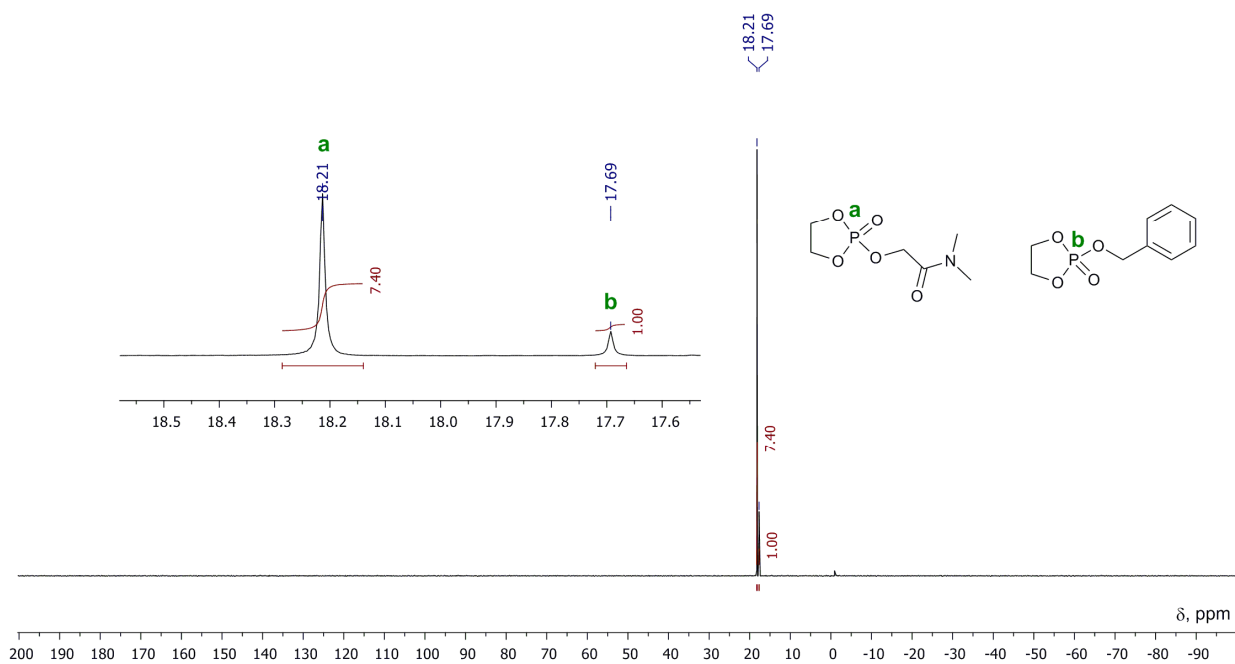
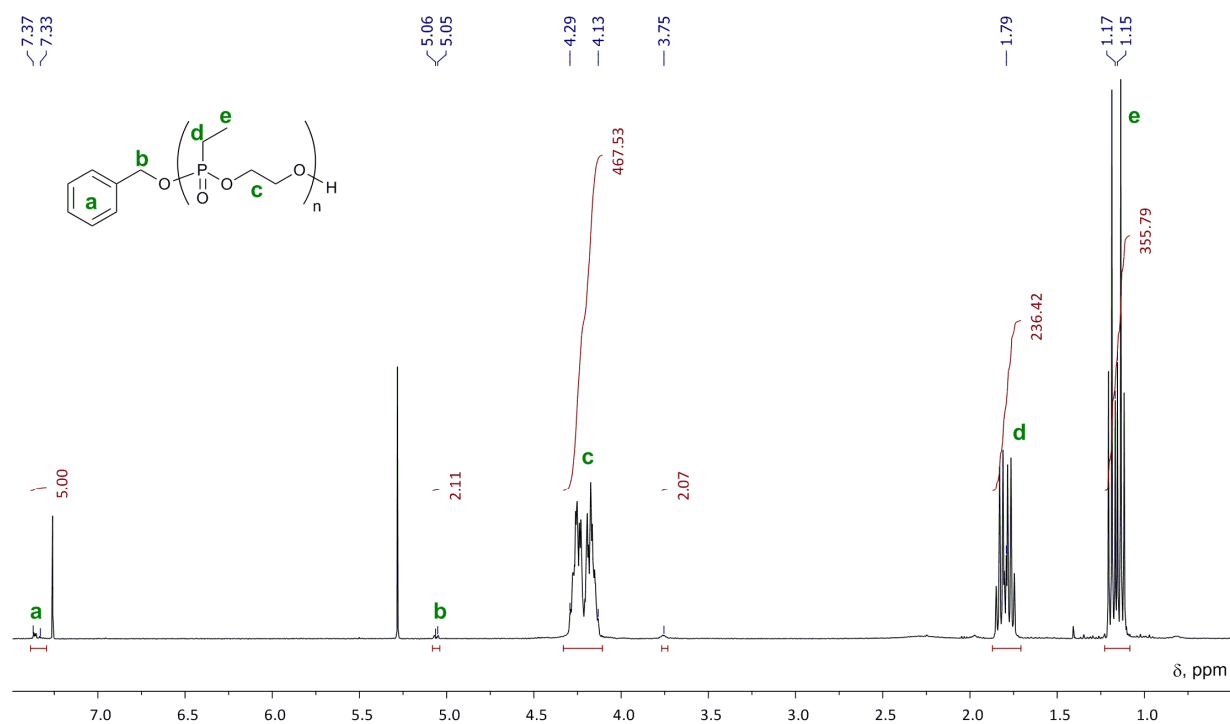


Fig. S45.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the reaction mixture obtained at [7]/[Mg] ratio of 30:1 followed by the addition of 3 eq. of BnOEP.

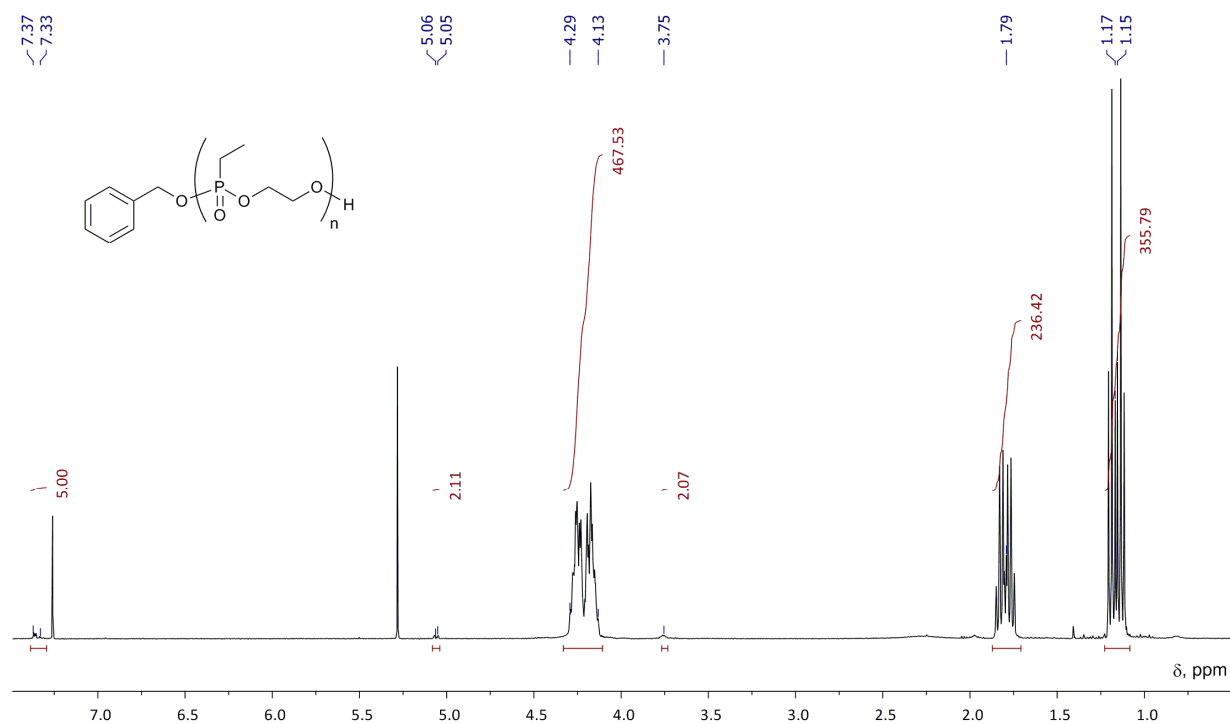


**Fig. S46.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the reaction mixture obtained at [7]/[Mg] ratio of 30:1 followed by the addition of 3 eq. of **BnOEP**.

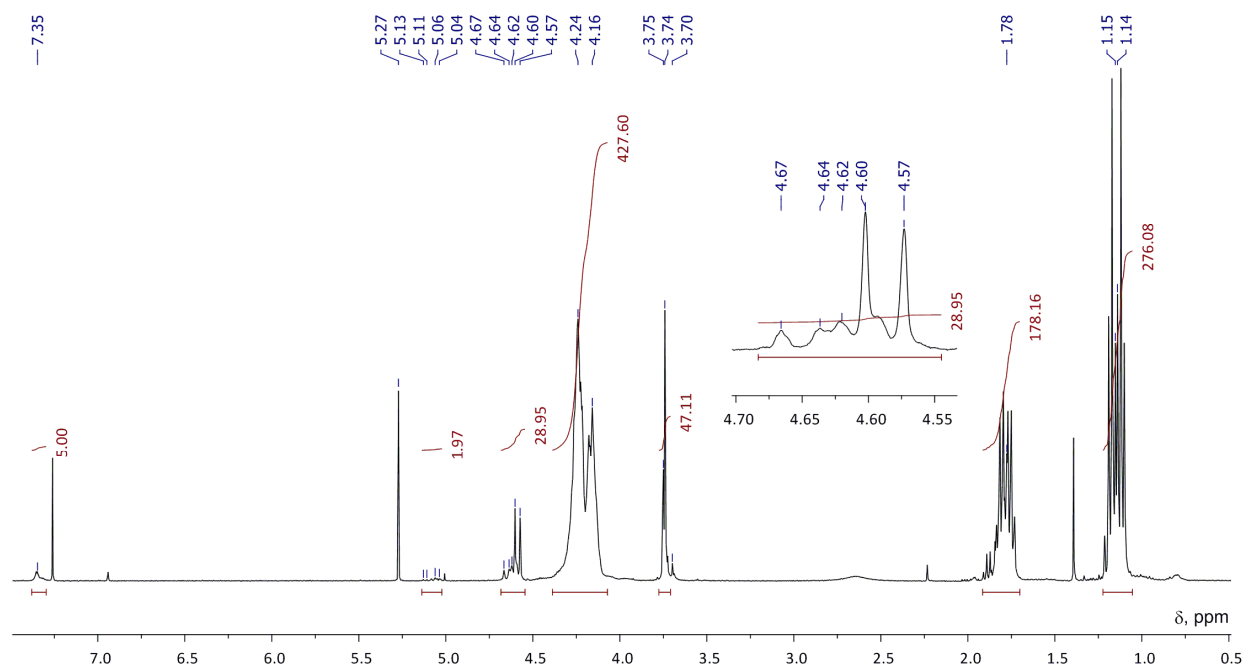
## S5. Copolymerization of 1 and EtEP



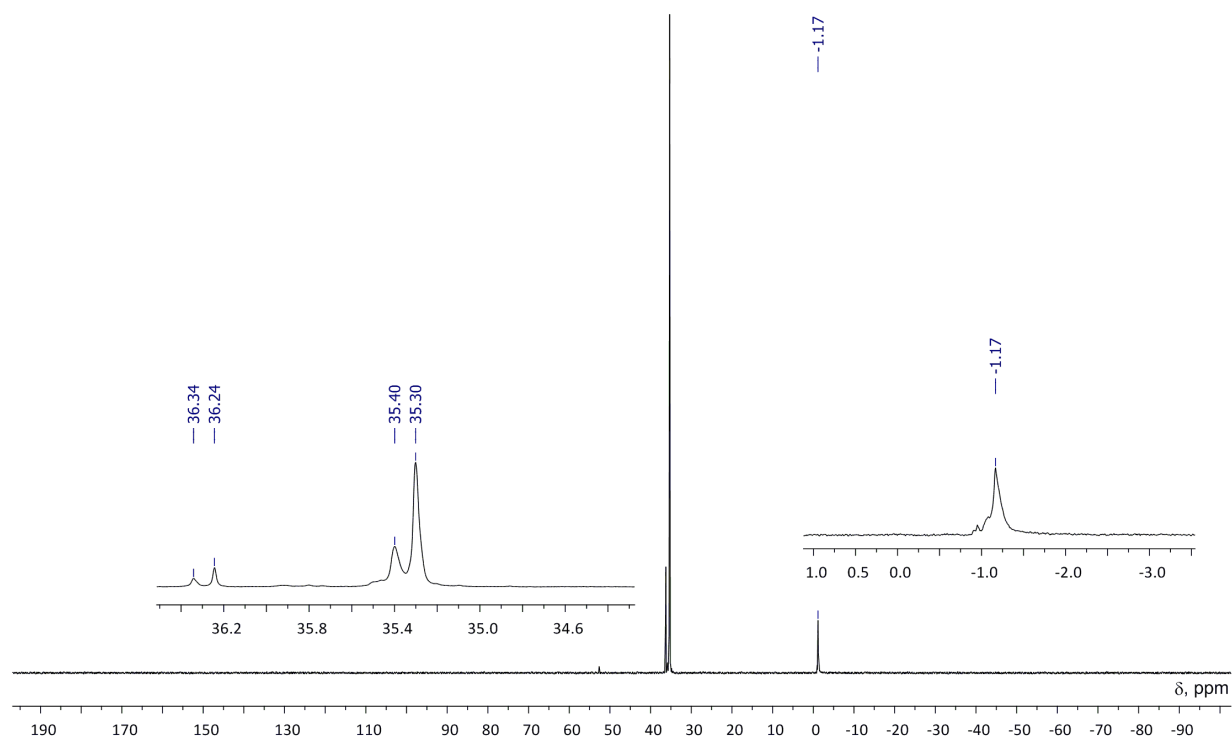
**Fig. S47.** <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 20 °C) of the homopolymer of EtEP (Table 3, Entry 1).



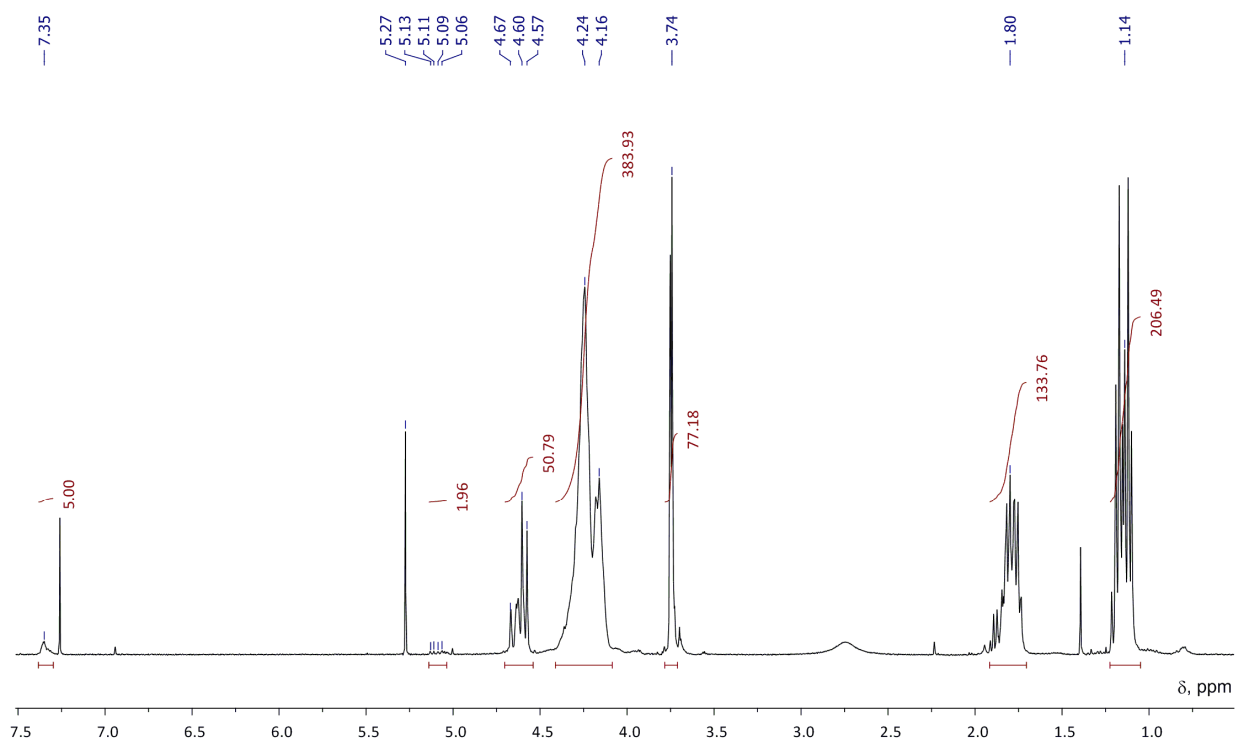
**Fig. S48.** <sup>31</sup>P {<sup>1</sup>H} NMR spectrum (162 MHz, CDCl<sub>3</sub>, 20 °C) of the homopolymer of EtEP (Table 3, Entry 1).



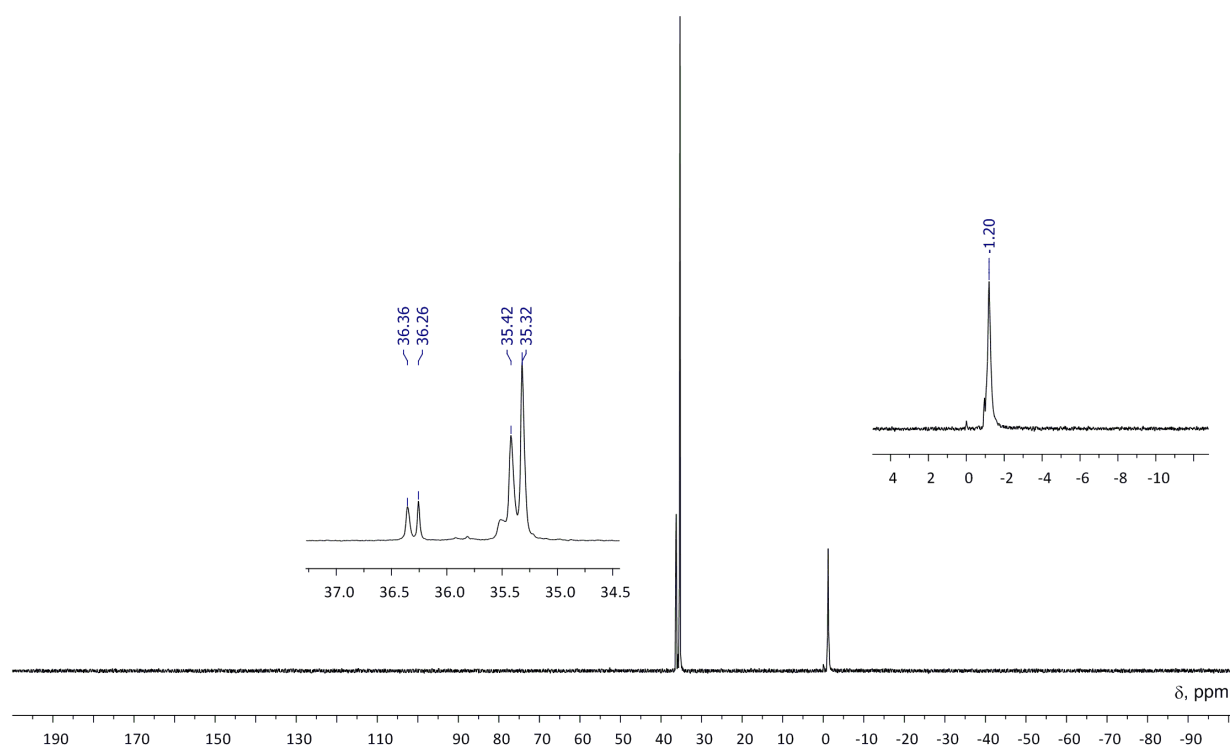
**Fig. S49.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and **EtEP** (initial **[1]**/**[EtEP]** ratio of 18:82, Table 3, Entry 2).



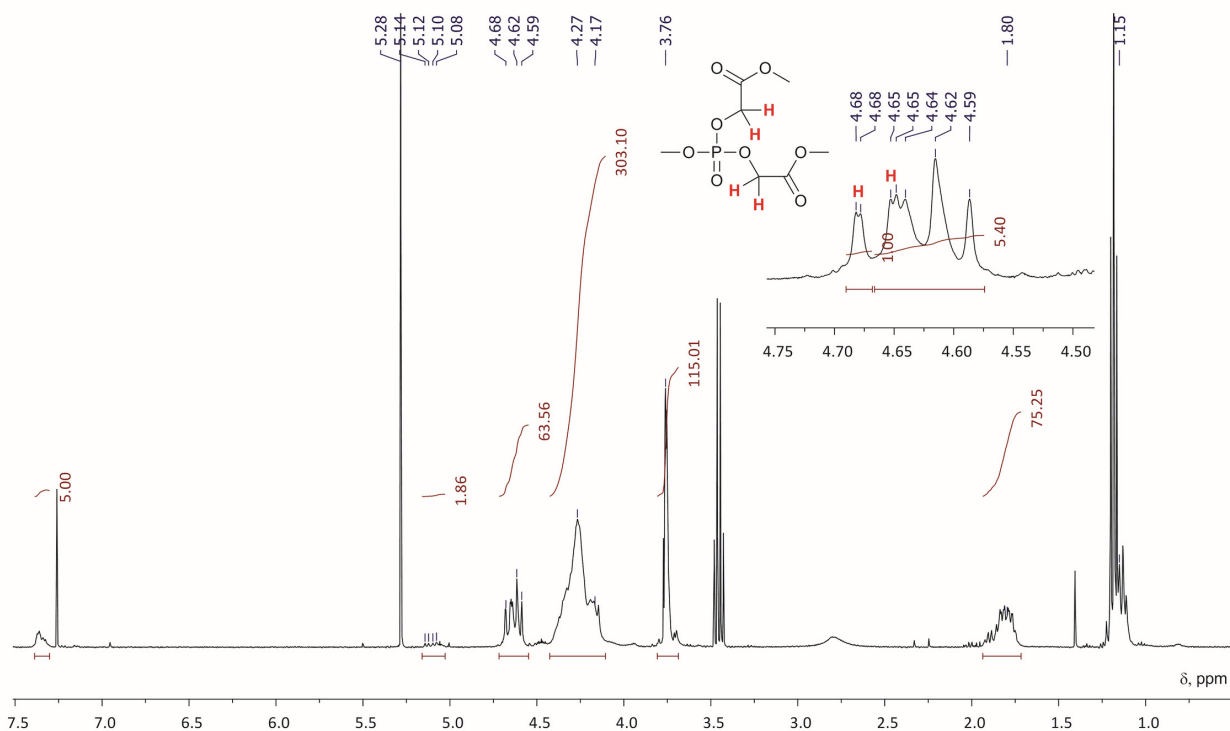
**Fig. S50.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and **EtEP** (initial **[1]**/**[EtEP]** ratio of 18:82, Table 3, Entry 2).



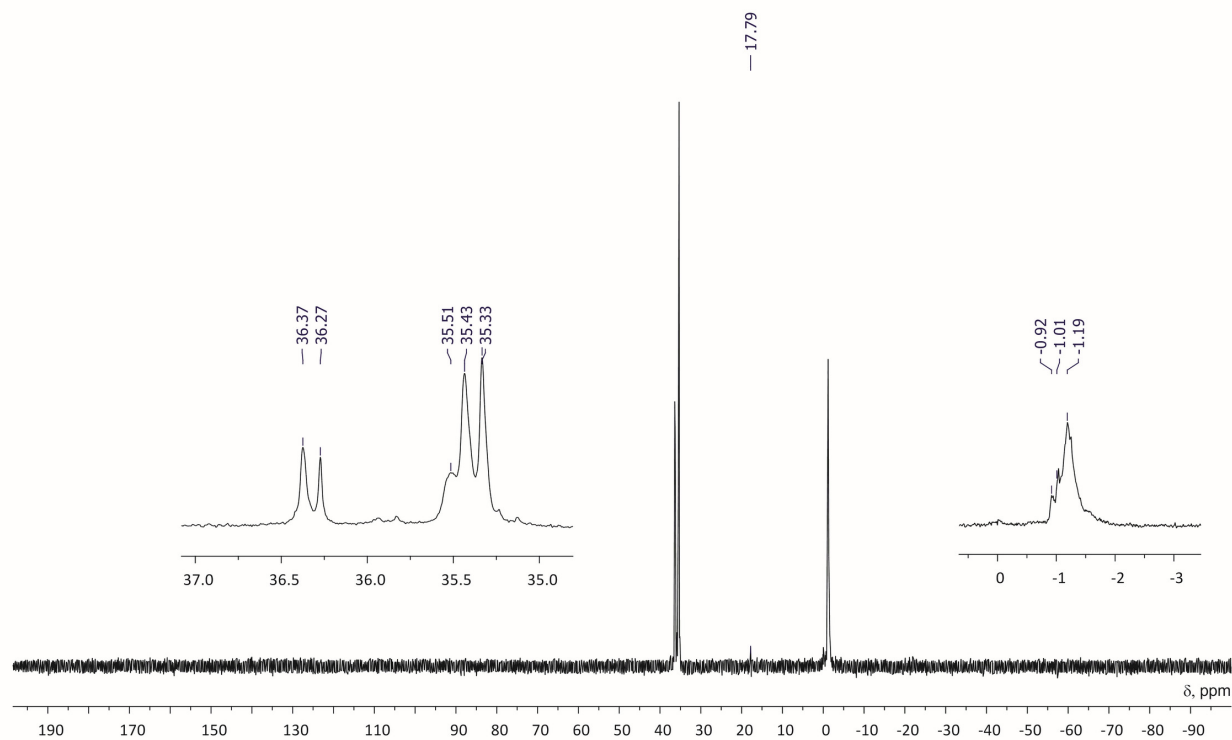
**Fig. S51.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and **EtEP** (initial **[1]**/**[EtEP]** ratio of 30:70, Table 3, Entry 3).



**Fig. S52.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and **EtEP** (initial **[1]**/**[EtEP]** ratio of 30:70, Table 3, Entry 3).



**Fig. S53.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and EtEP (initial [1]/[EtEP] ratio of 50:50, Table 3, Entry 4).



**Fig. S54.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20 °C) of the copolymer of **1** and EtEP (initial [1]/[EtEP] ratio of 50:50, Table 3, Entry 4).

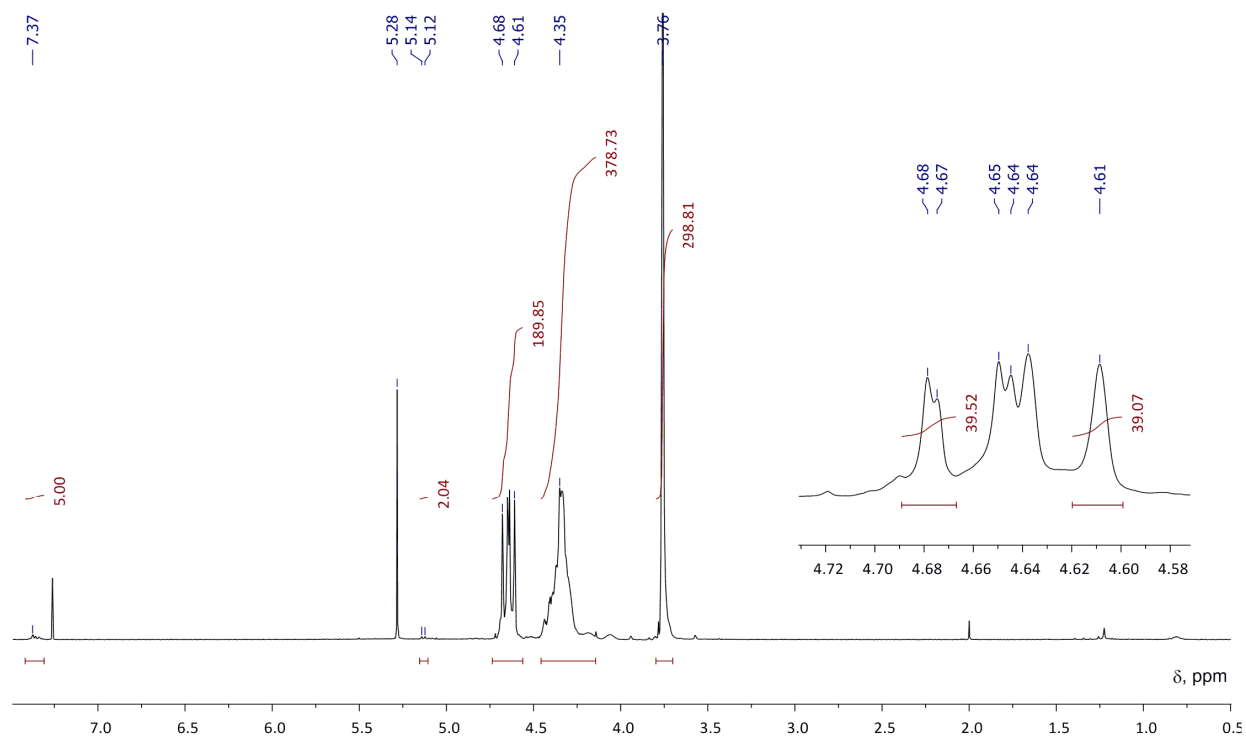


Fig. S55.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 20  $^\circ\text{C}$ ) of the homopolymer of **1** (Table 3, Entry 5).

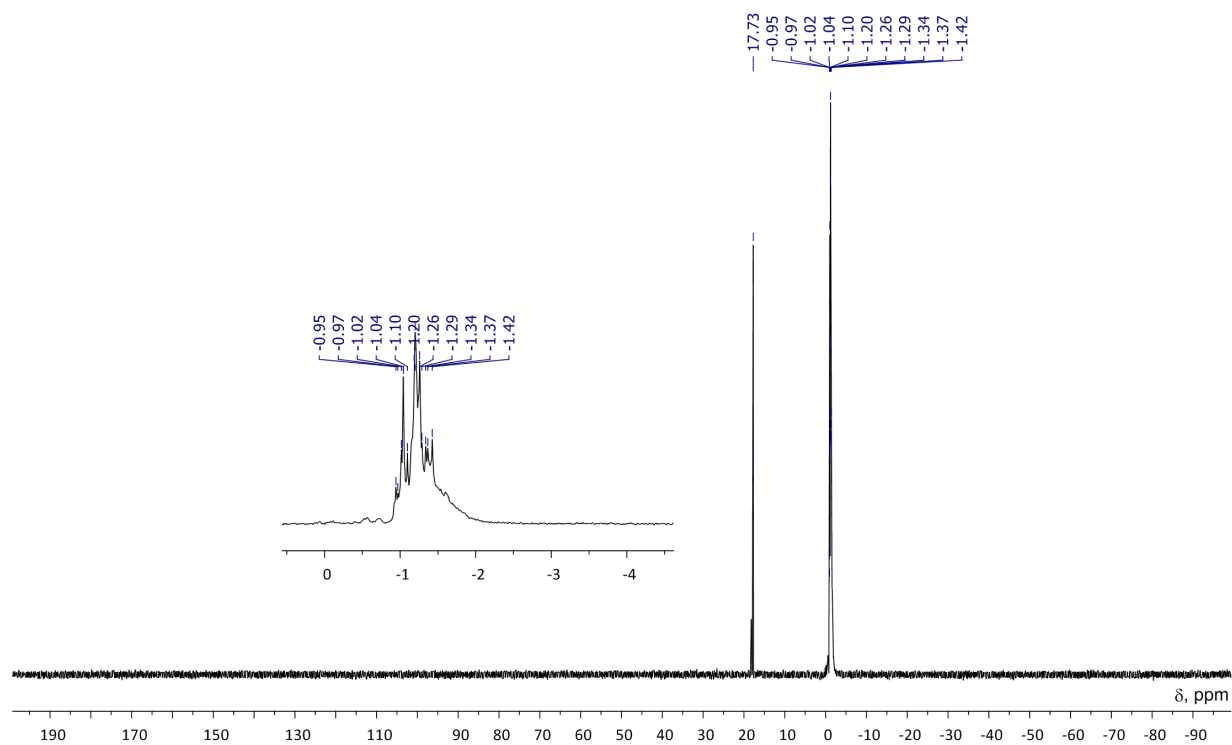
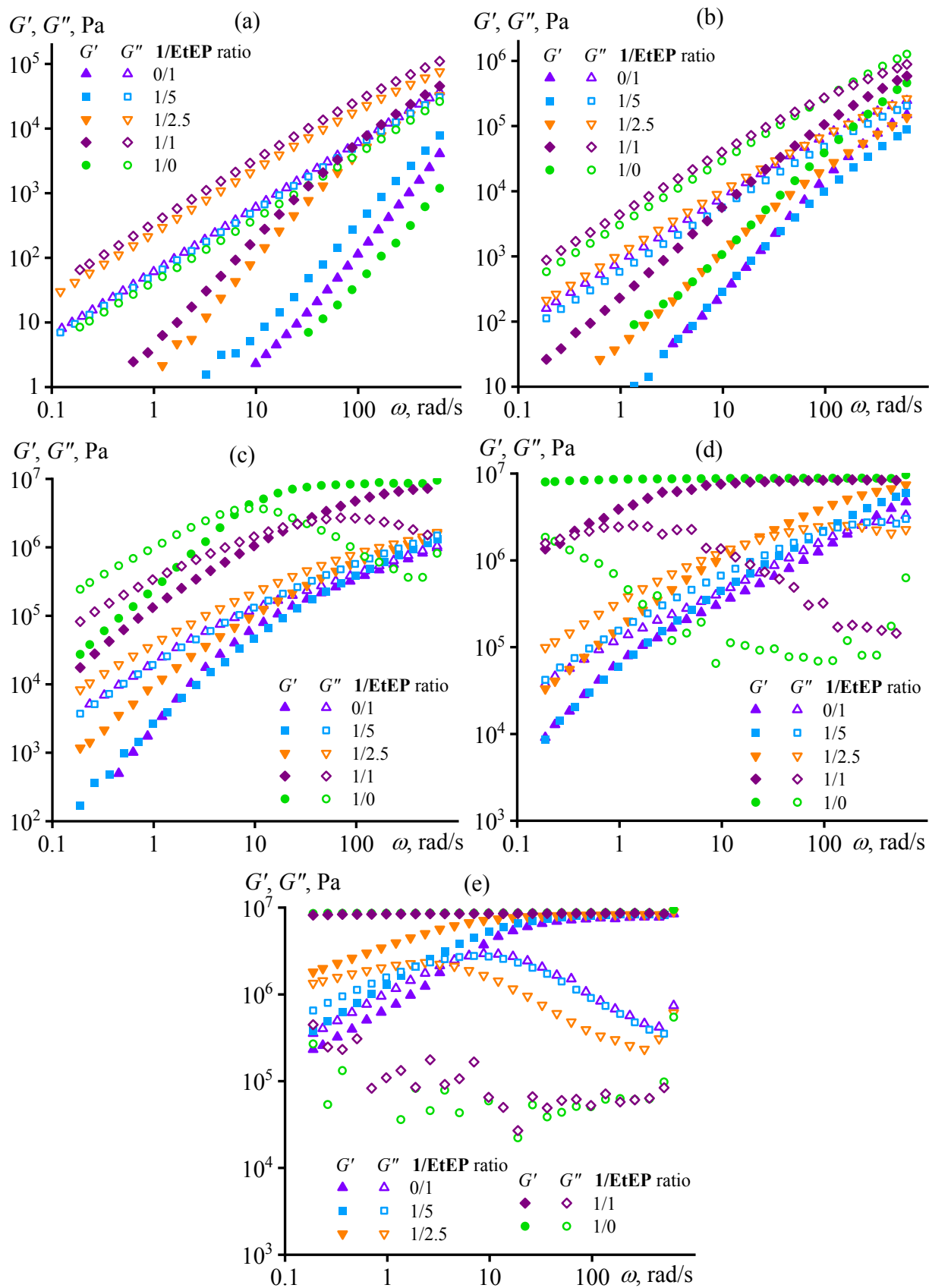
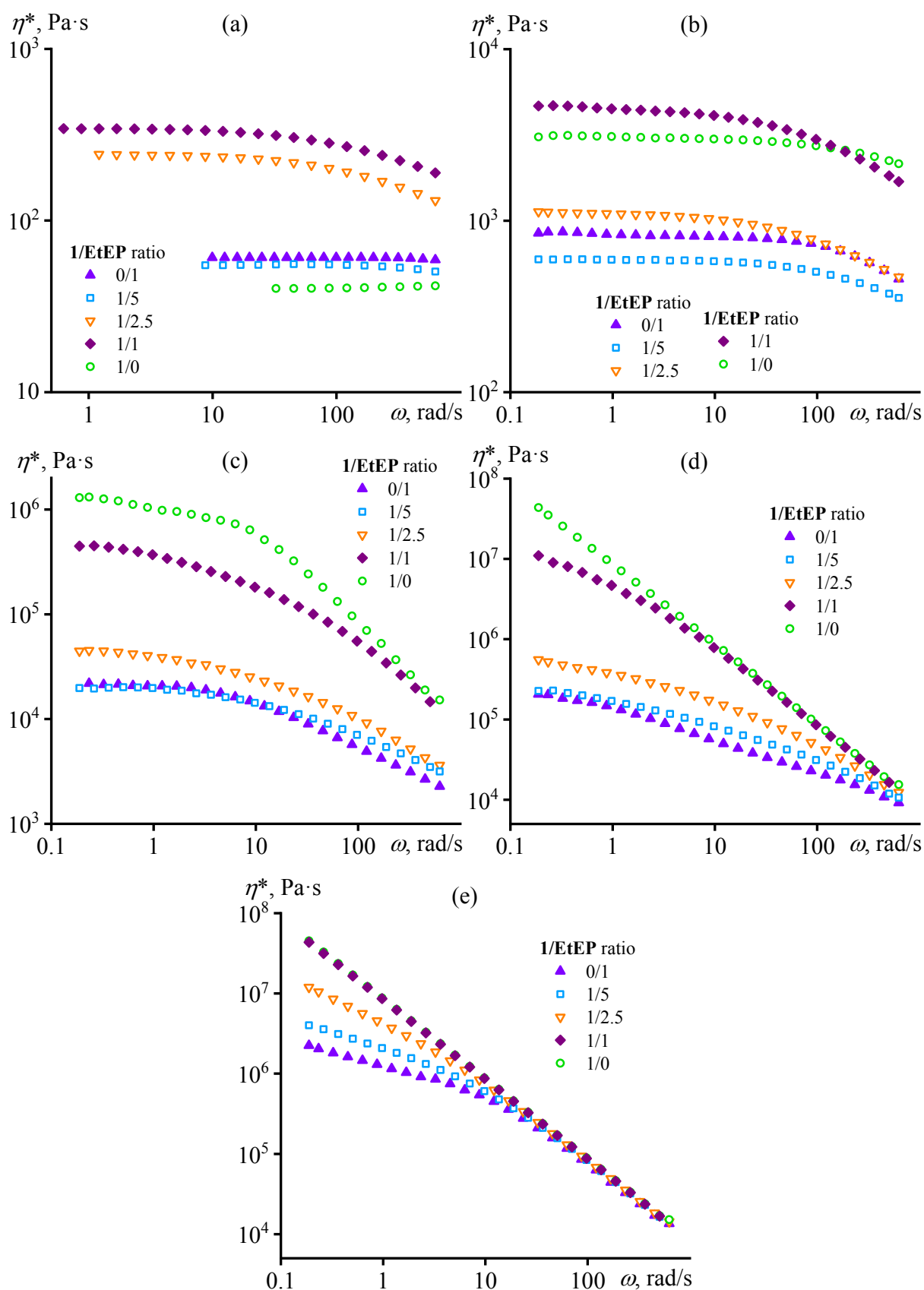


Fig. S56.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ , 20  $^\circ\text{C}$ ) of the homopolymer of **1** (Table 3, Entry 5).

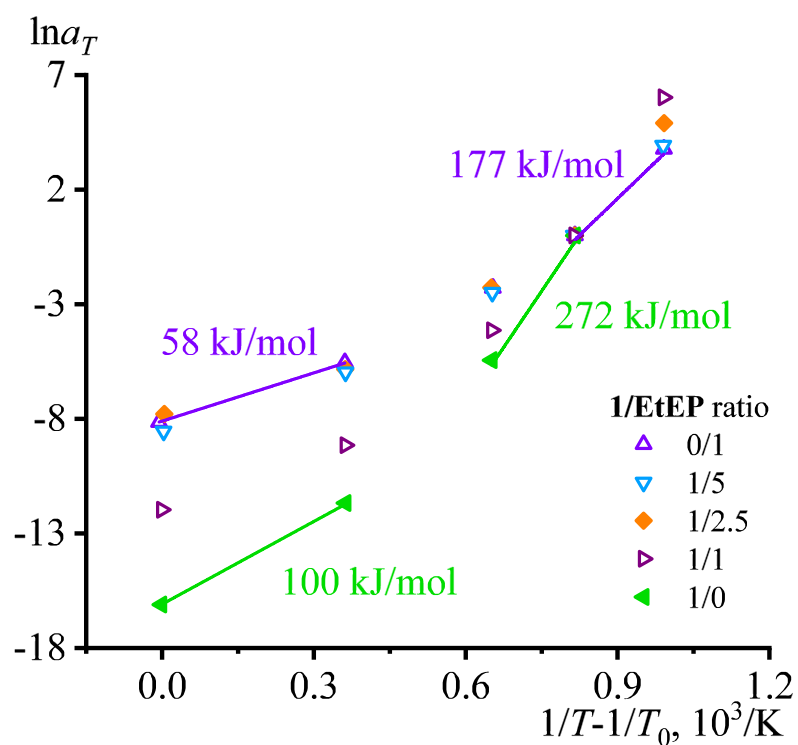


**Fig. S57.** Frequency dependences of storage (filled symbols) and loss (hollow symbols) moduli for **1** and **EtEP** copolymers at 30 (a), 0 (b), -20 (c), -30 (d), and -40 °C (e).





**Fig. S58.** Frequency dependences of complex viscosity for **1** and **EtEP** copolymers at 30 (a), 0 (b), -20 (c), -30 (d), and -40 °C (e).



**Fig. S59.** Temperature dependences of the shift factor for **1** and **EtEP** copolymers in the coordinates of the Arrhenius equation:

$$\ln a_T = \frac{E_A}{R \left( \frac{1}{T} - \frac{1}{T_0} \right)},$$

where  $a_T$  is the shift factor,  $E_A$  is the flow activation energy,  $R$  is the gas constant,  $T$  is the thermodynamic temperature, and  $T_0$  is the reference temperature (243.15 K).