

Prediction of ^1H NMR chemical shifts for clusters of imidazolium-based ionic liquids

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SUPPLEMENTARY INFORMATION

Table S1. The calculated proton chemical shifts and R² of all ion pairs

size		Chemical shifts								
		H2	H4	H5	H1	H3	H6	a	b	R2
		[C ₂ mim]Cl								
1IP	Expt ¹	10.55	7.75	7.73	4.13	4.44	1.61			
	Gas Phase	9.46	6.97	7.03	3.87	3.68	1.93	0.86	0.29	0.99
	EtOH	8.67	7.40	7.46	3.83	3.98	1.58	0.84	0.39	0.97
2P	CHCl ₃	8.58	7.50	7.58	3.84	3.91	1.66	0.84	0.45	0.97
	Gas Phase	13.16	6.83	6.90	4.18	3.90	1.69	1.18	1.00	0.91
	EtOH	11.49	7.45	7.47	4.03	4.13	1.65	1.07	-0.43	0.99
8IP	CHCl ₃	11.82	7.32	7.36	4.11	4.04	1.73	1.09	-0.50	0.97
	Gas Phase	12.11	7.03	8.17	4.04	4.16	1.59			
	EtOH	10.94	7.37	7.91	3.91	4.12	1.53			
Central ions	CHCl ₃	11.21	7.25	7.95	3.94	4.15	1.55			
	Gas Phase	11.15	7.80	7.36	4.35	3.48	1.71			
	EtOH	10.80	7.93	7.15	4.11	3.36	1.59			
16IP	CHCl ₃	10.81	7.81	7.23	4.31	3.55	1.65			
	Gas Phase	10.22	7.21	8.45	2.80	3.82	0.46			
	EtOH	10.05	8.66	9.47	3.02	4.13	0.70			
	CHCl ₃	10.32	7.48	8.44	2.79	3.81	0.45			
		[C ₂ mim]OAc								
1IP	Expt ²	10.32	8.00	7.92	3.85	4.19	1.42			
	Gas Phase	14.63	7.03	7.03	3.84	4.10	1.27	1.29	-1.36	0.86
	EtOH	12.12	7.53	7.59	3.86	4.09	1.43	1.12	-0.53	0.96
2P	CHCl ₃	13.04	7.38	7.40	4.24	3.96	1.38	1.17	-0.72	0.92
	Gas Phase	12.68	6.75	6.80	4.43	3.56	2.01	1.13	-0.21	0.87
	EtOH	11.97	7.19	7.32	4.43	3.78	1.92	1.03	-0.02	0.93
8IP	CHCl ₃	12.21	7.11	7.22	4.47	3.74	1.96	1.04	-0.06	0.92
	Gas Phase	13.65	8.16	7.98	5.44	4.86	1.71	1.17	0.03	0.92
	EtOH	13.34	8.19	8.09	5.35	4.77	1.64	1.16	0.00	0.94

	CHCl ₃	11.85	7.86	7.84	5.18	4.29	1.70	1.04	0.29	0.96
Central ions	Gas Phase	12.13	6.68	8.65	4.46	4.34	2.21			
	EtOH	11.87	7.07	8.59	4.44	4.42	2.10			
	CHCl ₃	11.28	6.87	9.31	3.97	4.03	2.22			
	[C ₂ mim][BF ₄]									
	Expt ³	8.55	7.41	7.35	3.83	4.14	1.41			
1IP	Gas Phase	9.46	7.21	7.32	3.79	3.98	1.62	1.05	-0.14	0.98
	EtOH	8.80	7.58	7.66	3.78	3.99	1.53	1.04	-0.11	1.00
	CHCl ₃	8.89	7.50	7.59	3.78	3.97	1.61	1.03	-0.06	1.00
2P	Gas Phase	10.47	6.95	7.09	3.87	4.09	1.52	1.11	-0.38	0.93
	EtOH	9.95	7.44	7.53	3.95	4.15	1.58	1.10	-0.24	0.98
	CHCl ₃	10.08	7.35	7.45	3.94	4.16	1.58	1.10	-0.25	0.97
8IP	Gas Phase	9.92	7.16	7.22	3.79	3.92	1.50			
	EtOH	9.74	7.34	7.42	3.81	3.92	1.45			
	CHCl ₃	9.75	7.30	7.37	3.80	3.91	1.50			
Central ions	Gas Phase	9.35	6.90	8.13	4.08	2.93	1.45			
	EtOH	9.40	7.16	8.13	4.18	2.99	1.39			
	CHCl ₃	9.38	7.11	8.12	4.16	2.97	1.40			
	[C ₂ mim][PF ₆]									
	Expt ⁴	8.82	7.29	7.24	3.97	4.26	1.59			
1IP	Gas Phase	9.28	7.23	7.36	3.78	3.91	1.68	-0.29	0.99	1.05
	EtOH	8.71	7.58	7.67	3.77	3.97	1.55	-0.24	0.99	1.05
	CHCl ₃	8.79	7.52	7.36	3.78	3.95	1.59	-0.21	1.00	1.03
2IP	Gas Phase	10.08	6.92	6.94	3.78	3.95	1.49	-0.62	0.97	1.11
	EtOH	9.63	7.43	7.45	3.90	4.10	1.51	-0.45	1.00	1.11
	CHCl ₃	9.75	7.34	7.37	4.08	3.88	1.52	-0.48	0.99	1.11
	[C ₂ mim][DCA]									
	Expt ⁵	8.76	7.23	7.23	3.71	4.01	1.30			
1IP	Gas Phase	10.28	7.36	7.28	4.02	4.10	1.97	1.05	0.17	0.97
	EtOH	8.94	7.64	7.68	4.08	3.93	1.80	0.99	0.35	0.99
	CHCl ₃	9.44	7.54	7.57	3.99	4.04	1.81	1.02	0.23	0.99
2IP	Gas Phase	11.32	7.40	7.13	4.24	3.73	1.84	1.15	-0.25	0.92

	EtOH	10.55	7.55	7.56	4.21	3.93	1.85	1.11	-0.02	0.97
	CHCl ₃	10.71	7.53	7.48	4.23	3.91	1.87	1.12	-0.04	0.96
	[C ₂ mim][TFA]									
	Expt ⁶	9.75	7.38	7.36	3.81	4.12	1.33			
1IP	Gas Phase	9.82	7.13	7.29	4.12	4.13	1.65	0.95	0.33	1.00
	EtOH	8.88	7.53	7.62	3.86	3.99	1.53	0.92	0.38	0.98
	CHCl ₃	9.08	7.46	7.56	3.91	4.02	1.56	0.93	0.36	0.99
2IP	Gas Phase	10.20	6.87	6.91	4.18	3.89	1.70	0.96	0.21	0.98
	EtOH	9.76	7.28	7.37	4.19	4.02	1.75	0.95	0.40	1.00
	CHCl ₃	9.87	7.20	7.29	4.21	4.01	1.76	0.95	0.38	0.99
	[C ₂ mim][OTs]									
	Expt ⁶	9.69	7.40	7.39	3.87	4.17	1.40			
1IP	Gas Phase	9.55	7.23	7.41	3.48	4.15	1.64	0.98	0.07	1.00
	EtOH	9.10	7.57	7.71	3.79	4.05	1.58	0.96	0.22	0.99
	CHCl ₃	9.20	7.50	7.64	3.71	4.06	1.59	0.96	0.18	0.99
2IP	Gas Phase	11.10	6.81	7.36	3.95	4.55	1.85	1.04	0.04	0.96
	EtOH	10.83	6.96	7.12	4.23	4.41	1.81	1.01	0.16	0.97
	CHCl ₃	10.84	6.87	7.01	4.24	4.41	1.81	1.01	0.18	0.96
	[C ₂ mim][EtSO ₄]									
	Expt ⁷	9.44	7.62	7.62	4.03	4.33	1.28			
1IP	Gas Phase	9.26	7.13	7.23	3.84	4.08	1.72	0.92	0.28	0.99
	EtOH	8.89	7.52	7.52	3.81	3.97	1.64	0.93	0.24	0.99
	CHCl ₃	8.97	7.44	7.46	3.83	4.01	1.66	0.93	0.26	1.00

Table S2. Calculated absolute errors (in ppm) of single and two ion-pairs cluster respect to experiment in gas phase and two solvents.

IL	Size	Solvent	Absolute errors					
			H2	H4	H5	H1	H3	H6
[C ₂ mim]Cl	1IP	Gas Phase	1.09	0.78	0.70	0.26	0.76	0.32
		EtOH	1.88	0.35	0.27	0.30	0.46	0.03
		CHCl ₃	1.97	0.25	0.15	0.29	0.53	0.05
	2IP	Gas Phase	2.61	0.91	0.83	0.04	0.54	0.08
		EtOH	0.94	0.30	0.26	0.10	0.31	0.04
		CHCl ₃	1.27	0.43	0.37	0.03	0.40	0.12
[C ₂ mim][OAc]	1IP	Gas Phase	4.31	0.97	0.89	0.01	0.09	0.15
		EtOH	1.80	0.47	0.33	0.01	0.10	0.01
		CHCl ₃	2.72	0.62	0.52	0.39	0.23	0.04
	2IP	Gas Phase	2.36	1.25	1.12	0.58	0.63	0.59
		EtOH	1.65	0.81	0.60	0.58	0.41	0.50
		CHCl ₃	1.89	0.89	0.70	0.62	0.45	0.54
[C ₂ mim][BF ₄]	1IP	Gas Phase	0.91	0.20	0.03	0.04	0.16	0.21
		EtOH	0.25	0.17	0.31	0.05	0.15	0.12
		CHCl ₃	0.34	0.09	0.24	0.05	0.17	0.20
	2IP	Gas Phase	1.92	0.46	0.26	0.04	0.05	0.11
		EtOH	1.40	0.03	0.18	0.12	0.01	0.17
		CHCl ₃	1.53	0.06	0.10	0.11	0.02	0.17
[C ₂ mim][PF ₆]	1IP	Gas Phase	0.46	0.06	0.12	0.19	0.35	0.09
		EtOH	0.11	0.29	0.43	0.20	0.29	0.04
		CHCl ₃	0.03	0.23	0.12	0.19	0.31	0.00
	2IP	Gas Phase	1.26	0.37	0.30	0.19	0.31	0.10
		EtOH	0.81	0.14	0.21	0.07	0.16	0.08
		CHCl ₃	0.93	0.05	0.13	0.11	0.38	0.07
[C ₂ mim][DCA]	1IP	Gas Phase	1.52	0.13	0.05	0.31	0.08	0.67
		EtOH	0.18	0.41	0.45	0.37	0.08	0.50

		CHCl ₃	0.68	0.31	0.34	0.28	0.03	0.51
	2IP	Gas Phase	2.56	0.17	0.10	0.53	0.28	0.54
		EtOH	1.79	0.32	0.33	0.50	0.08	0.55
		CHCl ₃	1.95	0.30	0.25	0.52	0.10	0.57
[C ₂ mim][TFA]	1IP	Gas Phase	0.07	0.25	0.07	0.31	0.00	0.32
		EtOH	0.87	0.15	0.26	0.05	0.13	0.20
		CHCl ₃	0.67	0.08	0.20	0.10	0.10	0.23
	2IP	Gas Phase	0.45	0.51	0.45	0.37	0.23	0.37
		EtOH	0.01	0.10	0.01	0.38	0.10	0.42
		CHCl ₃	0.12	0.18	0.07	0.40	0.11	0.43
[C ₂ mim][OTs]	1IP	Gas Phase	0.14	0.17	0.02	0.39	0.02	0.24
		EtOH	0.59	0.17	0.32	0.08	0.12	0.18
		CHCl ₃	0.49	0.10	0.25	0.16	0.11	0.19
	2IP	Gas Phase	1.41	0.59	0.03	0.08	0.38	0.45
		EtOH	1.14	0.44	0.27	0.36	0.24	0.41
		CHCl ₃	1.15	0.53	0.38	0.37	0.24	0.41
[C ₂ mim][EtSO ₄]	1IP	Gas Phase	0.18	0.49	0.39	0.18	0.26	0.44
		EtOH	0.55	0.10	0.10	0.22	0.36	0.37
		CHCl ₃	0.48	0.18	0.16	0.20	0.33	0.38

Table S3. Absolute errors (AEs) and mean absolute errors (MAEs) of each cation in the 8 and 16 ion paired cluster in in gas phase and two solvents

			AE					MAEs	
			H2	H4	H5	H3	H1	H6	
[C2mim]Cl-8IP	Gas Phase	A	0.60	0.05	0.37	0.22	0.96	0.10	0.38
		B	1.72	0.90	0.75	0.38	0.44	0.08	0.71
		C	1.12	1.34	1.12	0.13	0.47	0.37	0.76
		D	1.48	1.28	2.51	0.63	0.53	0.37	1.13
		E	3.94	1.80	0.90	0.37	0.04	0.27	1.22
		F	1.84	0.93	1.71	0.01	0.70	0.59	0.96
		G	2.19	0.91	0.84	0.10	0.68	0.26	0.83
		H	0.38	1.35	1.44	0.30	0.32	0.72	0.75
	EtOH	A	0.25	0.18	0.58	0.02	1.07	0.02	0.35
		B	0.66	0.50	0.38	0.32	0.13	0.01	0.33
		C	0.61	0.60	0.86	0.18	0.55	0.10	0.48
		D	0.49	0.61	1.59	0.18	0.34	0.44	0.61
		E	1.21	1.29	0.19	0.50	0.03	0.18	0.57
		F	0.71	0.50	1.00	0.21	0.58	0.32	0.55
		G	0.67	0.43	0.43	0.22	0.52	0.07	0.39
		H	1.03	0.73	0.87	0.57	0.25	0.69	0.69
	CHCl ₃	A	0.26	0.06	0.51	0.17	0.89	0.04	0.32
		B	0.76	0.60	0.45	0.36	0.21	0.02	0.40
		C	0.79	0.82	0.92	0.21	0.54	0.18	0.57
		D	0.58	0.82	1.78	0.30	0.42	0.37	0.71
		E	1.86	1.46	0.38	0.53	0.01	0.18	0.74
		F	0.97	0.57	1.16	0.14	0.60	0.38	0.64
		G	0.94	0.54	0.52	0.18	0.62	0.14	0.49
		H	0.91	0.78	0.85	0.57	0.29	0.74	0.69
[C2mim]Cl-16IP	Gas Phase	A	0.53	1.32	1.24	0.21	0.20	0.53	0.67
		B	0.03	0.69	1.17	0.43	0.25	0.82	0.57
		C	0.41	1.47	1.21	0.36	0.34	0.89	0.78
		D	0.03	1.35	1.26	1.15	0.60	0.27	0.78

EtOH	E	0.89	0.79	1.58	0.60	0.11	0.65	0.77
	F	0.48	1.69	1.54	0.29	0.32	1.02	0.89
	G	0.66	1.57	1.29	0.26	0.04	0.99	0.80
	H	0.77	1.63	1.32	0.72	0.22	1.05	0.95
	I	0.14	0.94	1.52	0.59	0.05	0.65	0.65
	J	1.33	1.62	1.36	0.42	0.01	1.13	0.98
	K	0.57	1.27	1.44	0.12	0.14	0.81	0.72
	L	0.51	0.78	1.56	1.00	0.51	0.60	0.83
	M	0.33	0.54	0.72	1.33	0.62	1.15	0.78
	N	0.01	1.58	1.32	0.29	0.11	1.04	0.72
	O	0.13	1.71	1.28	0.34	0.32	0.87	0.77
	P	0.77	1.37	1.29	0.47	0.04	0.56	0.75
	A	1.32	0.42	0.40	0.08	0.51	0.19	0.49
	B	0.47	0.02	1.55	0.00	0.01	0.31	0.39
	C	0.23	0.54	1.67	0.18	0.83	0.31	0.63
	D	0.02	1.07	0.37	1.07	0.21	0.42	0.53
CHCl ₃	E	1.08	1.12	0.80	0.23	0.29	0.23	0.62
	F	0.25	0.93	1.76	0.00	0.43	1.00	0.73
	G	0.44	0.68	1.24	0.06	0.23	0.41	0.51
	H	0.64	0.82	1.61	0.40	0.02	0.28	0.63
	I	0.60	1.56	0.65	0.09	0.21	0.03	0.52
	J	0.92	0.76	1.29	0.00	0.12	0.54	0.60
	K	0.69	0.23	1.42	0.49	0.47	0.22	0.59
	L	0.14	0.99	0.67	0.89	0.05	0.13	0.48
	M	0.50	0.91	1.74	1.11	0.30	0.91	0.91
	N	0.78	0.76	1.65	0.08	0.07	0.51	0.64
	O	0.35	0.92	1.34	0.06	0.06	0.14	0.48
	P	0.84	0.52	0.42	0.16	0.19	0.04	0.36
	A	1.61	0.39	1.25	0.22	0.21	0.54	0.70
	B	1.15	0.95	1.16	0.44	0.24	0.83	0.80
	C	1.80	0.42	1.20	0.37	0.35	0.90	0.84
	D	0.82	0.99	1.27	1.16	0.61	0.28	0.85

		E	1.02	0.97	1.59	0.61	0.12	0.66	0.83
		F	0.20	0.94	1.53	0.30	0.33	1.03	0.72
		G	0.21	0.71	1.28	0.27	0.03	1.00	0.58
		H	1.07	0.89	1.31	0.73	0.23	1.06	0.88
		I	0.68	1.90	1.53	0.60	0.06	0.66	0.91
		J	0.80	0.87	1.35	0.43	0.00	1.14	0.77
		K	0.42	0.83	1.43	0.13	0.13	0.82	0.63
		L	0.35	1.10	1.57	1.01	0.52	0.61	0.86
		M	0.23	0.27	0.71	1.34	0.63	1.16	0.72
		N	0.65	0.77	1.31	0.30	0.12	1.05	0.70
		O	0.22	1.15	1.27	0.35	0.33	0.88	0.70
		P	1.09	0.55	1.30	0.48	0.05	0.57	0.68
[C2mim][OAc]-8IP	Gas Phase	A	3.14	1.95	1.19	0.86	1.06	0.09	1.38
		B	1.90	1.43	2.63	0.59	0.52	1.03	1.35
		C	3.54	0.80	0.98	1.06	1.62	0.11	1.35
		D	5.35	0.95	0.79	0.47	1.07	0.34	1.49
		E	4.47	1.19	1.08	0.01	0.00	0.30	1.18
		F	3.54	0.22	2.24	0.20	0.83	0.18	1.20
		G	2.91	2.89	1.10	0.60	1.14	0.11	1.46
		H	1.81	1.32	0.73	0.61	0.15	0.79	0.90
	EtOH	A	2.90	1.86	0.77	0.83	1.01	0.01	1.23
		B	1.65	1.04	2.51	0.56	0.39	0.92	1.18
		C	3.38	0.77	0.64	0.95	1.47	0.01	1.20
		D	4.96	0.61	0.50	0.45	1.00	0.29	1.30
		E	4.19	0.94	0.74	0.05	0.02	0.27	1.03
		F	3.42	0.24	2.05	0.22	0.69	0.21	1.14
		G	2.63	2.77	0.69	0.58	1.09	0.06	1.30
		H	1.54	0.94	0.66	0.58	0.22	0.67	0.77
	CHCl ₃	A	0.25	0.20	0.96	1.17	0.02	0.03	0.44
		B	0.69	1.51	1.66	0.72	0.14	0.70	0.90
		C	1.95	0.56	1.12	0.58	0.41	0.28	0.82
		D	2.21	0.86	0.60	0.44	0.05	0.47	0.77

		E	3.24	0.59	0.80	0.04	0.06	0.34	0.85
		F	2.14	0.30	0.86	0.65	0.35	0.33	0.77
		G	0.79	1.74	1.06	0.57	0.37	0.06	0.76
		H	0.95	1.14	1.38	0.33	0.17	0.79	0.79
[C2mim][BF4]-8IP	Gas phase	A	0.47	0.35	0.49	1.45	0.72	0.51	0.66
		B	1.80	0.36	0.20	0.41	0.23	0.27	0.54
		C	0.94	1.63	0.07	0.29	0.21	0.23	0.56
		D	1.63	0.42	0.23	0.36	0.14	0.54	0.55
		E	1.88	0.41	0.30	0.02	0.31	0.11	0.51
		F	1.88	1.17	0.41	0.24	0.04	0.04	0.63
		G	1.67	0.10	0.21	0.23	0.29	0.56	0.51
		H	0.80	0.51	0.78	0.25	1.21	0.04	0.60
	EtOH	A	0.47	0.20	0.28	1.40	0.79	0.43	0.59
		B	1.44	0.13	0.01	0.29	0.17	0.27	0.39
		C	0.99	1.14	0.02	0.14	0.27	0.21	0.46
		D	1.58	0.08	0.04	0.33	0.19	0.04	0.38
		E	1.53	0.06	0.10	0.00	0.22	0.12	0.34
		F	1.61	0.96	0.03	0.23	0.08	0.04	0.49
		G	1.06	0.03	0.07	0.13	0.20	0.49	0.33
		H	0.85	0.25	0.78	0.35	1.15	0.02	0.56
	CHCl ₃	A	0.46	0.22	0.33	1.43	0.79	0.46	0.61
		B	1.51	0.18	0.05	0.32	0.17	0.27	0.42
		C	0.89	1.27	0.03	0.18	0.23	0.23	0.47
		D	1.47	0.17	0.08	0.32	0.20	0.48	0.45
		E	1.61	0.14	0.00	0.01	0.23	0.11	0.35
		F	1.66	0.99	0.12	0.23	0.09	0.04	0.52
		G	1.17	0.06	0.01	0.15	0.22	0.50	0.35
		H	0.83	0.30	0.77	0.33	1.17	0.01	0.57

Table S4. Optimized geometries in the form of the Cartesian coordinates.

Ionic liquids	Solvents	Atoms	X	Y	Z
[C ₂ mim]Cl 1IP	CHCl ₃				
		N	0.037558	-0.013939	0.014631
		C	0.123855	-0.205532	1.343468
		N	1.416048	-0.097746	1.703916
		C	2.168700	0.214990	0.590752
		C	1.292097	0.270121	-0.480447
		C	1.912971	-0.157168	3.091417
		C	2.269815	1.240203	3.594428
		C	-1.225368	0.106038	-0.722201
		H	-0.705526	-0.409252	2.010984
		H	3.245032	0.353415	0.636090
		H	1.467314	0.474141	-1.532640
		H	-1.571548	1.144653	-0.637644
		H	-1.046263	-0.172606	-1.767228
		H	-1.958369	-0.576150	-0.275657
		H	2.777837	-0.835529	3.100705
		H	1.109500	-0.608290	3.689315
		H	2.580957	1.174468	4.647807
		H	3.102160	1.663577	3.012378
		H	1.397712	1.903796	3.504444
		Cl	-0.780482	2.668812	1.743482
[C ₂ mim][BF ₄] 1IP					
		N	0.269867	-0.113436	-0.236128
		C	0.022112	0.292865	1.023150
		N	1.049024	-0.095928	1.801932
		C	1.979170	-0.753707	1.025072
		C	1.484395	-0.764308	-0.268486
		C	1.189402	0.221271	3.237320

		C	2.412512	1.101891	3.481012
		C	-0.571570	0.187723	-1.401575
		H	-0.832517	0.875775	1.345976
		H	2.896108	-1.166197	1.435107
		H	1.895068	-1.181298	-1.183429
		H	-1.543373	0.542456	-1.043089
		H	-0.088760	0.973695	-1.994288
		H	-0.694842	-0.728671	-1.991263
		H	1.252913	-0.732374	3.780811
		H	0.265241	0.737073	3.527132
		H	2.462895	1.349824	4.551770
		H	3.340590	0.578434	3.207359
		H	2.327313	2.027046	2.897122
		B	0.553068	3.318283	0.727213
		F	0.837123	4.700710	0.599112
		F	0.167049	3.020436	2.075744
		F	1.707876	2.544925	0.390991
		F	-0.521663	2.951509	-0.145565
[C ₂ mim][OAc] IIP		N	1.725477	-0.929141	-0.041428
		C	0.761798	-0.153984	0.495926
		N	1.135955	1.132892	0.331438
		C	2.348709	1.182160	-0.324386
		C	2.727940	-0.131763	-0.553953
		C	0.273861	2.280339	0.676445
		C	-0.792909	2.490632	-0.396474
		C	1.682306	-2.399629	-0.046095
		H	-0.192034	-0.482259	0.938405
		H	2.839504	2.119420	-0.570993
		H	3.613164	-0.543885	-1.029682
		H	2.242085	-2.784971	0.815857
		H	0.623523	-2.686212	0.000428

		H	2.135403	-2.753636	-0.979902
		H	0.935141	3.151187	0.780337
		H	-0.179202	2.060314	1.652540
		H	-1.410431	3.361511	-0.130209
		H	-0.328298	2.673581	-1.376946
		H	-1.442062	1.604679	-0.455540
		C	-3.519460	-0.693080	-0.668291
		C	-2.270251	-1.101436	0.119841
		O	-2.054140	-0.512552	1.237342
		O	-1.502192	-1.971243	-0.407457
		H	-4.217479	-0.117374	-0.045140
		H	-4.022894	-1.583281	-1.073820
		H	-3.210005	-0.070475	-1.524695
[C ₂ mim][DCA] 1IP		N	0.187963	-0.045553	-0.012972
		C	0.434982	0.815797	0.995482
		N	1.462243	0.324373	1.721936
		C	1.863172	-0.875539	1.175963
		C	1.052027	-1.111730	0.077253
		C	2.011419	0.927092	2.956681
		C	2.106841	2.444742	2.851062
		C	-0.924225	0.068711	-0.964490
		H	-0.112106	1.730707	1.196877
		H	2.677752	-1.457297	1.597319
		H	1.025140	-1.941190	-0.622767
		H	-1.681243	-0.678380	-0.692635
		H	-1.339938	1.080266	-0.890051
		H	-0.543153	-0.106121	-1.977824
		H	3.001290	0.471191	3.093217
		H	1.358959	0.617024	3.785355
		H	2.577179	2.828100	3.768555
		H	2.723670	2.740509	1.989365

		H	1.107607	2.896069	2.773570
		N	-1.098007	-0.561971	3.569993
		C	-1.228605	0.756651	3.526341
		C	-1.442959	-1.241326	2.481304
		N	-1.266205	1.957817	3.576511
		N	-1.712180	-1.948740	1.547500
[C ₂ mim][TFA] IIP		C	-2.040430	-0.093986	3.462602
		F	-1.307050	0.929862	2.901117
		F	-1.704254	-0.124324	4.778873
		F	-3.342264	0.287565	3.400561
		C	-1.738312	-1.419133	2.699854
		O	-2.409343	-1.569132	1.642316
		O	-0.803398	-2.110644	3.186337
		N	-0.197403	0.278740	0.060190
		C	0.329953	-0.707780	0.812133
		N	1.329998	-0.184897	1.549278
		C	1.445336	1.159688	1.264463
		C	0.476784	1.452744	0.317760
		C	2.114509	-0.932761	2.554140
		C	1.927450	-0.335543	3.946075
		C	-1.326738	0.109998	-0.865558
		H	-0.018984	-1.734208	0.852510
		H	2.183491	1.797177	1.741671
		H	0.221676	2.387609	-0.172676
		H	-0.949441	0.017244	-1.891806
		H	-1.875616	-0.787163	-0.557448
		H	-1.977142	0.988228	-0.775326
		H	3.165664	-0.909510	2.232681
		H	1.744214	-1.965045	2.518235
		H	2.518409	-0.923543	4.664196
		H	2.278699	0.706226	3.986970

		H	0.869303	-0.384313	4.233938
[C ₂ mim][PF ₆] IIP		N	-0.735057	-0.518451	0.153427
		C	-0.659212	-0.940427	1.429596
		N	0.297014	-0.227834	2.054251
		C	0.836302	0.677324	1.164691
		C	0.180218	0.493396	-0.041053
		C	0.644415	-0.346395	3.485151
		C	0.408009	0.973678	4.215129
		C	-1.714765	-0.987268	-0.835228
		H	-1.290910	-1.692384	1.887614
		H	1.632536	1.362833	1.438379
		H	0.298416	0.992831	-0.998301
		H	-1.194403	-1.180728	-1.780901
		H	-2.170271	-1.910040	-0.460368
		H	-2.485900	-0.218191	-0.963397
		H	1.694982	-0.665184	3.544171
		H	0.008072	-1.144345	3.888807
		H	0.645979	0.835000	5.280277
		H	1.058982	1.768142	3.821302
		H	-0.641449	1.278705	4.116815
		P	-3.526611	0.709935	2.683183
		F	-3.573375	-0.439930	1.482983
		F	-4.518547	1.683178	1.793096
		F	-3.453262	1.845793	3.879125
		F	-2.200509	1.395400	1.954487
		F	-2.518235	-0.278841	3.564547
		F	-4.836417	0.012786	3.404227
[C ₂ mim][OTs] IIP		C	-1.251809	1.350312	4.583266
		C	-0.350429	2.361038	4.190500
		C	0.851125	2.049569	3.522762
		C	1.150602	0.705977	3.248287

		C	0.269280	-0.324753	3.628070
		C	-0.923813	0.005407	4.291762
		H	-0.589827	3.407724	4.406843
		H	1.549836	2.831413	3.215279
		S	2.685274	0.269567	2.412575
		H	0.514220	-1.366874	3.403669
		H	-1.613318	-0.792898	4.588174
		C	-2.543081	1.683506	5.298295
		O	3.479105	-0.540155	3.424576
		O	3.352049	1.579879	2.046025
		O	2.282001	-0.554237	1.204111
		H	-3.413545	1.335470	4.718550
		H	-2.642063	2.768781	5.449623
		H	-2.583483	1.192587	6.284315
		N	5.244921	0.155916	-0.064556
		C	5.428935	-0.408483	1.144706
		N	6.194901	0.416971	1.883557
		C	6.488129	1.540578	1.143064
		C	5.883625	1.375414	-0.092903
		C	6.559079	0.183031	3.295556
		C	6.094303	1.341984	4.173729
		C	4.377074	-0.383906	-1.118399
		H	5.006263	-1.348710	1.479243
		H	7.094188	2.354583	1.528279
		H	5.864696	2.019326	-0.967222
		H	3.383260	0.069521	-1.023447
		H	4.831747	-0.158399	-2.090439
		H	4.299437	-1.468250	-0.981966
		H	7.648728	0.039983	3.340436
		H	6.055572	-0.748308	3.583572
		H	6.316765	1.099556	5.223837

		H	6.620872	2.274339	3.920835
		H	5.012292	1.481544	4.050678
[C ₂ mim][EtSO ₄] IIP		C	4.991424	-0.167350	0.544018
		H	5.355302	-0.480170	-0.445985
		H	5.652063	0.626984	0.925660
		C	3.569886	0.359767	0.450100
		H	3.186754	0.665490	1.436784
		H	3.500497	1.212286	-0.244370
		O	2.749270	-0.727908	-0.057027
		S	1.128558	-0.307837	-0.231388
		O	0.547484	-1.588807	-0.758760
		O	0.645678	0.076477	1.143275
		O	1.100415	0.839529	-1.209492
		H	5.042360	-1.025386	1.230709
		N	-1.841475	1.628700	-0.269306
		C	-1.855991	0.323644	-0.605116
		N	-2.270925	-0.380784	0.466717
		C	-2.500867	0.486327	1.511008
		C	-2.230256	1.762501	1.044401
		C	-2.294800	-1.854836	0.569705
		C	-2.640868	-2.511496	-0.760615
		C	-1.372672	2.711884	-1.141975
		H	-1.566494	-0.078541	-1.567945
		H	-2.830516	0.140491	2.486152
		H	-2.289778	2.728782	1.536487
		H	-0.348995	2.978642	-0.853978
		H	-1.379722	2.349074	-2.175479
		H	-2.053091	3.565437	-1.036819
		H	-3.041210	-2.089469	1.341032
		H	-1.296837	-2.160971	0.912733
		H	-2.717834	-3.597290	-0.603134

		H	-3.604107	-2.144889	-1.146243
		H	-1.847255	-2.334642	-1.499645
[C ₂ mim]Cl 1IP	EtOH	N	0.029433	-0.001253	0.021016
		C	0.122973	-0.209232	1.347163
		N	1.414889	-0.083028	1.704646
		C	2.159739	0.246451	0.591640
		C	1.278536	0.299802	-0.476549
		C	1.921907	-0.170224	3.087390
		C	2.271967	1.217433	3.620305
		C	-1.233194	0.077382	-0.722256
		H	-0.699640	-0.442965	2.014154
		H	3.235034	0.394137	0.633901
		H	1.448077	0.510717	-1.528476
		H	-1.586426	1.116280	-0.693574
		H	-1.051201	-0.250130	-1.752147
		H	-1.962838	-0.586329	-0.244075
		H	2.793303	-0.839283	3.074182
		H	1.127398	-0.642838	3.680227
		H	2.593815	1.128663	4.668572
		H	3.094570	1.662526	3.040897
		H	1.394588	1.877211	3.558673
		Cl	-0.738929	2.832683	1.642312
[C ₂ mim][BF ₄]1IP		N	0.272978	-0.113255	-0.238264
		C	0.025468	0.285556	1.023654
		N	1.057355	-0.099780	1.798028
		C	1.989415	-0.748883	1.015922
		C	1.491187	-0.757253	-0.276485
		C	1.193009	0.197755	3.237916
		C	2.401598	1.093972	3.496122
		C	-0.585987	0.164231	-1.396944
		H	-0.839525	0.848406	1.354531

		H	2.908218	-1.160792	1.422549
		H	1.900088	-1.171543	-1.193488
		H	-1.543478	0.549331	-1.031317
		H	-0.099485	0.917167	-2.028309
		H	-0.739253	-0.768608	-1.952552
		H	1.273997	-0.762965	3.765662
		H	0.259249	0.690428	3.537448
		H	2.451122	1.320970	4.571496
		H	3.336851	0.591021	3.209278
		H	2.300766	2.029509	2.931158
		B	0.564350	3.360774	0.718186
		F	0.849675	4.750494	0.596006
		F	0.157100	3.069990	2.058853
		F	1.727851	2.598356	0.398615
		F	-0.493550	3.003118	-0.175067
[C ₂ mim][OAc] 1IP		N	1.992400	-1.030470	0.054391
		C	0.809665	-0.471646	0.383695
		N	0.912794	0.857085	0.172389
		C	2.173686	1.151239	-0.305779
		C	2.861998	-0.048722	-0.376664
		C	-0.199988	1.812766	0.339162
		C	-0.829654	2.151055	-1.011094
		C	2.294065	-2.465013	0.150792
		H	-0.098083	-0.975969	0.741309
		H	2.484688	2.164325	-0.544946
		H	3.879323	-0.269151	-0.686882
		H	1.387081	-2.980654	0.485971
		H	2.592915	-2.834815	-0.837660
		H	3.103535	-2.616280	0.875466
		H	0.211708	2.702714	0.834948
		H	-0.919533	1.328692	1.013111

		H	-1.660609	2.855137	-0.855043
		H	-0.094473	2.624396	-1.678957
		H	-1.218992	1.237917	-1.484442
		C	-3.634328	0.109007	-0.035937
		C	-2.423261	-0.825908	0.068720
		O	-1.983821	-1.061799	1.250931
		O	-1.923592	-1.292096	-1.004275
		H	-3.413618	1.062876	0.469353
		H	-4.491312	-0.344739	0.487026
		H	-3.909085	0.301847	-1.082037
[C ₂ mim][DCA] 1IP		N	0.191800	-0.026748	-0.031107
		C	0.433144	0.823891	0.988051
		N	1.461842	0.328030	1.709137
		C	1.867621	-0.863546	1.149229
		C	1.055444	-1.093322	0.051018
		C	1.980532	0.902864	2.970917
		C	2.102949	2.420676	2.894624
		C	-0.970690	0.049539	-0.923010
		H	-0.141578	1.712493	1.235398
		H	2.673895	-1.454676	1.573046
		H	1.008898	-1.931410	-0.637003
		H	-1.691516	-0.710185	-0.588664
		H	-1.403645	1.054004	-0.840774
		H	-0.643048	-0.132423	-1.954555
		H	2.958300	0.425577	3.130209
		H	1.290995	0.589181	3.768439
		H	2.550593	2.782503	3.832388
		H	2.750294	2.724325	2.057409
		H	1.108915	2.881326	2.803731
		N	-1.129263	-0.497745	3.572336
		C	-1.211571	0.818553	3.430091

		C	-1.333489	-1.209981	2.467132
		N	-1.195408	2.020574	3.358018
		N	-1.473392	-1.922297	1.507485
[C ₂ mim][TFA] IIP		C	-2.045023	-0.102646	3.467869
		F	-1.308763	0.907822	2.895166
		F	-1.704355	-0.125674	4.783966
		F	-3.346140	0.288647	3.411061
		C	-1.767334	-1.442214	2.720127
		O	-2.449189	-1.596809	1.670143
		O	-0.848504	-2.148550	3.215580
		N	-0.197800	0.288312	0.063396
		C	0.334323	-0.697225	0.813178
		N	1.336569	-0.172591	1.546224
		C	1.447809	1.172343	1.261518
		C	0.474856	1.463684	0.318727
		C	2.132328	-0.918736	2.542702
		C	1.928843	-0.344833	3.942172
		C	-1.322572	0.117373	-0.867137
		H	-0.003751	-1.727266	0.844558
		H	2.189449	1.810070	1.733222
		H	0.218586	2.397346	-0.173462
		H	-0.942919	0.073922	-1.895495
		H	-1.840586	-0.809091	-0.595677
		H	-2.001544	0.969847	-0.746258
		H	3.183592	-0.868363	2.226125
		H	1.787654	-1.959190	2.488376
		H	2.532183	-0.927779	4.654027
		H	2.256078	0.703997	3.995323
		H	0.871319	-0.419299	4.227653
[C ₂ mim][OTs] IIP		N	-0.734473	-0.521383	0.152847
		C	-0.645367	-0.947962	1.426814

		N	0.301918	-0.221798	2.049982
		C	0.822794	0.695267	1.161440
		C	0.164203	0.505275	-0.042163
		C	0.669870	-0.351676	3.474448
		C	0.419651	0.954412	4.224370
		C	-1.695215	-1.018154	-0.840850
		H	-1.252241	-1.722589	1.881022
		H	1.611365	1.390362	1.433440
		H	0.272344	1.007383	-0.999227
		H	-1.158832	-1.230108	-1.773272
		H	-2.150763	-1.935337	-0.452488
		H	-2.467117	-0.256135	-1.001891
		H	1.726846	-0.650264	3.515707
		H	0.056020	-1.168182	3.876128
		H	0.678942	0.808314	5.283465
		H	1.047620	1.765939	3.828391
		H	-0.637211	1.240073	4.147341
		P	-3.551920	0.736608	2.688938
		F	-3.602703	-0.392009	1.473923
		F	-4.535799	1.732211	1.807732
		F	-3.490249	1.857906	3.903332
		F	-2.220500	1.427127	1.984308
		F	-2.564298	-0.267740	3.568083
		F	-4.878885	0.041440	3.390192
[C ₂ mim][EtSO ₄] 1IP		C	-1.266959	1.357801	4.607260
		C	-0.362008	2.366350	4.216459
		C	0.833747	2.052895	3.538867
		C	1.124505	0.709663	3.251845
		C	0.238934	-0.318650	3.629803
		C	-0.948210	0.013105	4.303682
		H	-0.593612	3.412771	4.441891

		H	1.533964	2.834588	3.234528
		S	2.650106	0.271346	2.399047
		H	0.474616	-1.361300	3.397536
		H	-1.640126	-0.783671	4.598251
		C	-2.550918	1.692587	5.334212
		O	3.437728	-0.569527	3.390097
		O	3.329847	1.580341	2.055467
		O	2.228524	-0.521604	1.175531
		H	-3.426240	1.335931	4.767440
		H	-2.651626	2.778582	5.478031
		H	-2.577628	1.208945	6.324230
		N	5.273174	0.151669	-0.077523
		C	5.451008	-0.407766	1.134955
		N	6.202485	0.426547	1.878529
		C	6.493727	1.550441	1.137190
		C	5.902779	1.376329	-0.104254
		C	6.569611	0.193701	3.289711
		C	6.075262	1.335079	4.174608
		C	4.439132	-0.410359	-1.147092
		H	5.045725	-1.357590	1.463443
		H	7.093349	2.368534	1.524154
		H	5.891335	2.015004	-0.982601
		H	3.444181	0.047876	-1.099636
		H	4.924885	-0.207935	-2.108871
		H	4.356233	-1.491380	-0.989072
		H	7.662269	0.079356	3.335313
		H	6.093738	-0.754134	3.571175
		H	6.307991	1.094718	5.222930
		H	6.575764	2.282020	3.923517
		H	4.989620	1.446740	4.054597

		C	4.991424	-0.167350	0.544018
		H	5.355302	-0.480170	-0.445985
		H	5.652063	0.626984	0.925660
		C	3.569886	0.359767	0.450100
		H	3.186754	0.665490	1.436784
		H	3.500497	1.212286	-0.244370
		O	2.749270	-0.727908	-0.057027
		S	1.128558	-0.307837	-0.231388
		O	0.547484	-1.588807	-0.758760
		O	0.645678	0.076477	1.143275
		O	1.100415	0.839529	-1.209492
		H	5.042360	-1.025386	1.230709
		N	-1.841475	1.628700	-0.269306
		C	-1.855991	0.323644	-0.605116
		N	-2.270925	-0.380784	0.466717
		C	-2.500867	0.486327	1.511008
		C	-2.230256	1.762501	1.044401
		C	-2.294800	-1.854836	0.569705
		C	-2.640868	-2.511496	-0.760615
		C	-1.372672	2.711884	-1.141975
		H	-1.566494	-0.078541	-1.567945
		H	-2.830516	0.140491	2.486152
		H	-2.289778	2.728782	1.536487
		H	-0.348995	2.978642	-0.853978
		H	-1.379722	2.349074	-2.175479
		H	-2.053091	3.565437	-1.036819
		H	-3.041210	-2.089469	1.341032
		H	-1.296837	-2.160971	0.912733
		H	-2.717834	-3.597290	-0.603134
		H	-3.604107	-2.144889	-1.146243

		H	-1.847255	-2.334642	-1.499645
[C ₂ mim]Cl 2IP	Gas phase	N	0.059630	-1.058797	0.214821
		C	0.268935	-0.682865	1.475959
		N	1.495962	-1.063873	1.826928
		C	2.109028	-1.649636	0.740950
		C	1.204003	-1.653202	-0.274897
		C	2.174778	-0.637415	3.054721
		C	1.181161	-0.149446	4.091208
		C	-1.168394	-0.778701	-0.517281
		H	-0.489620	-0.144858	2.072208
		H	3.133263	-2.000687	0.782285
		H	1.273081	-2.024979	-1.290340
		H	-1.870296	-0.306322	0.186001
		H	-0.943839	-0.092509	-1.343631
		H	-1.587570	-1.714828	-0.906910
		H	2.841549	0.183913	2.756385
		H	2.758146	-1.495402	3.418399
		H	1.728004	0.146732	4.996287
		H	0.630414	0.720865	3.705966
		H	0.454327	-0.929225	4.361208
		Cl	-2.312171	0.889193	2.518159
		N	-0.646840	3.979062	3.460546
		C	-0.889115	3.596593	2.206872
		N	-2.116385	3.996169	1.878850
		C	-2.696153	4.602356	2.972133
		C	-1.769760	4.598766	3.968466
		C	-2.825419	3.580449	0.664414
		C	-1.860104	3.082898	-0.393832
		C	0.596226	3.697097	4.166361
		H	-0.152327	3.043267	1.597741
		H	-3.714029	4.973182	2.948900

		H	-1.810092	4.980994	4.981551
		H	1.269913	3.193439	3.457157
		H	1.042682	4.636061	4.516342
		H	0.383116	3.038857	5.017976
		H	-3.406207	4.446104	0.315749
		H	-3.494452	2.765488	0.974300
		H	-2.428860	2.807961	-1.292244
		H	-1.120182	3.848492	-0.668575
		H	-1.324768	2.196072	-0.025667
		Cl	1.671366	2.018733	1.132537
[C ₂ mim][BF ₄] 2IP		N	0.134933	-0.908484	-0.245815
		C	-0.170126	-1.034867	1.042219
		N	0.939177	-0.890344	1.759625
		C	1.989126	-0.636367	0.905449
		C	1.481799	-0.647420	-0.358172
		C	0.965058	-0.880671	3.227158
		C	1.492532	0.444711	3.751534
		C	-0.850620	-0.917708	-1.319094
		H	-1.163066	-1.208383	1.444712
		H	2.997933	-0.466701	1.261255
		H	1.958747	-0.487418	-1.317729
		H	-1.769376	-1.357020	-0.915169
		H	-1.042765	0.114971	-1.630671
		H	-0.469440	-1.522934	-2.149972
		H	1.578667	-1.730820	3.557637
		H	-0.072573	-1.058011	3.535185
		H	1.405106	0.461907	4.846376
		H	2.553033	0.585713	3.496115
		H	0.904057	1.265275	3.324665
		B	-1.227948	1.753072	1.407341
		F	-1.751462	3.016016	1.566841

		F	-1.324403	1.017122	2.639949
		F	0.109676	1.761415	0.999926
		F	-2.001090	1.015329	0.443729
		N	-5.162295	-0.082062	1.506438
		C	-4.147434	0.106499	2.344707
		N	-4.602400	0.023659	3.590856
		C	-5.950828	-0.253494	3.552717
		C	-6.303192	-0.320817	2.239115
		C	-3.742788	0.088614	4.778769
		C	-3.826636	-1.199823	5.580757
		C	-5.017509	-0.151845	0.057957
		H	-3.114124	0.280087	2.061602
		H	-6.541717	-0.382615	4.451390
		H	-7.257913	-0.521372	1.767941
		H	-4.053727	0.302753	-0.196427
		H	-5.019890	-1.204431	-0.246269
		H	-5.838666	0.403405	-0.410273
		H	-4.050211	0.964060	5.368259
		H	-2.731119	0.264403	4.393462
		H	-3.098682	-1.163096	6.402493
		H	-4.825126	-1.336292	6.021244
		H	-3.599145	-2.050659	4.928192
		B	-3.029151	-2.673534	2.165096
		F	-2.479683	-3.931771	2.071256
		F	-2.232265	-1.850143	3.037103
		F	-4.343229	-2.682155	2.642837
		F	-3.005245	-2.026754	0.880681
[C ₂ mim][DCA] 2IP		N	1.025768	-0.648605	-0.274245
		C	1.291045	0.599146	0.115842
		N	1.602522	0.575884	1.412134
		C	1.516181	-0.722571	1.866657

		C	1.157486	-1.494454	0.804697
		C	1.846676	1.753596	2.256424
		C	2.131093	2.996684	1.435538
		C	0.574652	-1.038448	-1.607727
		H	1.266589	1.484568	-0.527622
		H	1.689275	-0.977477	2.905304
		H	0.930190	-2.551091	0.730305
		H	-0.384072	-1.561672	-1.497553
		H	0.443940	-0.135300	-2.213838
		H	1.323827	-1.684902	-2.080036
		H	2.691129	1.497528	2.910752
		H	0.947386	1.889864	2.874476
		H	2.376998	3.818614	2.120218
		H	2.977030	2.845029	0.750787
		H	1.245281	3.281431	0.853018
		N	-1.572459	0.318052	1.913781
		C	-1.373242	1.482090	1.344777
		C	-1.793078	-0.681265	1.076076
		N	-1.145416	2.543211	0.891844
		N	-1.962361	-1.599167	0.366929
		N	-2.502423	1.889378	-2.753807
		C	-1.874694	2.872028	-2.105572
		N	-1.789821	3.923795	-2.921389
		C	-2.363665	3.596116	-4.130528
		C	-2.816408	2.317488	-4.024812
		C	-1.051032	5.163467	-2.645654
		C	-0.780086	5.348103	-1.165340
		C	-2.736597	0.544684	-2.235152
		H	-1.505859	2.820417	-1.076034
		H	-2.373311	4.287638	-4.964475
		H	-3.280715	1.658703	-4.748758

		H	-2.274072	-0.166433	-2.931805
		H	-2.273648	0.457831	-1.246057
		H	-3.814231	0.363246	-2.145783
		H	-1.655211	5.984434	-3.055472
		H	-0.109806	5.098366	-3.210980
		H	-0.294341	6.321136	-1.016823
		H	-1.708373	5.325859	-0.576984
		H	-0.106238	4.562827	-0.798680
		N	0.620308	2.337617	-4.299871
		C	1.013084	2.581506	-3.073065
		C	0.006257	1.177747	-4.466811
		N	1.350203	2.876829	-1.985828
		N	-0.569762	0.173474	-4.649857
		c2mimpf6			
		N	-2.252460	-1.996618	-1.149016
		C	-1.455491	-1.637772	-0.149401
		N	-2.023519	-1.990810	0.998074
		C	-3.232728	-2.590518	0.727036
		C	-3.381408	-2.586744	-0.627520
		C	-1.407861	-1.810447	2.316836
		C	-0.541078	-3.003144	2.691507
		C	-2.005152	-1.672248	-2.548862
		H	-0.510993	-1.127826	-0.257216
		H	-3.880131	-2.958111	1.511204
		H	-4.187562	-2.940217	-1.254994
		H	-2.572201	-0.775220	-2.813689
		H	-0.935097	-1.484418	-2.664623
		H	-2.302988	-2.524452	-3.164715
		H	-2.227999	-1.651762	3.024046
		H	-0.824421	-0.889059	2.255617

		H	-0.102582	-2.835799	3.681371
		H	-1.136730	-3.923085	2.725267
		H	0.268836	-3.122186	1.964386
		P	2.204249	-1.773626	-0.268603
		F	1.289927	-0.944760	-1.385696
		F	3.027934	-2.482642	-1.464934
		F	3.049880	-2.554752	0.867082
		F	1.082366	-2.968610	-0.291941
		F	1.316285	-1.016211	0.921426
		F	3.259637	-0.524532	-0.243791
		N	2.252460	1.996555	-1.149003
		C	1.455415	1.637773	-0.149432
		N	2.023531	1.990551	0.998088
		C	3.232879	2.589996	0.727122
		C	3.381555	2.586350	-0.627437
		C	1.407741	1.810249	2.316798
		C	0.541303	3.003206	2.691461
		C	2.005134	1.672290	-2.548877
		H	0.510848	1.127926	-0.257141
		H	3.880368	2.957380	1.511317
		H	4.187777	2.939727	-1.254877
		H	2.572077	0.775201	-2.813715
		H	0.935059	1.484569	-2.664643
		H	2.303061	2.524494	-3.164684
		H	2.227786	1.651277	3.024052
		H	0.823984	0.889054	2.255515
		H	0.102608	2.835933	3.681249
		H	1.137251	3.922951	2.725371
		H	-0.268476	3.122557	1.964235
		P	-2.204287	1.773766	-0.268551
		F	-1.289799	0.945055	-1.385658

		F	-3.028333	2.482368	-1.464881
		F	-3.050088	2.554712	0.867121
		F	-1.082790	2.969075	-0.292100
		F	-1.315953	1.016774	0.921491
		F	-3.259270	0.524330	-0.243497
[C ₂ mim][OTs] 2IP		C	-5.967152	-1.770648	-0.665313
		C	-6.005914	-0.489289	-1.232461
		C	-5.005822	0.442149	-0.974558
		C	-3.945246	0.090779	-0.140898
		C	-3.893631	-1.166522	0.449353
		C	-4.900256	-2.093145	0.177615
		H	-6.840750	-0.218683	-1.883290
		H	-5.037378	1.445963	-1.400422
		S	-2.604577	1.263029	0.109772
		H	-3.073855	-1.402805	1.128641
		H	-4.858367	-3.083520	0.637430
		C	-7.071912	-2.758267	-0.937464
		O	-1.905289	0.820093	1.363203
		O	-3.233384	2.606002	0.199370
		O	-1.729500	1.087598	-1.103796
		H	-7.342562	-2.767274	-2.002922
		H	-7.978267	-2.495452	-0.370400
		H	-6.778636	-3.775919	-0.647123
		N	0.413728	2.910102	-1.425861
		C	0.620662	2.451693	-0.193887
		N	-0.025027	3.244001	0.665598
		C	-0.691689	4.217069	-0.043087
		C	-0.415990	4.004168	-1.358473
		C	-0.037668	3.035119	2.123494
		C	-1.277093	3.633433	2.762047
		C	0.756349	2.192205	-2.646580

		H	1.206516	1.569720	0.086152
		H	-1.344583	4.937205	0.431405
		H	-0.770611	4.509623	-2.248384
		H	-0.165491	1.727152	-3.019737
		H	1.165008	2.899962	-3.377783
		H	1.482757	1.410281	-2.395549
		H	0.886237	3.466268	2.534958
		H	-0.029826	1.948668	2.262931
		H	-1.306278	3.332565	3.817652
		H	-1.263918	4.733026	2.730392
		H	-2.176594	3.254605	2.256822
		C	7.052119	-0.438364	-0.466097
		C	6.415917	-1.666453	-0.684995
		C	5.037466	-1.797258	-0.546272
		C	4.282833	-0.683171	-0.188759
		C	4.890620	0.544390	0.052363
		C	6.271428	0.660334	-0.091720
		H	7.014780	-2.537446	-0.961072
		H	4.533341	-2.752348	-0.695275
		S	2.500566	-0.839087	-0.056705
		H	4.281810	1.393018	0.366429
		H	6.755619	1.620596	0.098799
		C	8.543287	-0.312034	-0.638746
		O	2.092895	0.067152	1.076342
		O	2.226746	-2.281041	0.188436
		O	1.934765	-0.338264	-1.357244
		H	8.818006	-0.361443	-1.703701
		H	9.071119	-1.128236	-0.125170
		H	8.913026	0.641561	-0.239498
		N	-0.862716	-2.122211	-0.862040
		C	-0.517117	-1.325017	0.143764

		N	-0.573295	-2.013410	1.279082
		C	-0.949927	-3.305957	0.991506
		C	-1.135672	-3.372918	-0.358009
		C	-0.194418	-1.467556	2.587176
		C	0.899695	-2.305287	3.226692
		C	-0.853800	-1.698539	-2.259335
		H	-0.251223	-0.281174	0.043666
		H	-1.052888	-4.063969	1.758393
		H	-1.435250	-4.196203	-0.995192
		H	0.182938	-1.452101	-2.524514
		H	-1.237469	-2.522458	-2.870423
		H	-1.489633	-0.808117	-2.344151
		H	-1.104412	-1.400812	3.200405
		H	0.167238	-0.454813	2.381913
		H	1.234480	-1.816933	4.151847
		H	0.544646	-3.313976	3.487075
		H	1.743510	-2.386773	2.528535
[C ₂ mim][TFA] 2IP		C	-5.243948	0.796047	3.174528
		F	-5.184441	1.520734	4.309074
		F	-5.841937	-0.362737	3.475970
		F	-6.066013	1.461812	2.341959
		C	-3.837718	0.570615	2.549304
		O	-3.826591	0.475632	1.307126
		O	-2.895827	0.536723	3.363111
		N	-0.657183	1.039503	-0.035871
		C	-0.710960	0.548629	1.200237
		N	0.483881	0.712832	1.770331
		C	1.307705	1.371892	0.888925
		C	0.589365	1.575898	-0.250160
		C	0.796897	0.372616	3.162007
		C	0.251880	1.408932	4.129690

		C	-1.762763	1.054352	-0.987622
		H	-1.599282	0.138557	1.684139
		H	2.321521	1.649949	1.151132
		H	0.842665	2.075594	-1.177091
		H	-1.502999	0.432272	-1.853360
		H	-2.643927	0.655382	-0.470510
		H	-1.924836	2.099384	-1.274711
		H	1.890090	0.282137	3.218038
		H	0.364714	-0.617495	3.357210
		H	0.563914	1.148500	5.150975
		H	0.612369	2.411394	3.864812
		H	-0.844921	1.400419	4.071951
		C	-1.031935	5.715310	1.417832
		F	-2.194745	5.969187	2.076791
		F	-1.039280	6.482681	0.323207
		F	-0.043112	6.141929	2.209628
		C	-0.965615	4.197863	1.109912
		O	-0.558431	3.492198	2.053971
		O	-1.436883	3.863504	0.007646
		N	-3.596828	3.795840	3.412910
		C	-3.484991	3.316250	2.176383
		N	-4.530133	3.729554	1.464773
		C	-5.335537	4.504016	2.266920
		C	-4.747729	4.541452	3.496048
		C	-4.763301	3.398566	0.057047
		C	-4.432831	4.575387	-0.846714
		C	-2.646764	3.515582	4.484794
		H	-2.670233	2.696871	1.815145
		H	-6.256757	4.942469	1.902517
		H	-5.053731	5.021693	4.417428
		H	-2.784915	2.472371	4.796729

		H	-1.638844	3.669422	4.078383
		H	-2.846829	4.209903	5.307546
		H	-5.812420	3.081500	-0.020439
		H	-4.141693	2.518520	-0.145749
		H	-4.606050	4.290345	-1.893938
		H	-5.073030	5.440526	-0.619010
		H	-3.377041	4.852489	-0.720954
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		N	-2.500530	5.205758	2.906925
		C	-2.707581	4.946743	1.617743
		N	-3.755011	5.660029	1.210787
		C	-4.265508	6.356732	2.281009
		C	-3.470907	6.075311	3.352386
		C	-4.348763	5.520560	-0.119965
		C	-4.633037	6.871558	-0.754352
		C	-1.464077	4.556979	3.698086
		H	-2.107248	4.248213	1.018584
		H	-5.145906	6.982606	2.200794
		H	-3.515195	6.412538	4.381193
		H	-1.945449	3.838037	4.372206
		H	-0.814737	4.025479	2.990740
		H	-0.894948	5.318258	4.245820
		H	-5.257719	4.915832	0.010902
		H	-3.609767	4.951388	-0.701839
		H	-5.041627	6.720432	-1.762364
		H	-5.370781	7.451376	-0.180749
		H	-3.710505	7.461991	-0.841056
		C	0.529596	3.012715	-1.382162
		C	-0.686193	3.320051	-0.503790
		O	-1.710334	3.786426	-1.062514

		O	-0.563081	3.098689	0.734323
		H	0.247616	2.961972	-2.440903
		H	1.008762	2.078424	-1.058513
		H	1.267363	3.819458	-1.252132
		N	-3.004250	1.257766	-0.228672
		C	-2.675876	1.138683	1.057612
		N	-1.610717	0.331909	1.133710
		C	-1.222829	-0.023199	-0.136673
		C	-2.103606	0.558764	-0.996618
		C	-0.923695	-0.039322	2.374592
		C	-0.580990	1.182745	3.208829
		C	-4.117050	2.046729	-0.745278
		H	-3.162062	1.647043	1.919204
		H	-0.360557	-0.653603	-0.318956
		H	-2.155462	0.557622	-2.078917
		H	-4.575702	2.560551	0.112770
		H	-3.701926	2.763400	-1.462722
		H	-4.840764	1.371063	-1.220472
		H	-0.021626	-0.585100	2.067671
		H	-1.569054	-0.738140	2.925804
		H	-0.009287	0.867325	4.093157
		H	0.004690	1.883064	2.597547
		H	-1.506609	1.677428	3.539419
		C	-5.629659	3.533238	4.271722
		C	-4.713952	3.062957	3.136447
		O	-3.652854	2.467457	3.481003
		O	-5.082940	3.284727	1.959016
		H	-5.034141	3.941681	5.100231
		H	-6.174177	2.661006	4.664848
		H	-6.356337	4.271650	3.911568
[C ₂ mim]Cl 2IP	CHCl ₃	N	0.000649	-0.999554	0.155752

		C	0.189546	-0.594644	1.411689
		N	1.426187	-0.922777	1.776965
		C	2.057696	-1.530750	0.716850
		C	1.158948	-1.583534	-0.306385
		C	2.073035	-0.547776	3.041050
		C	1.083753	0.066769	4.011697
		C	-1.242196	-0.823537	-0.590559
		H	-0.574735	-0.095794	2.010355
		H	3.083750	-1.868402	0.778099
		H	1.240557	-1.986748	-1.306777
		H	-1.987995	-0.414051	0.097752
		H	-1.069114	-0.132794	-1.421084
		H	-1.572459	-1.793036	-0.971987
		H	2.853170	0.174560	2.780356
		H	2.529846	-1.454289	3.451447
		H	1.613717	0.327604	4.933173
		H	0.651082	0.980305	3.586217
		H	0.272997	-0.628470	4.259184
		Cl	-2.648820	0.693226	2.616293
		N	-0.585759	3.912992	3.523121
		C	-0.801139	3.529349	2.264131
		N	-2.048422	3.854983	1.934323
		C	-2.658390	4.440697	3.019130
		C	-1.736184	4.481981	4.021752
		C	-2.721292	3.511316	0.674474
		C	-1.760221	2.888075	-0.318242
		C	0.678784	3.745308	4.234348
		H	-0.048894	3.042128	1.640685
		H	-3.688461	4.770018	2.988539
		H	-1.797759	4.865890	5.031106
		H	1.395680	3.299107	3.537900

		H	1.035846	4.722975	4.568584
		H	0.522739	3.088798	5.095251
		H	-3.163451	4.433661	0.283448
		H	-3.513559	2.802953	0.936357
		H	-2.309407	2.648469	-1.234170
		H	-0.938588	3.568582	-0.570830
		H	-1.343115	1.960752	0.092065
		Cl	1.990975	2.205657	0.995940
[C ₂ mim][BF ₄] 2IP		N	0.145532	-0.881729	-0.264842
		C	-0.134454	-1.002916	1.029917
		N	0.990053	-0.857595	1.724411
		C	2.025817	-0.625677	0.848303
		C	1.492919	-0.640920	-0.406595
		C	1.068626	-0.879302	3.190883
		C	1.651109	0.417993	3.728343
		C	-0.845596	-0.925589	-1.335261
		H	-1.115914	-1.179982	1.450536
		H	3.043680	-0.474382	1.179617
		H	1.952742	-0.499958	-1.375318
		H	-1.781658	-1.289844	-0.907335
		H	-0.984668	0.081334	-1.736369
		H	-0.495560	-1.606455	-2.114709
		H	1.673674	-1.745340	3.478380
		H	0.043592	-1.031731	3.538102
		H	1.627972	0.390586	4.822866
		H	2.692954	0.547136	3.414311
		H	1.056318	1.264680	3.374161
		B	-1.217744	1.843223	1.449969
		F	-1.748045	3.116015	1.678025
		F	-1.280408	1.081532	2.650842
		F	0.113059	1.920741	1.012667

		F	-1.996559	1.166232	0.469909
		N	-5.184129	-0.113585	1.494765
		C	-4.183985	0.072194	2.352042
		N	-4.662792	-0.010227	3.589740
		C	-6.013428	-0.266974	3.526784
		C	-6.342137	-0.332194	2.205236
		C	-3.843849	0.092525	4.804701
		C	-3.965561	-1.161226	5.655571
		C	-5.036971	-0.150398	0.043103
		H	-3.149432	0.249466	2.088222
		H	-6.625319	-0.377333	4.411153
		H	-7.289764	-0.515103	1.716985
		H	-4.040601	0.223544	-0.200225
		H	-5.144086	-1.181597	-0.302309
		H	-5.801032	0.488152	-0.406485
		H	-4.168009	0.985033	5.349695
		H	-2.818563	0.242480	4.457137
		H	-3.289987	-1.075055	6.513236
		H	-4.984877	-1.285567	6.038068
		H	-3.689713	-2.038075	5.063211
		B	-3.017420	-2.766147	2.196526
		F	-2.435830	-4.035509	2.132889
		F	-2.257778	-1.939477	3.071655
		F	-4.342283	-2.839212	2.652479
		F	-2.995895	-2.162766	0.908009
[C ₂ mim][DCA] 2IP		N	0.988476	-0.645030	-0.246962
		C	1.228466	0.606837	0.143195
		N	1.586814	0.586067	1.426200
		C	1.568817	-0.717231	1.871266
		C	1.194908	-1.494008	0.816288
		C	1.845713	1.764901	2.267321

		C	2.132304	3.002315	1.437226
		C	0.550065	-1.040844	-1.582532
		H	1.163725	1.484685	-0.494193
		H	1.812727	-0.976896	2.892394
		H	1.042023	-2.561142	0.733557
		H	-0.395424	-1.582410	-1.486423
		H	0.409640	-0.138615	-2.182347
		H	1.311729	-1.672577	-2.045957
		H	2.695114	1.506987	2.907348
		H	0.960424	1.909758	2.896944
		H	2.377958	3.824017	2.116952
		H	2.981658	2.837404	0.764439
		H	1.253783	3.290909	0.849435
		N	-1.603619	0.256925	1.900737
		C	-1.433808	1.443273	1.372167
		C	-1.865240	-0.747083	1.090645
		N	-1.241217	2.532670	0.981631
		N	-2.087724	-1.688597	0.430372
		N	-2.459160	1.898179	-2.776667
		C	-1.815305	2.873075	-2.134787
		N	-1.759332	3.937418	-2.934152
		C	-2.380004	3.631532	-4.125046
		C	-2.824204	2.347447	-4.025181
		C	-1.051408	5.194463	-2.646308
		C	-0.777859	5.364870	-1.163554
		C	-2.708591	0.561482	-2.244067
		H	-1.428521	2.806605	-1.121348
		H	-2.444271	4.343548	-4.936540
		H	-3.345867	1.715045	-4.730109
		H	-2.268255	-0.168226	-2.929707
		H	-2.238795	0.487525	-1.260532

		H	-3.785044	0.400453	-2.147643
		H	-1.683791	6.000198	-3.031688
		H	-0.117185	5.174251	-3.218990
		H	-0.309942	6.342049	-1.009484
		H	-1.707433	5.325490	-0.584272
		H	-0.090882	4.591801	-0.801610
		N	0.634809	2.260835	-4.337703
		C	1.048568	2.544551	-3.127773
		C	0.038149	1.103322	-4.529654
		N	1.425513	2.890443	-2.071988
		N	-0.512499	0.098327	-4.771905
[C ₂ mim][PF ₆] 2IP		N	2.180590	2.179051	-1.131672
		C	1.353627	1.815913	-0.156767
		N	1.903195	2.136272	1.010615
		C	3.125790	2.724341	0.778005
		C	3.304026	2.745294	-0.573799
		C	1.255436	1.951225	2.314159
		C	0.389396	3.148718	2.672866
		C	1.968884	1.895152	-2.547068
		H	0.396290	1.334585	-0.293805
		H	3.758167	3.070081	1.584501
		H	4.126997	3.102396	-1.177384
		H	2.586610	1.040760	-2.835829
		H	0.913176	1.655883	-2.690728
		H	2.235453	2.779879	-3.128873
		H	2.055731	1.789096	3.041254
		H	0.663989	1.035893	2.239638
		H	-0.076834	2.977337	3.648858
		H	0.993752	4.061294	2.728460
		H	-0.398188	3.280563	1.923067
		P	-2.427995	1.654905	-0.280057

		F	-1.426203	0.937580	-1.383349
		F	-3.325184	2.269081	-1.490605
		F	-3.388340	2.351043	0.833468
		F	-1.465668	2.979533	-0.300133
		F	-1.487764	1.019474	0.924555
		F	-3.351881	0.306263	-0.258610
		N	-2.021339	-2.219238	-1.118775
		C	-1.332311	-1.693411	-0.112321
		N	-1.788755	-2.197048	1.029414
		C	-2.809526	-3.078982	0.747109
		C	-2.961500	-3.086996	-0.607531
		C	-1.228486	-1.910474	2.354876
		C	-0.255670	-2.995292	2.789473
		C	-1.858793	-1.839750	-2.518603
		H	-0.541276	-0.967126	-0.210531
		H	-3.334865	-3.616630	1.524903
		H	-3.647781	-3.629776	-1.242946
		H	-2.625195	-1.106733	-2.784992
		H	-0.866084	-1.401344	-2.636967
		H	-1.948937	-2.735133	-3.137318
		H	-2.073380	-1.816698	3.043313
		H	-0.737022	-0.938425	2.275071
		H	0.144584	-2.743274	3.777323
		H	-0.759063	-3.966578	2.856248
		H	0.572221	-3.063969	2.076507
		P	2.294192	-1.618326	-0.300932
		F	1.346784	-0.828607	-1.399557
		F	3.143180	-2.295327	-1.513920
		F	3.203552	-2.386548	0.810090
		F	1.241616	-2.872992	-0.321594
		F	1.410230	-0.918382	0.908489

		F	3.316083	-0.343165	-0.279325
[C ₂ mim][OTs] 2IP		C	-5.688163	-1.587896	-0.182786
		C	-5.161203	-1.051792	-1.365650
		C	-4.144913	-0.100657	-1.333892
		C	-3.645337	0.328020	-0.104135
		C	-4.152428	-0.190721	1.084277
		C	-5.171660	-1.142405	1.038415
		H	-5.550464	-1.393401	-2.327767
		H	-3.727387	0.309847	-2.254530
		S	-2.329171	1.559139	-0.049093
		H	-3.742182	0.148052	2.037192
		H	-5.568775	-1.550727	1.970475
		C	-6.783885	-2.620033	-0.238834
		O	-1.497679	1.174770	1.141676
		O	-2.982879	2.888945	0.099087
		O	-1.594276	1.389189	-1.348492
		H	-6.490809	-3.467038	-0.876410
		H	-7.704115	-2.193627	-0.664975
		H	-7.018273	-3.007114	0.761361
		N	0.865051	2.939826	-1.478104
		C	0.932313	2.452029	-0.240979
		N	0.519623	3.394493	0.607525
		C	0.149521	4.509392	-0.110759
		C	0.364340	4.219992	-1.424836
		C	0.465150	3.220538	2.066421
		C	-0.771499	3.873757	2.656840
		C	1.082607	2.165915	-2.694171
		H	1.256578	1.448596	0.049690
		H	-0.235391	5.404819	0.361096

		H	0.196790	4.807543	-2.320052
		H	0.100146	1.905767	-3.107449
		H	1.658118	2.772166	-3.402792
		H	1.625447	1.253321	-2.423113
		H	1.388370	3.638858	2.491418
		H	0.450892	2.137247	2.225736
		H	-0.847189	3.594434	3.716367
		H	-0.714960	4.970574	2.606884
		H	-1.664644	3.523266	2.122789
		C	6.897418	-0.910712	-0.020217
		C	6.235165	-2.099957	-0.353222
		C	4.845257	-2.176357	-0.342165
		C	4.104972	-1.047008	0.001744
		C	4.737062	0.143250	0.349510
		C	6.129501	0.204969	0.333192
		H	6.820838	-2.982842	-0.618535
		H	4.324802	-3.103096	-0.584754
		S	2.312123	-1.121279	-0.028663
		H	4.140612	1.008449	0.641939
		H	6.631269	1.135006	0.608014
		C	8.401825	-0.845951	-0.046752
		O	1.843423	-0.239057	1.094517
		O	1.948763	-2.557335	0.135273
		O	1.890326	-0.559612	-1.358704
		H	8.776246	-0.937643	-1.077473
		H	8.840584	-1.669931	0.534172
		H	8.768299	0.102805	0.365487
		N	-1.287084	-1.937622	-1.259859
		C	-0.852868	-1.352089	-0.146724
		N	-1.346774	-2.005061	0.901098
		C	-2.131795	-3.042527	0.448398

		C	-2.096573	-2.998310	-0.914401
		C	-1.028532	-1.685256	2.296303
		C	-0.028701	-2.676623	2.868942
		C	-0.946312	-1.483571	-2.605095
		H	-0.233499	-0.465329	-0.096309
		H	-2.649393	-3.712676	1.125483
		H	-2.577506	-3.619395	-1.661129
		H	0.144682	-1.517192	-2.712412
		H	-1.436352	-2.146028	-3.325612
		H	-1.300214	-0.451054	-2.712438
		H	-1.977456	-1.683406	2.851047
		H	-0.633251	-0.663945	2.277448
		H	0.230037	-2.380302	3.894757
		H	-0.451116	-3.692022	2.901984
		H	0.877316	-2.682344	2.248471
[C ₂ mim][TFA] 2IP		C	3.677363	-0.549760	-0.011071
		F	3.691090	-0.030301	-1.253951
		F	4.788821	-1.305473	0.109500
		F	3.813249	0.484327	0.841364
		C	2.398104	-1.400739	0.266451
		O	2.011008	-1.401275	1.449120
		O	1.924847	-1.971033	-0.734276
		N	-1.541977	-2.101002	1.744804
		C	-0.899680	-2.600686	0.691057
		N	-1.804787	-3.096628	-0.155217
		C	-3.059085	-2.877630	0.358137
		C	-2.893777	-2.248301	1.556976
		C	-1.493641	-3.710360	-1.452607
		C	-0.957750	-2.681387	-2.434496
		C	-0.912400	-1.489238	2.911532
		H	0.178208	-2.590090	0.541132

		H	-3.954116	-3.178872	-0.168616
		H	-3.613800	-1.891938	2.280390
		H	-1.138800	-2.093383	3.794215
		H	0.165948	-1.463482	2.733500
		H	-1.314961	-0.478733	3.015450
		H	-2.423798	-4.164695	-1.804929
		H	-0.765932	-4.508191	-1.274656
		H	-0.764211	-3.168112	-3.396728
		H	-1.683186	-1.873046	-2.569039
		H	-0.018891	-2.264171	-2.053433
		C	-2.687102	2.193411	-0.584097
		F	-1.593933	2.869108	-1.027916
		F	-3.287221	2.985717	0.319068
		F	-3.523222	2.085027	-1.630494
		C	-2.230739	0.821056	-0.005556
		O	-2.088968	-0.077844	-0.854686
		O	-1.968927	0.832235	1.210442
		N	0.983185	1.229551	-1.499226
		C	0.671949	0.879673	-0.252421
		N	1.145785	1.804986	0.577932
		C	1.782661	2.778177	-0.156554
		C	1.682129	2.412559	-1.466855
		C	0.986789	1.785806	2.036044
		C	0.157833	2.968237	2.510577
		C	0.663791	0.437290	-2.683321
		H	0.104947	0.002811	0.031672
		H	2.257368	3.631659	0.306804
		H	2.048665	2.885307	-2.367278
		H	1.343388	-0.419063	-2.726976
		H	-0.374104	0.103999	-2.597091
		H	0.787531	1.075231	-3.560065

		H	1.991857	1.778383	2.469471
		H	0.499060	0.837029	2.267692
		H	0.040260	2.906521	3.597794
		H	0.649438	3.918772	2.274205
		H	-0.831731	2.934760	2.042724
[C ₂ mim][OAc] 2IP		N	-1.714793	-0.319845	1.625744
		C	-1.336660	0.701651	0.860777
		N	-2.410463	1.158545	0.215460
		C	-3.497646	0.387716	0.550584
		C	-3.058597	-0.544637	1.444081
		C	-2.373083	2.241708	-0.770714
		C	-3.464684	3.269536	-0.522722
		C	-0.819831	-1.089967	2.483438
		H	-0.328469	1.119832	0.793338
		H	-4.479071	0.546872	0.126671
		H	-3.581865	-1.340690	1.955919
		H	-0.801925	-2.119580	2.116682
		H	0.171988	-0.636807	2.402763
		H	-1.184543	-1.042236	3.513060
		H	-2.467689	1.783054	-1.761319
		H	-1.378833	2.688348	-0.677339
		H	-3.371209	4.070288	-1.263659
		H	-4.462695	2.829444	-0.625522
		H	-3.365362	3.703582	0.478225
		C	3.294797	2.593894	1.276014
		C	1.932572	1.934203	1.061351
		O	1.069579	2.587304	0.408246
		O	1.746476	0.796449	1.569152
		H	3.565823	3.212457	0.413920
		H	4.066534	1.841306	1.464688
		H	3.226464	3.250144	2.153995

		N	1.648191	0.341867	-1.649223
		C	1.533909	-0.804320	-0.978547
		N	2.756113	-1.172935	-0.582964
		C	3.664135	-0.224018	-0.986506
		C	2.964683	0.733882	-1.658288
		C	3.076932	-2.391999	0.171166
		C	2.126725	-2.587256	1.339937
		C	0.543218	1.087340	-2.245522
		H	0.600362	-1.349057	-0.789600
		H	4.718652	-0.306937	-0.762688
		H	3.285465	1.653096	-2.129033
		H	-0.369379	0.507265	-2.075324
		H	0.499929	2.062726	-1.753702
		H	0.729114	1.195770	-3.317894
		H	4.109226	-2.271074	0.511792
		H	3.040310	-3.239478	-0.521830
		H	2.430119	-3.477787	1.900954
		H	2.163880	-1.710240	1.994563
		H	1.100951	-2.729181	0.980138
		C	-3.096898	-2.912084	-1.030201
		C	-1.782335	-2.133797	-0.967156
		O	-0.860910	-2.616485	-0.248971
		O	-1.691198	-1.081279	-1.650815
		H	-3.301084	-3.404519	-0.073552
		H	-2.997746	-3.692887	-1.796065
		H	-3.927291	-2.256154	-1.309341
		EtOH			
		c2mimcl			
		N	-0.076407	-0.968143	0.095918
		C	0.095272	-0.550754	1.351368

		N	1.346606	-0.820616	1.715777
		C	2.000672	-1.410857	0.659771
		C	1.103977	-1.507443	-0.362507
		C	1.973647	-0.449098	2.991995
		C	0.979454	0.202169	3.932485
		C	-1.332060	-0.876824	-0.645295
		H	-0.687637	-0.087895	1.954134
		H	3.038992	-1.707851	0.722434
		H	1.202371	-1.913740	-1.360117
		H	-2.081661	-0.436623	0.018770
		H	-1.186057	-0.245076	-1.525806
		H	-1.642684	-1.879357	-0.949685
		H	2.780911	0.246360	2.743175
		H	2.393969	-1.362874	3.423847
		H	1.500258	0.481184	4.853555
		H	0.560936	1.108544	3.477998
		H	0.157263	-0.476272	4.187225
		Cl	-2.763252	0.604737	2.716761
		N	-0.536826	3.899999	3.589482
		C	-0.712732	3.481252	2.335060
		N	-1.963978	3.754632	1.973067
		C	-2.613691	4.348758	3.029627
		C	-1.714367	4.443937	4.049723
		C	-2.595134	3.383662	0.698719
		C	-1.606083	2.725350	-0.242285
		C	0.720358	3.806391	4.327841
		H	0.067311	3.014913	1.731370
		H	-3.651091	4.649301	2.968760
		H	-1.809199	4.852023	5.046946
		H	1.466525	3.360781	3.663503
		H	1.035645	4.808822	4.627768

		H	0.573987	3.178567	5.211086
		H	-3.011721	4.298605	0.265727
		H	-3.405348	2.692787	0.950531
		H	-2.130600	2.445676	-1.161061
		H	-0.781694	3.399447	-0.501407
		H	-1.190722	1.818536	0.214126
		Cl	2.143791	2.326988	0.967615
[C ₂ mim][BF ₄] 2IP		N	0.135395	-0.862987	-0.270859
		C	-0.127757	-0.989280	1.027029
		N	1.007370	-0.856232	1.706970
		C	2.033044	-0.628568	0.817766
		C	1.482887	-0.633647	-0.429929
		C	1.109378	-0.889055	3.171904
		C	1.688045	0.409178	3.710947
		C	-0.867836	-0.901793	-1.330801
		H	-1.104664	-1.162081	1.459961
		H	3.057210	-0.491040	1.136040
		H	1.930971	-0.496620	-1.404872
		H	-1.803329	-1.253949	-0.892026
		H	-1.000154	0.103860	-1.737163
		H	-0.532879	-1.589658	-2.110462
		H	1.728536	-1.750426	3.441709
		H	0.092310	-1.055063	3.535877
		H	1.696854	0.365850	4.805187
		H	2.718339	0.557330	3.368755
		H	1.071175	1.251988	3.386112
		B	-1.217288	1.856569	1.485166
		F	-1.750029	3.129859	1.730146
		F	-1.278363	1.082445	2.674348
		F	0.113724	1.950975	1.049682
		F	-1.993180	1.197225	0.494535

		N	-5.179719	-0.133295	1.484802
		C	-4.189985	0.053353	2.353853
		N	-4.686633	-0.011144	3.585754
		C	-6.038820	-0.255649	3.506851
		C	-6.349711	-0.332618	2.181384
		C	-3.887276	0.103094	4.812669
		C	-4.003787	-1.151561	5.663053
		C	-5.016736	-0.175767	0.034602
		H	-3.150772	0.221815	2.102628
		H	-6.663993	-0.346519	4.384477
		H	-7.292892	-0.507385	1.681495
		H	-4.011040	0.178903	-0.198617
		H	-5.141147	-1.204609	-0.311602
		H	-5.763530	0.475840	-0.424781
		H	-4.234023	0.990149	5.352146
		H	-2.858957	0.269025	4.481643
		H	-3.346919	-1.052154	6.533636
		H	-5.028590	-1.291974	6.024629
		H	-3.701316	-2.024729	5.077810
		B	-2.996769	-2.784576	2.226206
		F	-2.412023	-4.057628	2.176556
		F	-2.238261	-1.950391	3.090032
		F	-4.320237	-2.864998	2.686718
		F	-2.982627	-2.201066	0.931030
[C ₂ mim][DCA] 2IP		N	0.987350	-0.650373	-0.234636
		C	1.217264	0.603972	0.153688
		N	1.588047	0.587166	1.433172
		C	1.590378	-0.716134	1.877742
		C	1.215550	-1.497242	0.826033
		C	1.849624	1.767906	2.271293
		C	2.127992	3.004715	1.437755

		C	0.544706	-1.050660	-1.567165
		H	1.137945	1.480360	-0.483139
		H	1.853220	-0.973418	2.894860
		H	1.085554	-2.567427	0.742366
		H	-0.412721	-1.570721	-1.470860
		H	0.427754	-0.151601	-2.176655
		H	1.294261	-1.704902	-2.018686
		H	2.704013	1.512906	2.905255
		H	0.969205	1.911261	2.907839
		H	2.374197	3.828037	2.115191
		H	2.975729	2.840205	0.762944
		H	1.246564	3.290354	0.852585
		N	-1.602621	0.246086	1.905955
		C	-1.444454	1.435884	1.380521
		C	-1.886208	-0.756279	1.102732
		N	-1.263079	2.528889	0.995675
		N	-2.131631	-1.700254	0.453865
		N	-2.458269	1.903294	-2.789095
		C	-1.805639	2.872209	-2.146956
		N	-1.757827	3.943195	-2.937872
		C	-2.394317	3.648792	-4.122974
		C	-2.839503	2.364423	-4.028563
		C	-1.051593	5.200592	-2.645975
		C	-0.772993	5.363751	-1.163490
		C	-2.706078	0.564120	-2.262765
		H	-1.408326	2.796983	-1.138799
		H	-2.472815	4.370143	-4.925034
		H	-3.380803	1.743284	-4.728828
		H	-2.243863	-0.162478	-2.937163
		H	-2.258878	0.495836	-1.268376
		H	-3.783028	0.393665	-2.193085

		H	-1.687709	6.006475	-3.023894
		H	-0.120138	5.187127	-3.223122
		H	-0.305317	6.340527	-1.006691
		H	-1.701638	5.322212	-0.582995
		H	-0.084677	4.589589	-0.805980
		N	0.629259	2.259996	-4.348414
		C	1.054647	2.540484	-3.141316
		C	0.052168	1.095243	-4.549980
		N	1.443837	2.885241	-2.089961
		N	-0.479138	0.083567	-4.808006
[C ₂ mim][PF ₆] 2IP		N	1.998651	2.265538	-1.102492
		C	1.280129	1.790977	-0.090860
		N	1.835840	2.184121	1.051023
		C	2.951078	2.939121	0.763237
		C	3.058287	2.984047	-0.595471
		C	1.275489	1.919386	2.381208
		C	0.311037	3.017901	2.799461
		C	1.744797	1.975747	-2.510214
		H	0.394579	1.180686	-0.183221
		H	3.565466	3.374455	1.539857
		H	3.788563	3.458582	-1.236548
		H	2.470517	1.237765	-2.861975
		H	0.733236	1.574261	-2.595667
		H	1.832094	2.902090	-3.081659
		H	2.121053	1.832022	3.068838
		H	0.778504	0.948113	2.319935
		H	-0.089779	2.786352	3.791950
		H	0.822736	3.985698	2.845888
		H	-0.518632	3.079551	2.086730
		P	-2.446555	1.573468	-0.309124
		F	-1.415188	0.848181	-1.374256

		F	-3.309551	2.178442	-1.553607
		F	-3.446452	2.283356	0.764781
		F	-1.490179	2.902060	-0.313012
		F	-1.550510	0.953397	0.931672
		F	-3.374927	0.228587	-0.304341
		N	-1.980846	-2.261525	-1.104362
		C	-1.279656	-1.768650	-0.089371
		N	-1.810008	-2.203564	1.049289
		C	-2.890656	-3.005787	0.756131
		C	-3.003299	-3.035921	-0.602482
		C	-1.254856	-1.934711	2.380733
		C	-0.278229	-3.022657	2.798185
		C	-1.748609	-1.939511	-2.508873
		H	-0.425592	-1.114661	-0.175550
		H	-3.478365	-3.481757	1.529621
		H	-3.714067	-3.535229	-1.246651
		H	-2.492784	-1.209679	-2.838658
		H	-0.746282	-1.516337	-2.597625
		H	-1.823415	-2.856478	-3.096951
		H	-2.101888	-1.857795	3.067909
		H	-0.768885	-0.957865	2.320921
		H	0.121558	-2.786121	3.789911
		H	-0.779416	-3.995879	2.846644
		H	0.550454	-3.076047	2.083808
		P	2.423788	-1.564404	-0.323315
		F	1.400880	-0.814792	-1.379161
		F	3.277610	-2.167443	-1.575362
		F	3.416279	-2.298933	0.741354
		F	1.450968	-2.881036	-0.340095
		F	1.538610	-0.946489	0.925889
		F	3.369493	-0.231922	-0.305552

[C ₂ mim][OTs] 2IP		C	-5.751345	-1.382145	-0.243480
		C	-5.195468	-0.858968	-1.419314
		C	-4.133901	0.041065	-1.374790
		C	-3.617209	0.430134	-0.138926
		C	-4.151669	-0.077224	1.042978
		C	-5.215859	-0.977465	0.983923
		H	-5.595800	-1.172662	-2.386341
		H	-3.695506	0.438115	-2.291699
		S	-2.244496	1.595073	-0.065570
		H	-3.726184	0.227197	2.000658
		H	-5.631494	-1.379878	1.910370
		C	-6.896568	-2.358026	-0.312065
		O	-1.463300	1.197477	1.153276
		O	-2.837664	2.959252	0.040295
		O	-1.483577	1.374861	-1.342026
		H	-6.666222	-3.184446	-1.000390
		H	-7.807113	-1.865746	-0.686272
		H	-7.117903	-2.781255	0.676490
		N	1.051831	2.922089	-1.436344
		C	1.014171	2.422080	-0.202660
		N	0.696165	3.403597	0.641306
		C	0.502578	4.563666	-0.076671
		C	0.723949	4.257869	-1.386136
		C	0.563804	3.237063	2.095465
		C	-0.683868	3.926755	2.618342
		C	1.233443	2.131839	-2.648460
		H	1.216745	1.388059	0.087683
		H	0.234413	5.501217	0.395278
		H	0.678616	4.871188	-2.278665
		H	0.248878	1.977927	-3.106212
		H	1.900591	2.672737	-3.328652

		H	1.662012	1.165980	-2.357693
		H	1.474888	3.633977	2.564439
		H	0.514213	2.155015	2.258748
		H	-0.814939	3.667722	3.677739
		H	-0.597295	5.020827	2.553009
		H	-1.559124	3.589756	2.047100
		C	6.825864	-0.954560	-0.049932
		C	6.181895	-2.161439	-0.354793
		C	4.793414	-2.261801	-0.329993
		C	4.035885	-1.139613	0.000455
		C	4.650108	0.067993	0.321190
		C	6.041106	0.153598	0.291422
		H	6.780398	-3.038508	-0.610446
		H	4.288825	-3.202172	-0.553276
		S	2.244432	-1.241312	-0.024491
		H	4.042661	0.929558	0.602094
		H	6.528168	1.097467	0.544612
		C	8.328007	-0.860699	-0.098036
		O	1.765531	-0.357481	1.092959
		O	1.899984	-2.681018	0.155647
		O	1.816610	-0.702721	-1.361271
		H	8.685599	-0.920347	-1.137218
		H	8.792039	-1.689815	0.454637
		H	8.683017	0.085632	0.329475
		N	-1.403457	-1.977118	-1.217893
		C	-0.940209	-1.407473	-0.107804
		N	-1.450856	-2.043205	0.943193
		C	-2.276705	-3.051224	0.496132
		C	-2.249311	-3.007325	-0.866895
		C	-1.114709	-1.733264	2.336218
		C	-0.134028	-2.748978	2.899310

		C	-1.057663	-1.541104	-2.568362
		H	-0.291906	-0.541104	-0.055799
		H	-2.814612	-3.702038	1.176545
		H	-2.757764	-3.609753	-1.610886
		H	0.019187	-1.685805	-2.713972
		H	-1.637930	-2.137145	-3.279427
		H	-1.302796	-0.475030	-2.650017
		H	-2.058131	-1.709647	2.898914
		H	-0.691511	-0.723084	2.316090
		H	0.129262	-2.469084	3.928585
		H	-0.575497	-3.756376	2.920594
		H	0.772500	-2.763670	2.279304
[C ₂ mim][TFA 2IP		C	3.688899	-0.547663	-0.022766
		F	3.696144	-0.038757	-1.269018
		F	4.808332	-1.294247	0.100758
		F	3.819068	0.492128	0.822350
		C	2.421193	-1.411508	0.266311
		O	2.047275	-1.417181	1.453183
		O	1.947385	-1.990249	-0.729168
		N	-1.547679	-2.104808	1.743209
		C	-0.915243	-2.595093	0.679056
		N	-1.826097	-3.103218	-0.153492
		C	-3.074949	-2.904616	0.380670
		C	-2.899929	-2.272588	1.577100
		C	-1.525382	-3.723160	-1.450820
		C	-0.966686	-2.704117	-2.430265
		C	-0.907377	-1.486568	2.900676
		H	0.160251	-2.574937	0.514445
		H	-3.973579	-3.224928	-0.128685
		H	-3.613638	-1.933003	2.314879
		H	-1.127601	-2.084517	3.788851

		H	0.169436	-1.464895	2.713578
		H	-1.306151	-0.474540	3.003104
		H	-2.464089	-4.156352	-1.805958
		H	-0.815881	-4.537070	-1.272392
		H	-0.776909	-3.194085	-3.391407
		H	-1.679276	-1.885292	-2.569929
		H	-0.023096	-2.298876	-2.047304
		C	-2.680588	2.215907	-0.594256
		F	-1.579560	2.870382	-1.046849
		F	-3.267891	3.026822	0.301765
		F	-3.521819	2.111375	-1.638394
		C	-2.247634	0.840360	-0.003553
		O	-2.111764	-0.063805	-0.847995
		O	-2.000658	0.853633	1.215137
		N	0.979701	1.217870	-1.486994
		C	0.669986	0.875176	-0.237574
		N	1.147863	1.803934	0.586996
		C	1.785032	2.772139	-0.154002
		C	1.681035	2.399798	-1.462333
		C	0.992938	1.794106	2.045804
		C	0.162365	2.977411	2.515245
		C	0.653055	0.423902	-2.668102
		H	0.100775	0.001285	0.052417
		H	2.261874	3.627543	0.303952
		H	2.046072	2.867536	-2.366136
		H	1.349307	-0.417399	-2.732096
		H	-0.374596	0.067106	-2.560664
		H	0.742554	1.067978	-3.544300
		H	1.999025	1.795880	2.476756
		H	0.510187	0.844897	2.286875
		H	0.047148	2.921038	3.602907

		H	0.652757	3.926744	2.272414
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[C ₂ mim][OAc] 2IP		N	-1.680313	-0.287152	1.602066
		C	-1.323196	0.735865	0.828669
		N	-2.411638	1.182606	0.199875
		C	-3.487606	0.406316	0.558896
		C	-3.025861	-0.520160	1.446982
		C	-2.406052	2.274588	-0.778437
		C	-3.509581	3.283388	-0.507558
		C	-0.767622	-1.044406	2.453123
		H	-0.321017	1.166492	0.749840
		H	-4.478682	0.559849	0.155702
		H	-3.535659	-1.315624	1.973290
		H	-0.755277	-2.078866	2.100834
		H	0.221399	-0.590580	2.347598
		H	-1.113905	-0.984346	3.488375
		H	-2.507748	1.825508	-1.772659
		H	-1.418461	2.737517	-0.697000
		H	-3.434375	4.092739	-1.241099
		H	-4.501889	2.830048	-0.605611
		H	-3.405970	3.707805	0.497028
		C	3.363100	2.603841	1.191484
		C	1.981627	1.966521	1.044751
		O	1.104126	2.625259	0.415827
		O	1.793681	0.842992	1.582035
		H	3.612072	3.200088	0.307455
		H	4.128856	1.841646	1.364060
		H	3.341581	3.277911	2.058459
		N	1.605737	0.325140	-1.636888
		C	1.508775	-0.812612	-0.948562
		N	2.741271	-1.180020	-0.585523

		C	3.639540	-0.240267	-1.030093
		C	2.922792	0.711647	-1.692292
		C	3.087330	-2.397935	0.159996
		C	2.150516	-2.615212	1.335313
		C	0.486929	1.067869	-2.210485
		H	0.581476	-1.356983	-0.736463
		H	4.700557	-0.326358	-0.840494
		H	3.232477	1.620849	-2.189265
		H	-0.420261	0.484562	-2.025635
		H	0.449379	2.042882	-1.717447
		H	0.652694	1.180592	-3.285483
		H	4.120142	-2.262661	0.492848
		H	3.058927	-3.242027	-0.537291
		H	2.473737	-3.503887	1.887831
		H	2.179971	-1.743399	1.997321
		H	1.123162	-2.771598	0.986071
		C	-3.141211	-2.935217	-0.944958
		C	-1.804410	-2.194020	-0.925024
		O	-0.877678	-2.692350	-0.224330
		O	-1.699971	-1.153463	-1.625617
		H	-3.339173	-3.402754	0.025330
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[C ₂ mim]Cl 8IP	Gas phase	N	3.116742	0.162156	-0.948480
		C	3.116338	0.432550	0.356211
		N	2.172110	-0.309637	0.937288
		C	1.537096	-1.061464	-0.026363
		C	2.135414	-0.769155	-1.216067
		C	1.773491	-0.238052	2.342751
		C	2.793063	0.513925	3.176373
		C	4.022193	0.764950	-1.918309

		H	3.801528	1.138981	0.831687
		H	0.728404	-1.757314	0.178276
		H	1.943692	-1.184359	-2.200450
		H	4.793279	1.308465	-1.355322
		H	4.495392	-0.041186	-2.491511
		H	3.457545	1.454060	-2.561178
		H	1.641546	-1.275930	2.682717
		H	0.808795	0.288342	2.370652
		H	2.493851	0.473691	4.232603
		H	3.802163	0.085654	3.076943
		H	2.820141	1.566996	2.859555
		Cl	5.911063	2.225659	0.995612
		N	8.552391	-1.316930	0.329255
		C	7.968920	-0.163331	0.003845
		N	8.632053	0.369068	-1.019425
		C	9.633192	-0.498074	-1.402914
		C	9.578736	-1.561705	-0.556434
		C	8.209417	1.582724	-1.727382
		C	7.558968	1.217154	-3.053617
		C	7.979185	-2.286242	1.248538
		H	7.111830	0.315488	0.490646
		H	10.295559	-0.282209	-2.233107
		H	10.175829	-2.464587	-0.508446
		H	7.340068	-2.963667	0.665447
		H	8.786321	-2.824852	1.758455
		H	7.373593	-1.747327	1.985929
		H	9.097294	2.217861	-1.857360
		H	7.508554	2.094053	-1.050885
		H	7.108028	2.112894	-3.503383
		H	8.293727	0.808891	-3.763263
		H	6.789300	0.449691	-2.884424

		Cl	6.042928	-1.914029	-1.549533
		N	-3.144880	-5.088000	-0.655840
		C	-2.375269	-4.315807	0.108217
		N	-3.106963	-3.848216	1.114905
		C	-4.387816	-4.343445	1.003245
		C	-4.411534	-5.134170	-0.106182
		C	-2.557800	-3.147269	2.277740
		C	-1.347750	-2.319135	1.891051
		C	-2.616077	-5.863438	-1.768281
		H	-1.340634	-4.082149	-0.123777
		H	-5.164700	-4.044278	1.696972
		H	-5.211507	-5.708456	-0.558909
		H	-1.784212	-5.294559	-2.207852
		H	-2.242786	-6.822063	-1.384062
		H	-3.409224	-6.017413	-2.509599
		H	-2.281093	-3.927229	3.003687
		H	-3.358979	-2.501232	2.655005
		H	-1.026053	-1.730326	2.762297
		H	-0.516802	-2.972788	1.576366
		H	-1.611202	-1.624092	1.078649
		Cl	-0.034376	-3.238009	-1.926398
		N	2.336109	-3.925800	2.045588
		C	2.098061	-4.357020	0.798494
		N	3.067150	-3.887706	0.010372
		C	3.944435	-3.131205	0.756394
		C	3.483995	-3.159356	2.039085
		C	3.229464	-4.157160	-1.427268
		C	4.296543	-5.213617	-1.660129
		C	1.542967	-4.241451	3.231455
		H	1.244584	-4.992209	0.525713
		H	4.778677	-2.620689	0.265009

		H	3.861992	-2.698485	2.945505
		H	2.190419	-4.733192	3.968608
		H	1.140933	-3.310655	3.655624
		H	0.722930	-4.913140	2.927604
		H	3.540571	-3.206250	-1.881019
		H	2.237820	-4.429591	-1.809200
		H	4.375462	-5.409719	-2.738133
		H	5.273708	-4.845952	-1.315269
		H	4.044336	-6.155135	-1.150349
		Cl	-0.630571	-6.138585	1.492112
		N	-1.612354	3.580927	-2.289571
		C	-2.538842	4.266937	-1.618811
		N	-3.737381	3.926793	-2.100700
		C	-3.574956	2.997772	-3.109884
		C	-2.232281	2.783574	-3.228493
		C	-5.029110	4.420482	-1.594108
		C	-4.851113	5.571648	-0.622719
		C	-0.181025	3.669475	-2.013354
		H	-2.301283	4.978055	-0.798470
		H	-4.438172	2.538735	-3.587636
		H	-1.670206	2.121293	-3.877640
		H	-0.054917	4.227857	-1.075758
		H	0.219188	2.659030	-1.860027
		H	0.324657	4.170495	-2.849473
		H	-5.550807	3.560001	-1.150469
		H	-5.620323	4.713702	-2.471815
		H	-5.843398	5.906883	-0.293643
		H	-4.264835	5.291640	0.264979
		H	-4.333153	6.421950	-1.089028
		Cl	-1.484156	6.118511	0.753645
		N	1.622785	5.115069	2.838130

		C	1.646346	5.501058	1.566349
		N	2.861764	5.259005	1.074780
		C	3.629495	4.645157	2.044429
		C	2.844403	4.559771	3.154053
		C	3.238164	5.446329	-0.326485
		C	3.436533	4.108840	-1.024753
		C	0.398856	5.009242	3.621439
		H	0.771935	5.903194	1.038005
		H	4.633242	4.269863	1.845590
		H	3.045926	4.138587	4.132183
		H	0.105191	3.951041	3.633235
		H	0.577891	5.389470	4.634567
		H	-0.382869	5.586504	3.110325
		H	4.152671	6.055272	-0.352056
		H	2.428510	6.031210	-0.783839
		H	3.643517	4.280942	-2.091738
		H	4.285683	3.567125	-0.578455
		H	2.532716	3.491819	-0.902806
		Cl	0.841172	2.614654	1.085033
		N	-7.764940	-1.511869	-0.141402
		C	-7.484332	-0.271164	0.248302
		N	-7.772129	-0.157552	1.543212
		C	-8.194453	-1.382717	2.010389
		C	-8.193872	-2.236463	0.950342
		C	-7.374110	0.973853	2.387338
		C	-6.904569	2.153375	1.557167
		C	-7.456886	-2.026585	-1.469204
		H	-7.105727	0.500520	-0.432994
		H	-8.451238	-1.541180	3.051254
		H	-8.467884	-3.282551	0.877299
		H	-7.278238	-1.164712	-2.127726

		H	-6.550709	-2.644767	-1.405772
		H	-8.303841	-2.618416	-1.837209
		H	-6.544551	0.604657	3.007364
		H	-8.234622	1.234131	3.019457
		H	-6.668561	2.989537	2.228415
		H	-5.991680	1.872968	1.011750
		H	-7.667977	2.484237	0.837756
		Cl	-6.533297	1.424964	-2.386628
		N	-2.557326	1.347667	-0.212520
		C	-3.527315	0.813786	-0.952111
		N	-2.994733	-0.113428	-1.744035
		C	-1.641415	-0.209355	-1.481640
		C	-1.365675	0.714563	-0.515519
		C	-3.757577	-0.956591	-2.664068
		C	-3.746820	-2.396834	-2.178468
		C	-2.767788	2.287022	0.884181
		H	-4.579878	1.091734	-0.964874
		H	-1.011682	-0.966805	-1.952257
		H	-0.442767	1.013352	-0.016411
		H	-2.985948	1.709655	1.793587
		H	-1.868402	2.907693	1.008605
		H	-3.632736	2.917497	0.639326
		H	-3.298698	-0.864298	-3.659638
		H	-4.767139	-0.523544	-2.708397
		H	-4.379048	-3.017508	-2.832435
		H	-2.720510	-2.797428	-2.198639
		H	-4.130881	-2.430711	-1.145020
		Cl	-4.728248	-0.836335	1.263464
[C ₂ mim]Cl 8IP	CHCl ₃	N	2.994814	0.089285	-1.000951
		C	3.065066	0.351604	0.305069
		N	2.132580	-0.368737	0.930270

		C	1.437917	-1.105209	-0.003901
		C	1.982411	-0.819346	-1.221864
		C	1.832509	-0.331315	2.365363
		C	2.930020	0.354801	3.153670
		C	3.872965	0.669064	-2.013073
		H	3.792790	1.033588	0.750544
		H	0.629155	-1.786563	0.244649
		H	1.734390	-1.214519	-2.201560
		H	4.632577	1.262097	-1.488143
		H	4.368787	-0.145183	-2.554609
		H	3.281279	1.305074	-2.682993
		H	1.692711	-1.374674	2.680656
		H	0.887160	0.217159	2.476831
		H	2.694360	0.285650	4.223550
		H	3.910569	-0.112875	2.979211
		H	2.981133	1.417755	2.878470
		Cl	5.937533	2.093221	0.881280
		N	8.579189	-1.599707	0.360875
		C	8.119765	-0.381321	0.081814
		N	8.898217	0.160914	-0.851979
		C	9.862922	-0.754047	-1.214465
		C	9.659980	-1.864110	-0.451098
		C	8.650520	1.464241	-1.481222
		C	7.908219	1.292434	-2.797051
		C	7.899290	-2.564965	1.212439
		H	7.259350	0.122709	0.528155
		H	10.612400	-0.533874	-1.966288
		H	10.192600	-2.807145	-0.408098
		H	7.279408	-3.208470	0.574835
		H	8.644812	-3.150319	1.761280
		H	7.264493	-2.019638	1.919241

		H	9.625210	1.950867	-1.614409
		H	8.054131	2.041665	-0.762726
		H	7.666697	2.280266	-3.212783
		H	8.520135	0.746109	-3.529637
		H	6.982270	0.723110	-2.630341
		Cl	6.130462	-1.960807	-1.783621
		N	-3.559198	-5.029784	-0.675414
		C	-2.674616	-4.397245	0.094078
		N	-3.301045	-3.947780	1.177863
		C	-4.632405	-4.298306	1.101896
		C	-4.796901	-4.985975	-0.063649
		C	-2.648625	-3.307628	2.326605
		C	-1.393733	-2.567060	1.907996
		C	-3.217305	-5.674488	-1.936823
		H	-1.627019	-4.258042	-0.163710
		H	-5.340039	-4.004749	1.868659
		H	-5.675730	-5.435606	-0.511835
		H	-2.262903	-5.252884	-2.278537
		H	-3.118734	-6.756428	-1.784607
		H	-4.003895	-5.469244	-2.671770
		H	-2.411234	-4.105303	3.044994
		H	-3.386381	-2.611201	2.741426
		H	-0.984408	-2.044696	2.784331
		H	-0.635641	-3.271182	1.528845
		H	-1.632930	-1.819081	1.136601
		Cl	-0.216626	-3.318620	-1.889101
		N	2.521303	-3.966034	2.000008
		C	2.212036	-4.344495	0.754308
		N	3.133487	-3.845732	-0.070968
		C	4.054595	-3.123225	0.655424
		C	3.669070	-3.201678	1.961915

		C	3.209484	-4.068942	-1.521968
		C	4.176252	-5.194629	-1.848535
		C	1.784795	-4.335317	3.207303
		H	1.345820	-4.962871	0.498677
		H	4.875097	-2.614120	0.144837
		H	4.105261	-2.785606	2.864014
		H	2.457003	-4.882004	3.879405
		H	1.425427	-3.426644	3.707303
		H	0.939787	-4.970641	2.908603
		H	3.568772	-3.125551	-1.954593
		H	2.184039	-4.257822	-1.863857
		H	4.198698	-5.344433	-2.936608
		H	5.191389	-4.929568	-1.519882
		H	3.865926	-6.136118	-1.372799
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		C	-2.438412	4.311775	-1.634172
		N	-3.634805	4.038161	-2.160593
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		C	-4.913674	4.666046	-1.783727
		C	-4.730012	5.746223	-0.736974
		C	-0.104086	3.540948	-1.925662
		H	-2.205598	5.043288	-0.844314
		H	-4.355368	2.645805	-3.633861
		H	-1.621711	2.021301	-3.766537
		H	0.038765	3.993902	-0.936315
		H	0.249669	2.503194	-1.885468
		H	0.434941	4.098172	-2.702414
		H	-5.574337	3.854684	-1.446510
		H	-5.343853	5.077028	-2.706848

		H	-5.712995	6.176220	-0.506424
		H	-4.297522	5.353069	0.194042
		H	-4.071792	6.551240	-1.092731
		Cl	-1.406710	6.352269	0.773741
		N	1.936390	5.444415	2.708803
		C	1.826788	5.663205	1.401568
		N	2.970664	5.313407	0.816530
		C	3.830413	4.813721	1.772701
		C	3.175494	4.900033	2.965119
		C	3.200793	5.316105	-0.629758
		C	3.353321	3.896746	-1.152745
		C	0.824712	5.540174	3.645992
		H	0.919611	6.035539	0.915179
		H	4.804232	4.399473	1.520151
		H	3.480620	4.615747	3.965718
		H	0.507288	4.521773	3.903695
		H	1.143566	6.088615	4.539428
		H	0.001545	6.059490	3.140874
		H	4.096375	5.919514	-0.829862
		H	2.339995	5.828850	-1.078046
		H	3.451147	3.917499	-2.247631
		H	4.251287	3.425516	-0.723677
		H	2.477979	3.294611	-0.861574
		Cl	0.820048	2.680138	1.388541
		N	-7.815157	-1.568229	-0.210954
		C	-7.605507	-0.329359	0.231767
		N	-7.899470	-0.287452	1.528626
		C	-8.273890	-1.547548	1.938621
		C	-8.224909	-2.356058	0.843296
		C	-7.640608	0.846684	2.424470
		C	-7.225767	2.087278	1.659209

		C	-7.577318	-2.004520	-1.581864
		H	-7.254967	0.489118	-0.402708
		H	-8.538172	-1.759100	2.968530
		H	-8.452187	-3.408983	0.720941
		H	-7.294480	-1.121681	-2.169457
		H	-6.764800	-2.741549	-1.587134
		H	-8.492596	-2.450302	-1.988088
		H	-6.828404	0.524540	3.089752
		H	-8.554315	1.015361	3.009626
		H	-7.079602	2.907976	2.372864
		H	-6.275263	1.904983	1.137321
		H	-7.989067	2.393579	0.929308
		Cl	-6.589578	1.580313	-2.352301
		N	-2.610496	1.453030	-0.056440
		C	-3.575115	0.950180	-0.825553
		N	-3.051630	-0.004158	-1.590225
		C	-1.713296	-0.146894	-1.282437
		C	-1.434505	0.774024	-0.313040
		C	-3.808297	-0.812753	-2.547344
		C	-3.872753	-2.256372	-2.078280
		C	-2.818906	2.399344	1.034357
		H	-4.617289	1.265179	-0.868939
		H	-1.096262	-0.916403	-1.747521
		H	-0.516644	1.045991	0.210058
		H	-3.119215	1.833592	1.926766
		H	-1.882012	2.944515	1.209609
		H	-3.622759	3.091605	0.755270
		H	-3.309728	-0.726960	-3.523437
		H	-4.799977	-0.346044	-2.623195
		H	-4.506412	-2.840471	-2.762468
		H	-2.863975	-2.699420	-2.070100

		H	-4.293246	-2.294961	-1.059022
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[C ₂ mim]Cl 8IP	EtOH	N	2.850415	0.053523	-1.155867
		C	3.035682	0.247968	0.150824
		N	2.109984	-0.445185	0.816022
		C	1.303703	-1.095454	-0.092651
		C	1.770973	-0.783198	-1.335836
		C	1.916325	-0.451467	2.270711
		C	3.090621	0.171263	2.997449
		C	3.690618	0.614798	-2.209599
		H	3.835190	0.865312	0.568205
		H	0.476946	-1.739150	0.193118
		H	1.431791	-1.119531	-2.309878
		H	4.476531	1.207395	-1.726127
		H	4.158475	-0.206570	-2.764118
		H	3.076006	1.245920	-2.862390
		H	1.769837	-1.500039	2.563589
		H	0.998709	0.118345	2.468887
		H	2.926530	0.078819	4.078663
		H	4.036043	-0.332042	2.744306
		H	3.166508	1.239169	2.747656
		Cl	5.971937	1.941202	0.660872
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		C	8.281719	-0.514163	0.186214
		N	9.131123	0.007808	-0.696690
		C	10.068708	-0.946562	-1.031015
		C	9.773904	-2.060471	-0.303721
		C	8.987382	1.336634	-1.304503
		C	8.324456	1.235859	-2.668909
		C	7.907184	-2.702217	1.269749
		H	7.416633	0.015371	0.590274

		H	10.867661	-0.746342	-1.736237
		H	10.261069	-3.027417	-0.249974
		H	7.277780	-3.307454	0.605133
		H	8.603699	-3.330916	1.834222
		H	7.275650	-2.135873	1.962461
		H	9.990563	1.777390	-1.363729
		H	8.373139	1.926217	-0.612054
		H	8.187404	2.243031	-3.084971
		H	8.943037	0.653216	-3.366847
		H	7.346034	0.743193	-2.573764
		Cl	6.085718	-1.847497	-1.648402
		N	-3.839224	-4.904270	-0.745175
		C	-2.881881	-4.364404	0.008701
		N	-3.414139	-3.999791	1.172162
		C	-4.758012	-4.308591	1.163314
		C	-5.027576	-4.883130	-0.043386
		C	-2.669624	-3.459498	2.316665
		C	-1.412840	-2.738591	1.871090
		C	-3.611388	-5.452285	-2.077191
		H	-1.850726	-4.230955	-0.312660
		H	-5.400133	-4.079557	2.006126
		H	-5.950009	-5.271841	-0.460460
		H	-2.669352	-5.033662	-2.453952
		H	-3.542437	-6.545366	-2.018464
		H	-4.442026	-5.165333	-2.731497
		H	-2.429481	-4.306098	2.975153
		H	-3.352821	-2.763316	2.816277
		H	-0.939517	-2.280890	2.751056
		H	-0.699311	-3.439238	1.408475
		H	-1.672068	-1.939456	1.160205
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		N	3.026406	-3.787123	-0.105482
		C	3.970061	-3.186848	0.699427
		C	3.586434	-3.415124	1.989407
		C	3.088560	-3.851234	-1.573064
		C	3.899828	-5.051878	-2.031035
		C	1.656722	-4.620555	3.093765
		H	1.215474	-4.923291	0.334125
		H	4.810335	-2.650241	0.254768
		H	4.038415	-3.125726	2.932604
		H	2.311408	-5.236875	3.720325
		H	1.297933	-3.759546	3.671292
		H	0.813341	-5.215469	2.719446
		H	3.572215	-2.918996	-1.893809
		H	2.050049	-3.871386	-1.930653
		H	3.926392	-5.072218	-3.129026
		H	4.933001	-4.979205	-1.662640
		H	3.453745	-5.992173	-1.676371
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		C	-2.384833	4.361498	-1.606506
		N	-3.604623	4.189686	-2.123700
		C	-3.545358	3.219410	-3.101022
		C	-2.246838	2.806012	-3.168783
		C	-4.833366	4.898791	-1.724628
		C	-4.559182	5.987022	-0.707803
		C	-0.114104	3.427645	-1.955302
		H	-2.095760	5.057350	-0.805741
		H	-4.440894	2.887382	-3.617354
		H	-1.766915	2.060400	-3.793790

		H	0.071445	3.694411	-0.905697
		H	0.194435	2.386346	-2.111189
		H	0.436194	4.088989	-2.636608
		H	-5.529166	4.134955	-1.349713
		H	-5.263067	5.315682	-2.645000
		H	-5.507707	6.483028	-0.466426
		H	-4.130028	5.587634	0.221823
		H	-3.862131	6.740165	-1.101111
		Cl	-1.301216	6.322572	0.931985
		N	2.178439	5.422051	2.690208
		C	1.982195	5.628198	1.390792
		N	3.077405	5.255473	0.732367
		C	3.994558	4.757478	1.633976
		C	3.425690	4.865625	2.868373
		C	3.214713	5.254466	-0.726729
		C	3.351125	3.836553	-1.256661
		C	1.147198	5.576056	3.707920
		H	1.050798	6.007683	0.961880
		H	4.945094	4.333147	1.319725
		H	3.797712	4.594435	3.849902
		H	0.828828	4.578342	4.034705
		H	1.547102	6.148434	4.552227
		H	0.298845	6.098930	3.250946
		H	4.087958	5.867913	-0.984402
		H	2.320849	5.754767	-1.120384
		H	3.393820	3.859270	-2.354776
		H	4.272316	3.370280	-0.874820
		H	2.495436	3.226942	-0.926038
		Cl	0.919856	2.641103	1.417565
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		C	-7.554418	-0.326402	0.303809

		N	-7.754242	-0.375772	1.618444
		C	-8.065108	-1.669238	1.971946
		C	-8.072559	-2.407084	0.826212
		C	-7.525244	0.722141	2.566960
		C	-7.165904	2.012094	1.858820
		C	-7.678112	-1.878127	-1.619061
		H	-7.278427	0.543903	-0.297842
		H	-8.254241	-1.950003	3.001966
		H	-8.285435	-3.455909	0.652471
		H	-7.369259	-0.974564	-2.159615
		H	-6.943689	-2.678830	-1.761532
		H	-8.662333	-2.207528	-1.971672
		H	-6.695840	0.396717	3.207918
		H	-8.439180	0.827226	3.166188
		H	-7.029196	2.799554	2.610579
		H	-6.222488	1.888061	1.307698
		H	-7.954863	2.331842	1.162962
		Cl	-6.686801	1.853821	-2.153168
		N	-2.645945	1.594710	0.040453
		C	-3.639173	1.142344	-0.723854
		N	-3.168787	0.161323	-1.489643
		C	-1.838734	-0.048454	-1.188678
		C	-1.509255	0.856863	-0.219776
		C	-3.960881	-0.594589	-2.462011
		C	-4.078289	-2.047948	-2.036416
		C	-2.793420	2.555200	1.127540
		H	-4.663254	1.516437	-0.767222
		H	-1.260731	-0.839106	-1.668182
		H	-0.574693	1.084045	0.294731
		H	-3.070681	2.003177	2.035954
		H	-1.840092	3.082856	1.261960

		H	-3.591706	3.262667	0.871853
		H	-3.463552	-0.503154	-3.437969
		H	-4.934842	-0.089810	-2.521436
		H	-4.704652	-2.590788	-2.759330
		H	-3.082653	-2.519388	-2.016542
		H	-4.529801	-2.116003	-1.032309
		Cl	-4.506890	-0.613930	1.750508
[C ₂ mim][OAc]	Gas phase	N	2.399270	5.867380	-1.323020
		C	3.632338	6.172804	-0.903117
		N	3.545873	7.253695	-0.113181
		C	2.212918	7.627730	-0.012988
		C	1.489248	6.752901	-0.772603
		C	4.693007	7.930217	0.511704
		C	4.931429	9.321383	-0.069771
		C	2.058132	4.698717	-2.138652
		H	4.561445	5.636486	-1.175795
		H	1.898030	8.478295	0.581464
		H	0.424092	6.656106	-0.993970
		H	2.777320	4.619536	-2.965105
		H	2.107954	3.793241	-1.509251
		H	1.044307	4.852933	-2.528716
		H	5.572227	7.287223	0.337646
		H	4.493358	7.982439	1.594116
		H	5.803550	9.776147	0.425523
		H	5.149099	9.261110	-1.147656
		H	4.069032	9.992936	0.074500
		C	2.024453	2.553335	2.420629
		C	2.567193	2.903427	1.017840
		O	3.414617	3.828261	0.957645
		O	2.130564	2.212704	0.040207
		H	1.905593	3.465135	3.025861

		H	2.761506	1.915434	2.940580
		H	1.065630	2.014285	2.368248
		N	6.362370	3.122274	1.664098
		C	6.075279	2.848713	0.387525
		N	6.158271	1.521550	0.217250
		C	6.498984	0.920809	1.421153
		C	6.618612	1.934454	2.330013
		C	5.933463	0.797800	-1.046951
		C	4.988275	1.539504	-1.985032
		C	6.236092	4.459732	2.246289
		H	5.859000	3.599104	-0.386065
		H	6.618629	-0.167681	1.494173
		H	6.862383	1.912236	3.386683
		H	6.640379	5.185855	1.523475
		H	5.165604	4.650653	2.411681
		H	6.802741	4.489616	3.186354
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		C	-5.875879	4.403545	-4.933277
		C	-5.419087	4.319214	-3.474810
		O	-6.255190	4.563315	-2.576802
		O	-4.201223	4.014919	-3.285720
		H	-6.963319	4.526705	-5.001719
		H	-5.561582	3.504266	-5.481335
		H	-5.385030	5.263318	-5.414838
		N	-5.865862	2.661939	0.056497
		C	-5.124288	2.253206	-0.973757
		N	-5.219360	0.923388	-1.051768
		C	-6.049637	0.465019	-0.046291
		C	-6.454446	1.566926	0.648137
		C	-4.588137	0.074054	-2.074349

		C	-3.439298	0.782272	-2.769032
		C	-5.957741	4.053065	0.490504
		H	-4.562445	2.912923	-1.644339
		H	-6.263083	-0.598712	0.083901
		H	-7.101178	1.663959	1.513190
		H	-4.932850	4.404549	0.673861
		H	-6.428591	4.629108	-0.313883
		H	-6.551628	4.084531	1.409923
		H	-5.372944	-0.212985	-2.790046
		H	-4.260737	-0.844832	-1.567504
		H	-2.970900	0.079803	-3.471962
		H	-3.781727	1.666474	-3.326128
		H	-2.694464	1.109243	-2.026646
		C	-3.250131	1.818968	1.842745
		C	-2.561289	2.416074	0.615228
		O	-1.782028	1.643293	-0.019596
		O	-2.795885	3.614284	0.334254
		H	-2.501057	1.677256	2.637598
		H	-3.656251	0.826600	1.595061
		H	-4.049750	2.472087	2.218043
[C ₂ mim][OAc]	EtOH	N	5.206564	-1.655363	-1.274056
		C	5.987694	-2.603568	-1.787642
		N	7.183771	-2.533490	-1.204233
		C	7.170748	-1.493213	-0.296536
		C	5.922837	-0.943734	-0.338773
		C	8.299474	-3.436492	-1.503142
		C	9.135110	-2.926344	-2.665619
		C	3.821945	-1.430959	-1.686344
		H	5.652120	-3.332096	-2.520234
		H	8.039472	-1.243758	0.302206
		H	5.465049	-0.150203	0.236974

		H	3.522800	-2.301956	-2.282660
		H	3.201938	-1.336558	-0.780069
		H	3.799324	-0.514678	-2.289232
		H	7.845234	-4.415679	-1.706535
		H	8.895315	-3.515209	-0.585228
		H	9.964066	-3.621238	-2.855123
		H	8.526839	-2.854063	-3.578461
		H	9.554146	-1.935000	-2.441359
		C	1.998780	-1.133282	3.156788
		C	2.454331	-1.163158	1.690377
		O	3.682359	-0.990006	1.472428
		O	1.564618	-1.331404	0.810715
		H	2.840461	-1.327685	3.833825
		H	1.200131	-1.867325	3.331392
		H	1.596259	-0.131862	3.381927
		N	3.714155	-4.131719	1.276120
		C	3.070013	-4.196392	0.110802
		N	1.769858	-4.357552	0.368725
		C	1.572451	-4.380870	1.728013
		C	2.802483	-4.240252	2.301761
		C	0.690143	-4.447817	-0.619995
		C	0.989787	-3.599286	-1.842662
		C	5.138439	-3.849648	1.415503
		H	3.536713	-4.174889	-0.882883
		H	0.559544	-4.473753	2.120405
		H	3.104714	-4.191162	3.341925
		H	5.632949	-4.195723	0.497261
		H	5.252610	-2.767624	1.564712
		H	5.521874	-4.404817	2.279333
		H	-0.216002	-4.122144	-0.088091
		H	0.564292	-5.507730	-0.888818

		H	0.112422	-3.587427	-2.503688
		H	1.216542	-2.571134	-1.523741
		H	1.848999	-4.002447	-2.400029
		C	5.007430	-6.845125	-3.198410
		C	4.905666	-5.579340	-2.347277
		O	4.067983	-4.701512	-2.715271
		O	5.679506	-5.469341	-1.364538
		H	4.059771	-7.051066	-3.710941
		H	5.308077	-7.702729	-2.583589
		H	5.783271	-6.690724	-3.964439
		N	-2.000027	-1.581102	0.953233
		C	-3.223998	-1.985713	1.286273
		N	-3.379965	-1.800412	2.597817
		C	-2.213195	-1.287365	3.118831
		C	-1.342017	-1.146328	2.075082
		C	-4.619161	-2.090740	3.323970
		C	-5.244741	-0.821337	3.878357
		C	-1.451158	-1.564144	-0.396355
		H	-3.959207	-2.433758	0.610640
		H	-2.099665	-1.070645	4.175483
		H	-0.312577	-0.806777	1.999626
		H	-0.370672	-1.734811	-0.308172
		H	-1.951397	-2.348698	-0.979056
		H	-1.634172	-0.568738	-0.822116
		H	-4.371860	-2.823262	4.102102
		H	-5.278265	-2.574006	2.590027
		H	-6.166189	-1.075216	4.419727
		H	-4.566770	-0.313537	4.579985
		H	-5.493658	-0.123371	3.065919
		C	-6.574615	-3.632933	-2.027892
		C	-5.549534	-3.317764	-0.938223

		O	-6.004187	-2.949220	0.184296
		O	-4.328602	-3.393258	-1.230625
		H	-7.426737	-4.184762	-1.609021
		H	-6.123151	-4.195930	-2.853946
		H	-6.963239	-2.679440	-2.421458
		N	-5.382753	-5.856273	0.910803
		C	-4.074771	-5.704680	0.713445
		N	-3.752508	-6.290735	-0.438531
		C	-4.892209	-6.802774	-1.016180
		C	-5.921495	-6.528924	-0.163478
		C	-2.388429	-6.328766	-0.974143
		C	-2.297376	-5.655038	-2.333302
		C	-6.107338	-5.336248	2.066129
		H	-3.374886	-5.196744	1.385441
		H	-4.878754	-7.331635	-1.962318
		H	-6.978382	-6.762753	-0.223940
		H	-5.354118	-5.036888	2.806081
		H	-6.694214	-4.470042	1.739193
		H	-6.748533	-6.128366	2.469672
		H	-2.077038	-7.381348	-1.023175
		H	-1.772590	-5.821996	-0.218434
		H	-1.250553	-5.652927	-2.668291
		H	-2.882569	-6.205085	-3.084940
		H	-2.683468	-4.629080	-2.268857
		C	-0.947978	-4.285001	4.279546
		C	-1.967611	-4.516795	3.159378
		O	-1.523547	-4.496520	1.972006
		O	-3.158586	-4.735405	3.484567
		H	-0.308608	-3.425142	4.034313
		H	-0.297136	-5.170549	4.359448
		H	-1.443083	-4.122129	5.244410

		N	4.669236	4.843733	0.218518
		C	3.990107	5.392862	1.229835
		N	4.857412	5.664356	2.208648
		C	6.120242	5.281811	1.808968
		C	6.003720	4.760607	0.553717
		C	4.489981	6.260073	3.503700
		C	3.692279	7.536929	3.308481
		C	4.086130	4.446903	-1.060670
		H	2.908888	5.616450	1.258505
		H	6.983230	5.397169	2.455074
		H	6.713627	4.274634	-0.107839
		H	4.516667	3.482144	-1.361077
		H	3.000089	4.363579	-0.931079
		H	4.306519	5.212702	-1.815076
		H	5.432368	6.438407	4.035004
		H	3.886092	5.519987	4.041089
		H	3.442388	7.958158	4.291908
		H	4.272442	8.282051	2.745395
		H	2.756162	7.313394	2.775837
		C	-0.535117	4.697570	2.646299
		C	0.893735	5.218313	2.486614
		O	1.761569	4.867812	3.316514
		O	1.105024	5.993033	1.498076
		H	-1.189410	5.536613	2.932900
		H	-0.591723	3.925273	3.424438
		H	-0.928195	4.305396	1.694800
		N	3.277478	2.011692	1.146665
		C	3.049212	1.543881	-0.081684
		N	1.729522	1.489047	-0.264607
		C	1.093920	1.910780	0.883147
		C	2.072944	2.243318	1.774399

		C	1.061077	0.936110	-1.447632
		C	1.618819	1.522623	-2.734236
		C	4.591154	2.034520	1.775748
		H	3.819640	1.324900	-0.836125
		H	0.005856	1.924972	0.928020
		H	2.015802	2.685722	2.764417
		H	5.346182	2.121408	0.980643
		H	4.646632	2.893765	2.456440
		H	4.713334	1.089597	2.322601
		H	-0.006911	1.160421	-1.315355
		H	1.193199	-0.154841	-1.394136
		H	1.137173	1.033015	-3.591589
		H	1.410977	2.600806	-2.793576
		H	2.707300	1.378180	-2.812752
		C	7.304941	0.987503	-2.796025
		C	6.177355	1.583975	-1.953270
		O	5.000080	1.359740	-2.356676
		O	6.478228	2.241897	-0.926872
		H	8.287152	1.172687	-2.344927
		H	7.272662	1.418167	-3.807997
		H	7.141495	-0.096666	-2.902075
		N	-1.393484	5.492722	-0.997468
		C	-2.564876	5.392416	-1.620299
		N	-3.330007	6.416375	-1.242818
		C	-2.631059	7.185047	-0.334435
		C	-1.410611	6.596428	-0.172221
		C	-4.696010	6.644113	-1.728393
		C	-4.705859	7.124598	-3.170129
		C	-0.333380	4.491814	-1.054307
		H	-2.908631	4.607442	-2.296961
		H	-3.063403	8.072331	0.113816

		H	-0.557177	6.804531	0.472461
		H	-0.781336	3.512915	-0.822172
		H	0.121715	4.497202	-2.053152
		H	0.409816	4.767916	-0.294672
		H	-5.147492	7.378368	-1.049940
		H	-5.240857	5.693703	-1.650053
		H	-5.745941	7.259359	-3.498543
		H	-4.170507	8.078029	-3.281615
		H	-4.239857	6.364447	-3.814154
		C	-6.012781	4.028429	-5.038205
		C	-5.599280	3.968015	-3.565310
		O	-6.479082	4.155624	-2.695740
		O	-4.370574	3.747897	-3.336024
		H	-7.102473	3.968816	-5.147422
		H	-5.526713	3.223916	-5.606497
		H	-5.667627	4.984132	-5.463306
		N	-6.012063	2.356340	0.014227
		C	-5.232649	1.970913	-0.997117
		N	-5.242412	0.636548	-1.043439
		C	-6.055960	0.150596	-0.037106
		C	-6.538906	1.240602	0.625876
		C	-4.538157	-0.199035	-2.028165
		C	-3.444597	0.569487	-2.746482
		C	-6.193302	3.749174	0.413607
		H	-4.703799	2.649661	-1.675104
		H	-6.202204	-0.922371	0.109414
		H	-7.201438	1.317026	1.481094
		H	-5.194161	4.165784	0.601813
		H	-6.685323	4.278687	-0.409709
		H	-6.801741	3.767853	1.323477
		H	-5.290941	-0.579656	-2.734045

		H	-4.139015	-1.066292	-1.483460
		H	-2.923763	-0.118081	-3.426907
		H	-3.851109	1.407454	-3.330924
		H	-2.725660	0.973822	-2.016993
		C	-3.348421	1.698375	1.824097
		C	-2.684884	2.330509	0.600567
		O	-1.830135	1.616128	-0.004434
		O	-3.011679	3.500265	0.290604
		H	-2.602109	1.608267	2.628865
		H	-3.686494	0.679886	1.578568
		H	-4.194920	2.298709	2.184129
[C ₂ mim][BF ₄] 8IP	Gas phase	N	0.797724	-0.502352	-0.061921
		C	-0.228910	-1.333778	-0.226746
		N	-1.164910	-0.717775	-0.943371
		C	-0.727046	0.553307	-1.246010
		C	0.512294	0.690264	-0.693660
		C	-2.476282	-1.286833	-1.265512
		C	-2.698101	-1.380074	-2.764849
		C	1.980223	-0.800238	0.741021
		H	-0.311710	-2.327443	0.198909
		H	-1.354356	1.262083	-1.773400
		H	1.202742	1.527558	-0.672248
		H	1.723818	-0.760325	1.804601
		H	2.321157	-1.813245	0.499979
		H	2.764504	-0.076150	0.498376
		H	-3.221021	-0.631482	-0.796956
		H	-2.495276	-2.277739	-0.793868
		H	-3.711090	-1.767175	-2.949860
		H	-2.632043	-0.391498	-3.243795
		H	-1.971240	-2.067788	-3.216862
		B	-0.439253	-4.500733	-0.948955

		F	-0.488599	-5.878264	-1.153617
		F	-1.331606	-4.135224	0.099705
		F	-0.781097	-3.784435	-2.108315
		F	0.873984	-4.114914	-0.551836
		N	1.946877	-4.800840	2.079497
		C	0.639310	-5.014166	2.213505
		N	0.331411	-6.163832	1.611054
		C	1.470669	-6.683515	1.044913
		C	2.489848	-5.829280	1.343991
		C	-1.016547	-6.750291	1.560336
		C	-1.616780	-6.877335	2.950722
		C	2.684058	-3.665882	2.634867
		H	-0.068246	-4.349219	2.703087
		H	1.450201	-7.591610	0.454882
		H	3.544297	-5.852485	1.092248
		H	3.446483	-3.339885	1.919456
		H	1.973166	-2.857631	2.831082
		H	3.179377	-3.969252	3.566266
		H	-0.899914	-7.724992	1.071063
		H	-1.621491	-6.110739	0.910157
		H	-2.600112	-7.361458	2.874142
		H	-0.980438	-7.487062	3.607757
		H	-1.765699	-5.886385	3.401965
		B	-1.513272	-2.204252	2.795427
		F	-1.821258	-1.383440	3.880757
		F	-2.160922	-1.738253	1.632967
		F	-1.916295	-3.538999	3.049563
		F	-0.109201	-2.190599	2.559672
		N	2.639260	-0.166029	-2.946758
		C	3.453577	-0.823281	-2.125587
		N	2.989894	-2.061674	-1.969827

		C	1.832107	-2.205615	-2.706900
		C	1.613912	-1.009551	-3.322961
		C	3.718840	-3.123703	-1.264624
		C	4.328784	-4.094033	-2.263776
		C	2.843663	1.205292	-3.387347
		H	4.352478	-0.426601	-1.660884
		H	1.245669	-3.118663	-2.698708
		H	0.816294	-0.684493	-3.980764
		H	3.844858	1.515259	-3.075731
		H	2.770244	1.235525	-4.481061
		H	2.096037	1.864676	-2.929787
		H	2.997439	-3.622481	-0.603351
		H	4.492202	-2.620962	-0.673101
		H	4.962793	-4.815436	-1.729005
		H	3.547091	-4.650035	-2.802055
		H	4.946703	-3.537792	-2.980601
		B	6.272609	-0.903309	-3.229981
		F	7.553698	-0.970937	-3.784961
		F	6.246475	-1.658757	-2.016822
		F	5.299661	-1.410696	-4.095725
		F	5.954295	0.446298	-2.895966
		N	7.351232	1.704323	-0.862114
		C	7.561615	0.452349	-0.465696
		N	8.559052	-0.060047	-1.182686
		C	8.985377	0.887859	-2.085013
		C	8.227193	1.999104	-1.881230
		C	9.025136	-1.453122	-1.124320
		C	8.447754	-2.190194	0.068076
		C	6.245889	2.535373	-0.399652
		H	7.004461	-0.050487	0.318927
		H	9.752185	0.671474	-2.818537

		H	8.207924	2.952405	-2.395160
		H	5.654982	2.856506	-1.265427
		H	5.605407	1.920968	0.241093
		H	6.624977	3.405999	0.148662
		H	10.123005	-1.415758	-1.084346
		H	8.707731	-1.913767	-2.068354
		H	8.861711	-3.206924	0.085119
		H	8.700719	-1.697996	1.018179
		H	7.355558	-2.266284	-0.010718
		B	5.205871	-1.217226	1.685254
		F	4.118774	-1.070980	2.571168
		F	5.396233	-2.580558	1.389802
		F	6.369459	-0.652878	2.223762
		F	4.913750	-0.525790	0.470762
		N	-8.693699	2.663927	-0.150571
		C	-7.601015	2.268238	-0.797733
		N	-7.735168	2.568317	-2.084707
		C	-8.962885	3.163680	-2.275194
		C	-9.569676	3.216647	-1.056954
		C	-6.743754	2.244616	-3.115709
		C	-6.100279	3.498965	-3.680500
		C	-8.973410	2.350776	1.244958
		H	-6.767840	1.736831	-0.350939
		H	-9.301077	3.487160	-3.252556
		H	-10.545655	3.582439	-0.761504
		H	-9.575494	1.435466	1.278471
		H	-8.017798	2.181128	1.751766
		H	-9.498189	3.197954	1.701290
		H	-7.265765	1.653550	-3.880150
		H	-6.006531	1.598210	-2.626118
		H	-5.375031	3.215402	-4.455587

		H	-6.843801	4.168089	-4.138675
		H	-5.565788	4.030083	-2.882802
		B	-4.368983	1.881831	-0.206370
		F	-3.034165	1.575262	0.103025
		F	-4.951612	0.749973	-0.865628
		F	-4.441024	2.974931	-1.087006
		F	-5.107794	2.137184	0.958846
		N	-4.934884	-1.981727	0.827155
		C	-5.653352	-1.923827	-0.291477
		N	-5.584611	-3.102294	-0.907661
		C	-4.786594	-3.944775	-0.157602
		C	-4.373368	-3.237034	0.932143
		C	-6.335744	-3.431874	-2.123780
		C	-7.370465	-4.513271	-1.859482
		C	-4.773159	-0.844843	1.736153
		H	-6.179392	-1.049562	-0.659474
		H	-4.559783	-4.957757	-0.468905
		H	-3.696549	-3.500800	1.738894
		H	-3.939854	-0.218300	1.398573
		H	-5.706462	-0.273055	1.722152
		H	-4.552825	-1.230237	2.737021
		H	-5.610033	-3.738408	-2.891142
		H	-6.822649	-2.497754	-2.434470
		H	-7.914103	-4.728950	-2.789286
		H	-6.899636	-5.445359	-1.514718
		H	-8.087569	-4.156799	-1.109966
		B	-8.511927	-0.597722	-0.750386
		F	-9.697036	0.122813	-0.874139
		F	-7.648499	-0.302967	-1.856021
		F	-8.707158	-1.978393	-0.708163
		F	-7.838481	-0.177656	0.439281

		N	2.183434	6.528701	0.410082
		C	0.891497	6.306492	0.633005
		N	0.295930	6.041854	-0.528349
		C	1.244348	6.081279	-1.526859
		C	2.432553	6.384394	-0.935818
		C	-1.094351	5.589408	-0.661240
		C	-1.172741	4.090179	-0.895653
		C	3.165661	6.791783	1.456968
		H	0.413278	6.337486	1.609374
		H	1.009045	5.843896	-2.557530
		H	3.431483	6.457887	-1.347926
		H	2.633390	6.814371	2.413658
		H	3.876471	5.959539	1.464150
		H	3.662329	7.748698	1.254291
		H	-1.551699	6.164580	-1.478434
		H	-1.597318	5.858245	0.275885
		H	-2.224170	3.778454	-0.966193
		H	-0.642843	3.811853	-1.819801
		H	-0.695599	3.577336	-0.051492
		B	3.122530	3.340223	-0.645112
		F	3.359823	1.949129	-0.485738
		F	1.749645	3.560157	-0.365976
		F	3.425460	3.733419	-1.953618
		F	3.920589	4.066686	0.260421
		N	2.424583	1.509750	3.005481
		C	1.366295	1.852158	2.273923
		N	0.300661	1.197031	2.730605
		C	0.682150	0.420122	3.801931
		C	2.022225	0.614300	3.969401
		C	-1.061177	1.331695	2.192106
		C	-2.033236	1.832399	3.244164

		C	3.768234	2.048808	2.839349
		H	1.369292	2.588890	1.472633
		H	-0.029130	-0.221989	4.310830
		H	2.729518	0.175979	4.662848
		H	3.777111	2.673186	1.940802
		H	4.005241	2.673591	3.709019
		H	4.472377	1.213116	2.748164
		H	-1.364770	0.353331	1.792582
		H	-0.990962	2.041224	1.362722
		H	-2.999904	2.018367	2.754452
		H	-2.177498	1.078896	4.030624
		H	-1.655260	2.766653	3.679517
		B	0.777887	4.592537	3.208913
		F	0.585521	5.951772	3.543959
		F	-0.177918	4.245911	2.200556
		F	0.636375	3.752099	4.299999
		F	2.073034	4.465874	2.639658
[C ₂ mim][BF ₄] 8IP	CHCl ₃	N	-0.788180	0.567793	-0.057464
		C	0.262093	1.366654	-0.237140
		N	1.179295	0.711317	-0.943352
		C	0.704562	-0.551025	-1.226203
		C	-0.537622	-0.642775	-0.670307
		C	2.501302	1.242857	-1.289710
		C	2.714185	1.284322	-2.792743
		C	-1.967445	0.916142	0.729390
		H	0.372962	2.365403	0.169672
		H	1.300193	-1.280383	-1.762482
		H	-1.254632	-1.457777	-0.639521
		H	-1.723817	0.884841	1.796515
		H	-2.271655	1.936827	0.470076
		H	-2.771960	0.212426	0.490587

		H	3.236461	0.588179	-0.804569
		H	2.544097	2.246800	-0.847763
		H	3.725994	1.663141	-2.998666
		H	2.637804	0.281705	-3.238627
		H	1.984130	1.955734	-3.263577
		B	0.464417	4.488169	-1.043161
		F	0.533242	5.847294	-1.352020
		F	1.360044	4.182808	0.015876
		F	0.797827	3.701385	-2.163025
		F	-0.850925	4.148207	-0.624799
		N	-1.856542	4.981224	1.992086
		C	-0.541388	5.173579	2.076628
		N	-0.239057	6.320154	1.465632
		C	-1.392911	6.863031	0.951260
		C	-2.412864	6.022194	1.284353
		C	1.111162	6.896365	1.366805
		C	1.780455	6.975427	2.728364
		C	-2.590121	3.860965	2.577780
		H	0.170929	4.496764	2.541862
		H	-1.386939	7.788938	0.388589
		H	-3.477186	6.072058	1.083800
		H	-3.361681	3.522846	1.877677
		H	-1.878333	3.055567	2.781561
		H	-3.068833	4.186152	3.510103
		H	0.980462	7.889689	0.921438
		H	1.680013	6.274686	0.668094
		H	2.765744	7.447150	2.614916
		H	1.183334	7.576565	3.428221
		H	1.932198	5.971936	3.149984
		B	1.557343	2.267799	2.778242
		F	1.828309	1.452843	3.886165

		F	2.216299	1.767810	1.638228
		F	1.989272	3.590579	3.029502
		F	0.159740	2.277972	2.523478
		N	-2.596983	0.119645	-2.958767
		C	-3.428786	0.788325	-2.162887
		N	-2.986513	2.039624	-2.044622
		C	-1.824212	2.176307	-2.775333
		C	-1.580516	0.965302	-3.352465
		C	-3.722053	3.117621	-1.370729
		C	-4.422545	4.000493	-2.391215
		C	-2.760839	-1.274657	-3.345144
		H	-4.321413	0.388327	-1.688446
		H	-1.254093	3.099006	-2.790364
		H	-0.772924	0.631157	-3.994043
		H	-3.730311	-1.618232	-2.976394
		H	-2.719906	-1.344577	-4.438325
		H	-1.963177	-1.880924	-2.896988
		H	-2.987033	3.684211	-0.783299
		H	-4.438471	2.629358	-0.700536
		H	-5.028965	4.751141	-1.865465
		H	-3.694075	4.527375	-3.024630
		H	-5.078317	3.384355	-3.019430
		B	-6.327747	0.648482	-3.218006
		F	-7.634020	0.607850	-3.722566
		F	-6.286704	1.505753	-2.084263
		F	-5.431518	1.128079	-4.184092
		F	-5.926396	-0.651975	-2.804663
		N	-7.466681	-1.783094	-0.716474
		C	-7.586621	-0.490402	-0.428400
		N	-8.658625	-0.011165	-1.055271
		C	-9.231769	-1.027083	-1.786811

		C	-8.481707	-2.143780	-1.572958
		C	-9.083090	1.395913	-1.073977
		C	-8.428119	2.197793	0.032951
		C	-6.347458	-2.617526	-0.297699
		H	-6.904058	0.071462	0.202375
		H	-10.108654	-0.862209	-2.401870
		H	-8.577500	-3.152311	-1.957575
		H	-5.828956	-2.996671	-1.186056
		H	-5.648126	-1.994705	0.268293
		H	-6.707853	-3.448659	0.318820
		H	-10.176601	1.393584	-0.977267
		H	-8.807940	1.782961	-2.063121
		H	-8.823995	3.221332	0.003439
		H	-8.639788	1.769495	1.022772
		H	-7.340304	2.244311	-0.106431
		B	-5.213103	1.401877	1.685851
		F	-4.135556	1.250243	2.581339
		F	-5.362661	2.760773	1.351007
		F	-6.396678	0.897129	2.238106
		F	-4.933872	0.664530	0.495510
		N	8.700126	-2.805986	-0.057513
		C	7.625558	-2.394462	-0.724787
		N	7.753025	-2.747288	-1.999876
		C	8.956665	-3.399070	-2.161420
		C	9.555991	-3.429613	-0.937419
		C	6.766779	-2.444027	-3.043213
		C	6.110853	-3.706608	-3.573525
		C	8.979181	-2.474686	1.334520
		H	6.808469	-1.816928	-0.306049
		H	9.283954	-3.779606	-3.122277
		H	10.509223	-3.835760	-0.619571

		H	9.585449	-1.562328	1.359626
		H	8.025038	-2.301990	1.842737
		H	9.505608	-3.314597	1.799692
		H	7.293294	-1.887945	-3.829719
		H	6.035123	-1.776506	-2.574291
		H	5.382741	-3.434589	-4.349736
		H	6.848269	-4.387827	-4.021644
		H	5.580875	-4.221871	-2.762400
		B	4.375757	-1.901205	-0.124026
		F	3.047195	-1.554893	0.174108
		F	4.992994	-0.805805	-0.803665
		F	4.420466	-3.021912	-0.970727
		F	5.096219	-2.156735	1.056392
		N	5.013936	1.985022	0.759938
		C	5.704606	1.906264	-0.375515
		N	5.628498	3.077330	-1.005202
		C	4.856414	3.936421	-0.248207
		C	4.464385	3.245786	0.860642
		C	6.347866	3.392197	-2.245257
		C	7.426345	4.436637	-2.009351
		C	4.868509	0.870393	1.696619
		H	6.218090	1.022727	-0.740376
		H	4.641218	4.951003	-0.564033
		H	3.813699	3.525293	1.683031
		H	3.982669	0.282099	1.433852
		H	5.770490	0.254855	1.625048
		H	4.750089	1.282121	2.704172
		H	5.607771	3.729580	-2.983396
		H	6.786028	2.444767	-2.584759
		H	7.940413	4.643569	-2.957561
		H	6.996539	5.378565	-1.640535

		H	8.157737	4.055484	-1.285973
		B	8.570768	0.498412	-0.726433
		F	9.752088	-0.242849	-0.802535
		F	7.742961	0.203596	-1.848624
		F	8.816309	1.877063	-0.705476
		F	7.865314	0.129200	0.454447
		N	-2.239841	-6.498197	0.398135
		C	-0.950850	-6.249374	0.609067
		N	-0.364236	-6.005591	-0.561204
		C	-1.314836	-6.086282	-1.554498
		C	-2.495967	-6.395246	-0.950220
		C	1.022867	-5.553047	-0.718382
		C	1.096228	-4.047037	-0.909905
		C	-3.209536	-6.793367	1.447320
		H	-0.462224	-6.259182	1.579091
		H	-1.078808	-5.892584	-2.594492
		H	-3.490834	-6.527197	-1.358021
		H	-2.678527	-6.781818	2.404130
		H	-3.966291	-6.002954	1.440636
		H	-3.657870	-7.775849	1.259975
		H	1.451035	-6.100936	-1.567945
		H	1.554608	-5.859277	0.190654
		H	2.146833	-3.732895	-0.982129
		H	0.560693	-3.745506	-1.822855
		H	0.626439	-3.552885	-0.049611
		B	-3.203337	-3.279821	-0.545731
		F	-3.422933	-1.882995	-0.380416
		F	-1.822724	-3.509037	-0.326356
		F	-3.568408	-3.667602	-1.841338
		F	-3.967058	-4.000064	0.390711
		N	-2.452192	-1.384631	2.991714

		C	-1.392706	-1.756999	2.275312
		N	-0.320227	-1.114090	2.735004
		C	-0.699379	-0.314348	3.790489
		C	-2.044934	-0.481155	3.946436
		C	1.042170	-1.266581	2.204213
		C	2.009786	-1.750138	3.268183
		C	-3.818826	-1.830946	2.745722
		H	-1.400187	-2.504863	1.483503
		H	0.016397	0.321952	4.299951
		H	-2.748749	-0.022938	4.630843
		H	-3.770541	-2.783194	2.208508
		H	-4.316899	-1.964494	3.712587
		H	-4.341372	-1.068812	2.154423
		H	1.353135	-0.296932	1.790021
		H	0.972532	-1.987661	1.384794
		H	2.981830	-1.932217	2.788063
		H	2.143625	-0.988703	4.048730
		H	1.636160	-2.682616	3.710926
		B	-0.778122	-4.522364	3.241118
		F	-0.566769	-5.875217	3.593632
		F	0.169181	-4.168310	2.239162
		F	-0.629611	-3.684626	4.344984
		F	-2.077882	-4.404797	2.697103
[C ₂ mim][BF ₄] 16IP	EtOH	N	-0.777186	0.564312	-0.070376
		C	0.269250	1.367297	-0.254962
		N	1.187947	0.713769	-0.961051
		C	0.717978	-0.551228	-1.239870
		C	-0.522353	-0.647140	-0.680405
		C	2.505905	1.251539	-1.314899
		C	2.710207	1.294840	-2.819097
		C	-1.956628	0.910120	0.717373

		H	0.376067	2.367836	0.148649
		H	1.313227	-1.277870	-1.780438
		H	-1.236120	-1.465226	-0.647125
		H	-1.710816	0.885022	1.784242
		H	-2.266903	1.928172	0.454485
		H	-2.757380	0.200671	0.483489
		H	3.247350	0.600808	-0.833360
		H	2.546285	2.255433	-0.872542
		H	3.717817	1.681492	-3.030716
		H	2.636956	0.292260	-3.265225
		H	1.972444	1.960657	-3.285600
		B	0.443472	4.492824	-1.059983
		F	0.501337	5.851432	-1.376053
		F	1.340727	4.198864	-0.000609
		F	0.786159	3.707218	-2.178756
		F	-0.869330	4.143194	-0.644221
		N	-1.880660	5.000041	1.971367
		C	-0.565033	5.192657	2.049391
		N	-0.267804	6.346459	1.449996
		C	-1.426109	6.895830	0.952268
		C	-2.443110	6.049709	1.281318
		C	1.080774	6.926466	1.348789
		C	1.755421	7.000193	2.707852
		C	-2.607711	3.872041	2.549171
		H	0.149984	4.511269	2.503307
		H	-1.426185	7.832709	0.407740
		H	-3.509155	6.104068	1.091619
		H	-3.377276	3.532974	1.847098
		H	-1.890841	3.069742	2.747508
		H	-3.087150	4.188282	3.484117
		H	0.946133	7.922142	0.910253

		H	1.648537	6.309969	0.644432
		H	2.739602	7.473459	2.592082
		H	1.159800	7.597763	3.411860
		H	1.909174	5.995099	3.124907
		B	1.553235	2.284121	2.761675
		F	1.827688	1.469931	3.872172
		F	2.216649	1.785882	1.624289
		F	1.979205	3.607341	3.015374
		F	0.156528	2.285722	2.507355
		N	-2.559431	0.093286	-2.979988
		C	-3.399826	0.753484	-2.185633
		N	-2.974890	2.011393	-2.072675
		C	-1.814466	2.160535	-2.803745
		C	-1.553869	0.950497	-3.376274
		C	-3.727584	3.081058	-1.404368
		C	-4.438472	3.949720	-2.429845
		C	-2.702284	-1.306081	-3.358095
		H	-4.283422	0.339919	-1.705926
		H	-1.258155	3.091408	-2.824088
		H	-0.742062	0.624266	-4.016833
		H	-3.664741	-1.662206	-2.983162
		H	-2.660625	-1.382475	-4.450688
		H	-1.892130	-1.895624	-2.910045
		H	-3.003993	3.660860	-0.815761
		H	-4.438796	2.583727	-0.735298
		H	-5.054542	4.695561	-1.908595
		H	-3.716418	4.482687	-3.065359
		H	-5.085939	3.322031	-3.055515
		B	-6.343131	0.568426	-3.191788
		F	-7.662022	0.465143	-3.653380
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		H	-10.273598	1.437423	-1.026411
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		F	-4.134894	1.237376	2.567979
		F	-5.369943	2.713714	1.303893
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		C	7.649288	-2.392102	-0.695027
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		H	-3.757620	-2.801246	2.219627
		H	-4.304501	-1.969972	3.718077
		H	-4.330695	-1.090629	2.150111
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		H	2.998347	-1.898952	2.773399
		H	2.149219	-0.967127	4.034831
		H	1.661203	-2.666110	3.696217
		B	-0.728350	-4.530562	3.232825
		F	-0.489431	-5.879625	3.580203
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		H	0.261774	0.431960	0.824931
		H	2.423763	3.023835	2.376977
		H	1.262017	1.685411	2.714953
		H	3.002493	1.325663	2.418712
		H	3.278869	3.246518	-2.526439
		H	1.642044	3.036236	-3.205533
		H	3.321932	1.731036	-4.538783
		H	3.831735	0.878983	-3.053214
		H	2.179767	0.614039	-3.735631
		Cl	5.606822	1.883726	-1.104325
		N	7.136999	5.804211	-2.099493
		C	6.727806	5.026407	-1.096523
		N	7.780733	4.746788	-0.327680
		C	8.900600	5.358236	-0.852019
		C	8.494309	6.020479	-1.972900
		C	7.722057	3.947938	0.904573
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		C	6.273976	6.310767	-3.162128
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		H	8.763258	3.695233	1.153539
		H	7.164811	3.036060	0.648233
		H	7.014436	4.092182	2.928912
		H	7.583647	5.642937	2.256516
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		C	10.569625	-0.329307	3.463917
		H	11.264637	0.877253	1.032188
		H	7.068553	0.559235	0.500761
		H	7.787449	-0.518925	3.001369
		H	11.612232	-0.388140	3.123753
		H	10.465877	0.405262	4.272366
		H	10.233317	-1.313426	3.810392
		H	9.523693	2.606324	-0.724567
		H	8.276845	1.472893	-1.347568
		H	10.356136	1.376486	-2.753297
		H	11.344521	1.030070	-1.314711
		H	10.130712	-0.173728	-1.875973
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		C	14.484355	2.726775	0.870679

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		C	13.211811	2.405343	3.936170
		C	14.292012	3.850196	-1.318022
		H	14.178744	1.722521	0.566020
		H	15.274148	4.931955	3.093723
		H	15.140636	5.860743	0.467707
		H	13.231676	4.124725	-1.391621
		H	14.928698	4.588171	-1.817080
		H	14.455148	2.862593	-1.761929
		H	15.397724	2.391392	3.977764
		H	14.657182	1.163597	2.903701
		H	13.082769	1.688276	4.758762
		H	13.123412	3.423540	4.342456
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		C	-9.413535	-1.679081	-4.633303
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		H	-15.215229	-2.807220	-4.335143
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		N	-9.276839	-0.627336	0.448834
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		C	-7.462328	0.361497	-0.309863
		C	-10.216750	-1.284483	1.367622
		C	-10.974841	-0.263503	2.200410
		C	-8.333789	1.054378	-2.566795
		H	-10.507982	-0.257209	-1.306480
		H	-7.550547	-0.601448	1.724801
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		H	-9.340209	1.139595	-2.998665
		H	-7.865705	2.039200	-2.428184
		H	-7.694144	0.428392	-3.201279
		H	-9.605037	-1.937338	2.006968
		H	-10.885323	-1.897213	0.747482
		H	-11.654905	-0.787625	2.885362
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		N	-8.642143	-5.198660	2.762056
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		H	-7.810432	-4.346018	-2.536660
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		H	-5.215758	0.715354	6.012859
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		H	1.027996	4.205639	2.174908
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		N	1.863857	1.532686	0.843787
		C	0.779482	0.690614	0.967811
		C	0.760986	0.258946	2.262967
		C	2.258434	2.249116	-0.376116
		C	2.484410	1.281593	-1.523622
		C	2.255112	0.585860	4.269629
		H	3.379785	2.212330	2.203103
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		H	2.652592	1.512412	4.702049
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		H	3.029297	-0.191438	4.281321
		H	3.172758	2.796247	-0.118405
		H	1.462152	2.973779	-0.600357
		H	2.741163	1.849423	-2.429577
		H	3.325215	0.616773	-1.274274
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		C	6.840123	5.094418	-2.179004
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		H	6.782437	5.564936	-3.153902
		H	3.745097	5.199495	-0.830923
		H	4.332646	6.266706	-2.150898
		H	3.960116	4.547370	-2.500022
		H	9.188185	3.362604	0.415088
		H	7.703678	2.527143	0.997509
		H	8.724441	3.888337	2.844017
		H	8.606178	5.360710	1.842647
		H	7.123884	4.533348	2.404897
		Cl	3.551649	4.827724	1.888016
		N	10.970474	0.014153	1.323969
		C	10.713746	0.472099	0.097334
		N	9.390995	0.483196	-0.077288
		C	8.782019	0.014085	1.066215
		C	9.777235	-0.276942	1.952251
		C	8.702942	0.941400	-1.294158
		C	9.105637	0.114131	-2.502153
		C	12.304070	-0.120994	1.899947
		H	11.468190	0.775480	-0.627568
		H	7.697832	-0.047343	1.132182
		H	9.743762	-0.665961	2.963419
		H	13.031172	-0.069643	1.079477

		H	12.476497	0.685330	2.623221
		H	12.375962	-1.091824	2.403314
		H	8.984419	1.993756	-1.437087
		H	7.628699	0.872196	-1.072113
		H	8.570687	0.484004	-3.388564
		H	10.186611	0.206643	-2.693527
		H	8.855009	-0.943670	-2.339973
		Cl	13.569273	-0.292934	-1.586228
		N	13.854637	3.924475	-3.349676
		C	14.155619	2.933024	-2.512948
		N	14.865312	3.431701	-1.502824
		C	14.995840	4.792455	-1.678346
		C	14.356521	5.102085	-2.841643
		C	15.303632	2.660728	-0.333120
		C	14.383777	2.911278	0.850746
		C	12.960200	3.797761	-4.493439
		H	13.865881	1.883432	-2.597287
		H	15.544642	5.413970	-0.979605
		H	14.228843	6.048798	-3.353850
		H	11.928137	3.906922	-4.136432
		H	13.207529	4.575323	-5.222963
		H	13.100525	2.810862	-4.945870
		H	16.340593	2.949440	-0.119449
		H	15.277269	1.606123	-0.634291
		H	14.699713	2.287358	1.697928
		H	14.419549	3.964671	1.164957
		H	13.346798	2.665573	0.577557
		Cl	11.216545	3.454991	-1.376057

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