Supplementary Materials For:

Dicyclohexylammonium O,O'-diphenyl phosphate, $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$: spectroscopic study, crystal structure and Hirshfeld surface analysis

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Supplementary Table S1. Cambridge Structural Database (CSD) comparison study of bond lengths for cation moiety "dicyclohexylammonium". In the table, if the structures contain more than one molecule in the asymmetric unit, they are marked as Mol1, Mol2, etc.

No.	CSD REFCODE	C13-N1	C13-C14	C13-C18	C14-C15	C15-C16	C16-C17	C17-C18	C19-N1	C19-C24	C19-C20	C20-C21	C21-C22	C22-C23	C23-C24
1	CADGUJ-Mol1	1.529	1.502	1.506	1.520	1.503	1.540	1.497	1.505	1.510	1.501	1.495	1.524	1.521	1.504
2	CADGUJ-Mol2	1.512	1.497	1.506	1.526	1.496	1.537	1.524	1.507	1.510	1.555	1.506	1.537	1.525	1.522
3	EFUMEX	1.503	1.515	1.528	1.514	1.506	1.528	1.516	1.505	1.519	1.527	1.513	1.521	1.530	1.523
4	GAGQOV-Mol1	1.493	1.519	1.543	1.543	1.484	1.549	1.497	1.509	1.519	1.521	1.519	1.509	1.517	1.523
5	GAGQOV-Mol2	1.488	1.509	1.523	1.507	1.503	1.542	1.515	1.503	1.518	1.532	1.525	1.520	1.500	1.521
6	HAXRAZ	1.497	1.485	1.465	1.484	1.491	1.520	1.495	1.508	1.509	1.519	1.460	1.497	1.483	1.487
7	JOXMAK	1.504	1.521	1.533	1.504	1.512	1.528	1.538	1.519	1.529	1.539	1.501	1.504	1.531	1.526
8	LOKGUN	1.497	1.519	1.523	1.523	1.528	1.522	1.527	1.503	1.519	1.516	1.515	1.530	1.517	1.517
9	OBOTOQ	1.504	1.526	1.534	1.517	1.530	1.527	1.524	1.516	1.517	1.539	1.517	1.529	1.521	1.523
10	TEDFIR	1.494	1.530	1.521	1.497	1.499	1.524	1.504	1.517	1.506	1.536	1.503	1.523	1.536	1.500
11	WILCOR	1.498	1.514	1.530	1.512	1.490	1.517	1.499	1.501	1.502	1.534	1.481	1.502	1.534	1.491
12	YIWXOR	1.507	1.519	1.531	1.525	1.514	1.531	1.523	1.509	1.524	1.534	1.515	1.521	1.526	1.516
13	ZALTEL-Mol1	1.494	1.522	1.533	1.519	1.519	1.531	1.510	1.491	1.520	1.498	1.516	1.522	1.508	1.512
14	ZALTEL-Mol2	1.502	1.506	1.603	1.481	1.500	1.621	1.484	1.503	1.526	1.519	1.519	1.523	1.529	1.530
15	ZALTIP-Mol1	1.493	1.504	1.515	1.530	1.493	1.554	1.505	1.509	1.517	1.541	1.521	1.495	1.524	1.512
16	ZALTIP-Mol2	1.486	1.511	1.508	1.509	1.523	1.539	1.500	1.504	1.527	1.526	1.497	1.518	1.500	1.493
17	ZALTIP-Mol3	1.503	1.524	1.511	1.490	1.527	1.515	1.503	1.509	1.498	1.523	1.522	1.518	1.504	1.538
18	ZALTIP-Mol4	1.498	1.504	1.518	1.529	1.493	1.521	1.503	1.503	1.509	1.508	1.522	1.503	1.527	1.532
19	ZARGOQ	1.503	1.517	1.527	1.526	1.523	1.526	1.524	1.503	1.520	1.534	1.518	1.520	1.525	1.526
20	ZETHIP-Mol1	1.498	1.532	1.519	1.529	1.539	1.537	1.541	1.514	1.520	1.530	1.520	1.538	1.528	1.515
21	ZETHIP-Mol2	1.519	1.530	1.547	1.486	1.533	1.528	1.506	1.521	1.510	1.532	1.546	1.512	1.567	1.534
	Average	*1.501*	*1.515*	*1.525*	*1.513*	*1.510*	*1.535*	*1.511*	*1.508*	*1.516*	*1.527*	*1.511*	*1.517*	*1.522*	*1.516*
	Std-Dev	*0.010*	*0.012*	*0.025*	*0.017*	*0.016*	*0.022*	*0.015*	*0.007*	*0.008*	*0.014*	*0.018*	*0.012*	*0.017*	*0.014*
	Title Compound	**1.499(4)**	**1.516(4)**	**1.519(4)**	**1.522(4)**	**1.516(5)**	**1.508(5)**	**1.528(4)**	**1.506(4)**	**1.509(4)**	**1.517(4)**	**1.523(5)**	**1.512(5)**	**1.501(5)**	**1.524(4)**

Supplementary Table S2. Cambridge Structural Database (CSD) comparison study of selected bond angles for cation moiety "dicyclohexylammonium".

No.	CSD REFCODE	C13-N1-C19	N1-C13-C14	N1-C13-C18	N1-C19-C20	N1-C19-C24
1	CADGUJ-Mol1	118.18	111.75	107.35	108.40	109.05
2	CADGUJ-Mol2	117.53	112.42	108.21	107.75	111.30
3	EFUMEX	117.06	112.46	108.10	109.72	111.62
4	GAGQOV-Mol1	119.04	112.52	107.66	107.59	112.55
5	GAGQOV-Mol2	119.07	111.91	107.18	107.50	112.41
6	HAXRAZ	118.54	113.36	106.84	108.42	111.70
7	JOXMAK	119.25	112.01	105.98	105.76	109.30
8	LOKGUN	118.70	112.35	107.96	108.00	113.06
9	OBOTOQ	117.48	111.26	108.03	109.13	110.85
10	TEDFIR	118.31	112.32	108.30	107.62	112.09
11	WILCOR	117.36	111.93	109.79	108.86	111.27
12	YIWXOR	116.78	110.80	109.01	108.22	110.84
13	ZALTEL-Mol1	116.81	111.79	108.51	108.35	112.27
14	ZALTEL-Mol2	117.49	108.53	106.90	107.40	112.14
15	ZALTIP-Mol1	117.86	113.85	109.16	108.92	110.46
16	ZALTIP-Mol2	116.77	112.24	107.79	107.68	111.71
17	ZALTIP-Mol3	117.07	111.64	108.40	107.75	111.00
18	ZALTIP-Mol4	117.36	111.21	108.33	107.91	112.87
19	ZARGOQ	118.82	111.92	106.83	107.64	110.82
20	ZETHIP-Mol1	117.24	110.74	107.31	107.89	112.11
21	ZETHIP-Mol2	117.37	110.19	108.23	106.60	110.94
	Average	*117.81*	*111.77*	*107.90*	*107.96*	*111.45*
	Std-Dev	*0.8*	*1.1*	*0.9*	*0.9*	*1.0*
	Title Compound	**118.1(2)**	**111.2(2)**	**108.0(2)**	**107.1(2)**	**112.3(2)**

Supplementary Table S3. Cambridge Structural Database (CSD) comparison study of selected torsion angles for cation moiety "dicyclohexylammonium". In the table “sc” represents synclinal.

No.	CSD REFCODE	C14-C13-N1-C19			C24-C19-N1-C13		
1	Title Compound	–61.1(3)		–sc	–53.9(3)		–sc
2	CADGUJ-Mol1	–64.7		–sc	–61.2		–sc
3	CADGUJ-Mol2	–62.5		–sc	–59		–sc
4	GAGQOV-Mol1	–56.9		–sc	–56.18		–sc
5	LOKGUN	–56.5		–sc	–55.6		–sc
6	YIWXOR	–66.0		–sc	–65.3		–sc
7	ZALTEL-Mol1	–61.8		–sc	–55.6		–sc
8	ZALTIP-Mol4	–52.3		–sc	–51.2		–sc
9	ZARGOQ	–62.6		–sc	–53.3		–sc
10	ZETHIP-Mol1	–58.7		–sc	–54.8		–sc
11	ZALTIP-Mol2	–59.2		–sc	–53.2		–sc
12	EFUMEX		68.9	+sc		53.2	+sc
13	GAGQOV-Mol2		56.1	+sc		56.5	+sc
14	HAXRAZ		60.6	+sc		55.7	+sc
15	JOXMAK		60.8	+sc		52.9	+sc
16	OBOTOQ		59.6	+sc		59.2	+sc
17	TEDFIR		58.8	+sc		51.5	+sc
18	WILCOR		63.6	+sc		60.7	+sc
19	ZALTEL-Mol2		56.9	+sc		53.4	+sc
20	ZALTIP-Mol1		53.1	+sc		53	+sc
21	ZALTIP-Mol3		61.1	+sc		54.3	+sc
22	ZETHIP-Mol2		58.3	+sc		56.6	+sc
	Average	*–60.1*	*59.8*		*–56.5*	*55.2*	
	Std-Dev	*4.2*	*4.1*		*4.2*	*2.9*	
	Title Compound	**–61.1(3)**			**–53.9(3)**		

Supplementary Table S4. Cambridge Structural Database (CSD) comparison study of selected bond lengths for anion moiety "diphenyl phosphate".

No.	CSD REFCODE	O1-P1	P1-O2	O3-P1	O4-P1	C1-O4	C7-O3
1	CUVMUB	1.494	1.468	1.591	1.605	1.405	1.401
2	DUWWEX	1.484	1.482	1.599	1.608	1.409	1.390
3	ETADIM	1.475	1.464	1.628	1.632	1.393	1.383
4	FAGLEE-Mol1	1.484	1.475	1.589	1.620	1.402	1.383
5	FAGLEE-Mol2	1.478	1.477	1.599	1.612	1.398	1.383
6	FAGLEE-Mol3	1.489	1.474	1.596	1.608	1.400	1.387
7	FAGLEE-Mol4	1.482	1.482	1.607	1.612	1.398	1.391
8	FAWYOR-Mol1	1.487	1.473	1.603	1.608	1.407	1.389
9	FAWYOR-Mol2	1.504	1.488	1.579	1.588	1.400	1.405
10	HUHTEJ	1.477	1.472	1.600	1.602	1.402	1.391
11	OFESID	1.482	1.451	1.617	1.627	1.383	1.379
12	PABMUA	1.485	1.465	1.619	1.623	1.390	1.386
13	PABNAH	1.478	1.477	1.602	1.609	1.409	1.395
14	RUXWOY	1.492	1.482	1.619	1.619	1.406	1.405
15	VOVCOY	1.477	1.473	1.602	1.605	1.389	1.381
16	ZOXVEN-Mol1	1.477	1.460	1.575	1.633	1.399	1.356
17	ZOXVEN-Mol2	1.507	1.455	1.576	1.610	1.368	1.341
	Average	*1.485*	*1.472*	*1.600*	*1.613*	*1.398*	*1.385*
	Std-Dev	*0.009*	*0.010*	*0.015*	*0.012*	*0.011*	*0.016*
	Title Compound	**1.469(2)**	**1.459(2)**	**1.602(2)**	**1.623(2)**	**1.382(3)**	**1.374(3)**

Supplementary Table S5. Cambridge Structural Database (CSD) comparison study of selected bond angles for anion moiety "diphenyl phosphate".

No.	CSD REFCODE	O2-P1-O1	O2-P1-O3	O1-P1-O3	O2-P1-O4	O1-P1-O4	O3-P1-O4
1	CUVMUB	118.58	111.66	105.04	112.81	102.71	104.44
2	DUWWEX	118.86	111.25	105.34	110.66	105.66	104.20
3	ETADIM	121.46	109.30	106.14	111.01	104.86	102.52
4	FAGLEE-Mol1	119.48	108.59	110.18	109.58	107.59	99.55
5	FAGLEE-Mol2	121.45	110.49	105.35	110.62	103.78	103.91
6	FAGLEE-Mol3	119.65	109.48	107.09	109.76	109.33	99.64
7	FAGLEE-Mol4	121.42	110.10	105.13	110.20	104.78	103.97
8	FAWYOR-Mol1	119.96	113.37	102.76	110.83	104.57	104.48
9	FAWYOR-Mol2	118.30	111.59	103.86	111.22	104.53	106.97
10	HUHTEJ	120.30	110.65	104.25	111.08	105.07	104.52
11	OFESID	119.49	111.43	105.36	111.53	103.72	104.46
12	PABMUA	122.68	110.63	104.42	109.23	105.16	103.13
13	PABNAH	119.20	109.98	108.91	111.04	105.41	100.64
14	RUXWOY	118.17	112.17	104.67	111.55	104.92	104.69
15	VOVCOY	120.75	111.25	105.14	111.48	103.35	103.74
16	ZOXVEN-Mol1	122.40	111.52	109.96	111.73	100.11	97.79
17	ZOXVEN-Mol2	121.68	114.01	101.86	113.18	104.27	98.86
	Average	*120.23*	*111.03*	*105.62*	*111.03*	*104.70*	*102.79*
	Std-Dev	*1.43*	*1.39*	*2.29*	*1.03*	*1.95*	*2.55*
	Title Compound	**119.96(12)**	**111.27(13)**	**106.78(12)**	**110.05(15)**	**109.86(12)**	**96.31(11)**

Supplementary Table S6. Cambridge Structural Database (CSD) comparison study of selected torsion angles for anion moiety "diphenyl phosphate".

No.	CSD REFCODE	C7-O3-P1-O4			C1-O4-P1-O3		
1	**Title Compound**	**–72.5(2)**		**–sc**	**–163.3(2)**		**–ap**
2	FAGLEE-Mol1	–87.94		–sc	–152.22		–ap
3	CUVMUB	–61.35		–sc	–94.59		–ac
4	FAWYOR-Mol2	–59.37		–sc	–66.81		–sc
5	PABMUA	–67.93		–sc	–72.13		–sc
6	RUXWOY	–73.26		–sc	–62.28		–sc
7	FAGLEE-Mol4	–87.44		–sc	–69.70		–sc
8	ZOXVEN-Mol1	–75.25		–sc		151.57	+ap
9	FAGLEE-Mol3		89.63	+sc		155.48	+ap
10	DUWWEX		59.32	+sc		116.45	+ac
11	ETADIM		66.99	+sc		79.19	+sc
12	FAGLEE-Mol2		85.20	+sc		75.10	+sc
13	HUHTEJ		58.58	+sc		77.22	+sc
14	OFESID		74.29	+sc		43.63	+sc
15	FAWYOR-Mol1		83.25	+sc		51.59	+sc
16	VOVCOY		67.09	+sc		79.21	+sc
17	PABNAH		74.40	+sc	–134.38		–ac
18	ZOXVEN-Mol2		82.62	+sc	–125.05		–ac

sc: synclinal

ac: anticlinal

ap: antiperiplanar

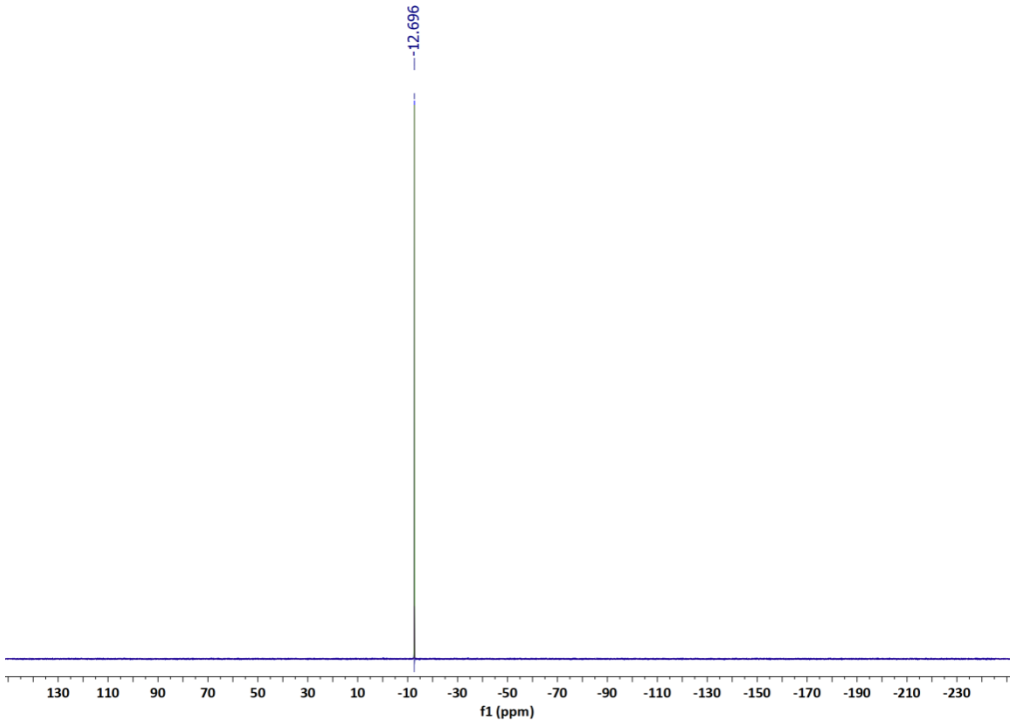

Figure S1. The $^{31}P\{^{1}H\}$ NMR spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ in DMSO-d_6.

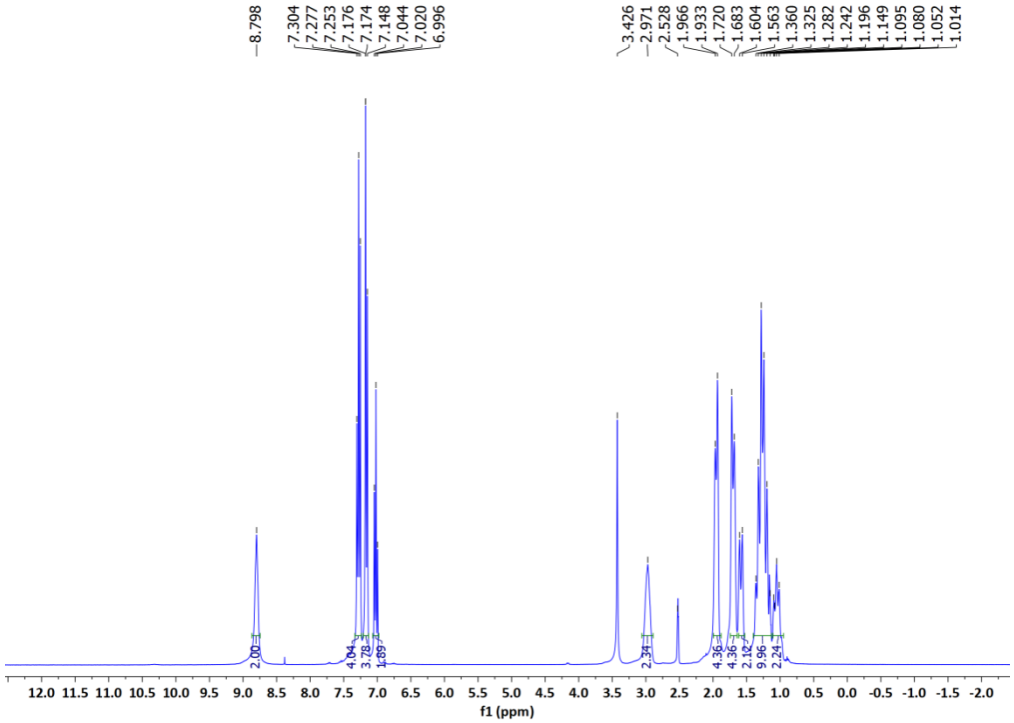

Figure S2. The ^{1}H NMR spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ in DMSO-d_6.

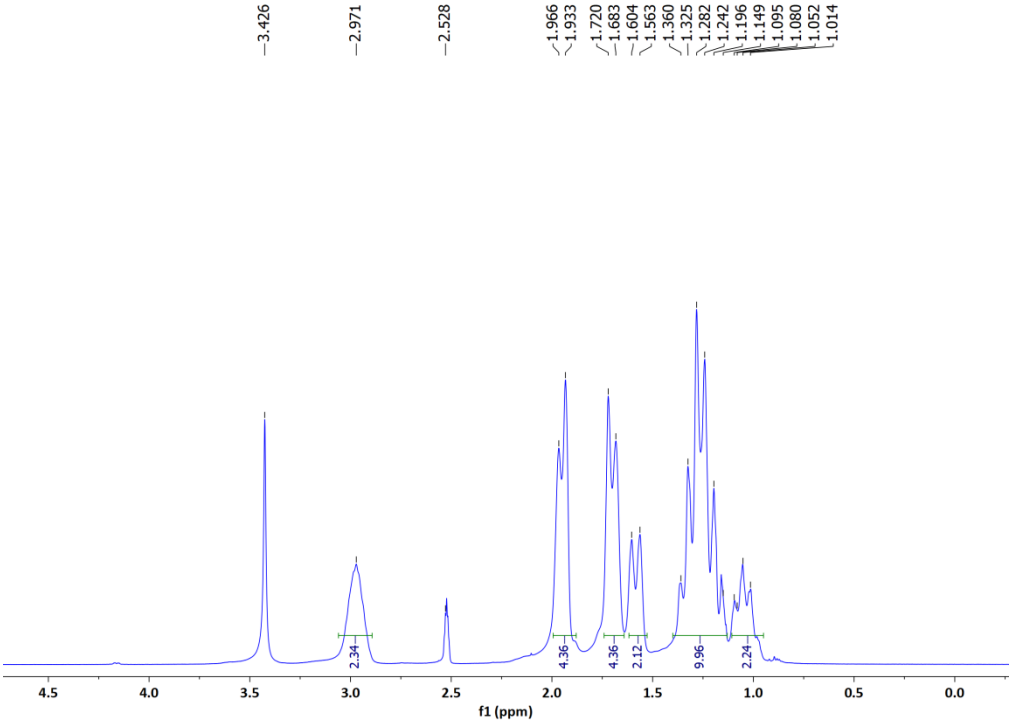

Figure S3. The aliphatic region of ^{1}H NMR spectrum.

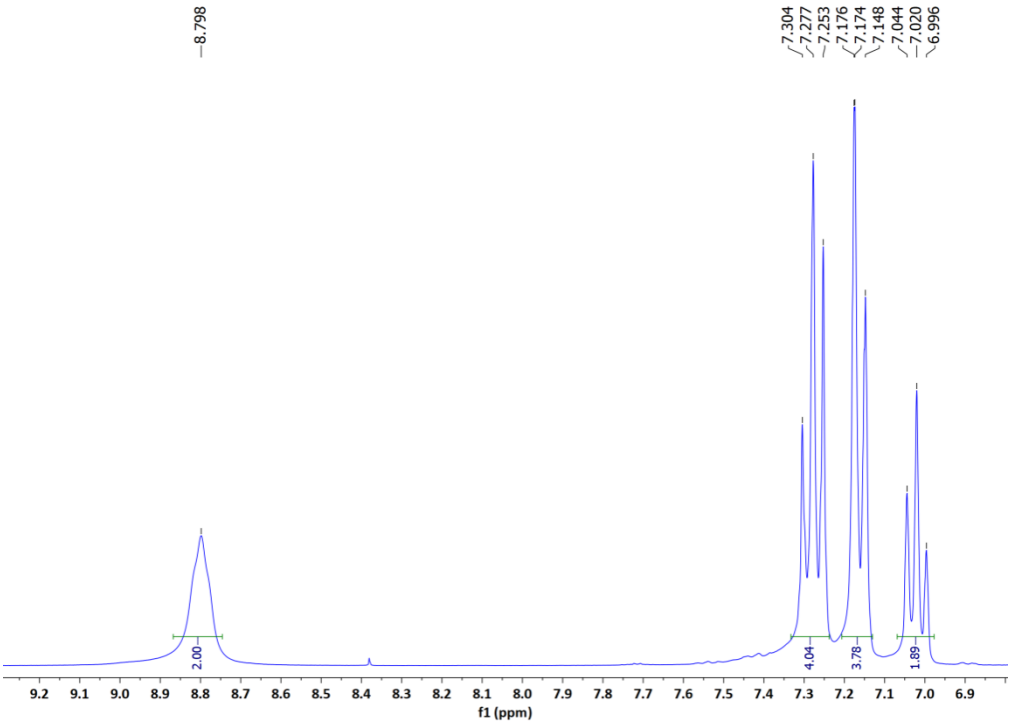

Figure S4. The ^{1}H NMR spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ within 6.9 to 9.2 ppm, showing the aromatic and NH hydrogen atoms.

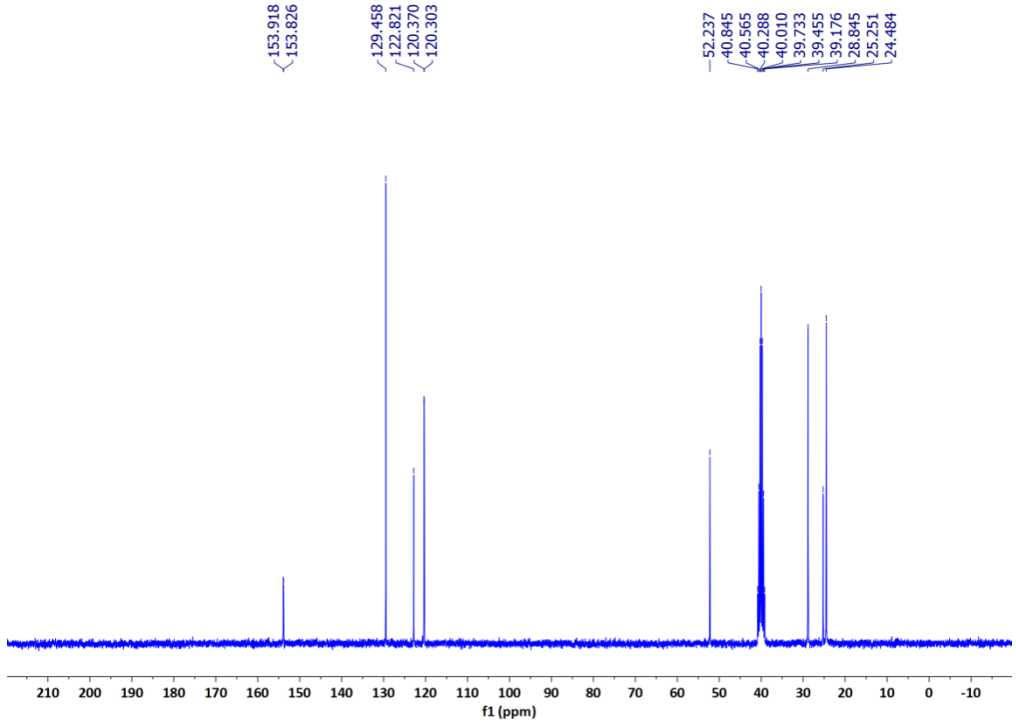

Figure S5. The $^{13}C\{^{1}H\}$ NMR spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ in DMSO-d_6.

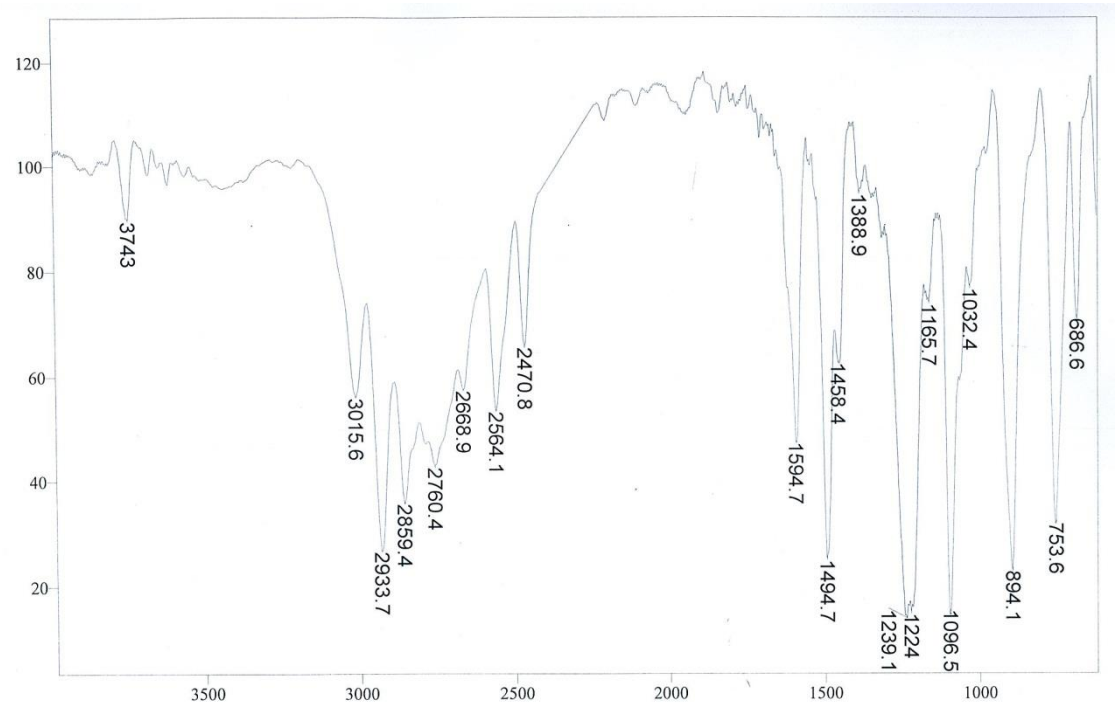

Figure S6. The IR spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ (KBr).

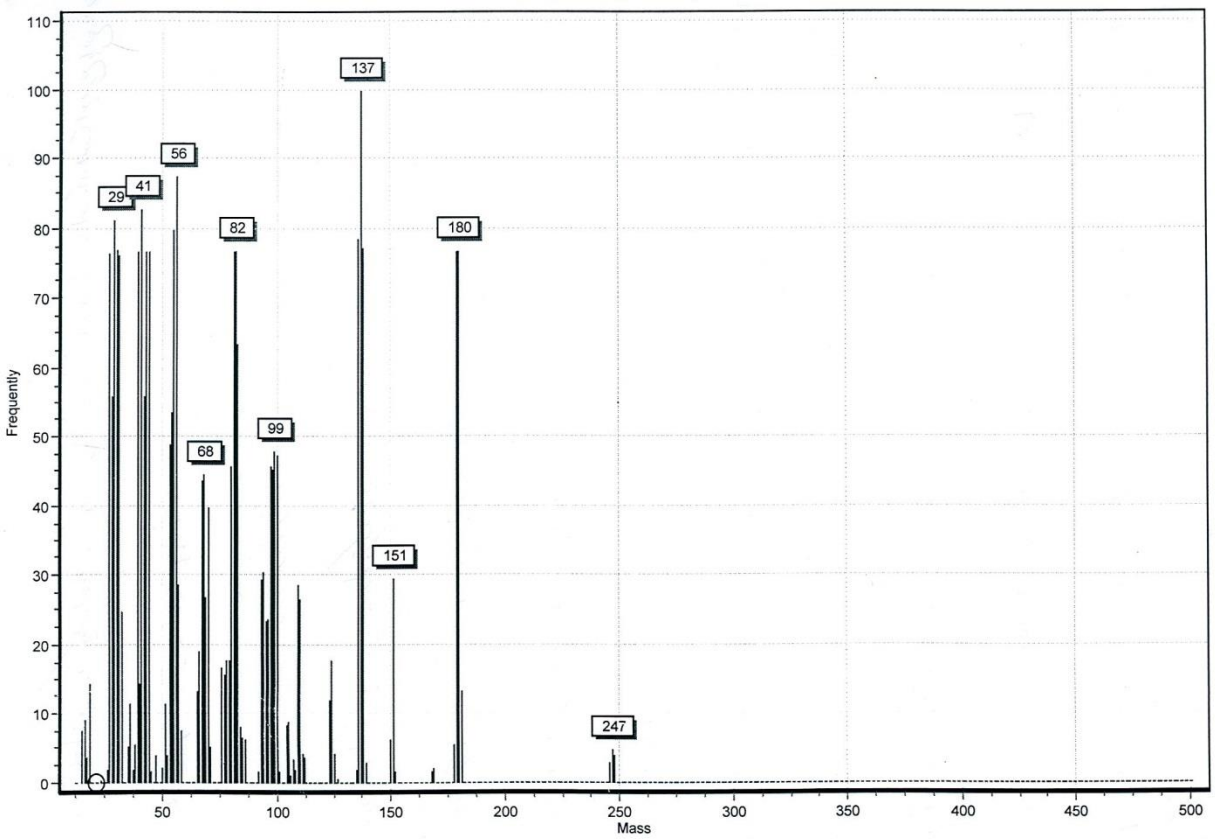

Figure S7. The Mass spectrum of $[(C_6H_{11})_2NH_2][(C_6H_5O)_2P(O)(O)]$ (70 eV).