Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Bulk and Gas Phase of 1-Ethyl-3-Methylimidazolium Ethylsulfate: Dispersion Interaction makes the Difference.

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1 Starting structures

To be able to reproduce our results, we provide all starting structures for our calculations.

Starting structure of one ion pair of$[C_2C_1im][C_2SO_4]$

C	13.381009822032812	9.030855362567177	11.439764763159445
N	12.510523222032813	8.770860662567177	10.384362463159444
C	11.256988422032812	8.672554662567176	10.869697663159446
N	11.302374822032814	8.868186362567178	12.202642463159446
C	12.624056322032812	9.096209662567176	12.579189163159445
C	12.852754222032813	8.685439662567177	8.946037263159445
C	10.095958722032814	8.971623462567177	13.076225863159445
C	9.743055022032813	10.427303962567176	13.410599263159446
O	8.621302422032812	9.019727962567178	9.620851163159445
S	8.968533922032812	10.424955762567176	9.152454663159446
O	7.738625222032812	10.709393062567177	7.993914363159446
C	7.791749422032813	12.023657562567177	7.359757263159445
C	6.568054022032813	12.135549662567177	6.455086563159446
O	8.823376022032813	11.489625862567177	10.214060263159444
O	10.289904822032813	10.485052662567178	8.398860163159444
H	10.331925822032813	8.536439362567178	10.292090363159446
H	12.907140022032813	9.285528262567176	13.605050163159445
H	14.445166922032813	9.148522662567178	11.289589963159445
H	12.032930022032813	9.150022162567177	8.383477163159444
H	13.778742822032813	9.243258062567177	8.779786463159445
H	12.991945022032812	7.637859562567177	8.655647463159445
H	9.279828122032812	8.495876262567178	12.522692163159444
H	10.301798322032813	8.377672362567177	13.975883463159445
H	6.572289122032813	13.109539662567176	5.944814763159446
H	6.569339322032813	11.345722762567178	5.692844463159446
H	5.642199422032813	12.053850762567176	7.038451163159445
H	7.784212922032813	12.803068062567178	8.135923463159445
H	8.724366022032813	12.110764462567177	6.782282263159445
H	8.853123422032812	10.433638862567177	14.053472563159445
H	10.556596022032814	10.926146462567177	13.954118663159445
H	9.510019322032813	10.988095862567178	12.496108363159445

Starting structure of 27 ion pairs of $[C_2C_1im][C_2SO_4]$

C	00.34	05.56	09.32

N	00.84	05.69	08.09
C	02.03	05.06	08.02
N	02.36	04.68	09.22
C	01.28	04.93	10.03
C	00.02	06.21	06.97
C	03.68	04.27	09.77
C	04.56	03.90	08.61
O	15.12	16.01	05.17
S	14.01	15.76	04.30
O	12.84	15.70	05.12
C	12.32	16.90	05.62
C	11.31	16.51	06.73
O	13.81	16.82	03.42
O	14.14	14.51	03.69
H	02.67	05.04	07.10
H	01.37	04.58	11.02
H	-00.58	05.86	09.67
H	00.62	06.82	06.31
H	-00.26	05.36	06.45
H	-00.88	06.81	07.30
H	04.10	05.14	10.28
H	03.50	03.53	10.54
H	10.52	17.06	06.40
H	11.10	15.48	06.46
H	11.51	16.72	07.81
H	13.11	17.50	06.14
H	11.76	17.59	04.91
H	04.91	04.85	08.32
H	05.36	03.36	09.08
H	03.94	03.32	07.93
C	00.93	02.19	13.01
N	02.10	01.48	13.08
C	02.53	01.17	11.92
N	01.67	01.56	11.03
C	00.63	02.26	11.71
C	02.81	01.16	14.38
C	01.78	01.25	09.56
C	01.20	-00.18	09.27
O	19.11	02.10	07.55
S	19.19	01.25	06.37
O	20.58	01.07	06.00
C	21.17	02.22	05.41
C	22.63	02.25	05.82
O	18.67	00.00	06.71
O	18.52	01.82	05.28

H	03.41	00.53	11.76
H	-00.24	02.60	11.12
H	00.56	02.70	13.93
H	03.54	00.36	14.36
H	03.41	02.04	14.54
H	02.05	00.91	15.17
H	01.31	02.02	08.92
H	02.92	01.29	09.38
H	23.12	02.98	05.18
H	22.71	02.48	06.90
H	22.96	01.21	05.71
H	21.07	02.19	04.33
H	20.65	03.08	05.86
H	01.85	-00.89	09.76
H	00.26	-00.29	09.61
H	01.34	-00.24	08.23
C	04.61	19.52	17.69
N	03.68	18.80	16.90
C	02.51	19.38	17.17
N	02.56	20.43	17.94
C	03.89	20.46	18.36
C	03.87	17.59	16.13
C	01.37	21.18	18.41
C	00.42	21.52	17.27
O	00.24	12.09	06.40
S	-01.07	11.63	06.71
O	-01.30	10.39	06.00
C	-01.89	10.39	04.65
C	-01.97	08.91	04.21
O	-01.22	11.50	08.08
O	-02.07	12.57	06.21
H	01.62	19.12	16.66
H	04.21	21.18	19.12
H	05.63	19.26	17.70
H	03.26	16.75	16.45
H	03.75	17.63	15.05
H	04.91	17.18	16.31
H	00.85	20.49	19.06
H	01.66	22.04	19.01
H	-01.97	08.83	03.21
H	-01.20	08.28	04.51
H	-02.84	08.58	04.61
H	-02.88	10.82	04.92
H	-01.34	11.07	04.05
H	00.51	20.95	16.41

H	-00.52	21.55	17.74
H	00.77	22.47	17.11
C	12.34	05.47	08.34
N	12.26	04.11	08.01
C	11.01	03.76	08.24
N	10.26	04.68	08.71
C	11.05	05.77	08.89
C	13.21	03.09	07.52
C	08.87	04.48	09.19
C	08.11	05.81	08.95
O	17.40	12.88	12.15
S	17.91	12.69	10.86
O	17.49	13.55	09.87
C	16.10	13.97	09.81
C	15.82	14.76	08.53
O	19.35	12.74	10.92
O	17.52	11.34	10.43
H	10.70	02.81	08.20
H	10.76	06.54	09.55
H	13.24	05.82	08.33
H	13.19	02.92	06.52
H	14.17	03.46	07.85
H	13.02	02.21	08.13
H	08.37	03.76	08.59
H	08.98	04.31	10.19
H	16.43	14.36	07.76
H	14.75	14.70	08.29
H	15.84	15.86	08.70
H	15.46	13.12	09.84
H	15.85	14.57	10.64
H	08.19	05.99	07.85
H	07.13	05.76	09.22
H	08.46	06.59	09.61
C	09.63	14.74	17.13
N	08.30	14.77	17.25
C	07.91	16.04	17.43
N	09.01	16.79	17.45
C	10.11	16.01	17.26
C	07.33	13.69	17.01
C	09.04	18.27	17.75
C	08.70	18.55	19.17
O	05.29	06.49	20.25
S	06.66	06.58	20.08
O	07.14	07.61	20.96
C	07.12	07.31	22.36

C	07.34	08.69	23.08
O	07.33	05.43	20.49
O	06.99	06.82	18.73
H	06.97	16.33	17.83
H	11.07	16.51	17.30
H	10.11	13.80	17.06
H	07.73	12.77	16.86
H	06.81	13.44	17.98
H	06.73	14.02	16.25
H	10.08	18.61	17.65
H	08.42	18.77	17.05
H	06.34	09.05	23.43
H	08.11	08.52	23.86
H	07.73	09.35	22.37
H	06.16	06.95	22.65
H	07.96	06.64	22.66
H	08.28	19.62	19.26
H	07.96	17.90	19.63
H	09.55	18.49	19.77
C	08.35	19.23	02.34
N	07.05	18.86	02.44
C	06.38	19.64	01.67
N	07.11	20.55	01.06
C	08.42	20.28	01.49
C	06.34	18.19	03.55
C	06.60	21.65	00.23
C	07.51	22.80	00.00
O	15.25	17.90	15.43
S	14.39	19.04	15.45
O	14.89	19.90	16.46
C	14.45	21.26	16.52
C	15.64	22.16	16.13
O	14.47	19.69	14.17
O	13.09	18.64	15.67
H	05.28	19.55	01.40
H	09.25	20.92	01.33
H	09.06	18.64	02.88
H	07.00	18.25	04.40
H	05.43	18.75	03.77
H	06.17	17.15	03.37
H	06.33	21.18	-00.68
H	05.66	22.00	00.66
H	16.48	22.04	16.83
H	15.90	21.90	15.12
H	15.44	23.23	16.17

H	13.53	21.46	15.94
H	14.07	21.51	17.51
H	08.54	22.50	-00.19
H	07.25	23.40	-00.84
H	07.49	23.29	00.94
C	09.94	19.90	07.75
N	08.77	19.80	07.07
C	08.15	18.76	07.52
N	08.72	18.22	08.56
C	09.90	18.94	08.74
C	08.43	20.59	05.93
C	08.17	17.08	09.35
C	09.05	15.84	09.34
O	01.33	07.98	02.99
S	01.70	09.29	03.18
O	02.82	09.73	02.43
C	02.68	09.56	01.04
C	04.04	09.91	00.24
O	00.63	10.09	02.88
O	01.97	09.41	04.56
H	07.17	18.49	07.08
H	10.48	18.78	09.60
H	10.55	20.70	07.63
H	09.22	20.57	05.26
H	07.57	20.17	05.44
H	08.21	21.64	06.13
H	07.81	17.37	10.36
H	07.38	16.74	08.75
H	03.92	10.09	-00.82
H	04.37	10.85	00.70
H	04.79	09.26	00.33
H	02.21	08.63	00.78
H	01.85	10.25	00.70
H	09.23	15.36	08.40
H	09.98	16.22	09.63
H	08.71	15.03	09.96
C	18.62	19.83	11.51
N	18.01	20.73	12.41
C	16.89	20.99	11.94
N	16.78	20.44	10.75
C	17.83	19.74	10.45
C	18.41	20.97	13.78
C	15.53	20.45	09.96
C	14.69	19.16	10.01
O	17.99	05.04	19.58

S	18.43	06.38	19.54
O	18.56	06.91	18.23
C	17.42	06.78	17.44
C	17.51	07.67	16.16
O	17.42	07.16	20.24
O	19.64	06.48	20.22
H	16.08	21.42	12.51
H	18.01	19.17	09.51
H	19.56	19.46	11.76
H	18.63	21.98	14.00
H	17.70	20.57	14.58
H	19.38	20.41	13.86
H	14.82	21.29	10.23
H	15.76	20.67	08.93
H	17.46	08.74	16.49
H	18.43	07.43	15.65
H	16.73	07.52	15.44
H	17.20	05.69	17.22
H	16.59	07.30	17.98
H	15.25	18.39	09.65
H	14.44	18.88	11.05
H	13.73	19.35	09.43
C	13.40	10.58	03.11
N	12.69	09.42	03.45
C	13.26	08.36	02.87
N	14.22	08.84	02.13
C	14.42	10.17	02.25
C	11.56	09.52	04.34
C	14.93	08.15	01.03
C	14.37	08.13	-00.37
O	19.05	17.83	18.62
S	17.89	17.91	17.86
O	16.75	18.05	18.75
C	16.80	19.14	19.56
C	15.70	18.86	20.63
O	17.94	18.91	16.83
O	17.74	16.70	17.27
H	12.79	07.42	02.57
H	14.97	10.64	01.56
H	12.97	11.52	03.43
H	11.63	08.68	05.05
H	11.77	10.39	04.93
H	10.62	09.77	03.83
H	15.82	08.61	00.92
H	14.91	07.16	01.45

H	15.33	17.82	20.54
H	15.95	19.09	21.67
H	14.89	19.55	20.34
H	17.73	19.41	20.08
H	16.50	19.97	19.08
H	13.51	07.49	-00.39
H	14.10	09.13	-00.50
H	15.02	07.91	-01.14
C	17.19	15.92	00.65
N	18.56	15.97	00.40
C	19.09	16.57	01.39
N	18.17	16.91	02.28
C	17.01	16.46	01.87
C	19.18	15.06	-00.68
C	18.40	17.06	03.67
C	17.79	18.32	04.17
O	03.21	08.13	16.23
S	03.31	08.00	17.65
O	02.43	08.88	18.28
C	01.12	08.86	17.88
C	00.21	09.69	18.84
O	03.14	06.66	18.07
O	04.60	08.32	18.09
H	20.14	16.73	01.59
H	16.13	16.33	02.45
H	16.56	15.39	-00.01
H	18.44	15.03	-01.48
H	20.05	15.48	-01.08
H	19.35	14.02	-00.35
H	18.05	16.17	04.09
H	19.49	17.16	03.89
H	00.04	09.16	19.78
H	00.66	10.70	18.88
H	-00.74	09.94	18.41
H	01.12	09.27	16.93
H	00.78	07.84	17.76
H	16.72	18.25	03.90
H	17.97	18.45	05.26
H	18.23	19.20	03.73
C	18.91	11.04	15.51
N	19.39	12.38	15.55
C	20.58	12.37	14.96
N	20.96	11.17	14.61
C	19.97	10.29	15.09
C	18.71	13.61	15.90

C	22.40	10.97	14.01
C	22.27	10.43	12.58
O	12.00	04.12	12.55
S	11.00	03.41	13.27
O	10.78	02.22	12.63
C	11.87	01.50	12.07
C	11.65	00.00	12.25
O	11.33	03.30	14.61
O	09.83	04.24	13.17
H	21.14	13.26	14.78
H	20.11	09.22	15.00
H	17.91	10.77	15.89
H	19.12	14.40	15.33
H	17.73	13.54	15.52
H	18.80	13.74	16.98
H	23.00	11.84	13.89
H	22.99	10.18	14.44
H	12.59	-00.48	11.80
H	11.60	-00.32	13.28
H	10.85	-00.28	11.59
H	11.92	01.85	11.04
H	12.82	01.84	12.55
H	21.42	09.71	12.48
H	22.16	11.32	11.90
H	23.21	10.04	12.19
C	04.67	19.83	07.75
N	04.68	18.88	08.76
C	05.35	19.27	09.81
N	05.80	20.46	09.53
C	05.36	20.85	08.24
C	04.12	17.50	08.81
C	06.49	21.32	10.53
C	07.96	21.43	10.40
O	11.69	05.53	01.21
S	11.39	04.85	-00.00
O	12.27	05.27	-00.98
C	12.24	04.71	-02.28
C	13.50	05.24	-03.08
O	11.43	03.44	00.14
O	10.08	05.20	-00.36
H	05.28	18.86	10.80
H	05.72	21.82	07.88
H	04.15	19.70	06.85
H	04.61	16.86	08.06
H	04.06	17.07	09.72

H	03.04	17.52	08.55
H	06.11	22.34	10.36
H	06.15	20.88	11.39
H	14.33	05.49	-02.44
H	13.72	04.48	-03.80
H	13.26	06.14	-03.72
H	12.39	03.62	-02.15
H	11.45	04.87	-03.02
H	08.25	21.76	09.46
H	08.42	22.01	11.14
H	08.40	20.47	10.42
C	01.77	13.94	01.67
N	01.33	13.97	02.98
C	02.33	13.63	03.78
N	03.37	13.47	03.06
C	03.06	13.61	01.74
C	00.02	14.47	03.44
C	04.63	13.34	03.72
C	05.41	12.00	03.46
O	09.53	01.07	15.37
S	09.67	01.25	16.81
O	10.64	00.35	17.31
C	11.17	00.62	18.58
C	12.18	-00.51	18.89
O	09.94	02.61	17.12
O	08.45	00.86	17.39
H	02.41	13.64	04.83
H	03.67	13.56	00.84
H	01.06	14.11	00.81
H	00.12	15.52	03.63
H	-00.76	14.26	02.70
H	-00.15	13.96	04.35
H	05.28	14.18	03.52
H	04.60	13.47	04.82
H	12.51	-00.39	19.86
H	11.61	-01.49	18.85
H	12.92	-00.62	18.10
H	11.65	01.54	18.66
H	10.37	00.53	19.25
H	04.84	11.07	03.70
H	05.70	12.01	02.41
H	06.37	12.06	03.92
C	03.03	10.29	07.48
N	02.86	09.19	08.29
C	03.87	08.33	08.08

N	04.57	08.76	07.08
C	04.13	10.05	06.74
C	01.76	09.06	09.19
C	06.00	08.32	06.92
C	07.09	09.22	07.43
O	10.99	08.13	00.53
S	10.50	09.50	00.23
O	09.33	09.39	-00.59
C	08.82	10.65	-00.81
C	07.57	10.38	-01.54
O	10.18	10.20	01.36
O	11.51	10.17	-00.48
H	03.91	07.48	08.78
H	04.70	10.54	06.00
H	02.31	11.04	07.57
H	00.87	09.07	08.54
H	01.88	08.07	09.63
H	01.72	09.86	09.91
H	06.13	07.35	07.32
H	06.30	08.02	05.85
H	07.28	11.24	-02.21
H	07.77	09.58	-02.26
H	06.76	10.09	-00.83
H	08.55	11.14	00.05
H	09.44	11.26	-01.46
H	08.08	08.78	07.36
H	07.13	10.19	06.91
H	06.89	09.53	08.44
C	03.83	02.47	02.19
N	02.64	02.43	01.46
C	02.11	01.23	01.52
N	02.96	00.45	02.14
C	04.02	01.19	02.57
C	01.89	03.61	00.99
C	02.96	-00.96	02.40
C	01.53	-01.43	02.60
O	14.51	11.37	15.56
S	13.68	10.28	15.92
O	12.41	10.33	15.30
C	11.61	11.48	15.58
C	10.58	11.83	14.48
O	14.28	09.07	15.57
O	13.53	10.35	17.30
H	01.13	00.88	01.09
H	04.67	00.82	03.30

H	04.41	03.39	02.38
H	00.89	03.42	00.64
H	01.87	04.20	01.86
H	02.59	04.16	00.31
H	03.37	-01.39	01.53
H	03.55	-01.10	03.36
H	11.08	11.75	13.56
H	09.67	11.23	14.64
H	10.29	12.90	14.63
H	11.14	11.49	16.62
H	12.28	12.30	15.67
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H	00.96	-01.32	01.67
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C	02.29	04.52	15.05
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O	09.53	12.41	03.38
S	09.16	12.61	04.71
O	08.35	13.70	04.80
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H	07.70	16.05	05.34
H	06.92	13.27	06.29
H	08.39	14.12	06.87
H	01.45	07.52	12.36
H	02.40	07.25	13.81
H	02.35	05.99	12.49

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C	11.31	09.46	08.15
C	12.63	09.25	08.79
O	05.57	18.99	13.45
S	06.71	19.35	14.19
O	07.31	18.12	14.69
C	07.87	17.32	13.66
C	08.58	16.07	14.15
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H	08.55	12.97	09.89
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H	10.83	08.40	08.06
H	11.41	09.75	07.15
H	07.96	15.46	14.75
H	08.85	15.47	13.35
H	09.45	16.37	14.67
H	07.06	17.06	12.96
H	08.68	17.79	13.09
H	13.26	10.04	08.70
H	12.42	09.17	09.87
H	13.19	08.37	08.53
C	15.36	03.61	12.87
N	16.64	04.10	13.10
C	17.43	03.90	11.98
N	16.59	03.50	11.01
C	15.35	03.26	11.58
C	17.09	04.62	14.42
C	16.98	03.31	09.64
C	16.98	04.53	08.79
O	05.39	02.62	12.93
S	06.53	03.40	13.17
O	06.43	04.11	14.43
C	06.11	03.37	15.58
C	05.96	04.27	16.77
O	07.65	02.57	13.21

O	06.63	04.26	12.14
H	18.47	03.91	11.98
H	14.62	02.92	10.94
H	14.53	03.68	13.58
H	16.42	05.39	14.73
H	17.22	03.82	15.16
H	18.05	04.90	14.28
H	18.07	03.22	09.72
H	16.34	02.52	09.28
H	06.19	03.71	17.70
H	06.61	05.17	16.77
H	04.96	04.67	16.80
H	05.25	02.69	15.42
H	06.89	02.67	15.78
H	17.57	05.34	09.13
H	17.48	04.25	07.83
H	16.00	04.98	08.73
C	14.34	13.18	12.66
N	13.33	12.53	11.90
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H	13.94	11.13	10.59
H	12.54	16.42	10.78
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H	09.55	06.95	06.47
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H	08.79	04.78	05.95

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H	13.46	12.77	17.50
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H	15.67	14.76	15.71
H	16.51	14.61	17.38
H	11.09	13.89	20.07
H	11.89	12.33	19.50
H	14.97	03.44	00.25
H	15.31	03.72	-01.49
H	14.21	02.49	-01.05
H	16.83	01.79	-01.49
H	15.91	01.12	-00.19
H	13.60	12.56	21.08
H	13.04	14.19	21.60
H	12.01	12.72	22.01
C	17.14	09.03	12.77
N	17.71	08.42	11.65
C	16.82	07.68	11.04
N	15.68	07.85	11.61
C	15.79	08.58	12.85
C	19.17	08.14	11.52
C	14.47	07.18	11.09
C	13.39	07.06	12.19
O	03.65	06.79	05.00
S	03.61	05.62	04.20
O	04.40	04.52	04.76

C	05.60	04.91	05.32
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O	02.25	05.19	04.03
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H	19.74	09.04	11.71
H	13.97	07.69	10.36
H	14.68	06.22	10.89
H	07.00	03.17	05.26
H	06.99	04.08	06.74
H	05.60	02.96	06.31
H	06.24	05.26	04.56
H	05.55	05.69	06.09
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H	13.18	08.08	12.57
H	12.43	06.90	11.73
C	02.89	15.21	06.72
N	02.53	16.21	05.85
C	01.20	16.45	05.95
N	00.67	15.67	06.90
C	01.72	14.89	07.41
C	03.43	16.83	04.80
C	-00.76	15.47	07.40
C	-01.29	16.80	07.84
O	11.23	06.79	15.40
S	10.11	07.39	16.04
O	08.97	07.41	15.16
C	09.27	08.04	13.88
C	09.06	07.25	12.61
O	09.80	06.62	17.17
O	10.42	08.73	16.44
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H	01.55	14.11	08.03
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H	04.45	16.69	05.15
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H	08.25	06.56	12.74

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N	15.99	08.89	06.91
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N	15.25	10.93	06.58
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C	14.59	12.21	06.11
C	13.25	12.36	06.91
O	00.29	17.17	16.77
S	00.23	17.21	15.37
O	-01.01	16.64	14.87
C	-01.84	17.40	14.03
C	-02.73	16.52	13.15
O	00.43	18.58	14.92
O	01.35	16.47	14.90
H	14.57	09.21	05.41
H	16.14	11.81	08.21
H	17.28	09.37	08.58
H	16.38	07.18	08.10
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C	04.69	07.83	11.61
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O	00.33	14.74	12.74
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H	06.23	07.94	15.96
H	06.49	11.57	14.61
H	05.72	11.08	16.14
H	07.26	10.60	15.72
H	04.23	06.89	11.71
H	04.01	08.55	11.21
H	02.98	18.11	13.09
H	03.70	17.62	11.54
H	02.54	19.06	11.63
H	01.28	17.39	10.79
H	00.89	17.28	12.42
H	05.77	07.25	09.81
H	06.35	08.84	10.45
H	06.61	07.27	11.26
C	14.71	00.37	04.45
N	13.73	-00.10	05.30
C	12.63	-00.26	04.62
N	12.83	00.03	03.35
C	14.14	00.49	03.23
C	13.89	-00.39	06.75
C	11.80	-00.18	02.34
C	11.73	-01.64	01.70
O	16.06	02.84	03.38
S	15.94	04.33	03.30
O	17.24	04.84	02.91
C	18.14	04.72	03.95
C	19.57	04.85	03.39
O	15.02	04.71	02.28
O	15.50	04.82	04.52
H	11.76	-00.72	04.96
H	14.57	00.84	02.27
H	15.64	00.77	04.82
H	13.68	-01.41	07.00
H	14.86	-00.09	07.05
H	13.20	00.40	07.23
H	10.89	-00.01	02.84

H	11.85	00.56	01.50
H	19.86	05.86	03.50
H	20.18	04.22	03.96
H	19.62	04.54	02.38
H	17.89	05.43	04.68
H	18.06	03.71	04.35
H	11.55	-02.37	02.44
H	10.75	-01.68	01.16
H	12.61	-01.79	01.11
C	18.29	12.04	01.64
N	17.21	12.73	02.12
C	16.33	12.79	01.12
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C	18.01	11.65	00.34
C	17.10	13.31	03.44
C	16.29	12.11	-01.32
C	16.58	10.72	-02.05
O	07.84	15.53	20.09
S	07.91	14.58	21.12
O	08.38	15.08	22.33
C	09.68	15.69	22.28
C	10.51	15.73	23.53
O	06.66	13.97	21.37
O	08.82	13.54	20.72
H	15.47	13.29	01.19
H	18.54	11.00	-00.30
H	19.13	12.03	02.26
H	17.94	13.51	04.11
H	16.67	14.30	03.06
H	16.27	12.77	03.95
H	15.31	12.43	-01.38
H	17.00	12.79	-01.89
H	10.19	16.44	24.24
H	10.39	14.74	23.93
H	11.56	15.97	23.43
H	10.26	15.10	21.63
H	09.67	16.72	21.83
H	17.60	10.75	-02.42
H	16.26	09.82	-01.54
H	16.05	10.85	-03.00
C	02.51	15.99	19.31
N	03.82	15.81	19.79
C	04.42	14.80	19.17
N	03.51	14.32	18.22
C	02.30	15.06	18.30

C	04.60	16.74	20.63
C	03.70	13.17	17.34
C	03.55	13.52	15.85
O	05.78	12.33	08.81
S	04.90	12.42	09.94
O	05.65	13.16	10.95
C	04.92	13.58	12.04
C	05.91	14.13	13.02
O	03.65	13.00	09.64
O	04.73	11.09	10.43
H	05.45	14.50	19.25
H	01.60	15.11	17.49
H	01.82	16.62	19.69
H	04.29	17.74	20.41
H	04.47	16.61	21.66
H	05.70	16.62	20.51
H	04.66	12.65	17.65
H	02.94	12.47	17.46
H	06.75	13.45	13.18
H	06.43	14.96	12.53
H	05.34	14.35	13.91
H	04.16	14.38	11.82
H	04.39	12.74	12.55
H	04.16	14.37	15.47
H	03.64	12.66	15.18
H	02.61	13.92	15.63

2 Computational Details

The simulations were performed in a cubic box with a cell vector of 1800 pm for the gas phase (1 ion pair) and 2049.85 pm for the bulk phase (27 ion pairs) and periodic boundary conditions, employing Born–Oppenheimer molecular dynamics simulations with an atom-centered Gaussian basis set to represent the Kohn–Sham orbitals and plane waves basis set for the electronic density using the program CP2k.[1,2] The simulations were carried out in the NVT ensemble, where the temperature was kept constant at 400 K by a Nose–Hoover chain thermostats.[3–5] A time step of 0.5 fs was chosen, and pseudopotentials from reference [6] replaced the core electrons of non-hydrogen atoms. The semi-empirical pair potential developed by Grimme et al.[7] was used to effectively account for dispersion effects (DFT-D2). The TZVP basis set represented the Kohn–Sham orbitals, and the plane wave representation was truncated with a cutoff of 280 Ry. The gradient-corrected BLYP functional[8,9] was used throughout the simulations. The systems were simulated for 325 ps (1 IP) and for 39 ps (27 IPs).

3 Additional Figures

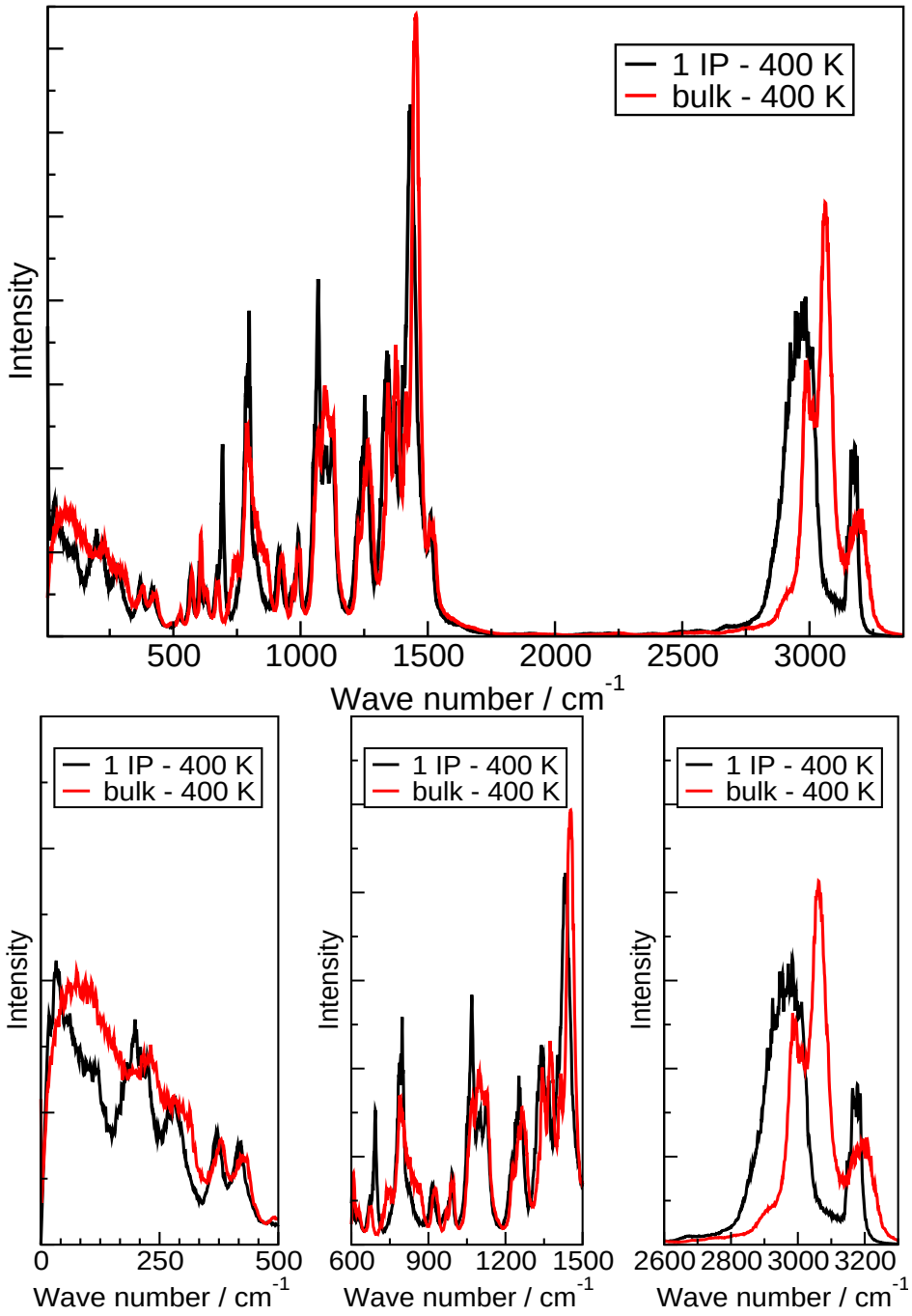

Figure **S1**: Comparison of the power spectrum obtained from the calculations with one ion pair (black curve) and of the bulk (red curve).

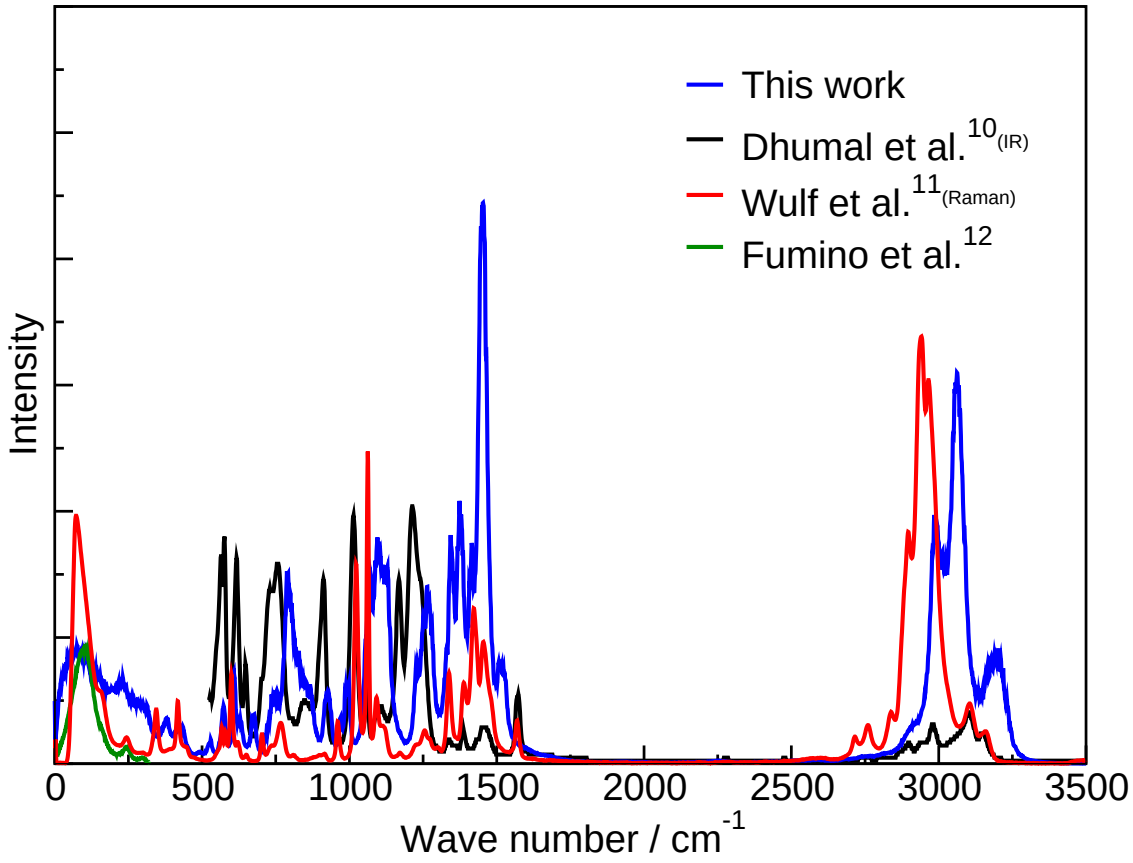

Figure **S2**: Comparison of the power spectrum obtained from the calculations of the bulk (blue curve) with the experimental IR-spectrum (black) provided by Dhumal et al.,[10] the experimental Raman-spectrum (red) provided by Wulf et al.[11]and the experimental far IR-spectrum (green) provided by Fumino et al.[12]

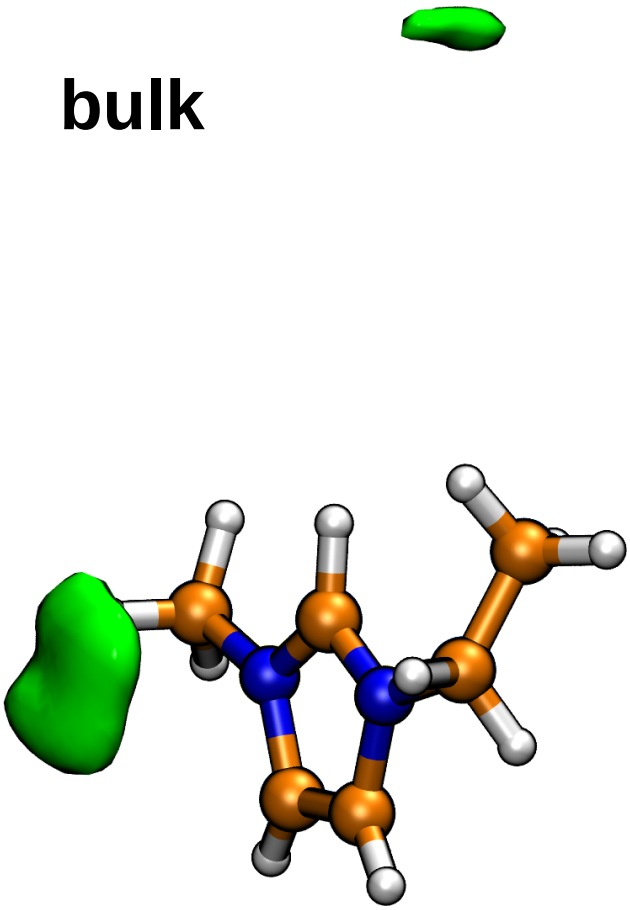

Figure **S3**: Spatial distribution function of the terminal carbon atom C7' (green) of the ethyl chain of the anion, which already interacts with the cation via the hydrogen atoms H2, H4 and H5 in the bulk phase.

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[2] *CP2k developers group (GNU General Public License) see http://cp2k.berlios.de/index.html.*

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