Electronic Supplementary Information

Cholinium-based ionic liquid catalysts for polyethylene terephthalate glycolysis: understanding the role of solvent and a reappraisal of the cation contribution

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2. Computational Section

2.1. Computational Details

The geometries of the isolated reactants and structures in the reaction pathways were optimised using the ωb97-xD[1] density functional theory (DFT) method, which is a long-range corrected hybrid density functional including empirical atom-atom dispersion correction, with the DFT standard split valence (SV) def2SVP[2] basis sets. Vibrational frequency calculations were performed to confirm that the optimised structures corresponded to a minimum in the free-energy profile or alternatively to a transition state. Single point energy calculations[3] of optimised structures were obtained to increase accuracy of the free energy values by using the higher level, triple zeta valence (TZV) def2TZVP[2] basis set. All calculations were carried out with the *Gaussian16* program[4]. The self-consistent reaction field (SCRF) calculations using the SMD solvation model[5] were carried out, along with the inclusion of some explicit solvent molecules. The dielectric constant in the SMD calculations was set to ε = 40.245 to simulate 1,2-EthaneDiol (ethylene glycol or more commonly glycol solvent).

To study and understand the nature of the non-covalent interactions involved this research, the Quantum Theory of Atoms in Molecules (QTAIM) analysis was applied using the *AIMAll* program[6]. The critical points (CPs), bond paths (BPs) and related properties were found for the transition states of the pathways of particular interest. This data was used to help identify the existence of various non-covalent interactions within the studied orientations.

2.2. Figures

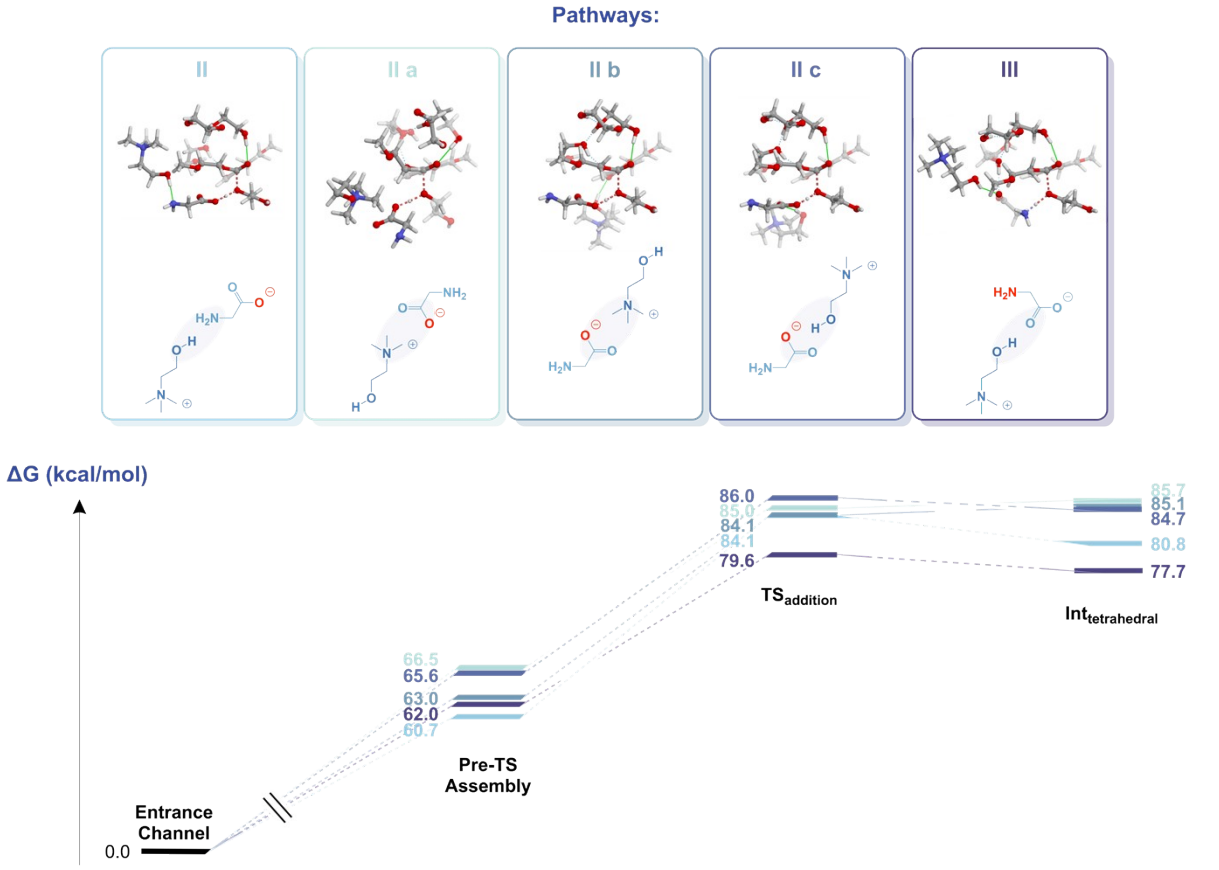


Fig. S1. Free energy profile of PET glycolysis with various orientations for new **Pathways: II** *(HB assisted catalysis: choline hydroxyl to base amine)*, **IIa** *(strict ion pair: choline hydroxyl not interacting)*, **IIb** *(strict ion pair reflected: choline hydroxyl interaction with PET carbonyl not involved in reaction)*, **IIc** *(HB assisted catalysis: choline hydroxyl to base carboxylate)* and **III** *(HB assisted catalysis: choline hydroxyl to base carboxylate with amine deprotonating)*.

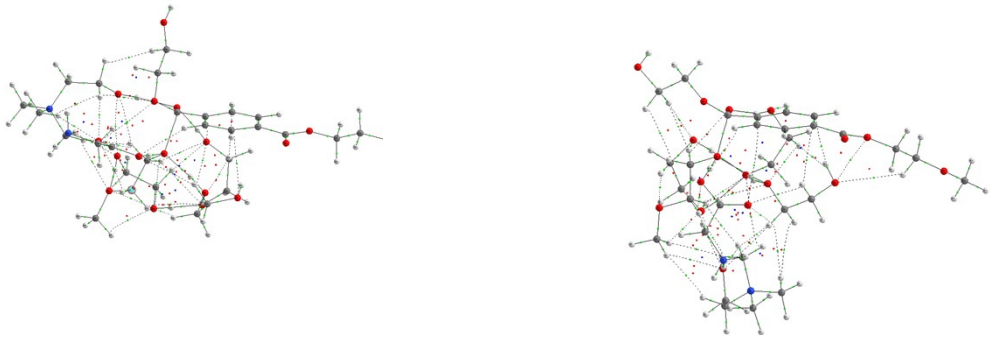
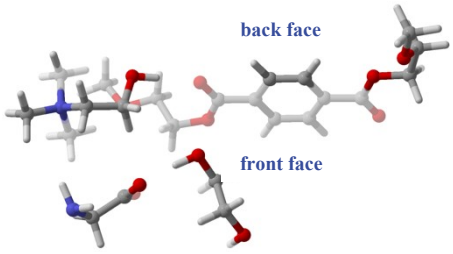


Fig. S2. Web of non-covalent interactions in TS-$I_{addition}$ (left) and TS-$II_{addition}$ (right).

(a)



(b)

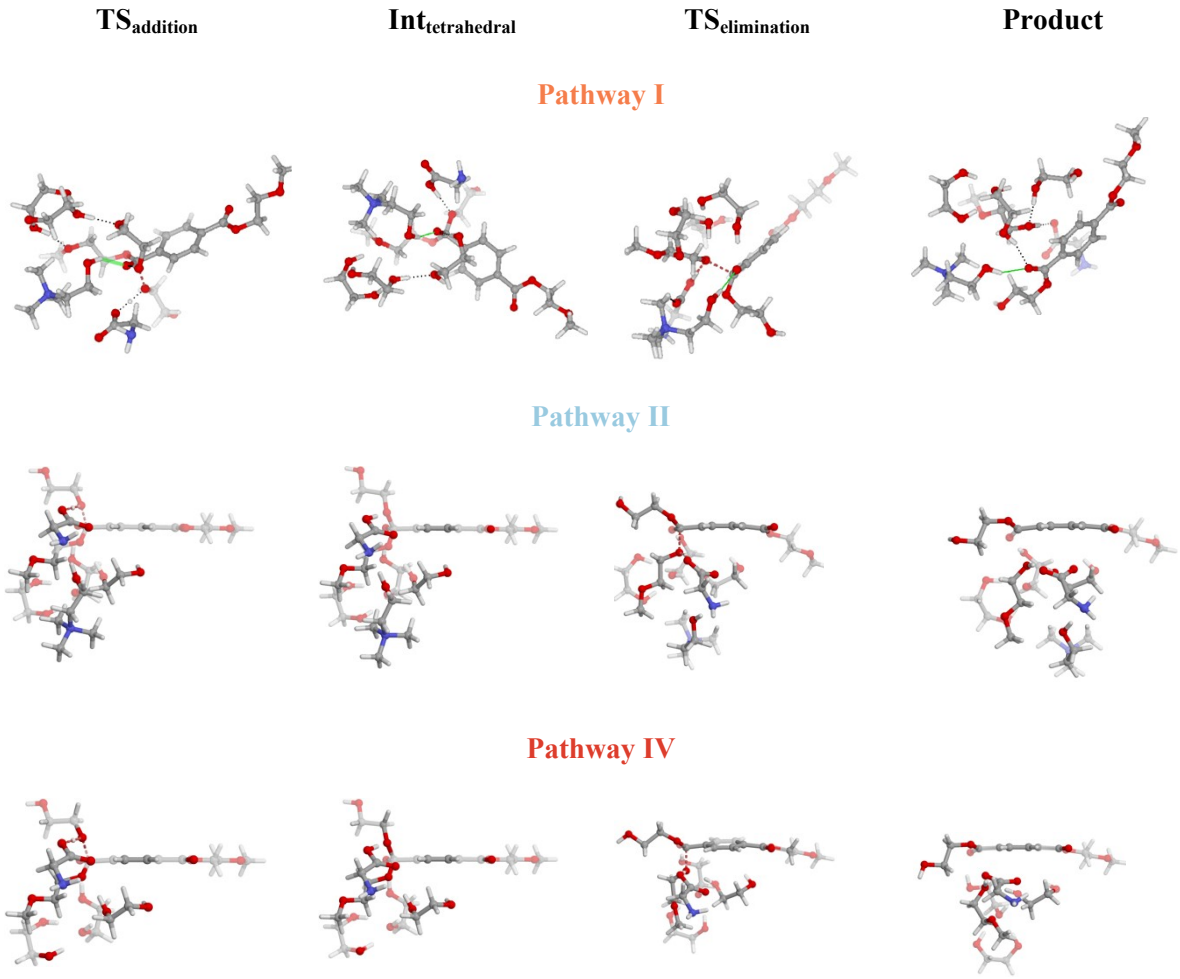


Fig. S3. Orientations of glycinate, attacking glycol, and cholinium species with respect to PET (a) in the pre-transition state assembly in absence of explicit solvent molecules (b) in the reaction pathway in the presence of explicit solvent molecules for Pathways: **I**, **II** and **IV**.

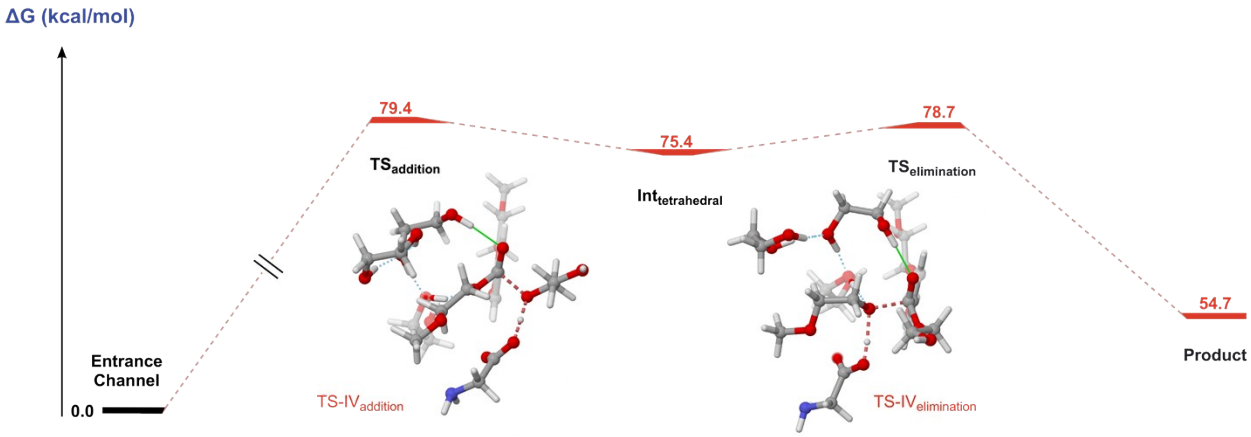


Fig. S4. Free energy profile of PET glycolysis for the new Pathway IV without choline present (red).

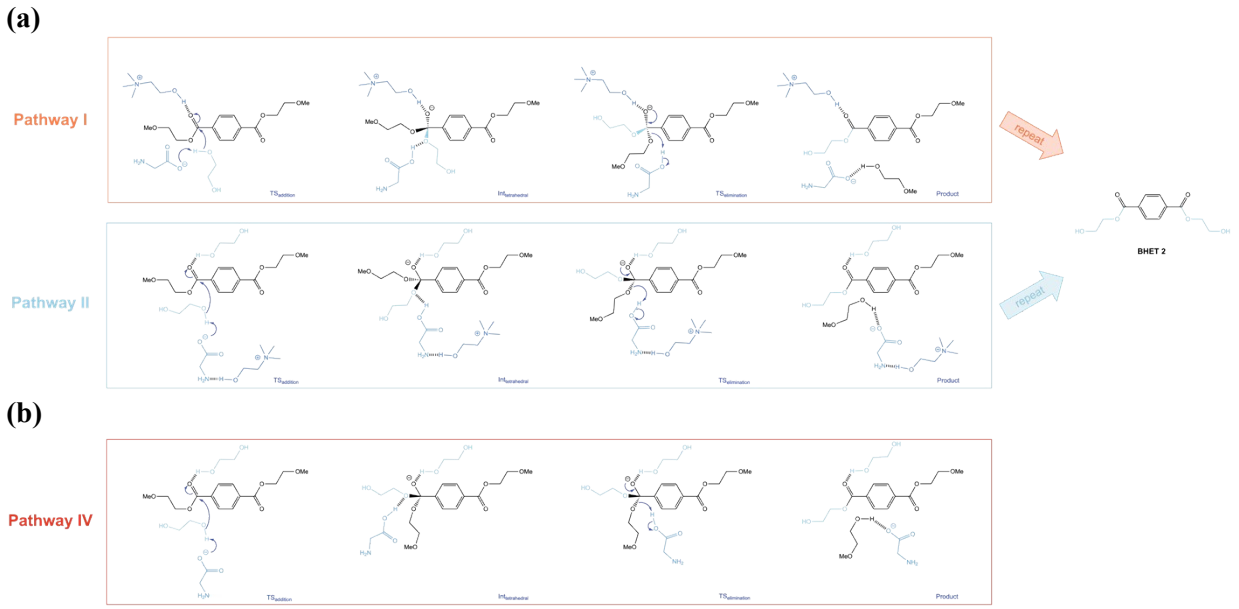


Fig. S5. (a) Mechanism of action of PET glycolysis for the literature **Pathway I** (orange) *versus* new **Pathway II** proposed (blue) and (b) **Pathway IV** where choline is removed from the calculations (red).

ΔG = 11.5 kcal mol^{-1} ΔG = 10.0 kcal mol^{-1}

Fig. S6. Competition in deprotonation of glycol (left) *versus* choline (right) by glycinate in $TS_{addition}$ in isolated calculations.

2.3. Reaction Coordinates & AIM Molecular Graphs

Table S1. Cartesian coordinates (in Å) of DFT optimised geometries for the entrance channel species and of the reaction pathways using cholinium glycinate catalyst in: **Pathway I, II, II a, II b, II c, III** and **IV** including molecular graphs (AIM) of the $\mathbf{TS_{addition}}$ and $\mathbf{TS_{elimination}}$. Green dots indicate bond critical points (BCPs):

Entrance Channel (EC)

Compound	Coordinates			
cholinium				
Imaginary frequencies=0	C	0.769943	-0.123616	1.486221
SCF energy=-328.4504698	N	0.769383	0.019980	0.003558
	C	2.067725	-0.485357	-0.530605
	C	0.641758	1.464813	-0.353035
	C	-0.337194	-0.792217	-0.631858
	C	-1.704946	-0.705142	0.005338
	O	-2.232338	0.595488	-0.090751
	H	0.773906	-1.189565	1.743898
	H	-0.116344	0.369330	1.900431
	H	1.672814	0.359654	1.877666
	H	2.038857	-0.445804	-1.625832
	H	2.214400	-1.518310	-0.193946
	H	2.875741	0.152480	-0.153422
	H	1.457246	2.014439	0.131388
	H	0.717444	1.564090	-1.442423
	H	-0.329623	1.829747	-0.009072
	H	-0.014666	-1.841149	-0.592668
	H	-0.378735	-0.480338	-1.684408
	H	-2.324163	-1.434581	-0.548304
	H	-1.669457	-1.053546	1.051534
	H	-3.068119	0.618906	0.389895
glycinate				
Imaginary frequencies=0	C	-0.658573	-0.746870	0.000194
SCF energy=-283.6675938	C	0.653946	0.059644	-0.000017
	O	0.573643	1.310105	0.000051
	O	1.714293	-0.612997	-0.000125
	N	-1.897140	0.012033	-0.000013
	H	-0.630146	-1.415008	0.877915
	H	-0.630151	-1.415473	-0.877176
	H	-1.868055	0.645689	-0.800340
	H	-1.867398	0.647053	0.799225
glycol				
Imaginary frequencies=0	C	0.686595	0.595300	-0.276261
SCF energy=-230.0224628	C	-0.722379	0.569691	0.281088
	O	-1.429204	-0.563294	-0.172566
	O	1.379523	-0.594884	0.043922
	H	0.646501	0.646052	-1.375860

	H	1.220151	1.493016	0.085009
	H	-0.677624	0.594170	1.388734
	H	-1.271216	1.466963	-0.044898
	H	-0.834977	-1.316737	-0.050652
	H	1.529312	-0.607987	0.997858
pet_dimer Imaginary frequencies=0 SCF energy=-994.6340496				
	C	-5.652531	-0.146535	0.528214
	C	-5.019934	0.272653	-0.785713
	O	-3.634969	0.564269	-0.605832
	C	-2.769384	-0.443382	-0.638754
	O	-3.091255	-1.597027	-0.817327
	C	-1.358132	0.001219	-0.438792
	C	-1.028840	1.345280	-0.230815
	C	0.299919	1.710077	-0.050531
	C	1.305184	0.738074	-0.076975
	C	0.975787	-0.606134	-0.284060
	C	-0.352825	-0.970919	-0.463795
	C	2.717819	1.180543	0.117883
	O	3.047211	2.332115	0.297548
	H	-5.194248	-1.086404	0.891274
	H	-5.145605	-0.510913	-1.546201
	H	-5.474638	1.204043	-1.146151
	H	-1.810956	2.104840	-0.209559
	H	0.567147	2.755760	0.111627
	H	1.757803	-1.365836	-0.305170
	H	-0.620034	-2.016584	-0.625877
	O	3.583294	0.176915	0.072639
	O	-7.023608	-0.315945	0.289561
	H	-5.471669	0.633387	1.293454
	C	4.964248	0.489460	0.239520
	H	5.288315	1.182286	-0.552088
	H	5.123163	0.973170	1.215365
	C	5.720689	-0.817225	0.154650
	H	5.368837	-1.506601	0.946803
	H	5.522914	-1.302078	-0.821257
	O	7.082492	-0.522790	0.307203
	C	-7.738861	-0.721398	1.428404
	H	-8.794837	-0.825701	1.142996
	H	-7.377427	-1.693781	1.812269
	H	-7.663633	0.022391	2.243735
	C	7.903963	-1.660804	0.249459
	H	7.812201	-2.181379	-0.722218
	H	8.944550	-1.331256	0.375700
	H	7.660184	-2.381095	1.052799

Pathway I

Compound	Coordinates			
PI_1_addition_pre_TS Imaginary frequencies=0 SCF energy=-2526.9903451				
	C	-1.933582	-0.509780	2.020810
	C	-1.157436	0.803226	2.031753
	O	0.244385	0.543533	1.932247

	C	0.777026	0.432658	0.726990
	O	0.116032	0.479061	-0.291350
	C	2.250902	0.220438	0.754454
	C	2.929617	-0.008913	1.955463
	C	4.307404	-0.191023	1.945801
	C	5.013826	-0.136758	0.740377
	C	4.334345	0.099253	-0.460204
	C	2.956670	0.276648	-0.451766
	C	6.492647	-0.335978	0.780775
	O	7.114861	-0.555531	1.796281
	H	-1.667251	-1.090204	1.127778
	H	-1.475268	1.462696	1.211798
	H	-1.276157	1.333945	2.984419
	H	2.379933	-0.047343	2.896380
	H	4.845541	-0.375107	2.877251
	H	4.883866	0.146470	-1.400772
	H	2.426365	0.468689	-1.385715
	O	7.054440	-0.241914	-0.419924
	O	-3.321590	-0.293407	1.946641
	H	-1.681132	-1.109500	2.914025
	C	-4.436791	1.996299	-0.097735
	N	-4.953256	1.270399	-1.294201
	C	-6.107214	2.025248	-1.858006
	C	-5.416839	-0.088961	-0.885561
	C	-3.897836	1.177232	-2.371021
	C	-2.531155	0.698318	-1.942727
	O	-2.560734	-0.640342	-1.525072
	H	-3.979946	2.939009	-0.423502
	H	-3.705026	1.362362	0.412676
	H	-5.281351	2.188929	0.574866
	H	-6.434970	1.535430	-2.782886
	H	-5.791075	3.054313	-2.066939
	H	-6.922070	2.022551	-1.124146
	H	-6.150185	0.021129	-0.078584
	H	-5.879350	-0.579147	-1.750465
	H	-4.552040	-0.663034	-0.546190
	H	-3.782049	2.190587	-2.776172
	H	-4.313246	0.524779	-3.151702
	H	-1.885958	0.823184	-2.831340
	H	-2.116881	1.346713	-1.156516
	H	-1.675703	-0.911706	-1.227018
	C	1.239853	5.113635	2.039070
	C	1.429638	3.604883	1.942847
	O	1.361144	3.159372	0.615180
	O	1.376475	5.588727	3.360077
	H	2.010607	5.613365	1.430935
	H	0.256103	5.381267	1.608186
	H	2.419883	3.338246	2.350449
	H	0.673121	3.106658	2.581890

	H	0.425357	3.283733	0.306511
	H	0.647899	5.232370	3.882800
	C	-0.239716	3.427122	-2.304073
	C	-1.388034	3.753824	-1.340161
	O	-2.471506	4.157347	-1.806927
	O	-1.152182	3.589667	-0.105165
	N	-0.542045	3.478158	-3.719701
	H	0.140910	2.427751	-2.040589
	H	0.582274	4.124127	-2.063648
	H	-1.036525	4.350683	-3.908597
	H	-1.227305	2.751543	-3.928914
	C	-4.468115	-4.062046	2.685762
	C	-5.413971	-2.878584	2.726976
	O	-5.320078	-2.069979	1.571524
	O	-3.114722	-3.670410	2.644774
	H	-4.630251	-4.671832	3.591053
	H	-4.723830	-4.693188	1.814213
	H	-6.451640	-3.242039	2.796209
	H	-5.209615	-2.274026	3.629977
	H	-4.469289	-1.585447	1.601518
	H	-2.890936	-3.514454	1.702799
	C	-3.306074	-4.171622	-0.940136
	C	-4.527917	-3.589589	-1.620657
	O	-5.639331	-3.444352	-0.769461
	O	-2.756885	-3.278182	0.012390
	H	-3.581094	-5.111670	-0.430440
	H	-2.551646	-4.418979	-1.706115
	H	-4.241287	-2.626624	-2.085281
	H	-4.826827	-4.269269	-2.435783
	H	-5.398704	-2.915774	0.020403
	H	-1.895895	-2.956136	-0.323557
	C	-0.075362	-2.607798	-2.386230
	C	0.966918	-1.634854	-2.897715
	O	0.526959	-0.297798	-2.908533
	O	-0.441668	-2.335254	-1.039895
	H	-1.001115	-2.515735	-2.973166
	H	0.299892	-3.640613	-2.485972
	H	1.890283	-1.745546	-2.294864
	H	1.222557	-1.914954	-3.931766
	H	0.386515	-0.015002	-1.985833
	H	0.338271	-2.371340	-0.469297
	C	8.466087	-0.418914	-0.525542
	H	8.763304	0.108309	-1.440927
	H	8.971201	0.038599	0.336726
	C	8.810598	-1.892795	-0.631993
	H	8.505631	-2.424644	0.289813
	H	8.256644	-2.343192	-1.478651
	C	-3.900024	0.396986	3.035628
	H	-3.649048	1.470600	3.021236

	H	-4.988945	0.291712	2.939784
	H	-3.577685	-0.036771	3.998226
	O	10.196019	-1.980216	-0.827265
	C	10.655967	-3.301871	-0.948703
	H	11.744050	-3.267173	-1.097886
	H	10.441007	-3.893514	-0.039190
	H	10.195644	-3.815965	-1.813241
PI_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.9669661				
	C	-1.998202	-0.604523	2.132376
	C	-1.358981	0.777644	2.203512
	O	0.050548	0.660425	2.097962
	C	0.599577	0.886256	0.870212
	O	-0.077800	0.674791	-0.161365
	C	2.075274	0.554268	0.884283
	C	2.691587	-0.009148	2.003369
	C	4.047559	-0.323734	1.970540
	C	4.800103	-0.073099	0.820797
	C	4.183086	0.496173	-0.301283
	C	2.830389	0.806235	-0.266334
	C	6.246860	-0.425871	0.831260
	O	6.821104	-0.902652	1.786260
	H	-1.617035	-1.134845	1.250676
	H	-1.756326	1.422944	1.407242
	H	-1.554044	1.260510	3.171513
	H	2.109031	-0.208275	2.903156
	H	4.529890	-0.768008	2.843310
	H	4.764081	0.695680	-1.202576
	H	2.353111	1.242767	-1.145055
	O	6.849297	-0.157985	-0.324929
	O	-3.396814	-0.535965	1.978547
	H	-1.738120	-1.197570	3.028310
	C	-4.596050	1.815891	-0.048937
	N	-5.018281	1.068927	-1.268507
	C	-6.273826	1.671137	-1.797616
	C	-5.284887	-0.355791	-0.907434
	C	-3.969928	1.155018	-2.352614
	C	-2.539281	0.929957	-1.923999
	O	-2.311177	-0.367057	-1.441845
	H	-4.272726	2.823413	-0.338260
	H	-3.782389	1.269673	0.437892
	H	-5.453677	1.871171	0.631975
	H	-6.538248	1.170921	-2.737040
	H	-6.111304	2.741411	-1.971967
	H	-7.071167	1.526271	-1.059130
	H	-6.004429	-0.376237	-0.081124
	H	-5.702019	-0.869107	-1.781598
	H	-4.341746	-0.820222	-0.611031
	H	-4.034436	2.170634	-2.765922
	H	-4.271667	0.439603	-3.130273

	H	-1.925717	1.138315	-2.820343
	H	-2.249991	1.667187	-1.164143
	H	-1.497408	-0.323761	-0.908493
	C	1.637579	4.736341	1.743049
	C	1.189188	3.314264	2.052163
	O	0.742665	2.695031	0.878685
	O	2.158334	5.388577	2.879039
	H	2.440221	4.701135	0.989674
	H	0.793361	5.298625	1.301230
	H	2.043955	2.755496	2.475791
	H	0.396701	3.336601	2.827034
	H	1.439553	5.512706	3.510790
	C	-0.356288	3.777125	-1.915950
	C	-1.548592	3.968925	-0.982443
	O	-2.621022	4.394347	-1.405511
	O	-1.371201	3.661706	0.263278
	N	-0.619239	3.992020	-3.320001
	H	0.032256	2.759565	-1.758483
	H	0.440033	4.454590	-1.562308
	H	-1.087685	4.891455	-3.431734
	H	-1.304940	3.303159	-3.631023
	C	-4.045112	-4.458140	2.303335
	C	-5.137018	-3.412796	2.415691
	O	-5.115562	-2.492939	1.343451
	O	-2.752527	-3.899696	2.358069
	H	-4.153877	-5.170580	3.138911
	H	-4.192451	-5.026476	1.365874
	H	-6.120229	-3.910096	2.411407
	H	-5.037172	-2.875878	3.377278
	H	-4.350123	-1.892705	1.469183
	H	-2.524747	-3.599924	1.451767
	C	-2.715054	-4.053561	-1.210893
	C	-3.974705	-3.592877	-1.913812
	O	-5.135309	-3.669943	-1.121188
	O	-2.323963	-3.151442	-0.191011
	H	-2.883152	-5.052142	-0.769264
	H	-1.907104	-4.154440	-1.954846
	H	-3.803560	-2.564699	-2.288164
	H	-4.137563	-4.238144	-2.792865
	H	-5.007594	-3.189488	-0.275901
	H	-1.449155	-2.776901	-0.433315
	C	0.270889	-2.169200	-2.450236
	C	1.192146	-1.043429	-2.877367
	O	0.635901	0.236697	-2.714040
	O	0.028793	-2.178627	-1.053009
	H	-0.711576	-2.045101	-2.929193
	H	0.695872	-3.134326	-2.778837
	H	2.151951	-1.138783	-2.329470
	H	1.420671	-1.176686	-3.947341

	H	0.443596	0.378513	-1.760505
	H	0.854220	-2.344623	-0.579252
	C	8.239100	-0.450222	-0.451078
	H	8.606269	0.198068	-1.256926
	H	8.766202	-0.202098	0.481075
	C	8.448205	-1.908079	-0.816461
	H	8.088861	-2.562730	0.000505
	H	7.861992	-2.150960	-1.724280
	C	-4.106048	0.044180	3.052240
	H	-3.962117	1.136611	3.097246
	H	-5.171979	-0.161824	2.885416
	H	-3.800745	-0.398293	4.016737
	O	9.821417	-2.086815	-1.035608
	C	10.164081	-3.411152	-1.353986
	H	11.250845	-3.448987	-1.511941
	H	9.899715	-4.108383	-0.536974
	H	9.659619	-3.752464	-2.277408
	H	-0.342552	3.182725	0.523967
PI_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.9791932				
	C	-2.284247	-0.402663	2.158947
	C	-1.693316	0.992519	2.329343
	O	-0.283851	0.906550	2.347790
	C	0.360808	1.316168	1.154399
	O	-0.221812	0.939685	0.046658
	C	1.809627	0.821857	1.240474
	C	2.126396	-0.364814	1.906819
	C	3.410190	-0.894679	1.827441
	C	4.397724	-0.238894	1.085201
	C	4.086651	0.958557	0.428596
	C	2.801449	1.481201	0.507697
	C	5.749865	-0.852790	1.010557
	O	6.059288	-1.883484	1.569575
	H	-1.746798	-0.916047	1.352649
	H	-2.042723	1.644337	1.513635
	H	-2.007674	1.445333	3.282829
	H	1.357811	-0.881093	2.484015
	H	3.654790	-1.826409	2.341603
	H	4.851047	1.477558	-0.151285
	H	2.558428	2.408161	-0.015214
	O	6.595151	-0.150069	0.258072
	O	-3.640759	-0.382346	1.772921
	H	-2.160381	-0.994101	3.085062
	C	-4.303833	1.701516	-0.791501
	N	-4.625299	0.763780	-1.905087
	C	-5.850249	1.241594	-2.605956
	C	-4.894115	-0.594777	-1.345808
	C	-3.500419	0.702729	-2.912160
	C	-2.098091	0.653560	-2.343564
	O	-1.883455	-0.433894	-1.488870

	H	-4.022111	2.673595	-1.213767
	H	-3.486021	1.280726	-0.198411
	H	-5.196303	1.805456	-0.163036
	H	-6.037154	0.596489	-3.472684
	H	-5.694891	2.276923	-2.931960
	H	-6.696470	1.188486	-1.910465
	H	-5.684424	-0.510458	-0.591598
	H	-5.221158	-1.253876	-2.158646
	H	-3.970590	-0.972579	-0.901272
	H	-3.577479	1.608086	-3.529566
	H	-3.708649	-0.169391	-3.546957
	H	-1.424104	0.619858	-3.220043
	H	-1.876935	1.591424	-1.818102
	H	-1.273430	-0.117232	-0.785276
	C	1.102986	4.883167	1.959353
	C	0.771933	3.448660	2.334825
	O	0.363765	2.779263	1.162121
	O	1.509273	5.631492	3.081012
	H	1.939515	4.889319	1.243360
	H	0.231419	5.340248	1.454595
	H	1.661940	2.965180	2.773375
	H	-0.030307	3.431609	3.094367
	H	0.751367	5.727314	3.670780
	C	0.025665	3.726777	-1.934440
	C	-1.401022	3.949888	-1.459781
	O	-2.303781	4.268622	-2.210559
	O	-1.630891	3.805105	-0.168456
	N	0.196336	3.675885	-3.364864
	H	0.396778	2.799300	-1.475368
	H	0.627184	4.541692	-1.494023
	H	-0.286534	4.467390	-3.790002
	H	-0.276193	2.845656	-3.722491
	C	-4.052255	-4.347682	2.298000
	C	-5.204974	-3.372979	2.159111
	O	-5.065901	-2.527503	1.035473
	O	-2.819800	-3.704012	2.524859
	H	-4.259448	-5.015340	3.151829
	H	-4.009690	-4.978357	1.390300
	H	-6.144890	-3.936285	2.041631
	H	-5.290503	-2.767745	3.080548
	H	-4.396012	-1.841158	1.244677
	H	-2.460372	-3.436457	1.651434
	C	-2.106893	-4.073952	-0.944882
	C	-3.279522	-3.803462	-1.863827
	O	-4.536083	-3.937889	-1.244833
	O	-1.979649	-3.071243	0.047507
	H	-2.238174	-5.057530	-0.458333
	H	-1.185580	-4.125548	-1.548994
	H	-3.147302	-2.796281	-2.304601

	H	-3.244928	-4.529982	-2.692365
	H	-4.597101	-3.359109	-0.455540
	H	-1.092108	-2.660895	-0.045576
	C	1.000924	-2.063620	-1.712792
	C	1.885256	-0.868428	-2.013238
	O	1.190342	0.346965	-2.102768
	O	0.461058	-2.033322	-0.401895
	H	0.140833	-2.068547	-2.398759
	H	1.574505	-2.993865	-1.873957
	H	2.690414	-0.822875	-1.251276
	H	2.377625	-1.048527	-2.983619
	H	0.727455	0.531117	-1.244271
	H	1.174982	-2.118095	0.243853
	C	7.922451	-0.641781	0.089859
	H	8.533923	0.233465	-0.164391
	H	8.288819	-1.078289	1.029747
	C	7.974836	-1.662179	-1.032234
	H	7.355959	-2.543554	-0.776032
	H	7.559927	-1.218271	-1.958250
	C	-4.528657	0.221950	2.686493
	H	-4.420876	1.319567	2.697381
	H	-5.549215	-0.025938	2.363930
	H	-4.373682	-0.162474	3.710311
	O	9.318791	-2.024972	-1.200095
	C	9.511156	-2.991641	-2.200704
	H	10.586950	-3.208321	-2.257090
	H	8.971909	-3.929621	-1.970494
	H	9.170078	-2.629846	-3.188854
	H	-0.846146	3.421764	0.324844
PI_4_elimination_TS Imaginary frequencies=1 SCF energy=-2526.9614896				
	C	2.174822	1.557592	1.696503
	C	1.588386	0.969975	0.421851
	O	0.542360	0.082037	0.688176
	C	0.092896	-0.848005	-1.017187
	O	0.453708	-0.058187	-1.896524
	C	-1.356943	-1.043999	-0.673504
	C	-1.734367	-1.817194	0.429391
	C	-3.074648	-1.940513	0.763841
	C	-4.050945	-1.289206	0.000360
	C	-3.677572	-0.550130	-1.126063
	C	-2.332437	-0.438153	-1.465460
	C	-5.466638	-1.377428	0.455050
	O	-5.826169	-1.986722	1.438786
	H	1.507547	2.333983	2.115022
	H	1.238292	1.795034	-0.220835
	H	2.403097	0.462606	-0.121372
	H	-0.970829	-2.300981	1.040376
	H	-3.374068	-2.520527	1.637866
	H	-4.435539	-0.052840	-1.732475

	H	-2.032923	0.135872	-2.343999
	O	-6.304303	-0.703947	-0.324252
	O	3.428814	2.113013	1.366967
	H	2.303900	0.771762	2.463727
	C	2.269037	4.783959	-1.063658
	C	3.641344	4.261707	-1.431067
	O	3.751956	2.868073	-1.263364
	O	2.045583	4.631436	0.319688
	H	2.202898	5.849569	-1.361302
	H	1.512769	4.228512	-1.644146
	H	3.838742	4.488331	-2.491350
	H	4.405062	4.798929	-0.833801
	H	3.616784	2.664318	-0.316338
	H	1.125068	4.324492	0.459074
	C	-1.396705	4.047246	-0.411387
	C	-1.554295	2.854551	-1.332227
	O	-0.375973	2.583568	-2.056106
	O	-0.493483	3.821880	0.648648
	H	-1.024791	4.915657	-0.979499
	H	-2.397020	4.314914	-0.021876
	H	-1.854706	1.985582	-0.725018
	H	-2.391179	3.068449	-2.024976
	H	-0.155370	1.634772	-1.992795
	H	-0.775136	3.008894	1.132245
	C	-1.294217	1.307765	3.136601
	C	-2.098918	0.078684	3.512471
	O	-3.420737	0.163551	3.026392
	O	-1.330435	1.515207	1.740274
	H	-1.732474	2.199110	3.614428
	H	-0.257400	1.201053	3.503213
	H	-1.588788	-0.824725	3.125653
	H	-2.147711	-0.014539	4.608545
	H	-3.349053	0.414363	2.094610
	H	-0.662497	0.903415	1.305962
	C	0.648861	-3.128356	-1.447265
	H	1.486069	-3.793349	-1.193139
	C	0.582790	-2.962442	-2.957154
	H	1.456221	-2.383788	-3.309015
	H	-0.322438	-2.394939	-3.240717
	O	0.559951	-4.264499	-3.493907
	H	0.430348	-4.197743	-4.446442
	O	0.909853	-1.918143	-0.749618
	N	6.090487	-0.987143	-0.810858
	C	5.354604	-1.508269	-2.023757
	H	5.607214	-0.841896	-2.859935
	H	5.785781	-2.496502	-2.228120
	C	7.481930	-0.657986	-1.230662
	H	7.933679	-1.544475	-1.691707
	H	7.447265	0.167020	-1.952050

	H	8.056999	-0.360423	-0.345973
	C	6.141437	-2.033902	0.251226
	H	6.705975	-1.633719	1.102107
	H	5.123954	-2.276670	0.577139
	H	6.646623	-2.920682	-0.149096
	C	3.845090	-1.596663	-1.918477
	H	3.526537	-1.891775	-0.905318
	H	3.540790	-2.414086	-2.596943
	O	3.272794	-0.372767	-2.310087
	H	2.310695	-0.382222	-2.143023
	C	5.446226	0.237731	-0.256100
	H	6.093210	0.637159	0.534324
	H	5.317838	0.977411	-1.053150
	H	4.476747	-0.033450	0.170786
	H	-0.280559	-3.598745	-1.081953
	C	2.249438	-2.188901	2.202063
	O	1.049527	-1.694583	2.306202
	O	3.131379	-1.699062	1.509143
	C	4.014475	2.883212	2.384128
	H	4.981511	3.246347	2.009575
	H	3.385062	3.751751	2.647015
	H	4.186954	2.279735	3.293355
	C	-7.682705	-0.703931	0.037139
	H	-7.804293	-0.288217	1.049056
	H	-8.070819	-1.734043	0.033103
	C	-8.402228	0.146968	-0.985221
	H	-8.245184	-0.270792	-1.998858
	H	-7.985237	1.172953	-0.979263
	O	-9.761780	0.150869	-0.644248
	C	-10.548794	0.920129	-1.516837
	H	-11.590299	0.860210	-1.171826
	H	-10.236773	1.981364	-1.519682
	H	-10.496740	0.541215	-2.554798
	H	0.875690	-0.895196	1.597043
	C	2.472939	-3.443357	3.026172
	H	2.222590	-3.190922	4.069722
	H	1.711193	-4.173953	2.708351
	N	3.791595	-4.024876	2.946141
	H	3.997617	-4.257617	1.974669
	H	4.484967	-3.322118	3.202872
PI_5_product Imaginary frequencies=0 SCF energy=-2526.9957065				
	C	-1.536745	-1.070892	2.147369
	C	-1.468791	-0.153035	0.938947
	O	-0.139142	0.119344	0.569827
	C	-0.204922	2.261442	-1.772458
	O	-0.865149	1.420625	-2.358143
	C	1.224515	2.063469	-1.410884
	C	1.870229	2.909430	-0.505146
	C	3.163055	2.611349	-0.091124

	C	3.823922	1.490737	-0.600227
	C	3.192439	0.670995	-1.542878
	C	1.894120	0.956257	-1.940985
	C	5.183506	1.171510	-0.077223
	O	5.660525	1.680347	0.913336
	H	-1.107735	-2.060725	1.903974
	H	-1.972807	-0.613124	0.078760
	H	-1.998210	0.786151	1.178906
	H	1.358722	3.777036	-0.084992
	H	3.662810	3.247470	0.641669
	H	3.710356	-0.198532	-1.949790
	H	1.389561	0.314514	-2.664122
	O	5.819585	0.270937	-0.813303
	O	-2.877901	-1.202503	2.544716
	H	-0.932901	-0.633084	2.967784
	C	-3.310020	-5.001209	0.715918
	C	-3.997291	-3.688611	0.389778
	O	-3.297116	-2.900924	-0.548653
	O	-2.119440	-4.848102	1.455953
	H	-3.999676	-5.610576	1.322471
	H	-3.123985	-5.554867	-0.224949
	H	-4.983155	-3.911550	-0.049630
	H	-4.171424	-3.127907	1.326905
	H	-2.366833	-2.819397	-0.271807
	H	-1.454507	-4.427779	0.874194
	C	-0.209702	-3.610948	-1.570190
	C	0.119132	-2.315758	-2.280650
	O	-1.009497	-1.475475	-2.277128
	O	-0.528491	-3.404641	-0.207538
	H	-1.090601	-4.079765	-2.036182
	H	0.640801	-4.307647	-1.675566
	H	0.977790	-1.840133	-1.775805
	H	0.440348	-2.559015	-3.312384
	H	-0.736154	-0.546173	-2.309198
	H	0.235913	-2.961188	0.232536
	C	2.083144	-1.874401	1.989771
	C	3.285462	-0.952522	2.012901
	O	4.280396	-1.381767	1.107848
	O	1.518548	-1.927120	0.693820
	H	2.396459	-2.896928	2.254832
	H	1.342028	-1.541663	2.737153
	H	2.961424	0.081225	1.790239
	H	3.731452	-0.950047	3.019324
	H	3.856493	-1.466695	0.243611
	H	0.936614	-1.131191	0.574683
	C	-2.053199	3.752008	-1.636939
	H	-2.085258	4.838060	-1.791660
	C	-2.887674	3.360827	-0.431466
	H	-2.502755	3.880560	0.459799

	H	-2.794452	2.274984	-0.260575
	O	-4.220834	3.729542	-0.712608
	H	-4.716100	3.727888	0.114350
	O	-0.678362	3.436418	-1.405563
	N	-6.155875	-0.014502	-0.485849
	C	-5.656513	-0.242492	-1.893344
	H	-5.267176	-1.269583	-1.919228
	H	-6.542353	-0.182039	-2.538262
	C	-7.078416	-1.138826	-0.156109
	H	-7.881569	-1.172744	-0.901912
	H	-6.509107	-2.075684	-0.169802
	H	-7.498341	-0.969436	0.842107
	C	-6.903934	1.269448	-0.391982
	H	-7.299482	1.366553	0.626033
	H	-6.223388	2.101828	-0.599536
	H	-7.726903	1.257167	-1.116716
	C	-4.583200	0.694244	-2.399947
	H	-4.832448	1.749820	-2.195059
	H	-4.582369	0.574217	-3.498727
	O	-3.348507	0.331105	-1.846586
	H	-2.637331	0.898267	-2.185494
	C	-5.039756	-0.009818	0.506213
	H	-5.476096	-0.016908	1.511994
	H	-4.423000	-0.900079	0.347012
	H	-4.440479	0.894544	0.367202
	H	-2.409565	3.250234	-2.547982
	C	0.513700	2.741870	2.339573
	O	0.939915	1.554078	2.446551
	O	-0.581991	3.065744	1.844058
	C	-3.044732	-2.064065	3.640371
	H	-4.116128	-2.099616	3.883592
	H	-2.697917	-3.086784	3.405640
	H	-2.492317	-1.701649	4.527959
	C	7.063732	-0.218808	-0.322745
	H	6.963372	-0.493130	0.737799
	H	7.834866	0.561789	-0.414591
	C	7.414441	-1.429569	-1.157576
	H	7.465234	-1.150015	-2.228077
	H	6.621176	-2.194961	-1.048407
	O	8.648875	-1.911036	-0.700542
	C	9.084972	-3.056033	-1.386918
	H	10.051699	-3.356775	-0.959846
	H	8.371907	-3.894405	-1.275979
	H	9.220799	-2.857724	-2.466733
	H	0.270969	0.686799	1.288880
	C	1.412463	3.843735	2.893770
	H	2.458650	3.512288	2.813338
	H	1.187479	3.898732	3.979955
	N	1.216689	5.094849	2.183355

	H	0.214466	5.279998	2.144849
	H	1.630524	5.862365	2.709619

Pathway II

Compound	Coordinates			
PII_1_addition_pre_TS Imaginary frequencies=0 SCF energy=-2526.9886377				
	C	2.708072	1.061060	0.125408
	C	1.609527	2.073975	0.367678
	O	0.367315	1.448967	0.035204
	C	-0.735036	1.816650	0.668825
	O	-0.742514	2.579268	1.614582
	C	-1.954144	1.136592	0.144096
	C	-1.979395	0.564801	-1.133548
	C	-3.127663	-0.079818	-1.574541
	C	-4.250615	-0.163394	-0.742970
	C	-4.227297	0.419606	0.527846
	C	-3.081974	1.075973	0.965794
	C	-5.450974	-0.887652	-1.254917
	O	-5.520380	-1.387677	-2.355931
	H	2.752196	0.327729	0.950103
	H	1.590114	2.416544	1.409446
	H	1.741561	2.931588	-0.305531
	H	-1.104185	0.625552	-1.783565
	H	-3.155872	-0.535193	-2.565841
	H	-5.101614	0.357889	1.176531
	H	-3.046192	1.517066	1.963667
	O	-6.441921	-0.933967	-0.374211
	O	3.914166	1.778118	0.037807
	H	2.507395	0.506435	-0.808536
	C	3.966888	0.391973	4.001037
	C	3.444880	1.757340	3.589697
	O	2.048504	1.904619	3.738227
	O	3.636372	-0.648263	3.105192
	H	5.066664	0.440045	4.047521
	H	3.602821	0.164573	5.022244
	H	3.918699	2.514814	4.234861
	H	3.762017	1.970322	2.550718
	H	1.601516	1.176231	3.266577
	H	2.662152	-0.692269	3.022158
	C	0.063023	-0.908935	3.810908
	C	-1.338024	-0.341919	3.707888
	O	-1.411653	1.037133	3.990257
	O	0.922827	-0.407037	2.802963

	H	0.508318	-0.629360	4.778525
	H	0.014774	-2.010998	3.761548
	H	-1.744416	-0.571855	2.704732
	H	-1.974738	-0.859473	4.443156
	H	-1.031045	1.536732	3.252612
	H	0.639810	-0.762015	1.925138
	C	0.717564	-2.472848	-0.146708
	C	0.221074	-2.668541	-1.562347
	O	-1.181087	-2.819303	-1.613205
	O	0.120507	-1.324035	0.433775
	H	0.428078	-3.326794	0.483701
	H	1.814190	-2.383520	-0.147711
	H	0.558089	-1.815997	-2.183059
	H	0.670979	-3.581218	-1.982962
	H	-1.564648	-2.089953	-1.107689
	H	0.347786	-0.541645	-0.094091
	C	-0.806276	4.958705	-1.545537
	H	-0.689220	5.392041	-2.558672
	C	0.348186	5.431396	-0.677683
	H	1.296304	5.045728	-1.098946
	H	0.234033	5.005081	0.337185
	O	0.332486	6.842282	-0.657858
	H	1.070274	7.145953	-0.117672
	O	-0.905023	3.561649	-1.583711
	C	3.191802	1.500954	-3.439621
	H	3.772831	1.833533	-2.563676
	H	3.398318	2.226867	-4.246553
	N	5.090590	-3.768482	-0.147875
	C	5.212787	-3.335489	-1.591500
	H	5.995608	-2.564380	-1.612794
	H	5.575952	-4.216525	-2.138407
	C	6.373121	-4.426740	0.235717
	H	6.502013	-5.335097	-0.364402
	H	7.198541	-3.730047	0.047219
	H	6.332460	-4.681827	1.301205
	C	3.979165	-4.743464	0.031231
	H	4.032155	-5.144568	1.050098
	H	3.019404	-4.236715	-0.109693
	H	4.091987	-5.554534	-0.698297
	C	3.952860	-2.829987	-2.272167
	H	3.167230	-3.606446	-2.242899
	H	4.233203	-2.727447	-3.336108
	O	3.474602	-1.620817	-1.762891
	H	3.477632	-0.938548	-2.503740
	C	4.870353	-2.597553	0.752674

	H	4.783645	-2.963151	1.782380
	H	5.729789	-1.923329	0.664288
	H	3.957869	-2.078611	0.448885
	H	-1.747377	5.359226	-1.132056
	C	1.713253	1.646314	-3.077762
	O	0.984015	0.633738	-3.086474
	O	1.350103	2.820362	-2.796655
	N	3.564484	0.136578	-3.788367
	H	2.944867	-0.201982	-4.525426
	H	4.506744	0.125170	-4.178309
	C	5.050122	0.947383	0.018167
	H	5.929872	1.588385	-0.131441
	H	5.160502	0.404335	0.973947
	H	4.993190	0.211658	-0.802491
	C	-7.635455	-1.608513	-0.764695
	H	-7.406987	-2.654757	-1.019100
	H	-8.068090	-1.119222	-1.650734
	C	-8.586249	-1.535466	0.408989
	H	-8.786715	-0.476851	0.665157
	H	-8.125288	-2.012038	1.296131
	O	-9.762881	-2.197383	0.031849
	C	-10.742191	-2.205583	1.038372
	H	-11.619266	-2.741463	0.649861
	H	-10.386459	-2.721724	1.949808
	H	-11.048568	-1.180240	1.318404
	H	-0.104237	3.207472	-2.047072
PII_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.96756				
	C	2.609981	0.989450	0.110795
	C	1.515749	2.020720	0.319150
	O	0.289450	1.406986	-0.049616
	C	-0.847756	2.199502	-0.030209
	O	-0.942883	3.110964	0.818106
	C	-2.042576	1.311401	-0.329731
	C	-2.010844	0.367711	-1.362309
	C	-3.102216	-0.462760	-1.576648
	C	-4.236272	-0.360874	-0.759443
	C	-4.271880	0.591076	0.263861
	C	-3.175693	1.424470	0.473821
	C	-5.375775	-1.283016	-1.018784
	O	-5.382697	-2.128450	-1.887869
	H	2.708297	0.331278	0.993778
	H	1.476487	2.368702	1.360879
	H	1.709222	2.882906	-0.336977
	H	-1.129817	0.295064	-2.004571
	H	-3.080668	-1.206248	-2.375204

	H	-5.153496	0.678956	0.900225
	H	-3.189925	2.166736	1.274246
	O	-6.399301	-1.090542	-0.193995
	O	3.817048	1.672480	-0.126570
	H	2.350547	0.348972	-0.751855
	C	4.471713	0.545133	3.841018
	C	4.032937	1.905918	3.331306
	O	2.694480	2.223480	3.645186
	O	3.872480	-0.541111	3.165724
	H	5.560525	0.452223	3.700154
	H	4.272636	0.489465	4.928997
	H	4.667784	2.671240	3.807042
	H	4.207704	1.967355	2.241433
	H	2.115506	1.515825	3.305646
	H	2.905728	-0.497355	3.297745
	C	0.084346	0.159480	4.086979
	C	-0.925718	1.137247	3.520656
	O	-0.354891	2.412080	3.353587
	O	1.166081	-0.053365	3.198242
	H	0.509242	0.557670	5.021925
	H	-0.420768	-0.794080	4.322961
	H	-1.301537	0.741350	2.560168
	H	-1.790650	1.177621	4.211120
	H	-0.565292	2.729661	2.450730
	H	0.802412	-0.458701	2.374275
	C	0.712094	-2.163676	0.434154
	C	0.088909	-2.565667	-0.884626
	O	-1.261814	-2.944140	-0.730952
	O	0.002917	-1.090272	1.028008
	H	0.662325	-3.002323	1.145697
	H	1.769802	-1.901830	0.276309
	H	0.197355	-1.736192	-1.608940
	H	0.632405	-3.430903	-1.295141
	H	-1.701179	-2.228638	-0.251400
	H	0.090502	-0.285593	0.477883
	C	-1.026414	4.297467	-1.715262
	H	-1.401013	4.498502	-2.734277
	C	0.128558	5.236302	-1.408054
	H	0.971755	5.015696	-2.089094
	H	0.475630	5.056558	-0.374579
	O	-0.341601	6.555445	-1.577412
	H	0.378762	7.162099	-1.374158
	O	-0.660421	2.945900	-1.619748
	C	3.112137	1.130134	-3.587200
	H	3.748333	1.485643	-2.761112

	H	3.269210	1.830470	-4.427532
	N	4.858076	-3.902129	-0.027532
	C	4.933624	-3.626366	-1.512403
	H	5.748060	-2.901130	-1.646174
	H	5.230455	-4.575215	-1.980633
	C	6.104820	-4.620973	0.363783
	H	6.128433	-5.595475	-0.137854
	H	6.969915	-4.019685	0.060159
	H	6.106040	-4.757594	1.451594
	C	3.684464	-4.757010	0.302480
	H	3.756739	-5.052386	1.355732
	H	2.761463	-4.189154	0.146146
	H	3.697610	-5.647021	-0.338332
	C	3.664955	-3.136989	-2.188605
	H	2.859495	-3.882314	-2.063652
	H	3.907336	-3.134363	-3.266621
	O	3.235868	-1.875452	-1.769316
	H	3.282878	-1.249415	-2.552670
	C	4.780947	-2.631876	0.753515
	H	4.721507	-2.880834	1.819168
	H	5.685140	-2.045380	0.553267
	H	3.896832	-2.073173	0.437928
	H	-1.852684	4.495370	-1.012114
	C	1.673449	1.295255	-3.134127
	O	0.898850	0.338624	-3.101365
	O	1.376678	2.501828	-2.807558
	N	3.437477	-0.249537	-3.906977
	H	2.813039	-0.586751	-4.640692
	H	4.381933	-0.300425	-4.287421
	C	4.926012	0.810081	-0.204700
	H	5.803741	1.415977	-0.469128
	H	5.113236	0.313977	0.764656
	H	4.776145	0.032628	-0.974377
	C	-7.540877	-1.926761	-0.358048
	H	-7.255040	-2.981682	-0.226644
	H	-7.955712	-1.800659	-1.369871
	C	-8.545263	-1.507708	0.691998
	H	-8.808257	-0.440515	0.556090
	H	-8.100490	-1.615515	1.700542
	O	-9.671125	-2.329791	0.544787
	C	-10.689192	-2.045683	1.469579
	H	-11.521612	-2.736435	1.276321
	H	-10.345501	-2.187383	2.511429
	H	-11.057964	-1.008054	1.364864
	H	0.322305	2.672915	-2.228128

PII_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.9759235				
	C	-2.635635	-0.968758	0.242190
	C	-1.543762	-1.998408	0.477052
	O	-0.326734	-1.437550	0.020782
	C	0.795822	-2.338422	-0.044188
	O	0.926578	-3.123784	0.967639
	C	1.993092	-1.422697	-0.358075
	C	1.985834	-0.591477	-1.484094
	C	3.058190	0.252965	-1.739161
	C	4.156877	0.275886	-0.869220
	C	4.175510	-0.569328	0.244940
	C	3.096386	-1.414487	0.492909
	C	5.272998	1.212309	-1.168926
	O	5.287955	1.976455	-2.110592
	H	-2.688836	-0.249093	1.080148
	H	-1.475485	-2.274143	1.539726
	H	-1.786591	-2.905633	-0.098983
	H	1.130116	-0.607424	-2.162239
	H	3.048378	0.911989	-2.609041
	H	5.031719	-0.564536	0.921076
	H	3.098247	-2.076539	1.360601
	O	6.268264	1.135609	-0.291015
	O	-3.864626	-1.640630	0.100588
	H	-2.404356	-0.391873	-0.672193
	C	-4.317040	-0.247961	4.007956
	C	-3.916085	-1.646818	3.575456
	O	-2.570606	-1.962973	3.859527
	O	-3.726082	0.781009	3.241950
	H	-5.408806	-0.146423	3.899059
	H	-4.078787	-0.124090	5.082440
	H	-4.541833	-2.368387	4.125791
	H	-4.133755	-1.778897	2.499543
	H	-1.996172	-1.294678	3.440979
	H	-2.755186	0.722756	3.335050
	C	0.066873	0.064088	4.075461
	C	1.063981	-0.933243	3.518548
	O	0.490589	-2.207000	3.384402
	O	-1.032192	0.248799	3.201254
	H	-0.340867	-0.302937	5.030755
	H	0.576623	1.024658	4.270923
	H	1.430307	-0.556377	2.546497
	H	1.938100	-0.957030	4.199656
	H	0.669565	-2.547550	2.468348
	H	-0.676891	0.576539	2.339419
	C	-0.669907	2.070559	0.267134

	C	-0.137032	2.337777	-1.124048
	O	1.214561	2.742370	-1.093351
	O	0.086736	1.069021	0.921217
	H	-0.587529	2.980818	0.881668
	H	-1.732839	1.789516	0.209342
	H	-0.274833	1.435498	-1.749420
	H	-0.717595	3.149506	-1.589537
	H	1.692525	2.080391	-0.574881
	H	-0.037790	0.202828	0.470020
	C	1.167893	-4.297106	-1.493707
	H	1.445260	-4.371122	-2.558166
	C	0.263617	-5.458722	-1.124549
	H	-0.688548	-5.359890	-1.680491
	H	0.031819	-5.403255	-0.046342
	O	0.937213	-6.652330	-1.456353
	H	0.379072	-7.395198	-1.201506
	O	0.509008	-3.066403	-1.303660
	C	-3.397781	-1.374935	-3.479099
	H	-4.010068	-1.652218	-2.606332
	H	-3.588862	-2.141744	-4.251726
	N	-4.658367	3.963471	-0.152629
	C	-4.960206	3.586661	-1.585620
	H	-5.811436	2.892835	-1.545204
	H	-5.286726	4.510719	-2.082227
	C	-5.770238	4.828832	0.335918
	H	-5.770436	5.765976	-0.233137
	H	-6.719616	4.299646	0.191166
	H	-5.614173	5.035037	1.401432
	C	-3.379760	4.719002	-0.049134
	H	-3.274352	5.078662	0.981071
	H	-2.542596	4.057717	-0.293133
	H	-3.407978	5.568168	-0.742728
	C	-3.819970	2.993210	-2.393098
	H	-2.999060	3.727202	-2.481098
	H	-4.231187	2.876910	-3.411922
	O	-3.344071	1.774018	-1.901852
	H	-3.427596	1.091129	-2.628719
	C	-4.587357	2.747277	0.711894
	H	-4.327095	3.056797	1.730435
	H	-5.568958	2.259265	0.706826
	H	-3.833217	2.069511	0.304792
	H	2.094287	-4.336858	-0.898214
	C	-1.957443	-1.518509	-3.057749
	O	-1.144890	-0.614897	-3.108664
	O	-1.688595	-2.730846	-2.631468

	N	-3.704454	-0.020116	-3.895955
	H	-3.139638	0.229103	-4.709031
	H	-4.677331	0.030919	-4.195951
	C	-4.957623	-0.759932	0.007102
	H	-5.859051	-1.361197	-0.176092
	H	-5.092604	-0.190850	0.944747
	H	-4.825694	-0.042403	-0.822164
	C	7.382302	2.001427	-0.485576
	H	7.052130	3.051039	-0.449886
	H	7.838084	1.812200	-1.469576
	C	8.364401	1.709331	0.626691
	H	8.674910	0.647112	0.584140
	H	7.880125	1.876002	1.608705
	O	9.460879	2.565168	0.451163
	C	10.462598	2.388150	1.419432
	H	11.271799	3.098493	1.200327
	H	10.083795	2.586050	2.439730
	H	10.875663	1.362237	1.396635
	H	-0.779512	-2.788686	-2.202201
PII_4_elimination_TS Imaginary frequencies=1 SCF energy=-2526.9689827				
	C	2.886445	0.164956	0.797582
	C	2.443398	-1.285397	0.896629
	O	1.051611	-1.385255	1.016230
	C	0.426631	-2.974559	0.332604
	O	0.872479	-3.092330	-0.821475
	C	-1.033168	-2.634999	0.559819
	C	-1.555062	-2.427579	1.839903
	C	-2.871646	-2.012647	1.996551
	C	-3.683900	-1.820095	0.873825
	C	-3.186868	-2.107333	-0.401199
	C	-1.865091	-2.509266	-0.553553
	C	-5.027222	-1.211557	1.064378
	O	-5.578946	-1.079678	2.135833
	H	2.711508	0.555465	-0.219656
	H	2.783980	-1.830978	0.001419
	H	2.949112	-1.730545	1.775664
	H	-0.918194	-2.552563	2.717014
	H	-3.269343	-1.799444	2.990759
	H	-3.825934	-1.991464	-1.277469
	H	-1.463711	-2.707720	-1.548337
	O	-5.544213	-0.772233	-0.076812
	O	4.257008	0.231672	1.115755
	H	2.304257	0.788195	1.501241
	C	4.997556	-0.057158	-2.868651
	C	4.799997	-1.310306	-2.033196

	O	3.628281	-2.032578	-2.348588
	O	4.156117	1.016867	-2.508508
	H	6.035566	0.288321	-2.735662
	H	4.872642	-0.319864	-3.937991
	H	5.650583	-1.986604	-2.215798
	H	4.823803	-1.029429	-0.962907
	H	2.857058	-1.439900	-2.254797
	H	3.224957	0.713668	-2.541877
	C	1.010345	-0.215205	-3.752019
	C	-0.159028	-1.178275	-3.679930
	O	0.219688	-2.498102	-3.378739
	O	1.682918	-0.090063	-2.513160
	H	1.751164	-0.580121	-4.481029
	H	0.646926	0.769402	-4.099071
	H	-0.897445	-0.794372	-2.950745
	H	-0.654055	-1.185426	-4.665034
	H	0.474916	-2.566547	-2.434275
	H	1.026972	0.141208	-1.803738
	C	-0.788130	1.519805	-0.321324
	C	-2.266529	1.304048	-0.073047
	O	-2.962933	0.923491	-1.242084
	O	-0.126527	0.323694	-0.674964
	H	-0.674608	2.214503	-1.168823
	H	-0.327663	1.981172	0.565729
	H	-2.400319	0.559665	0.732211
	H	-2.710741	2.250546	0.272536
	H	-2.595203	0.081738	-1.539674
	H	0.186273	-0.205573	0.101714
	C	1.691953	-4.925236	0.909760
	H	1.626660	-5.652158	1.732609
	C	3.162936	-4.598505	0.678087
	H	3.556277	-4.047789	1.546338
	H	3.283610	-3.962213	-0.214208
	O	3.912780	-5.788832	0.563322
	H	3.670177	-6.216275	-0.267037
	O	0.891847	-3.826593	1.314236
	C	0.700726	1.375733	4.579303
	H	1.791547	1.295927	4.688966
	H	0.255106	0.971328	5.508319
	N	1.927577	4.654286	-0.785544
	C	2.651178	4.957388	0.509575
	H	3.607001	4.418788	0.452743
	H	2.860387	6.035423	0.504478
	C	2.552015	5.472457	-1.864564
	H	2.356805	6.533454	-1.669220

	H	3.631683	5.281454	-1.872261
	H	2.113944	5.179096	-2.825950
	C	0.480645	4.993839	-0.695901
	H	0.035083	4.863674	-1.689105
	H	-0.006273	4.321948	0.018421
	H	0.377143	6.037407	-0.375119
	C	1.917598	4.638754	1.795789
	H	1.011076	5.265599	1.876987
	H	2.600547	4.983276	2.595990
	O	1.615281	3.279608	1.922519
	H	1.130462	3.143126	2.785512
	C	2.083841	3.211535	-1.140668
	H	1.487101	3.005559	-2.036922
	H	3.141643	3.014513	-1.347381
	H	1.742556	2.606165	-0.298686
	H	1.266381	-5.389970	0.004706
	C	0.267542	0.470262	3.449423
	O	-0.628644	0.783120	2.683434
	O	0.929541	-0.653069	3.377051
	N	0.328278	2.751271	4.291293
	H	-0.683580	2.813060	4.172178
	H	0.566711	3.347594	5.082496
	C	4.784037	1.529122	1.002973
	H	5.824278	1.502905	1.357342
	H	4.775835	1.879725	-0.044366
	H	4.215049	2.247634	1.621161
	C	-6.764436	-0.041287	-0.029736
	H	-6.717700	0.716278	0.766943
	H	-7.603842	-0.721998	0.181272
	C	-6.911682	0.619491	-1.382571
	H	-6.980299	-0.150373	-2.175840
	H	-6.008697	1.227430	-1.587477
	O	-8.067090	1.411781	-1.345665
	C	-8.313135	2.086187	-2.552621
	H	-9.227637	2.681937	-2.425410
	H	-7.480694	2.765136	-2.816705
	H	-8.463289	1.380631	-3.391308
	H	0.832215	-1.057574	2.408485
PII_5_product Imaginary frequencies=0 SCF energy=-2526.9996633				
	C	2.873626	0.773625	1.033604
	C	2.845779	-0.744205	1.037474
	O	1.583872	-1.263977	1.381827
	C	0.779564	-3.803899	-0.157255
	O	1.284720	-3.591471	-1.242761
	C	-0.591250	-3.355999	0.212732

	C	-0.918000	-3.040798	1.534654
	C	-2.157342	-2.483618	1.820997
	C	-3.085152	-2.276502	0.795948
	C	-2.780787	-2.656625	-0.516340
	C	-1.528207	-3.180221	-0.808573
	C	-4.349177	-1.556701	1.125033
	O	-4.619365	-1.133379	2.227565
	H	2.230706	1.162252	0.222628
	H	3.096303	-1.119147	0.035764
	H	3.623408	-1.105623	1.733789
	H	-0.183307	-3.174987	2.329114
	H	-2.399544	-2.173277	2.838197
	H	-3.509402	-2.509789	-1.314674
	H	-1.263403	-3.430450	-1.837388
	O	-5.133582	-1.388010	0.069480
	O	4.208452	1.175672	0.856976
	H	2.476298	1.157647	1.992156
	C	4.515747	0.622063	-2.916810
	C	4.758925	-0.693260	-2.197894
	O	3.714675	-1.633948	-2.339446
	O	3.587178	1.464565	-2.270181
	H	5.469603	1.171327	-2.964768
	H	4.206571	0.408237	-3.959364
	H	5.667526	-1.158451	-2.612728
	H	4.956425	-0.470579	-1.131754
	H	2.855652	-1.197283	-2.173851
	H	2.746755	0.976068	-2.159753
	C	0.682368	-0.031089	-3.350193
	C	-0.326505	-1.148590	-3.521938
	O	0.264950	-2.423254	-3.596658
	O	1.410952	-0.151972	-2.143422
	H	1.415970	-0.057789	-4.171322
	H	0.156846	0.940388	-3.394243
	H	-1.066970	-1.093357	-2.700865
	H	-0.874256	-0.979338	-4.462799
	H	0.642205	-2.657074	-2.730078
	H	0.776741	-0.200739	-1.378734
	C	-0.730595	1.141463	0.070511
	C	-2.198045	1.204528	0.431383
	O	-3.024471	0.764867	-0.629331
	O	-0.314060	-0.189552	-0.172605
	H	-0.575270	1.712918	-0.859166
	H	-0.127626	1.610726	0.862399
	H	-2.379893	0.618751	1.349355
	H	-2.470980	2.250321	0.643206

	H	-2.732890	-0.122791	-0.875069
	H	0.263986	-0.533913	0.550076
	C	2.674148	-5.040228	0.544799
	H	2.804663	-5.820712	1.304945
	C	3.787981	-4.010495	0.672313
	H	3.682364	-3.488328	1.634853
	H	3.713514	-3.264498	-0.135265
	O	5.043051	-4.649658	0.669301
	H	5.228868	-4.946797	-0.229646
	O	1.382843	-4.479427	0.804669
	C	0.609783	1.765543	4.426357
	H	1.685589	1.994857	4.398817
	H	0.336465	1.643167	5.491801
	N	0.738276	4.945651	-1.101615
	C	1.446364	5.541946	0.097902
	H	2.519445	5.381276	-0.074731
	H	1.249793	6.622106	0.075324
	C	0.872760	5.896261	-2.242065
	H	0.322779	6.815875	-2.009704
	H	1.935869	6.119208	-2.392673
	H	0.458244	5.426237	-3.141742
	C	-0.707939	4.722767	-0.824546
	H	-1.188410	4.380626	-1.748637
	H	-0.812450	3.959243	-0.047262
	H	-1.158780	5.667188	-0.496763
	C	1.029996	5.022034	1.458906
	H	-0.023396	5.289555	1.657462
	H	1.633827	5.611256	2.176908
	O	1.244833	3.649474	1.600682
	H	0.717808	3.332118	2.395368
	C	1.382167	3.654073	-1.488934
	H	0.807728	3.206577	-2.309040
	H	2.405001	3.859328	-1.823609
	H	1.393722	2.998585	-0.615670
	H	2.676790	-5.503727	-0.453301
	C	0.373705	0.408584	3.760315
	O	-0.718588	0.225722	3.188377
	O	1.303054	-0.440473	3.856164
	N	-0.153661	2.815917	3.763390
	H	-1.069679	2.430745	3.524323
	H	-0.315161	3.598795	4.395527
	C	4.381686	2.567958	0.811780
	H	5.458698	2.766788	0.717351
	H	3.864471	3.016061	-0.053856
	H	4.008149	3.054521	1.731157

	C	-6.273318	-0.546558	0.216234
	H	-6.002174	0.353361	0.787739
	H	-7.065909	-1.083520	0.760131
	C	-6.722032	-0.176886	-1.179791
	H	-6.949520	-1.092046	-1.760510
	H	-5.899876	0.354732	-1.697516
	O	-7.855248	0.638490	-1.054582
	C	-8.364657	1.071139	-2.289704
	H	-9.243241	1.700001	-2.089691
	H	-7.621263	1.667882	-2.850907
	H	-8.675043	0.219703	-2.924037
	H	1.431675	-1.092381	2.350456

Pathway II a

Compound	Coordinates			
PII_a_1_addition_pre_TS				
Imaginary frequencies=0	C	2.792866	1.297800	0.400205
SCF energy=-2526.97421	C	2.105173	0.308742	-0.521825
	O	0.769273	0.087802	-0.071644
	C	-0.254230	0.562200	-0.761518
	O	-0.137120	1.304768	-1.714034
	C	-1.566599	0.093985	-0.231175
	C	-1.639344	-0.861962	0.787904
	C	-2.879926	-1.298607	1.234084
	C	-4.051196	-0.790170	0.664288
	C	-3.978237	0.165243	-0.355024
	C	-2.737448	0.607118	-0.799676
	C	-5.358893	-1.297513	1.174104
	O	-5.467073	-2.112840	2.063251
	H	2.392090	2.316146	0.256831
	H	2.102770	0.665177	-1.559769
	H	2.602132	-0.669431	-0.466450
	H	-0.727111	-1.283973	1.209465
	H	-2.948473	-2.046863	2.025440
	H	-4.889640	0.567492	-0.797826
	H	-2.673742	1.362690	-1.584092
	O	-6.398397	-0.764303	0.547703
	O	4.164019	1.263034	0.104623
	H	2.609571	1.009408	1.453889
	C	3.386360	5.062179	-1.558721
	C	3.278967	3.723762	-2.266216
	O	1.952737	3.296380	-2.486783
	O	3.066364	5.018140	-0.184816
	H	4.427632	5.414614	-1.636021
	H	2.750505	5.796577	-2.091860
	H	3.755076	3.818113	-3.255997

	H	3.853628	2.966501	-1.698439
	H	1.446635	3.361416	-1.655084
	H	2.147377	4.696478	-0.087459
	C	-0.516510	4.857474	-0.376471
	C	-1.785090	4.167923	-0.835816
	O	-1.671633	3.588772	-2.114316
	O	0.554836	3.952447	-0.179413
	H	-0.185855	5.574571	-1.143778
	H	-0.722824	5.421273	0.550670
	H	-2.088142	3.422904	-0.075176
	H	-2.587832	4.921246	-0.882675
	H	-1.076773	2.821786	-2.049743
	H	0.330183	3.310398	0.532507
	C	-0.741581	2.687614	2.951287
	C	-2.038364	1.957519	3.226962
	O	-2.977159	2.123214	2.187883
	O	-0.126398	2.226255	1.761135
	H	-0.942102	3.758558	2.796057
	H	-0.060229	2.587730	3.813181
	H	-1.828886	0.884571	3.404393
	H	-2.487551	2.361461	4.147250
	H	-2.579895	1.771582	1.380734
	H	0.207695	1.327099	1.879317
	C	-0.828745	-2.729118	-2.829265
	H	-1.177627	-2.305516	-3.785912
	C	-2.032649	-3.030550	-1.951702
	H	-2.587708	-2.094709	-1.755019
	H	-1.676463	-3.419457	-0.978316
	O	-2.835785	-3.975928	-2.624280
	H	-3.603123	-4.165829	-2.073344
	O	0.049567	-1.810656	-2.236823
	C	2.377701	-4.075283	-1.635607
	H	2.344788	-3.145377	-2.225071
	H	1.550189	-4.706040	-2.023585
	N	5.543572	-2.052934	1.387755
	C	6.594113	-1.109953	1.920693
	H	6.130750	-0.115978	1.965811
	H	6.798066	-1.438667	2.947773
	C	4.277836	-1.770410	2.128267
	H	4.473470	-1.855867	3.204100
	H	3.956018	-0.751658	1.885981
	H	3.518847	-2.501319	1.822248
	C	5.934932	-3.470453	1.629902
	H	5.129468	-4.114213	1.257013
	H	6.864317	-3.689059	1.092457
	H	6.074881	-3.622828	2.706776
	C	7.888181	-1.010182	1.146288
	H	8.259428	-2.006321	0.847276
	H	8.630631	-0.592901	1.849614

	O	7.714675	-0.163285	0.033734
	H	8.531685	-0.161115	-0.478431
	C	5.300881	-1.860519	-0.072306
	H	4.498999	-2.543729	-0.375612
	H	5.019474	-0.816290	-0.246257
	H	6.212430	-2.109340	-0.625078
	H	-0.322434	-3.686018	-3.066201
	C	1.994775	-3.734625	-0.196055
	O	2.636776	-4.255895	0.737705
	O	1.013575	-2.949867	-0.043420
	N	3.688452	-4.686261	-1.736729
	H	3.714972	-5.501134	-1.124506
	H	3.830248	-5.035911	-2.682899
	C	4.929747	2.134048	0.900818
	H	5.979536	2.020694	0.598542
	H	4.616797	3.182998	0.758108
	H	4.835328	1.884803	1.974405
	C	-7.698286	-1.186161	0.953165
	H	-7.853177	-0.948430	2.016670
	H	-7.796314	-2.274314	0.819322
	C	-8.689150	-0.445346	0.083697
	H	-8.496896	-0.674835	-0.982584
	H	-8.563444	0.646797	0.217640
	O	-9.972110	-0.858788	0.467560
	C	-10.996243	-0.241088	-0.268797
	H	-11.956234	-0.627075	0.101054
	H	-10.983719	0.857810	-0.142818
	H	-10.915657	-0.466801	-1.348694
	H	0.408632	-2.221522	-1.406489
PII_a_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.950811				
	C	-2.677773	1.425601	-0.680975
	C	-2.038138	0.458290	0.295184
	O	-0.704716	0.204142	-0.119408
	C	0.281950	0.268643	0.840146
	O	0.242093	1.141512	1.720933
	C	1.601292	-0.174817	0.249224
	C	1.664000	-1.078937	-0.817122
	C	2.895556	-1.504270	-1.295588
	C	4.079272	-1.038885	-0.710300
	C	4.018237	-0.134212	0.353409
	C	2.782059	0.299179	0.825023
	C	5.376135	-1.524719	-1.257298
	O	5.475722	-2.302655	-2.181601
	H	-2.238994	2.433595	-0.574808
	H	-2.047422	0.877973	1.310302
	H	-2.589704	-0.495540	0.292474
	H	0.744837	-1.463516	-1.260139
	H	2.950389	-2.207494	-2.128681
	H	4.935568	0.239930	0.809234

	H	2.730417	1.020709	1.641490
	O	6.427402	-1.017326	-0.624767
	O	-4.055309	1.463230	-0.409530
	H	-2.493164	1.086012	-1.719814
	C	-3.188570	5.084346	1.445536
	C	-3.119622	3.727514	2.122926
	O	-1.809533	3.302701	2.428082
	O	-2.778554	5.079088	0.095202
	H	-4.235148	5.429313	1.463467
	H	-2.593938	5.807264	2.038704
	H	-3.666942	3.791513	3.077781
	H	-3.646859	2.984778	1.493442
	H	-1.255803	3.361800	1.625705
	H	-1.853061	4.762397	0.052858
	C	0.836455	4.759674	0.508990
	C	2.023073	3.931838	0.962179
	O	1.809041	3.281127	2.190100
	O	-0.298660	3.965985	0.217293
	H	0.540830	5.454415	1.310657
	H	1.125589	5.359333	-0.372974
	H	2.287342	3.214248	0.161161
	H	2.885376	4.608442	1.081850
	H	1.207796	2.522782	2.034872
	H	-0.083673	3.339228	-0.514162
	C	0.877837	2.466255	-2.983295
	C	2.108115	1.612806	-3.210665
	O	3.086465	1.822364	-2.217294
	O	0.331505	2.247425	-1.699202
	H	1.148944	3.532311	-3.021141
	H	0.133254	2.273933	-3.775143
	H	1.815568	0.546147	-3.258549
	H	2.555470	1.875015	-4.181771
	H	2.685439	1.591080	-1.368509
	H	-0.014319	1.347170	-1.588202
	C	0.590538	-1.686629	2.767186
	H	1.159165	-0.817575	3.149667
	C	1.552677	-2.812600	2.420503
	H	2.264480	-2.473155	1.645869
	H	0.980324	-3.658290	1.992854
	O	2.220094	-3.185471	3.605987
	H	2.860929	-3.871897	3.390482
	O	-0.182132	-1.289021	1.676070
	H	-0.606873	-2.162554	0.907421
	C	-2.535424	-3.316889	1.964168
	H	-2.517540	-2.235600	2.174157
	H	-1.721861	-3.754200	2.579544
	N	-5.597496	-1.910459	-1.293818
	C	-6.625756	-1.036512	-1.973007
	H	-6.407758	-0.007664	-1.655429

	H	-6.436045	-1.113713	-3.051875
	C	-4.288058	-1.656765	-1.962356
	H	-4.351180	-1.991297	-3.004671
	H	-4.081169	-0.582212	-1.921041
	H	-3.507257	-2.218807	-1.438815
	C	-5.930919	-3.356623	-1.415012
	H	-5.077163	-3.932548	-1.037613
	H	-6.818202	-3.575756	-0.810519
	H	-6.113996	-3.597343	-2.469474
	C	-8.080438	-1.371999	-1.738478
	H	-8.303004	-2.395966	-2.084004
	H	-8.641621	-0.687199	-2.400403
	O	-8.439779	-1.190418	-0.390256
	H	-9.356921	-1.468263	-0.280763
	C	-5.475152	-1.554361	0.154054
	H	-4.799205	-2.270560	0.640698
	H	-5.086124	-0.531619	0.223232
	H	-6.468197	-1.615008	0.608438
	H	-0.060694	-2.024152	3.596114
	C	-2.118612	-3.522209	0.518675
	O	-2.755229	-4.256463	-0.232195
	O	-1.047541	-2.905463	0.135717
	N	-3.850232	-3.856536	2.229692
	H	-3.858638	-4.850776	2.004628
	H	-4.052768	-3.783501	3.224918
	C	-4.758682	2.363185	-1.229180
	H	-5.811563	2.351597	-0.915522
	H	-4.363934	3.388987	-1.122319
	H	-4.697826	2.071385	-2.294177
	C	7.719986	-1.420649	-1.067617
	H	7.855784	-1.147893	-2.125382
	H	7.825220	-2.512239	-0.971576
	C	8.724418	-0.704325	-0.193010
	H	8.554528	-0.970494	0.868554
	H	8.590323	0.390971	-0.287442
	O	10.002187	-1.096526	-0.615075
	C	11.036535	-0.497240	0.122104
	H	11.991608	-0.865173	-0.277707
	H	11.015841	0.605139	0.032656
	H	10.977262	-0.758494	1.195370
PII_a_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.9593227				
	C	-2.346829	1.433599	-0.772136
	C	-1.870515	0.508261	0.330002
	O	-0.529629	0.151994	0.054246
	C	0.325186	-0.056833	1.204958
	O	0.347988	0.906919	2.049063
	C	1.670499	-0.484527	0.592729
	C	1.727008	-1.447522	-0.422537
	C	2.946987	-1.823572	-0.966078

	C	4.133721	-1.244335	-0.498627
	C	4.081819	-0.291362	0.522822
	C	2.853392	0.081238	1.064637
	C	5.413836	-1.647869	-1.138535
	O	5.505809	-2.483908	-2.012253
	H	-1.817179	2.402136	-0.717349
	H	-1.939544	1.015388	1.304166
	H	-2.502929	-0.396081	0.351061
	H	0.807915	-1.903513	-0.793869
	H	2.990935	-2.562452	-1.768439
	H	5.001095	0.165009	0.892778
	H	2.807404	0.831319	1.855486
	O	6.464926	-0.989782	-0.660504
	O	-3.730031	1.626492	-0.620911
	H	-2.122315	0.980336	-1.758646
	C	-2.800115	5.207292	1.188893
	C	-2.902912	3.878462	1.916639
	O	-1.668886	3.376791	2.382596
	O	-2.251903	5.117756	-0.108194
	H	-3.815423	5.622851	1.082269
	H	-2.221386	5.912754	1.817895
	H	-3.545125	4.020261	2.801437
	H	-3.409676	3.147609	1.257790
	H	-1.035931	3.345136	1.639535
	H	-1.354199	4.731014	-0.039113
	C	1.215084	4.575296	0.808305
	C	2.278737	3.668920	1.397466
	O	1.859408	2.993413	2.554281
	O	0.097681	3.852230	0.327076
	H	0.839411	5.261794	1.583412
	H	1.659765	5.183789	-0.000040
	H	2.615369	2.960992	0.614835
	H	3.149497	4.294412	1.658563
	H	1.280338	2.231858	2.295228
	H	0.390320	3.206436	-0.362737
	C	0.781259	1.942341	-2.757357
	C	1.481010	0.723445	-3.323229
	O	2.841042	0.685534	-2.953973
	O	0.901139	1.968457	-1.349280
	H	1.260141	2.858829	-3.135121
	H	-0.277028	1.953929	-3.073056
	H	0.951539	-0.189325	-2.985162
	H	1.431675	0.746592	-4.422747
	H	2.872158	0.778371	-1.991684
	H	0.371113	1.241502	-0.951483
	C	0.241609	-1.763607	2.991558
	H	0.826505	-0.972879	3.486677
	C	1.088569	-3.004600	2.765523
	H	2.000517	-2.744658	2.198481

	H	0.512096	-3.724593	2.153066
	O	1.403266	-3.534043	4.033648
	H	1.987312	-4.290373	3.909970
	O	-0.293203	-1.281159	1.779769
	H	-0.958000	-2.295363	0.766821
	C	-2.895245	-3.123348	1.957952
	H	-2.780074	-2.039905	2.122300
	H	-2.113806	-3.607478	2.579846
	N	-5.675836	-1.505652	-1.469813
	C	-6.584680	-0.540476	-2.195191
	H	-6.279520	0.464461	-1.874110
	H	-6.362598	-0.643920	-3.265537
	C	-4.330007	-1.417744	-2.108833
	H	-4.401842	-1.779086	-3.141474
	H	-4.007966	-0.371135	-2.093234
	H	-3.626878	-2.041052	-1.546382
	C	-6.170992	-2.906588	-1.563017
	H	-5.405026	-3.565747	-1.137327
	H	-7.098358	-2.999520	-0.986732
	H	-6.344238	-3.158583	-2.616503
	C	-8.073176	-0.732641	-2.017231
	H	-8.382864	-1.724550	-2.388115
	H	-8.539492	0.013449	-2.686591
	O	-8.462229	-0.536344	-0.679403
	H	-9.401833	-0.740895	-0.604117
	C	-5.550266	-1.124418	-0.028666
	H	-4.986151	-1.905140	0.497376
	H	-5.033038	-0.159252	0.026654
	H	-6.555299	-1.045043	0.395335
	H	-0.594547	-2.021342	3.662493
	C	-2.522706	-3.422823	0.524633
	O	-3.194694	-4.125655	-0.204926
	O	-1.394652	-2.899149	0.090558
	N	-4.248995	-3.533229	2.248923
	H	-4.336124	-4.540593	2.118363
	H	-4.451633	-3.350907	3.229934
	C	-4.270111	2.536046	-1.546558
	H	-5.341334	2.644103	-1.326625
	H	-3.786741	3.524793	-1.458455
	H	-4.151836	2.174365	-2.585042
	C	7.738826	-1.292440	-1.221092
	H	7.725985	-1.102151	-2.305263
	H	7.979347	-2.353930	-1.055642
	C	8.744362	-0.397578	-0.531864
	H	8.734680	-0.590136	0.558745
	H	8.467871	0.663827	-0.685401
	O	10.001671	-0.678184	-1.084762
	C	11.034406	0.098611	-0.534826
	H	11.972031	-0.188824	-1.030491

	H	10.863744	1.179205	-0.698650
	H	11.140827	-0.074198	0.552582

Pathway II b

Compound	Coordinates			
PII_b_1_addition_pre_TS Imaginary frequencies=0 SCF energy=-2526.99316				
	C	4.062304	-0.197318	0.792336
	C	3.125047	-0.115543	1.981630
	O	1.764332	-0.163593	1.547650
	C	1.159008	-1.328188	1.416386
	O	1.695512	-2.396245	1.640660
	C	-0.260036	-1.197011	0.979346
	C	-0.706319	-0.053673	0.310178
	C	-2.030633	0.026544	-0.101569
	C	-2.917157	-1.018549	0.176572
	C	-2.467627	-2.161911	0.847691
	C	-1.138798	-2.252436	1.242048
	C	-4.342677	-0.869753	-0.228933
	O	-4.808571	0.127476	-0.746415
	H	4.011203	-1.197121	0.332584
	H	3.318799	-0.923520	2.700899
	H	3.233647	0.855446	2.481182
	H	-0.016545	0.768145	0.113530
	H	-2.385676	0.910611	-0.631019
	H	-3.158529	-2.976580	1.066441
	H	-0.780254	-3.142082	1.761575
	O	-5.075684	-1.933809	0.039816
	O	5.360621	0.070262	1.258821
	H	3.763330	0.535481	0.024077
	C	5.944859	-3.742941	-0.992077
	C	5.442469	-3.682894	0.439328
	O	4.061195	-3.935895	0.569218
	O	5.572680	-2.638279	-1.786593
	H	7.046480	-3.771137	-0.976120
	H	5.597937	-4.693701	-1.443893
	H	5.966693	-4.457366	1.022510
	H	5.714850	-2.702754	0.880169
	H	3.566949	-3.332285	-0.015463
	H	4.599461	-2.540247	-1.763419
	C	2.033197	-3.275671	-2.205918
	C	0.706216	-3.557396	-1.532372
	O	0.837756	-4.291368	-0.337266
	O	2.859711	-2.429622	-1.426597
	H	2.585375	-4.218439	-2.345085
	H	1.854850	-2.834713	-3.202371
	H	0.177554	-2.599193	-1.364704
	H	0.086102	-4.154064	-2.220669

	H	1.217336	-3.713949	0.345430
	H	2.499381	-1.509411	-1.435168
	C	2.117011	0.378002	-3.115080
	C	1.107805	1.391125	-3.618697
	O	-0.217150	0.930608	-3.459433
	O	1.836234	0.018167	-1.776297
	H	2.055247	-0.544395	-3.713475
	H	3.137599	0.786296	-3.214812
	H	1.258202	2.350123	-3.088114
	H	1.274026	1.576627	-4.690844
	H	-0.295196	0.615439	-2.548291
	H	1.867384	0.833225	-1.215947
	C	-0.504534	2.312418	3.692916
	H	-0.014454	3.163194	4.204404
	C	0.139146	1.017768	4.160484
	H	1.210232	1.020524	3.885836
	H	-0.337264	0.168778	3.633506
	O	-0.032590	0.927068	5.557939
	H	0.398120	0.121848	5.865207
	O	-0.460359	2.448748	2.298540
	C	3.737478	3.224082	-0.005937
	H	4.450136	2.790234	0.715948
	H	3.805435	4.322827	0.124831
	N	-1.773000	4.425131	-0.859633
	C	-2.810832	3.819242	0.055752
	H	-2.341487	2.930490	0.496962
	H	-2.978046	4.547954	0.861511
	C	-0.691132	4.999907	-0.006673
	H	-1.084505	5.880261	0.515706
	H	-0.374247	4.246312	0.722114
	H	0.149701	5.287724	-0.648977
	C	-2.352223	5.506118	-1.702170
	H	-1.531612	6.012171	-2.224438
	H	-3.038399	5.070152	-2.436614
	H	-2.881033	6.220028	-1.058945
	C	-4.159595	3.497829	-0.569355
	H	-4.654382	4.429600	-0.886089
	H	-4.770622	3.087181	0.252851
	O	-4.123331	2.622255	-1.666976
	H	-4.288416	1.714504	-1.353578
	C	-1.180358	3.376004	-1.743050
	H	-0.461700	3.860794	-2.414536
	H	-0.663429	2.646537	-1.111353
	H	-1.984329	2.901936	-2.310601
	H	-1.562173	2.313254	4.006398
	C	2.335671	2.838040	0.454301
	O	1.570824	2.259319	-0.357023
	O	2.026382	3.150947	1.630856
	N	4.045520	2.757238	-1.343067

	H	3.340046	3.100736	-1.994060
	H	4.934195	3.151514	-1.646660
	C	6.284106	0.234852	0.207260
	H	7.279002	0.375857	0.651893
	H	6.302038	-0.649965	-0.452674
	H	6.033450	1.117484	-0.408527
	C	-6.465893	-1.882465	-0.280289
	H	-6.592136	-1.728559	-1.362548
	H	-6.938075	-1.043341	0.252441
	C	-7.062634	-3.202119	0.154108
	H	-6.892250	-3.351418	1.238172
	H	-6.564525	-4.034537	-0.379960
	O	-8.431394	-3.155382	-0.142521
	C	-9.115899	-4.329464	0.212323
	H	-10.173202	-4.196010	-0.055311
	H	-8.721737	-5.210669	-0.327662
	H	-9.047387	-4.529315	1.298108
	H	0.472042	2.652069	2.028283
PII_b_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.962430				
	C	4.004123	0.024279	-0.685596
	C	3.228801	-0.060908	0.612780
	O	1.849911	-0.103068	0.274672
	C	0.970701	-0.345685	1.304722
	O	1.332130	-1.045690	2.266952
	C	-0.440571	-0.454538	0.767459
	C	-0.854734	0.249930	-0.367389
	C	-2.160946	0.133150	-0.821485
	C	-3.072102	-0.683018	-0.138951
	C	-2.655270	-1.397966	0.987960
	C	-1.342731	-1.281063	1.436855
	C	-4.475339	-0.739377	-0.620431
	O	-4.955476	0.041631	-1.422611
	H	4.028063	-0.962225	-1.183984
	H	3.506562	-0.953058	1.189166
	H	3.428586	0.831626	1.225459
	H	-0.154645	0.911769	-0.879972
	H	-2.481487	0.688062	-1.704759
	H	-3.358288	-2.040105	1.520316
	H	-1.004205	-1.848018	2.305492
	O	-5.174367	-1.727122	-0.090800
	O	5.308968	0.450250	-0.387538
	H	3.512602	0.738538	-1.374395
	C	6.080031	-3.605307	-0.255740
	C	5.680840	-2.811526	0.974748
	O	4.407935	-3.148587	1.485724
	O	5.383919	-3.237757	-1.427374
	H	7.151198	-3.432476	-0.448463
	H	5.953592	-4.684765	-0.040523
	H	6.412029	-3.016953	1.773347

	H	5.745529	-1.731563	0.740032
	H	3.748175	-3.050666	0.772660
	H	4.426806	-3.365632	-1.272010
	C	1.874652	-4.368707	-0.479881
	C	0.738404	-4.011452	0.458332
	O	1.168461	-3.751123	1.773378
	O	2.749550	-3.277365	-0.702798
	H	2.477689	-5.179365	-0.041481
	H	1.460146	-4.731457	-1.437162
	H	0.184101	-3.153045	0.037224
	H	0.038141	-4.864657	0.483310
	H	1.306234	-2.791801	1.893489
	H	2.279096	-2.600458	-1.246000
	C	1.715774	-0.920912	-3.309450
	C	0.817875	0.238123	-3.687881
	O	-0.541237	-0.143214	-3.709444
	O	1.331080	-1.460892	-2.056481
	H	1.614319	-1.735176	-4.042890
	H	2.769938	-0.593935	-3.301800
	H	0.988726	1.077160	-2.986871
	H	1.085753	0.592989	-4.695105
	H	-0.701383	-0.651571	-2.902657
	H	1.449273	-0.796688	-1.349481
	C	0.673197	1.532854	3.272318
	H	0.064379	2.431803	3.486154
	C	2.005402	1.655953	3.995012
	H	2.574661	2.503980	3.568815
	H	2.595390	0.737402	3.823706
	O	1.736353	1.852714	5.366212
	H	2.576137	1.902196	5.835944
	O	0.827792	1.383320	1.893735
	C	3.576467	3.571300	-1.017544
	H	4.416438	3.040036	-0.542142
	H	3.656787	4.627884	-0.688962
	N	-2.205955	4.179595	0.180997
	C	-3.277987	3.181825	0.549806
	H	-2.800279	2.194623	0.512400
	H	-3.540410	3.395879	1.595029
	C	-1.068255	3.974270	1.125896
	H	-1.421122	4.167977	2.145675
	H	-0.710125	2.942040	1.039303
	H	-0.264017	4.673630	0.869117
	C	-2.704447	5.575705	0.322443
	H	-1.865412	6.261345	0.155302
	H	-3.484898	5.768365	-0.421470
	H	-3.102495	5.710264	1.335302
	C	-4.549797	3.184128	-0.282493
	H	-4.996298	4.190847	-0.302260
	H	-5.257955	2.545430	0.274204

	O	-4.401632	2.739689	-1.605876
	H	-4.512027	1.771383	-1.616277
	C	-1.713177	3.969815	-1.212427
	H	-0.871946	4.650801	-1.385443
	H	-1.379075	2.932614	-1.315249
	H	-2.523389	4.173136	-1.917553
	H	0.123336	0.665344	3.681898
	C	2.301768	3.035479	-0.400258
	O	1.346611	2.693702	-1.092316
	O	2.320125	2.987977	0.892985
	N	3.609807	3.369610	-2.450653
	H	2.804961	3.830325	-2.874766
	H	4.434579	3.826185	-2.835936
	C	6.149567	0.427018	-1.514968
	H	7.139709	0.788724	-1.205236
	H	6.249904	-0.597923	-1.916736
	H	5.763060	1.084354	-2.315692
	C	-6.547618	-1.844067	-0.461248
	H	-6.625705	-2.024466	-1.543998
	H	-7.079535	-0.911300	-0.220273
	C	-7.111886	-3.007575	0.322661
	H	-7.006704	-2.814641	1.408154
	H	-6.541852	-3.928232	0.090573
	O	-8.458868	-3.140095	-0.040619
	C	-9.112141	-4.187629	0.629447
	H	-10.152894	-4.214173	0.278186
	H	-8.640611	-5.165183	0.416034
	H	-9.111207	-4.034351	1.724914
	H	1.561466	2.253212	1.345335
PII_b_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.9623216				
	C	3.631085	0.347865	-0.888188
	C	3.137320	-0.273892	0.403649
	O	1.724080	-0.221211	0.393824
	C	1.075070	-0.878967	1.508640
	O	1.547791	-2.035548	1.804319
	C	-0.423316	-0.814239	1.163282
	C	-1.043758	0.412025	0.896865
	C	-2.398276	0.464469	0.598043
	C	-3.151770	-0.716009	0.545765
	C	-2.535293	-1.943038	0.812138
	C	-1.178415	-1.985317	1.127804
	C	-4.596345	-0.608635	0.209819
	O	-5.172196	0.438147	-0.003146
	H	3.550069	-0.374603	-1.721070
	H	3.483424	-1.311828	0.504953
	H	3.537359	0.301945	1.253203
	H	-0.456362	1.331789	0.929509
	H	-2.886588	1.424363	0.419928
	H	-3.115108	-2.866697	0.778264

	H	-0.690350	-2.937013	1.344868
	O	-5.210740	-1.786378	0.162019
	O	4.971489	0.731352	-0.707828
	H	3.009698	1.229523	-1.144366
	C	5.921852	-3.020899	-2.004352
	C	5.728518	-2.748889	-0.523337
	O	4.608417	-3.399439	0.038559
	O	4.983088	-2.370986	-2.834501
	H	6.919577	-2.656077	-2.297530
	H	5.908815	-4.116126	-2.171580
	H	6.617404	-3.113890	0.016473
	H	5.676054	-1.654012	-0.368820
	H	3.814579	-3.160701	-0.479227
	H	4.086380	-2.667492	-2.579730
	C	1.877023	-4.272104	-1.793267
	C	0.820662	-4.376151	-0.709484
	O	1.350872	-4.372563	0.590491
	O	2.569407	-3.037478	-1.745409
	H	2.630358	-5.064857	-1.661307
	H	1.403008	-4.413133	-2.781519
	H	0.088614	-3.558629	-0.849828
	H	0.274169	-5.323303	-0.863777
	H	1.437124	-3.444964	0.927763
	H	1.913115	-2.305241	-1.854525
	C	0.773782	-0.230513	-3.002996
	C	-0.105323	0.972140	-2.738621
	O	-1.454945	0.608028	-2.550840
	O	0.719844	-1.139143	-1.920607
	H	0.416171	-0.771233	-3.892762
	H	1.808046	0.103086	-3.200331
	H	0.289251	1.519025	-1.859469
	H	-0.060915	1.656045	-3.599922
	H	-1.483663	-0.014760	-1.811600
	H	1.028673	-0.698225	-1.094655
	C	1.314397	-0.346023	3.912115
	H	0.816246	0.401519	4.551360
	C	2.748399	-0.532390	4.373843
	H	3.302127	0.412360	4.211641
	H	3.223999	-1.312815	3.753667
	O	2.721842	-0.890614	5.737733
	H	3.627973	-1.041839	6.028725
	O	1.270891	0.125783	2.586200
	C	3.379118	3.794728	0.455610
	H	4.174757	3.066490	0.223454
	H	3.766131	4.403743	1.295717
	N	-1.871697	4.836595	-0.986382
	C	-2.002793	4.715733	0.513814
	H	-1.380510	3.858746	0.805622
	H	-1.557257	5.624321	0.940023

	C	-0.474452	5.270967	-1.286274
	H	-0.303359	6.256960	-0.837901
	H	0.220182	4.532742	-0.868847
	H	-0.352735	5.327652	-2.374448
	C	-2.824923	5.836225	-1.539317
	H	-2.605739	5.968544	-2.605348
	H	-3.850068	5.468285	-1.421312
	H	-2.694206	6.787501	-1.009192
	C	-3.403353	4.586096	1.068746
	H	-3.993634	5.492884	0.849545
	H	-3.273987	4.548500	2.164948
	O	-4.040884	3.430594	0.584001
	H	-4.876790	3.313581	1.050693
	C	-2.093585	3.512421	-1.641694
	H	-1.894019	3.620101	-2.714204
	H	-1.399872	2.792392	-1.198186
	H	-3.124702	3.193448	-1.471008
	H	0.764073	-1.295730	4.005610
	C	2.236265	2.976210	1.002067
	O	1.139618	2.890105	0.481267
	O	2.565594	2.342784	2.108663
	N	3.020742	4.526615	-0.736653
	H	2.435047	5.324152	-0.489468
	H	3.863113	4.918014	-1.153324
	C	5.582437	1.152181	-1.901455
	H	6.611401	1.456245	-1.664592
	H	5.611542	0.335229	-2.645213
	H	5.049899	2.014264	-2.345253
	C	-6.600391	-1.788346	-0.149845
	H	-6.764863	-1.325593	-1.135030
	H	-7.154800	-1.209166	0.604617
	C	-7.047988	-3.232854	-0.152921
	H	-6.849950	-3.689685	0.836381
	H	-6.469817	-3.803949	-0.905378
	O	-8.417716	-3.244322	-0.450928
	C	-8.966196	-4.536555	-0.487634
	H	-10.035084	-4.441903	-0.724173
	H	-8.485538	-5.162295	-1.262936
	H	-8.862776	-5.051721	0.485809
	H	1.930886	1.591231	2.308870

Pathway II c

Compound	Coordinates			
PII_c_1_addition_pre_TS Imaginary frequencies=0 SCF energy=-2526.987233				
	C	3.873372	0.279254	-0.438452
	C	3.311816	-0.412032	0.787360
	O	1.888081	-0.447179	0.645836

	C	1.204866	-1.545383	0.936167
	O	1.722298	-2.593743	1.262654
	C	-0.265414	-1.354603	0.782268
	C	-0.814690	-0.071526	0.699993
	C	-2.186360	0.082113	0.564853
	C	-3.016882	-1.040189	0.494478
	C	-2.467889	-2.324114	0.585251
	C	-1.094010	-2.479341	0.739669
	C	-4.480746	-0.815018	0.316000
	O	-4.982317	0.275012	0.142485
	H	3.843983	-0.394822	-1.311820
	H	3.701858	-1.431301	0.896847
	H	3.535155	0.176660	1.688055
	H	-0.172781	0.810065	0.745836
	H	-2.613325	1.082963	0.529242
	H	-3.112829	-3.202012	0.533353
	H	-0.655571	-3.477227	0.798980
	O	-5.185083	-1.936810	0.363287
	O	5.197823	0.646275	-0.149502
	H	3.270435	1.176010	-0.678291
	C	5.824611	-2.871289	-2.346148
	C	5.639815	-2.838013	-0.839628
	O	4.407351	-3.369605	-0.402732
	O	5.052502	-1.919559	-3.046903
	H	6.881623	-2.655897	-2.571055
	H	5.614067	-3.897576	-2.706668
	H	6.433873	-3.449039	-0.380653
	H	5.778689	-1.799042	-0.482409
	H	3.682143	-2.922055	-0.878630
	H	4.109013	-2.064824	-2.835299
	C	1.817498	-3.446821	-2.738541
	C	0.699718	-3.989474	-1.873497
	O	1.154246	-4.625534	-0.700946
	O	2.508643	-2.376216	-2.120652
	H	2.559781	-4.238577	-2.925413
	H	1.405376	-3.127755	-3.711805
	H	-0.005010	-3.168215	-1.642571
	H	0.143581	-4.739904	-2.457994
	H	1.478468	-3.954924	-0.080123
	H	1.937509	-1.571948	-2.095186
	C	1.216232	0.849075	-3.003838
	C	0.336152	2.051593	-2.738551
	O	-1.029949	1.695428	-2.689290
	O	0.998826	-0.150129	-2.021788
	H	0.961856	0.391119	-3.971177
	H	2.275568	1.159026	-3.033301
	H	0.658296	2.533981	-1.798227
	H	0.459865	2.784636	-3.549998
	H	-1.125728	0.999927	-2.024261

	H	1.243770	0.193571	-1.148126
	C	1.852788	-0.616994	4.195486
	H	1.426194	-1.524878	4.653724
	C	2.474573	0.242330	5.283388
	H	1.679106	0.574472	5.977683
	H	2.910069	1.147933	4.820532
	O	3.458184	-0.525714	5.941194
	H	3.892415	0.031474	6.596502
	O	0.820463	0.053553	3.521723
	C	3.195766	3.444516	0.804270
	H	4.065094	2.782952	0.945603
	H	3.358746	4.309337	1.480163
	N	-3.138707	4.467423	-1.289904
	C	-1.745843	4.621602	-0.725547
	H	-1.144658	3.816469	-1.168502
	H	-1.379222	5.584248	-1.105860
	C	-3.025273	4.492811	-2.778127
	H	-2.577983	5.446354	-3.083302
	H	-2.393255	3.654266	-3.092557
	H	-4.028961	4.393763	-3.208173
	C	-4.017739	5.588646	-0.856440
	H	-4.979102	5.494108	-1.374809
	H	-4.182393	5.533782	0.224809
	H	-3.539078	6.539165	-1.120708
	C	-1.603707	4.582055	0.789032
	H	-2.390048	5.179241	1.276388
	H	-0.650524	5.094804	1.007328
	O	-1.611295	3.293296	1.342257
	H	-0.702580	2.935605	1.214899
	C	-3.749265	3.169797	-0.882265
	H	-4.729183	3.080617	-1.365702
	H	-3.089669	2.361773	-1.216753
	H	-3.864861	3.148871	0.205875
	H	2.654611	-0.953039	3.509916
	C	1.967163	2.727600	1.356467
	O	0.909501	2.754449	0.676236
	O	2.091898	2.185489	2.480323
	N	3.067522	3.798410	-0.596547
	H	2.225233	4.358921	-0.722897
	H	3.850664	4.388365	-0.872458
	C	5.842210	1.234441	-1.253752
	H	6.863993	1.496922	-0.947214
	H	5.889836	0.534103	-2.107217
	H	5.318082	2.151735	-1.578931
	C	-6.597288	-1.838276	0.194971
	H	-6.826325	-1.400843	-0.788870
	H	-7.021600	-1.188087	0.975157
	C	-7.149184	-3.241964	0.303416
	H	-6.890810	-3.671244	1.291008

	H	-6.689747	-3.886871	-0.470970
	O	-8.537940	-3.158295	0.134589
	C	-9.182785	-4.402907	0.223000
	H	-10.258959	-4.235210	0.077886
	H	-8.825076	-5.103968	-0.554297
	H	-9.027145	-4.873747	1.211758
	H	1.202897	0.851844	3.087958
PII_c_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.9636871				
	C	3.796922	-0.138240	-0.321296
	C	3.002567	-0.626667	0.874315
	O	1.628635	-0.474939	0.541551
	C	0.712911	-0.776193	1.539649
	O	1.012633	-1.647568	2.387209
	C	-0.687765	-0.762279	0.950394
	C	-1.050969	0.131813	-0.059885
	C	-2.342973	0.125795	-0.566105
	C	-3.290156	-0.776071	-0.066383
	C	-2.927751	-1.675188	0.940896
	C	-1.629142	-1.664388	1.444419
	C	-4.664833	-0.731774	-0.635310
	O	-5.029963	0.072907	-1.466165
	H	3.845699	-0.920580	-1.100706
	H	3.227832	-1.677386	1.105432
	H	3.246303	-0.009844	1.752654
	H	-0.317050	0.845198	-0.436459
	H	-2.634014	0.823801	-1.353163
	H	-3.659431	-2.382417	1.333956
	H	-1.332059	-2.366036	2.225864
	O	-5.463638	-1.669755	-0.140719
	O	5.091986	0.203779	0.100033
	H	3.293647	0.741997	-0.766301
	C	6.091633	-3.512198	-1.456457
	C	5.787798	-3.193594	-0.004574
	O	4.571489	-3.746424	0.450533
	O	5.246836	-2.850209	-2.374219
	H	7.123148	-3.193919	-1.677838
	H	6.046319	-4.609763	-1.598898
	H	6.590472	-3.620345	0.618866
	H	5.805440	-2.097686	0.142304
	H	3.849040	-3.438571	-0.128616
	H	4.325915	-3.126111	-2.205109
	C	1.711064	-4.305226	-1.290555
	C	0.834400	-3.998438	-0.093648
	O	1.596107	-3.967981	1.089149
	O	2.664120	-3.283994	-1.522295
	H	2.273445	-5.235685	-1.113971
	H	1.076675	-4.456195	-2.181818
	H	0.325089	-3.034324	-0.268500
	H	0.043471	-4.771576	-0.036348

	H	1.362349	-3.168674	1.604686
	H	2.181978	-2.463279	-1.780631
	C	1.665246	-0.216442	-3.124900
	C	0.868163	1.069843	-3.122593
	O	-0.507272	0.834884	-3.336764
	O	1.198336	-1.108607	-2.127006
	H	1.542048	-0.736034	-4.087277
	H	2.737450	0.011635	-2.995064
	H	1.041333	1.605037	-2.169632
	H	1.228302	1.722638	-3.932521
	H	-0.768264	0.117977	-2.742974
	H	1.286749	-0.709564	-1.238798
	C	0.183654	0.820410	3.626883
	H	-0.358665	1.770611	3.774123
	C	1.293464	0.695241	4.656275
	H	2.035213	1.499577	4.489918
	H	1.809331	-0.271093	4.512780
	O	0.706055	0.790430	5.934810
	H	1.400122	0.690259	6.595820
	O	0.680179	0.778279	2.316423
	C	3.636613	3.396136	0.073557
	H	4.450037	2.712468	0.359787
	H	3.818725	4.342833	0.623808
	N	-2.161624	4.640061	-1.150090
	C	-1.293154	5.152426	-0.021799
	H	-0.266967	5.164038	-0.412916
	H	-1.600185	6.189345	0.170120
	C	-2.363845	5.753558	-2.120191
	H	-2.952306	6.544508	-1.640404
	H	-1.383401	6.142083	-2.420509
	H	-2.896799	5.365265	-2.996201
	C	-3.488696	4.174318	-0.657334
	H	-4.108458	3.921185	-1.525745
	H	-3.348274	3.284424	-0.033928
	H	-3.960965	4.979509	-0.082174
	C	-1.369691	4.396661	1.296704
	H	-2.363732	4.527936	1.749230
	H	-0.654981	4.916685	1.962357
	O	-1.117521	3.021787	1.231605
	H	-0.218024	2.882710	0.859341
	C	-1.481027	3.514774	-1.857834
	H	-2.148508	3.142055	-2.642696
	H	-0.550595	3.888035	-2.300924
	H	-1.265763	2.732298	-1.128764
	H	-0.543820	0.002057	3.767487
	C	2.351391	2.837197	0.641597
	O	1.295006	2.916258	-0.001188
	O	2.443437	2.320908	1.810667
	N	3.574175	3.532047	-1.367273

	H	2.782038	4.124554	-1.614921
	H	4.407147	4.017163	-1.695977
	C	5.920459	0.564654	-0.978934
	H	6.907571	0.826693	-0.574064
	H	6.032289	-0.271272	-1.693496
	H	5.510396	1.436414	-1.521621
	C	-6.803058	-1.714614	-0.624734
	H	-6.801912	-1.878224	-1.713306
	H	-7.309865	-0.760189	-0.414957
	C	-7.489093	-2.857581	0.089198
	H	-7.468806	-2.684221	1.182837
	H	-6.946962	-3.802808	-0.108821
	O	-8.804955	-2.918643	-0.389953
	C	-9.561352	-3.945901	0.197421
	H	-10.568655	-3.914541	-0.240483
	H	-9.120081	-4.941083	0.001170
	H	-9.646773	-3.814928	1.292500
	H	1.533435	1.583528	2.070996
PII_c_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.96702				
	C	3.919907	0.529607	-0.533514
	C	3.486801	-0.359196	0.614834
	O	2.071071	-0.391261	0.623651
	C	1.477222	-0.992974	1.795630
	O	2.025147	-2.098091	2.167379
	C	-0.028071	-1.067491	1.469445
	C	-0.781364	0.093604	1.283815
	C	-2.125096	0.018849	0.943894
	C	-2.738575	-1.227860	0.776206
	C	-1.997857	-2.395075	0.996197
	C	-0.653649	-2.308892	1.351065
	C	-4.169116	-1.258290	0.371506
	O	-4.837298	-0.269590	0.149410
	H	3.785964	0.015114	-1.502798
	H	3.904152	-1.371676	0.507327
	H	3.865120	0.072184	1.555842
	H	-0.318273	1.068639	1.426762
	H	-2.701975	0.935189	0.818254
	H	-2.471718	-3.372070	0.888999
	H	-0.072037	-3.213824	1.534779
	O	-4.655750	-2.489667	0.265295
	O	5.269427	0.874313	-0.349303
	H	3.288980	1.438659	-0.541176
	C	6.164988	-2.019753	-3.183602
	C	6.270830	-2.115820	-1.673164
	O	5.249251	-2.890613	-1.082414
	O	5.082107	-1.232292	-3.631197
	H	7.086463	-1.555090	-3.570387
	H	6.110184	-3.043145	-3.604194
	H	7.228803	-2.600454	-1.423107

	H	6.291498	-1.098826	-1.241080
	H	4.384775	-2.528667	-1.350422
	H	4.251558	-1.648796	-3.328880
	C	2.192057	-3.486460	-2.256601
	C	1.574186	-3.646341	-0.882725
	O	2.559881	-3.697383	0.115534
	O	2.860980	-2.245344	-2.389986
	H	2.942197	-4.274523	-2.428822
	H	1.406548	-3.591398	-3.026322
	H	0.877864	-2.806110	-0.719972
	H	0.961221	-4.570096	-0.888902
	H	2.310821	-3.113250	0.878221
	H	2.204633	-1.521405	-2.254010
	C	0.926087	0.862220	-2.433220
	C	-0.175196	1.724376	-1.854036
	O	-1.446206	1.140298	-2.040357
	O	0.969572	-0.408832	-1.816134
	H	0.732078	0.691583	-3.503550
	H	1.892641	1.388569	-2.346777
	H	0.015914	1.919388	-0.782512
	H	-0.180667	2.695822	-2.371733
	H	-1.443945	0.281051	-1.597258
	H	1.281166	-0.323606	-0.885753
	C	1.289305	-0.183305	4.104049
	H	0.762775	0.696877	4.509260
	C	2.513554	-0.479305	4.949810
	H	3.223052	0.365612	4.860965
	H	3.013440	-1.380318	4.552296
	O	2.081304	-0.659970	6.279645
	H	2.845532	-0.888505	6.819966
	O	1.652585	0.100148	2.774091
	C	1.936605	4.160409	0.313680
	H	2.375893	3.585185	-0.518416
	H	2.778634	4.719293	0.768231
	N	-3.761906	4.017741	-1.543620
	C	-2.537578	4.565180	-0.848247
	H	-1.688067	3.937816	-1.145317
	H	-2.383905	5.569121	-1.266864
	C	-3.414611	3.823816	-2.981441
	H	-3.042672	4.771289	-3.388770
	H	-2.645556	3.045599	-3.052536
	H	-4.315738	3.510326	-3.521965
	C	-4.890458	4.983910	-1.443964
	H	-5.752411	4.570084	-1.980217
	H	-5.153136	5.133493	-0.390959
	H	-4.586908	5.935120	-1.897128
	C	-2.594241	4.635669	0.668934
	H	-3.572621	5.007430	1.011701
	H	-1.855034	5.397750	0.967008

	O	-2.339352	3.412315	1.307604
	H	-1.373096	3.296540	1.366062
	C	-4.184031	2.702441	-0.978617
	H	-5.024758	2.330021	-1.576346
	H	-3.336245	2.012720	-1.048779
	H	-4.498616	2.834401	0.061312
	H	0.592584	-1.037606	4.145121
	C	1.490610	3.152991	1.340028
	O	0.347468	3.063702	1.756013
	O	2.460339	2.375574	1.756270
	N	0.839343	4.966862	-0.168752
	H	0.492629	5.563923	0.581588
	H	1.177897	5.592970	-0.896426
	C	5.771567	1.655631	-1.403459
	H	6.827664	1.873171	-1.191413
	H	5.701120	1.122803	-2.369516
	H	5.223076	2.612666	-1.492361
	C	-6.017238	-2.626625	-0.131067
	H	-6.175571	-2.138941	-1.105099
	H	-6.673441	-2.146283	0.610983
	C	-6.300036	-4.109518	-0.220504
	H	-6.111520	-4.588717	0.759999
	H	-5.617336	-4.577091	-0.956608
	O	-7.639395	-4.257026	-0.607356
	C	-8.029160	-5.598686	-0.751495
	H	-9.086099	-5.611707	-1.051590
	H	-7.433752	-6.115406	-1.527486
	H	-7.922881	-6.158808	0.196445
	H	2.105339	1.584752	2.265144

Pathway III

Compound	Coordinates			
PIII_1_addition_pre_TS				
Imaginary frequencies=0	C	3.035057	1.746470	0.608501
SCF energy=-2526.9960187	C	2.047607	2.386770	1.557815
	O	0.775125	1.881241	1.162600
	C	-0.302144	2.248882	1.834253
	O	-0.279574	2.906520	2.851395
	C	-1.537901	1.743740	1.168034
	C	-1.589230	1.679385	-0.225869
	C	-2.689421	1.110584	-0.851311
	C	-3.723357	0.569443	-0.082481
	C	-3.698150	0.686043	1.313313
	C	-2.614982	1.295491	1.936631
	C	-4.775331	-0.214748	-0.789401
	O	-4.834431	-0.337345	-1.993583
	H	3.041140	0.652320	0.755757

	H	2.250997	2.111083	2.602821
	H	2.052960	3.483204	1.457800
	H	-0.746765	2.050331	-0.808081
	H	-2.722201	1.036736	-1.939221
	H	-4.513353	0.278414	1.911966
	H	-2.584334	1.381783	3.024831
	O	-5.627418	-0.802302	0.040139
	O	4.308904	2.285463	0.847523
	H	2.715854	1.937441	-0.433165
	C	4.817235	-1.370920	2.954661
	C	4.338769	-0.022375	3.456914
	O	2.952134	0.021989	3.714936
	O	4.402072	-1.662842	1.638231
	H	5.918994	-1.376699	2.955461
	H	4.481585	-2.156430	3.659318
	H	4.849360	0.194094	4.409180
	H	4.634507	0.764488	2.737873
	H	2.466502	-0.208082	2.902683
	H	3.422646	-1.651668	1.597139
	C	0.815974	-2.147999	2.460247
	C	-0.409582	-1.366971	2.877812
	O	-0.010686	-0.240325	3.627399
	O	1.679824	-1.393981	1.632380
	H	1.395126	-2.435095	3.351980
	H	0.491911	-3.073870	1.952907
	H	-0.969717	-1.064555	1.975206
	H	-1.061788	-2.036549	3.468378
	H	-0.797522	0.227278	3.927814
	H	1.186448	-1.171594	0.802315
	C	-0.271158	-2.157776	-1.185585
	C	-1.759851	-2.239532	-1.463940
	O	-2.529893	-2.333260	-0.283053
	O	0.053722	-1.009851	-0.433587
	H	0.042943	-3.044672	-0.609259
	H	0.276200	-2.165378	-2.144616
	H	-2.061431	-1.365572	-2.069109
	H	-1.967944	-3.143120	-2.057915
	H	-2.342220	-1.550273	0.250570
	H	0.308683	-0.282097	-1.061068
	C	-0.558737	4.858831	-1.207001
	H	-0.352978	5.656420	-1.948491
	C	-1.152187	5.493089	0.033149
	H	-0.400070	6.168217	0.484543
	H	-1.373517	4.705646	0.778039
	O	-2.319370	6.188549	-0.344237
	H	-2.710473	6.575288	0.446798
	O	0.606207	4.169096	-0.847821
	C	0.640316	2.404485	-3.863815
	H	-0.276664	3.003841	-3.976809

	H	0.941123	2.102671	-4.884820
	N	4.385738	-3.662154	-1.490527
	C	4.873738	-2.231907	-1.572112
	H	5.023013	-1.900883	-0.535912
	H	5.846536	-2.277825	-2.077778
	C	5.248060	-4.371603	-0.501250
	H	6.297095	-4.264287	-0.801536
	H	5.088535	-3.917746	0.483792
	H	4.968895	-5.431615	-0.483687
	C	4.515441	-4.330220	-2.815400
	H	4.157459	-5.362582	-2.724338
	H	3.909237	-3.795192	-3.554925
	H	5.569992	-4.323386	-3.115213
	C	3.965969	-1.239532	-2.264933
	H	3.578428	-1.640779	-3.219757
	H	4.610378	-0.379581	-2.526760
	O	2.936284	-0.864075	-1.396107
	H	2.320185	-0.242402	-1.832035
	C	2.967313	-3.751321	-1.034655
	H	2.729091	-4.808772	-0.868011
	H	2.848474	-3.182315	-0.106934
	H	2.316007	-3.343608	-1.812718
	H	-1.317776	4.188311	-1.658265
	C	0.259451	1.121039	-3.132207
	O	0.958744	0.803498	-2.121936
	O	-0.698197	0.468507	-3.578448
	N	1.654478	3.183083	-3.169861
	H	2.464060	2.592171	-2.978360
	H	1.981453	3.940615	-3.768504
	C	5.297088	1.676459	0.054508
	H	6.258385	2.156630	0.284418
	H	5.375800	0.595029	0.269858
	H	5.084170	1.806055	-1.023315
	C	-6.621376	-1.646578	-0.533691
	H	-6.136320	-2.451388	-1.107111
	H	-7.260765	-1.065450	-1.215605
	C	-7.428674	-2.213388	0.612316
	H	-7.887297	-1.389224	1.192843
	H	-6.763290	-2.774164	1.297446
	O	-8.408428	-3.049738	0.059711
	C	-9.235927	-3.646220	1.025043
	H	-9.965551	-4.277427	0.499089
	H	-8.657397	-4.279675	1.723416
	H	-9.783759	-2.889189	1.617035
	H	1.023232	3.801722	-1.676842
PIII_2_addition_TS Imaginary frequencies=1 SCF energy=-2526.9681362				
	C	2.621865	1.795301	-0.280170
	C	1.425642	2.454735	0.369709
	O	0.324253	1.570897	0.234257

	C	-0.894338	2.103036	0.487430
	O	-1.023763	3.024858	1.306770
	C	-2.005079	1.109169	0.270092
	C	-1.813926	-0.063526	-0.464270
	C	-2.864553	-0.947013	-0.663281
	C	-4.126495	-0.669138	-0.124541
	C	-4.318287	0.497326	0.623311
	C	-3.259385	1.378962	0.821532
	C	-5.224946	-1.642888	-0.367101
	O	-5.096011	-2.670483	-0.997701
	H	2.989498	0.945701	0.321451
	H	1.618862	2.673448	1.430876
	H	1.204949	3.398994	-0.152603
	H	-0.826109	-0.288909	-0.855298
	H	-2.711568	-1.859064	-1.243388
	H	-5.296168	0.715000	1.055136
	H	-3.398525	2.282934	1.416512
	O	-6.378013	-1.275406	0.181173
	O	3.628352	2.769168	-0.417841
	H	2.327299	1.396721	-1.266585
	C	5.242449	0.592748	2.840409
	C	4.559593	1.947201	2.794807
	O	3.257897	1.945724	3.339542
	O	4.689051	-0.354052	1.950889
	H	6.299541	0.721499	2.557417
	H	5.221279	0.214599	3.880998
	H	5.159471	2.653333	3.392081
	H	4.551880	2.321266	1.754813
	H	2.715869	1.288350	2.864098
	H	3.749216	-0.493780	2.182995
	C	1.024378	-0.630263	3.358440
	C	-0.186555	0.276848	3.290856
	O	0.183516	1.620908	3.499953
	O	1.983585	-0.318108	2.368560
	H	1.522894	-0.514973	4.334142
	H	0.690838	-1.678402	3.265838
	H	-0.671195	0.147147	2.309303
	H	-0.913987	-0.059430	4.054619
	H	-0.295326	2.186195	2.869714
	H	1.652844	-0.582399	1.475091
	C	1.249490	-2.730317	-0.002686
	C	-0.163198	-3.271105	0.080931
	O	-0.838371	-2.817125	1.235185
	O	1.253651	-1.319979	0.043908
	H	1.841111	-3.094050	0.854101
	H	1.729178	-3.092215	-0.927367
	H	-0.709956	-2.989208	-0.837454
	H	-0.133303	-4.370793	0.126768
	H	-0.864021	-1.851956	1.191288

	H	1.255033	-0.950364	-0.868326
	C	-2.077609	3.802289	-1.476609
	H	-2.499598	3.724577	-2.501265
	C	-1.596477	5.229245	-1.261239
	H	-0.754801	5.429399	-1.953139
	H	-1.206029	5.320408	-0.230143
	O	-2.674359	6.112417	-1.487692
	H	-2.369296	7.011753	-1.325381
	O	-1.057962	2.888241	-1.285424
	C	-0.595725	0.554763	-3.722561
	H	-1.654151	0.527253	-3.429797
	H	-0.543942	0.420166	-4.812722
	N	6.090911	-2.840339	-0.546804
	C	6.033609	-1.471772	-1.186042
	H	5.903414	-0.756366	-0.363165
	H	7.019140	-1.312815	-1.642306
	C	7.077221	-2.769002	0.570819
	H	8.034177	-2.404079	0.179473
	H	6.689345	-2.082642	1.332760
	H	7.201894	-3.772071	0.995493
	C	6.545924	-3.859436	-1.532551
	H	6.592917	-4.833221	-1.031251
	H	5.832220	-3.908603	-2.362397
	H	7.538638	-3.578312	-1.903629
	C	4.943509	-1.239176	-2.209827
	H	4.886248	-2.072830	-2.933130
	H	5.259111	-0.347481	-2.782292
	O	3.726791	-1.025465	-1.553735
	H	2.997139	-0.880090	-2.181560
	C	4.768716	-3.250140	0.013309
	H	4.913682	-4.175720	0.583520
	H	4.402379	-2.451380	0.666664
	H	4.069018	-3.423502	-0.808885
	H	-2.927616	3.613861	-0.784096
	C	0.135300	-0.622107	-3.070222
	O	1.227961	-0.352723	-2.488116
	O	-0.394256	-1.736455	-3.165766
	N	-0.013954	1.848808	-3.342831
	H	0.986291	1.715390	-3.153730
	H	-0.105116	2.537760	-4.092437
	C	4.787572	2.267051	-1.031036
	H	5.507193	3.093129	-1.118797
	H	5.246240	1.458646	-0.432915
	H	4.571236	1.874835	-2.042287
	C	-7.491366	-2.147875	0.011460
	H	-7.263448	-3.134423	0.443474
	H	-7.706847	-2.277176	-1.060300
	C	-8.662345	-1.508058	0.722918
	H	-8.869226	-0.511593	0.286042

	H	-8.415423	-1.358620	1.792167
	O	-9.761192	-2.365377	0.572183
	C	-10.926284	-1.886785	1.193348
	H	-11.724501	-2.622719	1.024066
	H	-10.785453	-1.760970	2.283297
	H	-11.244495	-0.915114	0.771107
	H	-0.489874	2.296863	-2.403798
PIII_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2526.9776621				
	C	-2.745241	1.715800	0.071762
	C	-1.520272	2.442128	-0.441012
	O	-0.379617	1.677994	-0.116774
	C	0.852837	2.364421	-0.307144
	O	0.950583	3.017762	-1.418579
	C	1.972204	1.337481	-0.048795
	C	1.875916	0.394676	0.977489
	C	2.914417	-0.489594	1.232386
	C	4.074240	-0.450772	0.449071
	C	4.175712	0.486178	-0.584960
	C	3.130228	1.373742	-0.826305
	C	5.154430	-1.429449	0.740077
	O	5.100240	-2.264615	1.618099
	H	-2.960675	0.813189	-0.526770
	H	-1.595225	2.598398	-1.529173
	H	-1.475300	3.433468	0.043120
	H	0.960543	0.336691	1.557346
	H	2.825582	-1.222420	2.037025
	H	5.072829	0.519596	-1.205016
	H	3.197228	2.098446	-1.639326
	O	6.203326	-1.303960	-0.067195
	O	-3.836235	2.605083	0.016119
	H	-2.574529	1.380104	1.108880
	C	-4.886668	0.082532	-3.259315
	C	-4.279193	1.472127	-3.219512
	O	-2.906456	1.501910	-3.543255
	O	-4.456147	-0.756810	-2.209123
	H	-5.981219	0.174040	-3.171491
	H	-4.670494	-0.375607	-4.244124
	H	-4.800405	2.095887	-3.964157
	H	-4.460939	1.924661	-2.227567
	H	-2.422809	0.911563	-2.935421
	H	-3.484452	-0.861661	-2.266869
	C	-0.643471	-0.982974	-3.044362
	C	0.504875	-0.005109	-2.901438
	O	0.132831	1.289566	-3.299652
	O	-1.734167	-0.647228	-2.207943
	H	-1.019989	-0.978555	-4.079825
	H	-0.275844	-1.999720	-2.817628
	H	0.828629	-0.014790	-1.848165
	H	1.355757	-0.384490	-3.502250

	H	0.469825	1.944547	-2.635696
	H	-1.463953	-0.750777	-1.261690
	C	-0.911079	-2.605044	0.502917
	C	0.526237	-3.045118	0.686814
	O	1.328882	-2.702221	-0.422571
	O	-0.980587	-1.217484	0.254602
	H	-1.353263	-3.120839	-0.365769
	H	-1.499490	-2.874309	1.395781
	H	0.920541	-2.597678	1.618546
	H	0.566091	-4.139568	0.799874
	H	1.303367	-1.739138	-0.502115
	H	-1.116426	-0.733476	1.098848
	C	1.817563	4.278702	0.927849
	H	2.184605	4.370824	1.964150
	C	1.209293	5.599447	0.492375
	H	0.312036	5.799820	1.109515
	H	0.881238	5.514199	-0.558309
	O	2.188841	6.600600	0.657993
	H	1.831329	7.432943	0.329761
	O	0.865405	3.245775	0.894616
	C	0.042229	1.349824	3.924046
	H	1.136203	1.417395	3.890181
	H	-0.279518	1.460630	4.968754
	N	-5.753623	-3.185291	0.386215
	C	-5.882263	-1.774921	0.914561
	H	-5.725909	-1.112502	0.052949
	H	-6.921489	-1.677546	1.253461
	C	-6.625274	-3.286464	-0.820819
	H	-7.645219	-2.989662	-0.549485
	H	-6.225884	-2.619605	-1.593859
	H	-6.617468	-4.323653	-1.175455
	C	-6.216867	-4.171398	1.401571
	H	-6.129912	-5.177847	0.975450
	H	-5.590269	-4.098277	2.297011
	H	-7.262525	-3.958068	1.653518
	C	-4.935587	-1.364763	2.021800
	H	-4.898335	-2.123476	2.824556
	H	-5.381762	-0.457553	2.469084
	O	-3.670481	-1.104535	1.484358
	H	-3.043906	-0.802994	2.166304
	C	-4.350816	-3.506410	-0.012604
	H	-4.355634	-4.475002	-0.526666
	H	-3.985470	-2.720445	-0.682145
	H	-3.727097	-3.562768	0.883607
	H	2.686158	4.041001	0.289821
	C	-0.425147	-0.022039	3.419406
	O	-1.434519	-0.009426	2.656037
	O	0.208979	-1.011370	3.800844
	N	-0.543589	2.442353	3.123498

	H	-1.473411	2.141862	2.797705
	H	-0.649211	3.305621	3.664260
	C	-5.021539	2.034687	0.506717
	H	-5.817350	2.788936	0.429226
	H	-5.317570	1.145392	-0.079213
	H	-4.917213	1.736453	1.566963
	C	7.290472	-2.203554	0.125496
	H	6.945006	-3.241554	0.002570
	H	7.696777	-2.089198	1.142240
	C	8.334338	-1.859304	-0.913134
	H	8.659103	-0.808095	-0.786219
	H	7.899557	-1.953724	-1.927322
	O	9.406469	-2.745540	-0.737660
	C	10.452936	-2.536966	-1.650840
	H	11.239073	-3.274008	-1.436037
	H	10.115992	-2.672477	-2.695708
	H	10.882593	-1.522202	-1.554557
	H	0.024774	2.677399	2.265633
PIII_4_elimination_TS Imaginary frequencies=1 SCF energy=-2526.9775712				
	C	2.595351	0.118217	1.082878
	C	2.165455	-1.340465	1.020162
	O	0.785401	-1.478340	0.850016
	C	0.403413	-3.018059	-0.113548
	O	1.003089	-2.939472	-1.198673
	C	-1.094700	-2.808523	-0.047546
	C	-1.807895	-2.967403	1.143466
	C	-3.149363	-2.610866	1.206308
	C	-3.800776	-2.132868	0.063906
	C	-3.114863	-2.079049	-1.153521
	C	-1.765721	-2.408180	-1.203363
	C	-5.177091	-1.588173	0.205303
	O	-5.774043	-1.520066	1.258152
	H	2.657259	0.554664	0.070686
	H	2.699700	-1.827277	0.186463
	H	2.502168	-1.827634	1.956357
	H	-1.298813	-3.343901	2.032372
	H	-3.695348	-2.677126	2.149349
	H	-3.626613	-1.740492	-2.055684
	H	-1.219703	-2.340123	-2.144323
	O	-5.674473	-1.146919	-0.947625
	O	3.855466	0.167263	1.709194
	H	1.856944	0.713718	1.648334
	C	5.262963	0.248666	-2.227377
	C	4.914897	-1.061622	-1.544714
	O	3.789371	-1.706950	-2.101248
	O	4.381600	1.307647	-1.923163
	H	6.268002	0.559516	-1.899072
	H	5.312318	0.073871	-3.320547
	H	5.767154	-1.750508	-1.658365

	H	4.780536	-0.879625	-0.460883
	H	3.012356	-1.121757	-2.016925
	H	3.460532	1.010653	-2.068484
	C	1.400047	0.352639	-3.590641
	C	0.263179	-0.616352	-3.846696
	O	0.633600	-1.965056	-3.704145
	O	1.868325	0.288198	-2.256378
	H	2.256342	0.106360	-4.238014
	H	1.067929	1.377492	-3.837714
	H	-0.583253	-0.358081	-3.181983
	H	-0.084412	-0.470368	-4.882600
	H	0.774104	-2.178366	-2.757368
	H	1.120167	0.469629	-1.636224
	C	-0.838312	1.402890	0.199902
	C	-2.239757	1.019424	0.631564
	O	-3.168323	1.026762	-0.432622
	O	-0.239370	0.426367	-0.624621
	H	-0.897307	2.337264	-0.380167
	H	-0.224764	1.599679	1.093999
	H	-2.219317	0.029590	1.125999
	H	-2.595031	1.751820	1.373034
	H	-2.867139	0.385036	-1.088172
	H	0.108098	-0.319608	-0.054036
	C	1.712871	-4.963668	0.377062
	H	1.576134	-5.798071	1.080602
	C	3.183342	-4.562744	0.388309
	H	3.439460	-4.136070	1.370427
	H	3.380593	-3.797214	-0.379796
	O	3.999322	-5.698544	0.198159
	H	3.900214	-5.987730	-0.717160
	O	0.819283	-3.951386	0.811965
	C	0.762776	-0.524001	4.192097
	H	0.398025	-0.673519	5.218076
	H	1.624669	-1.181214	4.029581
	N	1.693827	4.843247	-0.924108
	C	1.545850	5.360242	0.488421
	H	2.564452	5.500043	0.876237
	H	1.070257	6.345162	0.395772
	C	2.654894	5.738123	-1.631901
	H	2.290946	6.770503	-1.573274
	H	3.636008	5.655988	-1.149734
	H	2.724190	5.422714	-2.679394
	C	0.388557	4.887493	-1.640268
	H	0.539112	4.518926	-2.661883
	H	-0.334324	4.247577	-1.124429
	H	0.028245	5.922510	-1.662042
	C	0.765923	4.500353	1.459748
	H	-0.186463	4.159306	1.013512
	H	0.493100	5.175694	2.292012

	O	1.550023	3.431413	1.905003
	H	1.039189	2.879627	2.546755
	C	2.229120	3.449854	-0.959441
	H	2.438833	3.195596	-2.004501
	H	3.149569	3.409804	-0.367618
	H	1.485313	2.764381	-0.544447
	H	1.428913	-5.311979	-0.629822
	C	1.170289	0.945185	4.031699
	O	0.306299	1.689933	3.486126
	O	2.282359	1.279265	4.459362
	N	-0.311157	-0.862077	3.240622
	H	-0.905953	-1.624047	3.575303
	H	-0.889946	-0.018981	3.115611
	C	4.433117	1.448386	1.697736
	H	5.377259	1.395130	2.258344
	H	4.650861	1.778989	0.665886
	H	3.776734	2.194516	2.177965
	C	-6.919981	-0.455142	-0.927838
	H	-7.606026	-0.920734	-0.206513
	H	-7.334991	-0.556642	-1.938683
	C	-6.696826	1.008655	-0.593622
	H	-5.973040	1.448211	-1.306741
	H	-6.264727	1.107344	0.421020
	O	-7.942542	1.647178	-0.673699
	C	-7.878263	3.021810	-0.393228
	H	-8.894375	3.431112	-0.479540
	H	-7.504863	3.212174	0.630459
	H	-7.220021	3.553148	-1.106066
	H	0.077983	-1.132117	2.276881
PIII_5_product Imaginary frequencies=0 SCF energy=-2526.9918200				
	C	3.014125	0.187789	0.048426
	C	2.477039	1.530426	0.507870
	O	1.208520	1.816546	-0.030460
	C	-0.297125	4.288130	0.640303
	O	0.060250	4.318353	1.801461
	C	-1.445826	3.479424	0.145617
	C	-1.742452	3.385782	-1.217867
	C	-2.785645	2.573816	-1.642623
	C	-3.551728	1.870449	-0.708456
	C	-3.276513	1.991551	0.657696
	C	-2.222049	2.791156	1.080569
	C	-4.616385	0.958313	-1.219769
	O	-4.817740	0.750735	-2.395990
	H	2.246243	-0.592834	0.201386
	H	2.376247	1.515805	1.602591
	H	3.205185	2.317917	0.248324
	H	-1.156162	3.943840	-1.947371
	H	-3.010942	2.476762	-2.705893
	H	-3.876860	1.448768	1.388995

	H	-1.993625	2.886008	2.143115
	O	-5.317191	0.388504	-0.249450
	O	4.167452	-0.107238	0.795964
	H	3.256758	0.209751	-1.029401
	C	2.042315	-3.697291	3.774715
	C	3.394706	-3.195245	3.303414
	O	3.560033	-1.799269	3.413395
	O	0.982349	-3.383775	2.898201
	H	2.085006	-4.795578	3.854493
	H	1.850025	-3.300147	4.791262
	H	4.176243	-3.660578	3.925608
	H	3.558569	-3.539206	2.263119
	H	2.830699	-1.352160	2.947729
	H	0.970544	-2.413227	2.775234
	C	0.572638	-0.171849	3.909788
	C	-0.062018	1.191246	3.749532
	O	0.912074	2.156070	3.429196
	O	1.140742	-0.660963	2.708559
	H	1.383315	-0.130977	4.654453
	H	-0.194244	-0.871758	4.288867
	H	-0.836161	1.126877	2.965393
	H	-0.578783	1.438900	4.696959
	H	0.500854	2.872842	2.919149
	H	0.532221	-0.480420	1.945801
	C	-0.446305	-1.191341	-0.313108
	C	-1.632300	-1.067597	-1.242707
	O	-2.853042	-1.212651	-0.548199
	O	-0.443122	-0.147024	0.644752
	H	-0.510158	-2.145293	0.236690
	H	0.484380	-1.198607	-0.898757
	H	-1.581935	-0.094066	-1.768193
	H	-1.591981	-1.858962	-2.006902
	H	-2.810580	-0.637275	0.226982
	H	0.075181	0.625037	0.296755
	C	1.367247	5.857161	0.026791
	H	1.429370	6.586379	-0.791138
	C	2.668441	5.085090	0.133697
	H	2.806729	4.479427	-0.781283
	H	2.622203	4.397014	0.994880
	O	3.688453	6.042776	0.290443
	H	4.517952	5.577383	0.446429
	O	0.277266	5.000989	-0.314547
	C	2.384403	2.176929	-3.357305
	H	2.378284	2.542500	-4.401406
	H	3.332453	2.518386	-2.913530
	N	1.498919	-5.000515	-1.377140
	C	2.519856	-4.600010	-2.419536
	H	3.501620	-4.708162	-1.938357
	H	2.447009	-5.337964	-3.229635

	C	1.573637	-6.479950	-1.207648
	H	1.258795	-6.964440	-2.139467
	H	2.607325	-6.757049	-0.968592
	H	0.908340	-6.773376	-0.387155
	C	0.120397	-4.628256	-1.798387
	H	-0.587503	-5.036573	-1.067488
	H	0.034385	-3.537711	-1.823055
	H	-0.078905	-5.050576	-2.790615
	C	2.363520	-3.217678	-3.014963
	H	1.412452	-3.145151	-3.571571
	H	3.167660	-3.133581	-3.771775
	O	2.464153	-2.221920	-2.041621
	H	2.075983	-1.387786	-2.417443
	C	1.797231	-4.360347	-0.059133
	H	1.035667	-4.675674	0.661920
	H	2.787552	-4.693566	0.273662
	H	1.785412	-3.274770	-0.184858
	H	1.147862	6.385728	0.965751
	C	2.433818	0.650370	-3.420649
	O	1.432740	0.012869	-2.982722
	O	3.462384	0.138508	-3.901205
	N	1.270502	2.676036	-2.567087
	H	1.234739	3.694698	-2.599671
	H	0.392668	2.336819	-2.962038
	C	4.765314	-1.318216	0.414632
	H	5.623426	-1.497067	1.077445
	H	4.062980	-2.167197	0.504674
	H	5.120814	-1.283395	-0.632499
	C	-6.247050	-0.624222	-0.620965
	H	-5.766761	-1.334641	-1.310322
	H	-7.112235	-0.170401	-1.128685
	C	-6.667936	-1.318578	0.654481
	H	-7.108126	-0.585052	1.357851
	H	-5.777703	-1.759926	1.144158
	O	-7.597885	-2.307758	0.306118
	C	-8.059897	-3.046202	1.407902
	H	-8.778242	-3.790223	1.036715
	H	-7.234136	-3.574979	1.919861
	H	-8.568795	-2.400266	2.147779
	H	1.276502	2.118024	-0.992416

Pathway IV

Compound	Coordinates			
PIV_1_addition_pre_TS				
Imaginary frequencies=0	C	-3.509756	0.100178	-0.640559
SCF energy=-2198.506561	C	-2.789967	-0.244230	0.646693
	O	-1.400577	-0.381542	0.332047

	C	-0.485458	-0.051527	1.232186
	O	-0.747997	0.476746	2.293335
	C	0.902800	-0.321439	0.760044
	C	1.161893	-1.238058	-0.265447
	C	2.468158	-1.430469	-0.698023
	C	3.516407	-0.712668	-0.111800
	C	3.255780	0.190927	0.924105
	C	1.950489	0.380231	1.362598
	C	4.899741	-0.943509	-0.621808
	O	5.172883	-1.716380	-1.513508
	H	-3.328463	1.153879	-0.915871
	H	-2.923456	0.531081	1.410950
	H	-3.141368	-1.212744	1.026899
	H	0.346449	-1.809058	-0.717499
	H	2.681821	-2.135769	-1.502690
	H	4.071907	0.749420	1.383456
	H	1.732243	1.099755	2.153816
	O	5.809623	-0.209116	0.004858
	O	-4.881634	-0.117916	-0.429052
	H	-3.137338	-0.536787	-1.464467
	C	-4.761990	3.994996	0.295558
	C	-4.552621	2.946814	1.373481
	O	-3.224916	2.874308	1.849354
	O	-4.223175	3.648210	-0.962195
	H	-5.845703	4.135457	0.153568
	H	-4.349055	4.959004	0.652994
	H	-5.188759	3.204355	2.235707
	H	-4.896753	1.965387	0.993219
	H	-2.625757	2.738932	1.090801
	H	-3.263768	3.489989	-0.858982
	C	-0.659526	3.983467	-0.180689
	C	0.504880	3.509473	0.663748
	O	0.158033	3.246952	2.004889
	O	-1.627644	2.969061	-0.381029
	H	-1.170352	4.817460	0.325495
	H	-0.282263	4.351513	-1.150671
	H	0.960422	2.624142	0.181652
	H	1.269360	4.302856	0.675309
	H	-0.341578	2.418993	2.053457
	H	-1.276871	2.290092	-1.005167
	C	-0.877932	0.727318	-3.301892
	C	0.007646	-0.414249	-3.756839
	O	1.374550	-0.120448	-3.565364
	O	-0.612585	1.037835	-1.943848
	H	-0.658448	1.638482	-3.878279
	H	-1.939347	0.464156	-3.453050
	H	-0.287257	-1.333319	-3.216325
	H	-0.151355	-0.595867	-4.831016
	H	1.467882	0.188130	-2.653816

	H	-0.872584	0.285712	-1.387405
	C	-1.222819	-3.235313	3.142069
	H	-1.383517	-4.331475	3.172910
	C	-2.522358	-2.545282	3.522768
	H	-3.291006	-2.778881	2.761326
	H	-2.365972	-1.450175	3.516536
	O	-2.905740	-3.010258	4.799008
	H	-3.737989	-2.587932	5.038776
	O	-0.737463	-2.813704	1.897362
	C	-3.798917	-3.123819	-1.878697
	H	-4.560614	-2.609661	-1.270795
	H	-4.130873	-4.179698	-1.956404
	H	-0.460800	-3.001967	3.904942
	C	-2.506609	-3.154730	-1.062690
	O	-1.430827	-2.863523	-1.626051
	O	-2.628114	-3.507154	0.143816
	N	-3.645364	-2.452646	-3.156227
	H	-2.850501	-2.860729	-3.647500
	H	-4.463811	-2.628324	-3.736469
	C	-5.663270	0.280681	-1.529703
	H	-6.713163	0.057809	-1.295049
	H	-5.558507	1.364161	-1.720990
	H	-5.374343	-0.269364	-2.443647
	C	7.167583	-0.353824	-0.402910
	H	7.267806	-0.095361	-1.468175
	H	7.490354	-1.396976	-0.263784
	C	7.984620	0.582340	0.458934
	H	7.847655	0.324282	1.527212
	H	7.633591	1.623487	0.319790
	O	9.324706	0.443485	0.072048
	C	10.199091	1.268303	0.798389
	H	11.217441	1.089112	0.426571
	H	9.956015	2.339088	0.664273
	H	10.171393	1.039959	1.880390
	H	-1.385386	-3.090219	1.199150
PIV_2_addition_TS Imaginary frequencies=1 SCF energy=-2198.4840781				
	C	-3.439826	0.232181	-0.474760
	C	-2.669845	-0.206819	0.756685
	O	-1.324527	-0.423299	0.355376
	C	-0.443340	-0.869702	1.326005
	O	-0.622147	-0.519425	2.511222
	C	0.959585	-0.867674	0.743536
	C	1.223011	-1.338002	-0.546780
	C	2.507191	-1.255054	-1.068383
	C	3.543820	-0.705146	-0.302993
	C	3.284594	-0.254505	0.995105
	C	1.994935	-0.338000	1.512905
	C	4.900127	-0.620760	-0.910295
	O	5.170728	-1.003935	-2.028242

	H	-3.292302	1.308860	-0.671248
	H	-2.717665	0.550625	1.551817
	H	-3.099540	-1.148225	1.132532
	H	0.415825	-1.779482	-1.135413
	H	2.715781	-1.607511	-2.080051
	H	4.088293	0.169050	1.598882
	H	1.778901	0.026462	2.518849
	O	5.799716	-0.073807	-0.099515
	O	-4.803969	-0.036797	-0.267459
	H	-3.070869	-0.318107	-1.359533
	C	-4.972127	4.070055	0.452182
	C	-4.845015	2.961686	1.480263
	O	-3.566375	2.892771	2.073308
	O	-4.241743	3.836713	-0.733105
	H	-6.032172	4.165244	0.166323
	H	-4.669332	5.026969	0.921145
	H	-5.567961	3.154529	2.289691
	H	-5.119729	1.995355	1.017268
	H	-2.897522	2.795598	1.369472
	H	-3.295118	3.753958	-0.507351
	C	-0.583649	3.738586	0.722253
	C	0.152937	2.711292	1.557013
	O	-0.665218	2.222265	2.592835
	O	-1.685568	3.171692	0.037912
	H	-0.983063	4.533948	1.371241
	H	0.120617	4.203877	0.009974
	H	0.488232	1.897285	0.892073
	H	1.065364	3.187280	1.965963
	H	-0.623392	1.245445	2.610863
	H	-1.343534	2.510184	-0.609958
	C	-0.878257	1.146917	-2.944333
	C	0.145014	0.246212	-3.607337
	O	1.458829	0.723718	-3.416536
	O	-0.564592	1.341764	-1.577165
	H	-0.862124	2.143807	-3.411054
	H	-1.888788	0.721741	-3.072793
	H	0.031164	-0.782815	-3.220866
	H	-0.047846	0.212771	-4.690844
	H	1.557923	0.882435	-2.467569
	H	-0.764175	0.541093	-1.053640
	C	-0.827933	-3.314231	2.408183
	H	-0.520277	-4.358550	2.223364
	C	-2.206584	-3.302705	3.047795
	H	-2.947160	-3.701747	2.329517
	H	-2.489748	-2.260132	3.279100
	O	-2.138805	-4.094799	4.213590
	H	-3.005325	-4.088834	4.634805
	O	-0.788436	-2.603961	1.198862
	C	-3.852090	-2.835512	-2.235807

	H	-4.609275	-2.413372	-1.556631
	H	-4.118064	-3.904577	-2.368991
	H	-0.098646	-2.872463	3.107998
	C	-2.525669	-2.826241	-1.499428
	O	-1.487348	-2.503010	-2.078877
	O	-2.596213	-3.194829	-0.269141
	N	-3.791179	-2.068879	-3.463914
	H	-3.009135	-2.404294	-4.025733
	H	-4.632698	-2.236909	-4.012124
	C	-5.601419	0.408622	-1.338507
	H	-6.645917	0.156531	-1.108977
	H	-5.515149	1.502363	-1.473753
	H	-5.309380	-0.085177	-2.283402
	C	7.131037	0.059177	-0.588717
	H	7.136891	0.686204	-1.493544
	H	7.536510	-0.931069	-0.847271
	C	7.940596	0.700678	0.515831
	H	7.906536	0.066417	1.423104
	H	7.502936	1.683329	0.779476
	O	9.253577	0.840837	0.045272
	C	10.118393	1.426045	0.984399
	H	11.115797	1.492200	0.528086
	H	9.788597	2.444145	1.264430
	H	10.189855	0.819549	1.906747
	H	-1.641252	-2.911614	0.429840
PIV_3_tetrahedral_int1 Imaginary frequencies=0 SCF energy=-2198.49286				
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	O	1.351769	-0.444206	-0.335068
	C	0.499295	-1.026262	-1.340547
	O	0.638956	-0.526211	-2.519119
	C	-0.918030	-0.955797	-0.741529
	C	-1.199237	-1.487753	0.521693
	C	-2.476327	-1.386292	1.058437
	C	-3.496886	-0.760619	0.330422
	C	-3.225055	-0.250608	-0.943388
	C	-1.940611	-0.350996	-1.471227
	C	-4.846355	-0.662884	0.947204
	O	-5.125524	-1.083070	2.050160
	H	3.277898	1.354628	0.669607
	H	2.716436	0.560146	-1.539345
	H	3.153123	-1.116889	-1.114191
	H	-0.406248	-1.982545	1.086000
	H	-2.692639	-1.785264	2.051181
	H	-4.016322	0.230577	-1.520131
	H	-1.714809	0.055916	-2.458408
	O	-5.734607	-0.060115	0.162622
	O	4.824232	0.044630	0.279727
	H	3.102545	-0.266437	1.378682

	C	4.900551	4.127363	-0.543803
	C	4.786347	2.992412	-1.544200
	O	3.506051	2.886717	-2.128171
	O	4.186260	3.908852	0.653845
	H	5.961229	4.250311	-0.270941
	H	4.574665	5.066516	-1.032947
	H	5.501161	3.178466	-2.362435
	H	5.080662	2.042429	-1.060058
	H	2.844149	2.785199	-1.418270
	H	3.239857	3.795613	0.438693
	C	0.531475	3.706427	-0.767041
	C	-0.205244	2.643700	-1.557490
	O	0.597693	2.117889	-2.582021
	O	1.644419	3.171943	-0.073370
	H	0.919668	4.481245	-1.447156
	H	-0.168626	4.192361	-0.063955
	H	-0.530349	1.855301	-0.857145
	H	-1.126763	3.102360	-1.968872
	H	0.582668	1.125817	-2.547403
	H	1.312689	2.507226	0.577325
	C	0.824015	1.100558	2.883256
	C	-0.214042	0.195349	3.517022
	O	-1.522104	0.683306	3.314622
	O	0.535546	1.318017	1.515542
	H	0.804035	2.089075	3.368114
	H	1.830335	0.669522	3.025560
	H	-0.102845	-0.828471	3.116098
	H	-0.037907	0.143583	4.602706
	H	-1.609778	0.843997	2.364867
	H	0.766149	0.535245	0.967636
	C	0.638992	-3.251480	-2.394720
	H	0.327682	-4.248744	-2.042348
	C	1.881835	-3.384330	-3.255854
	H	2.715702	-3.750287	-2.626163
	H	2.160681	-2.386206	-3.637014
	O	1.588074	-4.282472	-4.302943
	H	2.357588	-4.337554	-4.880161
	O	0.894694	-2.454185	-1.262636
	C	4.016588	-2.759369	2.339046
	H	4.763736	-2.302766	1.671456
	H	4.314211	-3.822014	2.454386
	H	-0.186544	-2.829571	-2.990602
	C	2.704836	-2.774305	1.597343
	O	1.643008	-2.476086	2.110306
	O	2.830803	-3.158728	0.345040
	N	3.914907	-2.009172	3.571497
	H	3.198028	-2.425951	4.165062
	H	4.791305	-2.087536	4.083962
	C	5.609524	0.536090	1.338745

	H	6.660509	0.305638	1.115833
	H	5.495028	1.630136	1.448341
	H	5.331123	0.058408	2.296390
	C	-7.060895	0.084999	0.660517
	H	-7.051190	0.677685	1.588186
	H	-7.489379	-0.904437	0.882737
	C	-7.857415	0.785879	-0.417176
	H	-7.836787	0.186641	-1.348348
	H	-7.399214	1.768540	-0.643180
	O	-9.167200	0.935411	0.059414
	C	-10.018768	1.576606	-0.854868
	H	-11.014386	1.647031	-0.395290
	H	-9.666181	2.597332	-1.094648
	H	-10.104143	1.008975	-1.800502
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PIV_4_elimination_TS Imaginary frequencies=1 SCF energy=-2198.4852620				
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	C	1.204307	-1.651286	-1.799608
	O	1.441086	-1.008188	-2.844007
	C	-0.222196	-1.836028	-1.311605
	C	-0.507983	-2.570222	-0.156216
	C	-1.801750	-2.602489	0.344894
	C	-2.825731	-1.904717	-0.305587
	C	-2.555925	-1.235706	-1.503858
	C	-1.258333	-1.213246	-2.005083
	C	-4.150640	-1.824499	0.364254
	O	-4.455870	-2.455381	1.353566
	H	3.890554	1.820317	0.160751
	H	2.640521	0.739157	-1.567661
	H	3.731094	-0.428683	-0.773521
	H	0.291997	-3.088406	0.373979
	H	-2.022021	-3.138999	1.269746
	H	-3.354159	-0.711039	-2.031040
	H	-1.035795	-0.681050	-2.931059
	O	-4.968469	-0.950774	-0.213213
	O	3.360319	0.496581	1.670642
	H	2.173377	1.811702	0.620402
	C	2.116248	5.318094	1.066433
	C	3.396598	4.709602	0.525536
	O	3.287285	4.218556	-0.792371
	O	1.108167	4.364458	1.325323
	H	2.344865	5.820955	2.019967
	H	1.757489	6.093528	0.361714
	H	4.179351	5.485710	0.518820
	H	3.729307	3.916148	1.223599
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	H	0.844018	3.974063	0.469708

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	H	-0.518114	2.488391	-4.084661
	H	1.261736	0.640020	-3.271825
	H	0.357258	2.258144	-0.639413
	C	-0.474363	1.262454	1.582391
	C	-1.616547	0.440008	2.141858
	O	-2.828067	0.704021	1.463591
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	H	-1.356980	-0.632511	2.083758
	H	-1.766744	0.691259	3.203174
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	H	6.015789	-2.856722	-3.027943
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	C	3.063330	-2.568625	3.632729
	H	4.106887	-2.379818	3.337441
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	H	2.536852	-3.041536	-3.527329
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	O	1.170667	-1.361997	2.786494
	O	2.594092	-2.299168	1.340962
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	H	4.316193	1.990362	2.765772
	H	2.526803	1.991442	2.852979
	C	-6.216154	-0.703710	0.426025
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	H	-6.829654	-1.617896	0.425213
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	H	-7.029779	0.093283	-1.405966
	H	-6.252283	1.305463	-0.348164
	O	-8.126619	0.653929	0.266110

	C	-8.856124	1.682157	-0.352619
	H	-9.799495	1.803695	0.197578
	H	-8.306860	2.642084	-0.330976
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	H	2.140769	-1.685642	0.644752
PIV_5_product				
Imaginary frequencies=0	C	2.948149	1.641557	0.801557
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	C	1.134753	-2.606455	-2.030051
	O	1.407697	-2.106262	-3.104448
	C	-0.176566	-2.433177	-1.344607
	C	-0.335897	-2.763728	0.003983
	C	-1.552035	-2.528546	0.631687
	C	-2.612680	-1.965149	-0.082855
	C	-2.459377	-1.654063	-1.438970
	C	-1.244506	-1.893609	-2.068173
	C	-3.868336	-1.651629	0.658805
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	H	4.011432	-0.010918	-0.042741
	H	0.504132	-3.166916	0.568338
	H	-1.676029	-2.761870	1.690207
	H	-3.287303	-1.217423	-1.998418
	H	-1.115182	-1.653615	-3.124770
	O	-4.769392	-1.032102	-0.091856
	O	2.903216	1.091659	2.092862
	H	2.042958	2.250025	0.617811
	C	1.527793	5.656180	-0.148652
	C	2.899442	5.007799	-0.162536
	O	3.102687	4.119041	-1.238829
	O	0.484557	4.763495	0.178174
	H	1.527416	6.452678	0.612953
	H	1.345530	6.137567	-1.129335
	H	3.661746	5.799690	-0.246210
	H	3.057193	4.504353	0.812175
	H	2.341094	3.510895	-1.304194
	H	0.422451	4.099011	-0.534651
	C	0.366143	2.488193	-2.932989
	C	0.525395	1.046903	-3.356784
	O	1.886074	0.680696	-3.370745
	O	0.762469	2.702120	-1.593415
	H	0.988764	3.142650	-3.563389
	H	-0.688257	2.782482	-3.080362
	H	-0.046365	0.414013	-2.655939
	H	0.064426	0.927627	-4.356497
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	H	0.328788	2.031057	-1.005320

	C	-0.500175	1.389528	1.339002
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	H	-0.558955	2.490444	1.287792
	H	0.355393	1.118012	1.975023
	H	-1.647981	-0.254704	2.103894
	H	-1.963251	1.299090	2.912852
	H	-2.626429	0.859065	0.206502
	H	0.475500	0.307001	-0.012975
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	H	3.593697	-4.575358	-1.445901
	C	4.221801	-2.512780	-1.472182
	H	4.180512	-2.394876	-0.374523
	H	3.901429	-1.560977	-1.931386
	O	5.502108	-2.896987	-1.915722
	H	6.127962	-2.212086	-1.654672
	O	1.963840	-3.386614	-1.357272
	C	2.886940	-1.675418	3.978226
	H	3.856580	-1.237700	3.691108
	H	3.086916	-2.744144	4.199542
	H	3.225914	-3.719046	-2.975236
	C	2.002485	-1.674743	2.734024
	O	0.805025	-1.353325	2.847128
	O	2.562481	-2.051832	1.660744
	N	2.295051	-0.942103	5.081446
	H	1.303187	-1.177124	5.116559
	H	2.698987	-1.251227	5.963445
	C	2.762516	2.050405	3.106877
	H	2.631800	1.507185	4.053509
	H	3.654347	2.702316	3.177801
	H	1.878576	2.694535	2.938319
	C	-5.953669	-0.573304	0.552533
	H	-5.683875	0.065749	1.407047
	H	-6.537515	-1.430114	0.922640
	C	-6.734496	0.208359	-0.479588
	H	-6.957942	-0.437437	-1.351273
	H	-6.124146	1.058625	-0.841780
	O	-7.912629	0.655368	0.134094
	C	-8.726850	1.415680	-0.721141
	H	-9.620731	1.715189	-0.156632
	H	-8.208638	2.326870	-1.074457
	H	-9.045073	0.833288	-1.606175
	H	2.136499	-1.059274	0.460589

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3. Experimental Section

3.1. General

Proton Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker DPX 400 MHz and Bruker Avance II 600MHz spectrometers, using $CDCl_3$, DMSO-d_6 and D_2O as solvents, and referenced relative to residual $CHCl_3$ (δ = 7.26 ppm), DMSO (δ = 2.50 ppm) or D_2O (δ = 4.79 ppm). Chemical shifts are reported in ppm and coupling constants (*J*) in Hertz. Carbon NMR spectra were recorded on the same instruments (100.6 MHz and 150.9 MHz respectively) with total proton decoupling. Phosphorus NMR spectra were recorded on the Bruker DPX400 machine (162 MHz). HSQC, HMBC, TOCSY, NOE, EXSY and ROESY NMR experiments were used to aid assignment of NMR peaks when required. Infrared spectra were obtained on a Perkin Elmer Spectrum 100 FT-IR spectrometer equipped with a universal ATR sampling accessory. ESI mass spectra were acquired using a Waters Micromass LCT- time of flight mass spectrometer (TOF), interfaced to a Waters 2690 HPLC. The instrument was operated in either positive or negative mode as required. APCI experiments were carried out on a Bruker microTOF-Q III spectrometer interfaced to a Dionex UltiMate 3000 LC or direct insertion probe. Agilent tuning mix APCI-TOF was used to calibrate the system. Glycolysis experiments were accomplished with Radleys Carousel 12 Plus Reaction Station. Polyethylene terephthalate (granule size 3-5 mm) was purchased from Goodfellow Cambridge Limited and was used as provided. Anion exchange resin Amberlite-OH IRN78 (Supelco, strongly basic, total exchange capacity (OH) 1.25 eq/L) was purchased from Sigma Aldrich. Unless otherwise noted, all commercially available compounds were used as provided, without any further purification.

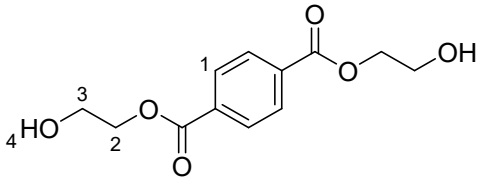
3.2. General procedure for PET glycolysis

An oven dried carousel flask was charged with polyethylene terephthalate granules (1.0000 g ± 0.0050 g), ethylene glycol (3.60 mL) and catalyst (X mol%).[a] The flask was placed under an atmosphere of nitrogen (balloon), and the reaction was stirred for 4 h at 180 °C.[b] The flask was removed from the carousel and was left to cool for 5 min. The reaction mixture was then filtered, and the residue was washed with H_2O (50 mL). The filtrate was cooled to 4 °C overnight to crystallise *bis*(2-hydroxyethyl)terephthalate (BHET). Residual polymer was left to dry overnight and weighed to obtain conversion data. BHET was filtered and was left to dry overnight and was weighed to obtain yield data. No appreciable weight loss of the product was recorded when filtered BHET was further dried for 4 h in vacuum oven at 60 °C.

[a]Mol% of catalyst is related to the number of moles of monomeric units (5.2 mmol) present in 1 g of polymer.

[b]Temperature was measured in an adjacent carousel flask filled with the equivalent amount of ethylene glycol and equipped with a thermometer.

Synthesis *bis*(2-hydroxyethyl)terephthalate (BHET)



BHET was synthesised following the General procedure A, polyethylene terephthalate granules (1.0000 g ± 0.0050 g) were used with ethylene glycol (3.60 mL) and **7** (0.0347 g, 0.104 mmol, 2 mol%).[a] BHET was isolated as a white solid (1.02 g, 77%). M.p. 103.0-104.5 °C (lit.,[1] M.p. 103.1-107.4 °C).

[a]Mol% of catalyst is related to the number of moles of monomeric units (5.2 mmol) present in 1 g of polymer.

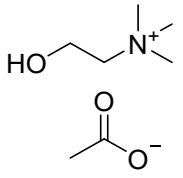
Spectral data for this compound were consistent with those in literature.[2]

δ_H (400 MHz, DMSO-d_6): 8.12 (s, 4H, *H*-1), 4.95 (t, 2H, *J* 5.6, *H*-4), 4.32 (t, 4H, *J* 4.7, *H*-2), 3.77-3.67 (m, 4H, *H*-3) ppm.

δ_C (100 MHz, DMSO-d_6): 165.2, 133.7, 129.5, 67.0, 59.0 ppm.

3.3. Synthesis of ionic catalysts: procedures

Cholinium acetate (4b)



To a 100 mL round-bottomed flask, choline chloride (0.70 g, 5.0 mmol) and MeOH (50 mL) were added. Amberlite-OH (bed volume ≈ 12 mL, 15 meq of total exchange capacity)[a] was added to the solution and the flask was shaken for 16 h on an orbital shaker. The resulting solution was passed through a plug of Amberlite-OH (bed volume ≈ 12 mL, 15 meq of total exchange capacity). Acetic acid (0.29 mL, 5.0 mmol) was added dropwise, and the resulting solution was stirred for 16 h. The solvent was removed under reduced pressure and the product dried under vacuum for 8 h at 60 °C to yield **4b** as a hygroscopic colourless amorphous solid (0.82 g, 99%).

[a]Bed volume (mL) is measured in a burette or graduate cylinder as packed resin beads soaked in methanol.

Spectral data for this compound were consistent with those in literature.[3]

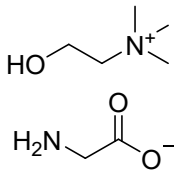
δ_H (400 MHz, DMSO-d_6): 3.87-3.81 (m, 2H, C$\underline{H}_2$OH), 3.44-3.39 (m, 2H, $(CH_3)_3NC\underline{H}_2$), 3.12 (s, 9H, $(C\underline{H}_3)_3NCH_2$), 1.57 (s, 3H, $C\underline{H}_3COO^-$) ppm.

δ_C (100 MHz, DMSO-d_6): 173.4 ($CH_3\underline{C}OO^-$), 67.3 (t, *J* 2.6, $(CH_3)_3N\underline{C}H_2$),[b] 54.9 ($\underline{C}H_2OH$), 53.1 (t, *J* 3.9, $(\underline{C}H_3)_3NCH_2$),[b] 25.7 ($\underline{C}H_3COO^-$) ppm.

HRMS (*m/z* – ESI^+): Found: 104.1071 (M^+) $C_5H_{14}NO^+$ Requires: 104.1070.

[b]The triplet originates from a spin-spin coupling between ^{14}N and ^{13}C.[4]

Cholinium glycinate (5)



To a 100 mL round-bottomed flask, choline chloride (0.70 g, 5.0 mmol) and MeOH (50 mL) were added. Amberlite-OH (bed volume ≈ 12 mL, 15 meq of total exchange capacity)[a] was added to the solution and the flask was shaken for 16 h on an orbital shaker. The resulting solution was passed through a plug of Amberlite-OH (bed volume ≈ 12 mL, 15 meq of total exchange capacity). Glycine (0.38 g, 5.0 mmol) was added, and the resulting solution was stirred for 16 h. The solvent was removed under reduced pressure and the product dried under vacuum for 8 h at 60 °C to yield **5** as a hygroscopic colourless gum (0.85 g, 95%).

[a]Bed volume (mL) is measured in a burette or graduate cylinder as packed resin beads soaked in methanol.

Spectral data for this compound were consistent with those in literature.[5]

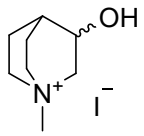
δ_H (400 MHz, D_2O): 4.10-4.04 (m, 2 H, C$\underline{H}_2$OH), 3.54-3.50 (m, 2 H, $(CH_3)_3NC\underline{H}_2$), 3.20 (s overlapped, 9 H, $(C\underline{H}_3)_3NCH_2$), 3.19 (s overlapped, 2 H, C$\underline{H}_2NH_2$) ppm.

δ_C (100 MHz, D_2O): 181.1 ($CH_2\underline{C}OO^-$) 67.4 (t, *J* 3.0, $(CH_3)_3N\underline{C}H_2$),[b] 55.6 ($\underline{C}H_2OH$), 53.8 (t, *J* 4.0, $(\underline{C}H_3)_3NCH_2$),[b] 44.5 ($\underline{C}H_2NH_2$) ppm.

HRMS (*m/z* – ESI^+): Found: 104.1070 (M^+) $C_5H_{14}NO^+$ Requires: 104.1070.

[b]The triplet originates from a spin-spin coupling between ^{14}N and ^{13}C.[4]

***N*-methylquinuclidin-3-olium iodide (S1)**



To a 100 mL round-bottomed flask, quinuclidin-3-ol (1.27 g, 10.0 mmol) and anhydrous THF (30 mL) were added. The solution was put under an argon atmosphere and stirred for 5 min. Methyl iodide (0.62 mL, 10.0 mmol) was added dropwise to the solution and the resulting mixture was stirred for 3 h. The reaction mixture was filtered and the resulting solid was washed three times with THF (10 mL). The product was dried under vacuum to yield **S1** as a white solid (2.31 g, 86%). M.p. 303.0-303.5 °C, compound turns brown at 290 °C. (Lit.,[6] M.p. 327-328 °C)

Spectral data for this compound were consistent with those in literature.[6]

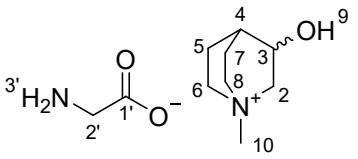
δ_H (400 MHz, DMSO-d_6): 5.52 (br. s, 1H), 4.09-4.01 (m, 1H), 3.69-3.60 (m, 1H), 3.41-3.33 (m, 3H), 3.27-3.17 (m, 1H), 3.10-3.03 (m, 1H), 2.92 (s, 3H), 2.18-2.06 (m, 1H), 2.05-1.98 (m, 1H), 1.97-1.86 (m, 1H), 1.83-1.66 (m, 2H) ppm.

δ_C (100 MHz, DMSO-d_6): 64.7 (t, *J* 2.5),[a] 63.4, 55.9 (t, *J* 2.6),[a] 55.0 (t, *J* 2.7),[a] 51.0 (t, *J* 4.1),[a] 26.0 (t, *J* 3.9),[a] 21.1, 17.4 ppm.

HRMS (*m/z* – ESI^+): Found: 142.1227 (M^+) $C_8H_{16}NO^+$ Requires: 142.1226.

[a]The triplet originates from a spin-spin coupling between ^{14}N and ^{13}C.[4]

***N*-methylquinuclidin-3-olium glycinate (6)**



To a 50 mL round-bottomed flask, *N*-methylquinuclidin-3-olium iodide (0.54 g, 2.0 mmol) and MeOH (20 mL) were added. Amberlite-OH (bed volume ≈ 5 mL, 6 meq of total exchange capacity)[a] was added to the solution and the flask was shaken for 16 h on an orbital shaker. The resulting solution was passed through a plug of Amberlite-OH (bed volume ≈ 5 mL, 6 meq of total exchange capacity). Glycine (0.15 g, 2.0 mmol) was added, and the resulting solution was stirred for 16 h. The solvent was removed under reduced pressure and the product was dried under vacuum for 8 h at 60 °C to yield **6** as a hygroscopic colourless gum (0.42 g, 98%).

[a]Bed volume (mL) is measured in a burette or graduate cylinder as packed resin beads soaked in methanol.

δ_H (600 MHz, DMSO-d_6):[b] 4.08-4.03 (m, 1H, *H*-3), 3.66-3.59 (m, 1H, *H*-2), 3.40-3.29 (m, 3H, *H*-8, *H*-6), 3.25-3.18 (m, 1H, *H*-6), 3.15-3.09 (m, 1H, *H*-2), 2.91 (s, 3H, *H*-10), 2.73 (s, 2H, *H*-2'), 2.18-2.09 (m, 1H, *H*-7), 2.05-2.00 (m, 1H, *H*-4), 1.95-1.86 (m, 1H, *H*-5), 1.80-1.67 (m, 2H, *H*-5, *H*-7) ppm.

δ_C (125 MHz, DMSO-d_6):[b] 175.6 (*C*-1'), 64.9 (t, *J* 2.5, *C*-2),[c] 63.4 (*C*-3), 56.1 (t, *J* 2.7, *C*-8),[c] 55.1 (t, *J* 2.8, *C*-6),[c] 51.1 (t, *J* 4.1, *C*-10),[c] 45.9 (*C*-2'), 26.1 (t, *J* 4.1, *C*-4),[c] 21.2 (*C*-5), 17.6 (*C*-7) ppm.

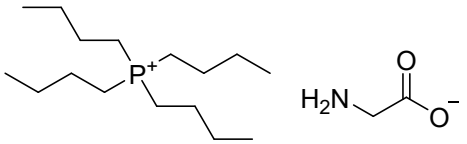
[b]A drop of D_2O was added to the DMSO-d_6.

[c]The triplet originates from a spin-spin coupling between ^{14}N and ^{13}C.[4]

ν_{max} (neat)/ cm^{-1}: 3361 (w), 3013 (w), 2954 (w), 2882 (w), 1575 (s), 1464 (w), 1380 (m), 1308 (m), 1125 (m), 1019 (m), 953 (m), 860 (m), 670 (w).

HRMS (*m/z* – ESI^+): Found: 142.1226 (M^+) $C_8H_{16}NO^+$ Requires: 142.1226.

Tetrabutylphosphonium glycinate (7)



To a 100 mL round-bottomed flask, glycine (0.38 g, 5.0 mmol) and MeOH (50 mL) were added. Tetrabutylphosphonium hydroxide in H_2O (40 *wt.*%, 3.50 mL, 5.0 mmol) was added dropwise to the solution and the resulting mixture was stirred for 16 h. The solvent was removed under reduced pressure and the product was dried under vacuum for 8 h at 60 °C to yield **7** as a hygroscopic colourless gum (1.65 g, 99%).

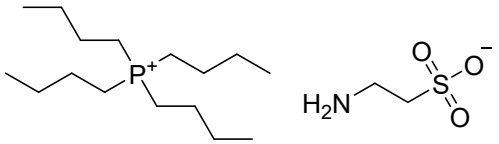
Spectral data for this compound were consistent with those in literature.[7]

δ_H (400 MHz, D_2O): 3.18 (s, 2H, $C\underline{H}_2NH_2$), 2.22-2.12 (m, 8H, $PC\underline{H}_2$), 1.62-1.41 (m, 16H), 0.93 (t, 12 H, *J* 7.2, $CH_2C\underline{H}_3$) ppm.

δ_C (100 MHz, D_2O): 181.3 ($CH_2\underline{C}OO^-$), 44.6 ($\underline{C}H_2COO^-$), 23.3 (d, *J* 15.3), 22.7 (d, *J* 4.4), 17.6 (d, *J* 48.3, $P\underline{C}H_2CH_2$), 12.5 ($CH_2\underline{C}H_3$) ppm.

HRMS (*m/z* – ESI^+): Found: 259.2549 (M^+) $C_{16}H_{36}P^+$ Requires: 259.2549.

Tetrabutylphosphonium taurinate (8)



To a 100 mL round-bottomed flask, taurine (0.63 g, 5.0 mmol) and MeOH (50 mL) were added. Tetrabutylphosphonium hydroxide in H_2O (40 *wt.*%, 3.50 mL, 5.0 mmol) was added dropwise to the solution and the resulting mixture was stirred for 16 h. The solvent was removed under reduced pressure and the product was dried under vacuum for 8 h at 60 °C to yield **8** as a hygroscopic colourless gum (1.88 g, 98%).

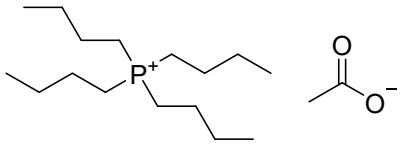
Spectral data for this compound were consistent with those in literature.[8]

δ_H (400 MHz, D_2O): 3.08-2.99 (m, 4H), 2.23-2.11 (m, 8H, PC$\underline{H}_2$), 1.63-1.41 (m, 16H), 0.94 (t, 12H, *J* 7.0, $CH_2C\underline{H}_3$) ppm.

δ_C (100 MHz, D_2O): 53.1, 36.5, 23.3 (d, *J* 15.3), 22.7 (d, *J* 4.5), 17.6 (d, *J* 48.3, P$\underline{C}H_2CH_2$), 12.5 ($CH_2\underline{C}H_3$) ppm.

HRMS (*m/z* – ESI^+): Found: 259.2548 (M^+) $C_{16}H_{36}P^+$ Requires: 259.2549.

Tetrabutylphosphonium acetate (9)



A 100 mL round-bottomed flask was charged with MeOH (50 mL). Tetrabutylphosphonium hydroxide in H_2O (40 *wt.*%, 3.50 mL, 5.0 mmol) was added dropwise to the solution and the resulting mixture was stirred for 5 min. Acetic acid (0.29 mL, 5.0 mmol) was added dropwise and the resulting solution was stirred for 16 h. The solvent was removed under reduced pressure and the product was dried under vacuum for 8 h at 60 °C to yield **8** as a hygroscopic colourless gum (1.54 g, 98%).

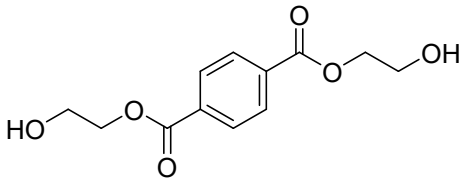
δ_H (400 MHz, $CDCl_3$): 2.50-2.35 (m, 8H, $PC\underline{H}_2$), 1.93 (s, 3H, $C\underline{H}_3COO^-$), 1.57-1.44 (m, 16H), 0.95 (t, 12H, *J* 7.0, $CH_2C\underline{H}_3$) ppm.

δ_C (100 MHz, $CDCl_3$): 176.9 ($CH_3\underline{C}OO^-$), 25.6 ($\underline{C}H_3COO^-$), 24.0 (d, *J* 15.3), 23.9 (d, *J* 4.9), 18.7 (d, *J* 47.3, $P\underline{C}H_2CH_2$), 13.5 ($CH_2\underline{C}H_3$) ppm.

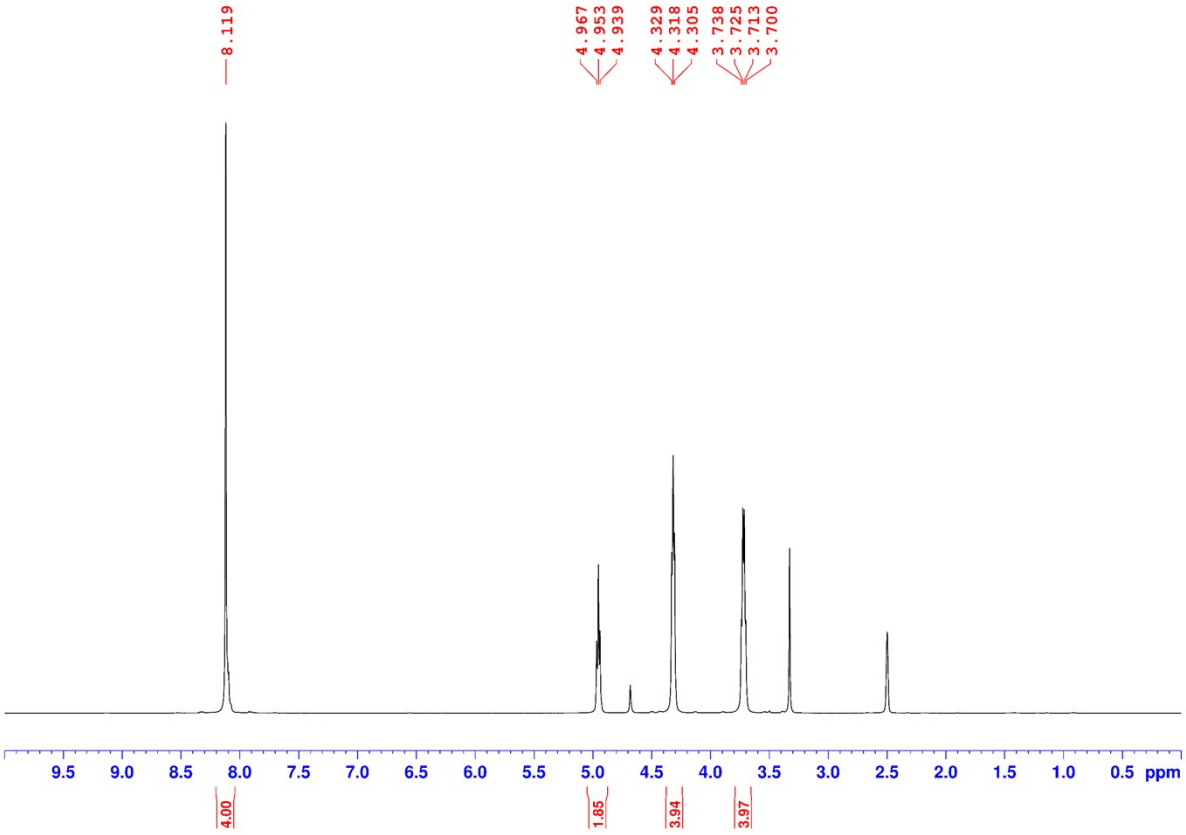
HRMS (*m/z* – ESI^+): Found: 259.2552 (M^+) $C_{16}H_{36}P^+$ Requires: 259.2549.

3.4. NMR spectra

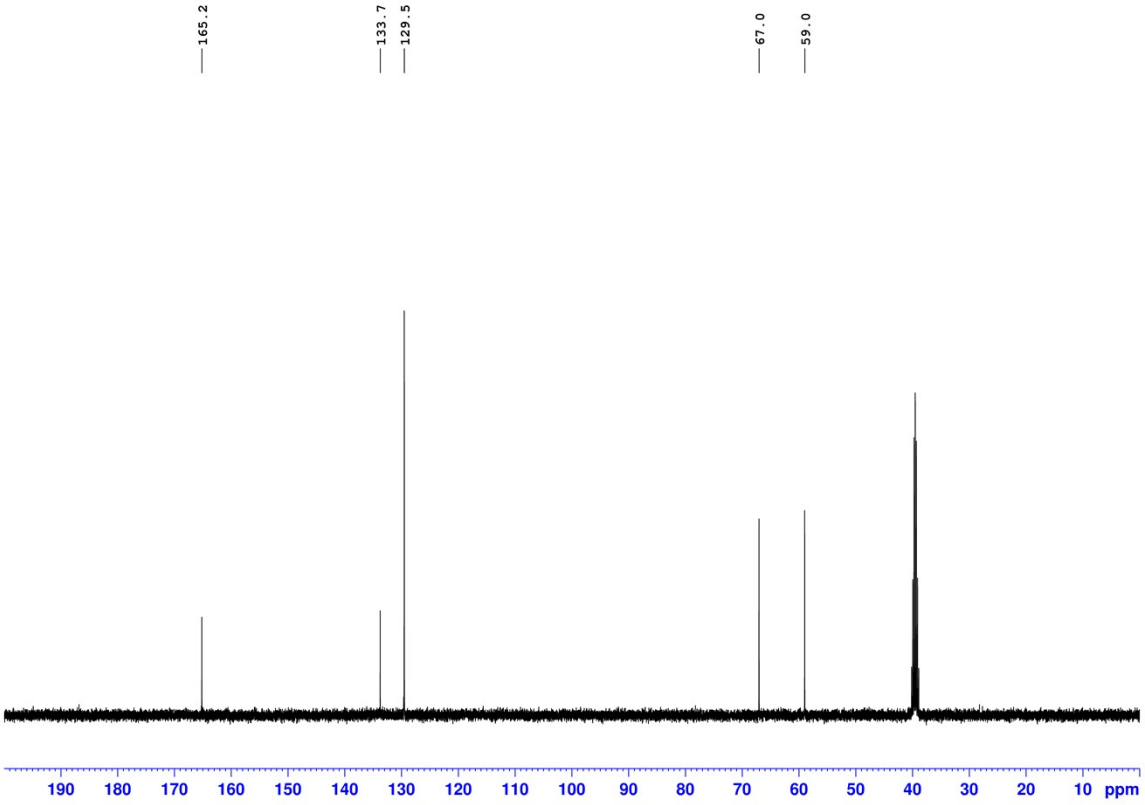
Product of the glycolysis reaction *bis*(2-hydroxyethyl)terephthalate (BHET).



^{1}H NMR spectrum (400MHz, DMSO-d_6) of **BHET**.

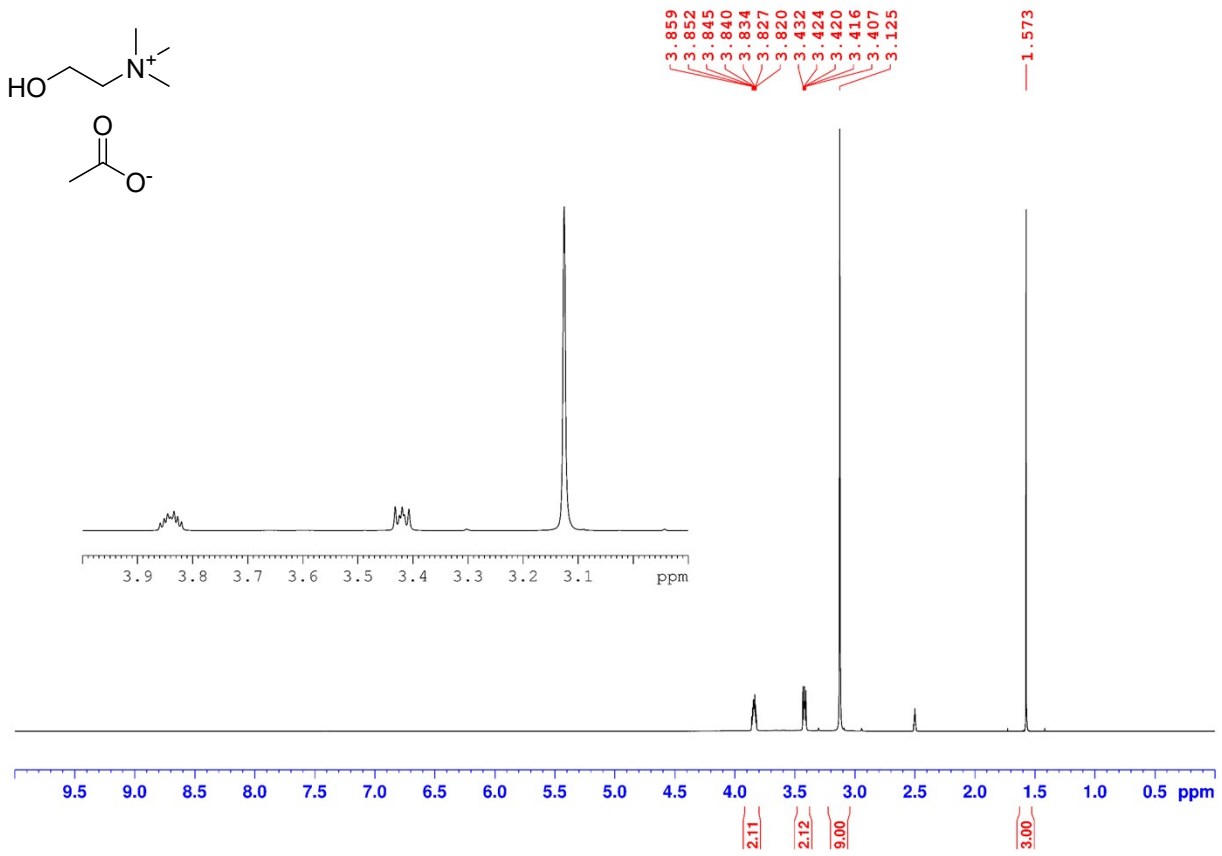


^{13}C NMR spectrum (100MHz, DMSO-d_6) of **BHET**.

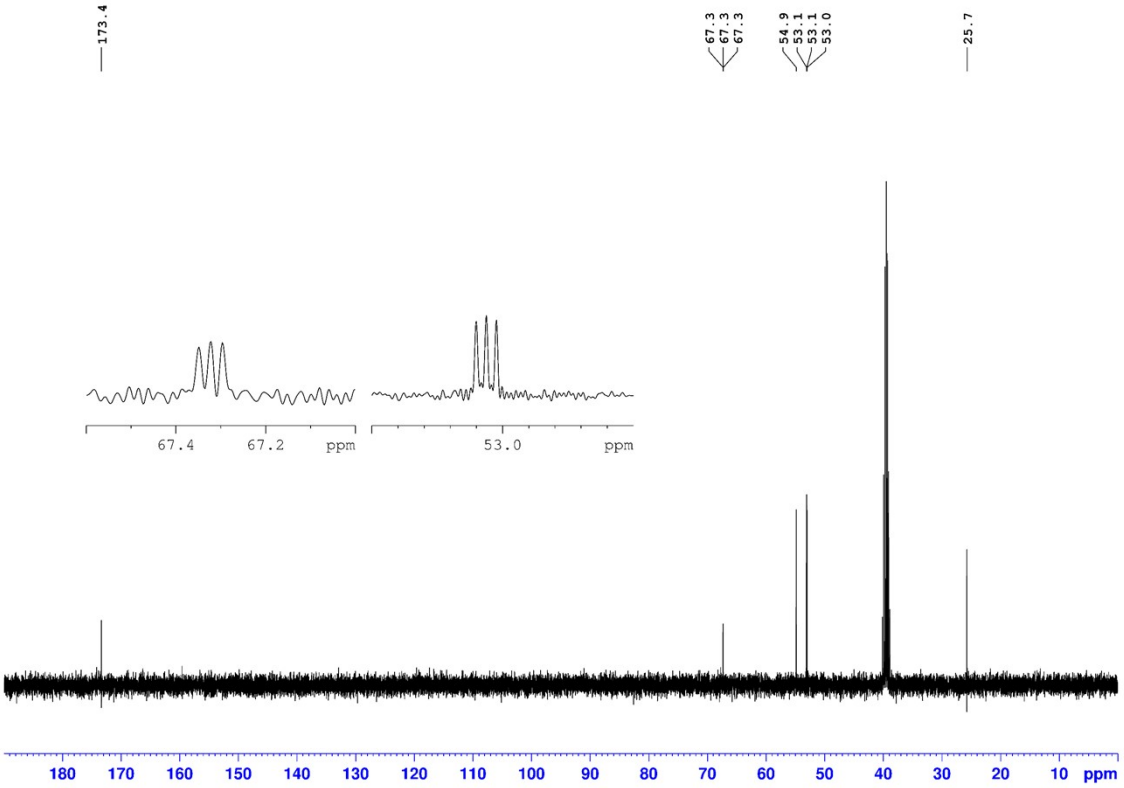


Cholinium acetate (4b)

^{1}H NMR spectrum (400MHz, DMSO-d_6) of **4b**.

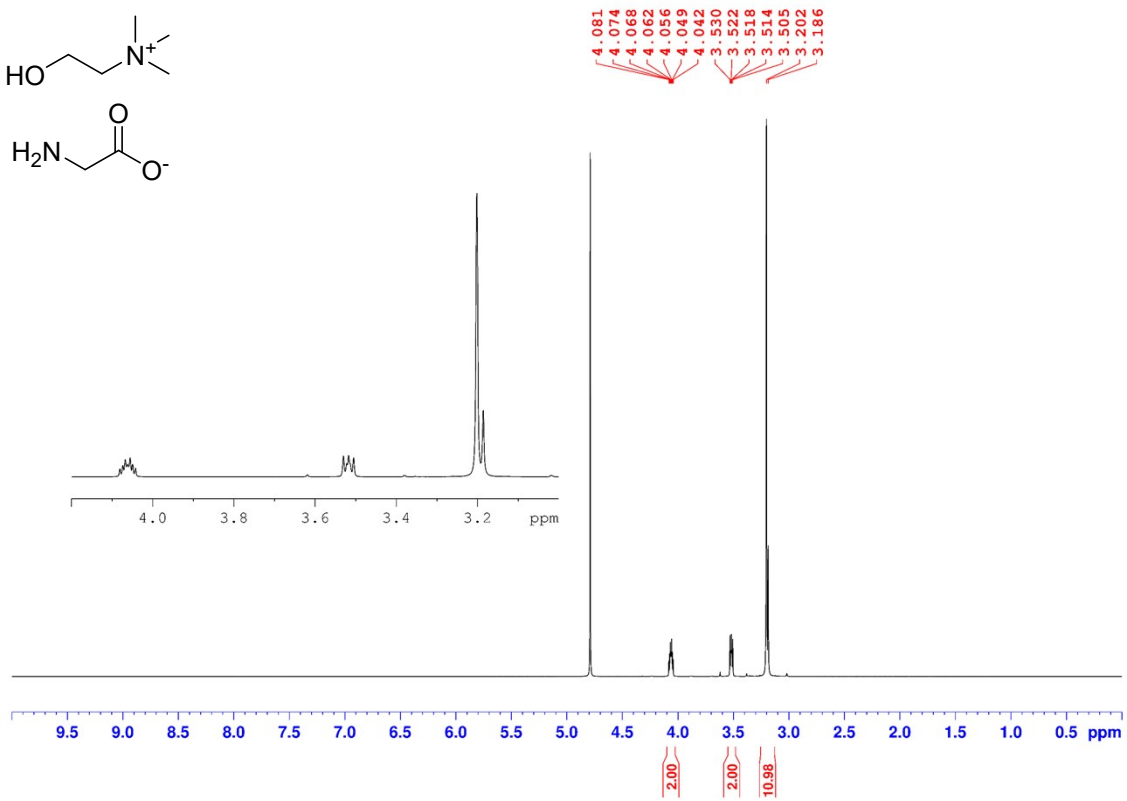


^{13}C NMR spectrum (100MHz, DMSO-d_6) of **4b**.

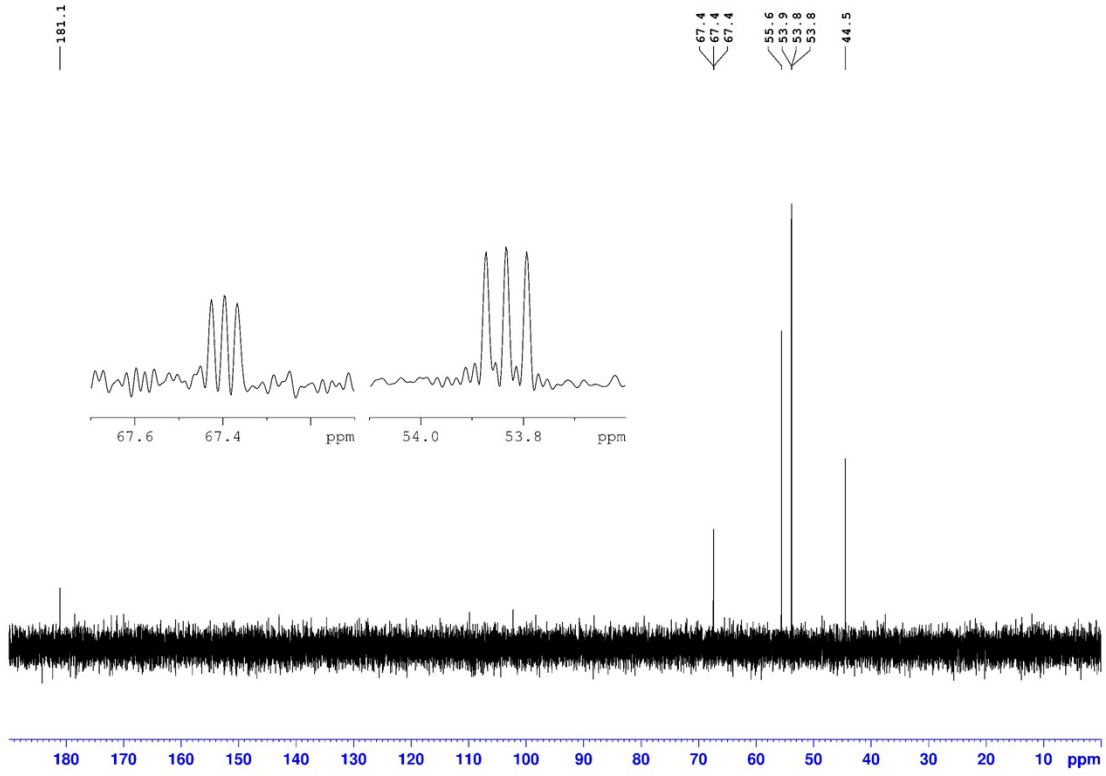


Cholinium glycinate (5)

^{1}H NMR spectrum (400MHz, D_2O) of **5**.

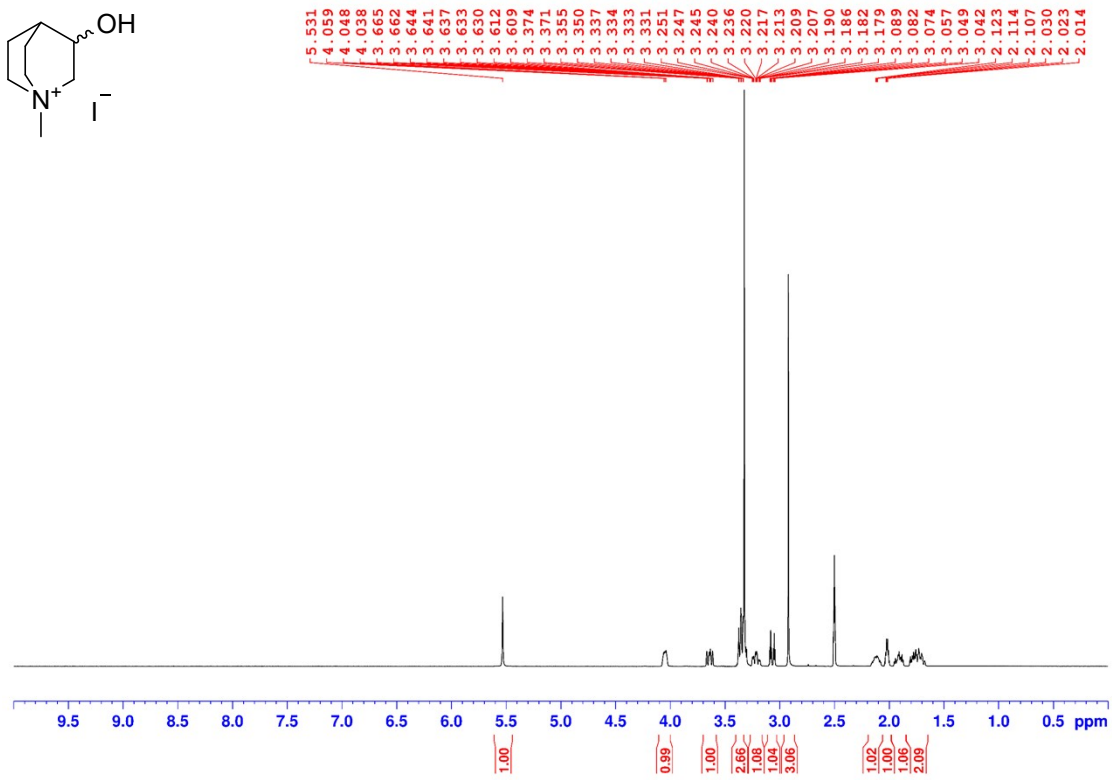


^{13}C NMR spectrum (100MHz, D_2O) of **5**.

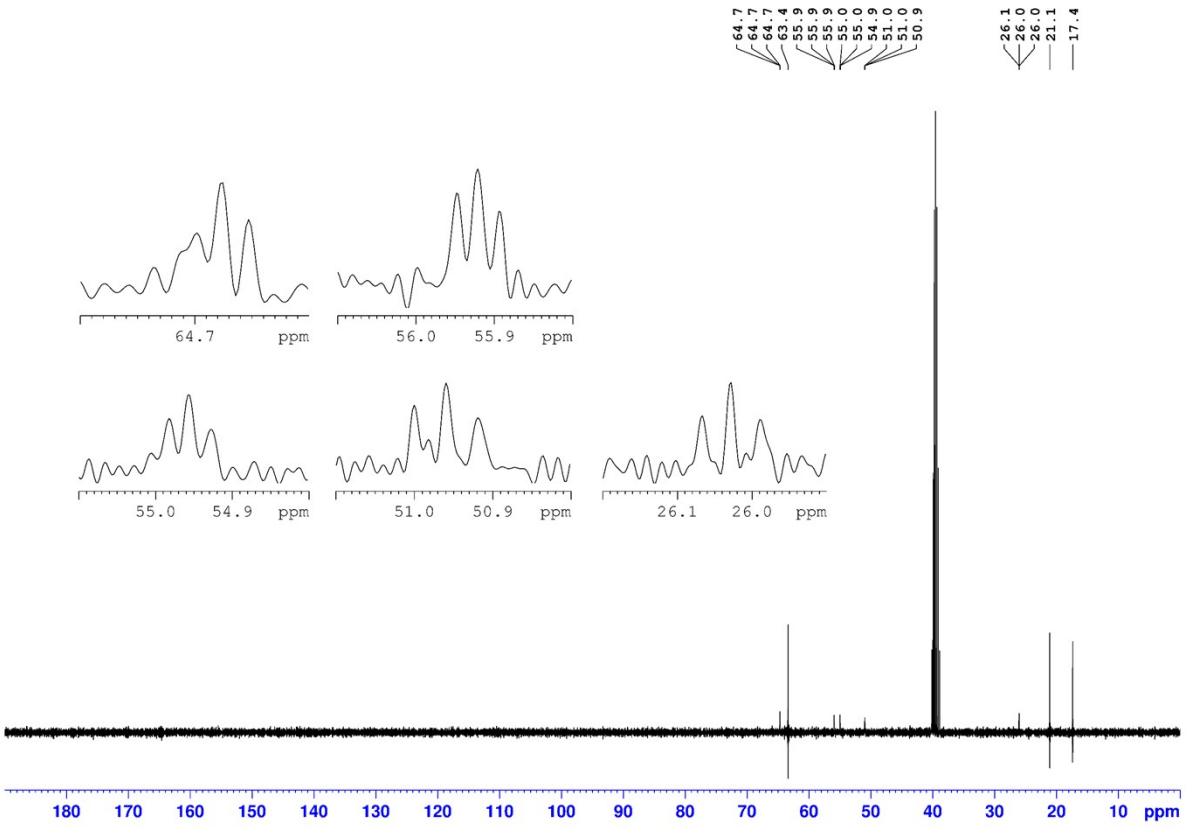


N-methylquinuclidin-3-olium iodide (S1)

^{1}H NMR spectrum (400MHz, DMSO-d_6) of **S1**.

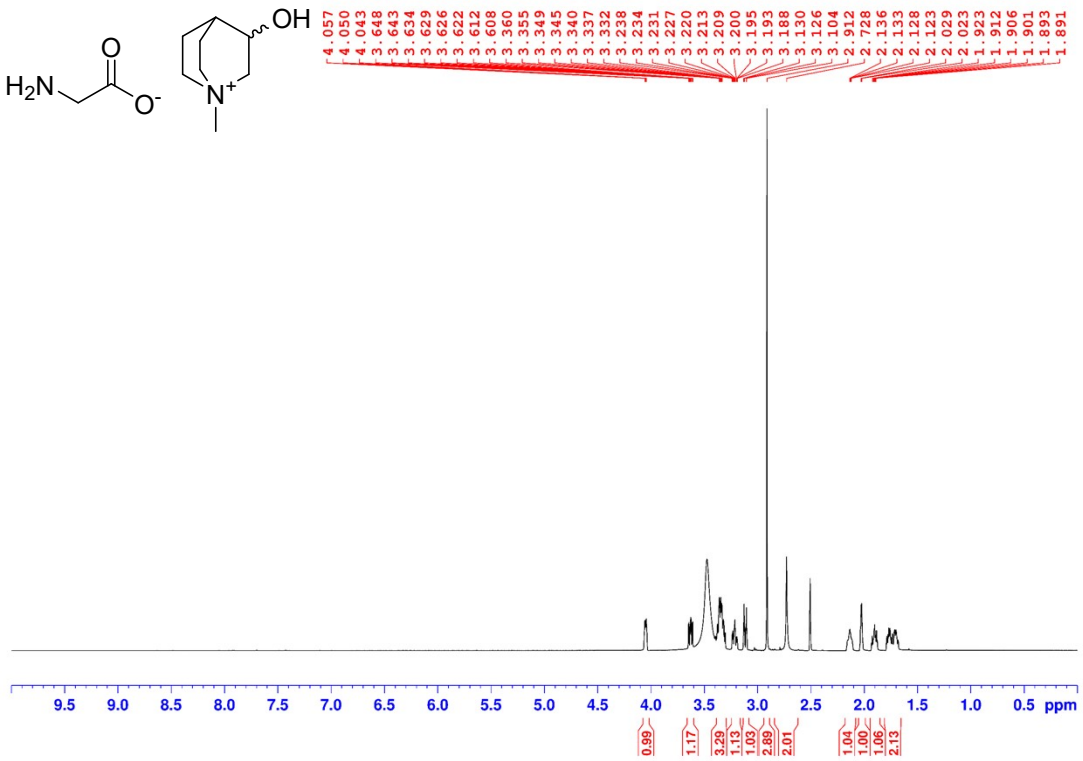


^{13}C NMR spectrum (100MHz, DMSO-d_6) of **S1**.

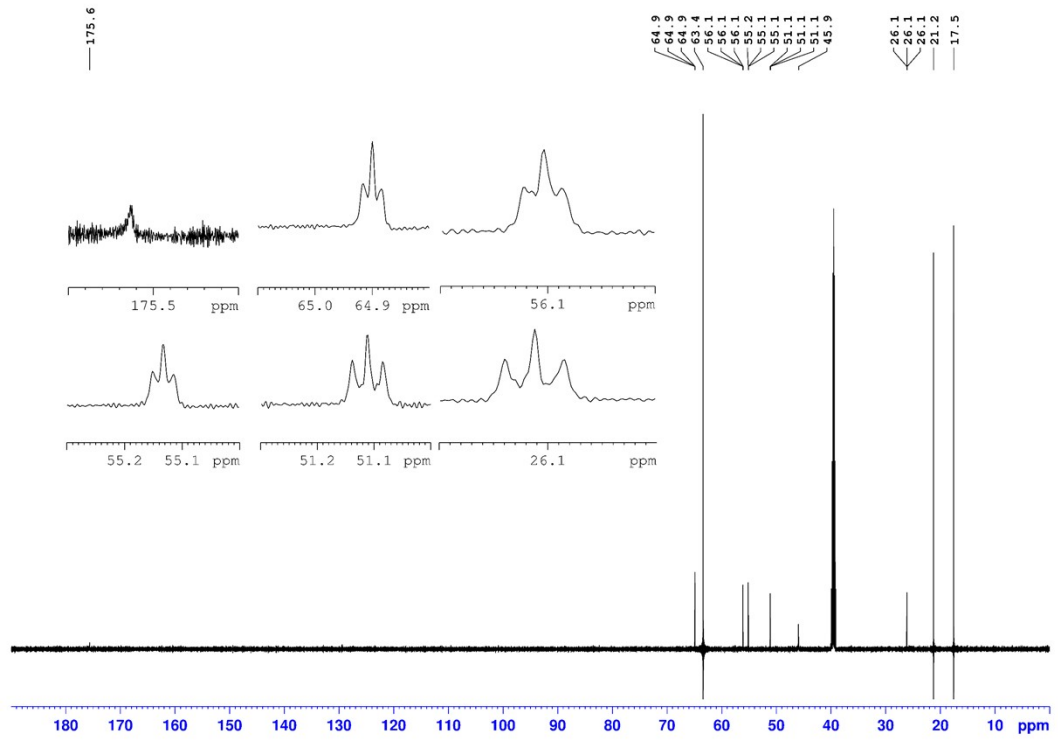


N-methylquinuclidin-3-olium glycinate (6)

^{1}H NMR spectrum (600MHz, DMSO-d_6) of **6**.

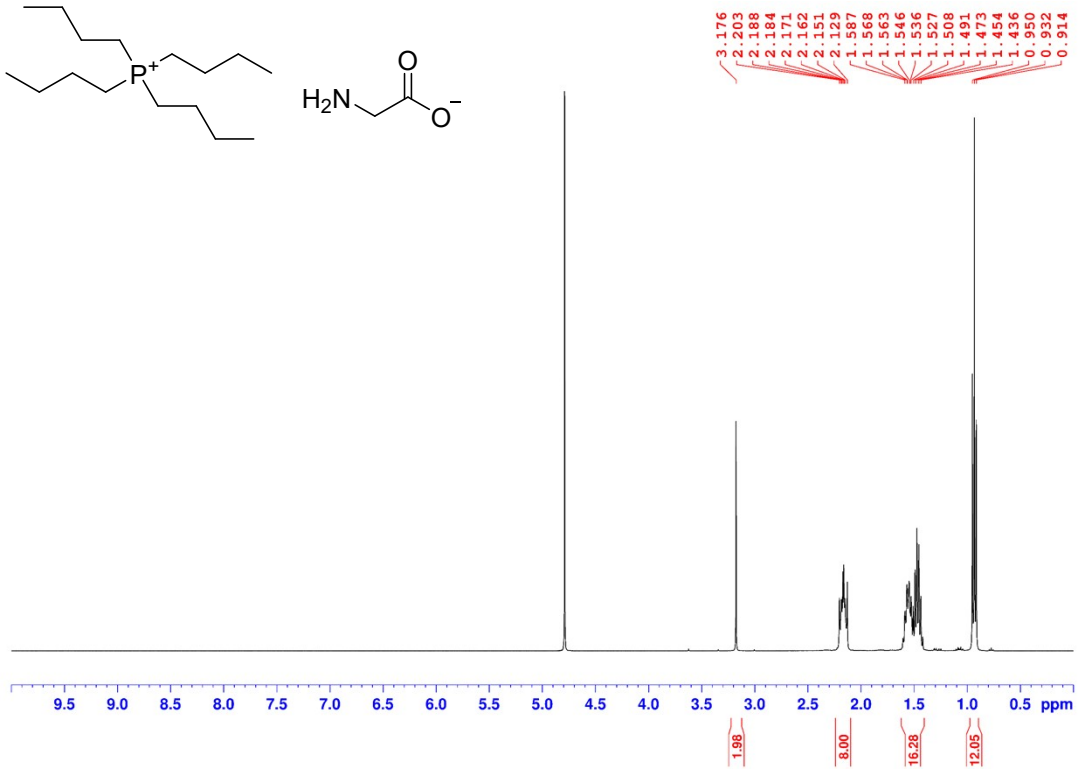


^{13}C NMR spectrum (150MHz, DMSO-d_6) of **6**.

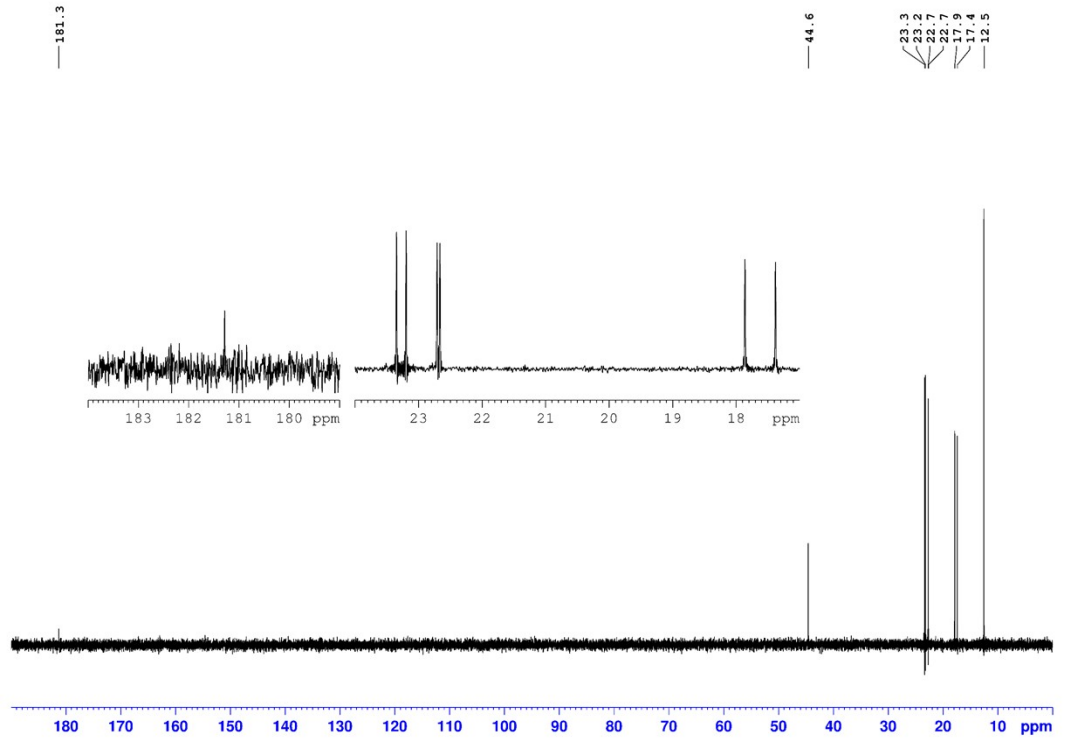


Tetrabutylphosphonium glycinate (7)

^{1}H NMR spectrum (400MHz, D_2O) of **7**.

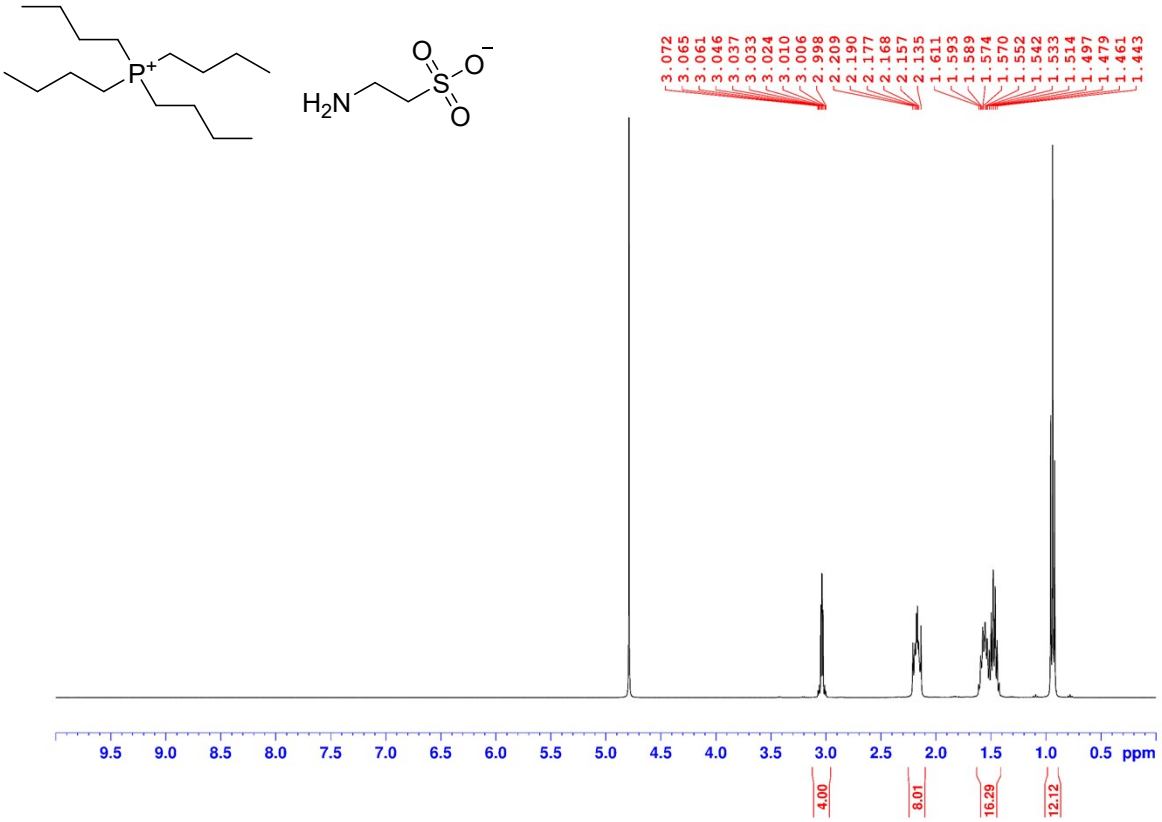


^{1}C NMR spectrum (100MHz, D_2O) of **7**.

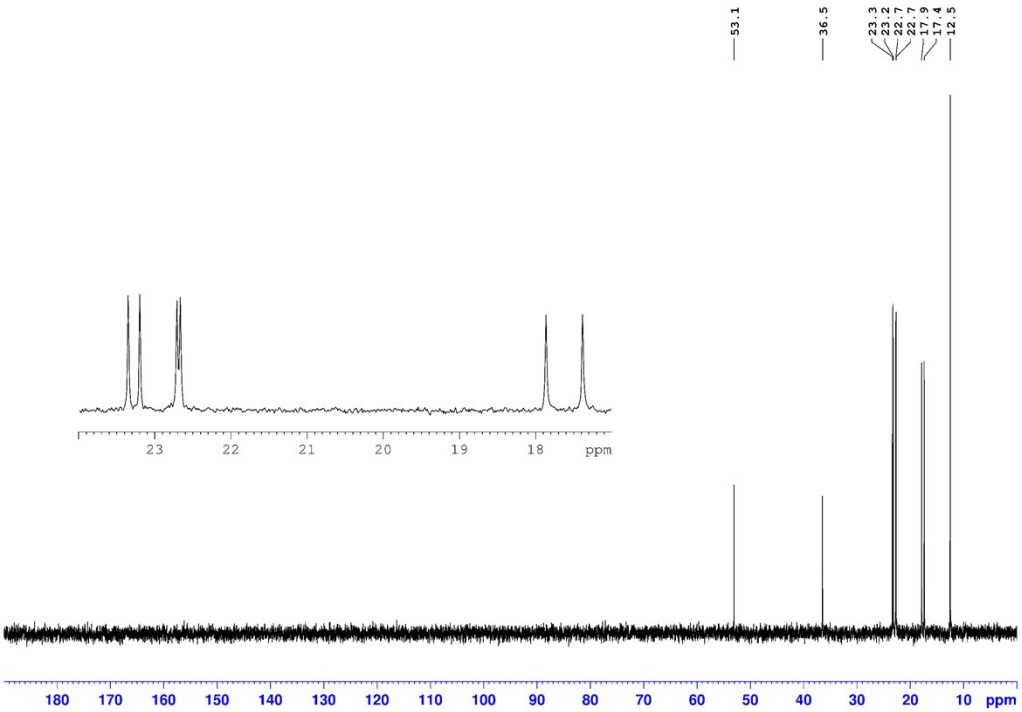


Tetrabutylphosphonium taurinate (8)

^{1}H NMR spectrum (400MHz, D_2O) of **8**.

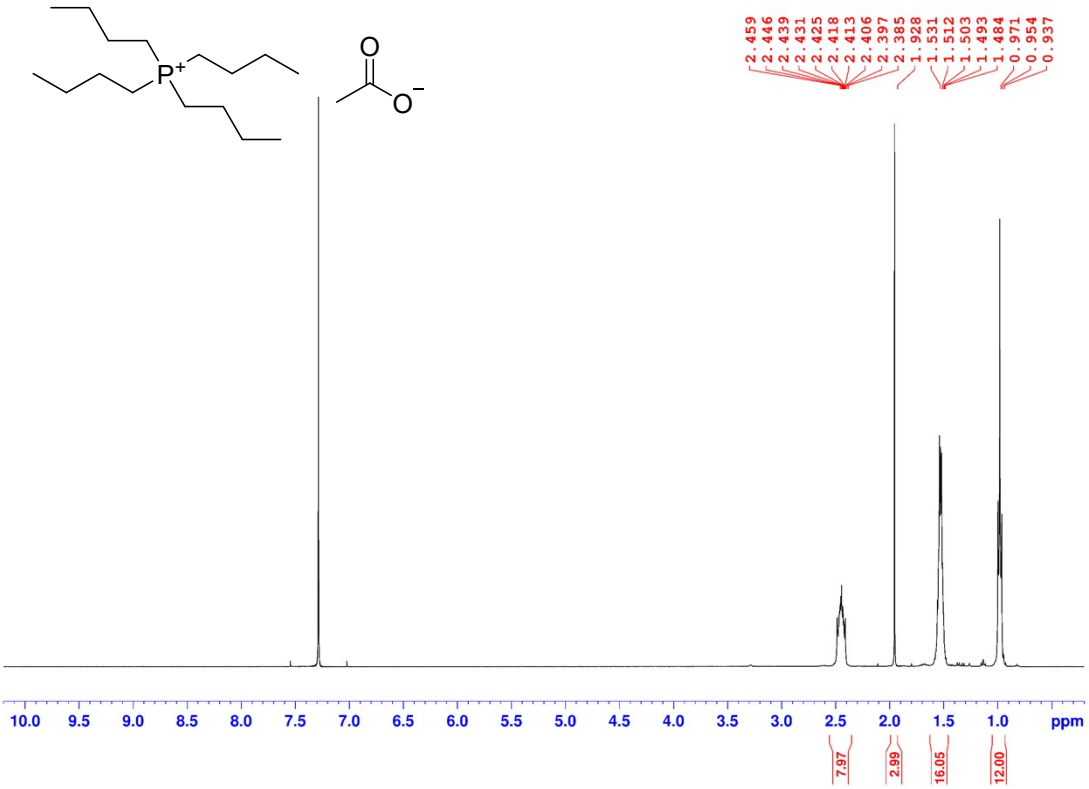


^{13}C NMR spectrum (100MHz, D_2O) of **8**.

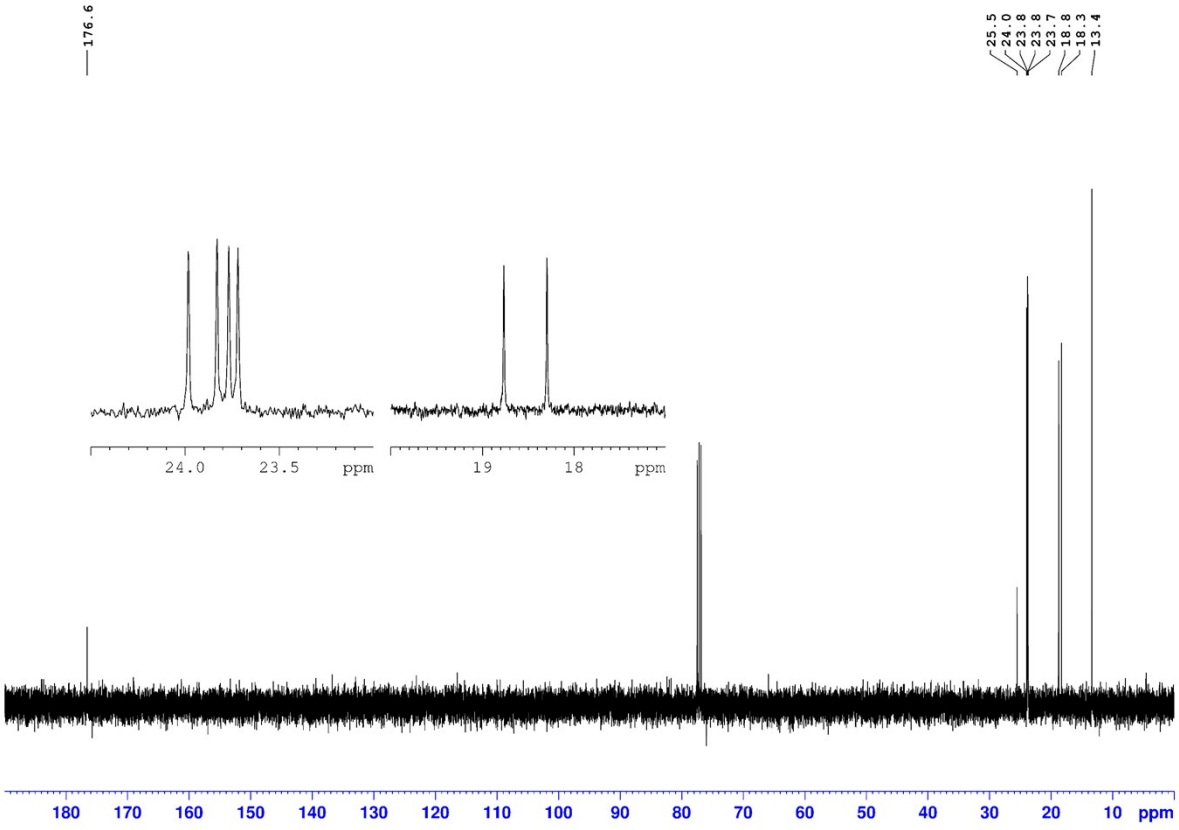


Tetrabutylphosphonium acetate (9)

*^1H NMR spectrum (400MHz, $CDCl_3$) of **9**.*

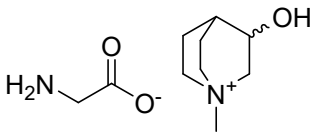


*^{13}C NMR spectrum (100MHz, $CDCl_3$) of **9**.*

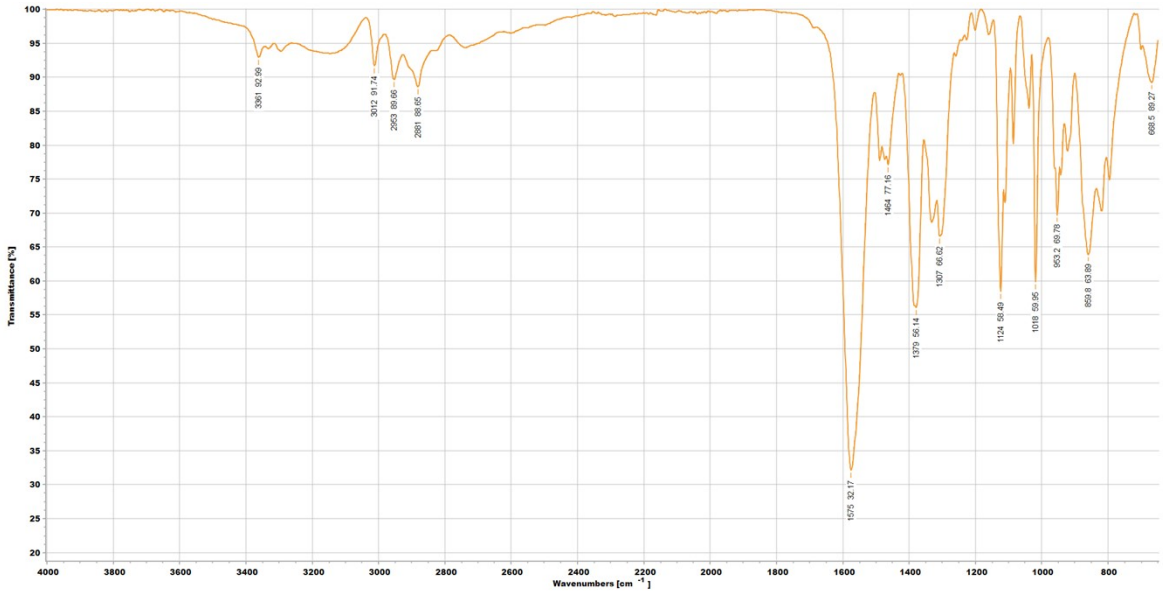


3.5. FT-IR Spectra

N-methylquinuclidin-3-olium glycinate (6)



FT-IR spectrum of **6**.



3.6. References

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