Supporting Information

The Effect of Mixture of Ionic Liquid and Organic Solvent on Oxygen Reduction Reaction Kinetics

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Force field parameters in Gromacs format

[atomtypes]

; name at.num mass charge ptype sigma epsilon

; DME

O	8	15.9994	-0.400	A	0.2900	0.58576
CT2	6	12.0112	0.140	A	0.3500	0.27614
CT3	6	12.0112	0.110	A	0.3500	0.27614
H	1	1.0079	0.030	A	0.2500	0.12552

; pyrrolidinium JPCB108(2004)16893

CT	6	12.011	-0.136	A	0.350	0.27614
HC	1	1.008	0.104	A	0.250	0.12552
NT	7	14.007	0.096	A	0.325	0.71128

; TFSI

SO	16	32.064	0.6	A	0.355	1.04600
OS	8	15.9994	-0.4	A	0.296	0.87864
FC	9	18.9984	-0.1	A	0.295	0.22175
CF	6	12.011	0.3	A	0.350	0.27614
NI	7	14.0027	-0.4	A	0.325	0.71128

; Li+ O2-

Li	3	6.941	0.7071	A	0.2126	0.07648
OA	8	15.9994	-0.35355	A	0.2960	0.87864
OAA	8	15.9994	-0.7071	A	0.2960	0.87864

; CO3 2-

CO	6	12.011	1.0227	A	0.3500	0.27614
OC	8	15.9994	-0.8123	A	0.2960	0.87864

[moleculetype]

;	molname	nrexcl
	DME	3

[atoms]

; nr	type	resnr	residu	atom	cgnr	charge	mass
1	CT3	1	DME	C1	1	0.110	12.0112
2	H	1	DME	H1	1	0.030	1.0079
3	H	1	DME	H2	1	0.030	1.0079
4	H	1	DME	H3	1	0.030	1.0079
5	CT2	1	DME	C2	1	0.140	12.0112
6	H	1	DME	H4	1	0.030	1.0079
7	H	1	DME	H5	1	0.030	1.0079
8	CT2	1	DME	C3	1	0.140	12.0112
9	H	1	DME	H6	1	0.030	1.0079
10	H	1	DME	H7	1	0.030	1.0079
11	CT3	1	DME	C4	1	0.110	12.0112
12	H	1	DME	H8	1	0.030	1.0079
13	H	1	DME	H9	1	0.030	1.0079
14	H	1	DME	H10	1	0.030	1.0079
15	O	1	DME	O1	1	-0.400	15.9994
16	O	1	DME	O2	1	-0.400	15.9994

[bonds]

; i	j	funct	length	force.c.
1	15	1	0.1410	267776
15	5	1	0.1410	267776
5	8	1	0.1529	224262.4
8	16	1	0.1410	267776

```
  16  11 1              0.1410  267776
   1   2  1              0.1090  284512
   1   3  1              0.1090  284512
   1   4  1              0.1090  284512
   5   6  1              0.1090  284512
   5   7  1              0.1090  284512
   8   9  1              0.1090  284512
   8  10  1              0.1090  284512
  11  12 1              0.1090  284512
  11  13 1              0.1090  284512
  11  14 1              0.1090  284512

[ angles ]
;  i    j   k    funct        angle       force.c.
   2   1   3       1              107.8   276.144
   3   1   4       1              107.8   276.144
   4   1   2       1              107.8   276.144
   1  15   5       1              109.5   502.08
  15   5   8       1              109.5   418.4
   5   8  16       1              109.5   418.4
   8  16  11       1              109.5   502.08
   2   1  15       1              109.5   292.88
   3   1  15       1              109.5   292.88
   4   1  15       1              109.5   292.88
  15   5   6       1              109.5   292.88
  15   5   7       1              109.5   292.88
   6   5   7       1              107.8   276.144
   6   5   8       1              110.7   313.8
   7   5   8       1              110.7   313.8
   5   8   9       1              110.7   313.8
   5   8  10       1              110.7   313.8
   9   8  16       1              109.5   292.88
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```
 10   8  16       1                109.5    292.88
  9   8  10       1                107.8    276.144
 16  11  12       1                109.5    292.88
 16  11  13       1                109.5    292.88
 16  11  14       1                109.5    292.88
 12  11  13       1                107.8    276.144
 13  11  14       1                107.8    276.144
 14  11  12       1                107.8    276.144

[ dihedrals ]
;  i    j   k    l       funct    C1          C2          C3          C4
   1  15   5   8    5     6.9781    -2.3652    -0.0138    -1.2263
  15   5   8  16    5    11.7980   -10.7136     3.4376    -3.8505
   5   8  16  11    5     6.9781    -2.3652    -0.0138    -1.2263
   2   1  15   5    5     0.0000     0.0000     3.1798     0.0000
   3   1  15   5    5     0.0000     0.0000     3.1798     0.0000
   4   1  15   5    5     0.0000     0.0000     3.1798     0.0000
   6   5  15   1    5     0.0000     0.0000     3.1798     0.0000
   7   5  15   1    5     0.0000     0.0000     3.1798     0.0000
   6   5   8   9    5     0.0000     0.0000     1.2552     0.0000
   7   5   8   9    5     0.0000     0.0000     1.2552     0.0000
   6   5   8  10    5     0.0000     0.0000     1.2552     0.0000
   7   5   8  10    5     0.0000     0.0000     1.2552     0.0000
  15   5   8   9    5     0.0000     0.0000     1.9581     0.0000
  15   5   8  10    5     0.0000     0.0000     1.9581     0.0000
   9   8  16  11    5     0.0000     0.0000     3.1798     0.0000
  10   8  16  11    5     0.0000     0.0000     3.1798     0.0000
   8  16  11  12    5     0.0000     0.0000     3.1798     0.0000
   8  16  11  13    5     0.0000     0.0000     3.1798     0.0000
   8  16  11  14    5     0.0000     0.0000     3.1798     0.0000
  16   8   5   6     5     0.0000     0.0000     1.9581     0.0000
  16   8   5   7     5     0.0000     0.0000     1.9581     0.0000
```

[moleculetype]

; Name nrexcl

PYR 3

[atoms]

; nr	type	resnr	residue	atom	cgnr	charge	mass
1	NT	1	PYR	N1	0	0.096	14.0067
2	CT	1	PYR	C2	1	-0.136	12.011
3	CT	1	PYR	C3	2	-0.136	12.011
4	CT	1	PYR	C4	3	0.008	12.011
5	CT	1	PYR	C5	4	0.008	12.011
6	CT	1	PYR	C6	5	-0.136	12.011
7	CT	1	PYR	C7	6	-0.136	12.011
8	HC	1	PYR	H8	7	0.104	1.008
9	HC	1	PYR	H9	8	0.104	1.008
10	HC	1	PYR	H10	9	0.104	1.008
11	HC	1	PYR	H11	10	0.104	1.008
12	HC	1	PYR	H12	11	0.048	1.008
13	HC	1	PYR	H13	12	0.048	1.008
14	HC	1	PYR	H14	13	0.048	1.008
15	HC	1	PYR	H15	14	0.048	1.008
16	HC	1	PYR	H16	15	0.104	1.008
17	HC	1	PYR	H17	16	0.104	1.008
18	HC	1	PYR	H18	17	0.104	1.008
19	HC	1	PYR	H19	18	0.104	1.008
20	HC	1	PYR	H20	19	0.104	1.008
21	CT	1	PYR	C21	20	0.008	12.011
22	HC	1	PYR	H22	21	0.048	1.008
23	HC	1	PYR	H23	22	0.048	1.008
24	CT	1	PYR	C24	23	-0.12	12.011
25	HC	1	PYR	H25	24	0.06	1.008

26	HC	1	PYR	H26	25	0.06	1.008
27	CT	1	PYR	C27	26	-0.18	12.011
28	HC	1	PYR	H28	27	0.06	1.008
29	HC	1	PYR	H29	28	0.06	1.008
30	HC	1	PYR	H30	29	0.06	1.008

[bonds]

; ai	aj	funct		
1	2	1	0.1471	307100.0
1	3	1	0.1471	307100.0
1	6	1	0.1471	307100.0
1	7	1	0.1471	307100.0
2	4	1	0.1529	224200
2	8	1	0.1090	284500
2	9	1	0.1090	284500
4	12	1	0.1090	284500
4	13	1	0.1090	284500
4	5	1	0.1529	224200
5	14	1	0.1090	284500
5	15	1	0.1090	284500
5	3	1	0.1529	224200
3	10	1	0.1090	284500
3	11	1	0.1090	284500
6	16	1	0.1090	284500
6	17	1	0.1090	284500
6	18	1	0.1090	284500
7	19	1	0.1090	284500
7	20	1	0.1090	284500
7	21	1	0.1529	224200
21	22	1	0.1090	284500
21	23	1	0.1090	284500
21	24	1	0.1529	224200

```
  24   25    1          0.1090  284500
  24   26    1          0.1090  284500
  24   27    1          0.1529  224200
  27   28    1          0.1090  284500
  27   29    1          0.1090  284500
  27   30    1          0.1090  284500

[ angles ]
;  ai   aj   ak funct       c0        c1        c2        c3
   2    4    5    1        112.7    488.3
   3    5    4    1        112.7    488.3
   7   21   24    1                 112.7    488.3
  21   24   27    1                 112.7    488.3

   2    4   12    1        110.7    313.8
   2    4   13    1        110.7    313.8
   4    2    8    1        110.7    313.8
   4    2    9    1        110.7    313.8
   4    5   14    1        110.7    313.8
   4    5   15    1        110.7    313.8
   5    4   12    1        110.7    313.8
   5    4   13    1        110.7    313.8
   5    3   10    1        110.7    313.8
   5    3   11    1        110.7    313.8
   3    5   14    1        110.7    313.8
   3    5   14    1        110.7    313.8
   7   21   22    1        110.7    313.8
   7   21   23    1        110.7    313.8
  21    7   19    1        110.7    313.8
  21    7   20    1        110.7    313.8
  21   24   25    1        110.7    313.8
  21   24   26    1        110.7    313.8
```

24	21	22	1	110.7	313.8
24	21	23	1	110.7	313.8
24	27	28	1	110.7	313.8
24	27	29	1	110.7	313.8
24	27	30	1	110.7	313.8
27	24	25	1	110.7	313.8
27	24	26	1	110.7	313.8
8	2	9	1	107.8	276.1
12	4	13	1	107.8	276.1
14	5	15	1	107.8	276.1
10	3	11	1	107.8	276.1
16	6	17	1	107.8	276.1
16	6	18	1	107.8	276.1
17	6	18	1	107.8	276.1
19	7	20	1	107.8	276.1
22	21	23	1	107.8	276.1
25	24	26	1	107.8	276.1
28	27	29	1	107.8	276.1
28	27	30	1	107.8	276.1
29	27	30	1	107.8	276.1
1	3	5	1	109.5	669.4
1	2	4	1	109.5	669.4
1	7	21	1	109.5	669.4
2	1	3	1	109.5	418.4
6	1	7	1	109.5	418.4
3	1	7	1	109.5	418.4
2	1	6	1	109.5	418.4
2	1	7	1	109.5	418.4
3	1	6	1	109.5	418.4

```
 10    3    1    1          109.5    209.2
 11    3    1    1          109.5    209.2
  8    2    1    1          109.5    209.2
  9    2    1    1          109.5    209.2
 16    6    1    1          109.5    209.2
 17    6    1    1          109.5    209.2
 18    6    1    1          109.5    209.2
 19    7    1    1          109.5    209.2
 20    7    1    1          109.5    209.2

[ dihedrals ]
;  ai    aj    ak    al funct         c0         c1         c2         c3         c4         c5
;HC-CT-CT-HC
  9    2    4   12    5     0.0000     0.0000     1.3305     0.0000
  9    2    4   13    5     0.0000     0.0000     1.3305     0.0000
  8    2    4   12    5     0.0000     0.0000     1.3305     0.0000
  8    2    4   13    5     0.0000     0.0000     1.3305     0.0000
 12    4    5   14    5     0.0000     0.0000     1.3305     0.0000
 12    4    5   15    5     0.0000     0.0000     1.3305     0.0000
 13    4    5   14    5     0.0000     0.0000     1.3305     0.0000
 13    4    5   15    5     0.0000     0.0000     1.3305     0.0000
 25   24   27   28    5     0.0000     0.0000     1.3305     0.0000
 25   24   27   29    5     0.0000     0.0000     1.3305     0.0000
 25   24   27   30    5     0.0000     0.0000     1.3305     0.0000
 26   24   27   28    5     0.0000     0.0000     1.3305     0.0000
 26   24   27   29    5     0.0000     0.0000     1.3305     0.0000
 26   24   27   30    5     0.0000     0.0000     1.3305     0.0000
 14    5    3   10    5     0.0000     0.0000     1.3305     0.0000
 14    5    3   11    5     0.0000     0.0000     1.3305     0.0000
 15    5    3   10    5     0.0000     0.0000     1.3305     0.0000
 15    5    3   11    5     0.0000     0.0000     1.3305     0.0000
```

19 7 21 23 5 0.0000 0.0000 1.3305 0.0000

19 7 21 22 5 0.0000 0.0000 1.3305 0.0000

20 7 21 23 5 0.0000 0.0000 1.3305 0.0000

20 7 21 22 5 0.0000 0.0000 1.3305 0.0000

22 21 24 25 5 0.0000 0.0000 1.3305 0.0000

22 21 24 26 5 0.0000 0.0000 1.3305 0.0000

23 21 24 25 5 0.0000 0.0000 1.3305 0.0000

23 21 24 26 5 0.0000 0.0000 1.3305 0.0000

;CT-CT-CT-HC

2 4 5 14 5 0.0000 0.0000 1.5313 0.0000

2 4 5 15 5 0.0000 0.0000 1.5313 0.0000

4 5 3 10 5 0.0000 0.0000 1.5313 0.0000

4 5 3 11 5 0.0000 0.0000 1.5313 0.0000

3 5 4 12 5 0.0000 0.0000 1.5313 0.0000

3 5 4 13 5 0.0000 0.0000 1.5313 0.0000

5 4 2 8 5 0.0000 0.0000 1.5313 0.0000

5 4 2 9 5 0.0000 0.0000 1.5313 0.0000

7 21 24 25 5 0.0000 0.0000 1.5313 0.0000

7 21 24 26 5 0.0000 0.0000 1.5313 0.0000

21 24 27 28 5 0.0000 0.0000 1.5313 0.0000

21 24 27 29 5 0.0000 0.0000 1.5313 0.0000

21 24 27 30 5 0.0000 0.0000 1.5313 0.0000

27 24 21 22 5 0.0000 0.0000 1.5313 0.0000

27 24 21 23 5 0.0000 0.0000 1.5313 0.0000

24 21 7 19 5 0.0000 0.0000 1.5313 0.0000

24 21 7 20 5 0.0000 0.0000 1.5313 0.0000

;CT-CT-CT-CT

2 4 5 3 5 7.2800 -0.6569 1.1673 0.0000

7 21 24 27 5 7.2800 -0.6569 1.1673 0.0000

;HC-CT-CT-NT

14 5 3 1 5 -4.2384 -2.9665 1.9790 0.0000

15 5 3 1 5 -4.2384 -2.9665 1.9790 0.0000

```
 12    4    2    1    5    -4.2384    -2.9665     1.9790     0.0000
 13    4    2    1    5    -4.2384    -2.9665     1.9790     0.0000
 22   21    7    1    5    -4.2384    -2.9665     1.9790     0.0000
 23   21    7    1    5    -4.2384    -2.9665     1.9790     0.0000
;CT-CT-CT-NT
  5    4    2    1    5    10.0081    -2.8200     2.3012     0.0000
  4    5    3    1    5    10.0081    -2.8200     2.3012     0.0000
 24   21    7    1    5    10.0081    -2.8200     2.3012     0.0000
;CT-NT-CT-CT
  2    1    3    5    5     1.7405    -0.5356     2.9079     0.0000
  2    1    7   21    5     1.7405    -0.5356     2.9079     0.0000
  3    1    2    4    5     1.7405    -0.5356     2.9079     0.0000
  3    1    7   21    5     1.7405    -0.5356     2.9079     0.0000
  7    1    3    5    5     1.7405    -0.5356     2.9079     0.0000
  7    1    2    4    5     1.7405    -0.5356     2.9079     0.0000
  6    1    2    4    5     1.7405    -0.5356     2.9079     0.0000
  6    1    3    5    5     1.7405    -0.5356     2.9079     0.0000
  6    1    7   21    5     1.7405    -0.5356     2.9079     0.0000
;HC-CT-NT-CT
  8    2    1    6    5     0.0000     0.0000     2.3430     0.0000
  9    2    1    6    5     0.0000     0.0000     2.3430     0.0000
  8    2    1    3    5     0.0000     0.0000     2.3430     0.0000
  9    2    1    3    5     0.0000     0.0000     2.3430     0.0000
  8    2    1    7    5     0.0000     0.0000     2.3430     0.0000
  9    2    1    7    5     0.0000     0.0000     2.3430     0.0000
 10    3    1    2    5     0.0000     0.0000     2.3430     0.0000
 11    3    1    2    5     0.0000     0.0000     2.3430     0.0000
 10    3    1    6    5     0.0000     0.0000     2.3430     0.0000
 11    3    1    6    5     0.0000     0.0000     2.3430     0.0000
 10    3    1    7    5     0.0000     0.0000     2.3430     0.0000
 11    3    1    7    5     0.0000     0.0000     2.3430     0.0000
 19    7    1    2    5     0.0000     0.0000     2.3430     0.0000
```

20	7	1	2	5	0.0000	0.0000	2.3430	0.0000
19	7	1	3	5	0.0000	0.0000	2.3430	0.0000
20	7	1	3	5	0.0000	0.0000	2.3430	0.0000
19	7	1	6	5	0.0000	0.0000	2.3430	0.0000
20	7	1	6	5	0.0000	0.0000	2.3430	0.0000
16	6	1	2	5	0.0000	0.0000	2.3430	0.0000
17	6	1	2	5	0.0000	0.0000	2.3430	0.0000
18	6	1	2	5	0.0000	0.0000	2.3430	0.0000
16	6	1	3	5	0.0000	0.0000	2.3430	0.0000
17	6	1	3	5	0.0000	0.0000	2.3430	0.0000
18	6	1	3	5	0.0000	0.0000	2.3430	0.0000
16	6	1	7	5	0.0000	0.0000	2.3430	0.0000
17	6	1	7	5	0.0000	0.0000	2.3430	0.0000
18	6	1	7	5	0.0000	0.0000	2.3430	0.0000

[moleculetype]

;	Name	nrexcl
	TFS	3

[atoms]

; nr	type	resnr	residue	atom	cgnr	charge	mass
1	NI	1	TFS	NI	1	-0.4	14.0067
2	SO	1	TFS	SO	2	0.6	32.06
3	SO	1	TFS	SO	3	0.6	32.06
4	OS	1	TFS	OS	4	-0.4	15.999
5	OS	1	TFS	OS	5	-0.4	15.999
6	OS	1	TFS	OS	6	-0.4	15.999
7	OS	1	TFS	OS	7	-0.4	15.999
8	CF	1	TFS	CF	8	0.3	12.011
9	CF	1	TFS	CF	9	0.3	12.011
10	FC	1	TFS	FC	10	-0.1	18.9984
11	FC	1	TFS	FC	11	-0.1	18.9984

12	FC	1	TFS	FC	12	-0.1	18.9984
13	FC	1	TFS	FC	13	-0.1	18.9984
14	FC	1	TFS	FC	14	-0.1	18.9984
15	FC	1	TFS	FC	15	-0.1	18.9984

[bonds]

1	2	1	0.1570	311300
1	3	1	0.1570	311300
2	6	1	0.1442	533100
2	7	1	0.1442	533100
2	9	1	0.1818	197000
3	8	1	0.1818	197000
3	4	1	0.1442	533100
3	5	1	0.1442	533100
8	10	1	0.1323	369700
8	11	1	0.1323	369700
8	12	1	0.1323	369700
9	13	1	0.1323	369700
9	14	1	0.1323	369700
9	15	1	0.1323	369700

[angles]

; FC-CF-FC

13	9	14	1	107.1	781	
13	9	15	1	107.1	781	
14	9	15	1	107.1	781	
10	8	11	1	107.1	781	
10	8	12	1	107.1	781	
11	8	12	1	107.1	781	

; FC-CF-SO

13	9	2	1	111.7	694	
14	9	2	1	111.7	694	

```
   15   9   2   1          111.7   694
    3   8  10   1          111.7   694
    3   8  11   1          111.7   694
    3   8  12   1          111.7   694
; CF-SO-OS
    9   2   6   1          102.6   870
    9   2   7   1          102.6   870
    9   2   1   1          102.6   870
    4   3   8   1          102.6   870
    5   3   8   1          102.6   870
; SO-NI-SO
    2   1   3   1          126.6   671
; OS-SO-NI
    6   2   1   1          113.6   789
    7   2   1   1          113.6   789
    1   3   4   1          113.6   789
    1   3   5   1          113.6   789
; NI-SO-CF
    1   3   8   1          100.2   816
; OS-SO-OS
    6   2   7   1          118.5   969
    4   3   5   1          118.5   969

[ dihedrals ]
; S-N-S-O
    3   1   2   6   5     0.0000    0.0000   -0.0150    0.0000
    3   1   2   7   5     0.0000    0.0000   -0.0150    0.0000
    2   1   3   4   5     0.0000    0.0000   -0.0150    0.0000
    2   1   3   5   5     0.0000    0.0000   -0.0150    0.0000
; N-S-C-F
    1   3   8  10   5     0.0000    0.0000    1.3220    0.0000
    1   3   8  11   5     0.0000    0.0000    1.3220    0.0000
```

```
   1    3    8   12    5     0.0000    0.0000    1.3220    0.0000
   1    2    9   13    5     0.0000    0.0000    1.3220    0.0000
   1    2    9   14    5     0.0000    0.0000    1.3220    0.0000
   1    2    9   15    5     0.0000    0.0000    1.3220    0.0000
; O-S-C-F
   5    3    8   10    5     0.0000    0.0000    1.4510    0.0000
   5    3    8   11    5     0.0000    0.0000    1.4510    0.0000
   5    3    8   12    5     0.0000    0.0000    1.4510    0.0000
   4    3    8   10    5     0.0000    0.0000    1.4510    0.0000
   4    3    8   11    5     0.0000    0.0000    1.4510    0.0000
   4    3    8   12    5     0.0000    0.0000    1.4510    0.0000
   6    2    9   13    5     0.0000    0.0000    1.4510    0.0000
   6    2    9   14    5     0.0000    0.0000    1.4510    0.0000
   6    2    9   15    5     0.0000    0.0000    1.4510    0.0000
   7    2    9   13    5     0.0000    0.0000    1.4510    0.0000
   7    2    9   14    5     0.0000    0.0000    1.4510    0.0000
   7    2    9   15    5     0.0000    0.0000    1.4510    0.0000
; S-N-S-C
   3    1    2    9    5    32.7730   -10.4200   -3.1950    0.0000
   2    1    3    8    5    32.7730   -10.4200   -3.1950    0.0000

[ moleculetype ]
;          molname                 nrexcl
           Li+                     1

[ atoms ]
;   nr     type              resnr          residu          atom          cgnr          charge  mass
    1      Li                3              Li+             Li1           1             0.7071  6.941

[ moleculetype ]
;          molname                 nrexcl
           O2-                     1
```

```
[ atoms ]
; OA - oxygen in superoxyde anion
;   nr     type          resnr          residu          atom          cgnr     charge  mass
     1      OA            4              O2-             OA1           1        -0.35355        15.9994
     2      OA            4              O2-             OA2           1        -0.35355        15.9994

[ bonds ]
;   i    j    funct          length   force.c.
     1    2    1              0.1340  357225.2

[ moleculetype ]
;          molname                 nrexcl
           O22-                    1

[ atoms ]
; OAA - oxygen in O2 2- ion
;   nr     type          resnr          residu          atom          cgnr                charge  mass
     1      OAA           4              O2-             OA1           1        -0.7071         15.9994
     2      OAA           4              O2-             OA2           1        -0.7071         15.9994

[ bonds ]
;   i    j    funct          length   force.c.
     1    2    1              0.1530  133826.7

[ moleculetype ]
;          molname                 nrexcl
           CO3                     1

[ atoms ]
; CO3 2-
;   nr     type          resnr          residu          atom          cgnr     charge  mass
```

```
   1      CO              4              CO3          CO          0       1.0227  12.011
   2      OC              4              CO3          OC1         1       -0.8123         15.9994
   3      OC              4              CO3          OC2         2       -0.8123         15.9994
   4      OC              4              CO3          OC3         3       -0.8123         15.9994

[ bonds ]
;  i    j    funct           length   force.c.
   1    2    1               0.130    612000
   1    3    1               0.130    612000
   1    4    1               0.130    612000

[ angles ]
;  ai   aj   ak   funct      c0       c1
; O-C-O
   2    1    3    1          120.0    1190
   3    1    4    1          120.0    1190
   4    1    2    1          120.0    1190

[ dihedrals ]
;  ai   aj   ak   al    funct   c0       c1
; O-C-O-O improper dihedral out of plane
   2    1    3    4     2       180.0      268
   4    1    2    3     2       180.0      268
   3    1    4    2     2       180.0      268
```