Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers

Supporting Information

Computation of Standard Equilibrium Acidity of C-H Acids in Ionic Media：Shedding Light on Predicting Changes of Chemical Behavior by Switching Solvent System from Molecular to Ionic

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Contents

Part 1. Conformal studies of complexes that formed from a [Bmim] cation and the conjugate base of carbon acids.

In principle, numerous conformers exist for the complexes formed from a [Bmim] cation and the conjugate anionic bases.[1] Inspired by previous studies,[1,2] several possible complexes were constructed and optimized. Their relative free energies (in kcal/mol) were evaluated with the SMD/M06-2x/cc-pVTZ//M06-2x/6-31+G(d,p) method. The most stable complexes were identified and used in the subsequent pK_a calculations. Structures were generated using CYLview.[3]

(1) (a) P. A. Hunt, B. Kirchner, T. Welton, *Chem. Eur. J.* **2006**, *12*, 6762. (b) P. A. Hunt, I. R. Gould, B. Kirchner, *Aust. J. Chem.* **2007**, *60*, 9.

(2) (a) S. Tsuzuki, H. Tokuda, K. Hayamizu, M. Watanabe, *J. Phys. Chem. B* **2005**, *109*, 16474. (b) K. Angenendt, P. Johansson, *J. Phys. Chem. C* **2010**, *114*, 20577.

(3) CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009.

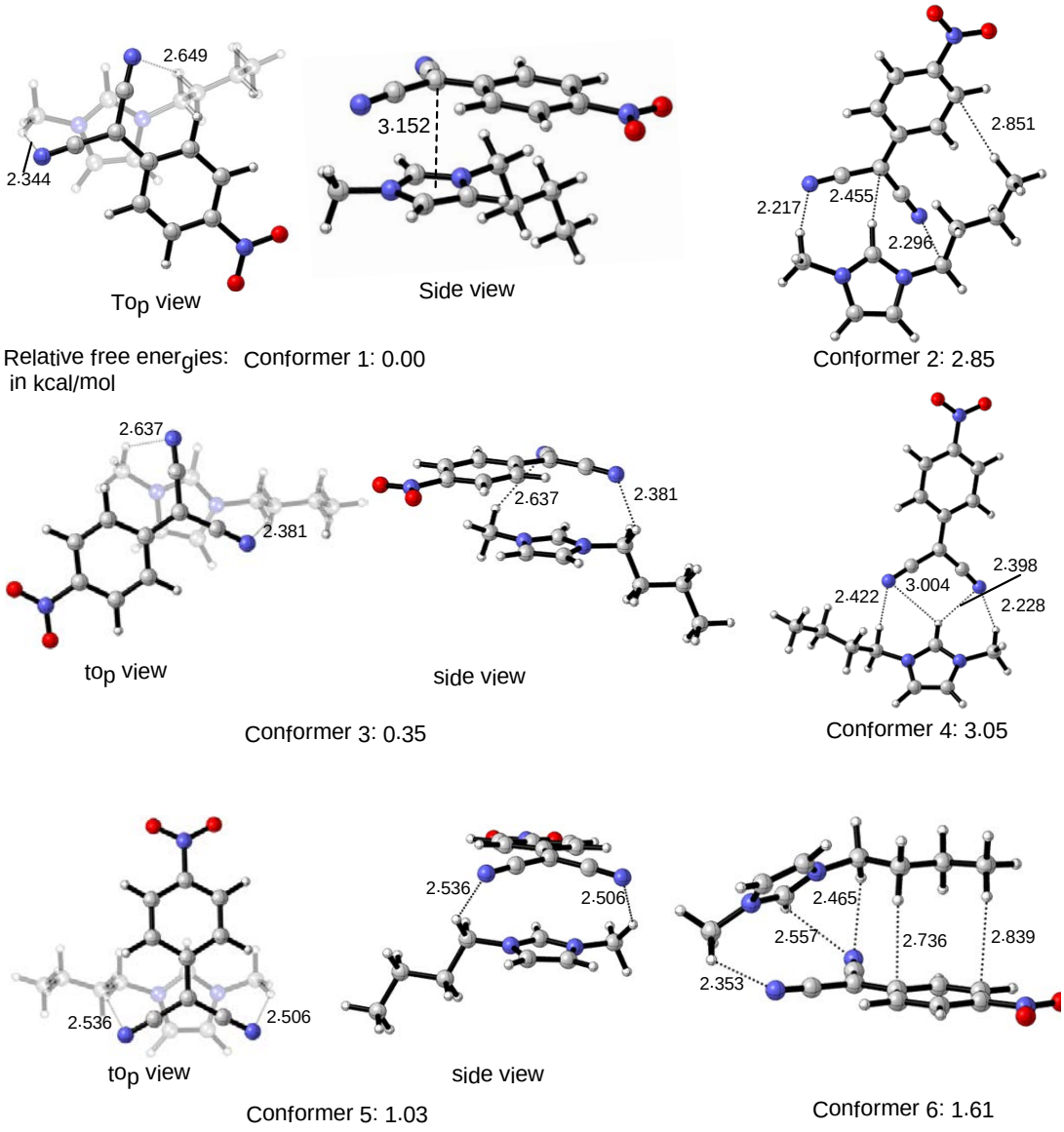


Figure S1. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-$NO_2PhCH(CN)_2$.

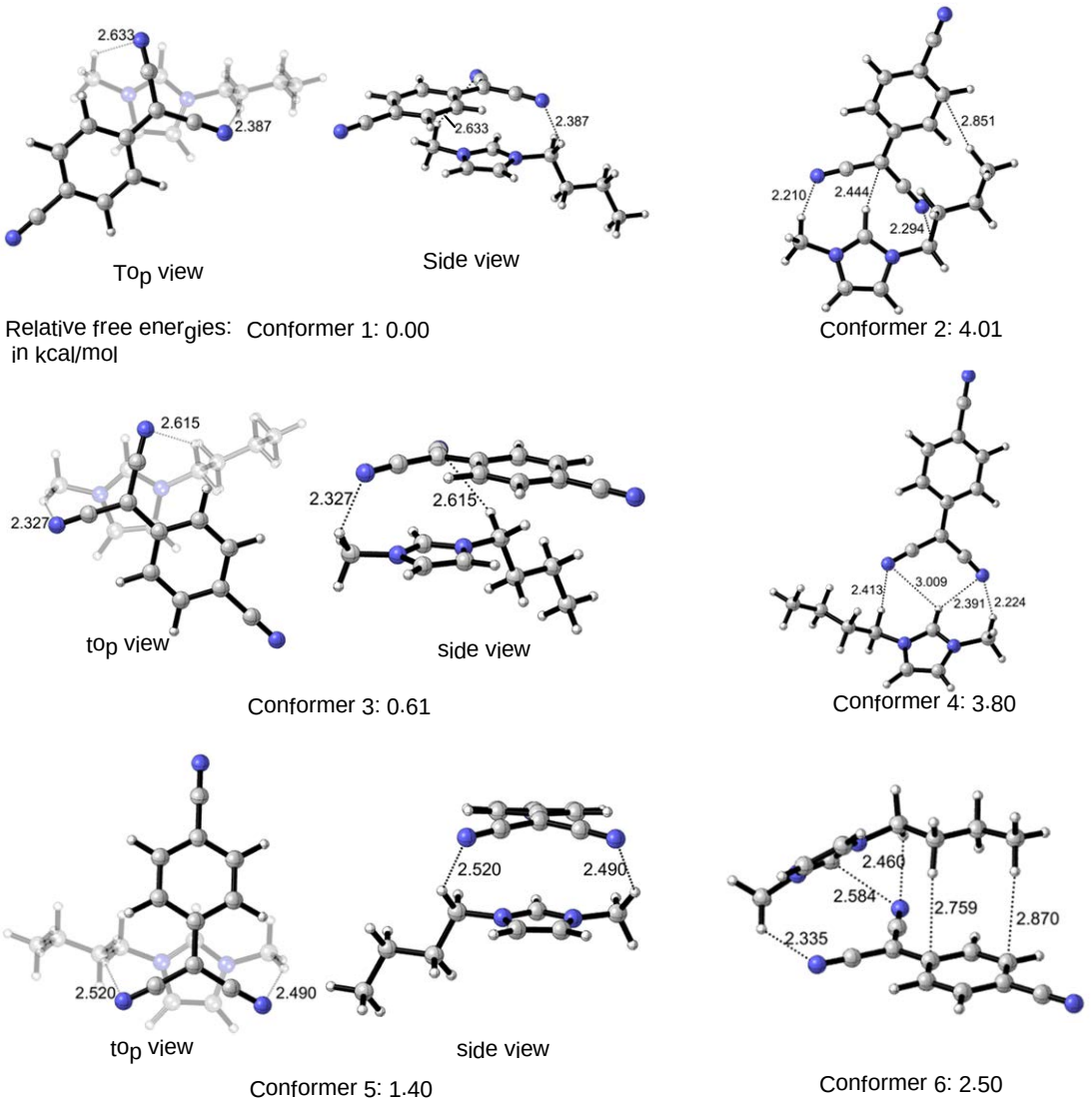


Figure S2. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-CNPhCH(CN)$_2$.

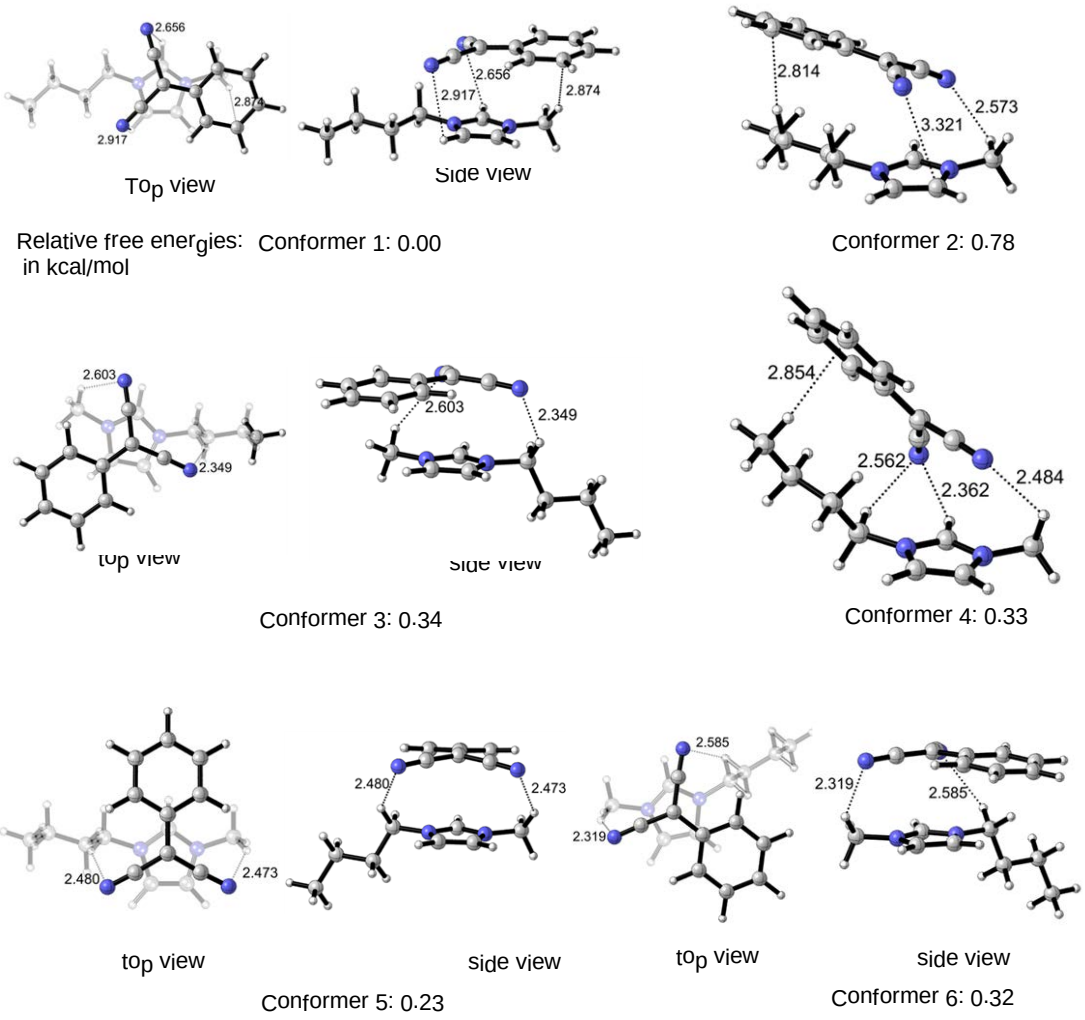


Figure S3. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of $PhCH(CN)_2$.

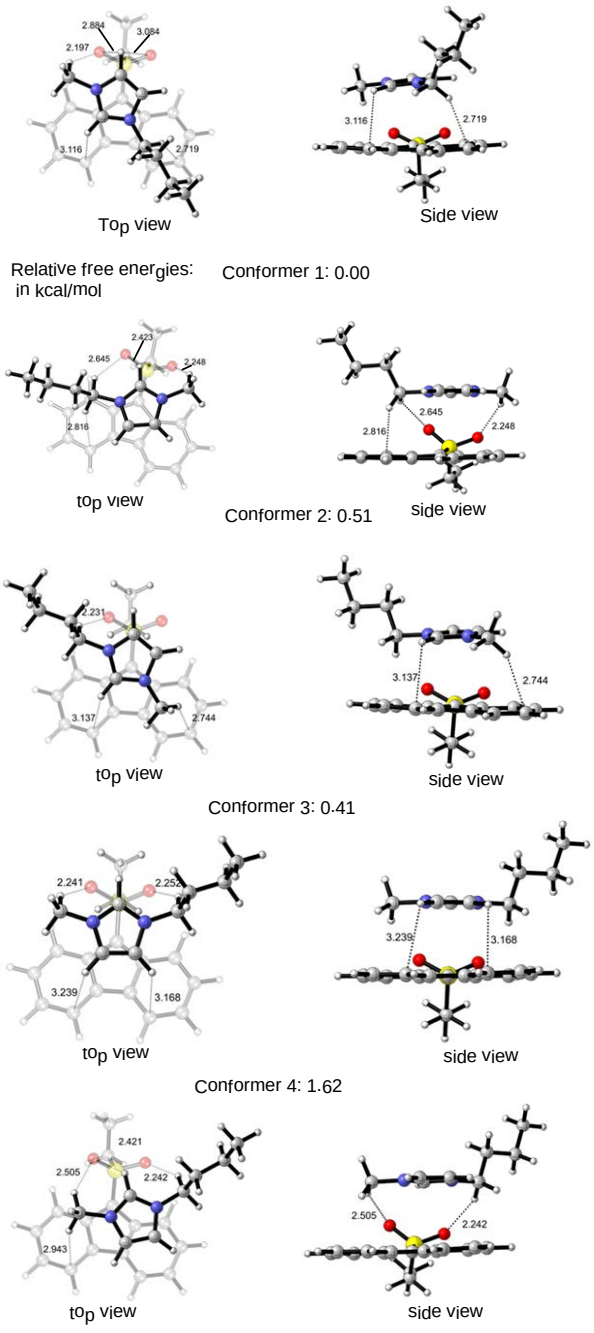


Figure S4. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of 9-EtSO$_2$Fl.

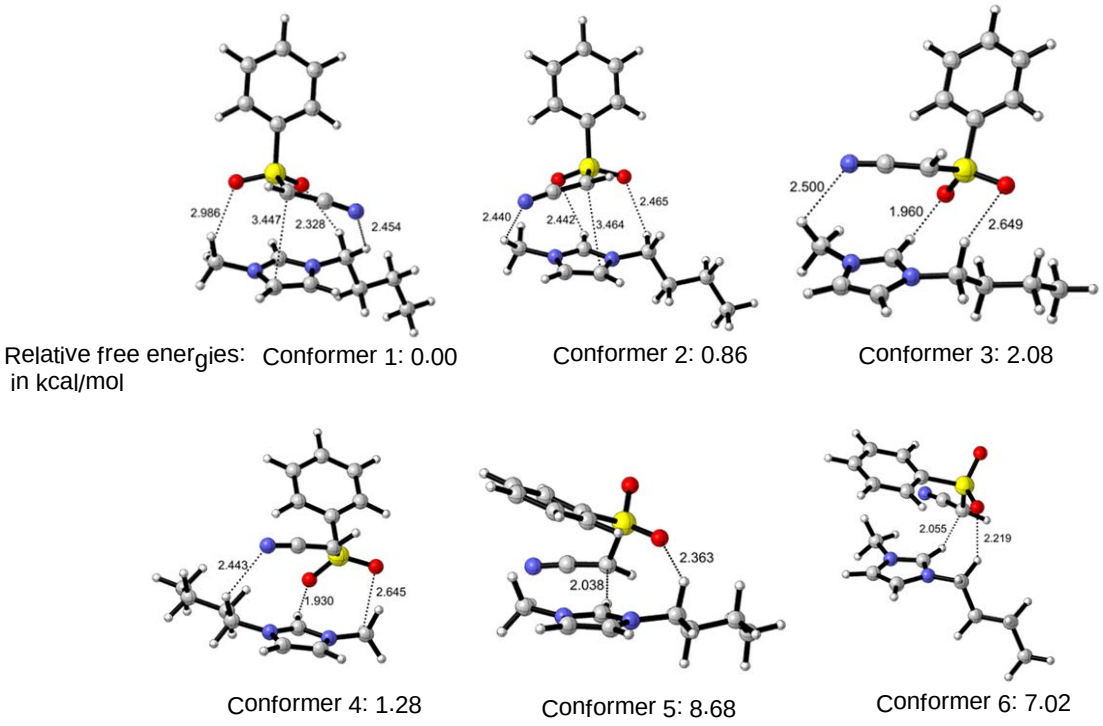


Figure S5. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of $PhSO_2CH_2CN$.

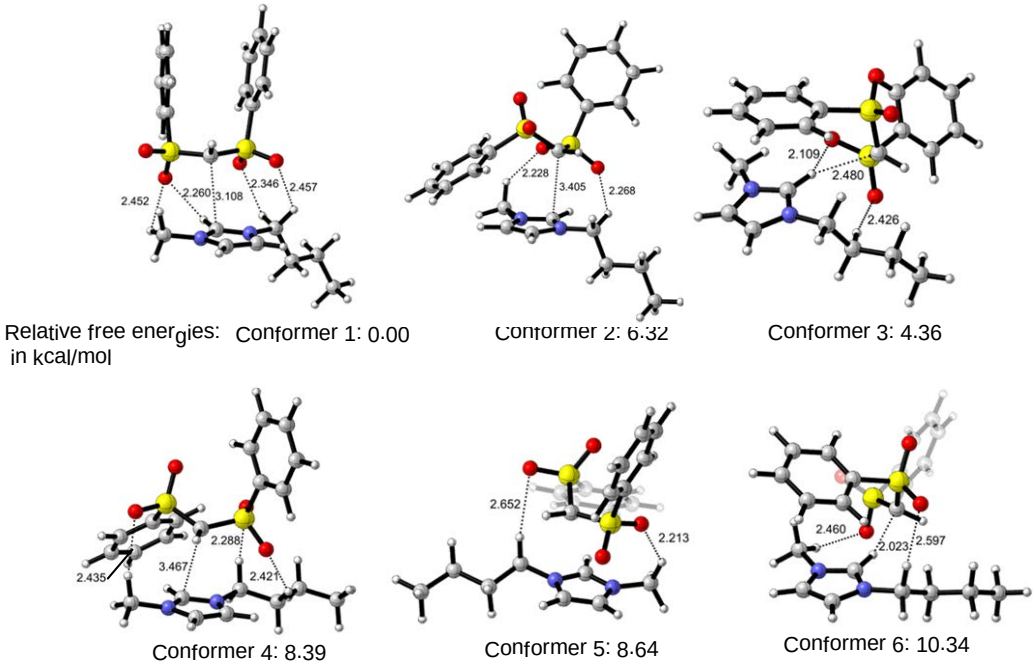


Figure S6. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of $PhSO_2CH_2SO_2Ph$

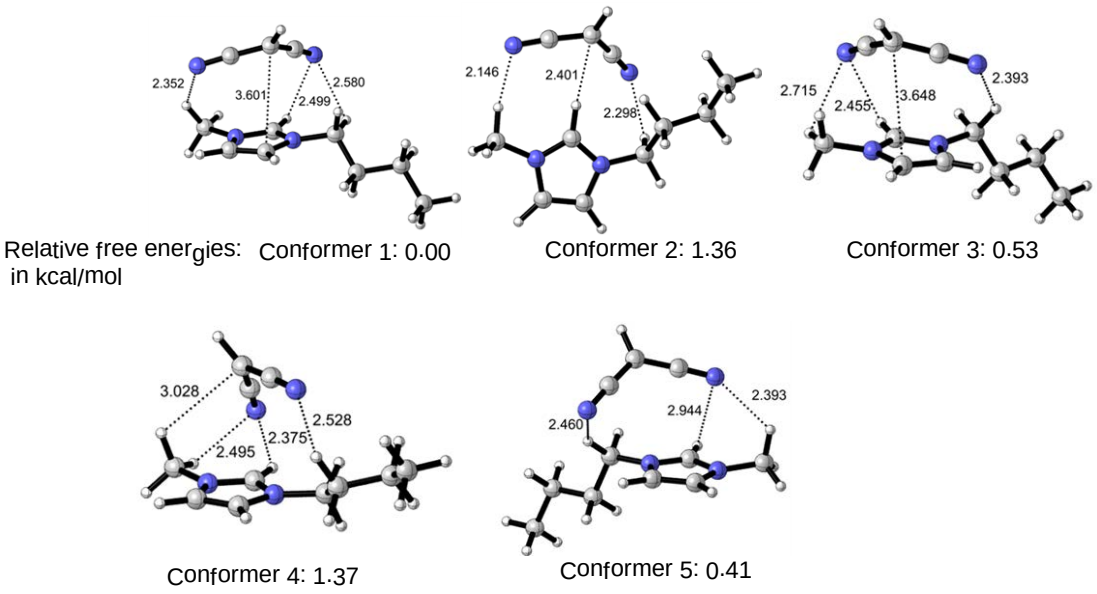
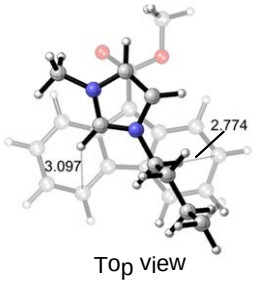
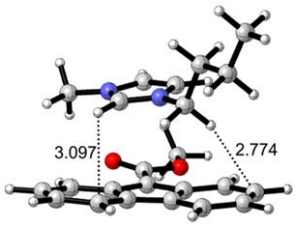


Figure S7. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of $CH_2(CN)_2$



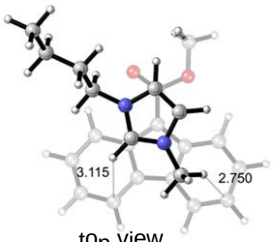
Top view



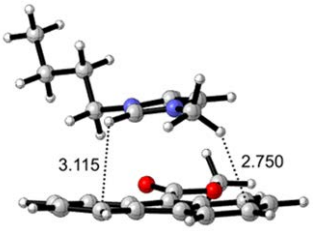
Side view

Relative free energies: in kcal/mol

Conformer 1: 0.00



top view



side view

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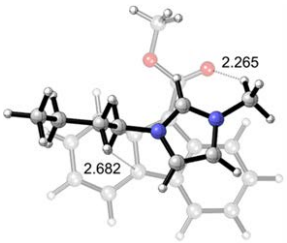
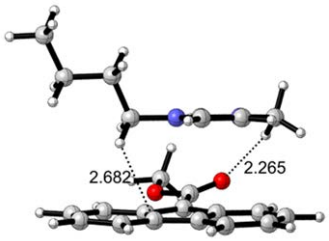
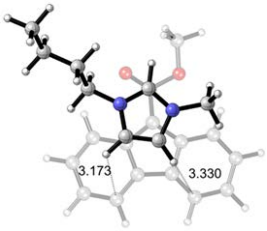


top view

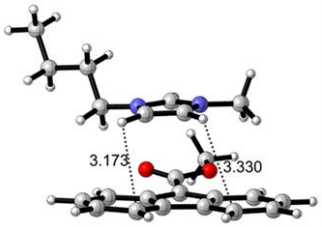


side view

Conformer 3: 0.63



top view



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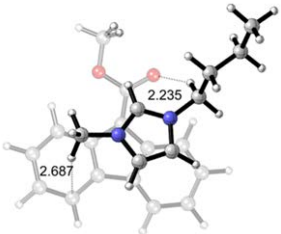
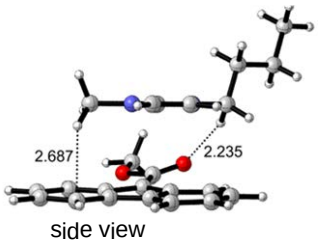


top view



side view

Conformer 4: 0.67

Figure S8. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of 9-COOMeFl.

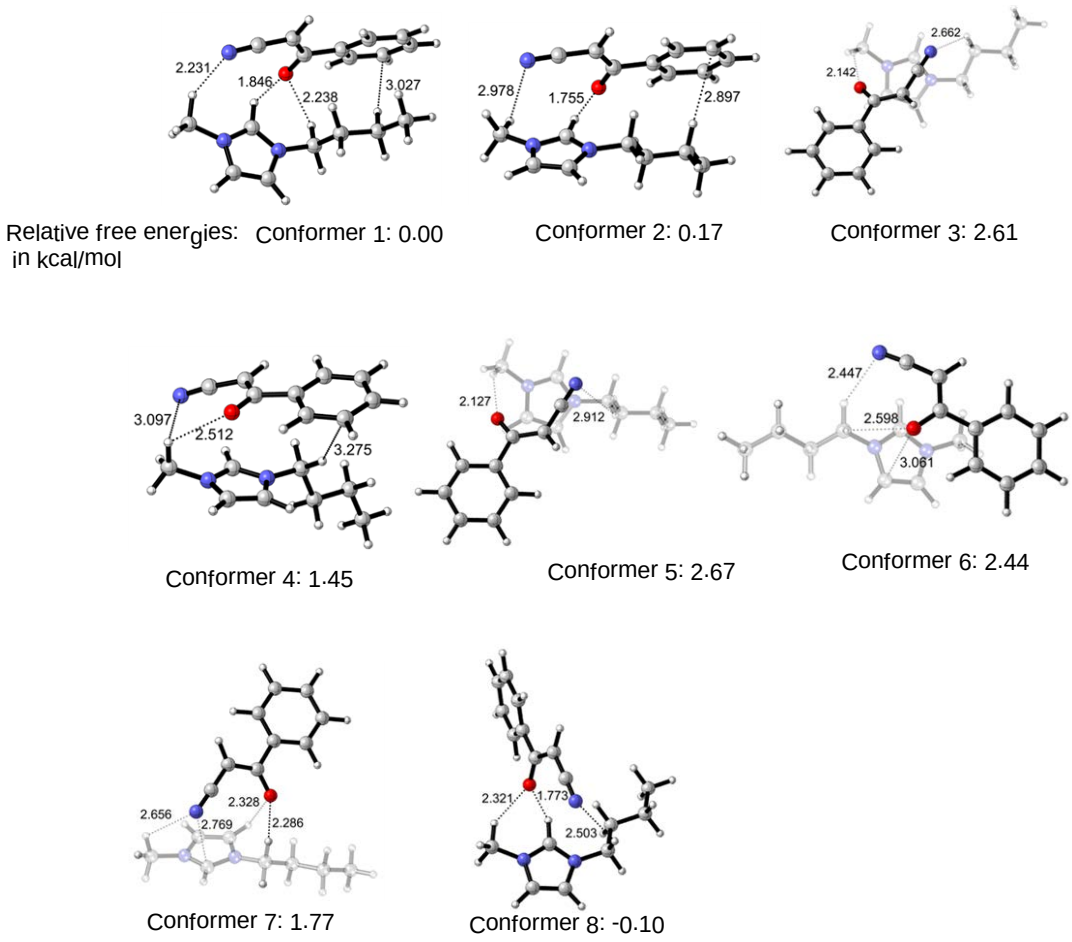


Figure S9. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of $PhCOCH_2CN$.

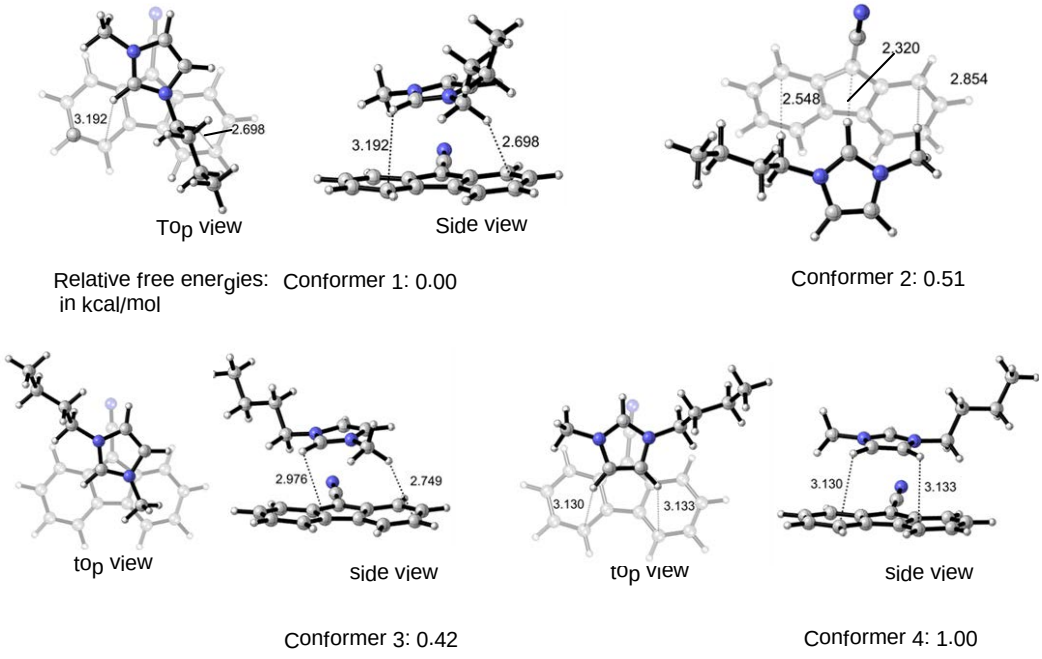
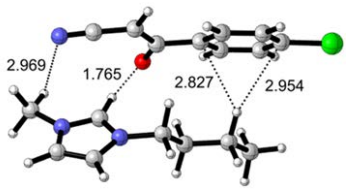
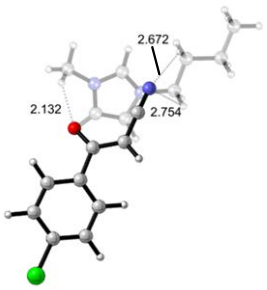


Figure S10. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of 9-CNFl.

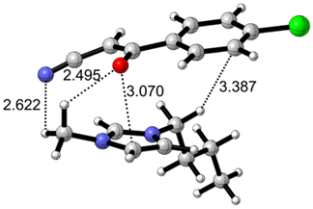




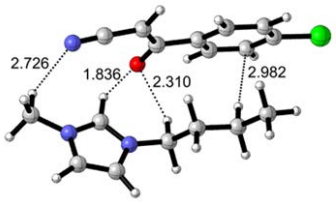
Relative free energies: in kcal/mol

Conformer 1: 0.00

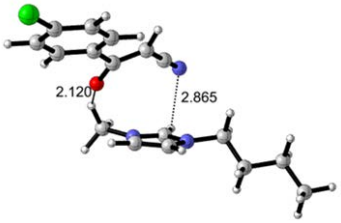
Conformer 2: 3.23



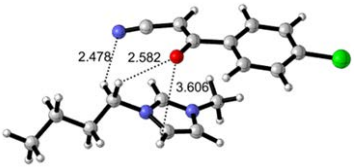
Conformer 3: 1.15



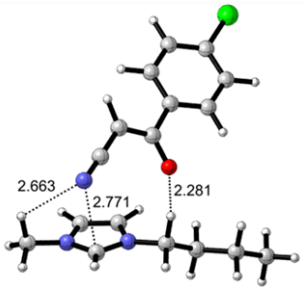
Conformer 4: 3.87



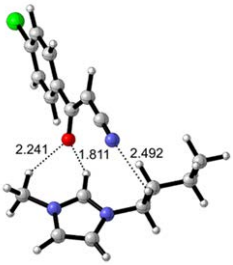
Conformer 5: 2.56



Conformer 6: 1.97



Conformer 7: 1.39



Conformer 8: 0.63

Figure S11. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-ClPhCOCH$_2$CN.

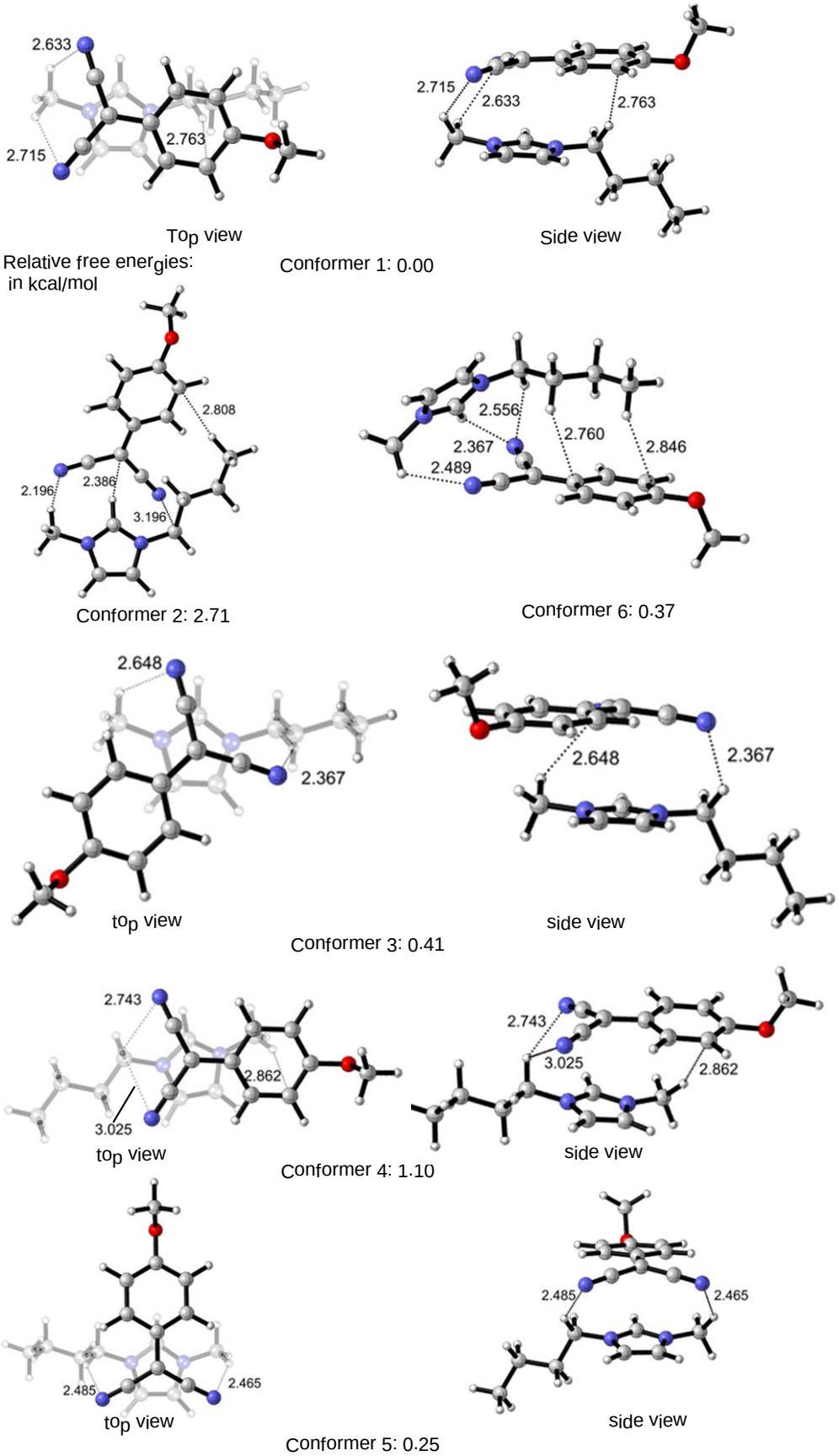


Figure S12. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-OMePhCH(CN)$_2$.

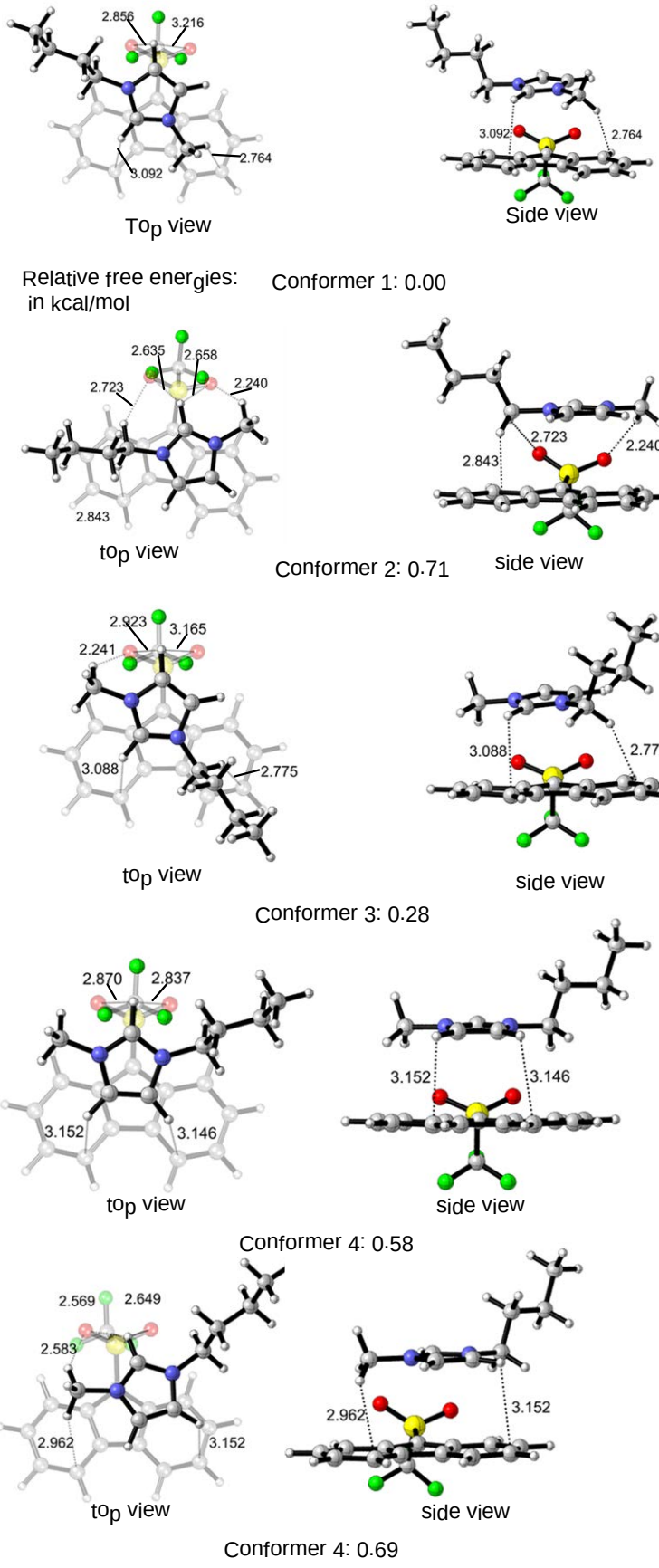


Figure S13. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of 9-CF_3SO_2Fl

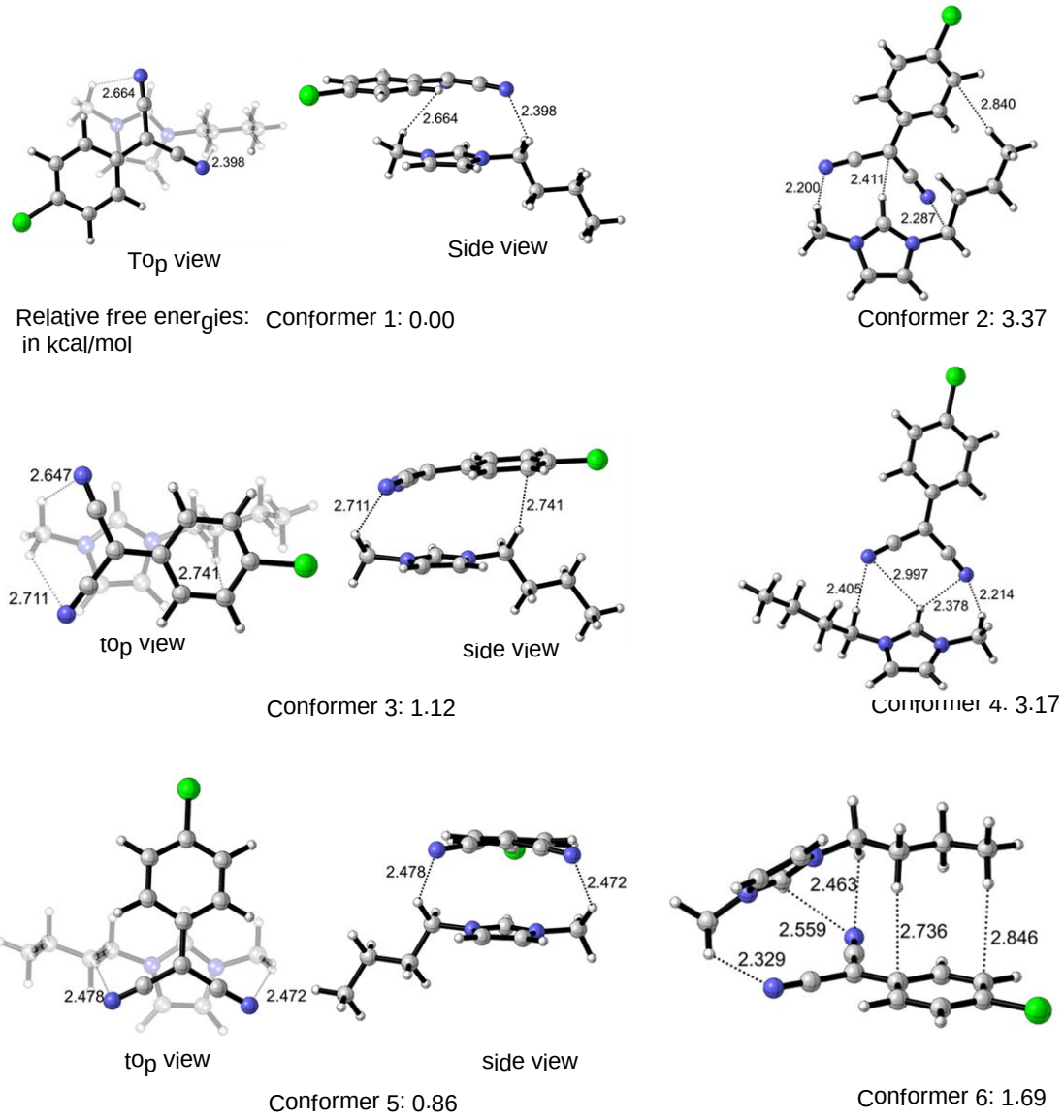


Figure S14. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-ClPhCH(CN)$_2$.

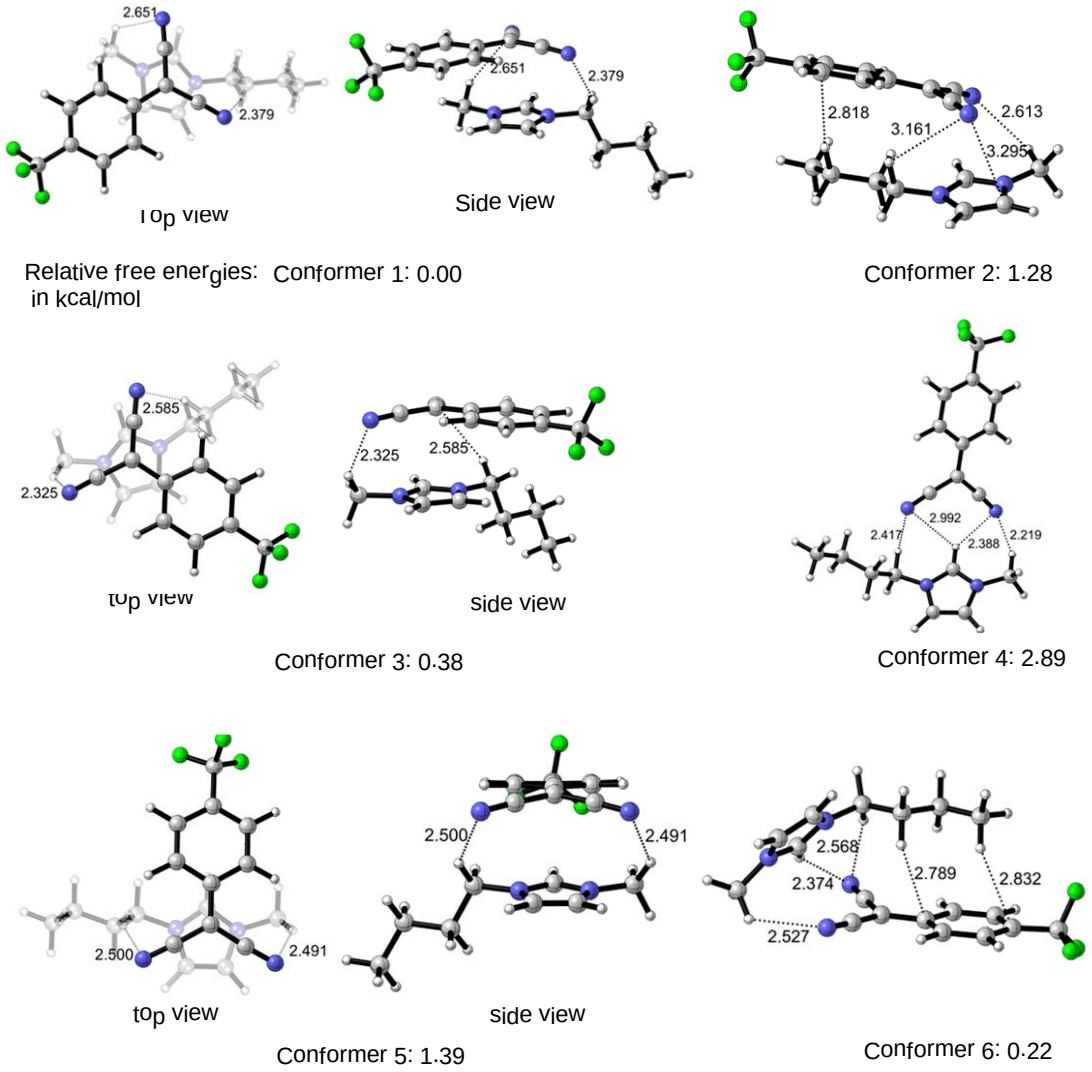


Figure S15. Optimized structures and relative Gibbs free energy values for complexes formed from a [Bmim] cation and the conjugate base anion of *p*-CNPhCH(CN)$_2$.

Part 2. M06-2x/6-31+G(d,p) calculated Cartesian Coordinates together with their energies for minima

p-NO_2PhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.218155	1.211208	0.214184
2	6	0	-0.908417	-0.000024	0.279270
3	6	0	-0.218065	-1.211244	0.214733
4	6	0	1.166864	-1.217530	0.087271
5	6	0	1.829723	0.000014	0.028172
6	6	0	1.166784	1.217531	0.086736
7	1	0	-0.756312	2.153427	0.249150
8	1	0	-0.756158	-2.153485	0.250129
9	1	0	1.728549	-2.141978	0.029253
10	1	0	1.728393	2.142001	0.028332
11	6	0	-2.427809	-0.000084	0.491725
12	1	0	-2.628481	-0.000277	1.572578
13	6	0	-3.069986	-1.207265	-0.057869
14	7	0	-3.544815	-2.179568	-0.459281
15	6	0	-3.070057	1.207239	-0.057463
16	7	0	-3.544897	2.179640	-0.458625
17	7	0	3.299681	0.000029	-0.112127
18	8	0	3.856799	1.080502	-0.164977
19	8	0	3.856818	-1.080434	-0.164993

Zero-point correction=	0.129938 (Hartree/Particle)
Thermal correction to Energy=	0.141687
Thermal correction to Enthalpy=	0.142631
Thermal correction to Gibbs Free Energy=	0.089089
Sum of electronic and zero-point Energies=	-660.161811
Sum of electronic and thermal Energies=	-660.150062
Sum of electronic and thermal Enthalpies=	-660.149117
Sum of electronic and thermal Free Energies=	-660.202660

The conjugate base anion of *p*-NO_2PhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.223746	-1.215508	0.000001
2	6	0	0.966942	0.000000	-0.000008
3	6	0	0.223746	1.215508	-0.000001
4	6	0	-1.153533	1.216051	0.000011
5	6	0	-1.850484	0.000000	0.000017
6	6	0	-1.153532	-1.216052	0.000012
7	1	0	0.762424	-2.158085	-0.000003
8	1	0	0.762423	2.158085	-0.000005
9	1	0	-1.712519	2.144611	0.000015
10	1	0	-1.712519	-2.144611	0.000016
11	6	0	2.391850	0.000000	-0.000015
12	6	0	3.118494	1.213955	-0.000004
13	7	0	3.683017	2.234215	0.000004
14	6	0	3.118493	-1.213956	-0.000004
15	7	0	3.683027	-2.234210	0.000004
16	7	0	-3.283931	-0.000001	0.000029
17	8	0	-3.874308	-1.080511	-0.000022
18	8	0	-3.874309	1.080510	-0.000020

Zero-point correction=	0.117333 (Hartree/Particle)
Thermal correction to Energy=	0.128698
Thermal correction to Enthalpy=	0.129643
Thermal correction to Gibbs Free Energy=	0.078738
Sum of electronic and zero-point Energies=	-659.688483
Sum of electronic and thermal Energies=	-659.677117
Sum of electronic and thermal Enthalpies=	-659.676173
Sum of electronic and thermal Free Energies=	-659.727077

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-NO_2PhCH$(CN)_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.729041	-0.281633	-0.293501
2	6	0	-1.515106	-1.191297	-1.888458
3	6	0	-0.881427	-0.062293	-1.468007
4	7	0	-1.656675	0.487604	-0.472240
5	1	0	-3.482984	-0.130467	0.465287
6	1	0	-1.228127	-1.943670	-2.605893
7	1	0	0.069374	0.364900	-1.750107
8	7	0	-2.669696	-1.304125	-1.144236
9	6	0	-1.359115	1.710340	0.286207

10	6	0	-1.916443	2.953259	-0.398740
11	1	0	-0.270807	1.756799	0.383441
12	1	0	-1.774317	1.567155	1.288679
13	6	0	-1.582626	4.219679	0.388804
14	1	0	-1.504611	3.026603	-1.413672
15	1	0	-3.005240	2.854810	-0.501388
16	1	0	-1.984611	4.129792	1.405397
17	1	0	-0.493813	4.306691	0.489903
18	6	0	-3.634483	-2.400682	-1.235452
19	1	0	-4.340988	-2.305577	-0.411332
20	1	0	-4.162101	-2.339534	-2.188280
21	1	0	-3.091251	-3.342433	-1.138292
22	6	0	-2.140656	5.474338	-0.278745
23	1	0	-3.230587	5.420028	-0.365510
24	1	0	-1.893928	6.370212	0.295914
25	1	0	-1.729216	5.597822	-1.285504
26	6	0	1.331870	-0.142017	1.466205
27	6	0	0.904169	-1.361530	0.883262
28	6	0	1.729407	-1.935646	-0.117155
29	6	0	2.882116	-1.304828	-0.545074
30	6	0	3.246292	-0.082086	0.022959
31	6	0	2.484633	0.493046	1.040788
32	1	0	0.744119	0.293931	2.269822
33	1	0	1.441141	-2.885349	-0.558685
34	1	0	3.509499	-1.739223	-1.315015
35	1	0	2.813151	1.425787	1.485732
36	6	0	-0.347597	-1.965651	1.253465
37	7	0	4.441955	0.596107	-0.442963
38	8	0	4.733313	1.667142	0.073537
39	8	0	5.091819	0.067969	-1.335209
40	6	0	-1.250546	-1.286783	2.094318
41	7	0	-2.008722	-0.651508	2.716935
42	6	0	-0.803806	-3.131080	0.604273
43	7	0	-1.177091	-4.062361	0.007072

Zero-point correction= 0.346954 (Hartree/Particle)
Thermal correction to Energy= 0.370834
Thermal correction to Enthalpy= 0.371778
Thermal correction to Gibbs Free Energy= 0.290390
Sum of electronic and zero-point Energies= -1082.574355
Sum of electronic and thermal Energies= -1082.550475
Sum of electronic and thermal Enthalpies= -1082.549531
Sum of electronic and thermal Free Energies= -1082.630920

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.960576	-0.324154	-0.422274
2	1	0	-1.995687	-0.714872	-0.119916
3	6	0	-5.027090	-0.197206	-1.175821
4	1	0	-5.958330	-0.557493	-1.582943
5	6	0	-4.627980	1.055488	-0.820282
6	1	0	-5.147866	1.999554	-0.852066
7	7	0	-3.972041	-1.041392	-0.917962
8	7	0	-3.337535	0.954049	-0.356168
9	6	0	-3.953819	-2.484803	-1.178924
10	1	0	-3.869510	-2.653427	-2.253501
11	1	0	-3.105811	-2.927477	-0.651816
12	1	0	-4.882123	-2.914176	-0.801884
13	6	0	-2.519936	2.067151	0.170861
14	1	0	-3.077132	2.978816	-0.059949
15	1	0	-2.450310	1.945737	1.255630
16	6	0	-0.742637	-0.190639	2.155490
17	7	0	-1.291398	0.648995	2.754264
18	6	0	-0.091145	-1.158325	1.364669
19	6	0	-0.805435	-2.334283	1.072001
20	7	0	-1.436746	-3.269110	0.766238
21	6	0	-1.132017	2.110838	-0.454859
22	6	0	-0.310870	3.252222	0.145686
23	1	0	-1.222897	2.236314	-1.541930
24	1	0	-0.603994	1.164640	-0.274357
25	6	0	1.016176	3.444023	-0.584406
26	1	0	-0.891448	4.183565	0.105560
27	1	0	-0.136847	3.035202	1.206797
28	1	0	1.617577	4.224541	-0.111377
29	1	0	1.600225	2.518826	-0.581722
30	1	0	0.849668	3.733615	-1.627147
31	6	0	1.236922	-0.928382	0.840640
32	6	0	1.859359	-1.874721	-0.005791
33	6	0	1.944929	0.256728	1.144959
34	6	0	3.115350	-1.643620	-0.535272
35	1	0	1.341775	-2.800450	-0.238901
36	6	0	3.203984	0.491778	0.620662
37	1	0	1.497298	0.988289	1.812776
38	6	0	3.778257	-0.456456	-0.223662
39	1	0	3.593329	-2.366128	-1.186347

40	1	0	3.751944	1.397440	0.854564
41	7	0	5.093932	-0.202523	-0.788993
42	8	0	5.649615	0.848949	-0.502517
43	8	0	5.574865	-1.051011	-1.526882

Zero-point correction= 0.347288 (Hartree/Particle)
Thermal correction to Energy= 0.371118
Thermal correction to Enthalpy= 0.372063
Thermal correction to Gibbs Free Energy= 0.290216
Sum of electronic and zero-point Energies= -1082.568758
Sum of electronic and thermal Energies= -1082.544928
Sum of electronic and thermal Enthalpies= -1082.543983
Sum of electronic and thermal Free Energies= -1082.625830

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.750363	1.125197	-1.060723
2	6	0	0.264739	-0.470731	-1.363338
3	6	0	1.305081	-0.990991	-0.656131
4	7	0	2.220285	0.023936	-0.481131
5	1	0	2.212187	2.101632	-1.034273
6	1	0	-0.676213	-0.905032	-1.665687
7	1	0	1.449638	-1.966464	-0.219218
8	7	0	0.565893	0.850790	-1.607014
9	6	0	3.496235	-0.090387	0.239773
10	6	0	4.537283	-0.846739	-0.577510
11	1	0	3.274342	-0.579827	1.192568
12	1	0	3.823843	0.929402	0.461684
13	6	0	5.868516	-0.942265	0.166935
14	1	0	4.164871	-1.855907	-0.796642
15	1	0	4.683195	-0.344235	-1.542577
16	1	0	6.239025	0.068634	0.377821
17	1	0	5.706383	-1.423497	1.138766
18	6	0	-0.280384	1.821446	-2.301657
19	1	0	0.002369	1.874371	-3.354289
20	1	0	-1.315848	1.496405	-2.203662
21	1	0	-0.161254	2.790039	-1.813032
22	6	0	6.914828	-1.719101	-0.628844
23	1	0	7.104951	-1.242512	-1.595923
24	1	0	7.863199	-1.772420	-0.088856
25	1	0	6.579407	-2.743367	-0.820222

26	6	0	-1.833298	-0.820009	1.384630
27	6	0	-1.497034	0.533309	1.125996
28	6	0	-2.413101	1.302797	0.365612
29	6	0	-3.568083	0.742967	-0.150445
30	6	0	-3.842011	-0.604152	0.089836
31	6	0	-2.986771	-1.383252	0.872424
32	1	0	-1.164947	-1.424458	1.990925
33	1	0	-2.205050	2.355608	0.194029
34	1	0	-4.268308	1.331446	-0.732717
35	1	0	-3.239881	-2.419635	1.064639
36	6	0	-0.245800	1.087616	1.569177
37	7	0	-5.039304	-1.200180	-0.473179
38	8	0	-5.263748	-2.378527	-0.231387
39	8	0	-5.758276	-0.496112	-1.170529
40	6	0	0.697485	0.284093	2.242342
41	7	0	1.474715	-0.427889	2.744300
42	6	0	0.165717	2.361393	1.131718
43	7	0	0.507225	3.379024	0.668913

Zero-point correction=	0.347457 (Hartree/Particle)
Thermal correction to Energy=	0.371175
Thermal correction to Enthalpy=	0.372119
Thermal correction to Gibbs Free Energy=	0.290997
Sum of electronic and zero-point Energies=	-1082.573716
Sum of electronic and thermal Energies=	-1082.549998
Sum of electronic and thermal Enthalpies=	-1082.549054
Sum of electronic and thermal Free Energies=	-1082.630176

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.075955	-1.406017	0.273159
2	6	0	4.573236	-2.115714	-1.178361
3	6	0	4.953619	-0.881091	-0.749439
4	7	0	4.006640	-0.459061	0.156379
5	1	0	2.198682	-1.373961	0.906693
6	1	0	5.025991	-2.793274	-1.884668
7	1	0	5.804888	-0.274038	-1.011647
8	7	0	3.400373	-2.424197	-0.526434
9	6	0	4.005767	0.839857	0.855218
10	6	0	4.093024	2.004190	-0.123211
11	1	0	4.841874	0.836003	1.561556

12	1	0	3.064493	0.893658	1.405402
13	6	0	3.842750	3.328657	0.595954
14	1	0	5.078627	2.023939	-0.608181
15	1	0	3.328622	1.863796	-0.893837
16	1	0	2.848390	3.283773	1.054472
17	1	0	4.573108	3.456997	1.405737
18	6	0	2.629225	-3.659987	-0.698114
19	1	0	2.296660	-3.726424	-1.734727
20	1	0	3.265926	-4.509731	-0.449559
21	1	0	1.764578	-3.625519	-0.032660
22	6	0	3.914889	4.515025	-0.361873
23	1	0	3.166191	4.413097	-1.153274
24	1	0	3.725683	5.456424	0.159879
25	1	0	4.900732	4.584919	-0.833997
26	6	0	-2.663590	1.042533	-0.161721
27	6	0	-2.202062	-0.216457	0.283413
28	6	0	-3.156361	-1.233067	0.511438
29	6	0	-4.504421	-1.006522	0.302725
30	6	0	-4.923466	0.247988	-0.139158
31	6	0	-4.010450	1.275913	-0.371550
32	1	0	-1.946731	1.838490	-0.340368
33	1	0	-2.823855	-2.206983	0.858419
34	1	0	-5.240499	-1.782664	0.475383
35	1	0	-4.369426	2.239518	-0.713186
36	6	0	-0.795235	-0.457092	0.497513
37	7	0	-6.339830	0.487898	-0.361278
38	8	0	-6.682922	1.599207	-0.741304
39	8	0	-7.118168	-0.434054	-0.157846
40	6	0	0.191647	0.519575	0.276915
41	7	0	1.057603	1.287245	0.107051
42	6	0	-0.283216	-1.691175	0.928754
43	7	0	0.226203	-2.686018	1.277396

Zero-point correction= 0.347417 (Hartree/Particle)
Thermal correction to Energy= 0.371383
Thermal correction to Enthalpy= 0.372327
Thermal correction to Gibbs Free Energy= 0.289837
Sum of electronic and zero-point Energies= -1082.566602
Sum of electronic and thermal Energies= -1082.542636
Sum of electronic and thermal Enthalpies= -1082.541691
Sum of electronic and thermal Free Energies= -1082.624182

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.310554	-1.557307	-0.581321
2	6	0	-0.545946	-0.429465	-1.259869
3	7	0	-1.675048	-0.334466	-0.560688
4	1	0	-3.217544	-1.733131	-0.024803
5	1	0	0.187841	0.356476	-1.380999
6	6	0	-2.156385	0.857561	0.151401
7	6	0	-3.393350	1.448867	-0.514335
8	1	0	-1.328752	1.572442	0.163295
9	1	0	-2.353250	0.546722	1.182902
10	6	0	-3.893667	2.683800	0.234717
11	1	0	-3.157407	1.710057	-1.553946
12	1	0	-4.188349	0.692801	-0.546984
13	1	0	-4.117623	2.410748	1.272944
14	1	0	-3.093627	3.433571	0.274246
15	6	0	-5.133394	3.287699	-0.420444
16	1	0	-5.954401	2.564168	-0.445020
17	1	0	-5.478800	4.168619	0.125901
18	1	0	-4.923024	3.592110	-1.450652
19	6	0	0.985701	0.474600	1.579793
20	6	0	1.261784	-0.843176	1.125371
21	6	0	2.379444	-1.014010	0.264470
22	6	0	3.115525	0.066984	-0.182501
23	6	0	2.765798	1.355487	0.230513
24	6	0	1.719268	1.557686	1.134345
25	1	0	0.175267	0.629683	2.286494
26	1	0	2.654105	-2.016889	-0.050286
27	1	0	3.961745	-0.064303	-0.847964
28	1	0	1.500161	2.563969	1.474125
29	6	0	0.396404	-1.939080	1.448156
30	7	0	3.514301	2.493866	-0.263881
31	8	0	3.183739	3.609009	0.118376
32	8	0	4.429960	2.283120	-1.048711
33	6	0	-0.805124	-1.705973	2.151230
34	7	0	-1.811383	-1.431672	2.674666
35	6	0	0.588981	-3.192860	0.828943
36	7	0	0.767613	-4.177130	0.227899
37	6	0	-1.533997	-2.396882	-1.317043
38	1	0	-1.627082	-3.449843	-1.530974
39	7	0	-0.439809	-1.670111	-1.734465
40	6	0	0.677982	-2.202685	-2.512770
41	1	0	1.016971	-3.122815	-2.032285

42	1	0	0.350407	-2.394284	-3.535779
43	1	0	1.483230	-1.468032	-2.506193

Zero-point correction=	0.346936	(Hartree/Particle)
Thermal correction to Energy=	0.369807	
Thermal correction to Enthalpy=	0.370751	
Thermal correction to Gibbs Free Energy=	0.293274	
Sum of electronic and zero-point Energies=	-1082.576217	
Sum of electronic and thermal Energies=	-1082.553345	
Sum of electronic and thermal Enthalpies=	-1082.552401	
Sum of electronic and thermal Free Energies=	-1082.629878	

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.658562	0.396479	0.206293
2	6	0	3.509809	-0.714243	-1.686774
3	6	0	2.726279	0.393987	-1.785352
4	7	0	2.836516	1.074378	-0.591705
5	1	0	3.888735	0.660586	1.228142
6	1	0	3.667219	-1.535853	-2.366616
7	1	0	2.088539	0.736743	-2.583429
8	7	0	4.091428	-0.685086	-0.440474
9	6	0	2.129863	2.313092	-0.219055
10	6	0	0.661577	2.272995	-0.627312
11	1	0	2.650858	3.153670	-0.688277
12	1	0	2.215945	2.392487	0.867510
13	6	0	-0.118875	3.399376	0.050834
14	1	0	0.568584	2.369040	-1.717161
15	1	0	0.231980	1.303736	-0.346475
16	1	0	-0.115859	3.220407	1.133399
17	1	0	0.393942	4.356904	-0.112041
18	6	0	4.928766	-1.743873	0.121571
19	1	0	4.354480	-2.672214	0.105240
20	1	0	5.843542	-1.830263	-0.466097
21	1	0	5.173866	-1.481004	1.150145
22	6	0	-1.553171	3.488285	-0.464434
23	1	0	-2.073002	2.534768	-0.329554
24	1	0	-2.116841	4.260393	0.065215
25	1	0	-1.570771	3.732277	-1.531667
26	6	0	-1.686649	0.035674	1.239728
27	6	0	-0.880045	-0.978561	0.672221

28	6	0	-1.484821	-1.869894	-0.245192
29	6	0	-2.818504	-1.747847	-0.587954
30	6	0	-3.579788	-0.727989	-0.016267
31	6	0	-3.022699	0.160239	0.902380
32	1	0	-1.251815	0.721623	1.962156
33	1	0	-0.889102	-2.664060	-0.685229
34	1	0	-3.282820	-2.428065	-1.292396
35	1	0	-3.644212	0.934126	1.338591
36	6	0	0.520845	-1.087137	1.003148
37	7	0	-4.978969	-0.587549	-0.383744
38	8	0	-5.617365	0.325061	0.123135
39	8	0	-5.445278	-1.385460	-1.185113
40	6	0	1.144483	-0.160888	1.857894
41	7	0	1.681020	0.641616	2.518676
42	6	0	1.336772	-2.094259	0.451474
43	7	0	2.017642	-2.914036	-0.027732

Zero-point correction= 0.347705 (Hartree/Particle)
Thermal correction to Energy= 0.371310
Thermal correction to Enthalpy= 0.372254
Thermal correction to Gibbs Free Energy= 0.292485
Sum of electronic and zero-point Energies= -1082.573577
Sum of electronic and thermal Energies= -1082.549973
Sum of electronic and thermal Enthalpies= -1082.549028
Sum of electronic and thermal Free Energies= -1082.628797

p-CNPhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.176936	1.209633	0.197690
2	6	0	-0.514371	0.000001	0.268423
3	6	0	0.176947	-1.209633	0.197776
4	6	0	1.560065	-1.212726	0.060174
5	6	0	2.252604	0.000000	-0.007113
6	6	0	1.560057	1.212722	0.060091
7	1	0	-0.359995	2.152589	0.237129
8	1	0	-0.359983	-2.152587	0.237279
9	1	0	2.103764	-2.149100	-0.000735
10	1	0	2.103749	2.149096	-0.000880
11	6	0	-2.032013	-0.000012	0.493274
12	1	0	-2.225676	-0.000043	1.575408
13	6	0	-2.678430	-1.207251	-0.051312

14	7	0	-3.155865	-2.180085	-0.448432
15	6	0	3.686187	0.000002	-0.152107
16	7	0	4.837608	0.000016	-0.266394
17	6	0	-2.678462	1.207239	-0.051249
18	7	0	-3.155882	2.180097	-0.448329

Zero-point correction= 0.125615 (Hartree/Particle)
Thermal correction to Energy= 0.136646
Thermal correction to Enthalpy= 0.137590
Thermal correction to Gibbs Free Energy= 0.086752
Sum of electronic and zero-point Energies= -547.949285
Sum of electronic and thermal Energies= -547.938254
Sum of electronic and thermal Enthalpies= -547.937310
Sum of electronic and thermal Free Energies= -547.988148

The conjugate base anion of *p*-CNPhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.172561	-1.211205	0.000001
2	6	0	0.570256	0.000000	-0.000002
3	6	0	-0.172561	1.211205	0.000001
4	6	0	-1.552889	1.209024	0.000006
5	6	0	-2.272201	0.000000	0.000009
6	6	0	-1.552889	-1.209024	0.000006
7	1	0	0.364628	-2.154951	-0.000001
8	1	0	0.364628	2.154951	-0.000002
9	1	0	-2.096014	2.149797	0.000008
10	1	0	-2.096014	-2.149797	0.000009
11	6	0	2.001991	0.000000	-0.000008
12	6	0	2.724098	1.214136	-0.000011
13	7	0	3.281451	2.239474	-0.000013
14	6	0	2.724098	-1.214136	-0.000010
15	7	0	3.281452	-2.239474	-0.000012
16	6	0	-3.701924	0.000000	0.000014
17	7	0	-4.864294	0.000000	0.000018

Zero-point correction= 0.112869 (Hartree/Particle)
Thermal correction to Energy= 0.123580
Thermal correction to Enthalpy= 0.124524
Thermal correction to Gibbs Free Energy= 0.075503
Sum of electronic and zero-point Energies= -547.470385
Sum of electronic and thermal Energies= -547.459675

Sum of electronic and thermal Enthalpies= -547.458731
Sum of electronic and thermal Free Energies= -547.507751

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-CNPhCH(CN)$_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.422091	1.144108	-1.016377
2	6	0	0.018634	-0.501639	-1.425289
3	6	0	1.071723	-1.008746	-0.727774
4	7	0	1.934961	0.037466	-0.485470
5	1	0	1.834844	2.138576	-0.928874
6	1	0	-0.898810	-0.961423	-1.760446
7	1	0	1.253835	-1.996263	-0.334098
8	7	0	0.260837	0.843258	-1.596743
9	6	0	3.196209	-0.051728	0.263730
10	6	0	4.301119	-0.698528	-0.563368
11	1	0	2.975488	-0.609922	1.178095
12	1	0	3.459954	0.968598	0.556691
13	6	0	5.609894	-0.773737	0.222396
14	1	0	3.991074	-1.708868	-0.860155
15	1	0	4.451998	-0.126593	-1.488282
16	1	0	5.917134	0.239036	0.511259
17	1	0	5.440219	-1.325121	1.154997
18	6	0	-0.626355	1.808643	-2.245577
19	1	0	-0.370487	1.896976	-3.302749
20	1	0	-1.650596	1.454238	-2.129653
21	1	0	-0.521260	2.766396	-1.732838
22	6	0	6.723850	-1.441910	-0.579917
23	1	0	6.920418	-0.896311	-1.508493
24	1	0	7.654813	-1.478166	-0.009041
25	1	0	6.452969	-2.468695	-0.845422
26	6	0	-2.149465	-1.053823	1.231876
27	6	0	-1.858098	0.321110	1.063728
28	6	0	-2.795418	1.102779	0.348172
29	6	0	-3.931640	0.535857	-0.204898
30	6	0	-4.185769	-0.836489	-0.060567
31	6	0	-3.284804	-1.619348	0.679573
32	1	0	-1.463296	-1.673939	1.801993
33	1	0	-2.622846	2.170915	0.242455
34	1	0	-4.639280	1.154501	-0.749042
35	1	0	-3.486527	-2.677356	0.816484

36	6	0	-0.627055	0.890966	1.556766
37	6	0	0.329097	0.081748	2.201633
38	7	0	1.118996	-0.634330	2.678817
39	6	0	-0.252163	2.197432	1.194650
40	7	0	0.058324	3.249901	0.789636
41	6	0	-5.349611	-1.427771	-0.654184
42	7	0	-6.283556	-1.907739	-1.146286

Zero-point correction= 0.342525 (Hartree/Particle)
Thermal correction to Energy= 0.365806
Thermal correction to Enthalpy= 0.366750
Thermal correction to Gibbs Free Energy= 0.285949
Sum of electronic and zero-point Energies= -970.358903
Sum of electronic and thermal Energies= -970.335622
Sum of electronic and thermal Enthalpies= -970.334678
Sum of electronic and thermal Free Energies= -970.415479

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.661151	-0.300122	-0.391999
2	1	0	-1.691546	-0.707667	-0.127641
3	6	0	-4.747784	-0.133277	-1.079992
4	1	0	-5.694675	-0.474221	-1.467078
5	6	0	-4.323681	1.106540	-0.708594
6	1	0	-4.833494	2.056600	-0.702617
7	7	0	-3.695357	-0.994603	-0.873108
8	7	0	-3.021066	0.980291	-0.286354
9	6	0	-3.700659	-2.431893	-1.166503
10	1	0	-3.643831	-2.577456	-2.246263
11	1	0	-2.845037	-2.895354	-0.670061
12	1	0	-4.625000	-2.858865	-0.777178
13	6	0	-2.175170	2.071253	0.241687
14	1	0	-2.728390	2.994522	0.050486
15	1	0	-2.072858	1.921662	1.320378
16	6	0	-0.359769	-0.244863	2.109967
17	7	0	-0.876087	0.585660	2.750067
18	6	0	0.251566	-1.196925	1.271348
19	6	0	-0.481667	-2.359030	0.975829
20	7	0	-1.129567	-3.282787	0.668959
21	6	0	-0.806517	2.114856	-0.425169
22	6	0	0.046876	3.229822	0.179809

23	1	0	-0.928669	2.270157	-1.505320
24	1	0	-0.285857	1.157922	-0.285141
25	6	0	1.353964	3.423468	-0.584900
26	1	0	-0.522184	4.169155	0.181183
27	1	0	0.249617	2.982400	1.229089
28	1	0	1.980725	4.182415	-0.109381
29	1	0	1.160704	3.744013	-1.613902
30	6	0	1.568398	-0.967306	0.708587
31	6	0	2.146284	-1.888975	-0.191467
32	6	0	2.306061	0.192270	1.029449
33	6	0	3.389821	-1.656557	-0.751522
34	1	0	1.605737	-2.796899	-0.442867
35	6	0	3.552945	0.423104	0.471816
36	1	0	1.893315	0.907762	1.736366
37	6	0	4.107733	-0.494374	-0.431080
38	1	0	3.818267	-2.375032	-1.443097
39	1	0	4.109098	1.318306	0.733179
40	6	0	5.394142	-0.249860	-1.018497
41	7	0	6.430990	-0.051136	-1.497835
42	1	0	1.923341	2.489824	-0.624863

Zero-point correction= 0.343162 (Hartree/Particle)
Thermal correction to Energy= 0.366259
Thermal correction to Enthalpy= 0.367203
Thermal correction to Gibbs Free Energy= 0.287793
Sum of electronic and zero-point Energies= -970.353400
Sum of electronic and thermal Energies= -970.330303
Sum of electronic and thermal Enthalpies= -970.329359
Sum of electronic and thermal Free Energies= -970.408769

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.234230	-1.037184	-0.266215
2	6	0	-0.820994	-1.490355	-1.891446
3	6	0	-0.585132	-0.217556	-1.470384
4	7	0	-1.478893	0.042967	-0.456718
5	1	0	-2.976762	-1.146511	0.510941
6	1	0	-0.317642	-2.103362	-2.621962
7	1	0	0.166893	0.499679	-1.764218
8	7	0	-1.860076	-1.979344	-1.129327
9	6	0	-1.587566	1.293504	0.306763

10	6	0	-2.539161	2.282036	-0.357907
11	1	0	-0.573982	1.697421	0.383932
12	1	0	-1.910359	1.018376	1.315713
13	6	0	-2.635144	3.583681	0.436753
14	1	0	-2.192584	2.492606	-1.378069
15	1	0	-3.533929	1.825789	-0.445849
16	1	0	-2.967654	3.360238	1.457862
17	1	0	-1.636419	4.028787	0.524266
18	6	0	-2.410130	-3.332584	-1.215583
19	1	0	-3.125096	-3.465648	-0.404193
20	1	0	-2.911325	-3.456596	-2.176543
21	1	0	-1.589864	-4.043332	-1.097390
22	6	0	-3.590366	4.583245	-0.211170
23	1	0	-4.600836	4.168477	-0.283668
24	1	0	-3.647917	5.507521	0.368672
25	1	0	-3.260356	4.841419	-1.222424
26	6	0	1.600733	0.442259	1.390412
27	6	0	1.567662	-0.851674	0.819186
28	6	0	2.497037	-1.133407	-0.210890
29	6	0	3.369246	-0.165189	-0.674633
30	6	0	3.360191	1.127308	-0.124941
31	6	0	2.474395	1.411340	0.925313
32	1	0	0.933128	0.672933	2.216801
33	1	0	2.516131	-2.127833	-0.648129
34	1	0	4.069409	-0.399979	-1.470614
35	1	0	2.484594	2.398363	1.378536
36	6	0	0.588678	-1.829002	1.230063
37	6	0	-0.462783	-1.472114	2.094080
38	7	0	-1.371741	-1.111252	2.735242
39	6	0	0.519195	-3.084058	0.593951
40	7	0	0.457996	-4.091537	0.005859
41	6	0	4.247404	2.138069	-0.622645
42	7	0	4.955623	2.959413	-1.033327

Zero-point correction= 0.342208 (Hartree/Particle)
Thermal correction to Energy= 0.365452
Thermal correction to Enthalpy= 0.366396
Thermal correction to Gibbs Free Energy= 0.286928
Sum of electronic and zero-point Energies= -970.359394
Sum of electronic and thermal Energies= -970.336150
Sum of electronic and thermal Enthalpies= -970.335206
Sum of electronic and thermal Free Energies= -970.414674

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.644932	-1.422150	0.295325
2	6	0	4.138776	-2.173800	-1.138533
3	6	0	4.538803	-0.942063	-0.719452
4	7	0	3.593663	-0.493665	0.175583
5	1	0	1.764224	-1.368664	0.922796
6	1	0	4.583528	-2.866252	-1.835385
7	1	0	5.402323	-0.352960	-0.982481
8	7	0	2.956091	-2.454150	-0.491763
9	6	0	3.611266	0.812294	0.861004
10	6	0	3.736820	1.963037	-0.129356
11	1	0	4.437441	0.798478	1.578865
12	1	0	2.663411	0.892282	1.396571
13	6	0	3.507401	3.301652	0.570133
14	1	0	4.728689	1.955034	-0.601809
15	1	0	2.979062	1.830049	-0.907833
16	1	0	2.506597	3.285160	1.016370
17	1	0	4.230432	3.424081	1.387399
18	6	0	2.162762	-3.676592	-0.657746
19	1	0	1.837956	-3.746857	-1.696581
20	1	0	2.780828	-4.535857	-0.395309
21	1	0	1.293053	-3.618438	-0.000291
22	6	0	3.618220	4.473440	-0.401925
23	1	0	2.876085	4.378629	-1.200392
24	1	0	3.445638	5.425931	0.105277
25	1	0	4.610608	4.513903	-0.863825
26	6	0	-3.035422	1.124928	-0.224062
27	6	0	-2.601803	-0.135656	0.236803
28	6	0	-3.577059	-1.129659	0.461532
29	6	0	-4.918770	-0.877066	0.234277
30	6	0	-5.335747	0.380285	-0.226311
31	6	0	-4.376782	1.378583	-0.451484
32	1	0	-2.302784	1.907102	-0.401044
33	1	0	-3.267830	-2.107347	0.820139
34	1	0	-5.657389	-1.652451	0.411135
35	1	0	-4.695143	2.353794	-0.806009
36	6	0	-1.198125	-0.400072	0.470557
37	6	0	-0.193560	0.556470	0.249408
38	7	0	0.685281	1.310119	0.078501
39	6	0	-0.714580	-1.636720	0.922733
40	7	0	-0.229166	-2.637593	1.289997

41	6	0	-6.726114	0.641993	-0.466022
42	7	0	-7.849131	0.853999	-0.662157

Zero-point correction= 0.343024 (Hartree/Particle)
Thermal correction to Energy= 0.366294
Thermal correction to Enthalpy= 0.367238
Thermal correction to Gibbs Free Energy= 0.286683
Sum of electronic and zero-point Energies= -970.351362
Sum of electronic and thermal Energies= -970.328092
Sum of electronic and thermal Enthalpies= -970.327148
Sum of electronic and thermal Free Energies= -970.407702

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.607357	-1.966351	-0.536877
2	6	0	-0.261920	-0.381210	-1.261348
3	7	0	-1.353775	-0.611812	-0.534949
4	1	0	-2.409759	-2.392025	0.044823
5	1	0	0.211633	0.582549	-1.397858
6	6	0	-2.142729	0.395886	0.186120
7	6	0	-3.497830	0.630310	-0.471886
8	1	0	-1.543883	1.310788	0.202232
9	1	0	-2.240788	0.035264	1.215547
10	6	0	-4.306636	1.682933	0.285392
11	1	0	-3.347708	0.948747	-1.511619
12	1	0	-4.058511	-0.312691	-0.503244
13	1	0	-4.442247	1.356312	1.323486
14	1	0	-3.736099	2.619348	0.323969
15	6	0	-5.666968	1.936182	-0.360058
16	1	0	-6.266406	1.020648	-0.382268
17	1	0	-6.230756	2.692698	0.191112
18	1	0	-5.552382	2.287887	-1.390396
19	6	0	0.998249	0.963727	1.531683
20	6	0	1.634816	-0.218584	1.075371
21	6	0	2.730291	-0.061268	0.188503
22	6	0	3.105204	1.186236	-0.278312
23	6	0	2.416751	2.341045	0.130425
24	6	0	1.374345	2.210234	1.063775
25	1	0	0.192798	0.882386	2.256719
26	1	0	3.278257	-0.942867	-0.133466
27	1	0	3.941174	1.280932	-0.965327

28	1	0	0.865131	3.101256	1.419760
29	6	0	1.133116	-1.520573	1.422849
30	6	0	-0.069685	-1.638952	2.149079
31	7	0	-1.103117	-1.661042	2.692098
32	6	0	1.669308	-2.666743	0.801398
33	7	0	2.117075	-3.560529	0.197912
34	6	0	-0.637751	-2.551333	-1.289582
35	1	0	-0.423775	-3.587917	-1.496684
36	7	0	0.188098	-1.542197	-1.736417
37	6	0	1.395384	-1.736730	-2.538147
38	1	0	2.002142	-2.505451	-2.054734
39	1	0	1.115949	-2.037721	-3.549015
40	1	0	1.946764	-0.796796	-2.564270
41	6	0	2.782499	3.629039	-0.381127
42	7	0	3.066570	4.668947	-0.808974

Zero-point correction=	0.342792 (Hartree/Particle)
Thermal correction to Energy=	0.365749
Thermal correction to Enthalpy=	0.366693
Thermal correction to Gibbs Free Energy=	0.289089
Sum of electronic and zero-point Energies=	-970.360390
Sum of electronic and thermal Energies=	-970.337433
Sum of electronic and thermal Enthalpies=	-970.336489
Sum of electronic and thermal Free Energies=	-970.414093

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.345453	0.432070	0.232021
2	6	0	3.205471	-0.660064	-1.672386
3	6	0	2.413912	0.443434	-1.759721
4	7	0	2.519735	1.112768	-0.559505
5	1	0	3.571990	0.686448	1.257075
6	1	0	3.368251	-1.474122	-2.359954
7	1	0	1.772750	0.789423	-2.553660
8	7	0	3.786703	-0.639387	-0.425616
9	6	0	1.803060	2.340784	-0.172550
10	6	0	0.333596	2.291622	-0.575418
11	1	0	2.314894	3.191031	-0.634495
12	1	0	1.890529	2.408844	0.914561
13	6	0	-0.453850	3.396569	0.129356
14	1	0	0.234194	2.406875	-1.662852

15	1	0	-0.083725	1.312475	-0.310735
16	1	0	-0.441078	3.195648	1.207976
17	1	0	0.048008	4.362413	-0.017953
18	6	0	4.636168	-1.695282	0.123544
19	1	0	4.071976	-2.629656	0.096386
20	1	0	5.551277	-1.764178	-0.465927
21	1	0	4.879263	-1.441532	1.154877
22	6	0	-1.892539	3.481027	-0.373889
23	1	0	-2.400853	2.519311	-0.253792
24	1	0	-2.459563	4.237865	0.174165
25	1	0	-1.920656	3.744215	-1.436326
26	6	0	-2.029447	-0.059843	1.141444
27	6	0	-1.186487	-1.050095	0.590925
28	6	0	-1.752709	-1.957054	-0.332359
29	6	0	-3.085722	-1.872293	-0.692008
30	6	0	-3.909524	-0.878428	-0.142116
31	6	0	-3.364937	0.022747	0.783529
32	1	0	-1.625100	0.640930	1.868000
33	1	0	-1.129069	-2.735181	-0.762824
34	1	0	-3.502985	-2.577851	-1.403488
35	1	0	-4.000059	0.787100	1.221378
36	6	0	0.215182	-1.123915	0.946722
37	6	0	0.799697	-0.190458	1.819128
38	7	0	1.306354	0.617864	2.497248
39	6	0	1.059528	-2.114298	0.410990
40	7	0	1.760747	-2.923055	-0.058882
41	6	0	-5.290351	-0.785828	-0.521026
42	7	0	-6.404831	-0.708792	-0.831748

Zero-point correction= 0.343442 (Hartree/Particle)
Thermal correction to Energy= 0.366342
Thermal correction to Enthalpy= 0.367286
Thermal correction to Gibbs Free Energy= 0.289700
Sum of electronic and zero-point Energies= -970.358177
Sum of electronic and thermal Energies= -970.335277
Sum of electronic and thermal Enthalpies= -970.334333
Sum of electronic and thermal Free Energies= -970.411919

p-$CF_3PhCH(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581281	-1.204270	-0.247890

2	6	0	-1.281205	0.002478	-0.289906
3	6	0	-0.596334	1.213771	-0.217010
4	6	0	0.791893	1.221521	-0.106292
5	6	0	1.485302	0.016585	-0.070333
6	6	0	0.804425	-1.197133	-0.137924
7	1	0	-1.113345	-2.149859	-0.291660
8	1	0	-1.138925	2.154062	-0.236937
9	1	0	1.329883	2.161402	-0.049588
10	1	0	1.354310	-2.132225	-0.105323
11	6	0	-2.802208	-0.006781	-0.491411
12	1	0	-3.012668	-0.016656	-1.570233
13	6	0	-3.448330	1.200685	0.052924
14	7	0	-3.927544	2.173074	0.449072
15	6	0	2.981767	0.004435	0.085901
16	9	0	3.345302	-0.280024	1.349771
17	9	0	3.552859	-0.925700	-0.698593
18	9	0	3.531265	1.187967	-0.225722
19	6	0	-3.434134	-1.213165	0.072191
20	7	0	-3.901523	-2.185311	0.482805

Zero-point correction=	0.132143 (Hartree/Particle)
Thermal correction to Energy=	0.144920
Thermal correction to Enthalpy=	0.145864
Thermal correction to Gibbs Free Energy=	0.090156
Sum of electronic and zero-point Energies=	-792.682718
Sum of electronic and thermal Energies=	-792.669941
Sum of electronic and thermal Enthalpies=	-792.668997
Sum of electronic and thermal Free Energies=	-792.724704

The conjugate base anion of *p*-$CF_3PhCH(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.606636	1.209034	-0.019589
2	6	0	-1.348810	-0.000005	-0.010673
3	6	0	-0.606644	-1.209045	-0.019617
4	6	0	0.776776	-1.205410	-0.034094
5	6	0	1.487310	-0.000014	-0.045218
6	6	0	0.776781	1.205391	-0.034063
7	1	0	-1.143078	2.153261	-0.018366
8	1	0	-1.143089	-2.153270	-0.018415
9	1	0	1.317142	-2.147966	-0.044828
10	1	0	1.317156	2.147942	-0.044772

11	6	0	-2.785069	0.000002	0.003227
12	6	0	-3.505382	-1.213726	0.010871
13	7	0	-4.060693	-2.240855	0.016906
14	6	0	-3.505372	1.213736	0.010851
15	7	0	-4.060672	2.240871	0.016864
16	6	0	2.970943	-0.000005	0.002497
17	9	0	3.474556	0.000039	1.267065
18	9	0	3.517069	-1.085037	-0.594355
19	9	0	3.517048	1.085017	-0.594396

Zero-point correction= 0.119148 (Hartree/Particle)
Thermal correction to Energy= 0.131618
Thermal correction to Enthalpy= 0.132562
Thermal correction to Gibbs Free Energy= 0.078636
Sum of electronic and zero-point Energies= -792.197811
Sum of electronic and thermal Energies= -792.185341
Sum of electronic and thermal Enthalpies= -792.184397
Sum of electronic and thermal Free Energies= -792.238323

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-$CF_3PhCH(CN)_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.107659	1.013229	-1.131972
2	6	0	0.596372	-0.577771	-1.307359
3	6	0	1.637512	-1.063532	-0.577602
4	7	0	2.569192	-0.052586	-0.483543
5	1	0	2.580337	1.983877	-1.173838
6	1	0	-0.356040	-1.015783	-1.564866
7	1	0	1.773076	-2.006840	-0.072804
8	7	0	0.913283	0.719282	-1.644874
9	6	0	3.841534	-0.126814	0.247875
10	6	0	4.895130	-0.909513	-0.527149
11	1	0	3.615100	-0.575711	1.219510
12	1	0	4.160204	0.903949	0.428997
13	6	0	6.215878	-0.971634	0.239221
14	1	0	4.528645	-1.927362	-0.713889
15	1	0	5.052919	-0.442214	-1.507941
16	1	0	6.574102	0.048281	0.426916
17	1	0	6.042704	-1.426196	1.221930
18	6	0	0.067179	1.657328	-2.382177

19	1	0	0.342419	1.656663	-3.438133
20	1	0	-0.969105	1.343522	-2.258510
21	1	0	0.194824	2.648263	-1.942795
22	6	0	7.281864	-1.760991	-0.517143
23	1	0	7.487036	-1.307268	-1.492141
24	1	0	8.220250	-1.794253	0.041665
25	1	0	6.956579	-2.791998	-0.689056
26	6	0	-1.560355	-0.636542	1.422578
27	6	0	-1.153493	0.676670	1.095156
28	6	0	-2.036592	1.455537	0.312570
29	6	0	-3.239381	0.937678	-0.143551
30	6	0	-3.607657	-0.373716	0.166802
31	6	0	-2.765067	-1.149764	0.966165
32	1	0	-0.913468	-1.253381	2.040186
33	1	0	-1.768909	2.482163	0.075495
34	1	0	-3.901656	1.556126	-0.743282
35	1	0	-3.053464	-2.163454	1.227033
36	6	0	0.139789	1.186121	1.497701
37	6	0	1.045934	0.368405	2.199413
38	7	0	1.790516	-0.359366	2.730074
39	6	0	0.608655	2.411923	0.993968
40	7	0	0.990677	3.389006	0.475530
41	6	0	-4.926083	-0.903077	-0.292812
42	9	0	-5.949188	-0.516657	0.500319
43	9	0	-4.955433	-2.249948	-0.319633
44	9	0	-5.240322	-0.477168	-1.535673

Zero-point correction= 0.349302 (Hartree/Particle)
Thermal correction to Energy= 0.374145
Thermal correction to Enthalpy= 0.375089
Thermal correction to Gibbs Free Energy= 0.291162
Sum of electronic and zero-point Energies= -1215.089497
Sum of electronic and thermal Energies= -1215.064654
Sum of electronic and thermal Enthalpies= -1215.063710
Sum of electronic and thermal Free Energies= -1215.147637

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.243020	0.627460	0.411598
2	1	0	2.741636	0.483595	1.357994
3	6	0	4.775634	0.499400	-1.164673

4	1	0	5.705896	0.203264	-1.621554
5	6	0	3.701596	1.162288	-1.670526
6	1	0	3.510962	1.547920	-2.659023
7	7	0	4.464152	0.173029	0.136451
8	7	0	2.758795	1.235145	-0.669766
9	6	0	5.273886	-0.633695	1.048832
10	1	0	6.167591	-0.079965	1.339376
11	1	0	4.666755	-0.873863	1.922937
12	1	0	5.545643	-1.559835	0.540897
13	6	0	1.360871	1.667684	-0.850799
14	1	0	1.384919	2.542476	-1.506931
15	1	0	0.842461	0.850878	-1.366643
16	6	0	1.815919	-1.753172	-0.884165
17	7	0	2.506738	-1.797156	-1.825696
18	6	0	0.985452	-1.613772	0.246984
19	6	0	1.629167	-1.638998	1.494918
20	7	0	2.216153	-1.569516	2.505452
21	6	0	0.660530	1.991423	0.459332
22	6	0	-0.794834	2.389646	0.208015
23	1	0	1.193173	2.798916	0.979431
24	1	0	0.663176	1.107453	1.109804
25	6	0	-1.520996	2.733232	1.505337
26	1	0	-0.830768	3.246944	-0.477052
27	1	0	-1.308025	1.558073	-0.290648
28	1	0	-2.574628	2.954348	1.317319
29	1	0	-1.476392	1.890174	2.202276
30	1	0	-1.069373	3.603483	1.993533
31	6	0	-0.421773	-1.298193	0.111883
32	6	0	-1.220480	-1.019590	1.244357
33	6	0	-1.032848	-1.216009	-1.157520
34	6	0	-2.550303	-0.658621	1.107099
35	1	0	-0.780941	-1.091802	2.236016
36	6	0	-2.367278	-0.854954	-1.290200
37	1	0	-0.449744	-1.450827	-2.044171
38	6	0	-3.131154	-0.562658	-0.161003
39	1	0	-3.145254	-0.440276	1.990163
40	1	0	-2.816851	-0.794597	-2.276065
41	6	0	-4.566806	-0.166083	-0.271977
42	9	0	-5.398459	-1.075171	0.280329
43	9	0	-4.960951	-0.003458	-1.547851
44	9	0	-4.821558	0.998718	0.367778

Zero-point correction= 0.350153 (Hartree/Particle)
Thermal correction to Energy= 0.374519

Thermal correction to Enthalpy=	0.375463
Thermal correction to Gibbs Free Energy=	0.295274
Sum of electronic and zero-point Energies=	-1215.092155
Sum of electronic and thermal Energies=	-1215.067789
Sum of electronic and thermal Enthalpies=	-1215.066845
Sum of electronic and thermal Free Energies=	-1215.147034

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.987588	-0.254191	-0.351856
2	6	0	-1.736015	-1.184221	-1.905066
3	6	0	-1.096252	-0.067749	-1.460859
4	7	0	-1.896094	0.496067	-0.493120
5	1	0	-3.760646	-0.092793	0.385403
6	1	0	-1.436942	-1.942243	-2.611382
7	1	0	-0.126230	0.339610	-1.704638
8	7	0	-2.917864	-1.276148	-1.202114
9	6	0	-1.605243	1.710739	0.280101
10	6	0	-2.188636	2.956431	-0.377730
11	1	0	-0.516445	1.769380	0.364190
12	1	0	-2.007078	1.546816	1.284895
13	6	0	-1.873788	4.212819	0.433165
14	1	0	-1.785695	3.056708	-1.393864
15	1	0	-3.276343	2.840660	-0.474537
16	1	0	-2.264744	4.093161	1.450938
17	1	0	-0.786080	4.320107	0.527010
18	6	0	-3.896766	-2.356601	-1.327451
19	1	0	-4.638134	-2.240993	-0.537341
20	1	0	-4.379842	-2.293959	-2.303621
21	1	0	-3.374929	-3.306651	-1.196712
22	6	0	-2.463603	5.469574	-0.202498
23	1	0	-3.553239	5.395407	-0.277712
24	1	0	-2.227766	6.358779	0.387054
25	1	0	-2.066894	5.620715	-1.211447
26	6	0	1.025098	-0.187479	1.484846
27	6	0	0.575661	-1.402856	0.919434
28	6	0	1.400511	-2.012117	-0.053335
29	6	0	2.583781	-1.418858	-0.464502
30	6	0	2.989728	-0.197699	0.079366
31	6	0	2.208718	0.403848	1.068761
32	1	0	0.432671	0.283924	2.265162

33	1	0	1.092117	-2.957842	-0.490459
34	1	0	3.197285	-1.901731	-1.219055
35	1	0	2.533429	1.339606	1.515830
36	6	0	-0.705508	-1.971740	1.277119
37	6	0	-1.605085	-1.259074	2.088813
38	7	0	-2.358240	-0.595113	2.689406
39	6	0	-1.176176	-3.131186	0.632248
40	7	0	-1.552729	-4.062109	0.034499
41	6	0	4.282036	0.427281	-0.331526
42	9	0	5.300029	0.123899	0.503167
43	9	0	4.670835	0.034499	-1.560933
44	9	0	4.210776	1.776150	-0.352745

Zero-point correction=	0.349238 (Hartree/Particle)
Thermal correction to Energy=	0.374062
Thermal correction to Enthalpy=	0.375006
Thermal correction to Gibbs Free Energy=	0.291731
Sum of electronic and zero-point Energies=	-1215.089642
Sum of electronic and thermal Energies=	-1215.064818
Sum of electronic and thermal Enthalpies=	-1215.063874
Sum of electronic and thermal Free Energies=	-1215.147148

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.474096	-1.381302	-0.274168
2	6	0	-4.957858	-2.078894	1.197185
3	6	0	-5.330946	-0.838915	0.777417
4	7	0	-4.392617	-0.424675	-0.140901
5	1	0	-2.605426	-1.356848	-0.920057
6	1	0	-5.407661	-2.753785	1.907880
7	1	0	-6.171697	-0.223337	1.053221
8	7	0	-3.798172	-2.398291	0.527072
9	6	0	-4.386083	0.876347	-0.835165
10	6	0	-4.444282	2.038407	0.148049
11	1	0	-5.232412	0.885306	-1.529252
12	1	0	-3.451986	0.920265	-1.398152
13	6	0	-4.180232	3.360667	-0.570090
14	1	0	-5.424064	2.072312	0.644095
15	1	0	-3.672738	1.883465	0.908708
16	1	0	-3.190185	3.301003	-1.036135
17	1	0	-4.915045	3.502001	-1.373758

18	6	0	-3.037496	-3.642398	0.684721
19	1	0	-2.684453	-3.711194	1.714404
20	1	0	-3.689290	-4.484909	0.450794
21	1	0	-2.186214	-3.618042	0.001252
22	6	0	-4.226868	4.545852	0.390743
23	1	0	-3.473924	4.430412	1.176253
24	1	0	-4.027045	5.485520	-0.130302
25	1	0	-5.207971	4.629774	0.870501
26	6	0	2.288852	0.959345	0.136814
27	6	0	1.804132	-0.282419	-0.320655
28	6	0	2.738370	-1.309196	-0.558677
29	6	0	4.093754	-1.104197	-0.347532
30	6	0	4.554837	0.130731	0.109691
31	6	0	3.643835	1.161535	0.347282
32	1	0	1.587357	1.766264	0.328938
33	1	0	2.389558	-2.275435	-0.912089
34	1	0	4.798847	-1.908614	-0.531972
35	1	0	3.999019	2.123253	0.705121
36	6	0	0.385266	-0.496991	-0.534622
37	6	0	-0.581518	0.493432	-0.300686
38	7	0	-1.432528	1.276494	-0.118637
39	6	0	-0.147943	-1.714874	-0.978633
40	7	0	-0.674824	-2.698352	-1.337380
41	6	0	6.017328	0.374516	0.290041
42	9	0	6.588172	0.942843	-0.797621
43	9	0	6.274957	1.207885	1.319031
44	9	0	6.703316	-0.762230	0.521832

Zero-point correction=	0.349363 (Hartree/Particle)
Thermal correction to Energy=	0.374410
Thermal correction to Enthalpy=	0.375354
Thermal correction to Gibbs Free Energy=	0.290118
Sum of electronic and zero-point Energies=	-1215.081893
Sum of electronic and thermal Energies=	-1215.056846
Sum of electronic and thermal Enthalpies=	-1215.055901
Sum of electronic and thermal Free Energies=	-1215.141138

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.841317	-1.069489	0.641490
2	6	0	0.841897	-0.379017	1.252421

3	7	0	1.938214	-0.029748	0.582282
4	1	0	3.778604	-1.035261	0.109070
5	1	0	-0.061545	0.211670	1.334821
6	6	0	2.143304	1.226801	-0.149910
7	6	0	3.215117	2.093608	0.501039
8	1	0	1.176110	1.737248	-0.176242
9	1	0	2.410660	0.950113	-1.175094
10	6	0	3.419873	3.395083	-0.273059
11	1	0	2.930331	2.313145	1.538015
12	1	0	4.160922	1.538029	0.539361
13	1	0	3.678406	3.159670	-1.312413
14	1	0	2.474562	3.951164	-0.304194
15	6	0	4.509906	4.266096	0.346915
16	1	0	5.470634	3.741566	0.355732
17	1	0	4.640414	5.195387	-0.212874
18	1	0	4.261609	4.528386	1.380371
19	6	0	-0.784380	0.114696	-1.599313
20	6	0	-0.750274	-1.226097	-1.145820
21	6	0	-1.808156	-1.648881	-0.302488
22	6	0	-2.783707	-0.763579	0.126126
23	6	0	-2.755322	0.575766	-0.277729
24	6	0	-1.763935	0.996896	-1.167407
25	1	0	-0.018016	0.457870	-2.289203
26	1	0	-1.843251	-2.686034	0.020317
27	1	0	-3.577123	-1.110008	0.783360
28	1	0	-1.759217	2.024439	-1.519261
29	6	0	0.360023	-2.094824	-1.447817
30	6	0	1.484321	-1.585976	-2.127778
31	7	0	2.405845	-1.078975	-2.635700
32	6	0	0.458688	-3.348915	-0.813081
33	7	0	0.505082	-4.341455	-0.198956
34	6	0	2.261838	-2.058530	1.372747
35	1	0	2.590084	-3.059046	1.605844
36	7	0	1.016460	-1.603220	1.748663
37	6	0	0.030209	-2.376611	2.501560
38	1	0	-0.104364	-3.335777	1.997106
39	1	0	0.385616	-2.519920	3.523176
40	1	0	-0.910432	-1.826001	2.503513
41	6	0	-3.826549	1.510154	0.177569
42	9	0	-4.980594	1.359087	-0.505833
43	9	0	-4.140768	1.324989	1.479213
44	9	0	-3.468442	2.801930	0.041263

Zero-point correction= 0.349917 (Hartree/Particle)

Thermal correction to Energy=	0.374302
Thermal correction to Enthalpy=	0.375246
Thermal correction to Gibbs Free Energy=	0.294416
Sum of electronic and zero-point Energies=	-1215.090911
Sum of electronic and thermal Energies=	-1215.066526
Sum of electronic and thermal Enthalpies=	-1215.065582
Sum of electronic and thermal Free Energies=	-1215.146412

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.927768	0.155658	0.487999
2	6	0	4.615761	0.296148	-1.596261
3	6	0	3.714958	1.293568	-1.382424
4	7	0	3.299898	1.186284	-0.074119
5	1	0	3.755009	-0.196471	1.498132
6	1	0	5.152028	0.003514	-2.484401
7	1	0	3.327692	2.049326	-2.045918
8	7	0	4.742183	-0.392006	-0.412898
9	6	0	2.265636	2.004310	0.585155
10	6	0	0.995651	2.087976	-0.256800
11	1	0	2.689687	2.994581	0.778587
12	1	0	2.061151	1.515719	1.542225
13	6	0	-0.182471	2.581811	0.582609
14	1	0	1.147887	2.758256	-1.113271
15	1	0	0.763838	1.091264	-0.650077
16	1	0	-0.311725	1.899179	1.431783
17	1	0	0.044079	3.572797	0.998401
18	6	0	5.436070	-1.666557	-0.247611
19	1	0	4.842463	-2.440876	-0.738684
20	1	0	6.431103	-1.590449	-0.686263
21	1	0	5.520563	-1.881455	0.817242
22	6	0	-1.473127	2.629066	-0.230069
23	1	0	-1.702263	1.639300	-0.639148
24	1	0	-2.321321	2.935615	0.387421
25	1	0	-1.388778	3.333997	-1.064243
26	6	0	-1.532098	-0.612488	1.437241
27	6	0	-0.666581	-1.054347	0.412537
28	6	0	-1.215322	-1.252787	-0.870804
29	6	0	-2.560357	-1.012402	-1.120223
30	6	0	-3.394922	-0.565106	-0.097259
31	6	0	-2.871840	-0.370079	1.184120

32	1	0	-1.138216	-0.469720	2.440100
33	1	0	-0.575013	-1.605761	-1.674491
34	1	0	-2.963750	-1.172275	-2.115019
35	1	0	-3.521768	-0.030747	1.985848
36	6	0	0.742943	-1.278230	0.669823
37	6	0	1.336442	-0.967769	1.904100
38	7	0	1.888991	-0.662602	2.890469
39	6	0	1.624295	-1.715575	-0.336816
40	7	0	2.383679	-2.041226	-1.165132
41	6	0	-4.827603	-0.233575	-0.358094
42	9	0	-5.644505	-0.691717	0.612681
43	9	0	-5.041099	1.102921	-0.416718
44	9	0	-5.272968	-0.739722	-1.522609

Zero-point correction=	0.349256 (Hartree/Particle)
Thermal correction to Energy=	0.373987
Thermal correction to Enthalpy=	0.374932
Thermal correction to Gibbs Free Energy=	0.292712
Sum of electronic and zero-point Energies=	-1215.091676
Sum of electronic and thermal Energies=	-1215.066944
Sum of electronic and thermal Enthalpies=	-1215.066000
Sum of electronic and thermal Free Energies=	-1215.148220

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.202265	-0.031050	1.206771
2	6	0	0.204567	0.667166	0.000000
3	6	0	0.202265	-0.031050	-1.206771
4	6	0	0.202265	-1.422777	-1.211157
5	6	0	0.204235	-2.107057	0.000000
6	6	0	0.202265	-1.422777	1.211157
7	1	0	0.188176	0.504266	2.151742
8	1	0	0.188176	0.504266	-2.151742
9	1	0	0.194648	-1.972858	-2.145460
10	1	0	0.194648	-1.972858	2.145460
11	6	0	0.282943	2.198760	0.000000
12	6	0	-0.321859	2.791303	-1.206509
13	7	0	-0.761281	3.231173	-2.178986
14	6	0	-0.321859	2.791303	1.206509
15	7	0	-0.761281	3.231173	2.178986
16	17	0	0.200578	-3.847176	0.000000

17	1	0	1.339941	2.499833	0.000000

Zero-point correction= 0.117442 (Hartree/Particle)
Thermal correction to Energy= 0.127807
Thermal correction to Enthalpy= 0.128752
Thermal correction to Gibbs Free Energy= 0.079827
Sum of electronic and zero-point Energies= -915.311731
Sum of electronic and thermal Energies= -915.301365
Sum of electronic and thermal Enthalpies= -915.300421
Sum of electronic and thermal Free Energies= -915.349346

The conjugate base anion of *p*-ClPhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.038623	1.204814	-0.000002
2	6	0	0.702598	0.000000	0.000001
3	6	0	-0.038623	-1.204814	-0.000001
4	6	0	-1.427505	-1.206438	-0.000006
5	6	0	-2.120564	0.000000	-0.000009
6	6	0	-1.427505	1.206438	-0.000007
7	1	0	0.494980	2.151045	0.000000
8	1	0	0.494980	-2.151045	0.000001
9	1	0	-1.973882	-2.144779	-0.000008
10	1	0	-1.973882	2.144779	-0.000009
11	6	0	2.147281	0.000000	0.000007
12	6	0	2.864084	-1.213058	0.000012
13	7	0	3.414499	-2.244124	0.000016
14	6	0	2.864084	1.213058	0.000011
15	7	0	3.414498	2.244125	0.000014
16	17	0	-3.882149	0.000000	-0.000013

Zero-point correction= 0.104596 (Hartree/Particle)
Thermal correction to Energy= 0.114718
Thermal correction to Enthalpy= 0.115662
Thermal correction to Gibbs Free Energy= 0.067755
Sum of electronic and zero-point Energies= -914.818590
Sum of electronic and thermal Energies= -914.808469
Sum of electronic and thermal Enthalpies= -914.807524
Sum of electronic and thermal Free Energies= -914.855431

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-ClPhCH(CN)$_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495534	1.348166	-0.998358
2	6	0	0.191464	-0.359051	-1.479229
3	6	0	1.282986	-0.834649	-0.820313
4	7	0	2.083503	0.249455	-0.532969
5	1	0	1.842957	2.361315	-0.856670
6	1	0	-0.701437	-0.856432	-1.826096
7	1	0	1.531630	-1.826821	-0.478466
8	7	0	0.347832	1.005837	-1.581616
9	6	0	3.349658	0.201743	0.210605
10	6	0	4.514941	-0.218166	-0.677754
11	1	0	3.189315	-0.484697	1.046898
12	1	0	3.504996	1.198375	0.633938
13	6	0	5.820084	-0.285276	0.114839
14	1	0	4.300857	-1.199532	-1.120955
15	1	0	4.618087	0.491819	-1.508789
16	1	0	6.016929	0.692265	0.572318
17	1	0	5.704006	-0.997230	0.940630
18	6	0	-0.616383	1.947044	-2.149875
19	1	0	-0.414830	2.091482	-3.212660
20	1	0	-1.614974	1.535487	-2.000751
21	1	0	-0.536416	2.887656	-1.601847
22	6	0	7.003567	-0.693202	-0.759495
23	1	0	7.153710	0.022957	-1.573699
24	1	0	7.927737	-0.738314	-0.178165
25	1	0	6.839272	-1.679098	-1.205917
26	6	0	-1.962337	-1.103310	1.124419
27	6	0	-1.716839	0.284628	1.065326
28	6	0	-2.699958	1.088103	0.452131
29	6	0	-3.848401	0.533982	-0.104775
30	6	0	-4.045159	-0.842533	-0.055139
31	6	0	-3.108677	-1.661074	0.571503
32	1	0	-1.237460	-1.750669	1.611088
33	1	0	-2.563762	2.166657	0.425784
34	1	0	-4.597372	1.170673	-0.565803
35	1	0	-3.279684	-2.731449	0.627417
36	6	0	-0.478415	0.856089	1.569585
37	6	0	0.511356	0.032594	2.135108
38	7	0	1.329680	-0.694906	2.545639
39	6	0	-0.149484	2.191380	1.289336

40	7	0	0.122292	3.278646	0.949229
41	17	0	-5.482918	-1.544738	-0.762393

Zero-point correction= 0.334132 (Hartree/Particle)
Thermal correction to Energy= 0.356815
Thermal correction to Enthalpy= 0.357759
Thermal correction to Gibbs Free Energy= 0.278697
Sum of electronic and zero-point Energies= -1337.714413
Sum of electronic and thermal Energies= -1337.691730
Sum of electronic and thermal Enthalpies= -1337.690786
Sum of electronic and thermal Free Energies= -1337.769848

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.764589	-0.315345	-0.380579
2	1	0	-1.799038	-0.713705	-0.085799
3	6	0	-4.834048	-0.164059	-1.123068
4	1	0	-5.770182	-0.513188	-1.528588
5	6	0	-4.423126	1.081891	-0.757356
6	1	0	-4.935485	2.030361	-0.777104
7	7	0	-3.784474	-1.019173	-0.878656
8	7	0	-3.131438	0.965052	-0.300545
9	6	0	-3.779231	-2.460399	-1.151129
10	1	0	-3.709479	-2.620701	-2.228093
11	1	0	-2.926348	-2.911977	-0.638340
12	1	0	-4.705819	-2.886722	-0.766223
13	6	0	-2.298821	2.063893	0.231807
14	1	0	-2.857118	2.982570	0.032969
15	1	0	-2.203865	1.917700	1.311829
16	6	0	-0.494167	-0.218483	2.132780
17	7	0	-1.012711	0.616310	2.767583
18	6	0	0.120211	-1.170621	1.300356
19	6	0	-0.598560	-2.342517	1.020664
20	7	0	-1.236145	-3.277603	0.721880
21	6	0	-0.924767	2.113635	-0.423615
22	6	0	-0.082127	3.234040	0.185978
23	1	0	-1.038905	2.266200	-1.505168
24	1	0	-0.400780	1.159471	-0.277122
25	6	0	1.229873	3.432683	-0.569048
26	1	0	-0.655964	4.170618	0.181565
27	1	0	0.113709	2.988635	1.236982

28	1	0	1.849002	4.195910	-0.090081
29	1	0	1.042499	3.750495	-1.600152
30	6	0	1.445787	-0.935520	0.735820
31	6	0	2.027415	-1.851483	-0.161116
32	6	0	2.180326	0.220668	1.056618
33	6	0	3.278570	-1.620377	-0.718673
34	1	0	1.490924	-2.760948	-0.417284
35	6	0	3.434781	0.455680	0.503051
36	1	0	1.767570	0.937939	1.762300
37	6	0	3.978111	-0.463242	-0.387943
38	1	0	3.713481	-2.337076	-1.407620
39	1	0	3.992095	1.349470	0.765482
40	1	0	1.804065	2.501732	-0.602442
41	17	0	5.553481	-0.168327	-1.088602

Zero-point correction=	0.334743 (Hartree/Particle)
Thermal correction to Energy=	0.357249
Thermal correction to Enthalpy=	0.358193
Thermal correction to Gibbs Free Energy=	0.279995
Sum of electronic and zero-point Energies=	-1337.709087
Sum of electronic and thermal Energies=	-1337.686580
Sum of electronic and thermal Enthalpies=	-1337.685636
Sum of electronic and thermal Free Energies=	-1337.763834

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.648324	1.561794	0.615334
2	6	0	-2.282131	1.455349	-1.490268
3	6	0	-0.923101	1.432429	-1.457580
4	7	0	-0.549175	1.504968	-0.132589
5	1	0	-1.686178	1.536865	1.696012
6	1	0	-2.975990	1.349907	-2.308977
7	1	0	-0.196116	1.331260	-2.247313
8	7	0	-2.713261	1.543739	-0.186500
9	6	0	0.832106	1.413402	0.355896
10	6	0	1.668145	2.629465	-0.020396
11	1	0	1.256279	0.495169	-0.062901
12	1	0	0.778792	1.285263	1.440276
13	6	0	3.107786	2.461703	0.466238
14	1	0	1.663086	2.757276	-1.110723
15	1	0	1.222885	3.535249	0.410422

16	1	0	3.108725	2.341794	1.556872
17	1	0	3.521710	1.533373	0.052887
18	6	0	-4.108998	1.469826	0.249177
19	1	0	-4.124671	1.320860	1.328688
20	1	0	-4.626248	2.389895	-0.026296
21	1	0	-4.567032	0.606477	-0.238413
22	6	0	3.990497	3.644935	0.076939
23	1	0	3.604928	4.578374	0.499593
24	1	0	5.012944	3.509994	0.437907
25	1	0	4.031388	3.761221	-1.010796
26	6	0	0.295278	-1.771214	1.300430
27	6	0	-0.550530	-1.741077	0.170560
28	6	0	0.060078	-1.866822	-1.096640
29	6	0	1.438964	-1.978999	-1.228733
30	6	0	2.247926	-1.972975	-0.092801
31	6	0	1.675451	-1.887474	1.172910
32	1	0	-0.142186	-1.706654	2.293239
33	1	0	-0.563569	-1.873103	-1.987039
34	1	0	1.890269	-2.074310	-2.211426
35	1	0	2.307664	-1.908641	2.055112
36	6	0	-1.981441	-1.542985	0.307823
37	6	0	-2.517107	-1.131281	1.539942
38	7	0	-2.907928	-0.688123	2.550137
39	6	0	-2.842065	-1.511173	-0.805568
40	7	0	-3.552661	-1.418214	-1.729097
41	17	0	3.986428	-2.079781	-0.262374

Zero-point correction=	0.334736 (Hartree/Particle)
Thermal correction to Energy=	0.357169
Thermal correction to Enthalpy=	0.358114
Thermal correction to Gibbs Free Energy=	0.281673
Sum of electronic and zero-point Energies=	-1337.716148
Sum of electronic and thermal Energies=	-1337.693715
Sum of electronic and thermal Enthalpies=	-1337.692771
Sum of electronic and thermal Free Energies=	-1337.769211

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.779709	-1.422020	0.292325
2	6	0	4.252625	-2.173403	-1.163303
3	6	0	4.663798	-0.945905	-0.742675

4	7	0	3.731542	-0.497643	0.165890
5	1	0	1.906503	-1.368191	0.930392
6	1	0	4.685599	-2.864464	-1.868844
7	1	0	5.526794	-0.359354	-1.012946
8	7	0	3.076449	-2.451363	-0.503663
9	6	0	3.760766	0.805864	0.855067
10	6	0	3.881283	1.958789	-0.133386
11	1	0	4.593385	0.786895	1.565404
12	1	0	2.817473	0.888342	1.398318
13	6	0	3.654063	3.295410	0.570395
14	1	0	4.870701	1.952264	-0.611211
15	1	0	3.118509	1.827016	-0.907128
16	1	0	2.654464	3.276244	1.019149
17	1	0	4.379717	3.416227	1.385676
18	6	0	2.273201	-3.667528	-0.667969
19	1	0	1.933356	-3.727284	-1.702656
20	1	0	2.889844	-4.532514	-0.421172
21	1	0	1.413308	-3.608711	0.002907
22	6	0	3.760840	4.469814	-0.398916
23	1	0	3.015957	4.376157	-1.194973
24	1	0	3.589188	5.421022	0.111143
25	1	0	4.751618	4.512200	-0.864261
26	6	0	-2.888367	1.098867	-0.206899
27	6	0	-2.448235	-0.152805	0.259003
28	6	0	-3.417711	-1.145967	0.485471
29	6	0	-4.766602	-0.902524	0.255315
30	6	0	-5.170995	0.345321	-0.207453
31	6	0	-4.235811	1.348556	-0.438886
32	1	0	-2.162032	1.886561	-0.387624
33	1	0	-3.107870	-2.122069	0.848940
34	1	0	-5.504131	-1.678168	0.433501
35	1	0	-4.561911	2.319233	-0.797903
36	6	0	-1.034671	-0.411258	0.498311
37	6	0	-0.035850	0.546102	0.271375
38	7	0	0.839398	1.304602	0.094365
39	6	0	-0.548900	-1.639756	0.961675
40	7	0	-0.062096	-2.638055	1.338663
41	17	0	-6.869552	0.654734	-0.501777

Zero-point correction= 0.334599 (Hartree/Particle)
Thermal correction to Energy= 0.357327
Thermal correction to Enthalpy= 0.358271
Thermal correction to Gibbs Free Energy= 0.278480
Sum of electronic and zero-point Energies= -1337.706448

Sum of electronic and thermal Energies= -1337.683720
Sum of electronic and thermal Enthalpies= -1337.682776
Sum of electronic and thermal Free Energies= -1337.762567

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.881395	-1.845996	-0.545961
2	6	0	-0.357051	-0.427066	-1.260646
3	7	0	-1.479709	-0.527275	-0.551923
4	1	0	-2.733359	-2.173338	0.028663
5	1	0	0.224234	0.476122	-1.396745
6	6	0	-2.155107	0.565326	0.159661
7	6	0	-3.485538	0.927118	-0.490919
8	1	0	-1.464871	1.414057	0.160712
9	1	0	-2.282090	0.229355	1.194396
10	6	0	-4.179642	2.062390	0.260292
11	1	0	-3.315685	1.216277	-1.536181
12	1	0	-4.137496	0.044353	-0.504877
13	1	0	-4.325350	1.767027	1.306347
14	1	0	-3.525168	2.942890	0.272077
15	6	0	-5.523245	2.427454	-0.366397
16	1	0	-6.202282	1.568904	-0.361031
17	1	0	-6.007419	3.241003	0.179242
18	1	0	-5.396788	2.748459	-1.405442
19	6	0	1.014606	0.816392	1.503888
20	6	0	1.514328	-0.435997	1.081329
21	6	0	2.624049	-0.419188	0.206540
22	6	0	3.155114	0.772799	-0.273788
23	6	0	2.598912	1.988776	0.117259
24	6	0	1.542585	2.010226	1.025229
25	1	0	0.193081	0.845470	2.215269
26	1	0	3.069418	-1.361905	-0.101422
27	1	0	4.008030	0.762054	-0.945729
28	1	0	1.141094	2.961321	1.361774
29	6	0	0.859967	-1.674983	1.451211
30	6	0	-0.353459	-1.639318	2.162527
31	7	0	-1.388429	-1.528652	2.694565
32	6	0	1.264792	-2.882118	0.853064
33	7	0	1.613927	-3.829900	0.264437
34	6	0	-0.971719	-2.542165	-1.278312
35	1	0	-0.868739	-3.598308	-1.470282

36	7	0	-0.032895	-1.634924	-1.720441
37	6	0	1.163066	-1.970516	-2.491224
38	1	0	1.682886	-2.779041	-1.972497
39	1	0	0.872930	-2.274605	-3.498206
40	1	0	1.802549	-1.088885	-2.533083
41	17	0	3.252541	3.488544	-0.498940

Zero-point correction= 0.334625 (Hartree/Particle)
Thermal correction to Energy= 0.356918
Thermal correction to Enthalpy= 0.357862
Thermal correction to Gibbs Free Energy= 0.281365
Sum of electronic and zero-point Energies= -1337.715719
Sum of electronic and thermal Energies= -1337.693426
Sum of electronic and thermal Enthalpies= -1337.692482
Sum of electronic and thermal Free Energies= -1337.768980

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.459899	0.415272	0.235290
2	6	0	3.302520	-0.686783	-1.662257
3	6	0	2.526990	0.427321	-1.755758
4	7	0	2.643665	1.102735	-0.559778
5	1	0	3.686794	0.670402	1.260014
6	1	0	3.450305	-1.509274	-2.343032
7	1	0	1.887925	0.776032	-2.550073
8	7	0	3.885226	-0.666393	-0.416052
9	6	0	1.934999	2.335593	-0.174744
10	6	0	0.465203	2.292840	-0.577243
11	1	0	2.451442	3.182523	-0.637853
12	1	0	2.022497	2.403676	0.912466
13	6	0	-0.317902	3.401584	0.126081
14	1	0	0.366200	2.407403	-1.664887
15	1	0	0.044151	1.315865	-0.310720
16	1	0	-0.308024	3.200131	1.204600
17	1	0	0.188251	4.365500	-0.020170
18	6	0	4.716614	-1.732442	0.140300
19	1	0	4.139591	-2.658935	0.109728
20	1	0	5.635463	-1.814330	-0.441834
21	1	0	4.954582	-1.480875	1.173396
22	6	0	-1.755450	3.491464	-0.379771
23	1	0	-2.266079	2.530478	-0.263356

24	1	0	-2.321535	4.248511	0.169269
25	1	0	-1.780069	3.758026	-1.441592
26	6	0	-1.907676	-0.019584	1.158707
27	6	0	-1.081609	-1.008574	0.592219
28	6	0	-1.664989	-1.890611	-0.337922
29	6	0	-3.004800	-1.787099	-0.689426
30	6	0	-3.794779	-0.795245	-0.115426
31	6	0	-3.250759	0.086486	0.811987
32	1	0	-1.493332	0.668099	1.892630
33	1	0	-1.056631	-2.671322	-0.786198
34	1	0	-3.438422	-2.476404	-1.406643
35	1	0	-3.876148	0.850251	1.263892
36	6	0	0.329924	-1.107898	0.942753
37	6	0	0.930197	-0.190755	1.817260
38	7	0	1.449110	0.608785	2.498982
39	6	0	1.151061	-2.112222	0.403474
40	7	0	1.834005	-2.934987	-0.072169
41	17	0	-5.482804	-0.661932	-0.558216

Zero-point correction=	0.334970 (Hartree/Particle)
Thermal correction to Energy=	0.357323
Thermal correction to Enthalpy=	0.358267
Thermal correction to Gibbs Free Energy=	0.281285
Sum of electronic and zero-point Energies=	-1337.713720
Sum of electronic and thermal Energies=	-1337.691367
Sum of electronic and thermal Enthalpies=	-1337.690423
Sum of electronic and thermal Free Energies=	-1337.767405

$PhCH(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.938179	1.193013	0.247891
2	6	0	-0.209611	0.002904	0.224317
3	6	0	-0.856130	-1.209353	-0.007025
4	6	0	-2.235226	-1.229343	-0.211876
5	6	0	-2.965998	-0.044677	-0.186308
6	6	0	-2.314613	1.166469	0.043083
7	1	0	-0.431862	2.140448	0.411713
8	1	0	-0.290135	-2.135638	-0.037276
9	1	0	-2.733526	-2.175332	-0.396764
10	1	0	-2.876252	2.094780	0.056575
11	6	0	1.295414	0.045983	0.520176

12	6	0	1.997960	-1.177124	0.095115
13	7	0	2.525641	-2.156570	-0.212374
14	6	0	1.942582	1.227088	-0.081395
15	7	0	2.421858	2.179453	-0.523907
16	1	0	-4.038484	-0.062640	-0.350530
17	1	0	1.440571	0.128451	1.606383

Zero-point correction= 0.127089 (Hartree/Particle)
Thermal correction to Energy= 0.136312
Thermal correction to Enthalpy= 0.137256
Thermal correction to Gibbs Free Energy= 0.090833
Sum of electronic and zero-point Energies= -455.734909
Sum of electronic and thermal Energies= -455.725686
Sum of electronic and thermal Enthalpies= -455.724741
Sum of electronic and thermal Free Energies= -455.771165

The conjugate base anion of $PhCH(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.899550	1.205399	0.000004
2	6	0	0.159461	0.000000	0.000001
3	6	0	0.899550	-1.205399	0.000003
4	6	0	2.288829	-1.198726	0.000008
5	6	0	3.006660	0.000000	0.000011
6	6	0	2.288829	1.198726	0.000009
7	1	0	0.361972	2.149802	0.000002
8	1	0	0.361972	-2.149802	0.000001
9	1	0	2.819968	-2.148204	0.000010
10	1	0	2.819968	2.148204	0.000011
11	6	0	-1.288022	0.000000	-0.000005
12	6	0	-2.007283	-1.211266	-0.000008
13	7	0	-2.564148	-2.239419	-0.000011
14	6	0	-2.007283	1.211266	-0.000007
15	7	0	-2.564147	2.239419	-0.000010
16	1	0	4.092429	0.000000	0.000015

Zero-point correction= 0.114004 (Hartree/Particle)
Thermal correction to Energy= 0.122906
Thermal correction to Enthalpy= 0.123850
Thermal correction to Gibbs Free Energy= 0.079310
Sum of electronic and zero-point Energies= -455.234218
Sum of electronic and thermal Energies= -455.225316

Sum of electronic and thermal Enthalpies= -455.224372
Sum of electronic and thermal Free Energies= -455.268912

Complexes formed from a [Bmim] cation and the conjugate base anion of $PhCH(CN)_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.266522	1.296974	1.161680
2	6	0	0.273050	1.960996	-0.863873
3	6	0	-0.987590	1.452644	-0.910534
4	7	0	-1.309508	1.053146	0.366925
5	1	0	-0.198685	1.003022	2.200916
6	1	0	0.911612	2.350389	-1.640166
7	1	0	-1.650068	1.294474	-1.744653
8	7	0	0.701755	1.856736	0.440245
9	6	0	-2.505391	0.291242	0.782501
10	6	0	-3.623803	0.361179	-0.243417
11	1	0	-2.824980	0.701721	1.744880
12	1	0	-2.188924	-0.744398	0.937838
13	6	0	-4.866898	-0.369023	0.266290
14	1	0	-3.873609	1.408781	-0.459747
15	1	0	-3.285627	-0.113954	-1.172114
16	1	0	-4.602259	-1.407835	0.496079
17	1	0	-5.202234	0.086824	1.206598
18	6	0	2.033501	2.224461	0.916133
19	1	0	2.775297	1.793720	0.239325
20	1	0	2.121982	3.311804	0.951299
21	1	0	2.178185	1.799580	1.908629
22	6	0	-6.001003	-0.341178	-0.755159
23	1	0	-5.693370	-0.821719	-1.688951
24	1	0	-6.883546	-0.866241	-0.381131
25	1	0	-6.295054	0.687920	-0.986757
26	6	0	2.426328	-0.587422	-1.469311
27	6	0	2.032686	-1.030764	-0.188158
28	6	0	3.000178	-0.991217	0.838423
29	6	0	4.285827	-0.517099	0.597040
30	6	0	4.655840	-0.059368	-0.668712
31	6	0	3.711996	-0.109591	-1.699222
32	1	0	1.707568	-0.627110	-2.284610
33	1	0	2.734410	-1.351114	1.829154
34	1	0	5.008621	-0.510850	1.408644

35	1	0	3.984239	0.219345	-2.698697
36	6	0	0.673372	-1.471456	0.080160
37	6	0	-0.302888	-1.560168	-0.929376
38	7	0	-1.135931	-1.576775	-1.750456
39	6	0	0.237188	-1.620888	1.407652
40	7	0	-0.119087	-1.632441	2.522712
41	1	0	5.660616	0.305043	-0.855231

Zero-point correction= 0.344100 (Hartree/Particle)
Thermal correction to Energy= 0.365274
Thermal correction to Enthalpy= 0.366218
Thermal correction to Gibbs Free Energy= 0.292313
Sum of electronic and zero-point Energies= -878.135420
Sum of electronic and thermal Energies= -878.114246
Sum of electronic and thermal Enthalpies= -878.113302
Sum of electronic and thermal Free Energies= -878.187206

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.125125	0.634603	0.534121
2	1	0	1.541844	0.441670	1.423225
3	6	0	3.796996	0.598135	-0.898867
4	1	0	4.772450	0.340683	-1.278088
5	6	0	2.755724	1.252285	-1.478763
6	1	0	2.644003	1.666226	-2.467749
7	7	0	3.377573	0.218658	0.357410
8	7	0	1.725014	1.268718	-0.566143
9	6	0	4.118733	-0.607512	1.309656
10	1	0	5.000431	-0.068023	1.658211
11	1	0	3.455517	-0.848089	2.141982
12	1	0	4.408167	-1.533575	0.811042
13	6	0	0.336484	1.671070	-0.853771
14	1	0	0.392027	2.552348	-1.499390
15	1	0	-0.123258	0.847211	-1.412368
16	6	0	0.841915	-1.693015	-0.982791
17	7	0	1.587128	-1.677254	-1.884243
18	6	0	-0.055087	-1.620851	0.100782
19	6	0	0.512489	-1.703708	1.380380
20	7	0	1.037214	-1.678699	2.428072
21	6	0	-0.464830	1.967620	0.403938
22	6	0	-1.903844	2.347749	0.053661

23	1	0	0.017253	2.775044	0.971745
24	1	0	-0.497223	1.074266	1.040198
25	6	0	-2.721168	2.663968	1.302936
26	1	0	-1.903347	3.213961	-0.621365
27	1	0	-2.369492	1.514493	-0.486838
28	1	0	-3.758958	2.891718	1.045588
29	1	0	-2.306911	3.523003	1.841948
30	6	0	-1.467353	-1.325187	-0.102993
31	6	0	-2.330614	-1.104646	0.988922
32	6	0	-2.009825	-1.210752	-1.399490
33	6	0	-3.667564	-0.777690	0.789698
34	1	0	-1.941447	-1.200008	2.000149
35	6	0	-3.348892	-0.883117	-1.588141
36	1	0	-1.371644	-1.398183	-2.260045
37	6	0	-4.191494	-0.657204	-0.498691
38	1	0	-4.307818	-0.614343	1.652638
39	1	0	-3.738512	-0.808060	-2.599653
40	1	0	-2.726636	1.803804	1.979901
41	1	0	-5.235714	-0.404598	-0.650327

Zero-point correction= 0.344485 (Hartree/Particle)
Thermal correction to Energy= 0.365371
Thermal correction to Enthalpy= 0.366315
Thermal correction to Gibbs Free Energy= 0.294640
Sum of electronic and zero-point Energies= -878.137427
Sum of electronic and thermal Energies= -878.116541
Sum of electronic and thermal Enthalpies= -878.115596
Sum of electronic and thermal Free Energies= -878.187271

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.856958	1.548876	-0.151009
2	6	0	-0.328122	0.369558	-1.583246
3	6	0	0.748143	-0.375660	-1.211632
4	7	0	1.474948	0.383301	-0.319769
5	1	0	1.144870	2.324504	0.543515
6	1	0	-1.179863	0.126293	-2.200651
7	1	0	1.023629	-1.391240	-1.447569
8	7	0	-0.236969	1.568443	-0.912173
9	6	0	2.699327	-0.047749	0.368125
10	6	0	3.897058	-0.075492	-0.574368
11	1	0	2.484317	-1.029287	0.802239

12	1	0	2.858123	0.652849	1.193001
13	6	0	5.169428	-0.500284	0.157912
14	1	0	3.697341	-0.772929	-1.398197
15	1	0	4.036090	0.916923	-1.022622
16	1	0	5.366103	0.201407	0.978051
17	1	0	5.010302	-1.482042	0.619491
18	6	0	-1.205346	2.663360	-0.955376
19	1	0	-0.884165	3.415230	-1.678460
20	1	0	-2.170321	2.244746	-1.241394
21	1	0	-1.284585	3.087597	0.047399
22	6	0	6.377563	-0.554800	-0.774324
23	1	0	6.564473	0.422446	-1.231110
24	1	0	7.280466	-0.851699	-0.235116
25	1	0	6.216069	-1.276645	-1.581245
26	6	0	-2.462532	-1.800678	-0.118946
27	6	0	-2.362729	-0.598807	0.613643
28	6	0	-3.350718	0.381834	0.388082
29	6	0	-4.360533	0.183506	-0.549675
30	6	0	-4.429470	-0.997811	-1.289850
31	6	0	-3.475421	-1.990507	-1.052133
32	1	0	-1.728104	-2.584312	0.049111
33	1	0	-3.324859	1.301589	0.968267
34	1	0	-5.110217	0.957450	-0.693560
35	1	0	-3.522114	-2.928184	-1.599454
36	6	0	-1.248725	-0.356232	1.518588
37	6	0	-0.231797	-1.315469	1.670857
38	7	0	0.618421	-2.116957	1.725244
39	6	0	-1.028172	0.925884	2.045440
40	7	0	-0.834609	2.030792	2.382858
41	1	0	-5.219551	-1.150925	-2.017342

Zero-point correction=	0.344485 (Hartree/Particle)
Thermal correction to Energy=	0.365634
Thermal correction to Enthalpy=	0.366578
Thermal correction to Gibbs Free Energy=	0.292922
Sum of electronic and zero-point Energies=	-878.134318
Sum of electronic and thermal Energies=	-878.113170
Sum of electronic and thermal Enthalpies=	-878.112226
Sum of electronic and thermal Free Energies=	-878.185882

Conformer 4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	2.754454	0.203438	0.666873
2	6	0	3.650337	0.397532	-1.332153
3	6	0	2.716054	1.377182	-1.192924
4	7	0	2.171396	1.236578	0.063635
5	1	0	2.483453	-0.171799	1.646866
6	1	0	4.275658	0.128459	-2.167813
7	1	0	2.384197	2.140508	-1.877569
8	7	0	3.666947	-0.312857	-0.155426
9	6	0	1.061040	2.022660	0.629534
10	6	0	-0.138101	2.060346	-0.314195
11	1	0	1.436024	3.027060	0.850250
12	1	0	0.795481	1.531578	1.570099
13	6	0	-1.399040	2.497224	0.430449
14	1	0	0.056618	2.744161	-1.151441
15	1	0	-0.295586	1.057905	-0.728531
16	1	0	-1.578119	1.788693	1.248777
17	1	0	-1.240522	3.483984	0.886434
18	6	0	4.352653	-1.585518	0.052034
19	1	0	3.799902	-2.357133	-0.488918
20	1	0	5.377102	-1.501099	-0.310752
21	1	0	4.358868	-1.808748	1.118489
22	6	0	-2.616867	2.526425	-0.488314
23	1	0	-2.789242	1.537417	-0.925831
24	1	0	-3.518479	2.807025	0.062570
25	1	0	-2.478263	3.246407	-1.302585
26	6	0	-2.772264	-0.758640	1.058060
27	6	0	-1.791349	-1.130474	0.118550
28	6	0	-2.198153	-1.314826	-1.216566
29	6	0	-3.527379	-1.138726	-1.589346
30	6	0	-4.489900	-0.767055	-0.650826
31	6	0	-4.096912	-0.579944	0.675636
32	1	0	-2.486098	-0.622127	2.098388
33	1	0	-1.462155	-1.609916	-1.960608
34	1	0	-3.811599	-1.294522	-2.626407
35	1	0	-4.831069	-0.295080	1.424430
36	6	0	-0.397410	-1.302547	0.511496
37	6	0	0.061765	-0.987127	1.798443
38	7	0	0.507259	-0.676130	2.837303
39	6	0	0.591751	-1.694878	-0.406507
40	7	0	1.437967	-1.983785	-1.162989
41	1	0	-5.525239	-0.629858	-0.944976

Zero-point correction= 0.344256 (Hartree/Particle)

Thermal correction to Energy=	0.365225
Thermal correction to Enthalpy=	0.366169
Thermal correction to Gibbs Free Energy=	0.294092
Sum of electronic and zero-point Energies=	-878.136341
Sum of electronic and thermal Energies=	-878.115372
Sum of electronic and thermal Enthalpies=	-878.114428
Sum of electronic and thermal Free Energies=	-878.186504

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.816751	-2.036921	-0.142651
2	6	0	0.005435	-0.337357	-1.276701
3	7	0	-0.978379	-0.704591	-0.457738
4	1	0	-1.460085	-2.530637	0.568288
5	1	0	0.178601	0.666567	-1.643918
6	6	0	-2.026816	0.167876	0.084998
7	6	0	-3.404537	-0.191737	-0.458641
8	1	0	-1.747748	1.193053	-0.174333
9	1	0	-1.979394	0.067236	1.174432
10	6	0	-4.482940	0.716712	0.130792
11	1	0	-3.400928	-0.111464	-1.553404
12	1	0	-3.633629	-1.237123	-0.215144
13	1	0	-4.459358	0.639521	1.224471
14	1	0	-4.250214	1.760887	-0.113227
15	6	0	-5.877183	0.365774	-0.382578
16	1	0	-6.142184	-0.663604	-0.121049
17	1	0	-6.634482	1.026189	0.047040
18	1	0	-5.929436	0.458914	-1.472169
19	6	0	0.769435	1.920673	1.007872
20	6	0	1.736688	0.908259	0.814546
21	6	0	2.742615	1.156431	-0.146972
22	6	0	2.733670	2.314307	-0.917785
23	6	0	1.736101	3.279603	-0.756476
24	6	0	0.769002	3.074970	0.231495
25	1	0	0.010582	1.783948	1.774607
26	1	0	3.532045	0.421632	-0.284974
27	1	0	3.522213	2.468981	-1.649984
28	1	0	0.006507	3.830070	0.405811
29	6	0	1.644621	-0.368001	1.498727
30	6	0	0.528103	-0.653029	2.305884
31	7	0	-0.456624	-0.844110	2.906774

32	6	0	2.498112	-1.422002	1.125102
33	7	0	3.196107	-2.265700	0.714753
34	6	0	0.290646	-2.469594	-0.801374
35	1	0	0.807375	-3.415922	-0.783282
36	7	0	0.783779	-1.393691	-1.508021
37	6	0	2.007785	-1.405448	-2.306666
38	1	0	2.811842	-1.806124	-1.685053
39	1	0	1.855066	-2.020687	-3.195048
40	1	0	2.241280	-0.380119	-2.592877
41	1	0	1.733838	4.182231	-1.358000

Zero-point correction= 0.344835 (Hartree/Particle)
Thermal correction to Energy= 0.365754
Thermal correction to Enthalpy= 0.366699
Thermal correction to Gibbs Free Energy= 0.294547
Sum of electronic and zero-point Energies= -878.136482
Sum of electronic and thermal Energies= -878.115563
Sum of electronic and thermal Enthalpies= -878.114619
Sum of electronic and thermal Free Energies= -878.186770

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.439246	-2.006117	-0.040194
2	6	0	0.777918	-1.346882	-1.751064
3	6	0	-0.112087	-0.358459	-1.461944
4	7	0	-0.862375	-0.793503	-0.393480
5	1	0	-0.793425	-2.561572	0.816153
6	1	0	1.583268	-1.392115	-2.466627
7	1	0	-0.229706	0.633177	-1.873856
8	7	0	0.549924	-2.368177	-0.853590
9	6	0	-1.935660	-0.048781	0.276191
10	6	0	-3.297049	-0.328868	-0.350611
11	1	0	-1.667603	1.008930	0.202895
12	1	0	-1.896872	-0.326480	1.334293
13	6	0	-4.404450	0.458183	0.348904
14	1	0	-3.269055	-0.066735	-1.416347
15	1	0	-3.512004	-1.404041	-0.291514
16	1	0	-4.421320	0.190590	1.412408
17	1	0	-4.172192	1.529309	0.301097
18	6	0	1.323116	-3.606800	-0.766160
19	1	0	1.035571	-4.127221	0.147051

20	1	0	1.106876	-4.230157	-1.635080
21	1	0	2.381195	-3.342819	-0.711207
22	6	0	-5.774887	0.199331	-0.272574
23	1	0	-6.036489	-0.862180	-0.215332
24	1	0	-6.556372	0.764611	0.241096
25	1	0	-5.787375	0.490810	-1.327711
26	6	0	0.636337	2.135132	0.969160
27	6	0	1.668459	1.273615	0.544438
28	6	0	2.442064	1.684608	-0.562166
29	6	0	2.164874	2.871644	-1.230270
30	6	0	1.115068	3.698514	-0.822350
31	6	0	0.364265	3.320897	0.292058
32	1	0	0.051638	1.866381	1.846172
33	1	0	3.261763	1.054203	-0.897434
34	1	0	2.779299	3.156771	-2.080010
35	1	0	-0.436482	3.963853	0.648905
36	6	0	1.885024	-0.018659	1.177431
37	6	0	0.967070	-0.516950	2.115806
38	7	0	0.129135	-0.931605	2.821265
39	6	0	2.861008	-0.900604	0.680696
40	7	0	3.643933	-1.625239	0.200908
41	1	0	0.904023	4.625530	-1.344770

Zero-point correction= 0.344485 (Hartree/Particle)
Thermal correction to Energy= 0.365641
Thermal correction to Enthalpy= 0.366585
Thermal correction to Gibbs Free Energy= 0.293039
Sum of electronic and zero-point Energies= -878.134578
Sum of electronic and thermal Energies= -878.113423
Sum of electronic and thermal Enthalpies= -878.112478
Sum of electronic and thermal Free Energies= -878.186024

9-CF_3SO_2Fl
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.985935	-1.532540	0.205386
2	6	0	3.128291	-2.511283	-0.301067
3	6	0	1.815687	-2.193636	-0.658741
4	6	0	1.396651	-0.880111	-0.502546
5	6	0	2.251485	0.107520	0.009179
6	6	0	3.557040	-0.214583	0.364997

7	1	0	5.001613	-1.801188	0.478302
8	1	0	3.483525	-3.529995	-0.415766
9	1	0	1.138342	-2.952702	-1.036273
10	1	0	4.231371	0.540062	0.758392
11	6	0	0.036940	-0.269354	-0.784908
12	1	0	-0.363123	-0.489454	-1.779176
13	6	0	0.237466	1.196452	-0.477567
14	6	0	-0.626846	2.267834	-0.655864
15	6	0	-0.192437	3.543341	-0.287345
16	6	0	1.085995	3.735752	0.238917
17	6	0	1.964308	2.663003	0.391935
18	6	0	1.534789	1.392193	0.026112
19	1	0	-1.617146	2.133304	-1.078531
20	1	0	-0.855843	4.392128	-0.416417
21	1	0	1.404014	4.734468	0.520736
22	1	0	2.965261	2.820928	0.781954
23	16	0	-1.107935	-1.105194	0.370167
24	8	0	-1.256216	-2.481120	-0.081775
25	8	0	-0.795581	-0.767767	1.745352
26	6	0	-2.770981	-0.326959	0.005930
27	9	0	-2.935283	0.801742	0.680800
28	9	0	-3.719909	-1.183108	0.346306
29	9	0	-2.863987	-0.067426	-1.303886

Zero-point correction=	0.205535 (Hartree/Particle)
Thermal correction to Energy=	0.221270
Thermal correction to Enthalpy=	0.222214
Thermal correction to Gibbs Free Energy=	0.161894
Sum of electronic and zero-point Energies=	-1386.441032
Sum of electronic and thermal Energies=	-1386.425297
Sum of electronic and thermal Enthalpies=	-1386.424353
Sum of electronic and thermal Free Energies=	-1386.484674

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.458483	-1.820014	0.438714
2	6	0	2.616499	-2.687708	-0.260296
3	6	0	1.437119	-2.221153	-0.845732
4	6	0	1.127733	-0.875824	-0.709897
5	6	0	1.968633	0.001797	-0.007158
6	6	0	3.143497	-0.467279	0.571273

7	1	0	4.370617	-2.203942	0.884655
8	1	0	2.879101	-3.736861	-0.347853
9	1	0	0.770010	-2.894045	-1.374710
10	1	0	3.802540	0.201378	1.117059
11	6	0	-0.064548	-0.107951	-1.233807
12	1	0	-0.185747	-0.182718	-2.323451
13	6	0	0.175067	1.307381	-0.755648
14	6	0	-0.596574	2.444691	-0.947244
15	6	0	-0.144901	3.645960	-0.396928
16	6	0	1.052007	3.696539	0.322327
17	6	0	1.824376	2.550899	0.510735
18	6	0	1.377395	1.349873	-0.032052
19	1	0	-1.534213	2.393281	-1.491902
20	1	0	-0.731096	4.549580	-0.528436
21	1	0	1.385123	4.641496	0.739928
22	1	0	2.753860	2.597958	1.070067
23	16	0	-1.665749	-0.771841	-0.694075
24	8	0	-2.718102	0.095298	-1.202756
25	8	0	-1.687458	-2.209486	-0.914752
26	6	0	-1.680105	-0.549493	1.163938
27	9	0	-0.567213	-1.039791	1.699635
28	9	0	-2.725224	-1.215081	1.635775
29	9	0	-1.794432	0.731597	1.485763

Zero-point correction= 0.205188 (Hartree/Particle)
Thermal correction to Energy= 0.220970
Thermal correction to Enthalpy= 0.221914
Thermal correction to Gibbs Free Energy= 0.161262
Sum of electronic and zero-point Energies= -1386.445098
Sum of electronic and thermal Energies= -1386.429316
Sum of electronic and thermal Enthalpies= -1386.428372
Sum of electronic and thermal Free Energies= -1386.489024

The conjugate base anion of 9-CF_3SO_2Fl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.835819	-3.008325	0.281339
2	6	0	-1.547796	-3.446669	-0.079010
3	6	0	-0.531639	-2.548782	-0.375072
4	6	0	-0.798816	-1.169528	-0.306728
5	6	0	-2.102091	-0.725023	0.065888
6	6	0	-3.112166	-1.648665	0.352490

7	1	0	-3.612673	-3.735363	0.501568
8	1	0	-1.344176	-4.513437	-0.130647
9	1	0	0.455928	-2.893555	-0.663253
10	1	0	-4.105564	-1.303779	0.632119
11	6	0	0.005590	-0.000058	-0.561024
12	6	0	-0.798609	1.169563	-0.306778
13	6	0	-0.531175	2.548765	-0.375159
14	6	0	-1.547163	3.446847	-0.079109
15	6	0	-2.835265	3.008748	0.281261
16	6	0	-3.111864	1.649141	0.352448
17	6	0	-2.101962	0.725306	0.065861
18	1	0	0.456458	2.893344	-0.663350
19	1	0	-1.343348	4.513577	-0.130768
20	1	0	-3.611983	3.735934	0.501481
21	1	0	-4.105322	1.304445	0.632097
22	16	0	1.655953	-0.000207	-0.839951
23	8	0	2.124465	-1.273017	-1.395429
24	8	0	2.124673	1.272391	-1.395740
25	6	0	2.485877	-0.000059	0.834892
26	9	0	3.820893	-0.000510	0.713154
27	9	0	2.139196	-1.081895	1.542672
28	9	0	2.139878	1.082360	1.542121

Zero-point correction= 0.191528 (Hartree/Particle)
Thermal correction to Energy= 0.207319
Thermal correction to Enthalpy= 0.208263
Thermal correction to Gibbs Free Energy= 0.146689
Sum of electronic and zero-point Energies= -1385.941250
Sum of electronic and thermal Energies= -1385.925458
Sum of electronic and thermal Enthalpies= -1385.924514
Sum of electronic and thermal Free Energies= -1385.986089

Complexes formed from a [Bmim] cation and the conjugate base anion of 9-CF_3SO_2Fl

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.329142	-2.018988	3.420754
2	6	0	1.019595	-0.810480	3.207202
3	6	0	0.639128	0.075647	2.208440
4	6	0	-0.452852	-0.251679	1.383856
5	6	0	-1.181087	-1.454947	1.629688

6	6	0	−0.778889	−2.334075	2.642653
7	1	0	0.648045	−2.690084	4.211956
8	1	0	1.861735	−0.559547	3.846694
9	1	0	1.173148	1.009099	2.058628
10	1	0	−1.332428	−3.252606	2.824545
11	6	0	−1.033809	0.381525	0.228365
12	6	0	−2.156684	−0.408489	−0.210314
13	6	0	−3.062828	−0.278717	−1.279936
14	6	0	−4.041389	−1.249775	−1.452654
15	6	0	−4.146856	−2.353967	−0.583794
16	6	0	−3.256858	−2.494914	0.472586
17	6	0	−2.254379	−1.536108	0.658720
18	1	0	−2.996492	0.573368	−1.948368
19	1	0	−4.750286	−1.147556	−2.269411
20	1	0	−4.932409	−3.087246	−0.736347
21	1	0	−3.337436	−3.342640	1.149415
22	16	0	−0.493619	1.804386	−0.479029
23	8	0	0.925563	2.048123	−0.169457
24	8	0	−0.965238	1.944082	−1.859931
25	6	0	−1.330324	3.215000	0.400581
26	6	0	1.136681	−1.880985	−0.633310
27	6	0	1.493152	−0.262597	−2.081158
28	6	0	0.448422	−1.007440	−2.532456
29	7	0	0.251150	−2.019433	−1.619504
30	1	0	1.186205	−2.488662	0.260847
31	1	0	1.919743	0.654354	−2.455383
32	1	0	−0.202382	−0.871679	−3.381560
33	7	0	1.912511	−0.831502	−0.899684
34	6	0	−0.763985	−3.066320	−1.725201
35	1	0	−1.734726	−2.602217	−1.911199
36	1	0	−0.810631	−3.601137	−0.777025
37	6	0	2.991222	−0.318807	−0.046548
38	1	0	2.735035	0.720096	0.182052
39	1	0	2.952173	−0.889892	0.884941
40	9	0	−0.918797	4.385051	−0.085369
41	9	0	−2.652020	3.129659	0.250493
42	9	0	−1.047293	3.169720	1.704030
43	1	0	−0.493710	−3.746757	−2.534935
44	6	0	4.352719	−0.444234	−0.720068
45	6	0	5.466588	0.073229	0.189538
46	1	0	4.354076	0.123137	−1.659482
47	1	0	4.538740	−1.494540	−0.979565
48	6	0	6.841784	−0.032602	−0.465343
49	1	0	5.260123	1.117241	0.454212

50	1	0	5.459416	-0.494165	1.128646
51	1	0	7.626199	0.338462	0.198968
52	1	0	7.077464	-1.071966	-0.715941
53	1	0	6.880080	0.552123	-1.389803

Zero-point correction= 0.422769 (Hartree/Particle)
Thermal correction to Energy= 0.450427
Thermal correction to Enthalpy= 0.451371
Thermal correction to Gibbs Free Energy= 0.363905
Sum of electronic and zero-point Energies= -1808.846827
Sum of electronic and thermal Energies= -1808.819169
Sum of electronic and thermal Enthalpies= -1808.818225
Sum of electronic and thermal Free Energies= -1808.905691

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.149653	-0.888769	3.233093
2	6	0	-1.722967	-2.018167	2.507303
3	6	0	-0.672654	-1.943819	1.603716
4	6	0	-0.030294	-0.708036	1.407830
5	6	0	-0.437190	0.427102	2.167270
6	6	0	-1.501852	0.330062	3.071733
7	1	0	-2.972010	-0.978922	3.935892
8	1	0	-2.224934	-2.969313	2.660381
9	1	0	-0.364954	-2.817635	1.037901
10	1	0	-1.813482	1.198024	3.648428
11	6	0	1.020249	-0.280002	0.516417
12	6	0	1.288993	1.116247	0.760620
13	6	0	2.194435	2.032290	0.196789
14	6	0	2.162012	3.356429	0.615330
15	6	0	1.251875	3.794894	1.595504
16	6	0	0.372141	2.892647	2.181834
17	6	0	0.385067	1.555699	1.772907
18	1	0	2.909425	1.700521	-0.549565
19	1	0	2.870112	4.065234	0.193143
20	1	0	1.259303	4.833259	1.912790
21	1	0	-0.317669	3.223745	2.954925
22	16	0	1.591232	-1.173221	-0.777876
23	8	0	0.609728	-2.177516	-1.214623
24	8	0	2.210238	-0.307073	-1.796662
25	6	0	3.019163	-2.213039	-0.199781

26	6	0	-0.693502	0.830642	-1.928985
27	6	0	-0.830279	2.899897	-1.188157
28	6	0	-1.778622	2.159256	-0.552619
29	7	0	-1.678398	0.874108	-1.033787
30	1	0	-0.354646	-0.057110	-2.446201
31	1	0	-0.528953	3.927019	-1.057961
32	1	0	-2.471809	2.416519	0.232802
33	7	0	-0.166038	2.049255	-2.044856
34	6	0	-2.480352	-0.278222	-0.598137
35	6	0	-3.850582	-0.310416	-1.262652
36	1	0	-2.564596	-0.214030	0.491634
37	1	0	-1.891248	-1.171817	-0.826385
38	6	0	-4.667934	-1.497378	-0.754081
39	1	0	-4.385304	0.625506	-1.051932
40	1	0	-3.732344	-0.374329	-2.352243
41	1	0	-4.121916	-2.425553	-0.962580
42	1	0	-4.756501	-1.430121	0.337488
43	6	0	0.976730	2.395008	-2.890088
44	1	0	0.628463	2.707014	-3.876328
45	1	0	1.516567	3.206774	-2.402450
46	1	0	1.627310	1.521052	-2.951581
47	6	0	-6.055666	-1.557454	-1.387522
48	1	0	-5.985419	-1.646813	-2.476451
49	1	0	-6.623874	-2.414565	-1.017352
50	1	0	-6.628564	-0.652086	-1.161932
51	9	0	2.624012	-3.014307	0.790360
52	9	0	3.489593	-2.961005	-1.195548
53	9	0	4.000168	-1.431011	0.250125

Zero-point correction= 0.422695 (Hartree/Particle)
Thermal correction to Energy= 0.450405
Thermal correction to Enthalpy= 0.451349
Thermal correction to Gibbs Free Energy= 0.364040
Sum of electronic and zero-point Energies= -1808.847699
Sum of electronic and thermal Energies= -1808.819989
Sum of electronic and thermal Enthalpies= -1808.819045
Sum of electronic and thermal Free Energies= -1808.906354

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.177064	2.533471	3.184687

2	6	0	−0.929470	2.884945	2.387051
3	6	0	−1.446867	2.011743	1.439007
4	6	0	−0.839609	0.754389	1.263820
5	6	0	0.251606	0.379187	2.106188
6	6	0	0.756530	1.276579	3.055033
7	1	0	0.558934	3.236880	3.917773
8	1	0	−1.396225	3.856654	2.525514
9	1	0	−2.303897	2.288957	0.833072
10	1	0	1.595042	0.992334	3.686950
11	6	0	−1.040467	−0.309133	0.314986
12	6	0	−0.091610	−1.357201	0.595098
13	6	0	0.194761	−2.581110	−0.038909
14	6	0	1.229019	−3.365520	0.453517
15	6	0	1.987957	−2.968175	1.572839
16	6	0	1.716039	−1.762531	2.205578
17	6	0	0.690555	−0.945524	1.714426
18	1	0	−0.388983	−2.898012	−0.896903
19	1	0	1.449112	−4.314452	−0.027388
20	1	0	2.778336	−3.612957	1.944274
21	1	0	2.300047	−1.452109	3.069397
22	16	0	−2.181692	−0.328880	−0.915387
23	8	0	−2.610731	1.033981	−1.272483
24	8	0	−1.823913	−1.273815	−1.977275
25	6	0	−3.742452	−1.058302	−0.211215
26	6	0	1.179250	1.867025	−0.665369
27	6	0	0.195064	1.255493	−2.538050
28	6	0	1.130377	0.318129	−2.227976
29	7	0	1.738565	0.724796	−1.061613
30	1	0	1.405447	2.397128	0.251426
31	1	0	−0.543332	1.288283	−3.323392
32	1	0	1.370051	−0.623472	−2.696292
33	7	0	0.251798	2.218830	−1.555571
34	6	0	2.833226	0.018394	−0.385544
35	6	0	4.166161	0.221852	−1.095122
36	1	0	2.556087	−1.039817	−0.340028
37	1	0	2.861275	0.388994	0.642700
38	6	0	5.284686	−0.535019	−0.379483
39	1	0	4.088143	−0.127893	−2.132868
40	1	0	4.402381	1.293315	−1.135634
41	1	0	5.346959	−0.188608	0.659796
42	1	0	5.026029	−1.600122	−0.334452
43	6	0	−0.616209	3.391084	−1.471740
44	1	0	−0.395734	4.061048	−2.304423
45	1	0	−1.650316	3.045579	−1.503885

46	1	0	-0.426952	3.890844	-0.521948
47	6	0	6.635718	-0.354398	-1.067404
48	1	0	6.922090	0.701909	-1.097429
49	1	0	7.424130	-0.900333	-0.543386
50	1	0	6.601524	-0.721128	-2.098265
51	9	0	-4.700408	-1.100946	-1.135784
52	9	0	-3.513578	-2.296805	0.224946
53	9	0	-4.170062	-0.317797	0.813218

Zero-point correction= 0.422947 (Hartree/Particle)
Thermal correction to Energy= 0.450548
Thermal correction to Enthalpy= 0.451492
Thermal correction to Gibbs Free Energy= 0.364797
Sum of electronic and zero-point Energies= -1808.847514
Sum of electronic and thermal Energies= -1808.819914
Sum of electronic and thermal Enthalpies= -1808.818969
Sum of electronic and thermal Free Energies= -1808.905664

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.687555	-2.840306	-0.796856
2	6	0	3.768918	-1.629447	-1.508569
3	6	0	2.969474	-0.540641	-1.181358
4	6	0	2.056222	-0.661042	-0.119850
5	6	0	1.993427	-1.878912	0.618982
6	6	0	2.807054	-2.961967	0.271941
7	1	0	4.327933	-3.672340	-1.072040
8	1	0	4.482236	-1.538610	-2.323369
9	1	0	3.043942	0.391848	-1.732500
10	1	0	2.753298	-3.890843	0.834822
11	6	0	1.050257	0.224036	0.417449
12	6	0	0.388477	-0.444912	1.512570
13	6	0	-0.656186	-0.067221	2.373678
14	6	0	-1.128525	-0.987064	3.301942
15	6	0	-0.579153	-2.278377	3.401529
16	6	0	0.471476	-2.654421	2.572790
17	6	0	0.962780	-1.744490	1.630818
18	1	0	-1.084941	0.928187	2.307637
19	1	0	-1.932971	-0.698124	3.973033
20	1	0	-0.965717	-2.973734	4.139941
21	1	0	0.910138	-3.645742	2.659048

22	16	0	0.637682	1.722492	-0.195971
23	8	0	1.060737	1.877676	-1.598266
24	8	0	-0.739852	2.096355	0.166501
25	6	0	1.645046	3.023120	0.672493
26	6	0	-0.260229	-2.004502	-1.700092
27	6	0	-1.306628	-0.083710	-1.946032
28	1	0	0.507315	-2.744161	-1.873017
29	1	0	-1.554595	0.913249	-2.280304
30	7	0	-0.337506	-0.850467	-2.445489
31	6	0	0.537427	-0.487065	-3.559190
32	1	0	0.051777	-0.729173	-4.506206
33	1	0	0.760604	0.577036	-3.480791
34	1	0	1.465042	-1.048814	-3.449909
35	6	0	-2.945341	-0.176938	-0.079463
36	6	0	-4.296208	-0.237105	-0.783780
37	1	0	-2.656289	0.845038	0.186192
38	1	0	-2.944491	-0.770993	0.837929
39	6	0	-5.412834	0.297613	0.111880
40	1	0	-4.255190	0.351885	-1.709710
41	1	0	-4.512211	-1.273720	-1.073199
42	6	0	-6.774958	0.253711	-0.576326
43	1	0	-5.446013	-0.290730	1.037262
44	1	0	-5.177657	1.327739	0.405828
45	1	0	-7.561912	0.636798	0.078080
46	1	0	-6.772446	0.859533	-1.488064
47	1	0	-7.039556	-0.771227	-0.855752
48	6	0	-1.223527	-1.922072	-0.740032
49	1	0	-1.457653	-2.573385	0.088650
50	7	0	-1.866161	-0.718204	-0.917021
51	9	0	2.943707	2.824536	0.445532
52	9	0	1.427750	2.961334	1.986713
53	9	0	1.316085	4.239589	0.240702

Zero-point correction= 0.422651 (Hartree/Particle)
Thermal correction to Energy= 0.450570
Thermal correction to Enthalpy= 0.451514
Thermal correction to Gibbs Free Energy= 0.362787
Sum of electronic and zero-point Energies= -1808.847339
Sum of electronic and thermal Energies= -1808.819420
Sum of electronic and thermal Enthalpies= -1808.818476
Sum of electronic and thermal Free Energies= -1808.907203

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.068333	-2.403291	-0.962754
2	6	0	4.129717	-1.109557	-1.515348
3	6	0	3.245603	-0.113463	-1.126144
4	6	0	2.266929	-0.411210	-0.161468
5	6	0	2.229124	-1.708147	0.426899
6	6	0	3.125385	-2.701077	0.013382
7	1	0	4.773713	-3.161664	-1.287781
8	1	0	4.887241	-0.886561	-2.261253
9	1	0	3.295472	0.875365	-1.571108
10	1	0	3.090382	-3.692813	0.458799
11	6	0	1.186747	0.357063	0.409484
12	6	0	0.506834	-0.462588	1.384351
13	6	0	-0.597974	-0.238319	2.224597
14	6	0	-1.062995	-1.279399	3.018132
15	6	0	-0.447372	-2.545071	3.005588
16	6	0	0.662633	-2.770509	2.200269
17	6	0	1.145200	-1.738206	1.390672
18	1	0	-1.075277	0.736475	2.249214
19	1	0	-1.908734	-1.106149	3.679101
20	1	0	-0.824676	-3.335102	3.647740
21	1	0	1.153639	-3.741203	2.202100
22	16	0	0.603732	1.790141	-0.225685
23	8	0	0.925891	1.921596	-1.656369
24	8	0	-0.782940	2.040732	0.203553
25	6	0	1.536929	3.207401	0.532591
26	6	0	-1.239054	-0.516360	-1.504469
27	6	0	-1.804620	-2.264337	-0.291725
28	6	0	-0.743750	-2.615326	-1.068906
29	7	0	-0.411708	-1.511977	-1.820689
30	1	0	-1.191644	0.488049	-1.903639
31	1	0	-2.322567	-2.804526	0.485024
32	1	0	-0.164060	-3.523840	-1.110546
33	7	0	-2.095147	-0.949586	-0.580259
34	6	0	0.693293	-1.414880	-2.776836
35	1	0	1.542840	-1.977657	-2.383990
36	1	0	0.978236	-0.364212	-2.858528
37	6	0	-3.147323	-0.138354	0.044259
38	1	0	-3.303945	-0.558901	1.041584
39	1	0	-2.736241	0.867973	0.165837
40	9	0	2.836702	3.093033	0.256211
41	9	0	1.097381	4.370265	0.055961

42	9	0	1.380000	3.199411	1.855910
43	1	0	0.375334	-1.813219	-3.742263
44	6	0	-4.432686	-0.147317	-0.776421
45	6	0	-5.536923	0.656694	-0.091694
46	1	0	-4.764015	-1.183119	-0.928130
47	1	0	-4.231362	0.273360	-1.770277
48	6	0	-6.827525	0.672057	-0.907659
49	1	0	-5.731616	0.231050	0.900750
50	1	0	-5.187756	1.683344	0.072130
51	1	0	-7.609416	1.244614	-0.402608
52	1	0	-6.662925	1.123719	-1.891030
53	1	0	-7.203734	-0.344133	-1.064531

Zero-point correction= 0.422008
(Hartree/Particle)
Thermal correction to Energy= 0.449847
Thermal correction to Enthalpy= 0.450791
Thermal correction to Gibbs Free Energy= 0.362552
Sum of electronic and zero-point Energies= -1808.847600
Sum of electronic and thermal Energies= -1808.819760
Sum of electronic and thermal Enthalpies= -1808.818816
Sum of electronic and thermal Free Energies= -1808.907055

p-MeOPhCH(CN)$_2$.

1	6	0	0.026895	-1.313021	-0.486638
2	6	0	0.670748	-0.083425	-0.299163
3	6	0	-0.082751	1.038947	0.014058
4	6	0	-1.471877	0.952264	0.139018
5	6	0	-2.106978	-0.274706	-0.051411
6	6	0	-1.346878	-1.411044	-0.365035
7	1	0	0.607298	-2.202602	-0.718653
8	1	0	0.399660	1.999556	0.168220
9	1	0	-2.033235	1.844285	0.387540
10	1	0	-1.859651	-2.356539	-0.503458
11	6	0	2.189142	-0.018476	-0.484526
12	6	0	2.750877	1.305528	-0.167945
13	7	0	3.169578	2.357778	0.055565
14	6	0	2.876921	-1.055136	0.311007
15	7	0	3.391801	-1.901249	0.904334
16	1	0	2.433182	-0.217987	-1.537009
17	8	0	-3.443487	-0.469728	0.047227
18	6	0	-4.254905	0.647351	0.357116
19	1	0	-4.167015	1.423123	-0.412276
20	1	0	-5.278128	0.275753	0.384770

21	1	0	-3.991017	1.066840	1.334863

Zero-point correction= 0.160410 (Hartree/Particle)
Thermal correction to Energy= 0.172128
Thermal correction to Enthalpy= 0.173072
Thermal correction to Gibbs Free Energy= 0.121000
Sum of electronic and zero-point Energies= -570.185358
Sum of electronic and thermal Energies= -570.173639
Sum of electronic and thermal Enthalpies= -570.172695
Sum of electronic and thermal Free Energies= -570.224767

The conjugate base anion of *p*-MeOPhCH(CN)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.033462	-1.204702	-0.152621
2	6	0	-0.703333	-0.000020	-0.086576
3	6	0	0.033532	1.204623	-0.152616
4	6	0	1.419087	1.202291	-0.266909
5	6	0	2.119729	-0.000098	-0.323573
6	6	0	1.419019	-1.202444	-0.266907
7	1	0	-0.501652	-2.149603	-0.114919
8	1	0	-0.501529	2.149554	-0.114915
9	1	0	1.970590	2.137922	-0.323666
10	1	0	1.970491	-2.138093	-0.323647
11	6	0	-2.147547	0.000025	0.039878
12	6	0	-2.860408	1.212242	0.107350
13	7	0	-3.408300	2.243998	0.160821
14	6	0	-2.860472	-1.212151	0.107428
15	7	0	-3.408430	-2.243869	0.160970
16	8	0	3.505644	-0.000162	-0.448937
17	6	0	4.163093	0.000193	0.801509
18	1	0	5.238035	0.000152	0.602037
19	1	0	3.899519	0.892032	1.385903
20	1	0	3.899528	-0.891336	1.386382

Zero-point correction= 0.146732 (Hartree/Particle)
Thermal correction to Energy= 0.158295
Thermal correction to Enthalpy= 0.159239
Thermal correction to Gibbs Free Energy= 0.108339
Sum of electronic and zero-point Energies= -569.679214
Sum of electronic and thermal Energies= -569.667651
Sum of electronic and thermal Enthalpies= -569.666706

Sum of electronic and thermal Free Energies= -569.717607

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-MeOPhCH(CN)$_2$

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.808597	1.448366	0.612069
2	6	0	-2.435274	1.266855	-1.490264
3	6	0	-1.081846	1.393367	-1.463270
4	7	0	-0.712909	1.510072	-0.140372
5	1	0	-1.839561	1.422699	1.692934
6	1	0	-3.116590	1.082850	-2.305604
7	1	0	-0.351149	1.370098	-2.255793
8	7	0	-2.868343	1.311542	-0.184948
9	6	0	0.672118	1.571762	0.342418
10	6	0	1.366333	2.871592	-0.041606
11	1	0	1.193506	0.703859	-0.073284
12	1	0	0.636966	1.442406	1.427248
13	6	0	2.815764	2.872390	0.445049
14	1	0	1.346826	2.991704	-1.132702
15	1	0	0.821595	3.723981	0.384097
16	1	0	2.829646	2.759040	1.536309
17	1	0	3.333409	1.995400	0.036708
18	6	0	-4.245340	1.086550	0.256988
19	1	0	-4.240134	0.939488	1.336845
20	1	0	-4.861430	1.943548	-0.018560
21	1	0	-4.607872	0.176868	-0.226314
22	6	0	3.556810	4.147210	0.049940
23	1	0	3.064843	5.032795	0.465193
24	1	0	4.586950	4.133792	0.414198
25	1	0	3.587950	4.260575	-1.038426
26	6	0	0.491745	-1.649222	1.298877
27	6	0	-0.354046	-1.716139	0.171646
28	6	0	0.261250	-1.776566	-1.097047
29	6	0	1.645858	-1.737915	-1.230398
30	6	0	2.460625	-1.645110	-0.101017
31	6	0	1.877300	-1.616157	1.163826
32	1	0	0.049474	-1.628481	2.291786
33	1	0	-0.363278	-1.852552	-1.984215
34	1	0	2.109294	-1.781103	-2.212520
35	1	0	2.517026	-1.562034	2.040704

36	6	0	-1.801882	-1.675441	0.314553
37	6	0	-2.374190	-1.320780	1.546631
38	7	0	-2.806984	-0.920273	2.558254
39	6	0	-2.664431	-1.741846	-0.794511
40	7	0	-3.383931	-1.729902	-1.716477
41	8	0	3.833291	-1.566510	-0.240723
42	6	0	4.469472	-2.837112	-0.220263
43	1	0	5.540106	-2.657335	-0.340568
44	1	0	4.285428	-3.349027	0.733129
45	1	0	4.105814	-3.467386	-1.042315

Zero-point correction= 0.376503 (Hartree/Particle)
Thermal correction to Energy= 0.400479
Thermal correction to Enthalpy= 0.401423
Thermal correction to Gibbs Free Energy= 0.321526
Sum of electronic and zero-point Energies= -992.582093
Sum of electronic and thermal Energies= -992.558117
Sum of electronic and thermal Enthalpies= -992.557173
Sum of electronic and thermal Free Energies= -992.637071

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.776315	-0.369127	-0.337720
2	1	0	-1.794975	-0.737361	-0.053631
3	6	0	-4.859529	-0.278992	-1.051850
4	1	0	-5.791647	-0.655711	-1.441566
5	6	0	-4.477198	0.980296	-0.701100
6	1	0	-5.015118	1.914438	-0.720082
7	7	0	-3.784045	-1.103856	-0.815810
8	7	0	-3.176593	0.901482	-0.261999
9	6	0	-3.743658	-2.546568	-1.076781
10	1	0	-3.673181	-2.713993	-2.152654
11	1	0	-2.877755	-2.972237	-0.562976
12	1	0	-4.658514	-2.992254	-0.685684
13	6	0	-2.363551	2.025802	0.246900
14	1	0	-2.953893	2.927171	0.061526
15	1	0	-2.235163	1.884620	1.324338
16	6	0	-0.456674	-0.185820	2.120843
17	7	0	-0.973762	0.639868	2.769532
18	6	0	0.151571	-1.125219	1.270706
19	6	0	-0.539411	-2.321709	1.033143

20	7	0	-1.158540	-3.279800	0.767897
21	6	0	-1.009571	2.113367	-0.445571
22	6	0	-0.186593	3.264889	0.131775
23	1	0	-1.157322	2.253108	-1.524864
24	1	0	-0.452748	1.177012	-0.305240
25	6	0	1.096591	3.498287	-0.661850
26	1	0	-0.790091	4.182766	0.136664
27	1	0	0.046388	3.034076	1.178452
28	1	0	1.704416	4.284742	-0.206384
29	1	0	1.698477	2.585502	-0.704418
30	1	0	0.869932	3.801159	-1.689589
31	6	0	1.447171	-0.851762	0.646025
32	6	0	2.007782	-1.746227	-0.284904
33	6	0	2.162676	0.322971	0.938855
34	6	0	3.226454	-1.476339	-0.896455
35	1	0	1.478065	-2.664097	-0.525945
36	6	0	3.384447	0.590964	0.327739
37	1	0	1.757862	1.027961	1.661740
38	6	0	3.918738	-0.304876	-0.594404
39	1	0	3.648928	-2.167530	-1.620360
40	1	0	3.930320	1.502761	0.555436
41	8	0	5.116932	-0.024213	-1.221055
42	6	0	6.243086	-0.527272	-0.520430
43	1	0	6.188260	-1.618910	-0.423485
44	1	0	7.125957	-0.255076	-1.101012
45	1	0	6.310838	-0.084300	0.481284

Zero-point correction= 0.376853 (Hartree/Particle)
Thermal correction to Energy= 0.400878
Thermal correction to Enthalpy= 0.401822
Thermal correction to Gibbs Free Energy= 0.320292
Sum of electronic and zero-point Energies= -992.574204
Sum of electronic and thermal Energies= -992.550179
Sum of electronic and thermal Enthalpies= -992.549235
Sum of electronic and thermal Free Energies= -992.630765

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.867034	1.470128	-0.341557
2	6	0	-0.316956	0.104813	-1.599145
3	6	0	0.759027	-0.582192	-1.127796

4	7	0	1.483842	0.291769	-0.346366
5	1	0	1.149488	2.331859	0.245338
6	1	0	-1.163711	-0.217452	-2.186207
7	1	0	1.037405	-1.619697	-1.223310
8	7	0	-0.226475	1.384570	-1.098247
9	6	0	2.704563	-0.041091	0.399624
10	6	0	3.921562	-0.130384	-0.513444
11	1	0	2.502154	-0.981634	0.920571
12	1	0	2.830337	0.735470	1.159589
13	6	0	5.184043	-0.470330	0.278162
14	1	0	3.748525	-0.898873	-1.277964
15	1	0	4.056038	0.821775	-1.043238
16	1	0	5.351892	0.300868	1.040146
17	1	0	5.029120	-1.411906	0.818414
18	6	0	-1.197183	2.461307	-1.288815
19	1	0	-0.907999	3.076399	-2.142831
20	1	0	-2.173777	2.007040	-1.456902
21	1	0	-1.232467	3.051636	-0.371376
22	6	0	6.413110	-0.583926	-0.620454
23	1	0	6.599099	0.355757	-1.150582
24	1	0	7.307232	-0.824767	-0.040215
25	1	0	6.277767	-1.370036	-1.370100
26	6	0	-2.519342	-1.783349	0.219250
27	6	0	-2.370998	-0.497543	0.779385
28	6	0	-3.348113	0.465180	0.457342
29	6	0	-4.400796	0.168623	-0.404952
30	6	0	-4.513156	-1.102504	-0.964658
31	6	0	-3.573321	-2.079646	-0.638488
32	1	0	-1.789640	-2.552567	0.459167
33	1	0	-3.278424	1.457420	0.897437
34	1	0	-5.145850	0.920967	-0.651355
35	1	0	-3.673210	-3.071112	-1.072093
36	6	0	-1.218341	-0.159323	1.606617
37	6	0	-0.218491	-1.113265	1.861189
38	7	0	0.617325	-1.919863	2.001615
39	6	0	-0.960114	1.176466	1.947266
40	7	0	-0.742120	2.314102	2.124426
41	8	0	-5.536557	-1.389448	-1.846123
42	6	0	-6.714559	-1.850266	-1.202249
43	1	0	-7.447231	-2.049913	-1.985840
44	1	0	-6.517118	-2.770878	-0.639058
45	1	0	-7.108093	-1.090466	-0.515524

Zero-point correction= 0.376774 (Hartree/Particle)

Thermal correction to Energy=	0.400780
Thermal correction to Enthalpy=	0.401724
Thermal correction to Gibbs Free Energy=	0.320931
Sum of electronic and zero-point Energies=	-992.579405
Sum of electronic and thermal Energies=	-992.555399
Sum of electronic and thermal Enthalpies=	-992.554455
Sum of electronic and thermal Free Energies=	-992.635248

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.987652	1.472362	1.032504
2	6	0	-0.310027	1.866417	-1.021547
3	6	0	-1.561995	1.338862	-1.086313
4	7	0	-1.971025	1.109065	0.207770
5	1	0	-0.992311	1.324951	2.104466
6	1	0	0.377763	2.160636	-1.797946
7	1	0	-2.163170	1.063586	-1.936180
8	7	0	0.027022	1.942892	0.311172
9	6	0	-3.190406	0.395179	0.641674
10	6	0	-4.220503	0.273844	-0.468440
11	1	0	-3.593390	0.945071	1.497364
12	1	0	-2.875195	-0.594314	0.985640
13	6	0	-5.480810	-0.424577	0.043784
14	1	0	-4.479908	1.269016	-0.854707
15	1	0	-3.793836	-0.317115	-1.287564
16	1	0	-5.205492	-1.407739	0.443541
17	1	0	-5.907975	0.147413	0.877358
18	6	0	1.325307	2.377970	0.822069
19	1	0	2.109043	1.843649	0.279931
20	1	0	1.427249	3.456666	0.691111
21	1	0	1.390027	2.116591	1.877694
22	6	0	-6.524932	-0.592308	-1.057359
23	1	0	-6.123731	-1.186095	-1.884334
24	1	0	-7.417789	-1.098400	-0.681562
25	1	0	-6.833078	0.379118	-1.457971
26	6	0	1.877604	-0.718512	-1.132272
27	6	0	1.411730	-0.997927	0.169820
28	6	0	2.315881	-0.811271	1.235577
29	6	0	3.612519	-0.355253	1.013020
30	6	0	4.042862	-0.063149	-0.279344
31	6	0	3.170145	-0.254824	-1.352223

32	1	0	1.205932	-0.863588	-1.975154
33	1	0	1.993101	-1.035506	2.249140
34	1	0	4.301337	-0.212567	1.841283
35	1	0	3.514706	-0.031980	-2.358827
36	6	0	0.037424	-1.415082	0.412117
37	6	0	-0.868889	-1.651232	-0.636968
38	7	0	-1.641871	-1.788660	-1.504375
39	6	0	-0.485041	-1.379672	1.715312
40	7	0	-0.916485	-1.239225	2.794788
41	8	0	5.314010	0.431339	-0.493844
42	6	0	6.259301	-0.576552	-0.820237
43	1	0	7.217324	-0.076615	-0.970430
44	1	0	6.347738	-1.305803	-0.005466
45	1	0	5.970986	-1.101845	-1.739175

Zero-point correction=	0.376456 (Hartree/Particle)
Thermal correction to Energy=	0.400404
Thermal correction to Enthalpy=	0.401349
Thermal correction to Gibbs Free Energy=	0.321645
Sum of electronic and zero-point Energies=	-992.580529
Sum of electronic and thermal Energies=	-992.556581
Sum of electronic and thermal Enthalpies=	-992.555637
Sum of electronic and thermal Free Energies=	-992.635340

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.068928	-1.726883	-0.413812
2	6	0	-0.465081	-0.483729	-1.269769
3	7	0	-1.567307	-0.447680	-0.523279
4	1	0	-2.920254	-1.948380	0.210130
5	1	0	0.180433	0.359212	-1.482541
6	6	0	-2.128272	0.738953	0.134268
7	6	0	-3.462703	1.148802	-0.478215
8	1	0	-1.382347	1.532957	0.037327
9	1	0	-2.224770	0.489200	1.196441
10	6	0	-4.031843	2.386610	0.213489
11	1	0	-3.328845	1.345323	-1.549840
12	1	0	-4.176318	0.319459	-0.391185
13	1	0	-4.143702	2.182223	1.285082
14	1	0	-3.314083	3.211844	0.125855
15	6	0	-5.375805	2.807967	-0.375914

16	1	0	-6.117936	2.010902	-0.265990
17	1	0	-5.765272	3.699040	0.122598
18	1	0	-5.281876	3.033769	-1.443055
19	6	0	1.070873	0.825545	1.356943
20	6	0	1.472639	-0.482013	1.005526
21	6	0	2.541956	-0.600129	0.090527
22	6	0	3.125186	0.521195	-0.492123
23	6	0	2.670677	1.800411	-0.172261
24	6	0	1.654006	1.945215	0.771996
25	1	0	0.280113	0.954858	2.091787
26	1	0	2.906802	-1.590701	-0.169816
27	1	0	3.937915	0.415431	-1.206364
28	1	0	1.323450	2.945538	1.040707
29	6	0	0.749042	-1.649862	1.481081
30	6	0	-0.435481	-1.483704	2.219806
31	7	0	-1.443043	-1.266270	2.772545
32	6	0	1.049628	-2.917642	0.953488
33	7	0	1.313365	-3.925158	0.421077
34	6	0	-1.242408	-2.539841	-1.123572
35	1	0	-1.228312	-3.611088	-1.246150
36	7	0	-0.252489	-1.741201	-1.655291
37	6	0	0.884163	-2.223349	-2.437334
38	1	0	1.365637	-3.025697	-1.873518
39	1	0	0.531133	-2.583097	-3.405164
40	1	0	1.583121	-1.398178	-2.573806
41	8	0	3.217670	2.908748	-0.787186
42	6	0	4.309721	3.465388	-0.069299
43	1	0	4.663173	4.322269	-0.644793
44	1	0	3.993448	3.796728	0.927495
45	1	0	5.119218	2.732947	0.037964

Zero-point correction=	0.377004 (Hartree/Particle)
Thermal correction to Energy=	0.400805
Thermal correction to Enthalpy=	0.401749
Thermal correction to Gibbs Free Energy=	0.322277
Sum of electronic and zero-point Energies=	-992.581455
Sum of electronic and thermal Energies=	-992.557655
Sum of electronic and thermal Enthalpies=	-992.556711
Sum of electronic and thermal Free Energies=	-992.636182

Conform 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.402113	0.058774	0.562910
2	6	0	4.185327	0.146792	-1.490157
3	6	0	3.328487	1.190715	-1.321429
4	7	0	2.853013	1.115528	-0.031579
5	1	0	3.166263	-0.275100	1.566747
6	1	0	4.741850	-0.180555	-2.353348
7	1	0	3.008395	1.959749	-2.005123
8	7	0	4.225529	-0.537083	-0.298403
9	6	0	1.830848	1.986006	0.577252
10	6	0	0.605044	2.120563	-0.320360
11	1	0	2.291920	2.957361	0.782499
12	1	0	1.561240	1.514695	1.527092
13	6	0	-0.576188	2.703871	0.453488
14	1	0	0.832713	2.757831	-1.185678
15	1	0	0.331337	1.128477	-0.697497
16	1	0	-0.784725	2.051884	1.311009
17	1	0	-0.309384	3.690641	0.855820
18	6	0	4.839976	-1.846718	-0.097993
19	1	0	4.222519	-2.589478	-0.608429
20	1	0	5.854694	-1.829457	-0.496085
21	1	0	4.868758	-2.058116	0.970462
22	6	0	-1.823557	2.804144	-0.419216
23	1	0	-2.096242	1.817460	-0.808328
24	1	0	-2.676428	3.182946	0.150118
25	1	0	-1.656806	3.475761	-1.268750
26	6	0	-2.120398	-0.424027	1.275237
27	6	0	-1.227336	-0.916765	0.304178
28	6	0	-1.718187	-1.100971	-1.001372
29	6	0	-3.043553	-0.816580	-1.319562
30	6	0	-3.908618	-0.327845	-0.344331
31	6	0	-3.441059	-0.130626	0.954369
32	1	0	-1.768907	-0.272817	2.293133
33	1	0	-1.051184	-1.479488	-1.771810
34	1	0	-3.417038	-0.958022	-2.329659
35	1	0	-4.118000	0.263438	1.707674
36	6	0	0.165947	-1.206433	0.633573
37	6	0	0.716953	-0.910619	1.887746
38	7	0	1.238799	-0.619539	2.896691
39	6	0	1.063075	-1.712774	-0.322112
40	7	0	1.835676	-2.096830	-1.114233
41	8	0	-5.210038	-0.009429	-0.677878
42	6	0	-6.145640	-1.007417	-0.303513
43	1	0	-7.129828	-0.650513	-0.611346

44	1	0	-5.923338	-1.957015	-0.806638
45	1	0	-6.138033	-1.169311	0.781594

Zero-point correction= 0.376557 (Hartree/Particle)
Thermal correction to Energy= 0.400463
Thermal correction to Enthalpy= 0.401407
Thermal correction to Gibbs Free Energy= 0.321744
Sum of electronic and zero-point Energies= -992.581180
Sum of electronic and thermal Energies= -992.557275
Sum of electronic and thermal Enthalpies= -992.556330
Sum of electronic and thermal Free Energies= -992.635993

p-ClPhCOCH$_2$CN.
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.056733	-0.093306	0.616830
2	6	0	3.103786	-1.262624	-0.263543
3	7	0	3.131803	-2.185200	-0.959011
4	8	0	2.366770	2.066188	-0.075185
5	6	0	0.568142	0.541459	0.128921
6	6	0	0.119588	-0.724277	0.519270
7	6	0	-0.355173	1.493039	-0.320728
8	6	0	-1.234148	-1.039268	0.463995
9	1	0	0.813511	-1.484900	0.862925
10	6	0	-1.707296	1.189354	-0.382732
11	1	0	0.008600	2.470625	-0.620201
12	6	0	-2.134181	-0.078171	0.013089
13	1	0	-1.590302	-2.018296	0.763423
14	1	0	-2.429348	1.918633	-0.732752
15	1	0	2.849825	-0.430330	1.638884
16	1	0	4.024741	0.411240	0.605357
17	6	0	2.003220	0.941133	0.183532
18	17	0	-3.826931	-0.464948	-0.056170

Zero-point correction= 0.128888 (Hartree/Particle)
Thermal correction to Energy= 0.139339
Thermal correction to Enthalpy= 0.140284
Thermal correction to Gibbs Free Energy= 0.091281
Sum of electronic and zero-point Energies= -936.391960
Sum of electronic and thermal Energies= -936.381508
Sum of electronic and thermal Enthalpies= -936.380564

Sum of electronic and thermal Free Energies= -936.429566

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710147	-0.848622	0.000019
2	6	0	-4.134672	-0.520978	-0.000025
3	7	0	-5.266060	-0.291216	-0.000061
4	8	0	-2.312645	1.510044	0.000072
5	6	0	-0.345462	0.194801	0.000057
6	6	0	0.242731	-1.073559	0.000010
7	6	0	0.470456	1.331775	0.000059
8	6	0	1.627130	-1.210052	-0.000032
9	1	0	-0.364648	-1.973299	0.000007
10	6	0	1.852665	1.209078	0.000017
11	1	0	-0.001495	2.309157	0.000096
12	6	0	2.419085	-0.065062	-0.000027
13	1	0	2.091328	-2.189807	-0.000067
14	1	0	2.491558	2.085126	0.000020
15	1	0	-2.482821	-1.457772	0.881761
16	1	0	-2.482750	-1.457700	-0.881756
17	6	0	-1.825563	0.404491	0.000107
18	17	0	4.149122	-0.228752	-0.000078

The conjugate base anion of *p*-ClPhCOCH$_2$CN.

Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.149273	-0.014970	0.029552
2	6	0	3.009004	1.354678	-0.255539
3	7	0	2.933947	2.500880	-0.484359
4	8	0	2.314951	-2.194981	0.285075
5	6	0	0.661686	-0.527533	0.096644
6	6	0	-0.266202	-1.474759	-0.350479
7	6	0	0.188152	0.719171	0.517706
8	6	0	-1.626551	-1.188535	-0.410128
9	1	0	0.113334	-2.450894	-0.635875
10	6	0	-1.173665	1.020832	0.476775
11	1	0	0.879960	1.468589	0.885323
12	6	0	-2.063973	0.064287	0.006896

13	1	0	-2.341552	-1.922969	-0.767156
14	1	0	-1.538488	1.987140	0.808796
15	1	0	4.162568	-0.396231	0.088121
16	6	0	2.119234	-0.964177	0.148098
17	17	0	-3.783224	0.437299	-0.048615

Zero-point correction= 0.115759 (Hartree/Particle)
Thermal correction to Energy= 0.125908
Thermal correction to Enthalpy= 0.126852
Thermal correction to Gibbs Free Energy= 0.078753
Sum of electronic and zero-point Energies= -935.872477
Sum of electronic and thermal Energies= -935.862328
Sum of electronic and thermal Enthalpies= -935.861384
Sum of electronic and thermal Free Energies= -935.909484

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.727438	-0.673924	-0.165266
2	6	0	-4.135089	-0.578727	-0.147494
3	7	0	-5.302936	-0.548581	-0.140413
4	8	0	-2.269510	1.603723	0.344123
5	6	0	-0.401903	0.186342	0.055764
6	6	0	0.425415	1.299318	-0.123561
7	6	0	0.201479	-1.065222	0.217370
8	6	0	1.811496	1.175697	-0.170325
9	1	0	-0.058803	2.266876	-0.215106
10	6	0	1.587471	-1.211040	0.182067
11	1	0	-0.414917	-1.940128	0.398793
12	6	0	2.377544	-0.085396	-0.018235
13	1	0	2.449232	2.041830	-0.317278
14	1	0	2.051484	-2.182739	0.316954
15	1	0	-2.312695	-1.630444	-0.453579
16	6	0	-1.907240	0.432495	0.097885
17	17	0	4.127761	-0.260139	-0.062889

Zero-point correction= 0.115400 (Hartree/Particle)
Thermal correction to Energy= 0.125710
Thermal correction to Enthalpy= 0.126654
Thermal correction to Gibbs Free Energy= 0.077955
Sum of electronic and zero-point Energies= -935.872055
Sum of electronic and thermal Energies= -935.861745

Sum of electronic and thermal Enthalpies= -935.860801
Sum of electronic and thermal Free Energies= -935.909500

Complexes formed from a [Bmim] cation and the conjugate base anion of *p*-ClPhCOCH$_2$CN.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.726853	-1.117948	1.484992
2	6	0	-2.797172	0.428696	0.363279
3	6	0	-4.582470	1.192439	-0.689027
4	6	0	-3.482351	1.729741	-1.284269
5	7	0	-2.382830	1.243157	-0.611140
6	1	0	-2.134967	-0.159066	1.022650
7	1	0	-5.632659	1.305908	-0.904632
8	1	0	-3.388148	2.406848	-2.117878
9	7	0	-4.128816	0.392419	0.335297
10	6	0	-0.970712	1.504517	-0.939054
11	6	0	-0.180844	2.027629	0.255109
12	1	0	-0.977147	2.232431	-1.755540
13	1	0	-0.543366	0.566443	-1.309646
14	6	0	1.263811	2.340844	-0.135277
15	1	0	-0.670412	2.929475	0.646737
16	1	0	-0.186299	1.267895	1.047517
17	1	0	1.734951	1.432688	-0.531197
18	1	0	1.276095	3.083736	-0.944325
19	6	0	-4.953135	-0.454995	1.195485
20	1	0	-4.303652	-0.908907	1.942958
21	1	0	-5.715888	0.159248	1.676213
22	1	0	-5.389095	-1.251731	0.592802
23	6	0	2.072607	2.858198	1.051377
24	1	0	2.046105	2.137225	1.874682
25	1	0	3.119778	3.014152	0.777285
26	1	0	1.670947	3.808024	1.420438
27	6	0	1.234007	-1.258444	0.173537
28	6	0	1.986959	-0.836596	1.273968
29	6	0	1.854664	-1.311172	-1.079729
30	6	0	3.323538	-0.474252	1.136685
31	1	0	1.491749	-0.786686	2.238835
32	6	0	3.188879	-0.944774	-1.236637
33	1	0	1.293325	-1.614087	-1.957901
34	6	0	3.910462	-0.523031	-0.123588

35	1	0	3.905233	-0.146345	1.992120
36	1	0	3.664175	-0.973458	-2.211332
37	6	0	-0.946111	-2.205532	-0.603445
38	6	0	-2.329418	-2.448274	-0.455016
39	7	0	-3.480245	-2.609918	-0.346314
40	1	0	-0.467115	-2.616974	-1.480461
41	6	0	-0.231872	-1.549443	0.400254
42	17	0	5.576435	-0.033891	-0.315651

Zero-point correction= 0.345473 (Hartree/Particle)
Thermal correction to Energy= 0.367688
Thermal correction to Enthalpy= 0.368632
Thermal correction to Gibbs Free Energy= 0.292872
Sum of electronic and zero-point Energies= -1358.787671
Sum of electronic and thermal Energies= -1358.765456
Sum of electronic and thermal Enthalpies= -1358.764512
Sum of electronic and thermal Free Energies= -1358.840272

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.779192	1.361683	-0.676013
2	6	0	-2.979086	1.404516	0.149108
3	6	0	-1.109881	1.620307	1.288995
4	6	0	-1.773203	0.532521	1.764137
5	7	0	-2.945624	0.421194	1.044534
6	1	0	-3.731109	1.541555	-0.609875
7	1	0	-0.138488	2.025028	1.520752
8	1	0	-1.504748	-0.183693	2.523763
9	7	0	-1.892890	2.157412	0.292621
10	6	0	-3.826053	-0.753726	1.078705
11	6	0	-5.056053	-0.604861	0.198604
12	1	0	-4.107438	-0.917017	2.124070
13	1	0	-3.223397	-1.597597	0.727528
14	6	0	-5.950232	-1.840655	0.303030
15	1	0	-5.627270	0.286146	0.493558
16	1	0	-4.728513	-0.483407	-0.840549
17	1	0	-5.368329	-2.726583	0.022306
18	1	0	-6.261739	-1.983458	1.345615
19	6	0	-1.495992	3.253012	-0.588582
20	1	0	-2.312381	3.448965	-1.283350
21	1	0	-1.300213	4.143381	0.010529

22	1	0	-0.598451	2.927069	-1.118339
23	6	0	-7.181258	-1.731119	-0.593358
24	1	0	-6.888588	-1.615635	-1.641475
25	1	0	-7.809213	-2.622259	-0.515960
26	1	0	-7.791427	-0.865057	-0.316880
27	6	0	2.595734	-0.132661	-0.415506
28	6	0	3.514434	0.912154	-0.549465
29	6	0	3.057394	-1.378012	0.021621
30	6	0	4.866246	0.721799	-0.279628
31	1	0	3.141848	1.878962	-0.871975
32	6	0	4.405295	-1.584934	0.304441
33	1	0	2.358291	-2.195490	0.166180
34	6	0	5.298406	-0.530649	0.145333
35	1	0	5.581065	1.529561	-0.395084
36	1	0	4.762031	-2.548967	0.650899
37	6	0	0.321350	-0.927917	-1.055439
38	6	0	-1.034977	-0.726793	-1.363201
39	7	0	-2.170961	-0.582510	-1.606328
40	1	0	0.713856	-1.926278	-1.188560
41	6	0	1.145069	0.156650	-0.727230
42	17	0	6.993168	-0.783479	0.494105

Zero-point correction=	0.345983 (Hartree/Particle)
Thermal correction to Energy=	0.368621
Thermal correction to Enthalpy=	0.369565
Thermal correction to Gibbs Free Energy=	0.290898
Sum of electronic and zero-point Energies=	-1358.777708
Sum of electronic and thermal Energies=	-1358.755069
Sum of electronic and thermal Enthalpies=	-1358.754125
Sum of electronic and thermal Free Energies=	-1358.832792

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.476263	-2.110250	-0.267471
2	6	0	-2.432841	0.540513	-0.253908
3	6	0	-2.282551	-0.024256	-2.371340
4	6	0	-1.140448	0.631918	-2.033043
5	7	0	-1.254636	0.973024	-0.703271
6	1	0	-2.790259	0.600256	0.765272
7	1	0	-2.582694	-0.494491	-3.293643
8	1	0	-0.256525	0.866708	-2.604588

9	7	0	-3.077348	-0.058884	-1.248975
10	6	0	-0.229028	1.639477	0.104909
11	6	0	-0.270742	3.155835	-0.041124
12	1	0	0.736134	1.229962	-0.211335
13	1	0	-0.391424	1.319603	1.139503
14	6	0	0.826354	3.826204	0.784608
15	1	0	-0.154297	3.423209	-1.099718
16	1	0	-1.255506	3.523768	0.274237
17	1	0	0.707461	3.546871	1.838819
18	1	0	1.803538	3.440122	0.468810
19	6	0	-4.252432	-0.913423	-1.070443
20	1	0	-4.809365	-0.571115	-0.199206
21	1	0	-4.865264	-0.857862	-1.970294
22	1	0	-3.886827	-1.925819	-0.882109
23	6	0	0.802336	5.346738	0.647883
24	1	0	-0.153815	5.755342	0.989976
25	1	0	1.595960	5.810361	1.239003
26	1	0	0.941562	5.647786	-0.395442
27	6	0	0.702179	-1.599208	0.499120
28	6	0	1.164524	-1.743550	-0.812728
29	6	0	1.619925	-1.237430	1.491229
30	6	0	2.497400	-1.509413	-1.141583
31	1	0	0.443122	-2.044491	-1.566552
32	6	0	2.957765	-1.003074	1.182627
33	1	0	1.301837	-1.132889	2.523155
34	6	0	3.382739	-1.131714	-0.136620
35	1	0	2.853585	-1.622876	-2.160366
36	1	0	3.667009	-0.723833	1.954535
37	6	0	-1.316078	-1.424442	1.982138
38	6	0	-2.716418	-1.374381	2.123263
39	7	0	-3.876620	-1.237262	2.159058
40	1	0	-0.710395	-1.174282	2.840528
41	6	0	-0.789072	-1.768449	0.726322
42	17	0	5.054990	-0.820032	-0.532139

Zero-point correction=	0.345406 (Hartree/Particle)
Thermal correction to Energy=	0.368067
Thermal correction to Enthalpy=	0.369011
Thermal correction to Gibbs Free Energy=	0.290029
Sum of electronic and zero-point Energies=	-1358.780001
Sum of electronic and thermal Energies=	-1358.757339
Sum of electronic and thermal Enthalpies=	-1358.756395
Sum of electronic and thermal Free Energies=	-1358.835378

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.002221	0.073184	-0.760210
2	1	0	2.428160	-0.813574	-1.057696
3	6	0	4.577465	1.441109	-0.037082
4	1	0	5.566225	1.736416	0.275457
5	6	0	3.418913	2.148815	-0.128827
6	1	0	3.202542	3.183556	0.084240
7	7	0	4.294130	0.154245	-0.439244
8	7	0	2.453068	1.277800	-0.585162
9	6	0	5.242637	-0.958934	-0.461104
10	1	0	5.505881	-1.225618	0.561749
11	1	0	4.751220	-1.817897	-0.914016
12	1	0	6.116842	-0.664151	-1.043536
13	6	0	1.037563	1.609446	-0.823549
14	1	0	1.017882	2.470317	-1.500151
15	1	0	0.599177	0.743362	-1.328274
16	6	0	0.731847	-1.935628	1.212805
17	1	0	0.164659	-2.051350	2.124944
18	6	0	2.122252	-2.158107	1.281372
19	7	0	3.280480	-2.297138	1.330044
20	6	0	0.298926	1.911963	0.475583
21	6	0	-1.152652	2.312140	0.209691
22	1	0	0.809857	2.721544	1.015575
23	1	0	0.334983	1.019209	1.113190
24	6	0	-1.896411	2.642448	1.501329
25	1	0	-1.176936	3.181315	-0.461280
26	1	0	-1.664382	1.494287	-0.312559
27	1	0	-2.948635	2.865862	1.304594
28	1	0	-1.858814	1.795160	2.193554
29	1	0	-1.450867	3.508297	2.002981
30	6	0	0.140620	-1.618264	-0.009118
31	8	0	0.749021	-1.552483	-1.120475
32	6	0	-1.327906	-1.263475	-0.033838
33	6	0	-2.070378	-0.944582	1.108171
34	6	0	-1.951132	-1.170260	-1.282767
35	6	0	-3.397863	-0.536156	1.010758
36	1	0	-1.609453	-0.982814	2.090254
37	6	0	-3.277926	-0.766212	-1.398926
38	1	0	-1.363527	-1.413312	-2.162015
39	6	0	-3.987970	-0.444321	-0.246017

40	1	0	-3.967244	-0.273640	1.896288
41	1	0	-3.758518	-0.692405	-2.368712
42	17	0	-5.643894	0.095998	-0.376463

Zero-point correction= 0.346185 (Hartree/Particle)
Thermal correction to Energy= 0.368306
Thermal correction to Enthalpy= 0.369250
Thermal correction to Gibbs Free Energy= 0.293076
Sum of electronic and zero-point Energies= -1358.787243
Sum of electronic and thermal Energies= -1358.765122
Sum of electronic and thermal Enthalpies= -1358.764178
Sum of electronic and thermal Free Energies= -1358.840352

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.822603	1.329101	0.010953
2	6	0	2.099728	1.840871	0.092853
3	6	0	0.577612	1.120166	-1.319518
4	6	0	1.478887	0.120247	-1.122093
5	7	0	2.429861	0.597350	-0.243423
6	1	0	2.608336	2.443308	0.828626
7	1	0	-0.350912	1.151189	-1.865912
8	1	0	1.504627	-0.887947	-1.501615
9	7	0	0.998064	2.190290	-0.562088
10	6	0	3.448856	-0.208183	0.432374
11	6	0	4.438497	-0.834520	-0.541265
12	1	0	2.915023	-0.958578	1.024226
13	1	0	3.955979	0.453117	1.139636
14	6	0	5.477886	-1.678824	0.194891
15	1	0	3.903435	-1.465000	-1.262957
16	1	0	4.935065	-0.043620	-1.117399
17	1	0	6.007884	-1.049553	0.920820
18	1	0	4.965468	-2.456710	0.774125
19	6	0	0.244715	3.427176	-0.365425
20	1	0	0.795590	4.058565	0.331162
21	1	0	0.136020	3.938859	-1.322626
22	1	0	-0.727460	3.143880	0.043243
23	6	0	6.482141	-2.322022	-0.758609
24	1	0	7.031296	-1.561000	-1.322065
25	1	0	7.211198	-2.927880	-0.214802
26	1	0	5.976178	-2.972452	-1.479175

27	6	0	-3.372416	-0.454070	0.143586
28	6	0	-4.379278	0.346088	-0.403801
29	6	0	-3.601218	-1.828308	0.263372
30	6	0	-5.596230	-0.198208	-0.801805
31	1	0	-4.183086	1.408076	-0.510593
32	6	0	-4.809928	-2.392211	-0.137054
33	1	0	-2.822750	-2.476653	0.652859
34	6	0	-5.799405	-1.567579	-0.662221
35	1	0	-6.380740	0.426050	-1.216205
36	1	0	-4.983972	-3.459390	-0.050017
37	6	0	-1.275187	-0.432794	1.491348
38	6	0	-0.065642	0.145437	1.915670
39	7	0	0.950465	0.604969	2.270993
40	1	0	-1.596041	-1.332581	1.997175
41	6	0	-2.080534	0.217652	0.549155
42	17	0	-7.321958	-2.267355	-1.164280

Zero-point correction= 0.345852 (Hartree/Particle)
Thermal correction to Energy= 0.368521
Thermal correction to Enthalpy= 0.369465
Thermal correction to Gibbs Free Energy= 0.289819
Sum of electronic and zero-point Energies= -1358.776583
Sum of electronic and thermal Energies= -1358.753914
Sum of electronic and thermal Enthalpies= -1358.752970
Sum of electronic and thermal Free Energies= -1358.832616

Conform 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.405517	0.531344	-1.236398
2	6	0	1.401889	0.100508	1.364654
3	6	0	1.592135	-1.828459	0.333408
4	6	0	0.425148	-1.843000	1.031684
5	7	0	0.325387	-0.625578	1.668790
6	1	0	1.587783	1.124609	1.659305
7	1	0	2.023635	-2.560393	-0.329009
8	1	0	-0.346536	-2.591558	1.114811
9	7	0	2.187933	-0.609939	0.565040
10	6	0	-0.807390	-0.162767	2.465480
11	1	0	-1.728023	-0.498241	1.984204
12	1	0	-0.795414	0.928135	2.467263
13	6	0	3.324383	-0.048469	-0.182880

14	1	0	3.528160	0.933383	0.251957
15	1	0	2.955305	0.124059	-1.199507
16	6	0	-1.874638	0.760899	-0.648776
17	6	0	-2.086373	-0.556982	-1.066365
18	6	0	-2.964596	1.484547	-0.153068
19	6	0	-3.339720	-1.155897	-0.968007
20	1	0	-1.234426	-1.095194	-1.471345
21	6	0	-4.226949	0.904473	-0.052607
22	1	0	-2.843612	2.516729	0.158390
23	6	0	-4.400437	-0.417699	-0.451925
24	1	0	-3.500703	-2.178931	-1.292454
25	1	0	-5.071261	1.468899	0.328859
26	6	0	-0.159597	2.491957	-0.053142
27	6	0	1.188548	2.876333	0.075316
28	7	0	2.322356	3.097871	0.253992
29	1	0	-0.912540	3.140301	0.370040
30	6	0	-0.448826	1.278885	-0.701201
31	1	0	-0.740013	-0.554004	3.482071
32	6	0	4.547793	-0.952459	-0.135891
33	6	0	5.724979	-0.317577	-0.876545
34	1	0	4.322642	-1.926987	-0.589247
35	1	0	4.823929	-1.142051	0.909406
36	6	0	6.967021	-1.205191	-0.852901
37	1	0	5.432281	-0.114437	-1.913723
38	1	0	5.952240	0.654579	-0.423320
39	1	0	7.800203	-0.734468	-1.380783
40	1	0	7.288895	-1.400885	0.175228
41	1	0	6.769359	-2.170210	-1.331031
42	17	0	-5.975647	-1.156775	-0.309300

Zero-point correction= 0.345432 (Hartree/Particle)
Thermal correction to Energy= 0.368095
Thermal correction to Enthalpy= 0.369039
Thermal correction to Gibbs Free Energy= 0.290479
Sum of electronic and zero-point Energies= -1358.778505
Sum of electronic and thermal Energies= -1358.755842
Sum of electronic and thermal Enthalpies= -1358.754898
Sum of electronic and thermal Free Energies= -1358.833459

Conformer 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.139203	0.402818	-0.355996
2	6	0	-4.090412	-0.526825	0.001774
3	6	0	-2.321912	-0.226527	1.268562
4	6	0	-2.893927	-1.412694	1.613418
5	7	0	-4.006428	-1.575035	0.817582
6	1	0	-4.815069	-0.408640	-0.788523
7	1	0	-1.410526	0.245383	1.595654
8	1	0	-2.593200	-2.159117	2.330475
9	7	0	-3.099521	0.316235	0.270352
10	6	0	-4.751549	-2.815267	0.644397
11	1	0	-4.205980	-3.441564	-0.065739
12	1	0	-5.742994	-2.585221	0.254198
13	6	0	-2.782143	1.503167	-0.542485
14	1	0	-3.720917	1.818148	-1.009383
15	1	0	-2.068852	1.169517	-1.300677
16	6	0	2.022866	-0.557645	-0.330222
17	6	0	2.607260	0.710279	-0.261162
18	6	0	2.831626	-1.678647	-0.121236
19	6	0	3.967556	0.864635	-0.013365
20	1	0	1.965729	1.573909	-0.405502
21	6	0	4.193619	-1.543335	0.135982
22	1	0	2.397515	-2.673273	-0.134446
23	6	0	4.749329	-0.269117	0.182456
24	1	0	4.421418	1.848956	0.031278
25	1	0	4.818868	-2.413196	0.307044
26	6	0	0.025260	-1.834846	-1.106217
27	6	0	-1.346978	-1.972334	-1.380585
28	7	0	-2.486810	-2.113657	-1.606704
29	1	0	0.664852	-2.659561	-1.387168
30	6	0	0.537526	-0.634604	-0.599679
31	1	0	-4.849878	-3.307812	1.611619
32	6	0	-2.175231	2.624254	0.284415
33	6	0	-1.877780	3.840488	-0.591523
34	1	0	-1.234857	2.264678	0.714333
35	1	0	-2.853501	2.902764	1.102251
36	6	0	-1.218656	4.967069	0.200527
37	1	0	-1.218082	3.530227	-1.410757
38	1	0	-2.806584	4.203983	-1.050537
39	1	0	-1.007986	5.831069	-0.435135
40	1	0	-1.863848	5.301318	1.019912
41	1	0	-0.272443	4.629866	0.635281
42	17	0	6.458855	-0.089122	0.503226

Zero-point correction= 0.345416 (Hartree/Particle)

Thermal correction to Energy=	0.368111
Thermal correction to Enthalpy=	0.369055
Thermal correction to Gibbs Free Energy=	0.288714
Sum of electronic and zero-point Energies=	-1358.779024
Sum of electronic and thermal Energies=	-1358.756329
Sum of electronic and thermal Enthalpies=	-1358.755385
Sum of electronic and thermal Free Energies=	-1358.835726

Conformer 8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.127320	-0.488228	-0.345133
2	6	0	2.627877	-1.069426	-0.404321
3	6	0	3.980956	-2.816238	-0.331311
4	6	0	4.735818	-1.690504	-0.210053
5	7	0	3.873397	-0.616344	-0.266067
6	1	0	1.682035	-0.513280	-0.421899
7	1	0	4.257362	-3.858390	-0.342948
8	1	0	5.799170	-1.560880	-0.086471
9	7	0	2.671927	-2.401620	-0.452686
10	6	0	4.243212	0.789898	-0.038277
11	6	0	3.239280	1.757244	-0.647292
12	1	0	5.235699	0.927871	-0.478302
13	1	0	4.291745	0.932655	1.044772
14	6	0	3.658517	3.204617	-0.392390
15	1	0	3.150111	1.573304	-1.726064
16	1	0	2.254724	1.589294	-0.196683
17	1	0	3.754238	3.360660	0.689019
18	1	0	4.649467	3.385504	-0.829105
19	6	0	1.485194	-3.248706	-0.575394
20	1	0	0.612623	-2.590247	-0.577542
21	1	0	1.539380	-3.819244	-1.503909
22	1	0	1.440726	-3.924362	0.279861
23	6	0	2.650239	4.197362	-0.966498
24	1	0	1.663342	4.047848	-0.518287
25	1	0	2.956021	5.229165	-0.774688
26	1	0	2.548846	4.071352	-2.049367
27	6	0	-2.337417	-0.004689	0.352309
28	6	0	-2.779992	-0.052538	-0.972693
29	6	0	-3.289074	0.053921	1.375175
30	6	0	-4.136683	-0.019373	-1.280300
31	1	0	-2.033251	-0.118888	-1.757054

32	6	0	-4.650627	0.081338	1.085969
33	1	0	-2.973962	0.054530	2.413670
34	6	0	-5.060983	0.048982	-0.242952
35	1	0	-4.479262	-0.048377	-2.309274
36	1	0	-5.388816	0.119564	1.879784
37	6	0	-0.363658	0.416250	1.822634
38	6	0	1.023279	0.362189	2.059457
39	7	0	2.180853	0.301401	2.208997
40	1	0	-0.994614	0.857906	2.579697
41	6	0	-0.851883	-0.043455	0.601055
42	17	0	-6.769094	0.082620	-0.611562

Zero-point correction= 0.345735 (Hartree/Particle)
Thermal correction to Energy= 0.368385
Thermal correction to Enthalpy= 0.369330
Thermal correction to Gibbs Free Energy= 0.289423
Sum of electronic and zero-point Energies= -1358.784135
Sum of electronic and thermal Energies= -1358.761485
Sum of electronic and thermal Enthalpies= -1358.760541
Sum of electronic and thermal Free Energies= -1358.840447

9-CNF1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.012172	-1.597229	-0.193674
2	6	0	3.455384	-0.302881	0.089713
3	6	0	2.540931	0.723084	0.338930
4	6	0	1.188390	0.422843	0.297220
5	6	0	0.736094	-0.871158	0.003516
6	6	0	1.650193	-1.893187	-0.240714
7	1	0	3.738505	-2.381178	-0.383597
8	1	0	4.519562	-0.091896	0.113466
9	1	0	2.882753	1.732489	0.550387
10	1	0	1.313303	-2.900020	-0.469095
11	6	0	-0.000042	1.338405	0.557804
12	1	0	-0.000047	1.668302	1.605683
13	6	0	-1.188348	0.422638	0.297258
14	6	0	-2.540939	0.722650	0.338998
15	6	0	-3.455224	-0.303467	0.089789
16	6	0	-3.011805	-1.597740	-0.193620
17	6	0	-1.649777	-1.893466	-0.240700
18	6	0	-0.735849	-0.871282	0.003523

19	1	0	-2.882926	1.732000	0.550453
20	1	0	-4.519437	-0.092662	0.113573
21	1	0	-3.738014	-2.381806	-0.383532
22	1	0	-1.312717	-2.900237	-0.469104
23	6	0	-0.000224	2.545845	-0.277922
24	7	0	-0.000959	3.506382	-0.921281

Zero-point correction= 0.188333 (Hartree/Particle)
Thermal correction to Energy= 0.199047
Thermal correction to Enthalpy= 0.199991
Thermal correction to Gibbs Free Energy= 0.151450
Sum of electronic and zero-point Energies= -593.252269
Sum of electronic and thermal Energies= -593.241555
Sum of electronic and thermal Enthalpies= -593.240611
Sum of electronic and thermal Free Energies= -593.289152

The conjugate base anion of 9-CNFl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.021932	-1.649232	-0.000029
2	6	0	-3.445486	-0.303220	0.000367
3	6	0	-2.532108	0.739345	0.000463
4	6	0	-1.152770	0.450101	0.000192
5	6	0	-0.722710	-0.917542	-0.000200
6	6	0	-1.664817	-1.951709	-0.000318
7	1	0	-3.758842	-2.447862	-0.000105
8	1	0	-4.510275	-0.080910	0.000520
9	1	0	-2.869648	1.773133	0.000614
10	1	0	-1.336481	-2.989803	-0.000547
11	6	0	-0.000016	1.294787	-0.000225
12	6	0	1.152772	0.450153	0.000192
13	6	0	2.532097	0.739459	0.000463
14	6	0	3.445521	-0.303065	0.000367
15	6	0	3.022025	-1.649096	-0.000028
16	6	0	1.664924	-1.951634	-0.000317
17	6	0	0.722770	-0.917508	-0.000199
18	1	0	2.869589	1.773263	0.000614
19	1	0	4.510300	-0.080708	0.000520
20	1	0	3.758971	-2.447694	-0.000104
21	1	0	1.336634	-2.989742	-0.000546
22	6	0	-0.000034	2.701867	-0.000368
23	7	0	-0.000239	3.870585	-0.000447

Complexes formed from a [Bmim] cation and the conjugate base anion of 9-CNFl.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.968448	-1.587687	-3.012766
2	6	0	3.019264	-0.795838	-2.503479
3	6	0	3.069482	-0.441862	-1.162719
4	6	0	2.039281	-0.863843	-0.299099
5	6	0	0.992005	-1.696281	-0.809444
6	6	0	0.967439	-2.048647	-2.165116
7	1	0	1.957645	-1.855643	-4.064519
8	1	0	3.812879	-0.473443	-3.172378
9	1	0	3.899274	0.146246	-0.776020
10	1	0	0.169663	-2.678182	-2.554212
11	6	0	1.757547	-0.559119	1.070936
12	6	0	0.533958	-1.218196	1.416641
13	6	0	-0.245602	-1.214126	2.591735
14	6	0	-1.428078	-1.938956	2.623853
15	6	0	-1.860230	-2.692141	1.509482
16	6	0	-1.108783	-2.700231	0.341644
17	6	0	0.072279	-1.950695	0.275885
18	1	0	0.085924	-0.657773	3.465489
19	1	0	-2.025273	-1.945410	3.531649
20	1	0	-2.775692	-3.272001	1.573845
21	1	0	-1.440620	-3.276563	-0.519724
22	6	0	0.308871	1.545033	-0.781441
23	6	0	0.570682	2.681749	1.088602
24	6	0	-0.612136	2.016142	1.160907
25	7	0	-0.757788	1.319988	-0.019396
26	1	0	0.510984	1.081653	-1.739158
27	1	0	1.100183	3.277736	1.814751
28	1	0	-1.337416	1.937411	1.954973
29	7	0	1.122365	2.383692	-0.137016
30	6	0	-1.900296	0.461076	-0.350396
31	6	0	-3.144252	1.273113	-0.690511
32	1	0	-2.066940	-0.193968	0.510944
33	1	0	-1.588070	-0.173887	-1.184097
34	6	0	-4.319673	0.354517	-1.022308
35	1	0	-3.408167	1.916246	0.159336

36	1	0	-2.932283	1.936083	-1.539499
37	1	0	-4.052449	-0.277086	-1.878549
38	1	0	-4.493497	-0.325607	-0.179187
39	6	0	2.441345	2.819279	-0.588233
40	1	0	2.445098	3.904955	-0.697418
41	1	0	3.176741	2.502629	0.154705
42	1	0	2.652622	2.341747	-1.544638
43	6	0	-5.594256	1.135635	-1.332839
44	1	0	-5.446449	1.804567	-2.186897
45	1	0	-6.422589	0.464229	-1.572341
46	1	0	-5.895338	1.747827	-0.476711
47	6	0	2.480196	0.369642	1.837428
48	7	0	3.068112	1.207300	2.403140

Zero-point correction= 0.405098 (Hartree/Particle)
Thermal correction to Energy= 0.427820
Thermal correction to Enthalpy= 0.428764
Thermal correction to Gibbs Free Energy= 0.352793
Sum of electronic and zero-point Energies= -1015.645424
Sum of electronic and thermal Energies= -1015.622702
Sum of electronic and thermal Enthalpies= -1015.621758
Sum of electronic and thermal Free Energies= -1015.697729

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.968448	-1.587687	-3.012766
2	6	0	3.019264	-0.795838	-2.503479
3	6	0	3.069482	-0.441862	-1.162719
4	6	0	2.039281	-0.863843	-0.299099
5	6	0	0.992005	-1.696281	-0.809444
6	6	0	0.967439	-2.048647	-2.165116
7	1	0	1.957645	-1.855643	-4.064519
8	1	0	3.812879	-0.473443	-3.172378
9	1	0	3.899274	0.146246	-0.776020
10	1	0	0.169663	-2.678182	-2.554212
11	6	0	1.757547	-0.559119	1.070936
12	6	0	0.533958	-1.218196	1.416641
13	6	0	-0.245602	-1.214126	2.591735
14	6	0	-1.428078	-1.938956	2.623853
15	6	0	-1.860230	-2.692141	1.509482
16	6	0	-1.108783	-2.700231	0.341644

17	6	0	0.072279	-1.950695	0.275885
18	1	0	0.085924	-0.657773	3.465489
19	1	0	-2.025273	-1.945410	3.531649
20	1	0	-2.775692	-3.272001	1.573845
21	1	0	-1.440620	-3.276563	-0.519724
22	6	0	0.308871	1.545033	-0.781441
23	6	0	0.570682	2.681749	1.088602
24	6	0	-0.612136	2.016142	1.160907
25	7	0	-0.757788	1.319988	-0.019396
26	1	0	0.510984	1.081653	-1.739158
27	1	0	1.100183	3.277736	1.814751
28	1	0	-1.337416	1.937411	1.954973
29	7	0	1.122365	2.383692	-0.137016
30	6	0	-1.900296	0.461076	-0.350396
31	6	0	-3.144252	1.273113	-0.690511
32	1	0	-2.066940	-0.193968	0.510944
33	1	0	-1.588070	-0.173887	-1.184097
34	6	0	-4.319673	0.354517	-1.022308
35	1	0	-3.408167	1.916246	0.159336
36	1	0	-2.932283	1.936083	-1.539499
37	1	0	-4.052449	-0.277086	-1.878549
38	1	0	-4.493497	-0.325607	-0.179187
39	6	0	2.441345	2.819279	-0.588233
40	1	0	2.445098	3.904955	-0.697418
41	1	0	3.176741	2.502629	0.154705
42	1	0	2.652622	2.341747	-1.544638
43	6	0	-5.594256	1.135635	-1.332839
44	1	0	-5.446449	1.804567	-2.186897
45	1	0	-6.422589	0.464229	-1.572341
46	1	0	-5.895338	1.747827	-0.476711
47	6	0	2.480196	0.369642	1.837428
48	7	0	3.068112	1.207300	2.403140

Zero-point correction= 0.404925 (Hartree/Particle)
Thermal correction to Energy= 0.428018
Thermal correction to Enthalpy= 0.428962
Thermal correction to Gibbs Free Energy= 0.350114
Sum of electronic and zero-point Energies= -1015.638641
Sum of electronic and thermal Energies= -1015.615548
Sum of electronic and thermal Enthalpies= -1015.614603
Sum of electronic and thermal Free Energies= -1015.693452

Conformer 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.710393	3.679265	-0.592066
2	6	0	-0.361856	3.402083	0.282352
3	6	0	-0.383995	2.246895	1.051294
4	6	0	0.675184	1.324375	0.940892
5	6	0	1.781990	1.625658	0.082691
6	6	0	1.785501	2.801678	-0.678272
7	1	0	0.704782	4.592573	-1.178351
8	1	0	-1.176266	4.116809	0.366327
9	1	0	-1.203628	2.056201	1.741142
10	1	0	2.623285	3.028410	-1.334788
11	6	0	0.865684	0.017956	1.492721
12	6	0	2.106138	-0.487615	0.986322
13	6	0	2.751779	-1.731087	1.139131
14	6	0	3.958208	-1.952389	0.491383
15	6	0	4.560267	-0.952120	-0.304162
16	6	0	3.932928	0.275316	-0.471510
17	6	0	2.697052	0.508451	0.145132
18	1	0	2.312179	-2.500507	1.769641
19	1	0	4.462797	-2.906687	0.615697
20	1	0	5.519881	-1.143140	-0.774171
21	1	0	4.393804	1.046469	-1.085666
22	6	0	-0.587287	-0.190405	-1.311862
23	6	0	-1.192571	-2.056722	-0.310144
24	6	0	-0.030498	-2.293167	-0.974343
25	7	0	0.323815	-1.117517	-1.599395
26	1	0	-0.543165	0.851048	-1.605473
27	1	0	-1.770517	-2.677447	0.355802
28	1	0	0.597327	-3.168460	-1.020982
29	7	0	-1.527246	-0.741406	-0.543680
30	6	0	1.518288	-0.931734	-2.420911
31	1	0	2.367887	-1.384582	-1.905599
32	1	0	1.704419	0.137739	-2.521566
33	6	0	-2.675747	-0.045940	0.048632
34	1	0	-2.599136	-0.184358	1.132399
35	1	0	-2.544808	1.017774	-0.168602
36	6	0	-0.096588	-0.679324	2.240933
37	7	0	-0.955798	-1.249091	2.792572
38	1	0	1.361110	-1.391707	-3.398604
39	6	0	-3.999245	-0.571500	-0.495108
40	6	0	-5.184681	0.147103	0.148098
41	1	0	-4.075606	-1.648710	-0.298930

42	1	0	-4.025795	-0.441315	-1.584674
43	6	0	-6.523403	-0.367134	-0.376054
44	1	0	-5.136678	0.017003	1.235944
45	1	0	-5.101724	1.224598	-0.041759
46	1	0	-7.359927	0.153241	0.096879
47	1	0	-6.603993	-0.219693	-1.457923
48	1	0	-6.636881	-1.437021	-0.174111

Zero-point correction= 0.405552 (Hartree/Particle)
Thermal correction to Energy= 0.428176
Thermal correction to Enthalpy= 0.429120
Thermal correction to Gibbs Free Energy= 0.352979
Sum of electronic and zero-point Energies= -1015.644701
Sum of electronic and thermal Energies= -1015.622077
Sum of electronic and thermal Enthalpies= -1015.621133
Sum of electronic and thermal Free Energies= -1015.697274

Confermer4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.470639	-0.294084	-0.975564
2	6	0	-4.240679	-1.276727	0.009332
3	6	0	-3.161420	-1.187458	0.878419
4	6	0	-2.277368	-0.096907	0.769190
5	6	0	-2.527913	0.913517	-0.213905
6	6	0	-3.621231	0.802028	-1.079142
7	1	0	-5.327272	-0.383703	-1.636121
8	1	0	-4.932595	-2.110499	0.099196
9	1	0	-3.004652	-1.942873	1.646053
10	1	0	-3.808323	1.569087	-1.827435
11	6	0	-1.067840	0.232504	1.464177
12	6	0	-0.584317	1.469137	0.924359
13	6	0	0.558807	2.235864	1.219139
14	6	0	0.833284	3.364285	0.458926
15	6	0	-0.019347	3.762331	-0.591277
16	6	0	-1.171382	3.035305	-0.870591
17	6	0	-1.465445	1.890976	-0.120073
18	1	0	1.208807	1.950224	2.043962
19	1	0	1.711116	3.963317	0.686927
20	1	0	0.214850	4.652869	-1.165941
21	1	0	-1.837097	3.354049	-1.669703
22	6	0	-0.435811	-1.115680	-1.582722

23	6	0	0.863131	-2.031121	-0.054582
24	1	0	-1.321363	-1.006719	-2.190718
25	1	0	1.227332	-2.681495	0.727156
26	7	0	-0.244545	-2.214447	-0.770866
27	6	0	-1.135513	-3.366460	-0.670126
28	1	0	-0.903958	-4.087070	-1.456620
29	1	0	-1.003481	-3.821396	0.312074
30	1	0	-2.162427	-3.010384	-0.758108
31	6	0	2.599644	-0.278339	0.212485
32	6	0	3.859666	-0.672632	-0.550550
33	1	0	2.624082	-0.607673	1.256621
34	1	0	2.451830	0.804965	0.211188
35	6	0	5.103380	-0.013671	0.043795
36	1	0	3.972243	-1.764729	-0.534678
37	1	0	3.749940	-0.377976	-1.602413
38	6	0	6.372825	-0.389143	-0.717267
39	1	0	4.973462	1.075543	0.032663
40	1	0	5.201138	-0.305101	1.096810
41	1	0	7.252722	0.091149	-0.282131
42	1	0	6.536333	-1.471395	-0.696415
43	1	0	6.305601	-0.080748	-1.765550
44	6	0	0.596949	-0.262732	-1.341616
45	1	0	0.790279	0.737572	-1.701842
46	7	0	1.393766	-0.857418	-0.387434
47	6	0	-0.332854	-0.624643	2.294350
48	7	0	0.340189	-1.374583	2.891799

Zero-point correction= 0.404679 (Hartree/Particle)
Thermal correction to Energy= 0.427691
Thermal correction to Enthalpy= 0.428636
Thermal correction to Gibbs Free Energy= 0.350616
Sum of electronic and zero-point Energies= -1015.641260
Sum of electronic and thermal Energies= -1015.618247
Sum of electronic and thermal Enthalpies= -1015.617303
Sum of electronic and thermal Free Energies= -1015.695323

$PhCOCH_2CN$
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.221068	0.231628	0.649756
2	6	0	2.522941	-0.881270	-0.253059

3	7	0	2.755153	-1.760263	-0.966622
4	8	0	1.146683	2.228766	-0.037360
5	6	0	-0.333450	0.384173	0.115853
6	6	0	-0.529315	-0.948687	0.491709
7	6	0	-1.415304	1.143936	-0.345552
8	6	0	-1.798651	-1.515419	0.408941
9	1	0	0.298259	-1.558646	0.840273
10	6	0	-2.679594	0.574801	-0.430007
11	1	0	-1.239753	2.176311	-0.630718
12	6	0	-2.871502	-0.755416	-0.051989
13	1	0	-1.947302	-2.550292	0.698699
14	1	0	-3.516691	1.164344	-0.789553
15	1	0	-3.859415	-1.200346	-0.120254
16	1	0	2.055003	-0.168706	1.656079
17	1	0	3.071143	0.915560	0.681199
18	6	0	0.997011	1.051835	0.202598

Zero-point correction= 0.138507 (Hartree/Particle)
Thermal correction to Energy= 0.147775
Thermal correction to Enthalpy= 0.148720
Thermal correction to Gibbs Free Energy= 0.102910
Sum of electronic and zero-point Energies= -476.814415
Sum of electronic and thermal Energies= -476.805147
Sum of electronic and thermal Enthalpies= -476.804203
Sum of electronic and thermal Free Energies= -476.850013

Conformer b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871268	-0.802227	0.000018
2	6	0	3.277991	-0.404971	-0.000251
3	7	0	4.397525	-0.122419	-0.000121
4	8	0	1.358591	1.532928	0.000206
5	6	0	-0.544148	0.121027	0.000094
6	6	0	-1.063273	-1.177837	0.000135
7	6	0	-1.416010	1.215670	-0.000045
8	6	0	-2.441539	-1.379109	0.000035
9	1	0	-0.406193	-2.042087	0.000225
10	6	0	-2.790643	1.012628	-0.000149
11	1	0	-0.992817	2.215081	-0.000078
12	6	0	-3.304636	-0.285134	-0.000108
13	1	0	-2.839774	-2.388458	0.000083

14	1	0	-3.463165	1.864165	-0.000254
15	1	0	-4.378494	-0.443854	-0.000198
16	1	0	1.674004	-1.421880	-0.881560
17	1	0	1.674455	-1.421989	0.881580
18	6	0	0.924420	0.405377	0.000171

Zero-point correction= 0.138387 (Hartree/Particle)
Thermal correction to Energy= 0.147702
Thermal correction to Enthalpy= 0.148646
Thermal correction to Gibbs Free Energy= 0.102863
Sum of electronic and zero-point Energies= -476.813230
Sum of electronic and thermal Energies= -476.803915
Sum of electronic and thermal Enthalpies= -476.802971
Sum of electronic and thermal Free Energies= -476.848754

The conjugate base anion of $PhCOCH_2CN$.
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.291646	0.431773	0.052258
2	6	0	-2.458355	-0.930285	-0.253306
3	7	0	-2.646628	-2.060145	-0.499280
4	8	0	-1.005283	2.376963	0.319736
5	6	0	0.248283	0.392198	0.092068
6	6	0	1.352657	1.108384	-0.384692
7	6	0	0.440529	-0.926358	0.517771
8	6	0	2.610576	0.517955	-0.466315
9	1	0	1.189570	2.142733	-0.671933
10	6	0	1.703277	-1.516531	0.448765
11	1	0	-0.396153	-1.497006	0.905842
12	6	0	2.791310	-0.801948	-0.049204
13	1	0	3.454217	1.087496	-0.849057
14	1	0	1.834455	-2.541267	0.786573
15	1	0	3.772399	-1.266652	-0.107939
16	1	0	-3.197517	1.023556	0.125019
17	6	0	-1.078015	1.134221	0.167416

Zero-point correction= 0.124939 (Hartree/Particle)
Thermal correction to Energy= 0.133929
Thermal correction to Enthalpy= 0.134873
Thermal correction to Gibbs Free Energy= 0.089806
Sum of electronic and zero-point Energies= -476.288461

Sum of electronic and thermal Energies=	-476.279471
Sum of electronic and thermal Enthalpies=	-476.278527
Sum of electronic and thermal Free Energies=	-476.323594

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.880829	-0.619753	-0.168600
2	6	0	-3.279898	-0.444010	-0.133624
3	7	0	-4.444494	-0.347844	-0.113126
4	8	0	-1.291279	1.617504	0.375583
5	6	0	0.494705	0.103479	0.040559
6	6	0	1.382172	1.167824	-0.150933
7	6	0	1.025423	-1.182803	0.192034
8	6	0	2.756877	0.954121	-0.218110
9	1	0	0.950962	2.161022	-0.234075
10	6	0	2.401753	-1.401087	0.135249
11	1	0	0.357267	-2.017649	0.380891
12	6	0	3.274867	-0.334108	-0.076330
13	1	0	3.429495	1.793773	-0.376355
14	1	0	2.794754	-2.406573	0.264351
15	1	0	4.347493	-0.504052	-0.121269
16	1	0	-1.524596	-1.593217	-0.477640
17	6	0	-0.994016	0.433266	0.104973

Zero-point correction=	0.125199 (Hartree/Particle)
Thermal correction to Energy=	0.134221
Thermal correction to Enthalpy=	0.135165
Thermal correction to Gibbs Free Energy=	0.090129
Sum of electronic and zero-point Energies=	-476.287790
Sum of electronic and thermal Energies=	-476.278768
Sum of electronic and thermal Enthalpies=	-476.277824
Sum of electronic and thermal Free Energies=	-476.322859

Complexes formed from a [Bmim] cation and the conjugate base anion of $PhCOCH_2CN$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.479365	0.033597	-0.618698

2	1	0	1.870728	-0.841617	-0.879582
3	6	0	4.107927	1.384932	0.017777
4	1	0	5.105632	1.660223	0.319841
5	6	0	2.983755	2.133272	-0.149039
6	1	0	2.808315	3.189011	-0.016123
7	7	0	3.769997	0.082561	-0.278573
8	7	0	1.985916	1.272945	-0.551467
9	6	0	4.680411	-1.063798	-0.263349
10	1	0	5.417116	-0.903949	0.523765
11	1	0	4.101911	-1.956747	-0.024914
12	1	0	5.176707	-1.149591	-1.231494
13	6	0	0.583196	1.650294	-0.802849
14	1	0	0.605684	2.558630	-1.413679
15	1	0	0.137128	0.832155	-1.375552
16	6	0	-0.100893	-2.096196	1.092825
17	1	0	-0.745407	-2.317066	1.931174
18	6	0	1.270455	-2.394793	1.212802
19	7	0	2.417999	-2.597711	1.290480
20	6	0	-0.178377	1.876540	0.498918
21	6	0	-1.603301	2.364197	0.235966
22	1	0	0.355587	2.612393	1.117076
23	1	0	-0.201580	0.932505	1.060106
24	6	0	-2.353974	2.644132	1.535443
25	1	0	-1.571960	3.276909	-0.374547
26	1	0	-2.143944	1.608529	-0.347047
27	1	0	-3.388076	2.939258	1.337506
28	1	0	-2.378113	1.748914	2.164770
29	1	0	-1.871918	3.446410	2.104718
30	6	0	-0.576032	-1.579141	-0.112566
31	8	0	0.130841	-1.394749	-1.150537
32	6	0	-2.022082	-1.157390	-0.203447
33	6	0	-2.809326	-0.872095	0.917317
34	6	0	-2.570333	-0.970419	-1.477451
35	6	0	-4.115323	-0.409455	0.768117
36	1	0	-2.392560	-0.980243	1.914380
37	6	0	-3.877761	-0.515299	-1.628956
38	1	0	-1.942328	-1.185182	-2.336374
39	6	0	-4.653690	-0.227909	-0.505444
40	1	0	-4.708643	-0.176449	1.647684
41	1	0	-4.292595	-0.380308	-2.623601
42	1	0	-5.669903	0.136834	-0.621085

Zero-point correction= 0.355428 (Hartree/Particle)
Thermal correction to Energy= 0.376519

Thermal correction to Enthalpy=	0.377464
Thermal correction to Gibbs Free Energy=	0.303732
Sum of electronic and zero-point Energies=	-899.207435
Sum of electronic and thermal Energies=	-899.186343
Sum of electronic and thermal Enthalpies=	-899.185399
Sum of electronic and thermal Free Energies=	-899.259130

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.094184	-1.106789	1.453444
2	6	0	-2.194456	0.429243	0.400081
3	6	0	-4.012478	1.185222	-0.601015
4	6	0	-2.931725	1.719380	-1.233519
5	7	0	-1.811468	1.237632	-0.591942
6	1	0	-1.509964	-0.156388	1.040155
7	1	0	-5.068942	1.296246	-0.784927
8	1	0	-2.864137	2.390747	-2.074310
9	7	0	-3.526393	0.392142	0.413733
10	6	0	-0.410115	1.498572	-0.963883
11	6	0	0.413354	2.027389	0.204756
12	1	0	-0.442415	2.223968	-1.782063
13	1	0	0.007633	0.559794	-1.343437
14	6	0	1.845089	2.344215	-0.227404
15	1	0	-0.067621	2.929265	0.607218
16	1	0	0.433900	1.270394	0.999460
17	1	0	2.311693	1.434891	-0.626330
18	1	0	1.830893	3.081352	-1.041935
19	6	0	-4.321906	-0.451859	1.303600
20	1	0	-3.649199	-0.896665	2.035853
21	1	0	-5.073317	0.162908	1.801326
22	1	0	-4.771183	-1.255599	0.720296
23	6	0	2.680011	2.875879	0.934415
24	1	0	2.697786	2.150511	1.753998
25	1	0	3.713605	3.057237	0.626809
26	1	0	2.269446	3.815309	1.320396
27	6	0	1.827961	-1.252066	0.081250
28	6	0	2.617687	-0.838355	1.159377
29	6	0	2.408331	-1.311935	-1.191887
30	6	0	3.955653	-0.499267	0.974732
31	1	0	2.149042	-0.783050	2.137245
32	6	0	3.745145	-0.966875	-1.380101

33	1	0	1.813367	-1.606783	-2.050859
34	6	0	4.524066	-0.557767	-0.297288
35	1	0	4.555179	-0.182998	1.823671
36	1	0	4.177623	-1.011719	-2.375296
37	6	0	-0.378796	-2.198274	-0.623643
38	6	0	-1.755748	-2.443699	-0.429902
39	7	0	-2.902293	-2.608590	-0.284212
40	1	0	0.071498	-2.609676	-1.515690
41	6	0	0.368688	-1.539221	0.354372
42	1	0	5.565103	-0.287215	-0.445832

Zero-point correction= 0.355231 (Hartree/Particle)
Thermal correction to Energy= 0.376172
Thermal correction to Enthalpy= 0.377116
Thermal correction to Gibbs Free Energy= 0.304985
Sum of electronic and zero-point Energies= -899.208055
Sum of electronic and thermal Energies= -899.187114
Sum of electronic and thermal Enthalpies= -899.186170
Sum of electronic and thermal Free Energies= -899.258301

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.593946	1.175416	-0.652121
2	6	0	-2.138123	1.460253	0.071087
3	6	0	-0.290313	1.643100	1.251692
4	6	0	-1.005765	0.596804	1.743551
5	7	0	-2.164158	0.506443	0.997880
6	1	0	-2.865385	1.599921	-0.711161
7	1	0	0.690943	2.015908	1.494521
8	1	0	-0.783172	-0.105095	2.530736
9	7	0	-1.027384	2.175648	0.218257
10	6	0	-3.091429	-0.630881	1.045497
11	6	0	-4.309973	-0.445289	0.156153
12	1	0	-3.385010	-0.764083	2.091823
13	1	0	-2.521635	-1.504532	0.712634
14	6	0	-5.265349	-1.631015	0.291206
15	1	0	-4.836443	0.481005	0.424729
16	1	0	-3.973820	-0.368495	-0.884451
17	1	0	-4.726364	-2.553556	0.044443
18	1	0	-5.591475	-1.723892	1.334943
19	6	0	-0.560756	3.217088	-0.693284

20	1	0	-1.339947	3.402847	-1.432064
21	1	0	-0.361502	4.128992	-0.128582
22	1	0	0.345235	2.837217	-1.169666
23	6	0	-6.482571	-1.489667	-0.619475
24	1	0	-6.177107	-1.427282	-1.668413
25	1	0	-7.157252	-2.343292	-0.515992
26	1	0	-7.048662	-0.583688	-0.379208
27	6	0	3.287923	-0.428435	-0.237932
28	6	0	4.281274	0.550124	-0.344355
29	6	0	3.638104	-1.691438	0.251214
30	6	0	5.598968	0.268720	0.006715
31	1	0	3.989576	1.529824	-0.709233
32	6	0	4.954544	-1.973747	0.610408
33	1	0	2.876120	-2.454862	0.373984
34	6	0	5.940917	-0.996153	0.484407
35	1	0	6.361495	1.035769	-0.093363
36	1	0	5.209858	-2.957362	0.993968
37	6	0	0.996203	-1.088943	-0.973844
38	6	0	-0.325302	-0.804737	-1.356139
39	7	0	-1.436047	-0.587159	-1.656763
40	1	0	1.321391	-2.116915	-1.050684
41	6	0	1.879520	-0.052158	-0.639977
42	1	0	6.967467	-1.218043	0.760825

Zero-point correction=	0.355354 (Hartree/Particle)
Thermal correction to Energy=	0.376793
Thermal correction to Enthalpy=	0.377737
Thermal correction to Gibbs Free Energy=	0.301676
Sum of electronic and zero-point Energies=	-899.197806
Sum of electronic and thermal Energies=	-899.176366
Sum of electronic and thermal Enthalpies=	-899.175422
Sum of electronic and thermal Free Energies=	-899.251483

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.053889	1.239969	-0.350618
2	6	0	1.315162	-1.469432	-0.056816
3	6	0	1.663306	-1.159347	-2.203234
4	6	0	0.331690	-1.010950	-1.971523
5	7	0	0.136648	-1.206846	-0.622183
6	1	0	1.502185	-1.604398	0.999835

7	1	0	2.242269	-1.046519	-3.105327
8	1	0	-0.483952	-0.758575	-2.630228
9	7	0	2.253696	-1.455649	-0.996577
10	6	0	-1.138214	-1.073173	0.089356
11	6	0	-1.977534	-2.343394	0.021949
12	1	0	-1.659975	-0.219475	-0.356524
13	1	0	-0.892989	-0.797015	1.119990
14	6	0	-3.312694	-2.164877	0.743529
15	1	0	-2.156126	-2.608393	-1.028584
16	1	0	-1.417425	-3.174200	0.469921
17	1	0	-3.124403	-1.891878	1.789204
18	1	0	-3.855133	-1.322895	0.295656
19	6	0	3.691313	-1.408529	-0.725280
20	1	0	3.884994	-1.887765	0.233298
21	1	0	4.216273	-1.921725	-1.531249
22	1	0	3.970739	-0.354408	-0.655568
23	6	0	-4.172798	-3.425163	0.685568
24	1	0	-3.659594	-4.270905	1.154080
25	1	0	-5.123760	-3.280522	1.204290
26	1	0	-4.394319	-3.700113	-0.350722
27	6	0	-0.078817	2.108926	0.203960
28	6	0	-0.323170	2.315440	-1.158308
29	6	0	-1.085554	2.435709	1.119786
30	6	0	-1.550236	2.808088	-1.599231
31	1	0	0.477784	2.073642	-1.850779
32	6	0	-2.312215	2.932914	0.683338
33	1	0	-0.920851	2.304496	2.184216
34	6	0	-2.553697	3.111796	-0.679252
35	1	0	-1.722668	2.963467	-2.660695
36	1	0	-3.080993	3.182329	1.408893
37	6	0	1.412817	1.023194	1.907035
38	6	0	2.525389	0.214170	2.206156
39	7	0	3.397076	-0.544898	2.382099
40	1	0	0.724015	1.250022	2.707076
41	6	0	1.238851	1.454725	0.580258
42	1	0	-3.510723	3.496243	-1.018942

Zero-point correction=	0.355111 (Hartree/Particle)
Thermal correction to Energy=	0.376466
Thermal correction to Enthalpy=	0.377410
Thermal correction to Gibbs Free Energy=	0.302723
Sum of electronic and zero-point Energies=	-899.200560
Sum of electronic and thermal Energies=	-899.179206
Sum of electronic and thermal Enthalpies=	-899.178262

Sum of electronic and thermal Free Energies= -899.252949

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.796295	1.358939	0.036314
2	6	0	2.078329	1.798356	0.095759
3	6	0	0.548441	1.111620	-1.325988
4	6	0	1.414321	0.085305	-1.108291
5	7	0	2.370251	0.541170	-0.223584
6	1	0	2.595525	2.389306	0.834774
7	1	0	-0.372513	1.165171	-1.882903
8	1	0	1.412073	-0.927639	-1.475951
9	7	0	0.995021	2.175763	-0.574618
10	6	0	3.378607	-0.282882	0.444027
11	6	0	4.406917	-0.838090	-0.533273
12	1	0	2.842073	-1.074774	0.976000
13	1	0	3.848522	0.346822	1.203842
14	6	0	5.447271	-1.703008	0.177218
15	1	0	3.901140	-1.434613	-1.303585
16	1	0	4.900695	-0.006073	-1.051058
17	1	0	5.947556	-1.106980	0.950750
18	1	0	4.941199	-2.525178	0.697826
19	6	0	0.267970	3.429223	-0.383223
20	1	0	0.862425	4.077440	0.260165
21	1	0	0.119107	3.906990	-1.352373
22	1	0	-0.688228	3.174394	0.080061
23	6	0	6.485171	-2.265757	-0.791016
24	1	0	7.018041	-1.459368	-1.304992
25	1	0	7.224833	-2.877457	-0.268464
26	1	0	6.009919	-2.891567	-1.553258
27	6	0	-3.340081	-0.433875	0.156536
28	6	0	-4.335967	0.350863	-0.433256
29	6	0	-3.565536	-1.806792	0.303485
30	6	0	-5.538181	-0.216462	-0.847401
31	1	0	-4.139018	1.411097	-0.556062
32	6	0	-4.764959	-2.378578	-0.116433
33	1	0	-2.793028	-2.440350	0.728304
34	6	0	-5.757616	-1.584656	-0.689487
35	1	0	-6.305889	0.408495	-1.294715
36	1	0	-4.922463	-3.447102	-0.001338
37	6	0	-1.262470	-0.384483	1.540117

38	6	0	-0.061575	0.204780	1.972644
39	7	0	0.949037	0.673452	2.332890
40	1	0	-1.584093	-1.280826	2.051329
41	6	0	-2.059769	0.250785	0.579227
42	1	0	-6.692919	-2.030096	-1.015547

Zero-point correction= 0.355203 (Hartree/Particle)
Thermal correction to Energy= 0.376591
Thermal correction to Enthalpy= 0.377535
Thermal correction to Gibbs Free Energy= 0.301409
Sum of electronic and zero-point Energies= -899.196707
Sum of electronic and thermal Energies= -899.175320
Sum of electronic and thermal Enthalpies= -899.174375
Sum of electronic and thermal Free Energies= -899.250501

Conform 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.242166	0.470822	-1.258561
2	6	0	0.741743	-0.051474	1.346733
3	6	0	1.144336	-1.857461	0.164276
4	6	0	-0.028404	-2.046057	0.825918
5	7	0	-0.262366	-0.903271	1.558698
6	1	0	0.816681	0.957247	1.730041
7	1	0	1.659496	-2.483087	-0.545617
8	1	0	-0.725568	-2.868477	0.819535
9	7	0	1.611069	-0.610736	0.513763
10	6	0	-1.455009	-0.621113	2.352676
11	1	0	-2.321567	-1.030473	1.829926
12	1	0	-1.569727	0.462139	2.414753
13	6	0	2.701784	0.118191	-0.152365
14	1	0	2.779847	1.087316	0.346980
15	1	0	2.349725	0.313861	-1.170757
16	6	0	-2.545500	0.426053	-0.705390
17	6	0	-2.619276	-0.883476	-1.193382
18	6	0	-3.713147	1.023203	-0.216142
19	6	0	-3.818768	-1.592270	-1.164785
20	1	0	-1.708924	-1.316245	-1.597574
21	6	0	-4.916030	0.319774	-0.192015
22	1	0	-3.695523	2.047524	0.141415
23	6	0	-4.971984	-0.994585	-0.656434
24	1	0	-3.858668	-2.607927	-1.548692

25	1	0	-5.813496	0.800385	0.186177
26	6	0	-1.018599	2.259314	0.069258
27	6	0	0.279361	2.768194	0.259821
28	7	0	1.381135	3.090856	0.482430
29	1	0	-1.839608	2.783137	0.535934
30	6	0	-1.175818	1.081605	-0.684255
31	1	0	-5.909491	-1.542007	-0.635294
32	1	0	-1.360716	-1.060839	3.347147
33	6	0	4.015599	-0.648627	-0.110052
34	6	0	5.133958	0.142954	-0.787924
35	1	0	3.908957	-1.620140	-0.611044
36	1	0	4.285214	-0.855934	0.933565
37	6	0	6.465758	-0.602691	-0.759697
38	1	0	4.848224	0.355809	-1.825085
39	1	0	5.239481	1.114618	-0.290994
40	1	0	7.254792	-0.024935	-1.247616
41	1	0	6.782154	-0.800304	0.269793
42	1	0	6.387155	-1.565386	-1.275788

Zero-point correction= 0.355450 (Hartree/Particle)
Thermal correction to Energy= 0.376712
Thermal correction to Enthalpy= 0.377657
Thermal correction to Gibbs Free Energy= 0.303420
Sum of electronic and zero-point Energies= -899.198766
Sum of electronic and thermal Energies= -899.177504
Sum of electronic and thermal Enthalpies= -899.176560
Sum of electronic and thermal Free Energies= -899.250796

Conformer 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.556206	0.392844	0.295572
2	6	0	3.404459	-0.494372	0.102165
3	6	0	1.687717	-0.208511	-1.237253
4	6	0	2.280645	-1.391934	-1.554809
5	7	0	3.360836	-1.545055	-0.713513
6	1	0	4.094155	-0.370010	0.922248
7	1	0	0.786554	0.255648	-1.601332
8	1	0	2.014291	-2.142568	-2.280983
9	7	0	2.420726	0.341956	-0.209816
10	6	0	4.104697	-2.780437	-0.505428
11	1	0	3.533178	-3.407191	0.183464

12	1	0	5.077841	-2.543823	-0.075077
13	6	0	2.060734	1.528191	0.586013
14	1	0	2.978798	1.857127	1.083673
15	1	0	1.325834	1.188260	1.320307
16	6	0	-2.700455	-0.602054	0.143538
17	6	0	-3.310115	0.654585	0.078869
18	6	0	-3.466837	-1.737208	-0.140932
19	6	0	-4.660275	0.775898	-0.238497
20	1	0	-2.697064	1.526563	0.284443
21	6	0	-4.816385	-1.618189	-0.467446
22	1	0	-3.003699	-2.719156	-0.130457
23	6	0	-5.419133	-0.361867	-0.511995
24	1	0	-5.122401	1.758290	-0.275219
25	1	0	-5.396572	-2.507737	-0.694809
26	6	0	-0.726880	-1.850825	1.023527
27	6	0	0.630132	-1.967126	1.371035
28	7	0	1.759378	-2.089042	1.656528
29	1	0	-1.368859	-2.686404	1.264458
30	6	0	-1.231223	-0.655616	0.494511
31	1	0	-6.471399	-0.270298	-0.764448
32	1	0	4.245433	-3.275157	-1.466273
33	6	0	1.468570	2.637338	-0.267361
34	6	0	1.132210	3.857534	0.588998
35	1	0	0.544851	2.265163	-0.721845
36	1	0	2.168885	2.916592	-1.066252
37	6	0	0.481667	4.968096	-0.232202
38	1	0	0.453000	3.546430	1.391810
39	1	0	2.043109	4.236744	1.070634
40	1	0	0.243223	5.835952	0.388281
41	1	0	1.144948	5.302076	-1.037214
42	1	0	-0.448209	4.614717	-0.688772

Zero-point correction= 0.355067 (Hartree/Particle)
Thermal correction to Energy= 0.376471
Thermal correction to Enthalpy= 0.377415
Thermal correction to Gibbs Free Energy= 0.301158
Sum of electronic and zero-point Energies= -899.198920
Sum of electronic and thermal Energies= -899.177516
Sum of electronic and thermal Enthalpies= -899.176572
Sum of electronic and thermal Free Energies= -899.252829

Conformer 8

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-0.731473	-0.714309	-0.459053
2	6	0	2.058638	-0.953833	-0.450236
3	6	0	3.669023	-2.451623	-0.232969
4	6	0	4.219756	-1.214677	-0.097715
5	7	0	3.200031	-0.298372	-0.246359
6	1	0	1.033822	-0.562727	-0.528967
7	1	0	4.111389	-3.433937	-0.190011
8	1	0	5.235829	-0.910419	0.096523
9	7	0	2.321491	-2.260352	-0.453797
10	6	0	3.302058	1.146116	0.013592
11	6	0	2.130593	1.922308	-0.569649
12	1	0	4.250082	1.482399	-0.418154
13	1	0	3.323582	1.264715	1.101347
14	6	0	2.253458	3.411718	-0.249844
15	1	0	2.083507	1.770977	-1.656092
16	1	0	1.192839	1.548011	-0.142351
17	1	0	2.309045	3.536085	0.838508
18	1	0	3.191457	3.805234	-0.663063
19	6	0	1.288561	-3.285012	-0.600603
20	1	0	0.325632	-2.770519	-0.658589
21	1	0	1.471952	-3.864703	-1.506716
22	1	0	1.306508	-3.935746	0.274690
23	6	0	1.070456	4.206921	-0.796861
24	1	0	0.130483	3.838886	-0.374339
25	1	0	1.159303	5.268943	-0.553592
26	1	0	1.006319	4.114566	-1.885937
27	6	0	-2.967862	-0.190910	0.125889
28	6	0	-3.350296	-0.236151	-1.218366
29	6	0	-3.961671	-0.116330	1.107821
30	6	0	-4.694612	-0.181629	-1.576782
31	1	0	-2.568678	-0.318129	-1.966695
32	6	0	-5.307500	-0.068794	0.751681
33	1	0	-3.687496	-0.120120	2.158146
34	6	0	-5.678421	-0.096049	-0.592255
35	1	0	-4.976912	-0.208693	-2.625311
36	1	0	-6.068290	-0.017648	1.525032
37	6	0	-1.060999	0.225131	1.682760
38	6	0	0.305599	0.141528	2.010772
39	7	0	1.448703	0.063980	2.244196
40	1	0	-1.727536	0.680748	2.400144
41	6	0	-1.495920	-0.247350	0.444236
42	1	0	-6.727785	-0.058436	-0.869237

Zero-point correction=	0.355064 (Hartree/Particle)
Thermal correction to Energy=	0.376574
Thermal correction to Enthalpy=	0.377519
Thermal correction to Gibbs Free Energy=	0.300234
Sum of electronic and zero-point Energies=	-899.204599
Sum of electronic and thermal Energies=	-899.183089
Sum of electronic and thermal Enthalpies=	-899.182145
Sum of electronic and thermal Free Energies=	-899.259429

9-COOMeFl
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553678	3.572308	0.285565
2	6	0	-1.758008	2.987605	-0.111986
3	6	0	-1.816866	1.632190	-0.447843
4	6	0	-0.652779	0.880055	-0.374704
5	6	0	0.559506	1.464315	0.026205
6	6	0	0.615785	2.815455	0.357135
7	1	0	-0.528279	4.626771	0.542515
8	1	0	-2.658213	3.592220	-0.160140
9	1	0	-2.751754	1.174534	-0.756385
10	1	0	1.550554	3.273647	0.667391
11	6	0	-0.430681	-0.592892	-0.697299
12	6	0	1.038753	-0.780962	-0.396263
13	6	0	1.806536	-1.933419	-0.480708
14	6	0	3.165006	-1.856493	-0.167504
15	6	0	3.738203	-0.644337	0.226058
16	6	0	2.965029	0.511949	0.319820
17	6	0	1.609753	0.434164	0.009104
18	1	0	1.359659	-2.879868	-0.770786
19	1	0	3.781177	-2.748290	-0.223385
20	1	0	4.796058	-0.605078	0.466794
21	1	0	3.412810	1.450686	0.633245
22	6	0	-1.346245	-1.504195	0.102325
23	8	0	-1.012374	-2.248565	0.988401
24	8	0	-2.618377	-1.375856	-0.316589
25	6	0	-3.576201	-2.162501	0.397684
26	1	0	-4.535757	-1.958723	-0.074066
27	1	0	-3.324980	-3.222450	0.322930
28	1	0	-3.592073	-1.871935	1.450159

29	1	0	-0.647870	-0.775600	-1.758304

Zero-point correction= 0.233284 (Hartree/Particle)
Thermal correction to Energy= 0.246675
Thermal correction to Enthalpy= 0.247619
Thermal correction to Gibbs Free Energy= 0.192476
Sum of electronic and zero-point Energies= -728.792939
Sum of electronic and thermal Energies= -728.779548
Sum of electronic and thermal Enthalpies= -728.778604
Sum of electronic and thermal Free Energies= -728.833747

Conformer b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.850382	-2.216612	0.464096
2	6	0	3.386684	-1.060918	-0.109153
3	6	0	2.549589	-0.057928	-0.605321
4	6	0	1.177552	-0.240104	-0.515460
5	6	0	0.633266	-1.394766	0.066744
6	6	0	1.469811	-2.393993	0.557601
7	1	0	3.517391	-2.984848	0.842706
8	1	0	4.463796	-0.941246	-0.169817
9	1	0	2.960400	0.845413	-1.048312
10	1	0	1.059521	-3.293875	1.006650
11	6	0	0.062569	0.689808	-0.974453
12	6	0	-1.181596	-0.071252	-0.569686
13	6	0	-2.512110	0.286103	-0.733470
14	6	0	-3.502426	-0.593283	-0.290799
15	6	0	-3.158254	-1.809667	0.304771
16	6	0	-1.821426	-2.169712	0.469430
17	6	0	-0.833965	-1.291524	0.029440
18	1	0	-2.781949	1.232997	-1.193793
19	1	0	-4.548830	-0.330677	-0.410079
20	1	0	-3.941274	-2.481467	0.642548
21	1	0	-1.559564	-3.116520	0.933144
22	6	0	0.251940	2.056119	-0.339381
23	8	0	0.864909	2.956555	-0.863578
24	8	0	-0.277696	2.131964	0.885465
25	6	0	-0.041065	3.359283	1.579911
26	1	0	-0.529553	3.247457	2.545878
27	1	0	1.031992	3.520208	1.704098
28	1	0	-0.467241	4.196770	1.023639
29	1	0	0.111905	0.848320	-2.057381

Zero-point correction=	0.233145 (Hartree/Particle)
Thermal correction to Energy=	0.246632
Thermal correction to Enthalpy=	0.247577
Thermal correction to Gibbs Free Energy=	0.191741
Sum of electronic and zero-point Energies=	-728.793110
Sum of electronic and thermal Energies=	-728.779623
Sum of electronic and thermal Enthalpies=	-728.778679
Sum of electronic and thermal Free Energies=	-728.834515

The conjugate base anion of 9-COOMeFl.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.363210	3.685218	-0.000078
2	6	0	-1.001122	3.337483	-0.000041
3	6	0	-1.413836	2.011432	0.000003
4	6	0	-0.450940	0.980246	0.000009
5	6	0	0.935694	1.343633	-0.000026
6	6	0	1.328831	2.684380	-0.000070
7	1	0	0.658130	4.731382	-0.000114
8	1	0	-1.750415	4.126659	-0.000046
9	1	0	-2.469269	1.762785	0.000040
10	1	0	2.386598	2.942804	-0.000100
11	6	0	-0.548397	-0.455798	0.000039
12	6	0	0.792196	-0.972738	0.000008
13	6	0	1.295826	-2.289357	0.000017
14	6	0	2.670014	-2.490037	-0.000001
15	6	0	3.573293	-1.408989	-0.000029
16	6	0	3.091959	-0.104028	-0.000041
17	6	0	1.712364	0.120879	-0.000024
18	1	0	0.603030	-3.124050	0.000032
19	1	0	3.059022	-3.506227	0.000008
20	1	0	4.643919	-1.596708	-0.000041
21	1	0	3.784762	0.735926	-0.000063
22	6	0	-1.710465	-1.276017	0.000072
23	8	0	-1.763039	-2.505924	-0.000003
24	8	0	-2.890832	-0.551759	0.000143
25	6	0	-4.065207	-1.336975	0.000025
26	1	0	-4.898753	-0.630873	-0.000070
27	1	0	-4.113193	-1.978123	-0.885949
28	1	0	-4.113388	-1.978101	0.886007

Zero-point correction=	0.219227 (Hartree/Particle)
Thermal correction to Energy=	0.232472
Thermal correction to Enthalpy=	0.233416
Thermal correction to Gibbs Free Energy=	0.179150
Sum of electronic and zero-point Energies=	-728.272678
Sum of electronic and thermal Energies=	-728.259433
Sum of electronic and thermal Enthalpies=	-728.258489
Sum of electronic and thermal Free Energies=	-728.312755

Complexes formed from a [Bmim] cation and the conjugate base anion of 9-COOMeFl.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.880810	3.931879	0.412618
2	6	0	-2.082888	3.400875	-0.096536
3	6	0	-2.409697	2.059749	0.063341
4	6	0	-1.509057	1.204428	0.729878
5	6	0	-0.316797	1.760049	1.291150
6	6	0	-0.007366	3.114195	1.122554
7	1	0	-0.653513	4.984416	0.274540
8	1	0	-2.776556	4.061065	-0.611682
9	1	0	-3.345786	1.662697	-0.315630
10	1	0	0.908150	3.526009	1.542578
11	6	0	-1.507032	-0.216694	0.945110
12	6	0	-0.303786	-0.534439	1.670935
13	6	0	0.270116	-1.753039	2.092384
14	6	0	1.503573	-1.742988	2.732235
15	6	0	2.194228	-0.541193	2.987473
16	6	0	1.646475	0.669262	2.580962
17	6	0	0.419175	0.677595	1.910277
18	1	0	-0.254855	-2.686581	1.923666
19	1	0	1.937625	-2.683597	3.061421
20	1	0	3.144866	-0.564091	3.511564
21	1	0	2.174218	1.601894	2.771191
22	6	0	-0.029283	0.618119	-1.757768
23	6	0	-0.873336	-1.359364	-2.226249
24	6	0	0.316803	-1.548858	-1.596282
25	7	0	0.831179	-0.301011	-1.323146
26	1	0	0.069416	1.688680	-1.625425
27	1	0	-1.618083	-2.059015	-2.570409
28	1	0	0.818261	-2.449021	-1.277868

29	7	0	-1.063467	0.000310	-2.327466
30	6	0	2.109011	-0.044986	-0.647004
31	6	0	3.301882	-0.325052	-1.552267
32	1	0	2.127715	-0.670019	0.251529
33	1	0	2.086831	0.996491	-0.314432
34	6	0	4.613764	-0.065083	-0.812298
35	1	0	3.271402	-1.369163	-1.891055
36	1	0	3.243835	0.304181	-2.450065
37	1	0	4.639797	0.980984	-0.482351
38	1	0	4.637959	-0.675752	0.098556
39	6	0	-2.254651	0.641758	-2.881229
40	1	0	-2.339036	0.382869	-3.938216
41	1	0	-3.116411	0.292659	-2.308235
42	1	0	-2.149209	1.719826	-2.762512
43	6	0	5.835885	-0.366400	-1.676131
44	1	0	5.838807	0.250357	-2.580730
45	1	0	6.763770	-0.169200	-1.133339
46	1	0	5.845920	-1.416093	-1.987175
47	6	0	-2.464103	-1.103879	0.380836
48	8	0	-3.388913	-0.806963	-0.384148
49	8	0	-2.263663	-2.418299	0.718896
50	6	0	-3.235012	-3.326152	0.223268
51	1	0	-2.956177	-4.304528	0.615882
52	1	0	-4.236535	-3.050325	0.562429
53	1	0	-3.238352	-3.346426	-0.871472

Zero-point correction=	0.450307 (Hartree/Particle)
Thermal correction to Energy=	0.475460
Thermal correction to Enthalpy=	0.476404
Thermal correction to Gibbs Free Energy=	0.395590
Sum of electronic and zero-point Energies=	-1151.185598
Sum of electronic and thermal Energies=	-1151.160445
Sum of electronic and thermal Enthalpies=	-1151.159501
Sum of electronic and thermal Free Energies=	-1151.240315

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.460287	3.769162	-0.997907
2	6	0	0.547654	3.024917	-1.642959
3	6	0	0.454258	1.645824	-1.785326
4	6	0	-0.662667	0.971154	-1.252519

5	6	0	−1.705596	1.736930	−0.643354
6	6	0	−1.595206	3.125983	−0.514344
7	1	0	−0.361465	4.846322	−0.904754
8	1	0	1.410008	3.545392	−2.052684
9	1	0	1.227373	1.082057	−2.297681
10	1	0	−2.389781	3.699181	−0.040536
11	6	0	−0.983316	−0.425437	−1.139894
12	6	0	−2.254112	−0.516766	−0.467379
13	6	0	−3.027311	−1.608514	−0.017706
14	6	0	−4.213468	−1.371047	0.666294
15	6	0	−4.675637	−0.062893	0.912896
16	6	0	−3.927128	1.025699	0.482384
17	6	0	−2.715963	0.807814	−0.182112
18	1	0	−2.700333	−2.622703	−0.218053
19	1	0	−4.809290	−2.215766	1.002265
20	1	0	−5.619411	0.090002	1.427143
21	1	0	−4.275008	2.039536	0.670836
22	6	0	0.602124	0.659933	1.405672
23	6	0	1.230651	−1.441390	1.239577
24	6	0	0.058111	−1.407427	1.927732
25	7	0	−0.309715	−0.084539	2.029967
26	1	0	0.550865	1.731928	1.260994
27	1	0	1.831154	−2.270185	0.900429
28	1	0	−0.569036	−2.198531	2.306714
29	7	0	1.556727	−0.139492	0.932902
30	6	0	−1.509271	0.405759	2.707061
31	1	0	−2.363286	−0.199061	2.394247
32	1	0	−1.682833	1.435905	2.396772
33	6	0	2.727941	0.279730	0.152421
34	1	0	2.652486	−0.233403	−0.811729
35	1	0	2.613607	1.352040	−0.026968
36	6	0	−0.095726	−1.473635	−1.506645
37	8	0	1.062203	−1.353312	−1.922471
38	8	0	−0.616591	−2.728745	−1.315802
39	6	0	0.220599	−3.799012	−1.724307
40	1	0	−0.349081	−4.710572	−1.540835
41	1	0	0.473919	−3.714480	−2.784051
42	1	0	1.153098	−3.815487	−1.150788
43	1	0	−1.361660	0.347699	3.787464
44	6	0	4.029532	−0.027841	0.883493
45	6	0	5.240763	0.422494	0.067591
46	1	0	4.101446	−1.106394	1.075083
47	1	0	4.029463	0.470662	1.861645
48	6	0	6.558613	0.114964	0.774637

49	1	0	5.219205	-0.070871	-0.911584
50	1	0	5.166360	1.500027	-0.125027
51	1	0	7.414468	0.444244	0.180059
52	1	0	6.609861	0.619016	1.745174
53	1	0	6.666549	-0.960289	0.950130

Zero-point correction= 0.450144 (Hartree/Particle)
Thermal correction to Energy= 0.475234
Thermal correction to Enthalpy= 0.476178
Thermal correction to Gibbs Free Energy= 0.395408
Sum of electronic and zero-point Energies= -1151.184801
Sum of electronic and thermal Energies= -1151.159711
Sum of electronic and thermal Enthalpies= -1151.158767
Sum of electronic and thermal Free Energies= -1151.239537

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.135596	-0.522461	3.089798
2	6	0	2.237174	0.837277	2.736060
3	6	0	1.226873	1.483866	2.036038
4	6	0	0.077693	0.762145	1.652508
5	6	0	-0.028765	-0.612847	2.036051
6	6	0	0.995470	-1.243258	2.750700
7	1	0	2.937528	-0.998769	3.645677
8	1	0	3.122961	1.395935	3.026845
9	1	0	1.319598	2.532790	1.777320
10	1	0	0.902380	-2.288960	3.036782
11	6	0	-1.070684	1.102790	0.849451
12	6	0	-1.908533	-0.067216	0.789806
13	6	0	-3.158799	-0.300887	0.185289
14	6	0	-3.722408	-1.568826	0.257667
15	6	0	-3.074749	-2.621802	0.933597
16	6	0	-1.858993	-2.396100	1.570758
17	6	0	-1.276852	-1.127091	1.507462
18	1	0	-3.669125	0.512587	-0.321398
19	1	0	-4.694205	-1.748429	-0.196960
20	1	0	-3.543494	-3.600135	0.985316
21	1	0	-1.370500	-3.199953	2.117818
22	6	0	-0.186585	0.097252	-1.859998
23	6	0	-1.049067	-1.925771	-1.924716
24	6	0	0.154030	-1.999059	-1.293825

25	7	0	0.680575	-0.726738	-1.274431
26	1	0	-0.081839	1.167891	-1.959211
27	1	0	-1.808185	-2.673466	-2.088544
28	1	0	0.652519	-2.825507	-0.812771
29	7	0	-1.236426	-0.607026	-2.278008
30	6	0	1.967795	-0.332479	-0.686943
31	6	0	3.146449	-0.757715	-1.553483
32	1	0	2.021380	-0.773091	0.313946
33	1	0	1.933282	0.751665	-0.550901
34	6	0	4.469079	-0.350048	-0.905478
35	1	0	3.125797	-1.846283	-1.697193
36	1	0	3.057231	-0.303163	-2.548994
37	1	0	4.477922	0.736942	-0.757448
38	1	0	4.530702	-0.795505	0.095068
39	6	0	-2.410821	-0.042904	-2.943628
40	1	0	-2.251535	-0.030405	-4.023821
41	1	0	-3.267951	-0.667521	-2.693550
42	1	0	-2.572502	0.961159	-2.545149
43	6	0	5.676234	-0.770037	-1.740620
44	1	0	5.643313	-0.312579	-2.734923
45	1	0	6.612562	-0.469088	-1.263885
46	1	0	5.701485	-1.856492	-1.873559
47	6	0	-1.279024	2.260029	0.054304
48	8	0	-2.116501	2.392114	-0.849622
49	8	0	-0.383607	3.270376	0.295232
50	6	0	-0.571190	4.447104	-0.478128
51	1	0	0.187102	5.151239	-0.134749
52	1	0	-0.442947	4.244551	-1.545914
53	1	0	-1.571187	4.859250	-0.323628

Zero-point correction= 0.449932 (Hartree/Particle)
Thermal correction to Energy= 0.475387
Thermal correction to Enthalpy= 0.476331
Thermal correction to Gibbs Free Energy= 0.394204
Sum of electronic and zero-point Energies= -1151.183997
Sum of electronic and thermal Energies= -1151.158542
Sum of electronic and thermal Enthalpies= -1151.157598
Sum of electronic and thermal Free Energies= -1151.239724

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	−0.317752	3.900243	−0.572326
2	6	0	0.623814	3.184872	−1.336295
3	6	0	0.450666	1.834967	−1.621905
4	6	0	−0.683536	1.167916	−1.122753
5	6	0	−1.656253	1.907096	−0.385149
6	6	0	−1.465546	3.263200	−0.108394
7	1	0	−0.160230	4.955367	−0.370255
8	1	0	1.496335	3.705102	−1.724800
9	1	0	1.174259	1.289257	−2.219267
10	1	0	−2.205620	3.818194	0.464229
11	6	0	−1.081186	−0.217226	−1.162423
12	6	0	−2.349789	−0.314748	−0.477357
13	6	0	−3.225541	−1.389820	−0.223763
14	6	0	−4.373071	−1.176118	0.530391
15	6	0	−4.688004	0.094634	1.044916
16	6	0	−3.853501	1.175073	0.779814
17	6	0	−2.697444	0.981280	0.018278
18	1	0	−3.004631	−2.374987	−0.620846
19	1	0	−5.048734	−2.006889	0.717391
20	1	0	−5.593792	0.233912	1.627105
21	1	0	−4.104335	2.165409	1.154024
22	6	0	1.051330	−1.221030	1.046311
23	6	0	−0.263434	0.192803	2.099485
24	6	0	0.766987	0.898752	1.556350
25	7	0	1.577999	−0.005540	0.911062
26	1	0	1.430402	−2.120541	0.583641
27	1	0	−1.153320	0.519785	2.614463
28	1	0	0.941519	1.963767	1.498664
29	7	0	−0.063179	−1.127874	1.769409
30	6	0	2.777814	0.303365	0.121070
31	6	0	4.053598	−0.146318	0.823944
32	1	0	2.765328	1.385185	−0.033873
33	1	0	2.639103	−0.175693	−0.854160
34	6	0	5.293611	0.218940	0.008906
35	1	0	4.108815	0.316432	1.817876
36	1	0	4.025331	−1.233302	0.978790
37	1	0	5.215666	−0.231731	−0.987905
38	1	0	5.318649	1.305284	−0.142070
39	6	0	−0.984601	−2.228329	2.047875
40	1	0	−0.659467	−2.774131	2.935493
41	1	0	−1.979018	−1.805565	2.192582
42	1	0	−1.018935	−2.875496	1.169731
43	6	0	6.583999	−0.237297	0.685312
44	1	0	6.592955	−1.323950	0.818251

45	1	0	7.460522	0.034671	0.091989
46	1	0	6.691947	0.221388	1.673537
47	6	0	-0.228106	-1.261287	-1.589486
48	8	0	0.927102	-1.160800	-2.022639
49	8	0	-0.755948	-2.525990	-1.392706
50	6	0	0.013722	-3.589679	-1.932613
51	1	0	-0.558791	-4.499062	-1.745048
52	1	0	0.169100	-3.453573	-3.005860
53	1	0	0.997297	-3.658353	-1.455318

Zero-point correction= 0.449565 (Hartree/Particle)
Thermal correction to Energy= 0.474994
Thermal correction to Enthalpy= 0.475938
Thermal correction to Gibbs Free Energy= 0.393361
Sum of electronic and zero-point Energies= -1151.180915
Sum of electronic and thermal Energies= -1151.155486
Sum of electronic and thermal Enthalpies= -1151.154542
Sum of electronic and thermal Free Energies= -1151.237119

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.656139	-0.043583	1.039718
2	6	0	-4.300136	1.310090	0.884210
3	6	0	-3.155325	1.686013	0.193778
4	6	0	-2.320482	0.692442	-0.357396
5	6	0	-2.699429	-0.680308	-0.212573
6	6	0	-3.860443	-1.037971	0.481378
7	1	0	-5.562243	-0.306346	1.576929
8	1	0	-4.942872	2.078346	1.305793
9	1	0	-2.900448	2.733492	0.077624
10	1	0	-4.139634	-2.084910	0.581638
11	6	0	-1.053439	0.746979	-1.044088
12	6	0	-0.684844	-0.608545	-1.362133
13	6	0	0.418471	-1.148463	-2.050961
14	6	0	0.538159	-2.527697	-2.167679
15	6	0	-0.427807	-3.396549	-1.622896
16	6	0	-1.544501	-2.877868	-0.976411
17	6	0	-1.680537	-1.492691	-0.847760
18	1	0	1.157798	-0.482847	-2.485681
19	1	0	1.384067	-2.947134	-2.707814
20	1	0	-0.314516	-4.470528	-1.738654

21	1	0	-2.306435	-3.546184	-0.580449
22	6	0	0.793358	0.272838	1.278773
23	6	0	1.168474	-1.892372	1.185684
24	6	0	0.043408	-1.691402	1.923609
25	7	0	-0.166744	-0.331128	1.978639
26	1	0	0.880807	1.335321	1.103422
27	1	0	1.641434	-2.801333	0.849643
28	1	0	-0.650064	-2.389841	2.363751
29	7	0	1.624671	-0.650829	0.801110
30	6	0	-1.266300	0.341881	2.670398
31	1	0	-2.208443	-0.140378	2.400673
32	1	0	-1.305539	1.375504	2.328493
33	6	0	2.814282	-0.373001	-0.015167
34	1	0	2.978411	-1.263699	-0.628168
35	1	0	2.549519	0.451552	-0.684942
36	6	0	-0.186359	1.859623	-1.206583
37	8	0	1.006175	1.823583	-1.539749
38	8	0	-0.754738	3.061668	-0.869647
39	6	0	0.075580	4.199554	-1.053572
40	1	0	-0.533260	5.059603	-0.774091
41	1	0	0.967928	4.146601	-0.422630
42	1	0	0.395512	4.282263	-2.095222
43	1	0	-1.095563	0.297662	3.747908
44	6	0	4.027573	-0.053575	0.852043
45	6	0	5.271443	0.197618	0.001429
46	1	0	4.211875	-0.880326	1.550866
47	1	0	3.812242	0.835652	1.459299
48	6	0	6.487350	0.558297	0.852088
49	1	0	5.489059	-0.697409	-0.594766
50	1	0	5.063549	1.004034	-0.712102
51	1	0	7.371004	0.726990	0.231396
52	1	0	6.303140	1.470821	1.428223
53	1	0	6.721546	-0.243076	1.560461

Zero-point correction= 0.449532 (Hartree/Particle)
Thermal correction to Energy= 0.474969
Thermal correction to Enthalpy= 0.475913
Thermal correction to Gibbs Free Energy= 0.393605
Sum of electronic and zero-point Energies= -1151.183621
Sum of electronic and thermal Energies= -1151.158184
Sum of electronic and thermal Enthalpies= -1151.157240
Sum of electronic and thermal Free Energies= -1151.239548

$CH_2(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.846127	0.000000
2	1	0	-0.000026	1.489040	0.885203
3	1	0	-0.000026	1.489040	-0.885203
4	6	0	-1.218897	0.025657	0.000000
5	7	0	-2.190051	-0.597350	0.000000
6	6	0	1.218943	0.025736	0.000000
7	7	0	2.190019	-0.597392	0.000000

Zero-point correction= 0.045444 (Hartree/Particle)
Thermal correction to Energy= 0.050253
Thermal correction to Enthalpy= 0.051198
Thermal correction to Gibbs Free Energy= 0.017781
Sum of electronic and zero-point Energies= -224.853087
Sum of electronic and thermal Energies= -224.848278
Sum of electronic and thermal Enthalpies= -224.847334
Sum of electronic and thermal Free Energies= -224.880750

The conjugate base anion of $CH_2(CN)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000023	0.726028	-0.000163
2	1	0	-0.000991	1.807457	0.000952
3	6	0	1.225348	0.052128	-0.000174
4	7	0	2.268991	-0.484821	0.000143
5	6	0	-1.225179	0.051771	-0.000137
6	7	0	-2.269013	-0.484754	0.000126

Zero-point correction= 0.031870 (Hartree/Particle)
Thermal correction to Energy= 0.036570
Thermal correction to Enthalpy= 0.037514
Thermal correction to Gibbs Free Energy= 0.004508
Sum of electronic and zero-point Energies= -224.328403
Sum of electronic and thermal Energies= -224.323703
Sum of electronic and thermal Enthalpies= -224.322759
Sum of electronic and thermal Free Energies= -224.355765.

Complexes formed from a [Bmim] cation and the conjugate base anion of $CH_2(CN)_2$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606869	-0.666755	0.991052
2	6	0	1.335579	-1.734627	-0.791515
3	6	0	0.134817	-1.174179	-1.095949
4	7	0	-0.305533	-0.519791	0.034758
5	1	0	0.569266	-0.189978	1.959612
6	1	0	2.046536	-2.270396	-1.398812
7	1	0	-0.422430	-1.155750	-2.018136
8	7	0	1.604365	-1.413686	0.520411
9	6	0	-1.492964	0.337934	0.119053
10	6	0	-2.782575	-0.447422	-0.079681
11	1	0	-1.364658	1.118911	-0.638468
12	1	0	-1.452690	0.833094	1.091734
13	6	0	-4.004488	0.467914	-0.006095
14	1	0	-2.766804	-0.956536	-1.052541
15	1	0	-2.854355	-1.229648	0.686718
16	1	0	-4.015144	0.978983	0.964319
17	1	0	-3.914721	1.251684	-0.768142
18	6	0	2.857990	-1.702560	1.212867
19	1	0	2.974349	-2.781976	1.319862
20	1	0	3.669079	-1.269393	0.623249
21	1	0	2.824318	-1.233600	2.195865
22	6	0	-5.310727	-0.297484	-0.202297
23	1	0	-5.432230	-1.068057	0.565714
24	1	0	-6.173823	0.370481	-0.146239
25	1	0	-5.332402	-0.792255	-1.178785
26	6	0	1.701608	2.056071	-0.820862
27	6	0	1.144174	2.218175	0.448706
28	7	0	0.650045	2.267559	1.512827
29	6	0	2.734861	1.127661	-0.987343
30	7	0	3.569530	0.313678	-1.113737
31	1	0	1.465987	2.751744	-1.613371

Zero-point correction= 0.261503 (Hartree/Particle)
Thermal correction to Energy= 0.278600
Thermal correction to Enthalpy= 0.279544
Thermal correction to Gibbs Free Energy= 0.214838
Sum of electronic and zero-point Energies= -647.234005
Sum of electronic and thermal Energies= -647.216908
Sum of electronic and thermal Enthalpies= -647.215964
Sum of electronic and thermal Free Energies= -647.280670

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.092779	-0.443445	-0.160741
2	1	0	0.674281	0.535741	-0.382487
3	6	0	2.517701	-2.105669	0.106129
4	1	0	3.475123	-2.601634	0.098516
5	6	0	1.277415	-2.554516	0.443275
6	1	0	0.943383	-3.517002	0.795816
7	7	0	2.379070	-0.789072	-0.267519
8	7	0	0.404999	-1.506438	0.265067
9	6	0	3.469099	0.075776	-0.731789
10	1	0	3.791477	-0.257511	-1.719459
11	1	0	3.111699	1.108767	-0.766323
12	1	0	4.293159	0.001328	-0.021619
13	6	0	-1.041049	-1.533783	0.566739
14	1	0	-1.300129	-2.588591	0.694814
15	1	0	-1.191719	-0.993736	1.505938
16	6	0	-0.894554	1.935580	1.035177
17	7	0	-1.277909	1.265283	1.917441
18	6	0	-0.417400	2.650519	-0.068734
19	1	0	-1.108303	3.184922	-0.705339
20	6	0	0.958012	2.864111	-0.196337
21	7	0	2.120320	2.958332	-0.318138
22	6	0	-1.869187	-0.890844	-0.536372
23	6	0	-3.336191	-0.796355	-0.119975
24	1	0	-1.765944	-1.465350	-1.466585
25	1	0	-1.497714	0.123132	-0.727373
26	6	0	-4.176214	-0.082517	-1.175979
27	1	0	-3.737435	-1.802547	0.060568
28	1	0	-3.389100	-0.248717	0.828114
29	1	0	-5.223570	-0.015628	-0.870808
30	1	0	-3.805927	0.935491	-1.334190
31	1	0	-4.137102	-0.608523	-2.135892

Zero-point correction= 0.261555 (Hartree/Particle)
Thermal correction to Energy= 0.278592
Thermal correction to Enthalpy= 0.279536
Thermal correction to Gibbs Free Energy= 0.214418
Sum of electronic and zero-point Energies= -647.232334
Sum of electronic and thermal Energies= -647.215297

Sum of electronic and thermal Enthalpies= -647.214353
Sum of electronic and thermal Free Energies= -647.279471

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.621945	-0.930237	0.619154
2	6	0	1.136824	-1.386038	-1.470506
3	6	0	-0.048901	-0.720995	-1.467383
4	7	0	-0.354724	-0.455698	-0.151140
5	1	0	0.712961	-0.800315	1.687794
6	1	0	1.745150	-1.747189	-2.283623
7	1	0	-0.663681	-0.361555	-2.276146
8	7	0	1.532340	-1.513940	-0.156372
9	6	0	-1.490849	0.354146	0.303577
10	6	0	-2.822949	-0.348745	0.071944
11	1	0	-1.420129	1.304625	-0.234957
12	1	0	-1.327692	0.555822	1.365909
13	6	0	-3.993505	0.510699	0.548256
14	1	0	-2.941942	-0.566350	-0.997435
15	1	0	-2.826934	-1.312878	0.596462
16	1	0	-3.872409	0.727027	1.617017
17	1	0	-3.966176	1.476722	0.030016
18	6	0	2.829781	-2.015401	0.288429
19	1	0	2.988072	-3.011740	-0.125923
20	1	0	3.597130	-1.317210	-0.053994
21	1	0	2.841995	-2.037101	1.376329
22	6	0	-5.340198	-0.167935	0.308987
23	1	0	-5.396163	-1.125240	0.837140
24	1	0	-6.166381	0.456620	0.657805
25	1	0	-5.495215	-0.363950	-0.756817
26	6	0	2.765247	1.629567	-0.221017
27	6	0	1.545623	2.001071	-0.798860
28	7	0	0.507833	2.266242	-1.276184
29	6	0	2.759546	1.094396	1.068258
30	7	0	2.703187	0.571152	2.117951
31	1	0	3.695573	1.925256	-0.684399

Zero-point correction= 0.261836 (Hartree/Particle)
Thermal correction to Energy= 0.278691
Thermal correction to Enthalpy= 0.279635
Thermal correction to Gibbs Free Energy= 0.215799

Sum of electronic and zero-point Energies=	-647.233850
Sum of electronic and thermal Energies=	-647.216995
Sum of electronic and thermal Enthalpies=	-647.216051
Sum of electronic and thermal Free Energies=	-647.279887

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002528	0.688809	0.739168
2	1	0	-1.332492	-0.073050	1.435309
3	6	0	-1.057260	2.228802	-0.829737
4	1	0	-1.503028	2.900985	-1.544970
5	6	0	0.247281	1.971629	-0.536465
6	1	0	1.154555	2.372894	-0.955322
7	7	0	-1.819068	1.422740	-0.016081
8	7	0	0.256808	1.012419	0.449358
9	6	0	-3.273154	1.272517	-0.075918
10	1	0	-3.523889	0.696965	-0.969521
11	1	0	-3.599676	0.711399	0.799636
12	1	0	-3.728183	2.262923	-0.101293
13	6	0	1.437938	0.340521	1.024416
14	1	0	1.662383	0.811152	1.987013
15	1	0	1.142235	-0.699577	1.182473
16	6	0	-0.707048	-1.816207	-1.016722
17	7	0	0.451584	-1.642782	-1.075560
18	6	0	-2.093007	-1.971291	-0.905751
19	1	0	-2.674301	-2.319940	-1.746747
20	6	0	-2.670267	-1.849382	0.359123
21	7	0	-3.106526	-1.651787	1.431317
22	6	0	2.636719	0.386849	0.088688
23	6	0	3.735701	-0.554704	0.580133
24	1	0	3.033727	1.409108	0.023261
25	1	0	2.307677	0.065622	-0.905223
26	6	0	4.973634	-0.497080	-0.311279
27	1	0	4.009188	-0.303864	1.613539
28	1	0	3.334743	-1.574717	0.590874
29	1	0	5.744813	-1.188594	0.037469
30	1	0	4.719318	-0.767692	-1.340608
31	1	0	5.405295	0.509463	-0.323073

Zero-point correction=	0.261969 (Hartree/Particle)
Thermal correction to Energy=	0.278938

Thermal correction to Enthalpy=	0.279882
Thermal correction to Gibbs Free Energy=	0.215500
Sum of electronic and zero-point Energies=	-647.233164
Sum of electronic and thermal Energies=	-647.216195
Sum of electronic and thermal Enthalpies=	-647.215251
Sum of electronic and thermal Free Energies=	-647.279634

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.412668	-0.443206	1.441682
2	6	0	0.770927	-1.212272	-0.589236
3	7	0	-0.048899	-0.462168	0.143169
4	1	0	-0.061144	0.164977	2.196934
5	1	0	0.702618	-1.359635	-1.655847
6	6	0	-1.262947	0.210193	-0.337806
7	6	0	-2.514742	-0.607128	-0.037869
8	1	0	-1.130777	0.376849	-1.410210
9	1	0	-1.287616	1.185909	0.156147
10	6	0	-3.773940	0.105525	-0.528722
11	1	0	-2.434887	-1.595110	-0.511114
12	1	0	-2.584920	-0.775334	1.044584
13	1	0	-3.832808	1.094995	-0.059833
14	1	0	-3.695823	0.277099	-1.609716
15	6	0	-5.041527	-0.688844	-0.222652
16	1	0	-5.153564	-0.844851	0.855079
17	1	0	-5.932848	-0.166921	-0.579861
18	1	0	-5.013078	-1.672784	-0.702297
19	6	0	1.348618	2.523609	-0.725350
20	6	0	0.728458	2.593743	0.523695
21	7	0	0.167798	2.591977	1.554214
22	6	0	2.213484	1.468923	-1.009768
23	7	0	2.905276	0.552501	-1.257960
24	6	0	1.534961	-1.212090	1.470254
25	1	0	2.219947	-1.433284	2.272390
26	7	0	1.729292	-1.698426	0.195305
27	6	0	2.929275	-2.378575	-0.283543
28	1	0	3.654289	-1.616712	-0.578177
29	1	0	3.309512	-3.015468	0.514784
30	1	0	2.666800	-2.994518	-1.143674
31	1	0	1.228627	3.328324	-1.436386

Zero-point correction=	0.261437 (Hartree/Particle)
Thermal correction to Energy=	0.278503
Thermal correction to Enthalpy=	0.279448
Thermal correction to Gibbs Free Energy=	0.214949
Sum of electronic and zero-point Energies=	-647.233639
Sum of electronic and thermal Energies=	-647.216572
Sum of electronic and thermal Enthalpies=	-647.215628
Sum of electronic and thermal Free Energies=	-647.280126

$PhSO_2CH_2SO_2Ph$

Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000010	0.000164	-1.413060
2	16	0	-0.916109	-1.244290	-0.465030
3	8	0	-1.280639	-2.248028	-1.461622
4	8	0	-0.117798	-1.591286	0.705630
5	6	0	-2.406427	-0.432388	0.067153
6	6	0	-3.503055	-0.444463	-0.792632
7	6	0	-2.446603	0.173454	1.319266
8	6	0	-4.674839	0.186263	-0.384720
9	1	0	-3.437053	-0.958374	-1.746752
10	6	0	-3.627786	0.795924	1.714177
11	1	0	-1.568862	0.158570	1.954803
12	6	0	-4.733292	0.805124	0.864240
13	1	0	-5.542855	0.185863	-1.035422
14	1	0	-3.683134	1.275802	2.685503
15	1	0	-5.649747	1.294369	1.179324
16	1	0	-0.701886	0.557026	-2.040261
17	1	0	0.701906	-0.556560	-2.040384
18	16	0	0.916130	1.244413	-0.464763
19	8	0	1.280686	2.248351	-1.461144
20	8	0	0.117811	1.591175	0.705961
21	6	0	2.406428	0.432379	0.067274
22	6	0	2.446591	-0.173662	1.319291
23	6	0	3.503048	0.444543	-0.792520
24	6	0	3.627751	-0.796242	1.714094
25	1	0	1.568855	-0.158837	1.954837
26	6	0	4.674809	-0.186296	-0.384718
27	1	0	3.437062	0.958609	-1.746558
28	6	0	4.733248	-0.805357	0.864145
29	1	0	3.683088	-1.276274	2.685345
30	1	0	5.542819	-0.185832	-1.035428

31	1	0	5.649684	-1.294693	1.179141

Zero-point correction= 0.232666 (Hartree/Particle)
Thermal correction to Energy= 0.249325
Thermal correction to Enthalpy= 0.250269
Thermal correction to Gibbs Free Energy= 0.186605
Sum of electronic and zero-point Energies= -1599.154797
Sum of electronic and thermal Energies= -1599.138138
Sum of electronic and thermal Enthalpies= -1599.137194
Sum of electronic and thermal Free Energies= -1599.200859

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000111	-0.007399	-0.000889
2	16	0	1.448061	-1.033368	0.413829
3	8	0	1.387461	-1.309326	1.842655
4	8	0	1.537663	-2.086894	-0.585528
5	6	0	2.780634	0.119489	0.133438
6	6	0	3.226664	0.902235	1.194644
7	6	0	3.333010	0.209745	-1.142059
8	6	0	4.256778	1.811512	0.964414
9	1	0	2.785954	0.776130	2.178843
10	6	0	4.362059	1.123022	-1.357100
11	1	0	2.971980	-0.441154	-1.933116
12	6	0	4.817935	1.922016	-0.307669
13	1	0	4.625571	2.426463	1.778726
14	1	0	4.813193	1.205982	-2.340397
15	1	0	5.621613	2.630736	-0.480913
16	1	0	0.227977	0.604109	-0.876422
17	1	0	-0.227521	0.606090	0.873325
18	16	0	-1.448224	-1.033804	-0.413319
19	8	0	-1.388579	-1.311560	-1.841832
20	8	0	-1.537191	-2.086099	0.587379
21	6	0	-2.780613	0.119391	-0.133488
22	6	0	-3.332573	0.210790	1.142111
23	6	0	-3.226926	0.901256	-1.195222
24	6	0	-4.361498	1.124322	1.356681
25	1	0	-2.971330	-0.439432	1.933627
26	6	0	-4.256888	1.810820	-0.965449
27	1	0	-2.786539	0.774300	-2.179456
28	6	0	-4.817648	1.922453	0.306715
29	1	0	-4.812311	1.208151	2.340051

30	1	0	-4.625876	2.425103	-1.780178
31	1	0	-5.621209	2.631390	0.479606

The conjugate base anion of $PhSO_2CH_2SO_2Ph$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000038	0.000355	-1.185604
2	16	0	-0.979916	-1.123547	-0.396907
3	8	0	-1.342827	-2.172275	-1.368025
4	8	0	-0.416835	-1.510038	0.908713
5	6	0	-2.561423	-0.353119	0.026098
6	6	0	-3.707859	-0.718176	-0.671797
7	6	0	-2.606872	0.600385	1.042784
8	6	0	-4.925809	-0.118441	-0.347823
9	1	0	-3.627355	-1.470728	-1.449667
10	6	0	-3.826444	1.193302	1.357410
11	1	0	-1.687875	0.879386	1.551166
12	6	0	-4.986370	0.836024	0.665507
13	1	0	-5.826353	-0.399616	-0.886993
14	1	0	-3.872523	1.941022	2.144214
15	1	0	-5.934548	1.304019	0.916283
16	1	0	0.000186	0.000333	-2.264156
17	16	0	0.980080	1.123997	-0.396662
18	8	0	1.343240	2.172907	-1.367491
19	8	0	0.417114	1.510231	0.909082
20	6	0	2.561404	0.353142	0.026217
21	6	0	2.606513	-0.600758	1.042545
22	6	0	3.707984	0.718175	-0.671454
23	6	0	3.825915	-1.194062	1.357094
24	1	0	1.687379	-0.879766	1.550696
25	6	0	4.925760	0.118045	-0.347561
26	1	0	3.627731	1.471019	-1.449064
27	6	0	4.985996	-0.836786	0.665446
28	1	0	3.871739	-1.942086	2.143622
29	1	0	5.826424	0.399202	-0.886540
30	1	0	5.934041	-1.305086	0.916156

Zero-point correction= 0.218871 (Hartree/Particle)
Thermal correction to Energy= 0.235539
Thermal correction to Enthalpy= 0.236483
Thermal correction to Gibbs Free Energy= 0.169709

Sum of electronic and zero-point Energies=	-1598.628986
Sum of electronic and thermal Energies=	-1598.612318
Sum of electronic and thermal Enthalpies=	-1598.611374
Sum of electronic and thermal Free Energies=	-1598.678148

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.635704	-1.218438	0.637209
2	16	0	2.215437	0.374480	0.482506
3	8	0	2.718501	0.758814	1.815750
4	8	0	3.083732	0.576869	-0.682296
5	6	0	0.804154	1.458642	0.161045
6	6	0	-0.117239	1.699083	1.179467
7	6	0	0.625560	1.992963	-1.109773
8	6	0	-1.223225	2.503089	0.924587
9	1	0	0.044017	1.252976	2.157338
10	6	0	-0.483548	2.804572	-1.357478
11	1	0	1.356619	1.759872	-1.877746
12	6	0	-1.404055	3.060973	-0.343907
13	1	0	-1.952081	2.685919	1.709065
14	1	0	-0.630741	3.229901	-2.346530
15	1	0	-2.271885	3.684343	-0.542598
16	1	0	1.524911	-1.553995	1.659324
17	16	0	0.581348	-1.914768	-0.481864
18	8	0	0.863963	-1.431198	-1.841397
19	8	0	0.487652	-3.358113	-0.205292
20	6	0	-1.099455	-1.313686	-0.150168
21	6	0	-1.728407	-1.663707	1.044495
22	6	0	-1.726905	-0.474870	-1.063594
23	6	0	-2.994859	-1.161411	1.327698
24	1	0	-1.221882	-2.328749	1.739278
25	6	0	-2.996223	0.027407	-0.774436
26	1	0	-1.205934	-0.223153	-1.981829
27	6	0	-3.630603	-0.312037	0.417910
28	1	0	-3.489405	-1.431526	2.256788
29	1	0	-3.481717	0.697364	-1.479028
30	1	0	-4.616636	0.085183	0.643228

Zero-point correction=	0.218713 (Hartree/Particle)
Thermal correction to Energy=	0.235148
Thermal correction to Enthalpy=	0.236092

Thermal correction to Gibbs Free Energy=	0.173913
Sum of electronic and zero-point Energies=	-1598.625830
Sum of electronic and thermal Energies=	-1598.609395
Sum of electronic and thermal Enthalpies=	-1598.608451
Sum of electronic and thermal Free Energies=	-1598.670630

Complexes formed from a [Bmim] cation and the conjugate base anion of $PhSO_2CH_2SO_2Ph$.

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.491534	1.417023	0.314663
2	1	0	1.943056	1.367424	1.246623
3	6	0	3.553601	0.813538	-1.516987
4	1	0	4.061036	0.143269	-2.191634
5	6	0	3.168938	2.109999	-1.661239
6	1	0	3.281083	2.796882	-2.484389
7	7	0	3.137275	0.408118	-0.270502
8	7	0	2.527429	2.472042	-0.499011
9	6	0	3.369320	-0.922439	0.304785
10	1	0	2.740395	-0.991918	1.193741
11	1	0	2.978843	-1.647043	-0.416023
12	6	0	1.832272	3.740965	-0.288410
13	1	0	0.943673	3.771431	-0.923850
14	1	0	1.507652	3.792547	0.749017
15	1	0	2.516778	4.557118	-0.524127
16	16	0	0.027636	-0.697417	-0.646507
17	8	0	0.921347	-1.231250	-1.692194
18	8	0	0.439856	-0.816979	0.766981
19	16	0	-1.035134	1.951468	0.151946
20	8	0	-0.184363	2.122344	1.347899
21	8	0	-1.433280	3.166442	-0.581220
22	6	0	4.843764	-1.144038	0.621328
23	6	0	5.075782	-2.519299	1.246139
24	1	0	5.191350	-0.359867	1.306626
25	1	0	5.442321	-1.052916	-0.294923
26	6	0	6.548037	-2.766750	1.566279
27	1	0	4.477081	-2.604308	2.161183
28	1	0	4.708246	-3.293894	0.562063
29	1	0	6.697067	-3.751791	2.015877
30	1	0	7.159507	-2.715824	0.659489
31	1	0	6.927481	-2.016698	2.267767

32	6	0	-2.539879	1.189710	0.765048
33	6	0	-2.617575	0.782363	2.091180
34	6	0	-3.590564	0.977137	-0.126599
35	6	0	-3.785136	0.161623	2.539019
36	1	0	-1.770034	0.955283	2.746235
37	6	0	-4.745755	0.350963	0.326807
38	1	0	-3.496882	1.300699	-1.159865
39	6	0	-4.844261	-0.052673	1.660629
40	1	0	-3.863060	-0.155803	3.574446
41	1	0	-5.567840	0.172942	-0.359406
42	1	0	-5.749048	-0.540658	2.010971
43	6	0	-1.484859	-1.660251	-0.779952
44	6	0	-2.096706	-2.141279	0.371755
45	6	0	-2.047052	-1.860182	-2.039807
46	6	0	-3.302437	-2.832675	0.258339
47	1	0	-1.628111	-1.965605	1.334476
48	6	0	-3.250099	-2.551810	-2.142598
49	1	0	-1.538232	-1.487503	-2.924642
50	6	0	-3.879032	-3.035840	-0.993337
51	1	0	-3.793619	-3.203854	1.152856
52	1	0	-3.696059	-2.717631	-3.118452
53	1	0	-4.819464	-3.572225	-1.076695
54	6	0	-0.281462	0.937778	-1.004817
55	1	0	-0.645261	1.106359	-2.012873

Zero-point correction=	0.448707 (Hartree/Particle)
Thermal correction to Energy=	0.477462
Thermal correction to Enthalpy=	0.478407
Thermal correction to Gibbs Free Energy=	0.385262
Sum of electronic and zero-point Energies=	-2021.544855
Sum of electronic and thermal Energies=	-2021.516100
Sum of electronic and thermal Enthalpies=	-2021.515155
Sum of electronic and thermal Free Energies=	-2021.608300

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.461782	-0.253401	-0.924090
2	16	0	-1.188371	1.180183	-1.527806
3	8	0	-0.868126	1.243546	-2.960952
4	8	0	-2.576137	1.345678	-1.070790
5	6	0	-0.336920	2.595272	-0.800918

6	6	0	0.602191	3.287572	-1.558837
7	6	0	-0.685702	3.016330	0.480371
8	6	0	1.209548	4.423460	-1.020842
9	1	0	0.818803	2.945342	-2.566428
10	6	0	-0.072899	4.150268	1.011423
11	1	0	-1.438979	2.461222	1.032590
12	6	0	0.872119	4.856287	0.262332
13	1	0	1.927470	4.983982	-1.612310
14	1	0	-0.353507	4.500814	2.000998
15	1	0	1.328374	5.753312	0.670751
16	1	0	-0.204806	-0.949036	-1.715407
17	16	0	-1.060489	-0.978957	0.489034
18	8	0	-0.192226	-2.154663	0.758159
19	8	0	-1.165734	0.043110	1.555868
20	6	0	-2.708610	-1.675779	0.334076
21	6	0	-3.822331	-0.861156	0.519303
22	6	0	-2.835289	-3.027706	0.025950
23	6	0	-5.090695	-1.420690	0.389265
24	1	0	-3.686984	0.190468	0.743912
25	6	0	-4.110155	-3.575352	-0.102319
26	1	0	-1.943291	-3.635059	-0.087045
27	6	0	-5.235440	-2.772864	0.078485
28	1	0	-5.968016	-0.796955	0.528641
29	1	0	-4.223180	-4.629417	-0.335994
30	1	0	-6.227741	-3.202148	-0.021615
31	6	0	2.844530	0.771701	-0.091853
32	6	0	2.412501	1.670229	0.833889
33	6	0	1.886270	-0.347354	1.540108
34	7	0	2.512115	-0.478859	0.373425
35	1	0	3.320954	0.916833	-1.048190
36	1	0	2.427900	2.749638	0.836822
37	1	0	1.431502	-1.154057	2.096383
38	6	0	2.701833	-1.740880	-0.348186
39	6	0	4.115722	-2.286277	-0.182799
40	1	0	2.469643	-1.534116	-1.397380
41	1	0	1.936643	-2.427119	0.024654
42	6	0	4.301325	-3.597472	-0.945146
43	1	0	4.843460	-1.544576	-0.538036
44	1	0	4.318670	-2.445212	0.884179
45	1	0	3.566506	-4.329079	-0.587871
46	1	0	4.085090	-3.432972	-2.008050
47	6	0	5.711498	-4.161384	-0.787305
48	1	0	5.939369	-4.353955	0.265956
49	1	0	5.826035	-5.101759	-1.332177

50	1	0	6.459247	-3.458639	-1.168700
51	6	0	1.120166	1.496900	3.004525
52	1	0	1.392276	0.926515	3.893136
53	1	0	1.426730	2.535183	3.126116
54	1	0	0.047200	1.421315	2.818124
55	7	0	1.826868	0.947753	1.848637

Zero-point correction= 0.449003 (Hartree/Particle)
Thermal correction to Energy= 0.477678
Thermal correction to Enthalpy= 0.478623
Thermal correction to Gibbs Free Energy= 0.388087
Sum of electronic and zero-point Energies= -2021.534327
Sum of electronic and thermal Energies= -2021.505651
Sum of electronic and thermal Enthalpies= -2021.504707
Sum of electronic and thermal Free Energies= -2021.595243

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758386	0.465221	0.849046
2	16	0	-0.508407	-0.928517	1.823455
3	8	0	-0.229442	-0.431237	3.178748
4	8	0	-1.503808	-1.989315	1.616539
5	6	0	1.040987	-1.658733	1.258103
6	6	0	2.234307	-1.251287	1.849063
7	6	0	1.028021	-2.606847	0.237717
8	6	0	3.442044	-1.762931	1.374326
9	1	0	2.198379	-0.557867	2.684767
10	6	0	2.237881	-3.133615	-0.212328
11	1	0	0.078435	-2.916616	-0.186698
12	6	0	3.444520	-2.701007	0.340886
13	1	0	4.378160	-1.452017	1.829269
14	1	0	2.236380	-3.893969	-0.988784
15	1	0	4.384773	-3.113942	-0.013764
16	1	0	-1.066029	1.327853	1.430748
17	16	0	-1.482310	0.339007	-0.686950
18	8	0	-1.409877	1.677702	-1.303692
19	8	0	-0.819648	-0.787985	-1.395285
20	6	0	-3.227151	-0.074547	-0.649965
21	6	0	-3.619588	-1.400197	-0.482360
22	6	0	-4.156760	0.954593	-0.774682
23	6	0	-4.979578	-1.694574	-0.438766

24	1	0	-2.869886	-2.174719	-0.368064
25	6	0	-5.515045	0.646241	-0.728580
26	1	0	-3.808581	1.971560	-0.923686
27	6	0	-5.924715	-0.675564	-0.560909
28	1	0	-5.301546	-2.722402	-0.305239
29	1	0	-6.251375	1.437188	-0.830840
30	1	0	-6.983617	-0.913264	-0.525820
31	6	0	4.094231	1.123149	-1.002821
32	6	0	4.039708	0.211162	-2.014903
33	6	0	2.046081	0.324029	-1.083997
34	7	0	2.839486	1.176470	-0.439655
35	1	0	4.909049	1.728956	-0.639778
36	1	0	4.795641	-0.131661	-2.702999
37	1	0	1.004158	0.128206	-0.862326
38	6	0	2.372879	2.046804	0.652870
39	6	0	1.442375	3.137013	0.136224
40	1	0	3.265643	2.452318	1.137225
41	1	0	1.836985	1.409378	1.362019
42	6	0	0.848885	3.944060	1.289549
43	1	0	1.985217	3.795930	-0.554529
44	1	0	0.624375	2.663619	-0.422365
45	1	0	0.403378	3.249566	2.013167
46	1	0	1.643119	4.484789	1.820957
47	6	0	-0.216628	4.919980	0.795831
48	1	0	-1.016729	4.377335	0.282638
49	1	0	-0.656617	5.480943	1.624500
50	1	0	0.207398	5.640016	0.087999
51	6	0	2.181101	-1.238230	-2.981977
52	1	0	1.131674	-1.381069	-2.712929
53	1	0	2.256525	-0.844702	-3.996832
54	1	0	2.724065	-2.180205	-2.895993
55	7	0	2.748186	-0.267142	-2.047653

Zero-point correction=	0.449077 (Hartree/Particle)
Thermal correction to Energy=	0.477795
Thermal correction to Enthalpy=	0.478739
Thermal correction to Gibbs Free Energy=	0.386914
Sum of electronic and zero-point Energies=	-2021.534518
Sum of electronic and thermal Energies=	-2021.505800
Sum of electronic and thermal Enthalpies=	-2021.504856
Sum of electronic and thermal Free Energies=	-2021.596681

Conformer 4

1	6	0	−0.401298	−0.829126	0.735681
2	16	0	0.104021	−2.251185	−0.062162
3	8	0	0.508458	−3.193427	1.001016
4	8	0	−0.798801	−2.691941	−1.131380
5	6	0	1.654698	−1.858683	−0.905531
6	6	0	2.824273	−2.485858	−0.487135
7	6	0	1.670380	−0.918580	−1.936797
8	6	0	4.042368	−2.124975	−1.068731
9	1	0	2.763591	−3.245782	0.285996
10	6	0	2.890200	−0.559825	−2.506292
11	1	0	0.738098	−0.461560	−2.257997
12	6	0	4.078668	−1.151076	−2.065946
13	1	0	4.959564	−2.611584	−0.749500
14	1	0	2.914523	0.177703	−3.303386
15	1	0	5.025585	−0.867365	−2.515271
16	1	0	−0.557807	−0.971136	1.798718
17	16	0	−1.426581	0.316660	0.006316
18	8	0	−1.434487	1.508204	0.886127
19	8	0	−1.032170	0.511321	−1.403166
20	6	0	−3.134055	−0.235444	−0.035006
21	6	0	−3.525484	−1.167083	−0.994413
22	6	0	−4.026794	0.264748	0.908525
23	6	0	−4.847256	−1.604459	−0.999108
24	1	0	−2.798423	−1.549408	−1.703467
25	6	0	−5.347635	−0.180654	0.890898
26	1	0	−3.682966	1.001548	1.626900
27	6	0	−5.756159	−1.113797	−0.060066
28	1	0	−5.168401	−2.331773	−1.738069
29	1	0	−6.056787	0.205651	1.616428
30	1	0	−6.785359	−1.459642	−0.071734
31	6	0	1.113600	1.829833	2.173829
32	6	0	1.517174	0.815305	2.986476
33	6	0	2.468017	0.534367	1.026270
34	7	0	1.729560	1.641231	0.960178
35	1	0	0.411954	2.627735	2.343358
36	1	0	1.258685	0.579931	4.006187
37	1	0	3.047811	0.117005	0.213374
38	6	0	1.475861	2.374335	−0.296508
39	6	0	0.786325	3.708845	−0.070192
40	1	0	0.843420	1.728837	−0.916375
41	1	0	2.446041	2.507473	−0.785972
42	6	0	0.554200	4.415810	−1.405734
43	1	0	−0.183135	3.524686	0.406171
44	1	0	1.390621	4.344110	0.591712

45	1	0	1.514710	4.568907	-1.915025
46	1	0	-0.048109	3.762548	-2.048117
47	6	0	-0.152641	5.757166	-1.225790
48	1	0	0.437319	6.430556	-0.595021
49	1	0	-0.313303	6.251835	-2.187143
50	1	0	-1.129024	5.619475	-0.751362
51	6	0	2.870041	-1.287845	2.662820
52	1	0	3.794550	-1.496974	2.124489
53	1	0	3.069717	-1.260538	3.734090
54	1	0	2.117983	-2.048016	2.423897
55	7	0	2.367474	0.021185	2.250736

Zero-point correction=	0.449919 (Hartree/Particle)
Thermal correction to Energy=	0.478431
Thermal correction to Enthalpy=	0.479375
Thermal correction to Gibbs Free Energy=	0.390023
Sum of electronic and zero-point Energies=	-2021.533338
Sum of electronic and thermal Energies=	-2021.504826
Sum of electronic and thermal Enthalpies=	-2021.503882
Sum of electronic and thermal Free Energies=	-2021.593234

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.482603	-0.715934	-0.383565
2	16	0	-0.357295	0.370972	-1.700545
3	8	0	0.446333	-0.327214	-2.720959
4	8	0	-1.625289	1.013427	-2.070351
5	6	0	0.682425	1.755782	-1.185055
6	6	0	1.971663	1.857310	-1.700722
7	6	0	0.174246	2.727117	-0.321870
8	6	0	2.784970	2.925207	-1.312770
9	1	0	2.312764	1.110322	-2.411541
10	6	0	0.991698	3.789039	0.059630
11	1	0	-0.840722	2.632564	0.051734
12	6	0	2.299302	3.886531	-0.426085
13	1	0	3.787868	3.016686	-1.719346
14	1	0	0.602515	4.553483	0.726392
15	1	0	2.926795	4.723041	-0.133626
16	1	0	-0.338246	-1.744232	-0.699148
17	16	0	-1.680336	-0.523785	0.815832
18	8	0	-1.511665	-1.639394	1.768126

19	8	0	-1.619953	0.862252	1.337413
20	6	0	-3.350927	-0.715512	0.182096
21	6	0	-4.022442	0.377097	-0.358783
22	6	0	-3.938154	-1.976616	0.238649
23	6	0	-5.309636	0.195082	-0.857757
24	1	0	-3.535693	1.344861	-0.396179
25	6	0	-5.226807	-2.146803	-0.262979
26	1	0	-3.392891	-2.798694	0.690822
27	6	0	-5.910192	-1.062790	-0.812142
28	1	0	-5.842373	1.037852	-1.286761
29	1	0	-5.698098	-3.123727	-0.217982
30	1	0	-6.913744	-1.197368	-1.204209
31	6	0	2.074050	0.732084	1.471941
32	6	0	0.982260	-0.554274	2.882742
33	1	0	2.448312	1.606796	0.956700
34	1	0	0.276756	-0.796201	3.660789
35	6	0	0.662405	1.930815	3.128797
36	1	0	0.693980	1.834506	4.214430
37	1	0	1.235396	2.804754	2.819779
38	1	0	-0.367040	1.995385	2.767560
39	7	0	1.268160	0.742995	2.532809
40	6	0	1.645998	-1.355814	2.007373
41	1	0	1.632899	-2.427064	1.903973
42	6	0	3.006494	-0.943673	-0.095243
43	6	0	3.720246	-2.280903	0.034989
44	1	0	3.716887	-0.149845	-0.345558
45	1	0	2.237510	-0.980305	-0.877789
46	6	0	4.490103	-2.610971	-1.244437
47	1	0	4.404808	-2.258559	0.892605
48	1	0	2.988598	-3.076492	0.220900
49	6	0	5.165661	-3.978049	-1.170836
50	1	0	3.800774	-2.581705	-2.096731
51	1	0	5.244028	-1.834231	-1.423617
52	1	0	5.716148	-4.197582	-2.088908
53	1	0	5.872242	-4.022576	-0.335651
54	1	0	4.425329	-4.771212	-1.026602
55	7	0	2.335745	-0.533907	1.146576

Zero-point correction= 0.448889 (Hartree/Particle)
Thermal correction to Energy= 0.476790
Thermal correction to Enthalpy= 0.477735
Thermal correction to Gibbs Free Energy= 0.389481
Sum of electronic and zero-point Energies= -2021.531700
Sum of electronic and thermal Energies= -2021.503799

Sum of electronic and thermal Enthalpies= -2021.502854
Sum of electronic and thermal Free Energies= -2021.591108

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.128954	-0.027060	-1.577293
2	8	0	-0.830263	1.017965	-2.007248
3	8	0	1.172393	-0.454838	-2.520204
4	6	0	-2.071527	0.408844	1.265486
5	6	0	-3.765601	-0.835354	1.929188
6	6	0	-4.268879	0.225981	1.237277
7	7	0	-3.193781	0.988712	0.833657
8	1	0	-1.034141	0.679416	1.006733
9	1	0	-4.258605	-1.662518	2.414587
10	1	0	-5.285339	0.503369	1.007151
11	7	0	-2.398022	-0.695343	1.934774
12	6	0	-3.243439	2.132134	-0.095775
13	6	0	-2.121563	3.129267	0.144819
14	1	0	-4.225219	2.596978	0.031749
15	1	0	-3.160832	1.733377	-1.112896
16	6	0	-2.148104	4.236945	-0.907464
17	1	0	-2.205954	3.550895	1.154505
18	1	0	-1.161504	2.609423	0.068294
19	1	0	-2.050297	3.776734	-1.897596
20	1	0	-3.116658	4.753802	-0.881055
21	6	0	-1.410937	-1.670828	2.411510
22	1	0	-0.489615	-1.143805	2.668024
23	1	0	-1.816507	-2.174215	3.289197
24	1	0	-1.205607	-2.387584	1.611452
25	6	0	-1.018212	5.241594	-0.696762
26	1	0	-0.045359	4.744606	-0.762247
27	1	0	-1.043400	6.029443	-1.453870
28	1	0	-1.090559	5.716052	0.287384
29	6	0	-0.865695	-1.505690	-1.293195
30	6	0	-2.250867	-1.381845	-1.233670
31	6	0	-0.252251	-2.754672	-1.207540
32	6	0	-3.034999	-2.516968	-1.025491
33	1	0	-2.701547	-0.406851	-1.388422
34	6	0	-1.041452	-3.883124	-1.002375
35	1	0	0.825518	-2.831499	-1.284714
36	6	0	-2.428643	-3.765778	-0.897260

37	1	0	-4.116508	-2.425879	-0.986013
38	1	0	-0.570697	-4.858092	-0.926414
39	1	0	-3.036990	-4.651699	-0.740594
40	6	0	0.685207	0.537883	-0.049198
41	1	0	0.882841	1.606716	-0.082471
42	16	0	1.746382	-0.339142	0.959911
43	8	0	1.562156	0.172156	2.332902
44	8	0	1.527567	-1.779284	0.734235
45	6	0	3.458171	0.006165	0.545760
46	6	0	4.305449	0.520291	1.521592
47	6	0	3.901694	-0.262713	-0.748156
48	6	0	5.639147	0.764904	1.192858
49	1	0	3.913043	0.718550	2.513624
50	6	0	5.234297	-0.012551	-1.062280
51	1	0	3.207686	-0.637166	-1.497034
52	6	0	6.101368	0.497648	-0.093930
53	1	0	6.314833	1.164740	1.942515
54	1	0	5.595378	-0.211787	-2.066292
55	1	0	7.139480	0.691877	-0.346346

Zero-point correction= 0.449085 (Hartree/Particle)
Thermal correction to Energy= 0.477733
Thermal correction to Enthalpy= 0.478677
Thermal correction to Gibbs Free Energy= 0.387823
Sum of electronic and zero-point Energies= -2021.529325
Sum of electronic and thermal Energies= -2021.500677
Sum of electronic and thermal Enthalpies= -2021.499733
Sum of electronic and thermal Free Energies= -2021.590586

$PhSO_2CH_2CN$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.617819	-0.000462	-1.073530
2	6	0	3.071293	-0.000009	-0.963461
3	7	0	4.223366	0.000701	-0.884322
4	16	0	0.853440	-0.000201	0.588234
5	8	0	1.185575	-1.275435	1.208074
6	8	0	1.185881	1.275156	1.207691
7	6	0	-0.878258	-0.000029	0.175223
8	6	0	-1.530147	-1.220159	0.013245
9	6	0	-1.530004	1.220242	0.013686
10	6	0	-2.879262	-1.211740	-0.332453
11	1	0	-0.991079	-2.147878	0.180583

12	6	0	-2.879138	1.212089	-0.331967
13	1	0	-0.990661	2.147764	0.181189
14	6	0	-3.547689	0.000253	-0.507469
15	1	0	-3.409268	-2.150257	-0.456029
16	1	0	-3.409079	2.150701	-0.455096
17	1	0	-4.599862	0.000362	-0.774035
18	1	0	1.270815	0.896778	-1.592102
19	1	0	1.271202	-0.898042	-1.591763

Zero-point correction= 0.138988 (Hartree/Particle)
Thermal correction to Energy= 0.149716
Thermal correction to Enthalpy= 0.150660
Thermal correction to Gibbs Free Energy= 0.101224
Sum of electronic and zero-point Energies= -912.002201
Sum of electronic and thermal Energies= -911.991473
Sum of electronic and thermal Enthalpies= -911.990529
Sum of electronic and thermal Free Energies= -912.039966

The conjugate base anion of $PhSO_2CH_2CN$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.997957	0.008657	-0.889599
2	6	0	2.267029	1.366717	-0.691703
3	7	0	2.497725	2.504582	-0.538089
4	16	0	1.069811	-0.832721	0.239547
5	8	0	1.001460	-2.250538	-0.164572
6	8	0	1.451326	-0.482182	1.617138
7	6	0	-0.645993	-0.260171	0.128087
8	6	0	-1.593469	-1.016981	-0.555659
9	6	0	-0.983442	0.974287	0.683601
10	6	0	-2.896001	-0.534032	-0.683694
11	1	0	-1.293984	-1.977363	-0.964445
12	6	0	-2.283886	1.453075	0.546586
13	1	0	-0.225086	1.540742	1.216402
14	6	0	-3.242295	0.700770	-0.135897
15	1	0	-3.642324	-1.123943	-1.209320
16	1	0	-2.551874	2.415259	0.974176
17	1	0	-4.256461	1.077104	-0.238555
18	1	0	2.026998	-0.432502	-1.875243

Zero-point correction= 0.125079 (Hartree/Particle)
Thermal correction to Energy= 0.135708

Thermal correction to Enthalpy=	0.136652
Thermal correction to Gibbs Free Energy=	0.087443
Sum of electronic and zero-point Energies=	-911.479213
Sum of electronic and thermal Energies=	-911.468584
Sum of electronic and thermal Enthalpies=	-911.467640
Sum of electronic and thermal Free Energies=	-911.516849

Complexes formed from a [Bmim] cation and the conjugate base anion of $PhSO_2CH_2CN$

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.360215	0.368793	-0.290613
2	8	0	0.429349	-0.666918	-0.794208
3	8	0	1.564629	1.571401	-1.128911
4	6	0	-1.636916	1.314045	-0.732957
5	6	0	-2.082225	2.630353	0.970769
6	6	0	-2.560406	1.389687	1.260604
7	7	0	-2.275756	0.587754	0.181211
8	1	0	-1.217002	0.931719	-1.651775
9	1	0	-2.069642	3.538744	1.550496
10	1	0	-3.021592	0.993045	2.150972
11	7	0	-1.526000	2.564132	-0.288923
12	6	0	-2.568456	-0.847751	0.074348
13	6	0	-3.990833	-1.095846	-0.414171
14	1	0	-2.388544	-1.268127	1.067886
15	1	0	-1.811819	-1.264622	-0.595335
16	6	0	-4.290045	-2.590341	-0.520605
17	1	0	-4.704323	-0.624427	0.274985
18	1	0	-4.131264	-0.618885	-1.393432
19	1	0	-3.572004	-3.053509	-1.208271
20	1	0	-4.131601	-3.060928	0.457303
21	6	0	-0.707881	3.601391	-0.910171
22	1	0	-0.637617	3.400516	-1.978330
23	1	0	-1.180703	4.569085	-0.741236
24	1	0	0.295699	3.554539	-0.483314
25	6	0	-5.714287	-2.860249	-1.000107
26	1	0	-5.885896	-2.415745	-1.985961
27	1	0	-5.911440	-3.932558	-1.077034
28	1	0	-6.447399	-2.432866	-0.308304
29	6	0	2.964517	-0.436640	-0.229096
30	6	0	3.049853	-1.696399	0.362515

31	6	0	4.087747	0.209310	-0.732406
32	6	0	4.290591	-2.319060	0.446290
33	1	0	2.152217	-2.175331	0.744033
34	6	0	5.327948	-0.424069	-0.642163
35	1	0	3.975262	1.184857	-1.193937
36	6	0	5.428943	-1.683088	-0.054645
37	1	0	4.372196	-3.301204	0.901250
38	1	0	6.213463	0.065847	-1.035151
39	1	0	6.395420	-2.173028	0.013916
40	6	0	0.861858	0.859110	1.251899
41	1	0	1.442437	1.653655	1.701714
42	6	0	0.104246	-0.017647	2.032362
43	7	0	-0.603821	-0.709622	2.657642

Zero-point correction=	0.355692 (Hartree/Particle)
Thermal correction to Energy=	0.378559
Thermal correction to Enthalpy=	0.379503
Thermal correction to Gibbs Free Energy=	0.298562
Sum of electronic and zero-point Energies=	-1334.391133
Sum of electronic and thermal Energies=	-1334.368266
Sum of electronic and thermal Enthalpies=	-1334.367322
Sum of electronic and thermal Free Energies=	-1334.448262

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.167381	-0.170241	-0.211671
2	8	0	0.301252	-1.358786	-0.381795
3	8	0	1.203391	0.810160	-1.321567
4	6	0	-1.614757	1.108225	-0.944895
5	6	0	-2.019870	2.636350	0.582770
6	6	0	-2.613422	1.477461	0.977648
7	7	0	-2.357484	0.539137	0.000354
8	1	0	-1.182854	0.602629	-1.795811
9	1	0	-1.924195	3.591941	1.072817
10	1	0	-3.164830	1.234024	1.871157
11	7	0	-1.410493	2.384330	-0.623757
12	6	0	-2.683174	-0.888010	0.077295
13	6	0	-4.184392	-1.136010	0.002009
14	1	0	-2.249617	-1.263092	1.009825
15	1	0	-2.138770	-1.379578	-0.731420
16	6	0	-4.507118	-2.626547	0.096835

17	1	0	-4.694097	-0.598761	0.812802
18	1	0	-4.571972	-0.728240	-0.940315
19	1	0	-3.988758	-3.160065	-0.709114
20	1	0	-4.108487	-3.024487	1.038172
21	6	0	-0.584427	3.326499	-1.381065
22	1	0	-1.219963	3.936759	-2.025063
23	1	0	-0.039669	3.937307	-0.660359
24	1	0	0.136905	2.745779	-1.956237
25	6	0	-6.007353	-2.898483	0.015364
26	1	0	-6.420193	-2.533433	-0.930551
27	1	0	-6.221200	-3.968044	0.084077
28	1	0	-6.540976	-2.396475	0.828893
29	6	0	2.836787	-0.823661	-0.107651
30	6	0	3.037073	-2.188502	0.065592
31	6	0	3.905056	0.070378	-0.160077
32	6	0	4.341000	-2.669724	0.188263
33	1	0	2.178032	-2.850951	0.088505
34	6	0	5.201102	-0.420261	-0.038577
35	1	0	3.713320	1.130638	-0.299551
36	6	0	5.418953	-1.788759	0.137300
37	1	0	4.512993	-3.733651	0.319126
38	1	0	6.042881	0.263658	-0.081358
39	1	0	6.432141	-2.167076	0.232144
40	6	0	0.735612	0.625854	1.218109
41	6	0	0.945623	2.001632	1.324965
42	7	0	1.035767	3.167496	1.390682
43	1	0	0.619385	-0.001415	2.091643

Zero-point correction= 0.355603 (Hartree/Particle)
Thermal correction to Energy= 0.378526
Thermal correction to Enthalpy= 0.379471
Thermal correction to Gibbs Free Energy= 0.299573
Sum of electronic and zero-point Energies= -1334.391126
Sum of electronic and thermal Energies= -1334.368203
Sum of electronic and thermal Enthalpies= -1334.367259
Sum of electronic and thermal Free Energies= -1334.447156

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.012198	0.273717	-0.150009
2	8	0	0.927602	1.670460	-0.616402

3	8	0	0.451879	-0.053613	1.185580
4	6	0	-2.371318	-0.717740	0.514296
5	6	0	-4.089010	-1.799016	-0.345731
6	6	0	-4.026611	-0.570456	-0.930014
7	7	0	-2.954478	0.089042	-0.373600
8	1	0	-1.452198	-0.500412	1.056520
9	1	0	-4.770429	-2.621288	-0.492194
10	1	0	-4.644723	-0.114165	-1.686298
11	7	0	-3.051616	-1.862884	0.555857
12	6	0	-2.436064	1.408058	-0.778044
13	6	0	-2.052903	2.272633	0.415504
14	1	0	-3.228310	1.879037	-1.367334
15	1	0	-1.560656	1.229533	-1.412603
16	6	0	-1.554806	3.639304	-0.051958
17	1	0	-2.916492	2.385411	1.084925
18	1	0	-1.248705	1.781373	0.975205
19	1	0	-0.750033	3.482270	-0.778165
20	1	0	-2.367778	4.173061	-0.562479
21	6	0	-2.694167	-3.021785	1.371827
22	1	0	-1.837566	-2.750420	1.987366
23	1	0	-3.543923	-3.291655	2.000900
24	1	0	-2.394678	-3.836542	0.713338
25	6	0	-1.028118	4.474114	1.111851
26	1	0	-0.178905	3.969193	1.582234
27	1	0	-0.690606	5.457285	0.773257
28	1	0	-1.800005	4.626599	1.874337
29	6	0	2.766431	-0.077566	-0.003349
30	6	0	3.693969	0.819767	-0.521321
31	6	0	3.161180	-1.275999	0.589789
32	6	0	5.051675	0.510567	-0.437486
33	1	0	3.343166	1.744665	-0.967561
34	6	0	4.517669	-1.574944	0.665748
35	1	0	2.412947	-1.956177	0.986500
36	6	0	5.462015	-0.682895	0.152796
37	1	0	5.787181	1.205038	-0.831412
38	1	0	4.840321	-2.503531	1.126139
39	1	0	6.519543	-0.920395	0.215710
40	6	0	0.275907	-0.725554	-1.307660
41	6	0	-0.062236	-2.034088	-0.946732
42	7	0	-0.413767	-3.103301	-0.624121
43	1	0	0.508190	-0.479525	-2.335724

Zero-point correction= 0.355924 (Hartree/Particle)
Thermal correction to Energy= 0.378572

Thermal correction to Enthalpy=	0.379516
Thermal correction to Gibbs Free Energy=	0.301676
Sum of electronic and zero-point Energies=	-1334.392183
Sum of electronic and thermal Energies=	-1334.369535
Sum of electronic and thermal Enthalpies=	-1334.368591
Sum of electronic and thermal Free Energies=	-1334.446431

Conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.248431	-1.055645	-0.336874
2	8	0	1.568548	-2.372626	-0.912037
3	8	0	0.474738	-0.094999	-1.165947
4	6	0	-2.310041	-0.751365	-0.495372
5	6	0	-4.130518	-0.946073	0.726796
6	6	0	-3.699419	-2.199247	0.414916
7	7	0	-2.567358	-2.051558	-0.354439
8	1	0	-1.430036	-0.350689	-0.994292
9	1	0	-4.971656	-0.611794	1.312691
10	1	0	-4.093856	-3.169411	0.671358
11	7	0	-3.252090	-0.059850	0.143204
12	6	0	-1.681605	-3.120798	-0.814725
13	1	0	-1.104794	-3.493862	0.033024
14	1	0	-0.978681	-2.708987	-1.538917
15	6	0	-3.271450	1.403171	0.323092
16	1	0	-4.288052	1.739494	0.094833
17	1	0	-3.039970	1.586872	1.375529
18	6	0	2.828680	-0.244015	-0.075400
19	6	0	4.008688	-0.944590	-0.296448
20	6	0	2.835906	1.072435	0.384670
21	6	0	5.226865	-0.307195	-0.057060
22	1	0	3.957078	-1.966634	-0.657445
23	6	0	4.055642	1.696856	0.623178
24	1	0	1.896808	1.593269	0.551790
25	6	0	5.250411	1.007616	0.401959
26	1	0	6.156820	-0.839300	-0.231856
27	1	0	4.076366	2.721522	0.980676
28	1	0	6.200354	1.499498	0.587436
29	6	0	0.425253	-1.283065	1.131447
30	6	0	-0.254373	-0.193076	1.683250
31	7	0	-0.878642	0.707366	2.097982
32	1	0	0.823853	-2.066026	1.762968

33	1	0	-2.283249	-3.907927	-1.270926
34	6	0	-2.248237	2.105975	-0.554935
35	6	0	-2.233357	3.606981	-0.268759
36	1	0	-2.473199	1.927591	-1.615239
37	1	0	-1.251254	1.697699	-0.351082
38	6	0	-1.223381	4.338661	-1.149600
39	1	0	-3.235438	4.028644	-0.422904
40	1	0	-1.981752	3.758876	0.787731
41	1	0	-1.194395	5.406508	-0.917624
42	1	0	-0.218433	3.930824	-1.003743
43	1	0	-1.475444	4.229831	-2.209420

Zero-point correction= 0.355448 (Hartree/Particle)
Thermal correction to Energy= 0.378370
Thermal correction to Enthalpy= 0.379314
Thermal correction to Gibbs Free Energy= 0.299823
Sum of electronic and zero-point Energies= -1334.391340
Sum of electronic and thermal Energies= -1334.368417
Sum of electronic and thermal Enthalpies= -1334.367473
Sum of electronic and thermal Free Energies= -1334.446965

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.142472	-1.828010	-0.537082
2	8	0	0.992419	-1.137955	-1.201586
3	8	0	-0.533548	-3.136886	-1.071446
4	6	0	0.552323	1.276502	0.843339
5	6	0	-0.379715	3.247308	0.501275
6	6	0	0.777083	3.196887	-0.217467
7	7	0	1.341087	1.960602	0.012479
8	1	0	0.646172	0.215537	1.142943
9	1	0	-1.118326	4.026376	0.603895
10	1	0	1.242927	3.926472	-0.860757
11	7	0	-0.493721	2.042476	1.155414
12	6	0	2.521106	1.405233	-0.676589
13	6	0	3.297005	0.432487	0.198087
14	1	0	3.138812	2.258485	-0.971209
15	1	0	2.158230	0.884482	-1.567903
16	6	0	4.413654	-0.237268	-0.601191
17	1	0	3.706286	0.957697	1.071026
18	1	0	2.615535	-0.348962	0.551114

19	1	0	3.960858	-0.761122	-1.451108
20	1	0	5.090778	0.524075	-1.010730
21	6	0	-1.651859	1.580376	1.924922
22	1	0	-1.423747	0.609216	2.368942
23	1	0	-1.877806	2.307095	2.706118
24	1	0	-2.500017	1.466695	1.244505
25	6	0	5.202722	-1.227788	0.251163
26	1	0	4.541833	-2.006138	0.645239
27	1	0	5.985907	-1.717733	-0.332781
28	1	0	5.678906	-0.727231	1.100770
29	6	0	-1.575601	-0.758174	-0.755636
30	6	0	-1.421277	0.455333	-1.421108
31	6	0	-2.829428	-1.187952	-0.320196
32	6	0	-2.535114	1.269494	-1.626841
33	1	0	-0.437778	0.734572	-1.790516
34	6	0	-3.934829	-0.364512	-0.520721
35	1	0	-2.936602	-2.153280	0.163714
36	6	0	-3.789437	0.862509	-1.170929
37	1	0	-2.425409	2.210861	-2.157420
38	1	0	-4.912407	-0.688391	-0.178785
39	1	0	-4.657578	1.493269	-1.337480
40	6	0	0.185646	-1.769507	1.157535
41	6	0	-0.893327	-1.904060	2.049507
42	7	0	-1.791355	-1.878024	2.798211
43	1	0	1.106216	-2.301686	1.384370

Zero-point correction=	0.355049 (Hartree/Particle)
Thermal correction to Energy=	0.377545
Thermal correction to Enthalpy=	0.378489
Thermal correction to Gibbs Free Energy=	0.302461
Sum of electronic and zero-point Energies=	-1334.379041
Sum of electronic and thermal Energies=	-1334.356546
Sum of electronic and thermal Enthalpies=	-1334.355602
Sum of electronic and thermal Free Energies=	-1334.431630

Conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.026339	-1.883594	-0.571453
2	8	0	0.283179	-1.632530	-1.226047
3	8	0	-1.861928	-2.953250	-1.126775
4	6	0	0.796024	0.717656	0.796652

5	6	0	0.570996	2.904017	0.603085
6	6	0	1.634721	2.521886	-0.157736
7	7	0	1.751057	1.154942	-0.025458
8	1	0	0.536937	-0.328195	1.043430
9	1	0	0.126398	3.873121	0.765253
10	1	0	2.306800	3.095931	-0.776038
11	7	0	0.071210	1.764650	1.191279
12	6	0	2.742497	0.290454	-0.681402
13	6	0	4.016774	0.156481	0.144333
14	1	0	2.950103	0.735769	-1.659114
15	1	0	2.247355	-0.671160	-0.847845
16	6	0	5.041562	-0.733322	-0.557884
17	1	0	4.447484	1.150406	0.326094
18	1	0	3.765159	-0.268250	1.124504
19	1	0	4.598806	-1.720516	-0.735353
20	1	0	5.271074	-0.312800	-1.545270
21	6	0	-1.167322	1.668908	1.969744
22	1	0	-1.263986	0.658343	2.369928
23	1	0	-1.133534	2.393579	2.784045
24	1	0	-2.013520	1.870867	1.307543
25	6	0	6.328196	-0.879068	0.250998
26	1	0	6.125723	-1.322439	1.231008
27	1	0	7.048628	-1.519620	-0.263686
28	1	0	6.800910	0.094818	0.414764
29	6	0	-1.976223	-0.364992	-0.768695
30	6	0	-1.387142	0.715970	-1.420035
31	6	0	-3.296332	-0.305512	-0.320417
32	6	0	-2.117245	1.891532	-1.593541
33	1	0	-0.375039	0.612298	-1.802275
34	6	0	-4.015884	0.875364	-0.491423
35	1	0	-3.751229	-1.169694	0.152759
36	6	0	-3.427983	1.973713	-1.122213
37	1	0	-1.668203	2.734544	-2.110725
38	1	0	-5.040697	0.933565	-0.139199
39	1	0	-3.998207	2.887244	-1.262046
40	6	0	-0.700631	-1.966894	1.119018
41	6	0	-1.770754	-1.793365	2.014478
42	7	0	-2.620013	-1.518791	2.769940
43	1	0	0.027143	-2.746636	1.327937

Zero-point correction= 0.354566 (Hartree/Particle)
Thermal correction to Energy= 0.377357
Thermal correction to Enthalpy= 0.378301
Thermal correction to Gibbs Free Energy= 0.299519

Sum of electronic and zero-point Energies= -1334.377222
Sum of electronic and thermal Energies= -1334.354431
Sum of electronic and thermal Enthalpies= -1334.353487
Sum of electronic and thermal Free Energies= -1334.432269

9-$EtSO_2Fl$

Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.370090	-2.028538	0.339336
2	6	0	2.406879	-2.859967	-0.236532
3	6	0	1.184666	-2.343223	-0.673586
4	6	0	0.960758	-0.981390	-0.528681
5	6	0	1.921863	-0.142717	0.055537
6	6	0	3.136435	-0.661698	0.491616
7	1	0	4.311569	-2.451842	0.675340
8	1	0	2.606949	-3.921467	-0.340878
9	1	0	0.421859	-2.987927	-1.098305
10	1	0	3.887979	-0.020213	0.942302
11	6	0	-0.271748	-0.174199	-0.875740
12	1	0	-0.622581	-0.311811	-1.903906
13	6	0	0.129911	1.239627	-0.529735
14	6	0	-0.548484	2.432882	-0.740103
15	6	0	0.045436	3.627447	-0.325236
16	6	0	1.301331	3.620168	0.283748
17	6	0	1.996856	2.425324	0.470247
18	6	0	1.407773	1.235515	0.054963
19	1	0	-1.516825	2.451615	-1.232782
20	1	0	-0.471074	4.568628	-0.483338
21	1	0	1.747414	4.556932	0.602840
22	1	0	2.983966	2.428513	0.923037
23	16	0	-1.633696	-0.827563	0.164196
24	8	0	-1.963762	-2.143661	-0.392340
25	8	0	-1.261902	-0.697469	1.570946
26	6	0	-3.041497	0.254020	-0.137712
27	1	0	-2.790573	1.216764	0.312209
28	1	0	-3.136831	0.357659	-1.223134
29	6	0	-4.283712	-0.370123	0.490709
30	1	0	-5.140398	0.287634	0.327972
31	1	0	-4.492616	-1.343686	0.043357
32	1	0	-4.143737	-0.499538	1.566319

Zero-point correction= 0.256956 (Hartree/Particle)

Thermal correction to Energy=	0.272050
Thermal correction to Enthalpy=	0.272995
Thermal correction to Gibbs Free Energy=	0.214492
Sum of electronic and zero-point Energies=	-1128.058329
Sum of electronic and thermal Energies=	-1128.043235
Sum of electronic and thermal Enthalpies=	-1128.042291
Sum of electronic and thermal Free Energies=	-1128.100794

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.330717	3.014449	0.432347
2	6	0	1.174677	3.455947	-0.216092
3	6	0	0.256403	2.543188	-0.742261
4	6	0	0.524824	1.187806	-0.603712
5	6	0	1.683510	0.738765	0.052288
6	6	0	2.596078	1.651990	0.573151
7	1	0	3.031149	3.740986	0.832275
8	1	0	0.986295	4.520422	-0.312002
9	1	0	-0.653224	2.877419	-1.231328
10	1	0	3.496341	1.314934	1.078780
11	6	0	-0.290143	-0.000696	-1.058200
12	6	0	0.528641	-1.186422	-0.603504
13	6	0	0.264680	-2.542693	-0.741999
14	6	0	1.186018	-3.452394	-0.215897
15	6	0	2.340655	-3.007052	0.432411
16	6	0	2.601547	-1.643721	0.573139
17	6	0	1.685899	-0.733538	0.052361
18	1	0	-0.643909	-2.879919	-1.230936
19	1	0	1.001140	-4.517490	-0.311736
20	1	0	3.043502	-3.731296	0.832262
21	1	0	3.500790	-1.303660	1.078567
22	16	0	-1.969764	-0.003101	-0.358037
23	8	0	-2.602617	1.261899	-0.740550
24	8	0	-2.598969	-1.270088	-0.740011
25	6	0	-1.726439	-0.002466	1.423256
26	1	0	-1.140203	-0.896524	1.653073
27	1	0	-1.142864	0.893382	1.652841
28	6	0	-3.087817	-0.004402	2.110446
29	1	0	-3.658359	-0.893474	1.833395
30	1	0	-2.944715	-0.004080	3.193109
31	1	0	-3.660921	0.882983	1.833256

32	1	0	-0.501605	-0.001134	-2.134886

Zero-point correction= 0.257435 (Hartree/Particle)
Thermal correction to Energy= 0.272486
Thermal correction to Enthalpy= 0.273431
Thermal correction to Gibbs Free Energy= 0.214868
Sum of electronic and zero-point Energies= -1128.065532
Sum of electronic and thermal Energies= -1128.050480
Sum of electronic and thermal Enthalpies= -1128.049536
Sum of electronic and thermal Free Energies= -1128.108098

The conjugate base anion of 9-EtSO_2Fl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.614055	3.012030	0.244878
2	6	0	1.298415	3.445272	-0.018047
3	6	0	0.269062	2.545146	-0.249717
4	6	0	0.544600	1.161729	-0.215503
5	6	0	1.880059	0.722902	0.062538
6	6	0	2.901777	1.653535	0.282031
7	1	0	3.400423	3.742563	0.414449
8	1	0	1.087098	4.511853	-0.047701
9	1	0	-0.736840	2.886098	-0.473966
10	1	0	3.915492	1.313064	0.486030
11	6	0	-0.269686	-0.000049	-0.414326
12	6	0	0.544764	-1.161708	-0.215475
13	6	0	0.269429	-2.545166	-0.249672
14	6	0	1.298917	-3.445137	-0.018001
15	6	0	2.614496	-3.011702	0.244912
16	6	0	2.902018	-1.653165	0.282049
17	6	0	1.880162	-0.722684	0.062551
18	1	0	-0.736424	-2.886268	-0.473903
19	1	0	1.087754	-4.511750	-0.047643
20	1	0	3.400970	-3.742119	0.414486
21	1	0	3.915684	-1.312540	0.486035
22	16	0	-1.972664	-0.000153	-0.448102
23	8	0	-2.484220	1.267688	-1.005179
24	8	0	-2.484057	-1.268171	-1.004926
25	6	0	-2.506467	-0.000007	1.283949
26	1	0	-2.055600	-0.891927	1.729445
27	1	0	-2.055686	0.892046	1.729267
28	6	0	-4.025483	-0.000071	1.385662

29	1	0	-4.436391	-0.886809	0.896081
30	1	0	-4.337862	0.000015	2.435013
31	1	0	-4.436479	0.886530	0.895908

Zero-point correction=	0.242843 (Hartree/Particle)
Thermal correction to Energy=	0.258015
Thermal correction to Enthalpy=	0.258959
Thermal correction to Gibbs Free Energy=	0.199257
Sum of electronic and zero-point Energies=	-1127.539664
Sum of electronic and thermal Energies=	-1127.524493
Sum of electronic and thermal Enthalpies=	-1127.523549
Sum of electronic and thermal Free Energies=	-1127.583251

Complexes formed from a [Bmim] cation and the conjugate base anion of 9-EtSO_2Fl

Conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.302068	3.266972	2.435837
2	6	0	-1.461280	3.262844	1.632243
3	6	0	-1.895684	2.112937	0.988730
4	6	0	-1.152963	0.921028	1.128072
5	6	0	-0.002553	0.917122	1.984439
6	6	0	0.415539	2.092083	2.621649
7	1	0	0.011989	4.182909	2.926379
8	1	0	-2.032626	4.181241	1.522651
9	1	0	-2.789107	2.125301	0.371913
10	1	0	1.296798	2.084299	3.259704
11	6	0	-1.254399	-0.374187	0.526348
12	6	0	-0.192782	-1.194883	1.030804
13	6	0	0.218927	-2.516172	0.749706
14	6	0	1.342522	-3.022302	1.387619
15	6	0	2.079757	-2.251860	2.312393
16	6	0	1.692263	-0.949348	2.594425
17	6	0	0.572046	-0.408095	1.950767
18	1	0	-0.338216	-3.117010	0.037636
19	1	0	1.657364	-4.040728	1.176307
20	1	0	2.944545	-2.684313	2.806054
21	1	0	2.260050	-0.349534	3.303019
22	16	0	-2.480985	-0.890326	-0.541447
23	8	0	-3.027466	0.278146	-1.274861
24	8	0	-2.000302	-2.030131	-1.346726

25	6	0	-3.847280	-1.518308	0.454031
26	1	0	-3.415785	-2.315231	1.066827
27	1	0	-4.142290	-0.687874	1.102212
28	6	0	-4.984721	-2.008032	-0.431278
29	1	0	-4.639126	-2.811119	-1.086346
30	1	0	-5.800439	-2.388499	0.189271
31	1	0	-5.366577	-1.192094	-1.049327
32	6	0	0.713175	1.593514	-1.146644
33	6	0	-0.281567	0.368125	-2.681701
34	6	0	0.764004	-0.345798	-2.185395
35	7	0	1.376223	0.441697	-1.236335
36	1	0	0.917740	2.386979	-0.439253
37	1	0	-1.060193	0.094505	-3.375556
38	1	0	1.078226	-1.360280	-2.372740
39	7	0	-0.283973	1.581133	-2.030462
40	6	0	2.562937	0.064008	-0.461098
41	6	0	3.829240	0.090686	-1.308379
42	1	0	2.375696	-0.931211	-0.045901
43	1	0	2.626442	0.759732	0.380100
44	6	0	5.050584	-0.290804	-0.472430
45	1	0	3.724194	-0.608478	-2.148275
46	1	0	3.964941	1.090923	-1.740073
47	1	0	5.151881	0.416565	0.360197
48	1	0	4.883626	-1.276589	-0.021102
49	6	0	-1.280373	2.632891	-2.216174
50	1	0	-1.205074	3.021261	-3.233357
51	1	0	-2.262240	2.194475	-2.028386
52	1	0	-1.083102	3.424396	-1.493695
53	6	0	6.334876	-0.304778	-1.298205
54	1	0	6.526903	0.678187	-1.740653
55	1	0	7.198986	-0.571200	-0.684428
56	1	0	6.266356	-1.031180	-2.114313

Zero-point correction= 0.473813 (Hartree/Particle)
Thermal correction to Energy= 0.500910
Thermal correction to Enthalpy= 0.501855
Thermal correction to Gibbs Free Energy= 0.416453
Sum of electronic and zero-point Energies= -1550.455780
Sum of electronic and thermal Energies= -1550.428682
Sum of electronic and thermal Enthalpies= -1550.427738
Sum of electronic and thermal Free Energies= -1550.513139

Conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.258935	-0.029883	3.211469
2	6	0	2.083916	1.278362	2.713889
3	6	0	1.001025	1.608766	1.913773
4	6	0	0.058341	0.612181	1.587810
5	6	0	0.220698	-0.706524	2.116545
6	6	0	1.325551	-1.016699	2.920573
7	1	0	3.116970	-0.259398	3.835674
8	1	0	2.816777	2.042273	2.959226
9	1	0	0.900830	2.611592	1.508550
10	1	0	1.450235	-2.022146	3.316939
11	6	0	-1.105009	0.608977	0.749049
12	6	0	-1.682960	-0.704197	0.775242
13	6	0	-2.807148	-1.276353	0.145262
14	6	0	-3.070784	-2.626420	0.326208
15	6	0	-2.246291	-3.436899	1.133350
16	6	0	-1.152668	-2.881817	1.785538
17	6	0	-0.863607	-1.523279	1.616752
18	1	0	-3.448138	-0.660069	-0.477304
19	1	0	-3.943049	-3.067082	-0.151136
20	1	0	-2.484329	-4.488062	1.265188
21	1	0	-0.524952	-3.499947	2.424105
22	16	0	-1.516144	1.870951	-0.315196
23	8	0	-0.282689	2.550445	-0.781599
24	8	0	-2.413650	1.351210	-1.376614
25	6	0	-2.456624	3.113392	0.585973
26	1	0	-3.346690	2.591863	0.949026
27	1	0	-1.831588	3.386247	1.441743
28	6	0	-2.789057	4.303129	-0.303656
29	1	0	-3.383241	3.984005	-1.163079
30	1	0	-3.363581	5.039908	0.263823
31	1	0	-1.873433	4.774902	-0.667100
32	6	0	0.139761	-0.383409	-1.972473
33	6	0	-0.189723	-2.538702	-1.655324
34	6	0	0.944082	-2.182462	-0.992844
35	7	0	1.133773	-0.836863	-1.210741
36	1	0	-0.004875	0.650498	-2.259546
37	1	0	-0.726129	-3.473380	-1.689593
38	1	0	1.594811	-2.749525	-0.346037
39	7	0	-0.671637	-1.399904	-2.263177
40	6	0	2.221450	-0.015271	-0.662601
41	6	0	3.525236	-0.208883	-1.426274

42	1	0	2.329966	-0.288080	0.392301
43	1	0	1.873696	1.021836	-0.697829
44	6	0	4.642333	0.630903	-0.808086
45	1	0	3.809138	-1.269846	-1.411033
46	1	0	3.382658	0.069542	-2.478715
47	1	0	4.348030	1.687504	-0.822950
48	1	0	4.752622	0.357006	0.248688
49	6	0	-1.897283	-1.296628	-3.051850
50	1	0	-1.678031	-1.484876	-4.104619
51	1	0	-2.601645	-2.036810	-2.672483
52	1	0	-2.310832	-0.298606	-2.900223
53	6	0	5.972453	0.451515	-1.535589
54	1	0	5.888243	0.749368	-2.585854
55	1	0	6.759976	1.056035	-1.078233
56	1	0	6.294847	-0.594620	-1.509681

Zero-point correction=	0.474248 (Hartree/Particle)
Thermal correction to Energy=	0.501274
Thermal correction to Enthalpy=	0.502218
Thermal correction to Gibbs Free Energy=	0.416948
Sum of electronic and zero-point Energies=	-1550.456518
Sum of electronic and thermal Energies=	-1550.429493
Sum of electronic and thermal Enthalpies=	-1550.428549
Sum of electronic and thermal Free Energies=	-1550.513819

Confermer3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088856	-2.506940	3.055095
2	6	0	0.785895	-1.400992	3.064040
3	6	0	0.550295	-0.281887	2.278945
4	6	0	-0.584656	-0.253992	1.440386
5	6	0	-1.495436	-1.360570	1.465954
6	6	0	-1.233380	-2.479246	2.267471
7	1	0	0.122626	-3.367819	3.681491
8	1	0	1.661471	-1.422642	3.707947
9	1	0	1.234682	0.561445	2.294449
10	1	0	-1.923785	-3.320140	2.276597
11	6	0	-1.054187	0.679768	0.461927
12	6	0	-2.275878	0.178746	-0.095376
13	6	0	-3.140816	0.653137	-1.105695
14	6	0	-4.257950	-0.097623	-1.444991

15	6	0	-4.550206	-1.321017	-0.805459
16	6	0	-3.704452	-1.806357	0.182312
17	6	0	-2.561740	-1.076267	0.533006
18	1	0	-2.924288	1.592216	-1.604773
19	1	0	-4.929129	0.270693	-2.216151
20	1	0	-5.441282	-1.875514	-1.082533
21	1	0	-3.924897	-2.749404	0.678382
22	16	0	-0.328163	2.179406	0.095003
23	8	0	1.131989	2.098294	0.348684
24	8	0	-0.759377	2.635904	-1.241169
25	6	0	0.746574	-1.646999	-0.914495
26	6	0	1.271459	0.191456	-2.003771
27	6	0	0.129985	-0.308298	-2.548350
28	7	0	-0.173513	-1.462016	-1.860334
29	1	0	0.739522	-2.433355	-0.170885
30	1	0	1.796153	1.114613	-2.190173
31	1	0	-0.522807	0.089219	-3.308891
32	7	0	1.645289	-0.667483	-0.995255
33	6	0	-1.322937	-2.325646	-2.122969
34	1	0	-2.219167	-1.706743	-2.201492
35	1	0	-1.445961	-3.004379	-1.279296
36	6	0	2.802581	-0.488093	-0.112242
37	1	0	2.691401	0.502965	0.337192
38	1	0	2.709865	-1.234858	0.681022
39	1	0	-1.150420	-2.884433	-3.044987
40	6	0	4.118934	-0.638859	-0.865502
41	6	0	5.311481	-0.478304	0.076626
42	1	0	4.177546	0.113586	-1.662351
43	1	0	4.155180	-1.622958	-1.350962
44	6	0	6.646540	-0.620578	-0.650124
45	1	0	5.255497	0.502658	0.563914
46	1	0	5.243306	-1.227353	0.875635
47	1	0	7.487273	-0.504038	0.038510
48	1	0	6.732961	-1.604785	-1.121909
49	1	0	6.747589	0.136380	-1.434391
50	6	0	-0.952116	3.392669	1.273337
51	6	0	-0.317940	4.756498	1.037371
52	1	0	-0.722480	2.984642	2.262299
53	1	0	-2.036889	3.400363	1.133196
54	1	0	-0.711861	5.478872	1.757122
55	1	0	0.766346	4.697999	1.156623
56	1	0	-0.540337	5.111538	0.028374

Zero-point correction= 0.474127 (Hartree/Particle)

Thermal correction to Energy=	0.501156
Thermal correction to Enthalpy=	0.502100
Thermal correction to Gibbs Free Energy=	0.416437
Sum of electronic and zero-point Energies=	-1550.454520
Sum of electronic and thermal Energies=	-1550.427491
Sum of electronic and thermal Enthalpies=	-1550.426547
Sum of electronic and thermal Free Energies=	-1550.512210

Conformer 4 (**This one has a very small imaginary frequencies: -2.7856i**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.387812	-1.465380	1.224317
2	6	0	-4.231503	-0.084660	1.455573
3	6	0	-3.201212	0.637412	0.869381
4	6	0	-2.288486	-0.027582	0.025150
5	6	0	-2.467035	-1.423969	-0.230732
6	6	0	-3.510776	-2.131033	0.377341
7	1	0	-5.204810	-2.002244	1.696125
8	1	0	-4.937847	0.428566	2.102978
9	1	0	-3.088586	1.699909	1.064676
10	1	0	-3.638343	-3.193641	0.182498
11	6	0	-1.113455	0.399768	-0.681447
12	6	0	-0.581615	-0.721179	-1.403173
13	6	0	0.542464	-0.887551	-2.237331
14	6	0	0.845767	-2.153049	-2.721216
15	6	0	0.052409	-3.273765	-2.404813
16	6	0	-1.076686	-3.120550	-1.609787
17	6	0	-1.405584	-1.855267	-1.112551
18	1	0	1.166279	-0.034231	-2.485557
19	1	0	1.710867	-2.280636	-3.367361
20	1	0	0.314243	-4.250241	-2.800161
21	1	0	-1.701339	-3.979479	-1.374564
22	16	0	-0.467103	1.970791	-0.649771
23	8	0	-0.804372	2.630166	0.637042
24	8	0	0.972424	1.930043	-1.005131
25	6	0	-0.111498	-1.301424	2.022939
26	6	0	1.112559	0.501743	1.718780
27	1	0	-0.961539	-1.874860	2.359313
28	1	0	1.435697	1.532586	1.721636
29	7	0	0.049009	0.022347	2.361993
30	6	0	-0.853301	0.813320	3.198281
31	1	0	-0.413076	0.954361	4.187109

32	1	0	-1.027211	1.764615	2.692050
33	1	0	-1.797609	0.274667	3.272665
34	6	0	2.832397	-0.338057	0.134989
35	6	0	4.126907	-0.316538	0.940999
36	1	0	2.683163	0.576397	-0.447893
37	1	0	2.804857	-1.184348	-0.556339
38	6	0	5.350093	-0.224435	0.030206
39	1	0	4.115880	0.539307	1.628880
40	1	0	4.187751	-1.222204	1.558497
41	6	0	6.655817	-0.188226	0.821207
42	1	0	5.355355	-1.081733	-0.654345
43	1	0	5.269181	0.673134	-0.595012
44	1	0	7.521498	-0.126737	0.156906
45	1	0	6.683250	0.678178	1.489797
46	1	0	6.766422	-1.088243	1.434857
47	6	0	0.898792	-1.617688	1.165862
48	1	0	1.102187	-2.521203	0.609964
49	7	0	1.655145	-0.480352	0.999932
50	6	0	-1.268314	2.956251	-1.927305
51	6	0	-0.738223	4.383122	-1.936290
52	1	0	-2.337996	2.902417	-1.703457
53	1	0	-1.073336	2.425385	-2.863695
54	1	0	-1.235688	4.957599	-2.722137
55	1	0	-0.926807	4.867442	-0.975502
56	1	0	0.337478	4.389382	-2.126628

Zero-point correction= 0.473575 (Hartree/Particle)
Thermal correction to Energy= 0.499925
Thermal correction to Enthalpy= 0.500870
Thermal correction to Gibbs Free Energy= 0.417004
Sum of electronic and zero-point Energies= -1550.456141
Sum of electronic and thermal Energies= -1550.429791
Sum of electronic and thermal Enthalpies= -1550.428847
Sum of electronic and thermal Free Energies= -1550.512712

Conformer 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.581275	-1.151129	-1.087701
2	6	0	4.389981	0.220301	-1.354315
3	6	0	3.322374	0.919668	-0.813561

4	6	0	2.408762	0.243059	0.020204
5	6	0	2.622160	-1.138947	0.316428
6	6	0	3.704085	-1.826449	-0.248894
7	1	0	5.425492	-1.672705	-1.527694
8	1	0	5.092785	0.738330	-2.000984
9	1	0	3.170831	1.967417	-1.057457
10	1	0	3.860325	-2.880285	-0.028195
11	6	0	1.199977	0.651678	0.675480
12	6	0	0.674893	-0.468205	1.404597
13	6	0	-0.468597	-0.647993	2.210014
14	6	0	-0.737190	-1.904337	2.734092
15	6	0	0.111251	-3.003202	2.488557
16	6	0	1.257971	-2.835690	1.723134
17	6	0	1.549471	-1.579699	1.180816
18	1	0	-1.129418	0.190278	2.407686
19	1	0	-1.614054	-2.040870	3.362980
20	1	0	-0.119025	-3.971483	2.922728
21	1	0	1.926679	-3.675678	1.546703
22	16	0	0.387601	2.109010	0.345968
23	8	0	0.614672	2.502529	-1.067542
24	8	0	-1.030550	1.988645	0.765120
25	6	0	1.107975	3.424821	1.341303
26	1	0	0.966750	3.110392	2.379038
27	1	0	2.177177	3.411256	1.108478
28	6	0	0.455054	4.764819	1.032504
29	1	0	-0.615197	4.727620	1.248593
30	1	0	0.908141	5.547439	1.646647
31	1	0	0.591258	5.021011	-0.020471
32	6	0	-0.997727	-0.180739	-1.466201
33	6	0	-1.287271	-2.227299	-0.705861
34	6	0	-0.168653	-2.219261	-1.480950
35	7	0	-0.012706	-0.935530	-1.951018
36	1	0	-1.101075	0.885580	-1.619842
37	1	0	-1.721490	-3.005243	-0.098062
38	1	0	0.554788	-2.991058	-1.690601
39	7	0	-1.786956	-0.943706	-0.710920
40	6	0	1.077940	-0.446273	-2.796427
41	1	0	2.006950	-0.924038	-2.477429
42	1	0	1.164889	0.630541	-2.638326
43	6	0	-2.960205	-0.462823	0.027418
44	1	0	-3.103471	-1.158419	0.859079
45	1	0	-2.686511	0.511714	0.443178
46	1	0	0.860022	-0.677156	-3.841142
47	6	0	-4.198210	-0.387640	-0.859781

48	6	0	-5.425629	0.060337	-0.067800
49	1	0	-4.384609	-1.369161	-1.315229
50	1	0	-4.012569	0.317078	-1.680784
51	6	0	-6.670173	0.166463	-0.946128
52	1	0	-5.607808	-0.649986	0.748475
53	1	0	-5.218396	1.029478	0.401980
54	1	0	-7.541404	0.479151	-0.365024
55	1	0	-6.520794	0.897698	-1.746887
56	1	0	-6.904304	-0.796580	-1.411546

Zero-point correction= 0.473497 (Hartree/Particle)
Thermal correction to Energy= 0.500652
Thermal correction to Enthalpy= 0.501596
Thermal correction to Gibbs Free Energy= 0.415471
Sum of electronic and zero-point Energies= -1550.456509
Sum of electronic and thermal Energies= -1550.429354
Sum of electronic and thermal Enthalpies= -1550.428410
Sum of electronic and thermal Free Energies= -1550.514535

Complexes formed from two [Bmim] cation and the conjugate base anion of $CH_2(CN)_2$.
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.724488	1.260480	-0.553250
2	6	0	4.080857	2.388797	-1.872888
3	6	0	4.591642	1.136047	-1.711972
4	7	0	3.731330	0.450743	-0.885664
5	1	0	1.896279	1.002869	0.096675
6	1	0	4.440532	3.234935	-2.436932
7	1	0	5.482131	0.678932	-2.113425
8	7	0	2.914965	2.442325	-1.143544
9	6	0	3.868767	-0.955216	-0.452077
10	6	0	3.870371	-1.090300	1.064995
11	1	0	4.806974	-1.314219	-0.882231
12	1	0	3.037102	-1.521417	-0.881201
13	6	0	3.968535	-2.559676	1.473149
14	1	0	4.703723	-0.515867	1.489008
15	1	0	2.940289	-0.669709	1.468468
16	1	0	3.152736	-3.111376	0.991399
17	1	0	4.909789	-2.980686	1.097779
18	6	0	2.042788	3.613941	-1.006530
19	1	0	2.502699	4.328565	-0.322728

20	1	0	1.914330	4.065526	-1.990087
21	1	0	1.073420	3.285964	-0.625936
22	6	0	3.889520	-2.735896	2.987407
23	1	0	2.937070	-2.357005	3.372333
24	1	0	3.967144	-3.789453	3.265752
25	1	0	4.696271	-2.195309	3.492337
26	6	0	0.001176	-0.002094	1.335021
27	6	0	-0.437792	1.110398	0.612803
28	7	0	-0.784208	2.018766	-0.043091
29	6	0	0.439074	-1.115379	0.613272
30	7	0	0.784730	-2.024415	-0.042073
31	1	0	0.001438	-0.001773	2.415665
32	6	0	-2.725675	-1.259683	-0.552774
33	6	0	-4.081550	-2.386393	-1.874252
34	6	0	-4.591902	-1.133532	-1.712774
35	7	0	-3.731903	-0.449233	-0.885316
36	1	0	-1.897726	-1.002624	0.097682
37	1	0	-4.441182	-3.231957	-2.439181
38	1	0	-5.481872	-0.675713	-2.114574
39	7	0	-2.916207	-2.440990	-1.144129
40	6	0	-3.868855	0.956577	-0.450999
41	6	0	-3.869837	1.090937	1.066127
42	1	0	-4.807162	1.315947	-0.880623
43	1	0	-3.037145	1.522716	-0.880151
44	6	0	-3.967168	2.560164	1.475032
45	1	0	-4.703291	0.516703	1.490207
46	1	0	-2.939796	0.669796	1.469107
47	1	0	-3.151037	3.111638	0.993578
48	1	0	-4.908147	2.981908	1.099793
49	6	0	-2.044874	-3.613209	-1.006826
50	1	0	-2.504083	-4.326348	-0.321009
51	1	0	-1.918721	-4.066468	-1.989904
52	1	0	-1.074528	-3.285439	-0.628579
53	6	0	-3.888178	2.735584	2.989381
54	1	0	-2.936065	2.355780	3.374245
55	1	0	-3.965041	3.789061	3.268246
56	1	0	-4.695389	2.195355	3.493953

Zero-point correction=	0.491891 (Hartree/Particle)
Thermal correction to Energy=	0.521418
Thermal correction to Enthalpy=	0.522362
Thermal correction to Gibbs Free Energy=	0.425502
Sum of electronic and zero-point Energies=	-1070.044544
Sum of electronic and thermal Energies=	-1070.015017

Sum of electronic and thermal Enthalpies= -1070.014073
Sum of electronic and thermal Free Energies= -1070.110933

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.546343	-0.934512	1.165810
2	6	0	-1.973270	-3.040450	0.872871
3	6	0	-2.748381	-2.660789	-0.179133
4	7	0	-3.102194	-1.346137	0.027871
5	1	0	-2.607870	0.064773	1.569012
6	1	0	-1.475950	-3.971731	1.092612
7	1	0	-3.071091	-3.205347	-1.052278
8	7	0	-1.866969	-1.947866	1.702519
9	6	0	-3.848244	-0.510156	-0.930481
10	6	0	-4.569819	0.653314	-0.268115
11	1	0	-4.559256	-1.176615	-1.426481
12	1	0	-3.127412	-0.146517	-1.669957
13	6	0	-5.371319	1.449294	-1.299805
14	1	0	-5.240328	0.275322	0.514759
15	1	0	-3.835092	1.322567	0.194201
16	1	0	-4.688635	1.816481	-2.075771
17	1	0	-6.091364	0.787212	-1.796501
18	6	0	-1.095859	-1.903765	2.944602
19	1	0	-1.512904	-2.620191	3.653106
20	1	0	-0.056715	-2.138873	2.707799
21	1	0	-1.164656	-0.897947	3.357875
22	6	0	-6.106141	2.626090	-0.662868
23	1	0	-5.401177	3.310928	-0.181515
24	1	0	-6.665693	3.191762	-1.411300
25	1	0	-6.815597	2.281755	0.096131
26	6	0	-0.025345	-0.567513	-1.129270
27	6	0	-0.703562	0.580820	-0.722860
28	7	0	-1.249633	1.541799	-0.326573
29	6	0	0.627251	-1.320593	-0.147928
30	7	0	1.187973	-1.903328	0.700715
31	1	0	-0.031574	-0.885780	-2.162186
32	6	0	2.415960	1.633901	0.056067
33	6	0	4.281237	2.214642	1.070853
34	6	0	3.516306	3.333039	0.926617
35	7	0	2.357334	2.946094	0.293683
36	1	0	1.653766	1.045005	-0.443976

37	1	0	5.254081	2.076502	1.515542
38	1	0	3.695910	4.356861	1.214652
39	7	0	3.577422	1.168579	0.520288
40	6	0	1.254580	3.833098	-0.092526
41	1	0	1.056669	4.517024	0.732771
42	1	0	0.366576	3.227069	-0.284938
43	6	0	4.008750	-0.243820	0.464773
44	1	0	5.019343	-0.268571	0.879884
45	1	0	3.340682	-0.825034	1.106424
46	1	0	1.537568	4.394839	-0.983693
47	6	0	3.981447	-0.791467	-0.955972
48	6	0	4.371653	-2.268896	-0.976822
49	1	0	4.657083	-0.205693	-1.592158
50	1	0	2.968867	-0.686491	-1.366687
51	6	0	4.292509	-2.854785	-2.384166
52	1	0	5.388861	-2.385432	-0.582066
53	1	0	3.700541	-2.818486	-0.306173
54	1	0	4.576451	-3.909645	-2.388746
55	1	0	3.273588	-2.779666	-2.778027
56	1	0	4.959337	-2.324779	-3.071715

Zero-point correction=	0.491216 (Hartree/Particle)
Thermal correction to Energy=	0.521068
Thermal correction to Enthalpy=	0.522012
Thermal correction to Gibbs Free Energy=	0.425305
Sum of electronic and zero-point Energies=	-1070.046459
Sum of electronic and thermal Energies=	-1070.016607
Sum of electronic and thermal Enthalpies=	-1070.015663
Sum of electronic and thermal Free Energies=	-1070.112370

Conformer c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.039992	-1.474626	-0.552722
2	6	0	2.043012	-2.416204	1.436771
3	6	0	3.015914	-1.464722	1.416581
4	7	0	2.998170	-0.893897	0.163967
5	1	0	1.762562	-1.195482	-1.558809
6	1	0	1.701811	-3.070235	2.223471
7	1	0	3.701631	-1.138665	2.182489
8	7	0	1.451559	-2.408940	0.193744
9	6	0	3.845223	0.220361	-0.286067

10	6	0	5.301044	−0.199162	−0.450399
11	1	0	3.734857	1.019495	0.454080
12	1	0	3.413562	0.583886	−1.221748
13	6	0	6.169991	0.974218	−0.904189
14	1	0	5.684013	−0.593684	0.499578
15	1	0	5.361480	−1.015111	−1.181453
16	1	0	5.779952	1.369431	−1.850029
17	1	0	6.093556	1.786598	−0.170814
18	6	0	0.325468	−3.251299	−0.207106
19	1	0	0.630196	−4.298109	−0.181359
20	1	0	−0.500369	−3.059424	0.480644
21	1	0	0.036348	−2.979956	−1.222274
22	6	0	7.632387	0.570694	−1.076379
23	1	0	7.736035	−0.217487	−1.828349
24	1	0	8.239586	1.420409	−1.396183
25	1	0	8.049106	0.195699	−0.136484
26	6	0	0.398147	0.872907	1.248463
27	6	0	0.638155	1.166435	−0.091477
28	7	0	0.803878	1.370230	−1.236991
29	6	0	−0.418060	−0.223995	1.540626
30	7	0	−1.108411	−1.149967	1.743287
31	1	0	0.846448	1.455997	2.040504
32	6	0	−2.281874	1.706696	−0.625930
33	6	0	−2.645107	2.663940	1.320264
34	6	0	−3.252079	1.445768	1.330943
35	7	0	−3.014454	0.868777	0.104269
36	1	0	−1.889162	1.513898	−1.613800
37	1	0	−2.569900	3.425245	2.080369
38	1	0	−3.796583	0.929650	2.105722
39	7	0	−2.053299	2.808695	0.085248
40	6	0	−3.487824	−0.457618	−0.315670
41	6	0	−4.982923	−0.461359	−0.614173
42	1	0	−3.218432	−1.149459	0.487819
43	1	0	−2.906537	−0.731157	−1.201306
44	6	0	−5.456392	−1.844545	−1.061349
45	1	0	−5.535994	−0.155968	0.283070
46	1	0	−5.202585	0.279905	−1.392920
47	1	0	−4.898847	−2.146098	−1.957138
48	1	0	−5.218593	−2.578295	−0.281331
49	6	0	−1.198489	3.920561	−0.327056
50	1	0	−1.774676	4.846129	−0.315373
51	1	0	−0.353568	3.983820	0.360796
52	1	0	−0.820416	3.715479	−1.327530
53	6	0	−6.954595	−1.870294	−1.355304

54	1	0	-7.210597	-1.161888	-2.149214
55	1	0	-7.276301	-2.863526	-1.676187
56	1	0	-7.532616	-1.601912	-0.465874

Zero-point correction= 0.491148 (Hartree/Particle)
Thermal correction to Energy= 0.520975
Thermal correction to Enthalpy= 0.521919
Thermal correction to Gibbs Free Energy= 0.425619
Sum of electronic and zero-point Energies= -1070.045343
Sum of electronic and thermal Energies= -1070.015516
Sum of electronic and thermal Enthalpies= -1070.014572
Sum of electronic and thermal Free Energies= -1070.110872

Complexes formed from two [Bmim] cation and the conjugate base anion of *p*-NO_2-PhCH(CN)2.
Conformer a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.609695	-1.476156	0.246728
2	6	0	-1.456860	-0.691593	1.083916
3	6	0	-0.997451	0.603552	1.465649
4	6	0	0.226156	1.074924	1.055357
5	6	0	1.040257	0.270240	0.238170
6	6	0	0.612524	-1.007022	-0.167594
7	1	0	-0.936267	-2.466601	-0.054634
8	1	0	-1.618228	1.214345	2.114742
9	1	0	0.578588	2.053574	1.359419
10	1	0	1.255133	-1.609001	-0.799696
11	6	0	-2.716400	-1.183346	1.519416
12	7	0	2.309258	0.741662	-0.163774
13	8	0	3.025903	0.025170	-0.879752
14	8	0	2.694547	1.857911	0.212663
15	6	0	-3.175710	-2.469431	1.148578
16	7	0	-3.563288	-3.512776	0.803945
17	6	0	-3.595860	-0.384730	2.286807
18	7	0	-4.350682	0.301357	2.851116
19	6	0	-5.805842	-0.481252	0.182775
20	6	0	-4.963299	-1.743580	-1.411847
21	6	0	-4.368062	-0.521778	-1.481296
22	7	0	-4.912652	0.250687	-0.479141
23	1	0	-6.354250	-0.156036	1.055286
24	1	0	-4.800098	-2.648732	-1.974783

25	1	0	−3.598851	−0.144855	−2.136543
26	7	0	−5.861544	−1.692863	−0.370005
27	6	0	−4.529383	1.634370	−0.161787
28	6	0	−4.988229	2.610140	−1.238802
29	1	0	−3.439870	1.641177	−0.043183
30	1	0	−4.963302	1.864825	0.814338
31	6	0	−4.580389	4.044267	−0.902171
32	1	0	−4.558858	2.322982	−2.207512
33	1	0	−6.078668	2.545577	−1.342354
34	1	0	−5.007764	4.323881	0.068492
35	1	0	−3.490147	4.094465	−0.789507
36	6	0	−6.654029	−2.824566	0.113497
37	1	0	−7.255478	−2.491859	0.958616
38	1	0	−7.306119	−3.173749	−0.687449
39	1	0	−5.966655	−3.610955	0.431184
40	6	0	−5.036118	5.034037	−1.971713
41	1	0	−6.124653	5.016160	−2.083275
42	1	0	−4.743063	6.054626	−1.715269
43	1	0	−4.595228	4.792307	−2.943993
44	6	0	5.723366	1.254080	−0.099954
45	6	0	7.670043	1.317425	0.936676
46	6	0	7.662397	0.230336	0.116121
47	7	0	6.441636	0.214652	−0.521734
48	1	0	4.705107	1.483691	−0.394318
49	1	0	8.427772	1.697868	1.603379
50	1	0	8.412964	−0.522802	−0.066396
51	7	0	6.448321	1.937951	0.786152
52	6	0	5.943130	−0.832846	−1.430252
53	6	0	5.407024	−2.033051	−0.657773
54	1	0	6.769643	−1.106698	−2.091577
55	1	0	5.149989	−0.377661	−2.026482
56	6	0	4.735141	−3.034403	−1.595839
57	1	0	6.222481	−2.518430	−0.106107
58	1	0	4.675057	−1.673799	0.075157
59	1	0	3.931886	−2.520625	−2.138392
60	1	0	5.455882	−3.380296	−2.347556
61	6	0	5.995713	3.148571	1.473514
62	1	0	4.941281	3.296734	1.240248
63	1	0	6.116255	3.015051	2.548724
64	1	0	6.579145	4.004466	1.132557
65	6	0	4.164898	−4.230911	−0.837864
66	1	0	3.421084	−3.907111	−0.102663
67	1	0	3.681635	−4.935484	−1.518748
68	1	0	4.952705	−4.770053	−0.302773

Zero-point correction=	0.576308 (Hartree/Particle)
Thermal correction to Energy=	0.613231
Thermal correction to Enthalpy=	0.614175
Thermal correction to Gibbs Free Energy=	0.497338
Sum of electronic and zero-point Energies=	-1505.380315
Sum of electronic and thermal Energies=	-1505.343392
Sum of electronic and thermal Enthalpies=	-1505.342448
Sum of electronic and thermal Free Energies=	-1505.459285

Conformer b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.790069	1.111235	-1.026385
2	6	0	0.362514	0.936676	0.306981
3	6	0	0.756421	1.896598	1.264490
4	6	0	1.546814	2.977650	0.910285
5	6	0	1.959826	3.108516	-0.413668
6	6	0	1.587640	2.187968	-1.387804
7	1	0	0.484067	0.394727	-1.785114
8	1	0	0.435679	1.783206	2.296872
9	1	0	1.850736	3.720397	1.639439
10	1	0	1.917898	2.331961	-2.410425
11	6	0	-0.436207	-0.213945	0.692406
12	7	0	2.804145	4.243328	-0.791004
13	8	0	3.179784	4.306700	-1.949755
14	8	0	3.083077	5.051805	0.077903
15	6	0	-0.643387	-1.286047	-0.183761
16	7	0	-0.824341	-2.191377	-0.907071
17	6	0	-0.902352	-0.377082	2.013223
18	7	0	-1.289156	-0.504887	3.107734
19	6	0	-3.947270	-1.134103	-0.823942
20	6	0	-5.933571	-0.206733	-0.638211
21	6	0	-6.042803	-1.261434	-1.494740
22	7	0	-4.789168	-1.823330	-1.594408
23	1	0	-2.890621	-1.350880	-0.718677
24	1	0	-6.671415	0.496125	-0.284128
25	1	0	-6.892927	-1.655686	-2.029178
26	7	0	-4.620116	-0.150242	-0.229597
27	6	0	-4.414888	-2.986597	-2.402257
28	1	0	-4.980697	-3.856590	-2.067953
29	1	0	-3.347092	-3.163329	-2.268512

30	6	0	-4.011617	0.869638	0.647297
31	1	0	-3.371439	0.350436	1.367184
32	1	0	-4.832960	1.333569	1.199028
33	6	0	1.600072	-2.732086	1.293930
34	6	0	2.189493	-1.215915	2.775320
35	6	0	2.757076	-0.883968	1.582476
36	7	0	2.372676	-1.841966	0.672856
37	1	0	1.118913	-3.576009	0.820687
38	1	0	2.208924	-0.722327	3.734450
39	1	0	3.364967	-0.038549	1.297130
40	7	0	1.476553	-2.376729	2.571871
41	6	0	2.754175	-1.891132	-0.747578
42	6	0	4.088358	-2.600055	-0.954801
43	1	0	2.790580	-0.854665	-1.095652
44	1	0	1.937046	-2.391140	-1.276403
45	6	0	4.473509	-2.639483	-2.433651
46	1	0	4.868513	-2.085052	-0.380038
47	1	0	4.020696	-3.621830	-0.559433
48	1	0	3.680428	-3.142302	-3.000933
49	1	0	4.534421	-1.614686	-2.820261
50	6	0	0.686619	-3.073218	3.589837
51	1	0	0.161922	-3.900242	3.112749
52	1	0	1.354007	-3.456295	4.362458
53	1	0	-0.038095	-2.370362	4.003334
54	6	0	5.803425	-3.355043	-2.659511
55	1	0	5.756958	-4.390024	-2.307044
56	1	0	6.064252	-3.373612	-3.719945
57	1	0	6.614723	-2.852686	-2.124040
58	1	0	-4.626926	-2.779509	-3.451406
59	6	0	-3.222934	1.899013	-0.154179
60	6	0	-2.584182	2.936913	0.766499
61	1	0	-3.885955	2.388180	-0.879348
62	1	0	-2.434015	1.385627	-0.720957
63	6	0	-1.759208	3.956072	-0.015182
64	1	0	-3.366731	3.450184	1.339427
65	1	0	-1.948257	2.419065	1.496565
66	1	0	-1.274011	4.668689	0.656446
67	1	0	-0.976650	3.458820	-0.598692
68	1	0	-2.389528	4.522548	-0.707927

Conformer c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.393995	0.121863	-1.151913
2	6	0	0.435807	-0.052235	-0.125824
3	6	0	0.334374	-1.328122	0.475927
4	6	0	1.148465	-2.375966	0.078288
5	6	0	2.085648	-2.161870	-0.930708
6	6	0	2.210719	-0.922084	-1.554544
7	1	0	1.479377	1.088545	-1.644087
8	1	0	-0.398205	-1.490273	1.262021
9	1	0	1.070962	-3.355688	0.536904
10	1	0	2.943572	-0.795459	-2.343493
11	6	0	-0.416082	1.039646	0.297247
12	7	0	2.972563	-3.252255	-1.326938
13	8	0	3.775820	-3.034234	-2.219611
14	8	0	2.867452	-4.311744	-0.729945
15	6	0	-0.380572	2.283336	-0.361145
16	7	0	-0.292298	3.306643	-0.916994
17	6	0	-1.378319	0.856877	1.305526
18	7	0	-2.183175	0.672961	2.131967
19	6	0	2.483599	2.862575	0.628378
20	6	0	4.271098	1.644146	0.229833
21	6	0	4.221670	2.638169	-0.700350
22	7	0	3.097841	3.386544	-0.432780
23	1	0	1.560714	3.225151	1.057505
24	1	0	4.977601	0.840865	0.356892
25	1	0	4.879992	2.870676	-1.522580
26	7	0	3.178230	1.805792	1.051482
27	6	0	2.663390	4.578190	-1.169641
28	1	0	3.243181	5.440818	-0.838468
29	1	0	1.597752	4.723416	-0.993159
30	6	0	2.792209	0.945690	2.192711
31	1	0	1.699238	0.886893	2.175368
32	1	0	3.107580	1.447487	3.112615
33	6	0	-4.951777	0.190657	0.872226
34	6	0	-6.182178	-0.133624	-0.927472
35	6	0	-6.939988	-0.451087	0.158297
36	7	0	-6.150787	-0.241282	1.268588
37	1	0	-4.103073	0.419695	1.514861
38	1	0	-6.413438	-0.152326	-1.981150
39	1	0	-7.958762	-0.797371	0.235608
40	7	0	-4.950731	0.268497	-0.458429
41	6	0	-6.550830	-0.453235	2.661008
42	1	0	-7.399089	0.189858	2.897154
43	1	0	-5.707935	-0.200001	3.302984

44	6	0	-3.791922	0.631024	-1.297743
45	1	0	-3.207328	1.376631	-0.751560
46	1	0	-4.197633	1.110264	-2.193066
47	1	0	2.825417	4.402055	-2.232969
48	6	0	3.402012	-0.444002	2.084048
49	6	0	2.825880	-1.396466	3.131822
50	1	0	4.490636	-0.391035	2.213029
51	1	0	3.203352	-0.843720	1.082177
52	6	0	3.424187	-2.795432	2.998237
53	1	0	3.016424	-1.001161	4.137321
54	1	0	1.736613	-1.443054	3.010298
55	1	0	2.993421	-3.481462	3.731222
56	1	0	3.240894	-3.209216	2.000283
57	1	0	4.507083	-2.775354	3.155782
58	1	0	-6.819496	-1.500271	2.804508
59	6	0	-2.948779	-0.589484	-1.654483
60	6	0	-1.907161	-0.262666	-2.724596
61	1	0	-3.607486	-1.390943	-2.014768
62	1	0	-2.449903	-0.959350	-0.747854
63	6	0	-1.067038	-1.485613	-3.085891
64	1	0	-2.415473	0.115023	-3.621051
65	1	0	-1.259225	0.547698	-2.367511
66	1	0	-0.298177	-1.232727	-3.820334
67	1	0	-0.565339	-1.889924	-2.200550
68	1	0	-1.691348	-2.277972	-3.511189

Zero-point correction=	0.576578 (Hartree/Particle)
Thermal correction to Energy=	0.612980
Thermal correction to Enthalpy=	0.613924
Thermal correction to Gibbs Free Energy=	0.502343
Sum of electronic and zero-point Energies=	-1505.379660
Sum of electronic and thermal Energies=	-1505.343258
Sum of electronic and thermal Enthalpies=	-1505.342314
Sum of electronic and thermal Free Energies=	-1505.453895

Conformer d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.301390	-1.377077	-0.469329
2	6	0	-1.013516	-0.763655	0.603008
3	6	0	-0.510680	0.470749	1.111812
4	6	0	0.629807	1.041132	0.598750

5	6	0	1.315531	0.400017	−0.447711
6	6	0	0.839246	−0.809895	−0.983975
7	1	0	−0.665281	−2.316130	−0.875504
8	1	0	−1.028407	0.952668	1.936206
9	1	0	1.016283	1.972932	0.994934
10	1	0	1.377775	−1.282122	−1.798263
11	6	0	−2.184476	−1.362162	1.139715
12	7	0	2.509914	0.967739	−0.953652
13	8	0	3.131651	0.368441	−1.843536
14	8	0	2.924111	2.035257	−0.483830
15	6	0	−2.680440	−2.588269	0.635442
16	7	0	−3.095831	−3.578517	0.183469
17	6	0	−2.940815	−0.730111	2.153492
18	7	0	−3.604822	−0.174279	2.933826
19	6	0	−5.412141	−0.552247	0.362223
20	6	0	−4.784659	−1.465374	−1.539770
21	6	0	−4.223445	−0.228091	−1.459957
22	7	0	−4.631615	0.324418	−0.266120
23	1	0	−5.838785	−0.413979	1.345443
24	1	0	−4.691675	−2.242761	−2.281297
25	1	0	−3.560806	0.294611	−2.131797
26	7	0	−5.526986	−1.643450	−0.394528
27	6	0	−4.231180	1.642640	0.247686
28	6	0	−4.906911	2.779120	−0.510540
29	1	0	−3.139305	1.692207	0.167580
30	1	0	−4.479972	1.655404	1.311614
31	6	0	−4.463311	4.141287	0.022815
32	1	0	−4.670506	2.706369	−1.580050
33	1	0	−5.995406	2.676637	−0.416730
34	1	0	−4.682311	4.198775	1.096053
35	1	0	−3.374663	4.232765	−0.079418
36	6	0	−6.237081	−2.871996	−0.034454
37	1	0	−6.685263	−2.737660	0.949237
38	1	0	−7.016313	−3.065186	−0.772212
39	1	0	−5.512311	−3.687670	−0.003148
40	6	0	−5.149666	5.294037	−0.706315
41	1	0	−6.236100	5.241691	−0.586013
42	1	0	−4.816142	6.259215	−0.318467
43	1	0	−4.928398	5.268007	−1.777893
44	6	0	5.637936	1.084175	−0.463972
45	6	0	6.724621	1.243038	1.446605
46	6	0	6.645736	−0.075191	1.114853
47	7	0	5.966112	−0.148600	−0.082509
48	1	0	5.055123	1.329678	−1.340734

49	1	0	7.175308	1.734388	2.294432
50	1	0	7.008994	-0.955485	1.621660
51	7	0	6.082836	1.946043	0.449586
52	6	0	5.525282	-1.380809	-0.758649
53	6	0	4.388804	-2.052455	0.004837
54	1	0	6.395856	-2.036031	-0.851453
55	1	0	5.195988	-1.087388	-1.757855
56	6	0	3.816240	-3.235330	-0.774861
57	1	0	4.747745	-2.389838	0.985817
58	1	0	3.596261	-1.314414	0.185064
59	1	0	3.414075	-2.867398	-1.727583
60	1	0	4.621465	-3.937658	-1.025207
61	6	0	5.883941	3.395028	0.391727
62	1	0	5.020924	3.591884	-0.244257
63	1	0	5.678055	3.758039	1.398305
64	1	0	6.776811	3.878319	-0.006740
65	6	0	2.725724	-3.958848	0.011562
66	1	0	1.912524	-3.273959	0.272845
67	1	0	2.301084	-4.782223	-0.567659
68	1	0	3.125069	-4.375034	0.941548

Zero-point correction=	0.576389 (Hartree/Particle)
Thermal correction to Energy=	0.613283
Thermal correction to Enthalpy=	0.614228
Thermal correction to Gibbs Free Energy=	0.499023
Sum of electronic and zero-point Energies=	-1505.381488
Sum of electronic and thermal Energies=	-1505.344593
Sum of electronic and thermal Enthalpies=	-1505.343649
Sum of electronic and thermal Free Energies=	-1505.458854

Conformer e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440918	1.130116	-0.935095
2	6	0	-0.053994	0.346454	0.132152
3	6	0	-0.657637	1.015700	1.221323
4	6	0	-0.764233	2.397661	1.244314
5	6	0	-0.262088	3.134117	0.174528
6	6	0	0.341070	2.512735	-0.916148
7	1	0	0.897052	0.638714	-1.791207
8	1	0	-1.034288	0.436135	2.060868
9	1	0	-1.224397	2.916340	2.077988

10	1	0	0.714732	3.119022	−1.733893
11	6	0	0.055039	−1.096588	0.111794
12	7	0	−0.372319	4.592253	0.195361
13	8	0	0.098830	5.206818	−0.747064
14	8	0	−0.927831	5.102909	1.153505
15	6	0	0.722148	−1.763907	−0.929071
16	7	0	1.305097	−2.304779	−1.786975
17	6	0	−0.497720	−1.884807	1.135140
18	7	0	−0.989063	−2.529321	1.978676
19	6	0	−2.743387	−2.463481	−0.807457
20	6	0	−2.075309	−1.376038	−2.600578
21	6	0	−2.679194	−0.485059	−1.766187
22	7	0	−3.084921	−1.185685	−0.653397
23	1	0	−2.897242	−3.242401	−0.074166
24	1	0	−1.597555	−1.243598	−3.558682
25	1	0	−2.829868	0.580228	−1.854579
26	7	0	−2.131070	−2.605908	−1.982238
27	6	0	−3.778648	−0.623455	0.516770
28	6	0	−5.289865	−0.579426	0.318658
29	1	0	−3.363952	0.377156	0.671045
30	1	0	−3.495322	−1.236801	1.377754
31	6	0	−5.990788	0.037861	1.529020
32	1	0	−5.522442	0.001462	−0.582966
33	1	0	−5.663474	−1.597456	0.149392
34	1	0	−5.740294	−0.540099	2.427119
35	1	0	−5.606156	1.052317	1.691326
36	6	0	−1.568891	−3.848327	−2.516922
37	1	0	−1.674214	−4.627417	−1.762615
38	1	0	−2.113322	−4.131975	−3.418143
39	1	0	−0.511290	−3.684634	−2.730674
40	6	0	−7.506513	0.083728	1.350357
41	1	0	−7.916593	−0.921974	1.216813
42	1	0	−7.990931	0.529752	2.221681
43	1	0	−7.780453	0.678358	0.473562
44	6	0	3.033170	−2.047443	0.997469
45	6	0	2.270456	−1.001432	2.777195
46	6	0	2.728162	−0.065419	1.900232
47	7	0	3.195768	−0.740771	0.796659
48	1	0	3.271499	−2.821927	0.282001
49	1	0	1.804747	−0.901552	3.745127
50	1	0	2.735450	1.012749	1.953256
51	7	0	2.475531	−2.232377	2.193644
52	6	0	3.786757	−0.130892	−0.405824
53	6	0	5.293344	0.059074	−0.265943

54	1	0	3.273153	0.824043	-0.551707
55	1	0	3.530394	-0.779729	-1.249103
56	6	0	5.888026	0.727934	-1.505245
57	1	0	5.503647	0.666748	0.623385
58	1	0	5.767777	-0.917751	-0.106168
59	1	0	5.649802	0.127100	-2.391576
60	1	0	5.413032	1.705774	-1.652101
61	6	0	2.099526	-3.521539	2.778887
62	1	0	2.284329	-4.301706	2.041134
63	1	0	2.702921	-3.704480	3.668666
64	1	0	1.035886	-3.495606	3.021667
65	6	0	7.400672	0.901817	-1.390183
66	1	0	7.898318	-0.065774	-1.273317
67	1	0	7.809521	1.382974	-2.281294
68	1	0	7.660149	1.520622	-0.525823

Zero-point correction=	0.576440 (Hartree/Particle)
Thermal correction to Energy=	0.613182
Thermal correction to Enthalpy=	0.614126
Thermal correction to Gibbs Free Energy=	0.501098
Sum of electronic and zero-point Energies=	-1505.378924
Sum of electronic and thermal Energies=	-1505.342183
Sum of electronic and thermal Enthalpies=	-1505.341238
Sum of electronic and thermal Free Energies=	-1505.454266