Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

FOR

Ion Mobility Calculations of Flexible All-Atom Systems at Arbitrary Fields Using Two-Temperature Theory.

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Explanation of Ion Mobility Types A-D.

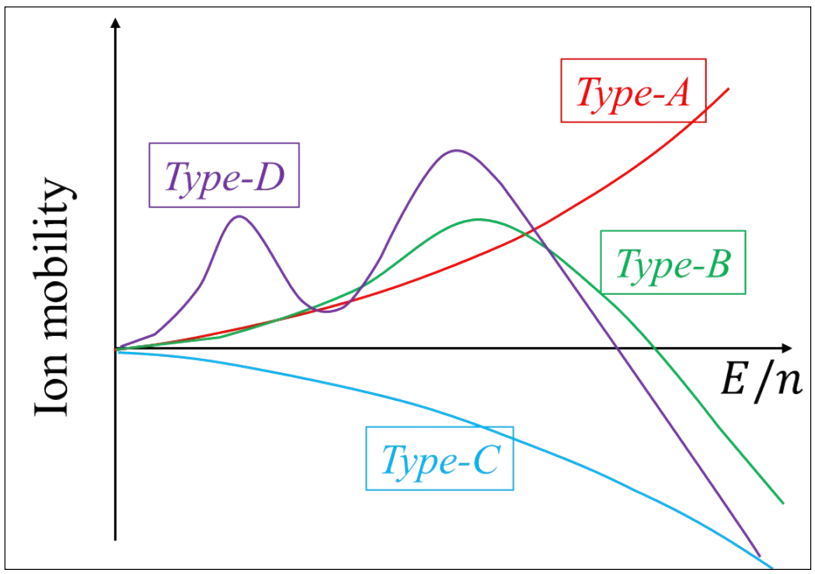

Figure S. 1: The plot illustrates the four distinct types of ion mobility as a function of electric field strength. Type-A mobility (red curve) shows a continuous increase with field strength, Type-B (green curve) demonstrates a peak before decreasing, Type-C (blue curve) represents a continuous decrease in mobility with increasing field strength, Type-D (purple curve) displays a complex behavior with multiple humps, reflecting intricate interactions between gas and ions. This supplementary figure aids in understanding the classification of ion mobility types mentioned in the manuscript. The figure is adapted from ref(1).

The ion mobility Vs E/n curve can be explained by a complex interplay of increasing collision energy (which reduces mobility) and diminishing capture effect of interatomic interactions (which increases mobility) as the field increases.

Type A mobility: At room temperature and low fields, the ion-induced dipole potential (r^{-4}) dominates the mobility behavior, particularly in small ions. As the relative velocity between ion and gas increases by increasing field, the "capture" effect of the ion-induced dipole interaction decreases which decreases the overall momentum transfer thus increasing the mobility.

Type B mobility: This is characterized by a singular distinctive peak in the mobility Vs E/n curve. At lower fields, Type B ions behave similarly to Type A, with mobility increasing due to diminishing capture effects of ion-induced dipole potential. However, as the electric field continues to increase, the ion reaches a point where the capture effect cannot diminish further. At this point, the mobility is dominated by the increased collision energy, which increases the drag on the ion leading to a reduction in mobility. It is shown in ref(2) that with given enough E/n range, all Type-A ion converts into Type-B ion.

Type C mobility: The mobility of these ions continuously decreases with increasing mobility. This behavior stems from the larger physical size of the ions, which inherently lacks the effects of the ion-induced dipole interaction. As the electric field is increased, these larger ions experience an increase in collision energy, leading to a continuous decrease in mobility.

Type D mobility: This behavior is only observed at cryogenic temperatures where the dispersion force component of the intermolecular forces, known by the r^{-6} component of the Lennard-Jones potential also moderately contributes to capture of gas along with r^{-4} potential at low field, an effect that is negligible at 300K, as demonstrated in ref(1). However, at cryogenic temperatures, the effect is observable. Here, as the relative velocity between ion and gas increases by increasing the field, the capture effect of the dispersion

force decreases, increasing mobility, consequently giving rise to the first peak. Subsequently, the collision energy increases with the field, decreasing the mobility until the r^{-4} potential influence decreases, giving rise to the second peak. The mobility peaks before being overtaken by hard sphere momentum transfer interactions, which lead to a subsequent continuous decrease in mobility.

The following sections contain the IMoS file results. In them, one can find the coordinates of the salts used, the mobility calculations for the two-temperature theory and the combined dispersion plots. It also includes the IMoS 1.13 Manual.

Independent Results for Three Structures of TDDA Salt:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_295_27.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_295_27.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_295_27.txt	295.00	312.0779	0.0000	0.0000	0.0000	0.0000	0.6657	0.6657	0.6657	0.6657
TDDA_295_27.txt	296.00	311.6951	16.6949	16.6897	16.6897	16.6897	0.6654	0.6656	0.6656	0.6656
TDDA_295_27.txt	297.00	311.4237	23.6294	23.6156	23.6155	23.6155	0.6649	0.6653	0.6653	0.6653
TDDA_295_27.txt	298.50	311.0390	31.2988	31.2676	31.2675	31.2675	0.6640	0.6647	0.6647	0.6647
TDDA_295_27.txt	300.00	310.6650	37.4580	37.4054	37.4051	37.4051	0.6631	0.6641	0.6641	0.6641
TDDA_295_27.txt	302.00	310.1155	44.3898	44.3035	44.3028	44.3028	0.6621	0.6635	0.6635	0.6635
TDDA_295_27.txt	305.00	309.1217	53.1480	53.0018	53.0002	53.0001	0.6610	0.6629	0.6629	0.6629
TDDA_295_27.txt	308.00	308.3246	60.7383	60.5236	60.5207	60.5204	0.6594	0.6619	0.6619	0.6619
TDDA_295_27.txt	312.00	307.2923	69.6724	69.3545	69.3491	69.3484	0.6574	0.6606	0.6606	0.6606
TDDA_295_27.txt	315.00	306.5770	75.7560	75.3537	75.3458	75.3448	0.6558	0.6595	0.6595	0.6595
TDDA_295_27.txt	320.00	305.3593	85.0283	84.4729	84.4597	84.4579	0.6532	0.6578	0.6579	0.6578
TDDA_295_27.txt	325.00	304.1019	93.4822	92.7596	92.7395	92.7366	0.6509	0.6563	0.6564	0.6563
TDDA_295_27.txt	330.00	302.7850	101.3054	100.4019	100.3732	100.3688	0.6487	0.6550	0.6551	0.6551
TDDA_295_27.txt	340.00	300.5196	115.7246	114.4338	114.3836	114.3751	0.6439	0.6518	0.6520	0.6519
TDDA_295_27.txt	350.00	298.3634	128.8748	127.1631	127.0857	127.0713	0.6393	0.6486	0.6489	0.6488
TDDA_295_27.txt	365.00	295.1132	146.8559	144.4541	144.3240	144.2974	0.6329	0.6444	0.6449	0.6447
TDDA_295_27.txt	380.00	292.0231	163.3901	160.2389	160.0426	159.9992	0.6268	0.6404	0.6412	0.6409
TDDA_295_27.txt	420.00	284.7625	203.1280	197.7798	197.3500	197.2399	0.6114	0.6298	0.6314	0.6309
TDDA_295_27.txt	470.00	277.3159	247.5996	239.2132	238.3907	238.1541	0.5935	0.6170	0.6196	0.6190
TDDA_295_27.txt	530.00	269.8743	296.5109	284.1489	282.7231	282.2732	0.5743	0.6029	0.6068	0.6062
TDDA_295_27.txt	600.00	262.6642	349.8112	332.5064	330.2322	329.4601	0.5546	0.5879	0.5934	0.5930
TDDA_295_27.txt	680.00	256.1431	408.0136	384.7830	381.3804	380.1548	0.5342	0.5718	0.5790	0.5788
TDDA_295_27.txt	770.00	250.3786	471.4077	441.3203	436.5107	434.6938	0.5136	0.5546	0.5635	0.5638
TDDA_295_27.txt	870.00	245.1286	539.7528	501.8632	495.3576	492.8011	0.4935	0.5374	0.5479	0.5487
TDDA_295_27.txt	980.00	240.4185	613.2442	566.6109	558.1067	554.6532	0.4741	0.5203	0.5323	0.5337
TDDA_295_27.txt	1100.00	236.3535	692.4105	636.2268	625.4757	620.9927	0.4552	0.5030	0.5163	0.5183

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_295_27.txt	0.0000	0.0000	0.0000	0.0000
TDDA_295_27.txt	16.6897	0.0006	-0.0002	16.6897
TDDA_295_27.txt	23.6155	0.0023	-0.0007	23.6155
TDDA_295_27.txt	31.2675	0.0062	-0.0015	31.2675
TDDA_295_27.txt	37.4051	0.0112	-0.0024	37.4051
TDDA_295_27.txt	44.3028	0.0187	-0.0034	44.3028
TDDA_295_27.txt	53.0001	0.0282	-0.0043	53.0001
TDDA_295_27.txt	60.5204	0.0399	-0.0057	60.5204
TDDA_295_27.txt	69.3484	0.0592	-0.0077	69.3484
TDDA_295_27.txt	75.3448	0.0762	-0.0093	75.3448
TDDA_295_27.txt	84.4579	0.1082	-0.0118	84.4579
TDDA_295_27.txt	92.7366	0.1437	-0.0141	92.7366
TDDA_295_27.txt	100.3688	0.1812	-0.0160	100.3688
TDDA_295_27.txt	114.3751	0.2695	-0.0208	114.3751
TDDA_295_27.txt	127.0713	0.3691	-0.0254	127.0713
TDDA_295_27.txt	144.2974	0.5271	-0.0316	144.2974
TDDA_295_27.txt	159.9992	0.6903	-0.0373	159.9992

TDDA_295_27.txt 197.2399 1.1838 -0.0522 197.2399
TDDA_295_27.txt 238.1541 1.9212 -0.0701 238.1541
TDDA_295_27.txt 282.2732 2.9140 -0.0894 282.2732
TDDA_295_27.txt 329.4601 4.1980 -0.1093 329.4601
TDDA_295_27.txt 380.1548 5.8279 -0.1306 380.1548
TDDA_295_27.txt 434.6938 7.8729 -0.1531 434.6938
TDDA_295_27.txt 492.8011 10.3182 -0.1758 492.8011
TDDA_295_27.txt 554.6532 13.1899 -0.1983 554.6532
TDDA_295_27.txt 620.9927 16.6185 -0.2215 620.9927

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 620.5757 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_390_25.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_390_25.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_390_25.txt	295.00	318.8685	0.0000	0.0000	0.0000	0.0000	0.6515	0.6515	0.6515	0.6515
TDDA_390_25.txt	296.00	318.5872	17.0640	17.0587	17.0587	17.0587	0.6510	0.6512	0.6512	0.6512
TDDA_390_25.txt	297.00	318.3619	24.1558	24.1415	24.1415	24.1415	0.6504	0.6508	0.6508	0.6508
TDDA_390_25.txt	298.50	317.9453	31.9938	31.9615	31.9614	31.9614	0.6496	0.6503	0.6503	0.6503
TDDA_390_25.txt	300.00	317.4760	38.2793	38.2248	38.2245	38.2245	0.6489	0.6499	0.6499	0.6499
TDDA_390_25.txt	302.00	316.8498	45.3538	45.2644	45.2637	45.2637	0.6480	0.6494	0.6494	0.6494
TDDA_390_25.txt	305.00	315.9245	54.3176	54.1662	54.1646	54.1645	0.6467	0.6486	0.6486	0.6486
TDDA_390_25.txt	308.00	315.1493	62.0827	61.8602	61.8574	61.8570	0.6452	0.6476	0.6476	0.6476
TDDA_390_25.txt	312.00	313.9666	71.1856	70.8557	70.8503	70.8496	0.6434	0.6466	0.6466	0.6466
TDDA_390_25.txt	315.00	313.1509	77.3804	76.9622	76.9541	76.9531	0.6420	0.6457	0.6458	0.6457
TDDA_390_25.txt	320.00	311.7680	86.8128	86.2347	86.2211	86.2193	0.6398	0.6444	0.6444	0.6444
TDDA_390_25.txt	325.00	310.7306	95.5198	94.7696	94.7491	94.7461	0.6370	0.6424	0.6425	0.6424
TDDA_390_25.txt	330.00	309.4283	103.5281	102.5907	102.5615	102.5569	0.6348	0.6410	0.6412	0.6411
TDDA_390_25.txt	340.00	307.0109	118.2243	116.8823	116.8311	116.8223	0.6303	0.6381	0.6384	0.6382
TDDA_390_25.txt	350.00	304.6815	131.6039	129.8191	129.7394	129.7244	0.6260	0.6353	0.6357	0.6355
TDDA_390_25.txt	365.00	301.3851	149.9770	147.4703	147.3361	147.3084	0.6197	0.6312	0.6318	0.6315
TDDA_390_25.txt	380.00	298.3437	166.9266	163.6433	163.4413	163.3963	0.6136	0.6270	0.6278	0.6276
TDDA_390_25.txt	420.00	290.9305	207.5277	201.9456	201.5008	201.3859	0.5985	0.6169	0.6184	0.6180
TDDA_390_25.txt	470.00	283.2816	252.9260	244.1529	243.2968	243.0487	0.5810	0.6045	0.6071	0.6066
TDDA_390_25.txt	530.00	275.9434	303.1791	290.2833	288.8077	288.3405	0.5617	0.5901	0.5941	0.5935
TDDA_390_25.txt	600.00	268.8544	358.0552	339.9953	337.6300	336.8258	0.5418	0.5750	0.5805	0.5800
TDDA_390_25.txt	680.00	262.3262	417.8629	393.6379	390.0951	388.8187	0.5216	0.5589	0.5661	0.5660
TDDA_390_25.txt	770.00	256.3943	482.7339	451.3467	446.3275	444.4310	0.5015	0.5423	0.5512	0.5515
TDDA_390_25.txt	870.00	251.1495	553.0102	513.4997	506.6939	504.0182	0.4817	0.5253	0.5358	0.5366
TDDA_390_25.txt	980.00	246.4533	628.6375	580.0780	571.1983	567.5907	0.4625	0.5083	0.5202	0.5216
TDDA_390_25.txt	1100.00	242.2431	709.6643	651.1015	639.8275	635.1169	0.4441	0.4916	0.5048	0.5069

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_390_25.txt	0.0000	0.0000	0.0000	0.0000
TDDA_390_25.txt	17.0587	0.0013	-0.0005	17.0587
TDDA_390_25.txt	24.1415	0.0038	-0.0012	24.1415

TDDA_390_25.txt	31.9614	0.0078	-0.0020	31.9614
TDDA_390_25.txt	38.2245	0.0116	-0.0025	38.2245
TDDA_390_25.txt	45.2637	0.0168	-0.0033	45.2637
TDDA_390_25.txt	54.1645	0.0254	-0.0045	54.1645
TDDA_390_25.txt	61.8570	0.0380	-0.0060	61.8570
TDDA_390_25.txt	70.8496	0.0563	-0.0076	70.8496
TDDA_390_25.txt	76.9531	0.0723	-0.0089	76.9531
TDDA_390_25.txt	86.2193	0.1012	-0.0110	86.2193
TDDA_390_25.txt	94.7461	0.1408	-0.0140	94.7461
TDDA_390_25.txt	102.5569	0.1817	-0.0160	102.5569
TDDA_390_25.txt	116.8223	0.2676	-0.0204	116.8223
TDDA_390_25.txt	129.7244	0.3607	-0.0246	129.7244
TDDA_390_25.txt	147.3084	0.5179	-0.0307	147.3084
TDDA_390_25.txt	163.3963	0.6920	-0.0368	163.3963
TDDA_390_25.txt	201.3859	1.1941	-0.0515	201.3859
TDDA_390_25.txt	243.0487	1.9320	-0.0690	243.0487
TDDA_390_25.txt	288.3405	2.9706	-0.0891	288.3405
TDDA_390_25.txt	336.8258	4.3243	-0.1097	336.8258
TDDA_390_25.txt	388.8187	6.0307	-0.1314	388.8187
TDDA_390_25.txt	444.4310	8.1383	-0.1536	444.4310
TDDA_390_25.txt	504.0182	10.6853	-0.1764	504.0182
TDDA_390_25.txt	567.5907	13.6884	-0.1994	567.5907
TDDA_390_25.txt	635.1169	17.1513	-0.2221	635.1169

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
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Total Trajectories = 900000

Max time step = 1.00e-13 second
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Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 639.9028 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_480_18.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_480_18.txt.

Results

Summary of ion calculations:
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Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_480_18.txt	295.00	333.5457	0.0000	0.0000	0.0000	0.0000	0.6229	0.6229	0.6229	0.6229
TDDA_480_18.txt	296.00	333.1468	17.8439	17.8383	17.8382	17.8382	0.6226	0.6228	0.6228	0.6228
TDDA_480_18.txt	297.00	332.9022	25.2591	25.2439	25.2439	25.2439	0.6220	0.6223	0.6223	0.6223
TDDA_480_18.txt	298.50	332.3186	33.4401	33.4059	33.4058	33.4058	0.6215	0.6221	0.6221	0.6221
TDDA_480_18.txt	300.00	331.8359	40.0107	39.9529	39.9526	39.9526	0.6208	0.6218	0.6218	0.6218
TDDA_480_18.txt	302.00	331.3505	47.4294	47.3347	47.3340	47.3340	0.6197	0.6210	0.6210	0.6210
TDDA_480_18.txt	305.00	330.4794	56.8200	56.6600	56.6583	56.6582	0.6183	0.6201	0.6201	0.6201
TDDA_480_18.txt	308.00	329.5636	64.9223	64.6868	64.6837	64.6833	0.6169	0.6193	0.6193	0.6193
TDDA_480_18.txt	312.00	328.5058	74.4821	74.1336	74.1277	74.1270	0.6150	0.6180	0.6180	0.6180
TDDA_480_18.txt	315.00	327.6319	80.9587	80.5170	80.5083	80.5072	0.6137	0.6172	0.6173	0.6172
TDDA_480_18.txt	320.00	326.2020	90.8320	90.2204	90.2056	90.2036	0.6115	0.6159	0.6160	0.6159
TDDA_480_18.txt	325.00	324.8557	99.8620	99.0649	99.0424	99.0391	0.6093	0.6145	0.6146	0.6146
TDDA_480_18.txt	330.00	323.5544	108.2544	107.2589	107.2268	107.2217	0.6071	0.6131	0.6133	0.6132
TDDA_480_18.txt	340.00	320.9892	123.6071	122.1796	122.1230	122.1132	0.6029	0.6105	0.6107	0.6106
TDDA_480_18.txt	350.00	318.5176	137.5802	135.6776	135.5888	135.5722	0.5988	0.6079	0.6083	0.6081
TDDA_480_18.txt	365.00	315.1478	156.8256	154.1558	154.0064	153.9756	0.5927	0.6038	0.6044	0.6042
TDDA_480_18.txt	380.00	312.1096	174.6287	171.1358	170.9118	170.8619	0.5865	0.5996	0.6005	0.6002
TDDA_480_18.txt	420.00	304.4636	217.1812	211.2444	210.7505	210.6233	0.5719	0.5898	0.5914	0.5909
TDDA_480_18.txt	470.00	296.8104	265.0052	255.7122	254.7695	254.4972	0.5545	0.5773	0.5799	0.5794
TDDA_480_18.txt	530.00	288.9906	317.5139	303.8326	302.1982	301.6808	0.5363	0.5640	0.5679	0.5674
TDDA_480_18.txt	600.00	281.6128	375.0466	355.9210	353.3149	352.4283	0.5173	0.5494	0.5549	0.5546

TDDA_480_18.txt	680.00	275.0276	438.0952	412.5102	408.6338	407.2366	0.4975	0.5335	0.5407	0.5406
TDDA_480_18.txt	770.00	268.9201	506.3172	473.2116	467.7380	465.6684	0.4782	0.5175	0.5262	0.5266
TDDA_480_18.txt	870.00	263.5271	580.2646	538.6434	531.2510	528.3431	0.4591	0.5010	0.5113	0.5122
TDDA_480_18.txt	980.00	258.7479	659.9976	608.9260	599.3188	595.4165	0.4405	0.4844	0.4961	0.4975
TDDA_480_18.txt	1100.00	254.4165	745.3269	683.8427	671.6956	666.6222	0.4229	0.4683	0.4811	0.4832

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_480_18.txt	0.0000	0.0000	0.0000	0.0000
TDDA_480_18.txt	17.8382	0.0015	-0.0002	17.8382
TDDA_480_18.txt	25.2439	0.0044	-0.0008	25.2439
TDDA_480_18.txt	33.4058	0.0066	-0.0012	33.4058
TDDA_480_18.txt	39.9526	0.0088	-0.0018	39.9526
TDDA_480_18.txt	47.3340	0.0149	-0.0030	47.3340
TDDA_480_18.txt	56.6582	0.0274	-0.0045	56.6582
TDDA_480_18.txt	64.6833	0.0420	-0.0057	64.6833
TDDA_480_18.txt	74.1270	0.0670	-0.0078	74.1270
TDDA_480_18.txt	80.5072	0.0864	-0.0091	80.5072
TDDA_480_18.txt	90.2036	0.1184	-0.0111	90.2036
TDDA_480_18.txt	99.0391	0.1524	-0.0133	99.0391
TDDA_480_18.txt	107.2217	0.1900	-0.0155	107.2217
TDDA_480_18.txt	122.1132	0.2736	-0.0197	122.1132
TDDA_480_18.txt	135.5722	0.3649	-0.0237	135.5722
TDDA_480_18.txt	153.9756	0.5184	-0.0300	153.9756
TDDA_480_18.txt	170.8619	0.7012	-0.0365	170.8619
TDDA_480_18.txt	210.6233	1.2400	-0.0513	210.6233
TDDA_480_18.txt	254.4972	2.0549	-0.0698	254.4972
TDDA_480_18.txt	301.6808	3.1615	-0.0891	301.6808
TDDA_480_18.txt	352.4283	4.5675	-0.1097	352.4283
TDDA_480_18.txt	407.2366	6.3900	-0.1321	407.2366
TDDA_480_18.txt	465.6684	8.6204	-0.1545	465.6684
TDDA_480_18.txt	528.3431	11.2881	-0.1777	528.3431
TDDA_480_18.txt	595.4165	14.4889	-0.2012	595.4165
TDDA_480_18.txt	666.6222	18.2358	-0.2243	666.6222

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 650.696 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.130
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000

P 0.4167763200 3.5000000000
Ca 0.4167763200 3.5000000000
Li 0.4167763200 3.5000000000
S 0.4167763200 3.5000000000
Other 0.4167763200 3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_295_27.txt	295.00	312.0779	0.0000	0.0000	0.0000	0.0000	0.6657	0.6657	0.6657	0.6657
TDDA_295_27.txt	296.00	311.6951	16.6949	16.6897	16.6897	16.6897	0.6654	0.6656	0.6656	0.6656
TDDA_295_27.txt	297.00	311.4237	23.6294	23.6156	23.6155	23.6155	0.6649	0.6653	0.6653	0.6653
TDDA_295_27.txt	298.50	311.0390	31.2988	31.2676	31.2675	31.2675	0.6640	0.6647	0.6647	0.6647
TDDA_295_27.txt	300.00	310.6650	37.4580	37.4054	37.4051	37.4051	0.6631	0.6641	0.6641	0.6641
TDDA_295_27.txt	302.00	310.1155	44.3898	44.3035	44.3028	44.3028	0.6621	0.6635	0.6635	0.6635
TDDA_295_27.txt	305.00	309.1217	53.1480	53.0018	53.0002	53.0001	0.6610	0.6629	0.6629	0.6629
TDDA_295_27.txt	308.00	308.3246	60.7383	60.5236	60.5207	60.5204	0.6594	0.6619	0.6619	0.6619
TDDA_295_27.txt	312.00	307.2923	69.6724	69.3545	69.3491	69.3484	0.6574	0.6606	0.6606	0.6606
TDDA_295_27.txt	315.00	306.5770	75.7560	75.3537	75.3458	75.3448	0.6558	0.6595	0.6595	0.6595
TDDA_295_27.txt	320.00	305.3593	85.0283	84.4729	84.4597	84.4579	0.6532	0.6578	0.6579	0.6578
TDDA_295_27.txt	325.00	304.1019	93.4822	92.7596	92.7395	92.7366	0.6509	0.6563	0.6564	0.6563
TDDA_295_27.txt	330.00	302.7850	101.3054	100.4019	100.3732	100.3688	0.6487	0.6550	0.6551	0.6551
TDDA_295_27.txt	340.00	300.5196	115.7246	114.4338	114.3836	114.3751	0.6439	0.6518	0.6520	0.6519
TDDA_295_27.txt	350.00	298.3634	128.8748	127.1631	127.0857	127.0713	0.6393	0.6486	0.6489	0.6488
TDDA_295_27.txt	365.00	295.1132	146.8559	144.4541	144.3240	144.2974	0.6329	0.6444	0.6449	0.6447
TDDA_295_27.txt	380.00	292.0231	163.3901	160.2389	160.0426	159.9992	0.6268	0.6404	0.6412	0.6409
TDDA_295_27.txt	420.00	284.7625	203.1280	197.7798	197.3500	197.2399	0.6114	0.6298	0.6314	0.6309
TDDA_295_27.txt	470.00	277.3159	247.5996	239.2132	238.3907	238.1541	0.5935	0.6170	0.6196	0.6190
TDDA_295_27.txt	530.00	269.8743	296.5109	284.1489	282.7231	282.2732	0.5743	0.6029	0.6068	0.6062
TDDA_295_27.txt	600.00	262.6642	349.8112	332.5064	330.2322	329.4601	0.5546	0.5879	0.5934	0.5930
TDDA_295_27.txt	680.00	256.1431	408.0136	384.7830	381.3804	380.1548	0.5342	0.5718	0.5790	0.5788
TDDA_295_27.txt	770.00	250.3786	471.4077	441.3203	436.5107	434.6938	0.5136	0.5546	0.5635	0.5638
TDDA_295_27.txt	870.00	245.1286	539.7528	501.8632	495.3576	492.8011	0.4935	0.5374	0.5479	0.5487
TDDA_295_27.txt	980.00	240.4185	613.2442	566.6109	558.1067	554.6532	0.4741	0.5203	0.5323	0.5337
TDDA_295_27.txt	1100.00	236.3535	692.4105	636.2268	625.4757	620.9927	0.4552	0.5030	0.5163	0.5183
TDDA_390_25.txt	295.00	318.8685	0.0000	0.0000	0.0000	0.0000	0.6515	0.6515	0.6515	0.6515
TDDA_390_25.txt	296.00	318.5872	17.0640	17.0587	17.0587	17.0587	0.6510	0.6512	0.6512	0.6512
TDDA_390_25.txt	297.00	318.3619	24.1558	24.1415	24.1415	24.1415	0.6504	0.6508	0.6508	0.6508
TDDA_390_25.txt	298.50	317.9453	31.9938	31.9615	31.9614	31.9614	0.6496	0.6503	0.6503	0.6503
TDDA_390_25.txt	300.00	317.4760	38.2793	38.2248	38.2245	38.2245	0.6489	0.6499	0.6499	0.6499
TDDA_390_25.txt	302.00	316.8498	45.3538	45.2644	45.2637	45.2637	0.6480	0.6494	0.6494	0.6494
TDDA_390_25.txt	305.00	315.9245	54.3176	54.1662	54.1646	54.1645	0.6467	0.6486	0.6486	0.6486
TDDA_390_25.txt	308.00	315.1493	62.0827	61.8602	61.8574	61.8570	0.6452	0.6476	0.6476	0.6476
TDDA_390_25.txt	312.00	313.9666	71.1856	70.8557	70.8503	70.8496	0.6434	0.6466	0.6466	0.6466
TDDA_390_25.txt	315.00	313.1509	77.3804	76.9622	76.9541	76.9531	0.6420	0.6457	0.6458	0.6457
TDDA_390_25.txt	320.00	311.7680	86.8128	86.2347	86.2211	86.2193	0.6398	0.6444	0.6444	0.6444
TDDA_390_25.txt	325.00	310.7306	95.5198	94.7696	94.7491	94.7461	0.6370	0.6424	0.6425	0.6424
TDDA_390_25.txt	330.00	309.4283	103.5281	102.5907	102.5615	102.5569	0.6348	0.6410	0.6412	0.6411
TDDA_390_25.txt	340.00	307.0109	118.2243	116.8823	116.8311	116.8223	0.6303	0.6381	0.6384	0.6382
TDDA_390_25.txt	350.00	304.6815	131.6039	129.8191	129.7394	129.7244	0.6260	0.6353	0.6357	0.6355
TDDA_390_25.txt	365.00	301.3851	149.9770	147.4703	147.3361	147.3084	0.6197	0.6312	0.6318	0.6315
TDDA_390_25.txt	380.00	298.3437	166.9266	163.6433	163.4413	163.3963	0.6136	0.6270	0.6278	0.6276
TDDA_390_25.txt	420.00	290.9305	207.5277	201.9456	201.5008	201.3859	0.5985	0.6169	0.6184	0.6180
TDDA_390_25.txt	470.00	283.2816	252.9260	244.1529	243.2968	243.0487	0.5810	0.6045	0.6071	0.6066
TDDA_390_25.txt	530.00	275.9434	303.1791	290.2833	288.8077	288.3405	0.5617	0.5901	0.5941	0.5935
TDDA_390_25.txt	600.00	268.8544	358.0552	339.9953	337.6300	336.8258	0.5418	0.5750	0.5805	0.5800
TDDA_390_25.txt	680.00	262.3262	417.8629	393.6379	390.0951	388.8187	0.5216	0.5589	0.5661	0.5660
TDDA_390_25.txt	770.00	256.3943	482.7339	451.3467	446.3275	444.4310	0.5015	0.5423	0.5512	0.5515
TDDA_390_25.txt	870.00	251.1495	553.0102	513.4997	506.6939	504.0182	0.4817	0.5253	0.5358	0.5366
TDDA_390_25.txt	980.00	246.4533	628.6375	580.0780	571.1983	567.5907	0.4625	0.5083	0.5202	0.5216

TDDA_390_25.txt	1100.00	242.2431	709.6643	651.1015	639.8275	635.1169	0.4441	0.4916	0.5048	0.5069
TDDA_480_18.txt	295.00	333.5457	0.0000	0.0000	0.0000	0.0000	0.6229	0.6229	0.6229	0.6229
TDDA_480_18.txt	296.00	333.1468	17.8439	17.8383	17.8382	17.8382	0.6226	0.6228	0.6228	0.6228
TDDA_480_18.txt	297.00	332.9022	25.2591	25.2439	25.2439	25.2439	0.6220	0.6223	0.6223	0.6223
TDDA_480_18.txt	298.50	332.3186	33.4401	33.4059	33.4058	33.4058	0.6215	0.6221	0.6221	0.6221
TDDA_480_18.txt	300.00	331.8359	40.0107	39.9529	39.9526	39.9526	0.6208	0.6218	0.6218	0.6218
TDDA_480_18.txt	302.00	331.3505	47.4294	47.3347	47.3340	47.3340	0.6197	0.6210	0.6210	0.6210
TDDA_480_18.txt	305.00	330.4794	56.8200	56.6600	56.6583	56.6582	0.6183	0.6201	0.6201	0.6201
TDDA_480_18.txt	308.00	329.5636	64.9223	64.6868	64.6837	64.6833	0.6169	0.6193	0.6193	0.6193
TDDA_480_18.txt	312.00	328.5058	74.4821	74.1336	74.1277	74.1270	0.6150	0.6180	0.6180	0.6180
TDDA_480_18.txt	315.00	327.6319	80.9587	80.5170	80.5083	80.5072	0.6137	0.6172	0.6173	0.6172
TDDA_480_18.txt	320.00	326.2020	90.8320	90.2204	90.2056	90.2036	0.6115	0.6159	0.6160	0.6159
TDDA_480_18.txt	325.00	324.8557	99.8620	99.0649	99.0424	99.0391	0.6093	0.6145	0.6146	0.6146
TDDA_480_18.txt	330.00	323.5544	108.2544	107.2589	107.2268	107.2217	0.6071	0.6131	0.6133	0.6132
TDDA_480_18.txt	340.00	320.9892	123.6071	122.1796	122.1230	122.1132	0.6029	0.6105	0.6107	0.6106
TDDA_480_18.txt	350.00	318.5176	137.5802	135.6776	135.5888	135.5722	0.5988	0.6079	0.6083	0.6081
TDDA_480_18.txt	365.00	315.1478	156.8256	154.1558	154.0064	153.9756	0.5927	0.6038	0.6044	0.6042
TDDA_480_18.txt	380.00	312.1096	174.6287	171.1358	170.9118	170.8619	0.5865	0.5996	0.6005	0.6002
TDDA_480_18.txt	420.00	304.4636	217.1812	211.2444	210.7505	210.6233	0.5719	0.5898	0.5914	0.5909
TDDA_480_18.txt	470.00	296.8104	265.0052	255.7122	254.7695	254.4972	0.5545	0.5773	0.5799	0.5794
TDDA_480_18.txt	530.00	288.9906	317.5139	303.8326	302.1982	301.6808	0.5363	0.5640	0.5679	0.5674
TDDA_480_18.txt	600.00	281.6128	375.0466	355.9210	353.3149	352.4283	0.5173	0.5494	0.5549	0.5546
TDDA_480_18.txt	680.00	275.0276	438.0952	412.5102	408.6338	407.2366	0.4975	0.5335	0.5407	0.5406
TDDA_480_18.txt	770.00	268.9201	506.3172	473.2116	467.7380	465.6684	0.4782	0.5175	0.5262	0.5266
TDDA_480_18.txt	870.00	263.5271	580.2646	538.6434	531.2510	528.3431	0.4591	0.5010	0.5113	0.5122
TDDA_480_18.txt	980.00	258.7479	659.9976	608.9260	599.3188	595.4165	0.4405	0.4844	0.4961	0.4975
TDDA_480_18.txt	1100.00	254.4165	745.3269	683.8427	671.6956	666.6222	0.4229	0.4683	0.4811	0.4832

TAA_multiTemperature_candidate2.xlsx - Sheet #1

x	y	z	Radius	Charge	Atom
11.245000	-6.793640	-0.613950	1.55000	0.0067114000	14
10.755000	-8.171380	-1.111000	1.70000	0.0067114000	1 12
11.074100	-9.373160	-0.230350	1.70000	0.0067114000	12
10.337900	-10.63610	-0.759200	1.70000	0.0067114000	690 12
10.563300	-11.80610	0.135020	1.70000	0.0067114000	12
10.045100	-11.73810	1.580600	1.70000	0.0067114000	12
11.086800	-11.35550	2.577000	1.70000	0.0067114000	12
10.487900	-10.76280	3.853000	1.70000	0.0067114000	12
11.591700	-10.34290	4.918300	1.70000	0.0067114000	12
12.404300	-9.177060	4.381900	1.70000	0.0067114000	12
11.677600	-7.817870	4.437000	1.70000	0.0067114000	12
12.565600	-6.567150	4.075300	1.70000	0.0067114000	12
11.837200	-5.313840	4.591300	1.70000	0.0067114000	12
11.132300	-5.784770	-1.749000	1.70000	0.0067114000	12
9.770790	-5.562390	-2.466500	1.70000	0.0067114000	12
9.846020	-4.717950	-3.785200	1.70000	0.0067114000	12
10.210600	-3.268330	-3.639700	1.70000	0.0067114000	12
9.717580	-2.337030	-4.734600	1.70000	0.0067114000	12
10.209700	-0.879950	-4.716800	1.70000	0.0067114000	12
9.754270	-0.237051	-3.438000	1.70000	0.0067114000	12
10.329900	1.092930	-3.128800	1.70000	0.0067114000	12
10.017100	1.493740	-1.674200	1.70000	0.0067114000	12
8.639990	2.126520	-1.656400	1.70000	0.0067114000	12
8.056250	2.105870	-0.172420	1.70000	0.0067114000	12
6.763250	2.998650	-0.177120	1.70000	0.0067114000	12
10.570800	-6.312920	0.674460	1.70000	0.0067114000	12
9.085290	-6.097140	0.621600	1.70000	0.0067114000	12
8.485170	-5.793630	2.043000	1.70000	0.0067114000	12
6.979520	-5.655650	2.046800	1.70000	0.0067114000	12
6.175460	-6.807870	1.342800	1.70000	0.0067114000	12
6.594590	-8.210990	1.785500	1.70000	0.0067114000	12
6.373430	-8.478130	3.291600	1.70000	0.0067114000	12
6.397300	-10.02350	3.574100	1.70000	0.0067114000	12
6.300080	-10.20640	5.089700	1.70000	0.0067114000	12
6.384840	-11.66690	5.541500	1.70000	0.0067114000	12
6.267410	-12.06850	7.094100	1.70000	0.0067114000	12
6.328690	-13.62620	7.248400	1.70000	0.0067114000	12
12.732700	-6.891870	-0.076261	1.70000	0.0067114000	12
13.749900	-7.165220	-1.216400	1.70000	0.0067114000	12
15.200200	-7.213800	-0.728150	1.70000	0.0067114000	12
15.840700	-6.039180	-0.007511	1.70000	0.0067114000	12
16.088000	-4.736920	-0.868340	1.70000	0.0067114000	12
14.849200	-3.725560	-0.744260	1.70000	0.0067114000	12
15.294300	-2.432400	-1.521000	1.70000	0.0067114000	12
14.222900	-1.315250	-1.607800	1.70000	0.0067114000	12

14.850700	-0.020165	-2.066100	1.70000	0.0067114000	12
15.808100	0.601212	-0.933120	1.70000	0.0067114000	12
16.296700	2.024960	-1.369400	1.70000	0.0067114000	12
17.163100	2.537690	-0.219520	1.70000	0.0067114000	12
9.705510	-8.292010	-1.371400	1.10000	0.0067114000	1
11.273500	-8.246130	-2.037400	1.10000	0.0067114000	1
12.175500	-9.543910	-0.128880	1.10000	0.0067114000	1
10.725600	-9.182930	0.856550	1.10000	0.0067114000	1
9.207590	-10.34100	-0.746940	1.10000	0.0067114000	1
10.595400	-11.01170	-1.784700	1.10000	0.0067114000	1
10.035800	-12.68230	-0.396700	1.10000	0.0067114000	1
11.697500	-12.07980	0.105180	1.10000	0.0067114000	1
9.234440	-10.99850	1.687200	1.10000	0.0067114000	1
9.619540	-12.68090	1.944500	1.10000	0.0067114000	1
11.831100	-12.11830	2.757900	1.10000	0.0067114000	1
11.703000	-10.53710	2.021200	1.10000	0.0067114000	1
9.747380	-9.915310	3.724100	1.10000	0.0067114000	1
9.824700	-11.59580	4.309600	1.10000	0.0067114000	1
11.228300	-9.858010	5.812100	1.10000	0.0067114000	1
12.152200	-11.23830	5.310100	1.10000	0.0067114000	1
13.324300	-9.179270	5.030900	1.10000	0.0067114000	1
12.857200	-9.568620	3.369100	1.10000	0.0067114000	1
10.925500	-7.884370	3.614900	1.10000	0.0067114000	1
11.297900	-7.666900	5.429100	1.10000	0.0067114000	1
13.503900	-6.770060	4.671800	1.10000	0.0067114000	1
12.746700	-6.356510	2.998500	1.10000	0.0067114000	1
12.467000	-4.415900	4.459600	1.10000	0.0067114000	1
10.866800	-5.102440	4.154300	1.10000	0.0067114000	1
11.637700	-5.508350	5.693000	1.10000	0.0067114000	1
11.551300	-4.790270	-1.538200	1.10000	0.0067114000	1
11.785700	-6.144590	-2.643400	1.10000	0.0067114000	1
9.350650	-6.548400	-2.635600	1.10000	0.0067114000	1
8.983280	-5.027110	-1.872400	1.10000	0.0067114000	1
10.647400	-5.137810	-4.331200	1.10000	0.0067114000	1
8.946800	-4.786040	-4.457500	1.10000	0.0067114000	1
9.680150	-3.031070	-2.715500	1.10000	0.0067114000	1
11.268700	-3.079880	-3.428400	1.10000	0.0067114000	1
10.181600	-2.862610	-5.727700	1.10000	0.0067114000	1
8.575520	-2.253570	-4.661700	1.10000	0.0067114000	1
11.323800	-0.896496	-4.669900	1.10000	0.0067114000	1
9.854320	-0.180062	-5.501500	1.10000	0.0067114000	1
8.615810	-0.071302	-3.399000	1.10000	0.0067114000	1
9.924540	-0.810896	-2.513600	1.10000	0.0067114000	1
11.406500	1.163810	-3.420900	1.10000	0.0067114000	1
10.048100	1.995200	-3.702900	1.10000	0.0067114000	1
10.067100	0.530019	-1.097800	1.10000	0.0067114000	1
10.826200	2.043150	-1.225500	1.10000	0.0067114000	1
7.776990	1.755960	-2.294100	1.10000	0.0067114000	1
8.813140	3.223520	-1.859500	1.10000	0.0067114000	1
7.971090	1.062110	0.176570	1.10000	0.0067114000	1
8.842930	2.468290	0.559310	1.10000	0.0067114000	1
6.950450	4.092980	-0.289510	1.10000	0.0067114000	1
6.047750	2.609320	-0.982650	1.10000	0.0067114000	1
6.171990	2.806810	0.679100	1.10000	0.0067114000	1
10.631700	-7.117250	1.431800	1.10000	0.0067114000	1
10.987700	-5.357770	1.027000	1.10000	0.0067114000	1
8.848700	-5.202500	0.023456	1.10000	0.0067114000	1
8.581500	-6.969910	0.185380	1.10000	0.0067114000	1
8.973650	-6.604670	2.594800	1.10000	0.0067114000	1
8.867220	-4.838450	2.401300	1.10000	0.0067114000	1
6.513110	-5.492720	3.028900	1.10000	0.0067114000	1
6.661570	-4.653880	1.539500	1.10000	0.0067114000	1
5.119080	-6.627720	1.736600	1.10000	0.0067114000	1
6.174110	-6.563210	0.316660	1.10000	0.0067114000	1
5.909680	-8.940360	1.354500	1.10000	0.0067114000	1
7.578420	-8.491480	1.471300	1.10000	0.0067114000	1
7.265700	-8.148800	3.783500	1.10000	0.0067114000	1
5.469470	-7.972900	3.810300	1.10000	0.0067114000	1
5.682660	-10.65050	3.039800	1.10000	0.0067114000	1
7.481080	-10.37510	3.227600	1.10000	0.0067114000	1
7.073190	-9.617860	5.507000	1.10000	0.0067114000	1
5.317630	-9.655180	5.459200	1.10000	0.0067114000	1
5.549570	-12.17450	5.096200	1.10000	0.0067114000	1
7.206010	-12.07260	4.967700	1.10000	0.0067114000	1
5.329430	-11.61780	7.565400	1.10000	0.0067114000	1
7.091620	-11.62700	7.642600	1.10000	0.0067114000	1
6.218060	-13.85040	8.287900	1.10000	0.0067114000	1
7.382260	-13.87390	6.959900	1.10000	0.0067114000	1
5.528260	-14.11390	6.660200	1.10000	0.0067114000	1
12.965600	-5.862770	0.338100	1.10000	0.0067114000	1

12.807600	-7.617020	0.709390	1.10000	0.0067114000	1
13.459500	-8.113830	-1.621700	1.10000	0.0067114000	1
13.680000	-6.331540	-1.981200	1.10000	0.0067114000	1
15.449700	-8.103840	-0.069326	1.10000	0.0067114000	1
15.792900	-7.454130	-1.650500	1.10000	0.0067114000	1
15.170000	-5.939420	0.937610	1.10000	0.0067114000	1
16.878100	-6.279270	0.340140	1.10000	0.0067114000	1
17.010600	-4.262360	-0.481660	1.10000	0.0067114000	1
16.311200	-5.025020	-1.922600	1.10000	0.0067114000	1
13.951200	-4.051120	-1.332100	1.10000	0.0067114000	1
14.559300	-3.404120	0.286800	1.10000	0.0067114000	1
16.130600	-2.183680	-0.895880	1.10000	0.0067114000	1
15.551100	-2.577520	-2.590800	1.10000	0.0067114000	1
13.475900	-1.571870	-2.388300	1.10000	0.0067114000	1
13.838000	-1.075040	-0.488690	1.10000	0.0067114000	1
15.537300	-0.279990	-2.882400	1.10000	0.0067114000	1
14.131200	0.680190	-2.534300	1.10000	0.0067114000	1
15.202200	0.638080	-0.015153	1.10000	0.0067114000	1
16.749100	0.001803	-0.743200	1.10000	0.0067114000	1
16.864300	2.097060	-2.329400	1.10000	0.0067114000	1
15.439000	2.680370	-1.430100	1.10000	0.0067114000	1
18.039500	1.792880	-0.214130	1.10000	0.0067114000	1
17.633300	3.535310	-0.491640	1.10000	0.0067114000	1
16.751300	2.483970	0.841370	1.10000	0.0067114000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #2

x	y	z	Radius	Charge	Atom		
9.861900	-4.248160	-1.183800	1.55000	0.0067114000			14
10.018700	-4.754160	0.252220	1.70000	0.0067114000		1	12
8.689220	-4.990170	1.109400	1.70000	0.0067114000			12
8.657960	-6.403790	1.617300	1.70000	0.0067114000		690	12
9.851520	-7.010100	2.336700	1.70000	0.0067114000			12
9.410420	-8.163950	3.232400	1.70000	0.0067114000			12
8.824350	-9.330680	2.345100	1.70000	0.0067114000			12
8.420220	-10.53670	3.156400	1.70000	0.0067114000			12
8.114860	-11.86670	2.371600	1.70000	0.0067114000			12
9.349980	-12.81820	2.447200	1.70000	0.0067114000			12
9.288560	-14.16500	1.636900	1.70000	0.0067114000			12
10.743100	-14.78920	1.896700	1.70000	0.0067114000			12
11.857500	-14.10920	1.031500	1.70000	0.0067114000			12
11.211600	-4.253770	-1.898900	1.70000	0.0067114000			12
12.358300	-3.341710	-1.378600	1.70000	0.0067114000			12
13.617300	-4.108460	-1.794800	1.70000	0.0067114000			12
13.986700	-5.306800	-0.725440	1.70000	0.0067114000			12
14.318800	-5.091940	0.761180	1.70000	0.0067114000			12
15.475300	-4.069120	0.853900	1.70000	0.0067114000			12
16.127700	-3.883260	2.278500	1.70000	0.0067114000			12
16.563800	-5.155020	3.064400	1.70000	0.0067114000			12
17.672300	-5.998460	2.322600	1.70000	0.0067114000			12
17.900100	-7.464430	2.844500	1.70000	0.0067114000			12
19.398800	-7.770900	2.926900	1.70000	0.0067114000			12
20.057600	-7.670190	1.455500	1.70000	0.0067114000			12
8.933670	-5.170270	-2.007900	1.70000	0.0067114000			12
9.519190	-6.576290	-1.963600	1.70000	0.0067114000			12
8.328780	-7.609040	-2.080400	1.70000	0.0067114000			12
8.807090	-8.975820	-2.596100	1.70000	0.0067114000			12
9.617670	-9.653180	-1.547100	1.70000	0.0067114000			12
10.370400	-10.88980	-1.994500	1.70000	0.0067114000			12
11.470400	-10.72700	-3.056100	1.70000	0.0067114000			12
12.467700	-9.591820	-2.720700	1.70000	0.0067114000			12
13.361800	-9.943700	-1.424400	1.70000	0.0067114000			12
14.706800	-9.234990	-1.436200	1.70000	0.0067114000			12
15.592200	-9.586190	-0.188800	1.70000	0.0067114000			12
15.912300	-11.02170	0.005199	1.70000	0.0067114000			12
9.161330	-2.777330	-1.208500	1.70000	0.0067114000			12
9.692230	-1.608470	-0.366830	1.70000	0.0067114000			12
8.920310	-0.327402	-0.629790	1.70000	0.0067114000			12
9.570630	0.891276	0.056550	1.70000	0.0067114000			12
8.595680	2.063280	-0.016932	1.70000	0.0067114000			12
7.388460	2.100300	1.006800	1.70000	0.0067114000			12
6.155400	2.882420	0.628880	1.70000	0.0067114000			12
5.002880	2.793360	1.652800	1.70000	0.0067114000			12
4.234700	4.079430	1.915200	1.70000	0.0067114000			12
3.095560	4.007560	2.952600	1.70000	0.0067114000			12
2.702640	5.493730	3.241800	1.70000	0.0067114000			12
2.229990	5.678640	4.761400	1.70000	0.0067114000			12
10.764200	-5.579030	0.344120	1.10000	0.0067114000			1
10.609500	-3.993420	0.743120	1.10000	0.0067114000			1

8.734950	-4.257950	1.974100	1.10000	0.0067114000	1
7.735860	-4.686940	0.536730	1.10000	0.0067114000	1
7.770000	-6.686860	2.313700	1.10000	0.0067114000	1
8.475100	-6.962060	0.597840	1.10000	0.0067114000	1
10.616200	-7.364380	1.646400	1.10000	0.0067114000	1
10.207700	-6.270170	3.069200	1.10000	0.0067114000	1
10.225100	-8.664180	3.790300	1.10000	0.0067114000	1
8.532180	-7.919610	4.005300	1.10000	0.0067114000	1
7.906970	-9.150260	1.813600	1.10000	0.0067114000	1
9.686040	-9.661330	1.653400	1.10000	0.0067114000	1
9.220820	-10.80480	3.843800	1.10000	0.0067114000	1
7.476590	-10.29720	3.695100	1.10000	0.0067114000	1
7.215840	-12.45710	2.784300	1.10000	0.0067114000	1
7.704650	-11.66840	1.300100	1.10000	0.0067114000	1
10.088500	-12.28430	1.839400	1.10000	0.0067114000	1
9.505750	-13.12190	3.527300	1.10000	0.0067114000	1
8.527860	-14.88170	2.119800	1.10000	0.0067114000	1
9.018930	-13.95670	0.538100	1.10000	0.0067114000	1
10.923500	-14.86640	2.958500	1.10000	0.0067114000	1
10.623300	-15.86680	1.535400	1.10000	0.0067114000	1
11.411800	-14.01450	0.053579	1.10000	0.0067114000	1
11.964300	-13.04910	1.421100	1.10000	0.0067114000	1
12.812300	-14.66460	0.948310	1.10000	0.0067114000	1
11.540100	-5.232320	-1.867500	1.10000	0.0067114000	1
11.203500	-4.263890	-2.991900	1.10000	0.0067114000	1
12.477500	-2.342320	-1.783500	1.10000	0.0067114000	1
12.392000	-3.194660	-0.255730	1.10000	0.0067114000	1
13.512800	-4.740500	-2.744500	1.10000	0.0067114000	1
14.559500	-3.515220	-1.922800	1.10000	0.0067114000	1
13.285600	-6.120320	-0.753960	1.10000	0.0067114000	1
14.904900	-5.679150	-1.236600	1.10000	0.0067114000	1
13.444200	-4.846800	1.426800	1.10000	0.0067114000	1
14.865400	-6.029670	1.025800	1.10000	0.0067114000	1
16.392200	-4.231010	0.202810	1.10000	0.0067114000	1
15.005800	-3.151720	0.461540	1.10000	0.0067114000	1
17.013300	-3.243600	2.130400	1.10000	0.0067114000	1
15.355800	-3.330930	2.889800	1.10000	0.0067114000	1
16.997400	-5.033210	4.102500	1.10000	0.0067114000	1
15.564300	-5.736170	3.112900	1.10000	0.0067114000	1
17.466100	-5.924290	1.198200	1.10000	0.0067114000	1
18.560000	-5.373210	2.457000	1.10000	0.0067114000	1
17.245600	-8.054110	2.198400	1.10000	0.0067114000	1
17.409800	-7.456270	3.873100	1.10000	0.0067114000	1
19.785300	-6.969200	3.646400	1.10000	0.0067114000	1
19.337500	-8.747490	3.430400	1.10000	0.0067114000	1
20.892400	-8.398090	1.245900	1.10000	0.0067114000	1
19.386900	-8.127010	0.713990	1.10000	0.0067114000	1
20.394300	-6.606500	1.221100	1.10000	0.0067114000	1
8.002220	-5.192370	-1.498700	1.10000	0.0067114000	1
8.626610	-4.827540	-3.038300	1.10000	0.0067114000	1
10.136900	-6.705130	-2.821800	1.10000	0.0067114000	1
10.250000	-6.890200	-1.161500	1.10000	0.0067114000	1
7.735710	-7.734710	-1.099500	1.10000	0.0067114000	1
7.777830	-7.105050	-2.939500	1.10000	0.0067114000	1
8.009190	-9.549670	-3.032400	1.10000	0.0067114000	1
9.504290	-8.820220	-3.519100	1.10000	0.0067114000	1
10.323200	-9.025130	-1.066900	1.10000	0.0067114000	1
8.927750	-9.919600	-0.776110	1.10000	0.0067114000	1
10.893400	-11.50700	-1.203900	1.10000	0.0067114000	1
9.545500	-11.52890	-2.449200	1.10000	0.0067114000	1
11.855700	-11.70200	-3.350800	1.10000	0.0067114000	1
10.958800	-10.40330	-4.012900	1.10000	0.0067114000	1
13.228300	-9.634930	-3.514700	1.10000	0.0067114000	1
11.976600	-8.600040	-2.680200	1.10000	0.0067114000	1
12.836700	-9.617340	-0.485470	1.10000	0.0067114000	1
13.631900	-10.99320	-1.243800	1.10000	0.0067114000	1
15.325300	-9.503430	-2.344400	1.10000	0.0067114000	1
14.573800	-8.089620	-1.615800	1.10000	0.0067114000	1
15.069800	-9.056930	0.710900	1.10000	0.0067114000	1
16.586200	-9.117740	-0.186310	1.10000	0.0067114000	1
14.905100	-11.32640	0.426710	1.10000	0.0067114000	1
16.630700	-11.31170	0.798100	1.10000	0.0067114000	1
16.278200	-11.57870	-0.869780	1.10000	0.0067114000	1
9.360760	-2.488020	-2.241800	1.10000	0.0067114000	1
8.109870	-2.892920	-1.138300	1.10000	0.0067114000	1
9.591300	-1.877080	0.730920	1.10000	0.0067114000	1
10.742100	-1.404050	-0.479960	1.10000	0.0067114000	1
8.954720	-0.281748	-1.703700	1.10000	0.0067114000	1
7.915920	-0.573113	-0.322470	1.10000	0.0067114000	1
9.851350	0.675906	1.104900	1.10000	0.0067114000	1

10.541300	1.045390	-0.424580	1.10000	0.0067114000	1
9.283490	2.944610	-0.015158	1.10000	0.0067114000	1
8.202780	2.021610	-1.107100	1.10000	0.0067114000	1
7.052380	1.061760	1.215200	1.10000	0.0067114000	1
7.697980	2.563950	1.911100	1.10000	0.0067114000	1
6.418540	3.921720	0.265490	1.10000	0.0067114000	1
5.666100	2.334820	-0.221540	1.10000	0.0067114000	1
4.259620	1.995340	1.584600	1.10000	0.0067114000	1
5.458930	2.451910	2.643900	1.10000	0.0067114000	1
5.009450	4.773470	2.411800	1.10000	0.0067114000	1
4.061920	4.792870	1.000900	1.10000	0.0067114000	1
2.287310	3.334320	2.483100	1.10000	0.0067114000	1
3.528930	3.437310	3.789700	1.10000	0.0067114000	1
3.469320	6.241280	2.995100	1.10000	0.0067114000	1
1.909410	5.720220	2.508800	1.10000	0.0067114000	1
1.979880	4.741030	5.276600	1.10000	0.0067114000	1
3.008440	6.132260	5.452900	1.10000	0.0067114000	1
1.333080	6.359490	4.627200	1.10000	0.0067114000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #3

x	y	z	Radius	Charge	Atom	
10.703900	-6.105630	-0.796950	1.55000	0.0067114000		14
11.809700	-7.090090	-1.098800	1.70000	0.0067114000	1	12
13.194300	-6.836570	-0.287470	1.70000	0.0067114000		12
14.144200	-8.033550	-0.665960	1.70000	0.0067114000	690	12
15.015400	-8.006270	-1.896800	1.70000	0.0067114000		12
16.383500	-7.435310	-1.691500	1.70000	0.0067114000		12
16.516300	-5.963490	-1.380600	1.70000	0.0067114000		12
17.740400	-5.244390	-1.967100	1.70000	0.0067114000		12
19.051000	-5.886290	-1.568300	1.70000	0.0067114000		12
19.048600	-5.720160	0.016875	1.70000	0.0067114000		12
20.353100	-5.921630	0.705390	1.70000	0.0067114000		12
21.253500	-7.138240	0.323390	1.70000	0.0067114000		12
20.724300	-8.524250	0.585410	1.70000	0.0067114000		12
9.554630	-6.364670	-1.803300	1.70000	0.0067114000		12
8.939120	-7.778290	-1.653300	1.70000	0.0067114000		12
7.544710	-7.991510	-2.544700	1.70000	0.0067114000		12
6.981130	-9.462120	-2.343300	1.70000	0.0067114000		12
6.803370	-10.00710	-0.772040	1.70000	0.0067114000		12
5.592430	-9.339530	-0.124760	1.70000	0.0067114000		12
5.731110	-9.231320	1.549100	1.70000	0.0067114000		12
4.828310	-8.147780	2.091700	1.70000	0.0067114000		12
3.315320	-8.402210	2.161800	1.70000	0.0067114000		12
2.475780	-7.591260	3.144200	1.70000	0.0067114000		12
2.720040	-7.765150	4.593900	1.70000	0.0067114000		12
2.369430	-6.619680	5.580300	1.70000	0.0067114000		12
10.269500	-6.230000	0.584870	1.70000	0.0067114000		12
9.202750	-5.308140	1.313000	1.70000	0.0067114000		12
8.751600	-6.073080	2.482500	1.70000	0.0067114000		12
7.687370	-5.232850	3.215700	1.70000	0.0067114000		12
7.070310	-5.792580	4.465400	1.70000	0.0067114000		12
8.165580	-6.092100	5.553300	1.70000	0.0067114000		12
8.582080	-7.566050	5.879200	1.70000	0.0067114000		12
7.387870	-8.422240	6.505100	1.70000	0.0067114000		12
6.391140	-9.190050	5.693400	1.70000	0.0067114000		12
5.743620	-10.46010	6.202600	1.70000	0.0067114000		12
4.859190	-10.97410	5.061700	1.70000	0.0067114000		12
3.818240	-11.99260	5.731000	1.70000	0.0067114000		12
11.123100	-4.560680	-0.824650	1.70000	0.0067114000		12
11.633800	-3.957720	-2.198800	1.70000	0.0067114000		12
11.651100	-2.398540	-2.178000	1.70000	0.0067114000		12
12.978200	-1.761170	-1.860800	1.70000	0.0067114000		12
12.754800	-0.211492	-2.141400	1.70000	0.0067114000		12
12.295300	0.544744	-0.870460	1.70000	0.0067114000		12
12.304000	2.040380	-0.910100	1.70000	0.0067114000		12
13.687000	2.760200	-1.147400	1.70000	0.0067114000		12
13.727000	3.211870	-2.596500	1.70000	0.0067114000		12
15.186500	3.468790	-3.059300	1.70000	0.0067114000		12
15.216400	3.944560	-4.561100	1.70000	0.0067114000		12
14.884900	5.401240	-4.699200	1.70000	0.0067114000		12
11.359200	-8.103260	-1.115700	1.10000	0.0067114000		1
12.142600	-6.949370	-2.198100	1.10000	0.0067114000		1
13.666600	-5.909270	-0.640860	1.10000	0.0067114000		1
12.987900	-6.728140	0.876340	1.10000	0.0067114000		1
14.915300	-8.179880	0.189250	1.10000	0.0067114000		1
13.576000	-8.963660	-0.776290	1.10000	0.0067114000		1
15.265100	-9.037220	-2.136500	1.10000	0.0067114000		1
14.434000	-7.724150	-2.772500	1.10000	0.0067114000		1

17.157200	-7.932830	-1.214700	1.10000	0.0067114000	1
16.787100	-7.533700	-2.719100	1.10000	0.0067114000	1
15.703700	-5.368470	-1.705800	1.10000	0.0067114000	1
16.476300	-5.840670	-0.287680	1.10000	0.0067114000	1
17.646000	-5.391820	-3.053300	1.10000	0.0067114000	1
17.691700	-4.123840	-1.739900	1.10000	0.0067114000	1
19.181700	-6.907180	-1.952300	1.10000	0.0067114000	1
19.889500	-5.433300	-2.091900	1.10000	0.0067114000	1
18.380400	-4.877370	0.531190	1.10000	0.0067114000	1
18.552300	-6.631110	0.392920	1.10000	0.0067114000	1
20.923700	-4.930250	0.469650	1.10000	0.0067114000	1
20.103300	-5.891270	1.807300	1.10000	0.0067114000	1
21.394700	-7.001420	-0.740200	1.10000	0.0067114000	1
22.290800	-7.080640	0.764720	1.10000	0.0067114000	1
21.005900	-8.763790	1.606200	1.10000	0.0067114000	1
19.621900	-8.666720	0.385660	1.10000	0.0067114000	1
21.085300	-9.258470	-0.100200	1.10000	0.0067114000	1
8.799730	-5.624640	-1.582100	1.10000	0.0067114000	1
9.922350	-6.222330	-2.831600	1.10000	0.0067114000	1
9.711400	-8.473510	-2.053800	1.10000	0.0067114000	1
8.737260	-7.998240	-0.637460	1.10000	0.0067114000	1
6.747130	-7.286000	-2.174300	1.10000	0.0067114000	1
7.883720	-7.925410	-3.668400	1.10000	0.0067114000	1
6.020530	-9.501830	-2.824700	1.10000	0.0067114000	1
7.584360	-10.13850	-2.928300	1.10000	0.0067114000	1
6.690010	-11.16210	-0.843260	1.10000	0.0067114000	1
7.771310	-9.919520	-0.188180	1.10000	0.0067114000	1
5.790890	-8.341930	-0.519280	1.10000	0.0067114000	1
4.550020	-9.862620	-0.267190	1.10000	0.0067114000	1
5.553470	-10.13400	2.237000	1.10000	0.0067114000	1
6.859650	-9.187750	1.684900	1.10000	0.0067114000	1
5.316430	-7.839240	3.119000	1.10000	0.0067114000	1
5.046280	-7.268210	1.436900	1.10000	0.0067114000	1
3.008250	-8.456540	1.105700	1.10000	0.0067114000	1
3.295960	-9.455050	2.655600	1.10000	0.0067114000	1
1.427360	-7.695770	2.820100	1.10000	0.0067114000	1
2.272260	-6.521050	2.880800	1.10000	0.0067114000	1
2.664350	-8.803930	4.956200	1.10000	0.0067114000	1
3.780560	-7.417630	4.579200	1.10000	0.0067114000	1
2.485310	-5.608290	5.059100	1.10000	0.0067114000	1
1.274430	-6.814830	5.745400	1.10000	0.0067114000	1
2.947210	-6.692710	6.528600	1.10000	0.0067114000	1
9.942060	-7.325320	0.739740	1.10000	0.0067114000	1
11.170900	-6.162440	1.228400	1.10000	0.0067114000	1
9.789840	-4.390360	1.615700	1.10000	0.0067114000	1
8.279010	-5.060390	0.744680	1.10000	0.0067114000	1
8.415350	-7.050230	1.991900	1.10000	0.0067114000	1
9.488890	-6.270600	3.271200	1.10000	0.0067114000	1
8.174870	-4.279410	3.584300	1.10000	0.0067114000	1
6.920040	-4.896620	2.480800	1.10000	0.0067114000	1
6.288030	-5.121030	4.827200	1.10000	0.0067114000	1
6.477850	-6.679510	4.265000	1.10000	0.0067114000	1
9.068380	-5.575300	5.173500	1.10000	0.0067114000	1
7.800070	-5.533710	6.441800	1.10000	0.0067114000	1
9.072840	-7.993310	4.965300	1.10000	0.0067114000	1
9.395570	-7.521520	6.673600	1.10000	0.0067114000	1
7.837720	-9.333110	6.950400	1.10000	0.0067114000	1
7.035650	-7.863320	7.421900	1.10000	0.0067114000	1
5.588390	-8.449710	5.575800	1.10000	0.0067114000	1
6.983250	-9.538040	4.762000	1.10000	0.0067114000	1
6.496470	-11.17680	6.764400	1.10000	0.0067114000	1
5.117920	-10.19150	7.035300	1.10000	0.0067114000	1
5.440090	-11.64670	4.376900	1.10000	0.0067114000	1
4.272160	-10.12480	4.496300	1.10000	0.0067114000	1
4.342110	-12.76200	6.346900	1.10000	0.0067114000	1
3.224260	-12.46810	5.004000	1.10000	0.0067114000	1
3.158360	-11.77900	6.692200	1.10000	0.0067114000	1
10.270000	-3.991200	-0.567460	1.10000	0.0067114000	1
11.751700	-4.428120	0.121010	1.10000	0.0067114000	1
12.584100	-4.487280	-2.477000	1.10000	0.0067114000	1
10.818800	-4.301140	-2.845300	1.10000	0.0067114000	1
11.157300	-2.125920	-3.188100	1.10000	0.0067114000	1
10.859200	-2.146540	-1.302100	1.10000	0.0067114000	1
13.323900	-1.924080	-0.801500	1.10000	0.0067114000	1
13.781500	-2.041130	-2.623500	1.10000	0.0067114000	1
13.832100	0.131644	-2.246600	1.10000	0.0067114000	1
12.338900	0.143044	-3.094000	1.10000	0.0067114000	1
11.269600	0.124644	-0.675910	1.10000	0.0067114000	1
12.846400	0.065015	0.000800	1.10000	0.0067114000	1
11.708000	2.573770	-1.673400	1.10000	0.0067114000	1

11.746300	2.457920	-0.016151	1.10000	0.0067114000	1
13.693100	3.783610	-0.480750	1.10000	0.0067114000	1
14.610000	2.378730	-0.785970	1.10000	0.0067114000	1
13.170400	2.384230	-3.225800	1.10000	0.0067114000	1
12.928900	3.899010	-2.632800	1.10000	0.0067114000	1
15.706500	4.264320	-2.528800	1.10000	0.0067114000	1
15.903200	2.578110	-2.847300	1.10000	0.0067114000	1
16.246400	3.689980	-4.938800	1.10000	0.0067114000	1
14.467200	3.398480	-5.271000	1.10000	0.0067114000	1
15.479800	5.637210	-5.655600	1.10000	0.0067114000	1
13.796500	5.664970	-4.744100	1.10000	0.0067114000	1
15.362500	5.967870	-3.827900	1.10000	0.0067114000	1

IMoS.cla

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excelfile Savefile Gas
/filefolder/TAA_multiTemperature_candidate2.xlsx /savefolder/TDDA_SI.txt N2

DNRCustomRange 0 0
interface 0
fromvalue 1
tovalue 3
red_coef 1.13
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 690
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0
qpol 1
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1
ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

Result of Multistructures Calculation for TDDA Salt:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_295_27.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_295_27.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_295_27.txt	295.00	312.0779	0.0000	0.0000	0.0000	0.0000	0.6657	0.6657	0.6657	0.6657
TDDA_295_27.txt	296.00	311.6951	16.6949	16.6897	16.6897	16.6897	0.6654	0.6656	0.6656	0.6656
TDDA_295_27.txt	297.00	311.4237	23.6294	23.6156	23.6155	23.6155	0.6649	0.6653	0.6653	0.6653
TDDA_295_27.txt	298.50	311.0390	31.2988	31.2676	31.2675	31.2675	0.6640	0.6647	0.6647	0.6647
TDDA_295_27.txt	300.00	310.6650	37.4580	37.4054	37.4051	37.4051	0.6631	0.6641	0.6641	0.6641
TDDA_295_27.txt	302.00	310.1155	44.3898	44.3035	44.3028	44.3028	0.6621	0.6635	0.6635	0.6635
TDDA_295_27.txt	305.00	309.1217	53.1480	53.0018	53.0002	53.0001	0.6610	0.6629	0.6629	0.6629
TDDA_295_27.txt	308.00	308.3246	60.7383	60.5236	60.5207	60.5204	0.6594	0.6619	0.6619	0.6619
TDDA_295_27.txt	312.00	307.2923	69.6724	69.3545	69.3491	69.3484	0.6574	0.6606	0.6606	0.6606
TDDA_295_27.txt	315.00	306.5770	75.7560	75.3537	75.3458	75.3448	0.6558	0.6595	0.6595	0.6595
TDDA_295_27.txt	320.00	305.3593	85.0283	84.4729	84.4597	84.4579	0.6532	0.6578	0.6579	0.6578
TDDA_295_27.txt	325.00	304.1019	93.4822	92.7596	92.7395	92.7366	0.6509	0.6563	0.6564	0.6563
TDDA_295_27.txt	330.00	302.7850	101.3054	100.4019	100.3732	100.3688	0.6487	0.6550	0.6551	0.6551
TDDA_295_27.txt	340.00	300.5196	115.7246	114.4338	114.3836	114.3751	0.6439	0.6518	0.6520	0.6519
TDDA_295_27.txt	350.00	298.3634	128.8748	127.1631	127.0857	127.0713	0.6393	0.6486	0.6489	0.6488
TDDA_295_27.txt	365.00	295.1132	146.8559	144.4541	144.3240	144.2974	0.6329	0.6444	0.6449	0.6447
TDDA_295_27.txt	380.00	292.0231	163.3901	160.2389	160.0426	159.9992	0.6268	0.6404	0.6412	0.6409

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_295_27.txt	0.0000	0.0000	0.0000	0.0000
TDDA_295_27.txt	16.6897	0.0006	-0.0002	16.6897
TDDA_295_27.txt	23.6155	0.0023	-0.0007	23.6155
TDDA_295_27.txt	31.2675	0.0062	-0.0015	31.2675
TDDA_295_27.txt	37.4051	0.0112	-0.0024	37.4051
TDDA_295_27.txt	44.3028	0.0187	-0.0034	44.3028
TDDA_295_27.txt	53.0001	0.0282	-0.0043	53.0001
TDDA_295_27.txt	60.5204	0.0399	-0.0057	60.5204
TDDA_295_27.txt	69.3484	0.0592	-0.0077	69.3484
TDDA_295_27.txt	75.3448	0.0762	-0.0093	75.3448
TDDA_295_27.txt	84.4579	0.1082	-0.0118	84.4579
TDDA_295_27.txt	92.7366	0.1437	-0.0141	92.7366
TDDA_295_27.txt	100.3688	0.1812	-0.0160	100.3688
TDDA_295_27.txt	114.3751	0.2695	-0.0208	114.3751
TDDA_295_27.txt	127.0713	0.3691	-0.0254	127.0713
TDDA_295_27.txt	144.2974	0.5272	-0.0316	144.2974
TDDA_295_27.txt	159.9992	0.6902	-0.0373	159.9992

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 439.1385 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_390_25.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_390_25.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff	CCS	E/n1	E/n2	E/n3	E/n4	<Ko1>	<Ko2>	<Ko3>	<Ko4>

	(K)	(A2)	(Td)	(Td)	(Td)	(Td)	(cm2/Vs)	(cm2/Vs)	(cm2/Vs)	(cm2/Vs)
TDDA_390_25.txt	295.00	318.8685	0.0000	0.0000	0.0000	0.0000	0.6515	0.6515	0.6515	0.6515
TDDA_390_25.txt	296.00	318.5872	17.0640	17.0587	17.0587	17.0587	0.6510	0.6512	0.6512	0.6512
TDDA_390_25.txt	297.00	318.3619	24.1558	24.1415	24.1415	24.1415	0.6504	0.6508	0.6508	0.6508
TDDA_390_25.txt	298.50	317.9453	31.9938	31.9615	31.9614	31.9614	0.6496	0.6503	0.6503	0.6503
TDDA_390_25.txt	300.00	317.4760	38.2793	38.2248	38.2245	38.2245	0.6489	0.6499	0.6499	0.6499
TDDA_390_25.txt	302.00	316.8498	45.3538	45.2644	45.2637	45.2637	0.6480	0.6494	0.6494	0.6494
TDDA_390_25.txt	305.00	315.9245	54.3176	54.1662	54.1646	54.1645	0.6467	0.6486	0.6486	0.6486
TDDA_390_25.txt	308.00	315.1493	62.0827	61.8602	61.8574	61.8570	0.6452	0.6476	0.6476	0.6476
TDDA_390_25.txt	312.00	313.9666	71.1856	70.8557	70.8503	70.8496	0.6434	0.6466	0.6466	0.6466
TDDA_390_25.txt	315.00	313.1509	77.3804	76.9622	76.9541	76.9531	0.6420	0.6457	0.6458	0.6457
TDDA_390_25.txt	320.00	311.7680	86.8128	86.2347	86.2211	86.2193	0.6398	0.6444	0.6444	0.6444
TDDA_390_25.txt	325.00	310.7306	95.5198	94.7696	94.7491	94.7461	0.6370	0.6424	0.6425	0.6424
TDDA_390_25.txt	330.00	309.4283	103.5281	102.5907	102.5615	102.5569	0.6348	0.6410	0.6412	0.6411
TDDA_390_25.txt	340.00	307.0109	118.2243	116.8823	116.8311	116.8223	0.6303	0.6381	0.6384	0.6382
TDDA_390_25.txt	350.00	304.6815	131.6039	129.8191	129.7394	129.7244	0.6260	0.6353	0.6357	0.6355
TDDA_390_25.txt	365.00	301.3851	149.9770	147.4703	147.3361	147.3084	0.6197	0.6312	0.6318	0.6315
TDDA_390_25.txt	380.00	298.3437	166.9266	163.6433	163.4413	163.3963	0.6136	0.6270	0.6278	0.6276
TDDA_390_25.txt	390.00	296.5243	177.6894	173.8656	173.6121	173.5530	0.6094	0.6241	0.6251	0.6247
TDDA_390_25.txt	420.00	290.9305	207.5277	201.9456	201.5008	201.3859	0.5985	0.6169	0.6184	0.6180
TDDA_390_25.txt	470.00	283.2816	252.9260	244.1529	243.2968	243.0487	0.5810	0.6045	0.6071	0.6066

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_390_25.txt	0.0000	0.0000	0.0000	0.0000
TDDA_390_25.txt	17.0587	0.0013	-0.0005	17.0587
TDDA_390_25.txt	24.1415	0.0038	-0.0012	24.1415
TDDA_390_25.txt	31.9614	0.0078	-0.0020	31.9614
TDDA_390_25.txt	38.2245	0.0116	-0.0025	38.2245
TDDA_390_25.txt	45.2637	0.0168	-0.0033	45.2637
TDDA_390_25.txt	54.1645	0.0254	-0.0045	54.1645
TDDA_390_25.txt	61.8570	0.0380	-0.0060	61.8570
TDDA_390_25.txt	70.8496	0.0563	-0.0076	70.8496
TDDA_390_25.txt	76.9531	0.0723	-0.0089	76.9531
TDDA_390_25.txt	86.2193	0.1012	-0.0110	86.2193
TDDA_390_25.txt	94.7461	0.1408	-0.0140	94.7461
TDDA_390_25.txt	102.5569	0.1817	-0.0160	102.5569
TDDA_390_25.txt	116.8223	0.2676	-0.0204	116.8223
TDDA_390_25.txt	129.7244	0.3607	-0.0246	129.7244
TDDA_390_25.txt	147.3084	0.5180	-0.0307	147.3084
TDDA_390_25.txt	163.3963	0.6916	-0.0368	163.3963
TDDA_390_25.txt	173.5530	0.8214	-0.0411	173.5530
TDDA_390_25.txt	201.3859	1.2004	-0.0515	201.3859
TDDA_390_25.txt	243.0487	1.9252	-0.0690	243.0487

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 515.5814 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDDA_480_18.txt

Number of atoms: 149
Molecular Weight: 690.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_480_18.txt.

Results

Summary of ion calculations:

Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_480_18.txt	295.00	333.5457	0.0000	0.0000	0.0000	0.0000	0.6229	0.6229	0.6229	0.6229
TDDA_480_18.txt	420.00	304.4636	217.1812	211.2444	210.7505	210.6233	0.5719	0.5898	0.5914	0.5909
TDDA_480_18.txt	470.00	296.8104	265.0052	255.7122	254.7695	254.4972	0.5545	0.5773	0.5799	0.5794
TDDA_480_18.txt	480.00	295.3888	274.0361	264.0365	262.9889	262.6808	0.5514	0.5750	0.5778	0.5773
TDDA_480_18.txt	530.00	288.9906	317.5139	303.8326	302.1982	301.6808	0.5363	0.5640	0.5679	0.5674
TDDA_480_18.txt	600.00	281.6128	375.0466	355.9210	353.3149	352.4283	0.5173	0.5494	0.5549	0.5546
TDDA_480_18.txt	680.00	275.0276	438.0952	412.5102	408.6338	407.2366	0.4975	0.5335	0.5407	0.5406
TDDA_480_18.txt	770.00	268.9201	506.3172	473.2116	467.7380	465.6684	0.4782	0.5175	0.5262	0.5266
TDDA_480_18.txt	870.00	263.5271	580.2646	538.6434	531.2510	528.3431	0.4591	0.5010	0.5113	0.5122
TDDA_480_18.txt	980.00	258.7479	659.9976	608.9260	599.3188	595.4165	0.4405	0.4844	0.4961	0.4975
TDDA_480_18.txt	1100.00	254.4165	745.3269	683.8427	671.6956	666.6222	0.4229	0.4683	0.4811	0.4832

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDDA_480_18.txt	0.0000	0.0000	0.0000	0.0000
TDDA_480_18.txt	210.6233	1.3346	-0.0513	210.6233
TDDA_480_18.txt	254.4972	2.1909	-0.0698	254.4972
TDDA_480_18.txt	262.6808	2.3692	-0.0732	262.6808
TDDA_480_18.txt	301.6808	3.2992	-0.0891	301.6808
TDDA_480_18.txt	352.4283	4.7064	-0.1097	352.4283
TDDA_480_18.txt	407.2366	6.4951	-0.1321	407.2366
TDDA_480_18.txt	465.6684	8.6608	-0.1545	465.6684
TDDA_480_18.txt	528.3431	11.2949	-0.1777	528.3431
TDDA_480_18.txt	595.4165	14.4777	-0.2012	595.4165
TDDA_480_18.txt	666.6222	18.1991	-0.2243	666.6222

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
MULTI STRUCTURE Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Teff	Ed (Td)	Ec (Td)	alpha (Td)	Kho (Td)
295	0.0000	0.0000	0.0000	0.6657
296	16.6936	0.0010	-0.0004	0.6655
297	23.6266	0.0035	-0.0011	0.6650
298.5	31.2931	0.0090	-0.0023	0.6642
300	37.4482	0.0160	-0.0035	0.6634
302	44.3736	0.0264	-0.0049	0.6624
305	53.1226	0.0414	-0.0065	0.6614
308	60.7033	0.0599	-0.0087	0.6600
312	69.6171	0.0889	-0.0114	0.6581
315	75.6834	0.1140	-0.0137	0.6566
320	84.9214	0.1602	-0.0171	0.6543
325	93.3712	0.2137	-0.0207	0.6519
330	101.1749	0.2711	-0.0237	0.6499
340	115.5343	0.4015	-0.0305	0.6454
350	128.6073	0.5463	-0.0370	0.6411
365	146.5160	0.7842	-0.0461	0.6350
380	163.0387	1.0454	-0.0552	0.6290
390	173.5530	1.2391	-0.0616	0.6247
420	204.4650	2.0151	-0.0853	0.6090
470	253.2251	3.8270	-0.1252	0.5824
480	262.6808	4.2475	-0.1328	0.5773
530	301.6808	5.7576	-0.1477	0.5674
600	352.4283	7.6822	-0.1670	0.5546
680	407.2366	9.7929	-0.1880	0.5406
770	465.6684	11.8929	-0.2090	0.5266

870	528.3431	14.0293	-0.2306	0.5122
980	595.4165	16.3395	-0.2526	0.4975
1100	666.6222	19.7103	-0.2742	0.4832

Time taken is a mere 257.9334 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.130
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDDA_295_27.txt	295.00	312.0779	0.0000	0.0000	0.0000	0.0000	0.6657	0.6657	0.6657	0.6657
TDDA_295_27.txt	296.00	311.6951	16.6949	16.6897	16.6897	16.6897	0.6654	0.6656	0.6656	0.6656
TDDA_295_27.txt	297.00	311.4237	23.6294	23.6156	23.6155	23.6155	0.6649	0.6653	0.6653	0.6653
TDDA_295_27.txt	298.50	311.0390	31.2988	31.2676	31.2675	31.2675	0.6640	0.6647	0.6647	0.6647
TDDA_295_27.txt	300.00	310.6650	37.4580	37.4054	37.4051	37.4051	0.6631	0.6641	0.6641	0.6641
TDDA_295_27.txt	302.00	310.1155	44.3898	44.3035	44.3028	44.3028	0.6621	0.6635	0.6635	0.6635
TDDA_295_27.txt	305.00	309.1217	53.1480	53.0018	53.0002	53.0001	0.6610	0.6629	0.6629	0.6629
TDDA_295_27.txt	308.00	308.3246	60.7383	60.5236	60.5207	60.5204	0.6594	0.6619	0.6619	0.6619
TDDA_295_27.txt	312.00	307.2923	69.6724	69.3545	69.3491	69.3484	0.6574	0.6606	0.6606	0.6606
TDDA_295_27.txt	315.00	306.5770	75.7560	75.3537	75.3458	75.3448	0.6558	0.6595	0.6595	0.6595
TDDA_295_27.txt	320.00	305.3593	85.0283	84.4729	84.4597	84.4579	0.6532	0.6578	0.6579	0.6578
TDDA_295_27.txt	325.00	304.1019	93.4822	92.7596	92.7395	92.7366	0.6509	0.6563	0.6564	0.6563
TDDA_295_27.txt	330.00	302.7850	101.3054	100.4019	100.3732	100.3688	0.6487	0.6550	0.6551	0.6551
TDDA_295_27.txt	340.00	300.5196	115.7246	114.4338	114.3836	114.3751	0.6439	0.6518	0.6520	0.6519
TDDA_295_27.txt	350.00	298.3634	128.8748	127.1631	127.0857	127.0713	0.6393	0.6486	0.6489	0.6488
TDDA_295_27.txt	365.00	295.1132	146.8559	144.4541	144.3240	144.2974	0.6329	0.6444	0.6449	0.6447
TDDA_295_27.txt	380.00	292.0231	163.3901	160.2389	160.0426	159.9992	0.6268	0.6404	0.6412	0.6409
TDDA_390_25.txt	295.00	318.8685	0.0000	0.0000	0.0000	0.0000	0.6515	0.6515	0.6515	0.6515
TDDA_390_25.txt	296.00	318.5872	17.0640	17.0587	17.0587	17.0587	0.6510	0.6512	0.6512	0.6512
TDDA_390_25.txt	297.00	318.3619	24.1558	24.1415	24.1415	24.1415	0.6504	0.6508	0.6508	0.6508
TDDA_390_25.txt	298.50	317.9453	31.9938	31.9615	31.9614	31.9614	0.6496	0.6503	0.6503	0.6503
TDDA_390_25.txt	300.00	317.4760	38.2793	38.2248	38.2245	38.2245	0.6489	0.6499	0.6499	0.6499

TDDA_390_25.txt	302.00	316.8498	45.3538	45.2644	45.2637	45.2637	0.6480	0.6494	0.6494	0.6494
TDDA_390_25.txt	305.00	315.9245	54.3176	54.1662	54.1646	54.1645	0.6467	0.6486	0.6486	0.6486
TDDA_390_25.txt	308.00	315.1493	62.0827	61.8602	61.8574	61.8570	0.6452	0.6476	0.6476	0.6476
TDDA_390_25.txt	312.00	313.9666	71.1856	70.8557	70.8503	70.8496	0.6434	0.6466	0.6466	0.6466
TDDA_390_25.txt	315.00	313.1509	77.3804	76.9622	76.9541	76.9531	0.6420	0.6457	0.6458	0.6457
TDDA_390_25.txt	320.00	311.7680	86.8128	86.2347	86.2211	86.2193	0.6398	0.6444	0.6444	0.6444
TDDA_390_25.txt	325.00	310.7306	95.5198	94.7696	94.7491	94.7461	0.6370	0.6424	0.6425	0.6424
TDDA_390_25.txt	330.00	309.4283	103.5281	102.5907	102.5615	102.5569	0.6348	0.6410	0.6412	0.6411
TDDA_390_25.txt	340.00	307.0109	118.2243	116.8823	116.8311	116.8223	0.6303	0.6381	0.6384	0.6382
TDDA_390_25.txt	350.00	304.6815	131.6039	129.8191	129.7394	129.7244	0.6260	0.6353	0.6357	0.6355
TDDA_390_25.txt	365.00	301.3851	149.9770	147.4703	147.3361	147.3084	0.6197	0.6312	0.6318	0.6315
TDDA_390_25.txt	380.00	298.3437	166.9266	163.6433	163.4413	163.3963	0.6136	0.6270	0.6278	0.6276
TDDA_390_25.txt	390.00	296.5243	177.6894	173.8656	173.6121	173.5530	0.6094	0.6241	0.6251	0.6247
TDDA_390_25.txt	420.00	290.9305	207.5277	201.9456	201.5008	201.3859	0.5985	0.6169	0.6184	0.6180
TDDA_390_25.txt	470.00	283.2816	252.9260	244.1529	243.2968	243.0487	0.5810	0.6045	0.6071	0.6066
TDDA_480_18.txt	295.00	333.5457	0.0000	0.0000	0.0000	0.0000	0.6229	0.6229	0.6229	0.6229
TDDA_480_18.txt	420.00	304.4636	217.1812	211.2444	210.7505	210.6233	0.5719	0.5898	0.5914	0.5909
TDDA_480_18.txt	470.00	296.8104	265.0052	255.7122	254.7695	254.4972	0.5545	0.5773	0.5799	0.5794
TDDA_480_18.txt	480.00	295.3888	274.0361	264.0365	262.9889	262.6808	0.5514	0.5750	0.5778	0.5773
TDDA_480_18.txt	530.00	288.9906	317.5139	303.8326	302.1982	301.6808	0.5363	0.5640	0.5679	0.5674
TDDA_480_18.txt	600.00	281.6128	375.0466	355.9210	353.3149	352.4283	0.5173	0.5494	0.5549	0.5546
TDDA_480_18.txt	680.00	275.0276	438.0952	412.5102	408.6338	407.2366	0.4975	0.5335	0.5407	0.5406
TDDA_480_18.txt	770.00	268.9201	506.3172	473.2116	467.7380	465.6684	0.4782	0.5175	0.5262	0.5266
TDDA_480_18.txt	870.00	263.5271	580.2646	538.6434	531.2510	528.3431	0.4591	0.5010	0.5113	0.5122
TDDA_480_18.txt	980.00	258.7479	659.9976	608.9260	599.3188	595.4165	0.4405	0.4844	0.4961	0.4975
TDDA_480_18.txt	1100.00	254.4165	745.3269	683.8427	671.6956	666.6222	0.4229	0.4683	0.4811	0.4832

TAA_multiTemperature_candidate2.xlsx - Sheet #1

x	y	z	Radius	Charge	Atom		
11.245000	-6.793640	-0.613950	1.55000	0.0067114000			14
10.755000	-8.171380	-1.111000	1.70000	0.0067114000		1	12
11.074100	-9.373160	-0.230350	1.70000	0.0067114000			12
10.337900	-10.63610	-0.759200	1.70000	0.0067114000		690	12
10.563300	-11.80610	0.135020	1.70000	0.0067114000			12
10.045100	-11.73810	1.580600	1.70000	0.0067114000			12
11.086800	-11.35550	2.577000	1.70000	0.0067114000			12
10.487900	-10.76280	3.853000	1.70000	0.0067114000			12
11.591700	-10.34290	4.918300	1.70000	0.0067114000			12
12.404300	-9.177060	4.381900	1.70000	0.0067114000			12
11.677600	-7.817870	4.437000	1.70000	0.0067114000			12
12.565600	-6.567150	4.075300	1.70000	0.0067114000			12
11.837200	-5.313840	4.591300	1.70000	0.0067114000			12
11.132300	-5.784770	-1.749000	1.70000	0.0067114000			12
9.770790	-5.562390	-2.466500	1.70000	0.0067114000			12
9.846020	-4.717950	-3.785200	1.70000	0.0067114000			12
10.210600	-3.268330	-3.639700	1.70000	0.0067114000			12
9.717580	-2.337030	-4.734600	1.70000	0.0067114000			12
10.209700	-0.879950	-4.716800	1.70000	0.0067114000			12
9.754270	-0.237051	-3.438000	1.70000	0.0067114000			12
10.329900	1.092930	-3.128800	1.70000	0.0067114000			12
10.017100	1.493740	-1.674200	1.70000	0.0067114000			12
8.639990	2.126520	-1.656400	1.70000	0.0067114000			12
8.056250	2.105870	-0.172420	1.70000	0.0067114000			12
6.763250	2.998650	-0.177120	1.70000	0.0067114000			12
10.570800	-6.312920	0.674460	1.70000	0.0067114000			12
9.085290	-6.097140	0.621600	1.70000	0.0067114000			12
8.485170	-5.793630	2.043000	1.70000	0.0067114000			12
6.979520	-5.655650	2.046800	1.70000	0.0067114000			12
6.175460	-6.807870	1.342800	1.70000	0.0067114000			12
6.594590	-8.210990	1.785500	1.70000	0.0067114000			12
6.373430	-8.478130	3.291600	1.70000	0.0067114000			12
6.397300	-10.02350	3.574100	1.70000	0.0067114000			12
6.300080	-10.20640	5.089700	1.70000	0.0067114000			12
6.384840	-11.66690	5.541500	1.70000	0.0067114000			12
6.267410	-12.06850	7.094100	1.70000	0.0067114000			12
6.328690	-13.62620	7.248400	1.70000	0.0067114000			12
12.732700	-6.891870	-0.076261	1.70000	0.0067114000			12
13.749900	-7.165220	-1.216400	1.70000	0.0067114000			12
15.200200	-7.213800	-0.728150	1.70000	0.0067114000			12
15.840700	-6.039180	-0.007511	1.70000	0.0067114000			12
16.088000	-4.736920	-0.868340	1.70000	0.0067114000			12
14.849200	-3.725560	-0.744260	1.70000	0.0067114000			12
15.294300	-2.432400	-1.521000	1.70000	0.0067114000			12
14.222900	-1.315250	-1.607800	1.70000	0.0067114000			12
14.850700	-0.020165	-2.066100	1.70000	0.0067114000			12

15.808100	0.601212	-0.933120	1.70000	0.0067114000	12
16.296700	2.024960	-1.369400	1.70000	0.0067114000	12
17.163100	2.537690	-0.219520	1.70000	0.0067114000	12
9.705510	-8.292010	-1.371400	1.10000	0.0067114000	1
11.273500	-8.246130	-2.037400	1.10000	0.0067114000	1
12.175500	-9.543910	-0.128880	1.10000	0.0067114000	1
10.725600	-9.182930	0.856550	1.10000	0.0067114000	1
9.207590	-10.34100	-0.746940	1.10000	0.0067114000	1
10.595400	-11.01170	-1.784700	1.10000	0.0067114000	1
10.035800	-12.68230	-0.396700	1.10000	0.0067114000	1
11.697500	-12.07980	0.105180	1.10000	0.0067114000	1
9.234440	-10.99850	1.687200	1.10000	0.0067114000	1
9.619540	-12.68090	1.944500	1.10000	0.0067114000	1
11.831100	-12.11830	2.757900	1.10000	0.0067114000	1
11.703000	-10.53710	2.021200	1.10000	0.0067114000	1
9.747380	-9.915310	3.724100	1.10000	0.0067114000	1
9.824700	-11.59580	4.309600	1.10000	0.0067114000	1
11.228300	-9.858010	5.812100	1.10000	0.0067114000	1
12.152200	-11.23830	5.310100	1.10000	0.0067114000	1
13.324300	-9.179270	5.030900	1.10000	0.0067114000	1
12.857200	-9.568620	3.369100	1.10000	0.0067114000	1
10.925500	-7.884370	3.614900	1.10000	0.0067114000	1
11.297900	-7.666900	5.429100	1.10000	0.0067114000	1
13.503900	-6.770060	4.671800	1.10000	0.0067114000	1
12.746700	-6.356510	2.998500	1.10000	0.0067114000	1
12.467000	-4.415900	4.459600	1.10000	0.0067114000	1
10.866800	-5.102440	4.154300	1.10000	0.0067114000	1
11.637700	-5.508350	5.693000	1.10000	0.0067114000	1
11.551300	-4.790270	-1.538200	1.10000	0.0067114000	1
11.785700	-6.144590	-2.643400	1.10000	0.0067114000	1
9.350650	-6.548400	-2.635600	1.10000	0.0067114000	1
8.983280	-5.027110	-1.872400	1.10000	0.0067114000	1
10.647400	-5.137810	-4.331200	1.10000	0.0067114000	1
8.946800	-4.786040	-4.457500	1.10000	0.0067114000	1
9.680150	-3.031070	-2.715500	1.10000	0.0067114000	1
11.268700	-3.079880	-3.428400	1.10000	0.0067114000	1
10.181600	-2.862610	-5.727700	1.10000	0.0067114000	1
8.575520	-2.253570	-4.661700	1.10000	0.0067114000	1
11.323800	-0.896496	-4.669900	1.10000	0.0067114000	1
9.854320	-0.180062	-5.501500	1.10000	0.0067114000	1
8.615810	-0.071302	-3.399000	1.10000	0.0067114000	1
9.924540	-0.810896	-2.513600	1.10000	0.0067114000	1
11.406500	1.163810	-3.420900	1.10000	0.0067114000	1
10.048100	1.995200	-3.702900	1.10000	0.0067114000	1
10.067100	0.530019	-1.097800	1.10000	0.0067114000	1
10.826200	2.043150	-1.225500	1.10000	0.0067114000	1
7.776990	1.755960	-2.294100	1.10000	0.0067114000	1
8.813140	3.223520	-1.859500	1.10000	0.0067114000	1
7.971090	1.062110	0.176570	1.10000	0.0067114000	1
8.842930	2.468290	0.559310	1.10000	0.0067114000	1
6.950450	4.092980	-0.289510	1.10000	0.0067114000	1
6.047750	2.609320	-0.982650	1.10000	0.0067114000	1
6.171990	2.806810	0.679100	1.10000	0.0067114000	1
10.631700	-7.117250	1.431800	1.10000	0.0067114000	1
10.987700	-5.357770	1.027000	1.10000	0.0067114000	1
8.848700	-5.202500	0.023456	1.10000	0.0067114000	1
8.581500	-6.969910	0.185380	1.10000	0.0067114000	1
8.973650	-6.604670	2.594800	1.10000	0.0067114000	1
8.867220	-4.838450	2.401300	1.10000	0.0067114000	1
6.513110	-5.492720	3.028900	1.10000	0.0067114000	1
6.661570	-4.653880	1.539500	1.10000	0.0067114000	1
5.119080	-6.627720	1.736600	1.10000	0.0067114000	1
6.174110	-6.563210	0.316660	1.10000	0.0067114000	1
5.909680	-8.940360	1.354500	1.10000	0.0067114000	1
7.578420	-8.491480	1.471300	1.10000	0.0067114000	1
7.265700	-8.148800	3.783500	1.10000	0.0067114000	1
5.469470	-7.972900	3.810300	1.10000	0.0067114000	1
5.682660	-10.65050	3.039800	1.10000	0.0067114000	1
7.481080	-10.37510	3.227600	1.10000	0.0067114000	1
7.073190	-9.617860	5.507000	1.10000	0.0067114000	1
5.317630	-9.655180	5.459200	1.10000	0.0067114000	1
5.549570	-12.17450	5.096200	1.10000	0.0067114000	1
7.206010	-12.07260	4.967700	1.10000	0.0067114000	1
5.329430	-11.61780	7.565400	1.10000	0.0067114000	1
7.091620	-11.62700	7.642600	1.10000	0.0067114000	1
6.218060	-13.85040	8.287900	1.10000	0.0067114000	1
7.382260	-13.87390	6.959900	1.10000	0.0067114000	1
5.528260	-14.11390	6.660200	1.10000	0.0067114000	1
12.965600	-5.862770	0.338100	1.10000	0.0067114000	1
12.807600	-7.617020	0.709390	1.10000	0.0067114000	1

13.459500	-8.113830	-1.621700	1.10000	0.0067114000	1
13.680000	-6.331540	-1.981200	1.10000	0.0067114000	1
15.449700	-8.103840	-0.069326	1.10000	0.0067114000	1
15.792900	-7.454130	-1.650500	1.10000	0.0067114000	1
15.170000	-5.939420	0.937610	1.10000	0.0067114000	1
16.878100	-6.279270	0.340140	1.10000	0.0067114000	1
17.010600	-4.262360	-0.481660	1.10000	0.0067114000	1
16.311200	-5.025020	-1.922600	1.10000	0.0067114000	1
13.951200	-4.051120	-1.332100	1.10000	0.0067114000	1
14.559300	-3.404120	0.286800	1.10000	0.0067114000	1
16.130600	-2.183680	-0.895880	1.10000	0.0067114000	1
15.551100	-2.577520	-2.590800	1.10000	0.0067114000	1
13.475900	-1.571870	-2.388300	1.10000	0.0067114000	1
13.838000	-1.075040	-0.488690	1.10000	0.0067114000	1
15.537300	-0.279990	-2.882400	1.10000	0.0067114000	1
14.131200	0.680190	-2.534300	1.10000	0.0067114000	1
15.202200	0.638080	-0.015153	1.10000	0.0067114000	1
16.749100	0.001803	-0.743200	1.10000	0.0067114000	1
16.864300	2.097060	-2.329400	1.10000	0.0067114000	1
15.439000	2.680370	-1.430100	1.10000	0.0067114000	1
18.039500	1.792880	-0.214130	1.10000	0.0067114000	1
17.633300	3.535310	-0.491640	1.10000	0.0067114000	1
16.751300	2.483970	0.841370	1.10000	0.0067114000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #2

x	y	z	Radius	Charge	Atom		
9.861900	-4.248160	-1.183800	1.55000	0.0067114000			14
10.018700	-4.754160	0.252220	1.70000	0.0067114000		1	12
8.689220	-4.990170	1.109400	1.70000	0.0067114000			12
8.657960	-6.403790	1.617300	1.70000	0.0067114000		690	12
9.851520	-7.010100	2.336700	1.70000	0.0067114000			12
9.410420	-8.163950	3.232400	1.70000	0.0067114000			12
8.824350	-9.330680	2.345100	1.70000	0.0067114000			12
8.420220	-10.53670	3.156400	1.70000	0.0067114000			12
8.114860	-11.86670	2.371600	1.70000	0.0067114000			12
9.349980	-12.81820	2.447200	1.70000	0.0067114000			12
9.288560	-14.16500	1.636900	1.70000	0.0067114000			12
10.743100	-14.78920	1.896700	1.70000	0.0067114000			12
11.857500	-14.10920	1.031500	1.70000	0.0067114000			12
11.211600	-4.253770	-1.898900	1.70000	0.0067114000			12
12.358300	-3.341710	-1.378600	1.70000	0.0067114000			12
13.617300	-4.108460	-1.794800	1.70000	0.0067114000			12
13.986700	-5.306800	-0.725440	1.70000	0.0067114000			12
14.318800	-5.091940	0.761180	1.70000	0.0067114000			12
15.475300	-4.069120	0.853900	1.70000	0.0067114000			12
16.127700	-3.883260	2.278500	1.70000	0.0067114000			12
16.563800	-5.155020	3.064400	1.70000	0.0067114000			12
17.672300	-5.998460	2.322600	1.70000	0.0067114000			12
17.900100	-7.464430	2.844500	1.70000	0.0067114000			12
19.398800	-7.770900	2.926900	1.70000	0.0067114000			12
20.057600	-7.670190	1.455500	1.70000	0.0067114000			12
8.933670	-5.170270	-2.007900	1.70000	0.0067114000			12
9.519190	-6.576290	-1.963600	1.70000	0.0067114000			12
8.328780	-7.609040	-2.080400	1.70000	0.0067114000			12
8.807090	-8.975820	-2.596100	1.70000	0.0067114000			12
9.617670	-9.653180	-1.547100	1.70000	0.0067114000			12
10.370400	-10.88980	-1.994500	1.70000	0.0067114000			12
11.470400	-10.72700	-3.056100	1.70000	0.0067114000			12
12.467700	-9.591820	-2.720700	1.70000	0.0067114000			12
13.361800	-9.943700	-1.424400	1.70000	0.0067114000			12
14.706800	-9.234990	-1.436200	1.70000	0.0067114000			12
15.592200	-9.586190	-0.188800	1.70000	0.0067114000			12
15.912300	-11.02170	0.005199	1.70000	0.0067114000			12
9.161330	-2.777330	-1.208500	1.70000	0.0067114000			12
9.692230	-1.608470	-0.366830	1.70000	0.0067114000			12
8.920310	-0.327402	-0.629790	1.70000	0.0067114000			12
9.570630	0.891276	0.056550	1.70000	0.0067114000			12
8.595680	2.063280	-0.016932	1.70000	0.0067114000			12
7.388460	2.100300	1.006800	1.70000	0.0067114000			12
6.155400	2.882420	0.628880	1.70000	0.0067114000			12
5.002880	2.793360	1.652800	1.70000	0.0067114000			12
4.234700	4.079430	1.915200	1.70000	0.0067114000			12
3.095560	4.007560	2.952600	1.70000	0.0067114000			12
2.702640	5.493730	3.241800	1.70000	0.0067114000			12
2.229990	5.678640	4.761400	1.70000	0.0067114000			12
10.764200	-5.579030	0.344120	1.10000	0.0067114000			1
10.609500	-3.993420	0.743120	1.10000	0.0067114000			1
8.734950	-4.257950	1.974100	1.10000	0.0067114000			1

7.735860	-4.686940	0.536730	1.10000	0.0067114000	1
7.770000	-6.686860	2.313700	1.10000	0.0067114000	1
8.475100	-6.962060	0.597840	1.10000	0.0067114000	1
10.616200	-7.364380	1.646400	1.10000	0.0067114000	1
10.207700	-6.270170	3.069200	1.10000	0.0067114000	1
10.225100	-8.664180	3.790300	1.10000	0.0067114000	1
8.532180	-7.919610	4.005300	1.10000	0.0067114000	1
7.906970	-9.150260	1.813600	1.10000	0.0067114000	1
9.686040	-9.661330	1.653400	1.10000	0.0067114000	1
9.220820	-10.80480	3.843800	1.10000	0.0067114000	1
7.476590	-10.29720	3.695100	1.10000	0.0067114000	1
7.215840	-12.45710	2.784300	1.10000	0.0067114000	1
7.704650	-11.66840	1.300100	1.10000	0.0067114000	1
10.088500	-12.28430	1.839400	1.10000	0.0067114000	1
9.505750	-13.12190	3.527300	1.10000	0.0067114000	1
8.527860	-14.88170	2.119800	1.10000	0.0067114000	1
9.018930	-13.95670	0.538100	1.10000	0.0067114000	1
10.923500	-14.86640	2.958500	1.10000	0.0067114000	1
10.623300	-15.86680	1.535400	1.10000	0.0067114000	1
11.411800	-14.01450	0.053579	1.10000	0.0067114000	1
11.964300	-13.04910	1.421100	1.10000	0.0067114000	1
12.812300	-14.66460	0.948310	1.10000	0.0067114000	1
11.540100	-5.232320	-1.867500	1.10000	0.0067114000	1
11.203500	-4.263890	-2.991900	1.10000	0.0067114000	1
12.477500	-2.342320	-1.783500	1.10000	0.0067114000	1
12.392000	-3.194660	-0.255730	1.10000	0.0067114000	1
13.512800	-4.740500	-2.744500	1.10000	0.0067114000	1
14.559500	-3.515220	-1.922800	1.10000	0.0067114000	1
13.285600	-6.120320	-0.753960	1.10000	0.0067114000	1
14.904900	-5.679150	-1.236600	1.10000	0.0067114000	1
13.444200	-4.846800	1.426800	1.10000	0.0067114000	1
14.865400	-6.029670	1.025800	1.10000	0.0067114000	1
16.392200	-4.231010	0.202810	1.10000	0.0067114000	1
15.005800	-3.151720	0.461540	1.10000	0.0067114000	1
17.013300	-3.243600	2.130400	1.10000	0.0067114000	1
15.355800	-3.330930	2.889800	1.10000	0.0067114000	1
16.997400	-5.033210	4.102500	1.10000	0.0067114000	1
15.564300	-5.736170	3.112900	1.10000	0.0067114000	1
17.466100	-5.924290	1.198200	1.10000	0.0067114000	1
18.560000	-5.373210	2.457000	1.10000	0.0067114000	1
17.245600	-8.054110	2.198400	1.10000	0.0067114000	1
17.409800	-7.456270	3.873100	1.10000	0.0067114000	1
19.785300	-6.969200	3.646400	1.10000	0.0067114000	1
19.337500	-8.747490	3.430400	1.10000	0.0067114000	1
20.892400	-8.398090	1.245900	1.10000	0.0067114000	1
19.386900	-8.127010	0.713990	1.10000	0.0067114000	1
20.394300	-6.606500	1.221100	1.10000	0.0067114000	1
8.002220	-5.192370	-1.498700	1.10000	0.0067114000	1
8.626610	-4.827540	-3.038300	1.10000	0.0067114000	1
10.136900	-6.705130	-2.821800	1.10000	0.0067114000	1
10.250000	-6.890200	-1.161500	1.10000	0.0067114000	1
7.735710	-7.734710	-1.099500	1.10000	0.0067114000	1
7.777830	-7.105050	-2.939500	1.10000	0.0067114000	1
8.009190	-9.549670	-3.032400	1.10000	0.0067114000	1
9.504290	-8.820220	-3.519100	1.10000	0.0067114000	1
10.323200	-9.025130	-1.066900	1.10000	0.0067114000	1
8.927750	-9.919600	-0.776110	1.10000	0.0067114000	1
10.893400	-11.50700	-1.203900	1.10000	0.0067114000	1
9.545500	-11.52890	-2.449200	1.10000	0.0067114000	1
11.855700	-11.70200	-3.350800	1.10000	0.0067114000	1
10.958800	-10.40330	-4.012900	1.10000	0.0067114000	1
13.228300	-9.634930	-3.514700	1.10000	0.0067114000	1
11.976600	-8.600040	-2.680200	1.10000	0.0067114000	1
12.836700	-9.617340	-0.485470	1.10000	0.0067114000	1
13.631900	-10.99320	-1.243800	1.10000	0.0067114000	1
15.325300	-9.503430	-2.344400	1.10000	0.0067114000	1
14.573800	-8.089620	-1.615800	1.10000	0.0067114000	1
15.069800	-9.056930	0.710900	1.10000	0.0067114000	1
16.586200	-9.117740	-0.186310	1.10000	0.0067114000	1
14.905100	-11.32640	0.426710	1.10000	0.0067114000	1
16.630700	-11.31170	0.798100	1.10000	0.0067114000	1
16.278200	-11.57870	-0.869780	1.10000	0.0067114000	1
9.360760	-2.488020	-2.241800	1.10000	0.0067114000	1
8.109870	-2.892920	-1.138300	1.10000	0.0067114000	1
9.591300	-1.877080	0.730920	1.10000	0.0067114000	1
10.742100	-1.404050	-0.479960	1.10000	0.0067114000	1
8.954720	-0.281748	-1.703700	1.10000	0.0067114000	1
7.915920	-0.573113	-0.322470	1.10000	0.0067114000	1
9.851350	0.675906	1.104900	1.10000	0.0067114000	1
10.541300	1.045390	-0.424580	1.10000	0.0067114000	1

9.283490	2.944610	-0.015158	1.10000	0.0067114000		1
8.202780	2.021610	-1.107100	1.10000	0.0067114000		1
7.052380	1.061760	1.215200	1.10000	0.0067114000		1
7.697980	2.563950	1.911100	1.10000	0.0067114000		1
6.418540	3.921720	0.265490	1.10000	0.0067114000		1
5.666100	2.334820	-0.221540	1.10000	0.0067114000		1
4.259620	1.995340	1.584600	1.10000	0.0067114000		1
5.458930	2.451910	2.643900	1.10000	0.0067114000		1
5.009450	4.773470	2.411800	1.10000	0.0067114000		1
4.061920	4.792870	1.000900	1.10000	0.0067114000		1
2.287310	3.334320	2.483100	1.10000	0.0067114000		1
3.528930	3.437310	3.789700	1.10000	0.0067114000		1
3.469320	6.241280	2.995100	1.10000	0.0067114000		1
1.909410	5.720220	2.508800	1.10000	0.0067114000		1
1.979880	4.741030	5.276600	1.10000	0.0067114000		1
3.008440	6.132260	5.452900	1.10000	0.0067114000		1
1.333080	6.359490	4.627200	1.10000	0.0067114000		1

TAA_multiTemperature_candidate2.xlsx - Sheet #3

x	y	z	Radius	Charge	Atom	
10.703900	-6.105630	-0.796950	1.55000	0.0067114000		14
11.809700	-7.090090	-1.098800	1.70000	0.0067114000	1	12
13.194300	-6.836570	-0.287470	1.70000	0.0067114000		12
14.144200	-8.033550	-0.665960	1.70000	0.0067114000	690	12
15.015400	-8.006270	-1.896800	1.70000	0.0067114000		12
16.383500	-7.435310	-1.691500	1.70000	0.0067114000		12
16.516300	-5.963490	-1.380600	1.70000	0.0067114000		12
17.740400	-5.244390	-1.967100	1.70000	0.0067114000		12
19.051000	-5.886290	-1.568300	1.70000	0.0067114000		12
19.048600	-5.720160	0.016875	1.70000	0.0067114000		12
20.353100	-5.921630	0.705390	1.70000	0.0067114000		12
21.253500	-7.138240	0.323390	1.70000	0.0067114000		12
20.724300	-8.524250	0.585410	1.70000	0.0067114000		12
9.554630	-6.364670	-1.803300	1.70000	0.0067114000		12
8.939120	-7.778290	-1.653300	1.70000	0.0067114000		12
7.544710	-7.991510	-2.544700	1.70000	0.0067114000		12
6.981130	-9.462120	-2.343300	1.70000	0.0067114000		12
6.803370	-10.00710	-0.772040	1.70000	0.0067114000		12
5.592430	-9.339530	-0.124760	1.70000	0.0067114000		12
5.731110	-9.231320	1.549100	1.70000	0.0067114000		12
4.828310	-8.147780	2.091700	1.70000	0.0067114000		12
3.315320	-8.402210	2.161800	1.70000	0.0067114000		12
2.475780	-7.591260	3.144200	1.70000	0.0067114000		12
2.720040	-7.765150	4.593900	1.70000	0.0067114000		12
2.369430	-6.619680	5.580300	1.70000	0.0067114000		12
10.269500	-6.230000	0.584870	1.70000	0.0067114000		12
9.202750	-5.308140	1.313000	1.70000	0.0067114000		12
8.751600	-6.073080	2.482500	1.70000	0.0067114000		12
7.687370	-5.232850	3.215700	1.70000	0.0067114000		12
7.070310	-5.792580	4.465400	1.70000	0.0067114000		12
8.165580	-6.092100	5.553300	1.70000	0.0067114000		12
8.582080	-7.566050	5.879200	1.70000	0.0067114000		12
7.387870	-8.422240	6.505100	1.70000	0.0067114000		12
6.391140	-9.190050	5.693400	1.70000	0.0067114000		12
5.743620	-10.46010	6.202600	1.70000	0.0067114000		12
4.859190	-10.97410	5.061700	1.70000	0.0067114000		12
3.818240	-11.99260	5.731000	1.70000	0.0067114000		12
11.123100	-4.560680	-0.824650	1.70000	0.0067114000		12
11.633800	-3.957720	-2.198800	1.70000	0.0067114000		12
11.651100	-2.398540	-2.178000	1.70000	0.0067114000		12
12.978200	-1.761170	-1.860800	1.70000	0.0067114000		12
12.754800	-0.211492	-2.141400	1.70000	0.0067114000		12
12.295300	0.544744	-0.870460	1.70000	0.0067114000		12
12.304000	2.040380	-0.910100	1.70000	0.0067114000		12
13.687000	2.760200	-1.147400	1.70000	0.0067114000		12
13.727000	3.211870	-2.596500	1.70000	0.0067114000		12
15.186500	3.468790	-3.059300	1.70000	0.0067114000		12
15.216400	3.944560	-4.561100	1.70000	0.0067114000		12
14.884900	5.401240	-4.699200	1.70000	0.0067114000		12
11.359200	-8.103260	-1.115700	1.10000	0.0067114000		1
12.142600	-6.949370	-2.198100	1.10000	0.0067114000		1
13.666600	-5.909270	-0.640860	1.10000	0.0067114000		1
12.987900	-6.728140	0.876340	1.10000	0.0067114000		1
14.915300	-8.179880	0.189250	1.10000	0.0067114000		1
13.576000	-8.963660	-0.776290	1.10000	0.0067114000		1
15.265100	-9.037220	-2.136500	1.10000	0.0067114000		1
14.434000	-7.724150	-2.772500	1.10000	0.0067114000		1
17.157200	-7.932830	-1.214700	1.10000	0.0067114000		1

16.787100	-7.533700	-2.719100	1.10000	0.0067114000	1
15.703700	-5.368470	-1.705800	1.10000	0.0067114000	1
16.476300	-5.840670	-0.287680	1.10000	0.0067114000	1
17.646000	-5.391820	-3.053300	1.10000	0.0067114000	1
17.691700	-4.123840	-1.739900	1.10000	0.0067114000	1
19.181700	-6.907180	-1.952300	1.10000	0.0067114000	1
19.889500	-5.433300	-2.091900	1.10000	0.0067114000	1
18.380400	-4.877370	0.531190	1.10000	0.0067114000	1
18.552300	-6.631110	0.392920	1.10000	0.0067114000	1
20.923700	-4.930250	0.469650	1.10000	0.0067114000	1
20.103300	-5.891270	1.807300	1.10000	0.0067114000	1
21.394700	-7.001420	-0.740200	1.10000	0.0067114000	1
22.290800	-7.080640	0.764720	1.10000	0.0067114000	1
21.005900	-8.763790	1.606200	1.10000	0.0067114000	1
19.621900	-8.666720	0.385660	1.10000	0.0067114000	1
21.085300	-9.258470	-0.100200	1.10000	0.0067114000	1
8.799730	-5.624640	-1.582100	1.10000	0.0067114000	1
9.922350	-6.222330	-2.831600	1.10000	0.0067114000	1
9.711400	-8.473510	-2.053800	1.10000	0.0067114000	1
8.737260	-7.998240	-0.637460	1.10000	0.0067114000	1
6.747130	-7.286000	-2.174300	1.10000	0.0067114000	1
7.883720	-7.925410	-3.668400	1.10000	0.0067114000	1
6.020530	-9.501830	-2.824700	1.10000	0.0067114000	1
7.584360	-10.13850	-2.928300	1.10000	0.0067114000	1
6.690010	-11.16210	-0.843260	1.10000	0.0067114000	1
7.771310	-9.919520	-0.188180	1.10000	0.0067114000	1
5.790890	-8.341930	-0.519280	1.10000	0.0067114000	1
4.550020	-9.862620	-0.267190	1.10000	0.0067114000	1
5.553470	-10.13400	2.237000	1.10000	0.0067114000	1
6.859650	-9.187750	1.684900	1.10000	0.0067114000	1
5.316430	-7.839240	3.119000	1.10000	0.0067114000	1
5.046280	-7.268210	1.436900	1.10000	0.0067114000	1
3.008250	-8.456540	1.105700	1.10000	0.0067114000	1
3.295960	-9.455050	2.655600	1.10000	0.0067114000	1
1.427360	-7.695770	2.820100	1.10000	0.0067114000	1
2.272260	-6.521050	2.880800	1.10000	0.0067114000	1
2.664350	-8.803930	4.956200	1.10000	0.0067114000	1
3.780560	-7.417630	4.579200	1.10000	0.0067114000	1
2.485310	-5.608290	5.059100	1.10000	0.0067114000	1
1.274430	-6.814830	5.745400	1.10000	0.0067114000	1
2.947210	-6.692710	6.528600	1.10000	0.0067114000	1
9.942060	-7.325320	0.739740	1.10000	0.0067114000	1
11.170900	-6.162440	1.228400	1.10000	0.0067114000	1
9.789840	-4.390360	1.615700	1.10000	0.0067114000	1
8.279010	-5.060390	0.744680	1.10000	0.0067114000	1
8.415350	-7.050230	1.991900	1.10000	0.0067114000	1
9.488890	-6.270600	3.271200	1.10000	0.0067114000	1
8.174870	-4.279410	3.584300	1.10000	0.0067114000	1
6.920040	-4.896620	2.480800	1.10000	0.0067114000	1
6.288030	-5.121030	4.827200	1.10000	0.0067114000	1
6.477850	-6.679510	4.265000	1.10000	0.0067114000	1
9.068380	-5.575300	5.173500	1.10000	0.0067114000	1
7.800070	-5.533710	6.441800	1.10000	0.0067114000	1
9.072840	-7.993310	4.965300	1.10000	0.0067114000	1
9.395570	-7.521520	6.673600	1.10000	0.0067114000	1
7.837720	-9.333110	6.950400	1.10000	0.0067114000	1
7.035650	-7.863320	7.421900	1.10000	0.0067114000	1
5.588390	-8.449710	5.575800	1.10000	0.0067114000	1
6.983250	-9.538040	4.762000	1.10000	0.0067114000	1
6.496470	-11.17680	6.764400	1.10000	0.0067114000	1
5.117920	-10.19150	7.035300	1.10000	0.0067114000	1
5.440090	-11.64670	4.376900	1.10000	0.0067114000	1
4.272160	-10.12480	4.496300	1.10000	0.0067114000	1
4.342110	-12.76200	6.346900	1.10000	0.0067114000	1
3.224260	-12.46810	5.004000	1.10000	0.0067114000	1
3.158360	-11.77900	6.692200	1.10000	0.0067114000	1
10.270000	-3.991200	-0.567460	1.10000	0.0067114000	1
11.751700	-4.428120	0.121010	1.10000	0.0067114000	1
12.584100	-4.487280	-2.477000	1.10000	0.0067114000	1
10.818800	-4.301140	-2.845300	1.10000	0.0067114000	1
11.157300	-2.125920	-3.188100	1.10000	0.0067114000	1
10.859200	-2.146540	-1.302100	1.10000	0.0067114000	1
13.323900	-1.924080	-0.801500	1.10000	0.0067114000	1
13.781500	-2.041130	-2.623500	1.10000	0.0067114000	1
13.832100	0.131644	-2.246600	1.10000	0.0067114000	1
12.338900	0.143044	-3.094000	1.10000	0.0067114000	1
11.269600	0.124644	-0.675910	1.10000	0.0067114000	1
12.846400	0.065015	0.000800	1.10000	0.0067114000	1
11.708000	2.573770	-1.673400	1.10000	0.0067114000	1
11.746300	2.457920	-0.016151	1.10000	0.0067114000	1

13.693100	3.783610	-0.480750	1.10000	0.0067114000	1
14.610000	2.378730	-0.785970	1.10000	0.0067114000	1
13.170400	2.384230	-3.225800	1.10000	0.0067114000	1
12.928900	3.899010	-2.632800	1.10000	0.0067114000	1
15.706500	4.264320	-2.528800	1.10000	0.0067114000	1
15.903200	2.578110	-2.847300	1.10000	0.0067114000	1
16.246400	3.689980	-4.938800	1.10000	0.0067114000	1
14.467200	3.398480	-5.271000	1.10000	0.0067114000	1
15.479800	5.637210	-5.655600	1.10000	0.0067114000	1
13.796500	5.664970	-4.744100	1.10000	0.0067114000	1
15.362500	5.967870	-3.827900	1.10000	0.0067114000	1

IMoS.cla

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excelfile Savefile Gas
/filefolder/TAA_multiTemperature_candidate2.xlsx /savefolder/TDDA_SI2.txt N2

DNRCustomRange 0 0
interface 0
fromvalue 1
tovalue 3
red_coef 1.13
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 690
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0
qpol 0
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1
ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
MultiT 1
MultiTval 295
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

Independent Result for One Structure (295K) of THA:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: THA_295_11.txt

Number of atoms: 89
Molecular Weight: 410.00 Da
Total Charge: 1

The TM Method used is High Field

Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule THA_295_11.txt.

Results

Summary of ion calculations:

Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_295_11.txt	295.00	239.4260	0.0000	0.0000	0.0000	0.0000	0.8792	0.8792	0.8792	0.8792
THA_295_11.txt	296.00	239.1768	12.6434	12.6397	12.6397	12.6397	0.8786	0.8789	0.8789	0.8789
THA_295_11.txt	297.00	238.9365	17.8927	17.8833	17.8833	17.8833	0.8780	0.8785	0.8785	0.8785
THA_295_11.txt	298.50	238.5663	23.6927	23.6724	23.6723	23.6723	0.8772	0.8780	0.8780	0.8780
THA_295_11.txt	300.00	238.1443	28.3391	28.3052	28.3051	28.3051	0.8765	0.8776	0.8776	0.8776
THA_295_11.txt	302.00	237.5882	33.5643	33.5092	33.5089	33.5089	0.8757	0.8772	0.8772	0.8772
THA_295_11.txt	305.00	236.8985	40.1987	40.1064	40.1056	40.1055	0.8739	0.8760	0.8760	0.8760
THA_295_11.txt	308.00	236.4286	45.9671	45.8325	45.8311	45.8309	0.8714	0.8741	0.8741	0.8741
THA_295_11.txt	312.00	235.4980	52.6974	52.4983	52.4956	52.4953	0.8692	0.8727	0.8728	0.8727
THA_295_11.txt	315.00	234.7817	57.2578	57.0052	57.0012	57.0006	0.8677	0.8718	0.8719	0.8718
THA_295_11.txt	320.00	233.7584	64.2410	63.8918	63.8851	63.8841	0.8646	0.8698	0.8698	0.8698
THA_295_11.txt	325.00	232.6763	70.5918	70.1364	70.1261	70.1245	0.8619	0.8680	0.8682	0.8681
THA_295_11.txt	330.00	231.7007	76.5100	75.9413	75.9267	75.9242	0.8590	0.8660	0.8662	0.8661
THA_295_11.txt	340.00	229.6358	87.2740	86.4553	86.4291	86.4243	0.8539	0.8628	0.8630	0.8629
THA_295_11.txt	350.00	227.7851	97.1048	96.0133	95.9723	95.9642	0.8484	0.8591	0.8595	0.8593
THA_295_11.txt	365.00	225.0796	110.5430	109.0017	108.9315	108.9164	0.8408	0.8540	0.8546	0.8544
THA_295_11.txt	380.00	222.5090	122.8708	120.8388	120.7314	120.7067	0.8336	0.8492	0.8501	0.8498
THA_295_11.txt	420.00	216.4968	152.4162	148.9189	148.6744	148.6105	0.8149	0.8366	0.8382	0.8377
THA_295_11.txt	470.00	210.2252	185.2476	179.6738	179.1837	179.0411	0.7933	0.8216	0.8244	0.8237
THA_295_11.txt	530.00	204.1505	221.3717	213.0654	212.1873	211.9089	0.7693	0.8042	0.8086	0.8078
THA_295_11.txt	600.00	198.3652	260.7299	248.9750	247.5266	247.0338	0.7441	0.7854	0.7918	0.7910
THA_295_11.txt	680.00	193.2082	303.7458	287.8750	285.6687	284.8734	0.7176	0.7645	0.7730	0.7725
THA_295_11.txt	770.00	188.5881	350.4340	329.7758	326.6062	325.4074	0.6909	0.7426	0.7532	0.7532
THA_295_11.txt	870.00	184.4675	400.8789	374.7673	370.4274	368.7192	0.6645	0.7201	0.7328	0.7333
THA_295_11.txt	980.00	180.8231	455.2102	423.0070	417.2938	414.9696	0.6387	0.6974	0.7120	0.7133
THA_295_11.txt	1100.00	177.5703	513.4101	474.4896	467.2000	464.1517	0.6139	0.6750	0.6913	0.6932

Dispersion plot

alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
THA_295_11.txt	0.0000	0.0000	0.0000	0.0000
THA_295_11.txt	12.6397	0.0005	-0.0004	12.6397
THA_295_11.txt	17.8833	0.0017	-0.0008	17.8833
THA_295_11.txt	23.6723	0.0039	-0.0014	23.6723
THA_295_11.txt	28.3051	0.0060	-0.0018	28.3051
THA_295_11.txt	33.5089	0.0087	-0.0023	33.5089
THA_295_11.txt	40.1055	0.0146	-0.0036	40.1055
THA_295_11.txt	45.8309	0.0263	-0.0058	45.8309
THA_295_11.txt	52.4953	0.0425	-0.0074	52.4953
THA_295_11.txt	57.0006	0.0545	-0.0084	57.0006
THA_295_11.txt	63.8841	0.0791	-0.0107	63.8841
THA_295_11.txt	70.1245	0.1055	-0.0126	70.1245
THA_295_11.txt	75.9242	0.1349	-0.0149	75.9242
THA_295_11.txt	86.4243	0.1906	-0.0186	86.4243
THA_295_11.txt	95.9642	0.2487	-0.0227	95.9642
THA_295_11.txt	108.9164	0.3507	-0.0283	108.9164
THA_295_11.txt	120.7067	0.4609	-0.0335	120.7067
THA_295_11.txt	148.6105	0.7963	-0.0472	148.6105
THA_295_11.txt	179.0411	1.2916	-0.0631	179.0411
THA_295_11.txt	211.9089	1.9751	-0.0812	211.9089
THA_295_11.txt	247.0338	2.8740	-0.1003	247.0338
THA_295_11.txt	284.8734	4.0446	-0.1213	284.8734
THA_295_11.txt	325.4074	5.5164	-0.1434	325.4074
THA_295_11.txt	368.7192	7.3176	-0.1659	368.7192
THA_295_11.txt	414.9696	9.4685	-0.1888	414.9696
THA_295_11.txt	464.1517	11.9872	-0.2115	464.1517

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 384.3458 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.070
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_295_11.txt	295.00	239.4260	0.0000	0.0000	0.0000	0.0000	0.8792	0.8792	0.8792	0.8792
THA_295_11.txt	296.00	239.1768	12.6434	12.6397	12.6397	12.6397	0.8786	0.8789	0.8789	0.8789
THA_295_11.txt	297.00	238.9365	17.8927	17.8833	17.8833	17.8833	0.8780	0.8785	0.8785	0.8785
THA_295_11.txt	298.50	238.5663	23.6927	23.6724	23.6723	23.6723	0.8772	0.8780	0.8780	0.8780
THA_295_11.txt	300.00	238.1443	28.3391	28.3052	28.3051	28.3051	0.8765	0.8776	0.8776	0.8776
THA_295_11.txt	302.00	237.5882	33.5643	33.5092	33.5089	33.5089	0.8757	0.8772	0.8772	0.8772
THA_295_11.txt	305.00	236.8985	40.1987	40.1064	40.1056	40.1055	0.8739	0.8760	0.8760	0.8760
THA_295_11.txt	308.00	236.4286	45.9671	45.8325	45.8311	45.8309	0.8714	0.8741	0.8741	0.8741
THA_295_11.txt	312.00	235.4980	52.6974	52.4983	52.4956	52.4953	0.8692	0.8727	0.8728	0.8727
THA_295_11.txt	315.00	234.7817	57.2578	57.0052	57.0012	57.0006	0.8677	0.8718	0.8719	0.8718
THA_295_11.txt	320.00	233.7584	64.2410	63.8918	63.8851	63.8841	0.8646	0.8698	0.8698	0.8698
THA_295_11.txt	325.00	232.6763	70.5918	70.1364	70.1261	70.1245	0.8619	0.8680	0.8682	0.8681
THA_295_11.txt	330.00	231.7007	76.5100	75.9413	75.9267	75.9242	0.8590	0.8660	0.8662	0.8661
THA_295_11.txt	340.00	229.6358	87.2740	86.4553	86.4291	86.4243	0.8539	0.8628	0.8630	0.8629
THA_295_11.txt	350.00	227.7851	97.1048	96.0133	95.9723	95.9642	0.8484	0.8591	0.8595	0.8593
THA_295_11.txt	365.00	225.0796	110.5430	109.0017	108.9315	108.9164	0.8408	0.8540	0.8546	0.8544
THA_295_11.txt	380.00	222.5090	122.8708	120.8388	120.7314	120.7067	0.8336	0.8492	0.8501	0.8498
THA_295_11.txt	420.00	216.4968	152.4162	148.9189	148.6744	148.6105	0.8149	0.8366	0.8382	0.8377
THA_295_11.txt	470.00	210.2252	185.2476	179.6738	179.1837	179.0411	0.7933	0.8216	0.8244	0.8237
THA_295_11.txt	530.00	204.1505	221.3717	213.0654	212.1873	211.9089	0.7693	0.8042	0.8086	0.8078
THA_295_11.txt	600.00	198.3652	260.7299	248.9750	247.5266	247.0338	0.7441	0.7854	0.7918	0.7910
THA_295_11.txt	680.00	193.2082	303.7458	287.8750	285.6687	284.8734	0.7176	0.7645	0.7730	0.7725

THA_295_11.txt	770.00	188.5881	350.4340	329.7758	326.6062	325.4074	0.6909	0.7426	0.7532	0.7532
THA_295_11.txt	870.00	184.4675	400.8789	374.7673	370.4274	368.7192	0.6645	0.7201	0.7328	0.7333
THA_295_11.txt	980.00	180.8231	455.2102	423.0070	417.2938	414.9696	0.6387	0.6974	0.7120	0.7133
THA_295_11.txt	1100.00	177.5703	513.4101	474.4896	467.2000	464.1517	0.6139	0.6750	0.6913	0.6932

TAA_multiTemperature_candidate2.xlsx - Sheet #7

x	y	z	Radius	Charge	Atom		
8.167250	-1.147400	0.380760	1.55000	-0.4466500000			14
9.576010	-1.385500	1.008700	1.70000	-0.0721640000		1	12
9.628080	-1.907400	2.491800	1.70000	-0.2161900000			12
11.034600	-2.328800	2.794100	1.70000	-0.1968800000		410	12
11.250700	-2.685800	4.223500	1.70000	-0.1816200000			12
10.484700	-3.893700	4.676900	1.70000	-0.1794900000			12
10.790200	-5.313500	3.984600	1.70000	-0.1808300000			12
10.008700	-6.360900	4.696300	1.70000	-0.3215500000			12
2.288060	2.518000	-0.594710	1.70000	-0.3196800000			12
2.675800	1.689700	0.634210	1.70000	-0.1779000000			12
3.594550	2.414400	1.628600	1.70000	-0.1746400000			12
4.918910	2.943500	1.111500	1.70000	-0.1870200000			12
6.143420	2.088000	1.524500	1.70000	-0.1875700000			12
6.375490	0.893180	0.598550	1.70000	-0.2162500000			12
7.596920	0.081910	1.155700	1.70000	-0.0603870000			12
7.294830	-2.405800	0.574490	1.70000	-0.0548790000			12
5.752720	-2.249700	0.382760	1.70000	-0.2106000000			12
5.107000	-3.605300	0.644620	1.70000	-0.2030700000			12
4.914990	-3.834700	2.203900	1.70000	-0.1862200000			12
4.016610	-5.117900	2.529400	1.70000	-0.1806800000			12
3.801730	-5.355200	4.022500	1.70000	-0.1798900000			12
3.012140	-6.657100	4.294200	1.70000	-0.3220400000			12
8.496250	-0.863880	-1.090500	1.70000	-0.0531930000			12
7.316000	-1.042000	-2.092500	1.70000	-0.2183500000			12
7.658340	-0.659300	-3.519400	1.70000	-0.1924000000			12
6.527750	-0.802120	-4.430100	1.70000	-0.1895400000			12
5.535710	0.321630	-4.630400	1.70000	-0.1745600000			12
4.477490	0.118990	-5.720500	1.70000	-0.1789000000			12
3.443330	1.313600	-5.697600	1.70000	-0.3197700000			12
10.123500	-2.179100	0.487460	1.10000	0.1510800000			1
10.183700	-0.485920	0.752560	1.10000	0.1501400000			1
9.103560	-2.805100	2.681600	1.10000	0.1455200000			1
9.214420	-1.041800	3.105800	1.10000	0.1472600000			1
11.368200	-3.219900	2.191100	1.10000	0.1457500000			1
11.734200	-1.520100	2.500800	1.10000	0.1573400000			1
12.321300	-2.977400	4.354600	1.10000	0.1500500000			1
11.071500	-1.803000	4.904700	1.10000	0.1478500000			1
10.614400	-4.037600	5.784900	1.10000	0.1322400000			1
9.402470	-3.749400	4.492900	1.10000	0.1246200000			1
10.461800	-5.058100	2.954700	1.10000	0.1098300000			1
11.846900	-5.286900	3.801300	1.10000	0.1073300000			1
8.984160	-6.110700	4.804000	1.10000	0.1145800000			1
10.031800	-7.280400	4.113100	1.10000	0.1025100000			1
10.569100	-6.797400	5.638200	1.10000	0.0843780000			1
1.769090	3.500100	-0.279630	1.10000	0.0941700000			1
3.129290	2.792000	-1.212700	1.10000	0.1039900000			1
1.588170	2.005700	-1.238000	1.10000	0.1052400000			1
1.758960	1.306900	1.250100	1.10000	0.1204000000			1
3.202360	0.795080	0.245750	1.10000	0.1058200000			1
3.138750	3.275600	2.081400	1.10000	0.0996690000			1
3.909050	1.600500	2.305800	1.10000	0.1088100000			1
4.901270	3.189000	0.028309	1.10000	0.1133800000			1
5.024310	3.917900	1.608500	1.10000	0.1112700000			1
7.038360	2.781200	1.591000	1.10000	0.0881070000			1
5.923600	1.601900	2.519300	1.10000	0.0961400000			1
5.457180	0.256650	0.436690	1.10000	0.1067200000			1
6.757680	1.336300	-0.330510	1.10000	0.0956700000			1
7.403020	-0.262950	2.163300	1.10000	0.0989680000			1
8.332610	0.817690	1.258200	1.10000	0.0969550000			1
7.675530	-3.142800	-0.138140	1.10000	0.1065500000			1
7.448470	-2.803200	1.611900	1.10000	0.1099000000			1
5.318410	-1.613600	1.158600	1.10000	0.1271700000			1
5.352780	-1.928700	-0.622540	1.10000	0.1265100000			1
4.171280	-3.634700	0.060715	1.10000	0.1266000000			1
5.554620	-4.475400	0.179090	1.10000	0.1209000000			1
5.975230	-3.793600	2.653000	1.10000	0.1249100000			1
4.490260	-2.849600	2.624800	1.10000	0.1068400000			1
2.951100	-5.158900	2.058300	1.10000	0.1008200000			1
4.490860	-6.082800	2.159800	1.10000	0.1194100000			1

4.785300	-5.439800	4.475300	1.10000	0.0686190000	1
3.127660	-4.518900	4.496800	1.10000	0.1159600000	1
3.421670	-7.584900	3.795500	1.10000	0.1155700000	1
2.835180	-6.931900	5.353200	1.10000	0.0745290000	1
2.060360	-6.513300	3.857700	1.10000	0.1227700000	1
9.026630	0.092079	-1.050400	1.10000	0.1175900000	1
9.212210	-1.634800	-1.529500	1.10000	0.0902110000	1
6.984150	-2.108300	-2.044800	1.10000	0.1254900000	1
6.576020	-0.374110	-1.747600	1.10000	0.1215900000	1
8.094840	0.407340	-3.652600	1.10000	0.1102900000	1
8.385700	-1.407900	-3.866100	1.10000	0.1227700000	1
7.011110	-0.879300	-5.461800	1.10000	0.0959550000	1
6.270010	-1.837900	-4.371000	1.10000	0.0881460000	1
5.117130	0.523970	-3.604900	1.10000	0.1018500000	1
6.227050	1.162700	-4.897400	1.10000	0.1050900000	1
4.882740	-0.037622	-6.753700	1.10000	0.0910520000	1
3.914710	-0.850620	-5.655100	1.10000	0.0935530000	1
4.045500	2.267800	-5.901200	1.10000	0.1117100000	1
2.683660	1.210400	-6.544500	1.10000	0.1124100000	1
2.918420	1.558400	-4.730400	1.10000	0.1123700000	1

IMoS.cla

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excelfile Savefile Gas
/filefolder/TAA_multiTemperature_candidate2.xlsx /savefolder/THA_SI.txt N2

DNRCustomRange 0 0
interface 0
fromvalue 7
tovalue 7
red_coef 1.07
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 410
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0
qpol 0
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1
ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

Result of Multistructures Calculation for THA Salt:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: THA_295_11.txt

Number of atoms: 89

Molecular Weight: 410.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule THA_295_11.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_295_11.txt	295.00	239.4260	0.0000	0.0000	0.0000	0.0000	0.8792	0.8792	0.8792	0.8792
THA_295_11.txt	296.00	239.1768	12.6434	12.6397	12.6397	12.6397	0.8786	0.8789	0.8789	0.8789
THA_295_11.txt	297.00	238.9365	17.8927	17.8833	17.8833	17.8833	0.8780	0.8785	0.8785	0.8785
THA_295_11.txt	298.50	238.5663	23.6927	23.6724	23.6723	23.6723	0.8772	0.8780	0.8780	0.8780
THA_295_11.txt	300.00	238.1443	28.3391	28.3052	28.3051	28.3051	0.8765	0.8776	0.8776	0.8776
THA_295_11.txt	302.00	237.5882	33.5643	33.5092	33.5089	33.5089	0.8757	0.8772	0.8772	0.8772
THA_295_11.txt	305.00	236.8985	40.1987	40.1064	40.1056	40.1055	0.8739	0.8760	0.8760	0.8760
THA_295_11.txt	308.00	236.4286	45.9671	45.8325	45.8311	45.8309	0.8714	0.8741	0.8741	0.8741
THA_295_11.txt	312.00	235.4980	52.6974	52.4983	52.4956	52.4953	0.8692	0.8727	0.8728	0.8727
THA_295_11.txt	315.00	234.7817	57.2578	57.0052	57.0012	57.0006	0.8677	0.8718	0.8719	0.8718
THA_295_11.txt	320.00	233.7584	64.2410	63.8918	63.8851	63.8841	0.8646	0.8698	0.8698	0.8698
THA_295_11.txt	325.00	232.6763	70.5918	70.1364	70.1261	70.1245	0.8619	0.8680	0.8682	0.8681
THA_295_11.txt	330.00	231.7007	76.5100	75.9413	75.9267	75.9242	0.8590	0.8660	0.8662	0.8661
THA_295_11.txt	340.00	229.6358	87.2740	86.4553	86.4291	86.4243	0.8539	0.8628	0.8630	0.8629
THA_295_11.txt	350.00	227.7851	97.1048	96.0133	95.9723	95.9642	0.8484	0.8591	0.8595	0.8593
THA_295_11.txt	365.00	225.0796	110.5430	109.0017	108.9315	108.9164	0.8408	0.8540	0.8546	0.8544
THA_295_11.txt	380.00	222.5090	122.8708	120.8388	120.7314	120.7067	0.8336	0.8492	0.8501	0.8498
THA_295_11.txt	420.00	216.4968	152.4162	148.9189	148.6744	148.6105	0.8149	0.8366	0.8382	0.8377

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
THA_295_11.txt	0.0000	0.0000	0.0000	0.0000
THA_295_11.txt	12.6397	0.0005	-0.0004	12.6397
THA_295_11.txt	17.8833	0.0017	-0.0008	17.8833
THA_295_11.txt	23.6723	0.0039	-0.0014	23.6723
THA_295_11.txt	28.3051	0.0060	-0.0018	28.3051
THA_295_11.txt	33.5089	0.0087	-0.0023	33.5089
THA_295_11.txt	40.1055	0.0146	-0.0036	40.1055
THA_295_11.txt	45.8309	0.0263	-0.0058	45.8309
THA_295_11.txt	52.4953	0.0425	-0.0074	52.4953
THA_295_11.txt	57.0006	0.0545	-0.0084	57.0006
THA_295_11.txt	63.8841	0.0791	-0.0107	63.8841
THA_295_11.txt	70.1245	0.1055	-0.0126	70.1245
THA_295_11.txt	75.9242	0.1349	-0.0149	75.9242
THA_295_11.txt	86.4243	0.1906	-0.0186	86.4243
THA_295_11.txt	95.9642	0.2487	-0.0227	95.9642
THA_295_11.txt	108.9164	0.3507	-0.0283	108.9164
THA_295_11.txt	120.7067	0.4609	-0.0335	120.7067
THA_295_11.txt	148.6105	0.7957	-0.0472	148.6105

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 282.6917 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: THA_460_1.txt

Number of atoms: 89
Molecular Weight: 410.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule THA_460_1.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_460_1.txt	295.00	241.1359	0.0000	0.0000	0.0000	0.0000	0.8730	0.8730	0.8730	0.8730
THA_460_1.txt	296.00	240.8824	12.7336	12.7299	12.7299	12.7299	0.8724	0.8726	0.8726	0.8726
THA_460_1.txt	297.00	240.6748	18.0229	18.0138	18.0137	18.0137	0.8717	0.8721	0.8721	0.8721
THA_460_1.txt	298.50	240.2677	23.8617	23.8418	23.8418	23.8418	0.8710	0.8717	0.8717	0.8717
THA_460_1.txt	300.00	239.8981	28.5478	28.5148	28.5146	28.5146	0.8701	0.8712	0.8712	0.8712
THA_460_1.txt	302.00	239.3984	33.8200	33.7664	33.7661	33.7660	0.8691	0.8705	0.8705	0.8705
THA_460_1.txt	305.00	238.6529	40.4964	40.4062	40.4055	40.4055	0.8675	0.8695	0.8695	0.8695
THA_460_1.txt	308.00	237.9950	46.2716	46.1396	46.1383	46.1381	0.8656	0.8683	0.8683	0.8683
THA_460_1.txt	312.00	236.9745	53.0278	52.8316	52.8292	52.8288	0.8638	0.8672	0.8672	0.8672
THA_460_1.txt	315.00	236.2994	57.6279	57.3794	57.3758	57.3753	0.8621	0.8661	0.8662	0.8661
THA_460_1.txt	320.00	235.1733	64.6298	64.2854	64.2793	64.2783	0.8594	0.8644	0.8645	0.8644
THA_460_1.txt	325.00	234.0593	71.0114	70.5615	70.5521	70.5505	0.8569	0.8628	0.8629	0.8628
THA_460_1.txt	330.00	232.9711	76.9295	76.3668	76.3533	76.3509	0.8543	0.8612	0.8613	0.8612
THA_460_1.txt	340.00	230.9447	87.7715	86.9608	86.9367	86.9322	0.8490	0.8577	0.8579	0.8578
THA_460_1.txt	350.00	229.0109	97.6273	96.5442	96.5061	96.4985	0.8439	0.8543	0.8547	0.8545
THA_460_1.txt	365.00	226.2130	111.0997	109.5647	109.4990	109.4847	0.8366	0.8496	0.8501	0.8499
THA_460_1.txt	380.00	223.5961	123.4711	121.4416	121.3401	121.3165	0.8295	0.8450	0.8458	0.8454
THA_460_1.txt	420.00	217.4094	153.0586	149.5439	149.3074	149.2451	0.8115	0.8330	0.8346	0.8341
THA_460_1.txt	460.00	212.2263	179.6469	174.4651	174.0397	173.9178	0.7943	0.8213	0.8238	0.8231
THA_460_1.txt	470.00	211.0396	185.9653	180.3415	179.8605	179.7202	0.7902	0.8184	0.8212	0.8205
THA_460_1.txt	530.00	204.8515	222.1318	213.7105	212.8332	212.5544	0.7667	0.8016	0.8061	0.8053

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
THA_460_1.txt	0.0000	0.0000	0.0000	0.0000
THA_460_1.txt	12.7299	0.0010	-0.0004	12.7299
THA_460_1.txt	18.0137	0.0027	-0.0010	18.0137
THA_460_1.txt	23.8418	0.0047	-0.0014	23.8418
THA_460_1.txt	28.5146	0.0068	-0.0021	28.5146
THA_460_1.txt	33.7660	0.0103	-0.0028	33.7660
THA_460_1.txt	40.4055	0.0167	-0.0039	40.4055
THA_460_1.txt	46.1381	0.0262	-0.0054	46.1381
THA_460_1.txt	52.8288	0.0387	-0.0066	52.8288
THA_460_1.txt	57.3753	0.0494	-0.0078	57.3753
THA_460_1.txt	64.2783	0.0694	-0.0098	64.2783
THA_460_1.txt	70.5505	0.0912	-0.0116	70.5505
THA_460_1.txt	76.3509	0.1149	-0.0134	76.3509
THA_460_1.txt	86.9322	0.1675	-0.0173	86.9322
THA_460_1.txt	96.4985	0.2265	-0.0212	96.4985
THA_460_1.txt	109.4847	0.3271	-0.0264	109.4847
THA_460_1.txt	121.3165	0.4338	-0.0315	121.3165
THA_460_1.txt	149.2451	0.7608	-0.0446	149.2451
THA_460_1.txt	173.9178	1.1400	-0.0571	173.9178
THA_460_1.txt	179.7202	1.2402	-0.0601	179.7202
THA_460_1.txt	212.5544	1.8993	-0.0776	212.5544

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 327.3725 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: THA_600_28.txt

Number of atoms: 89
Molecular Weight: 410.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule THA_600_28.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_600_28.txt	295.00	246.5516	0.0000	0.0000	0.0000	0.0000	0.8538	0.8538	0.8538	0.8538
THA_600_28.txt	470.00	216.2376	190.5457	184.7504	184.2378	184.0882	0.7712	0.7990	0.8018	0.8011
THA_600_28.txt	530.00	209.8664	227.5698	218.9245	218.0039	217.7106	0.7483	0.7827	0.7871	0.7863
THA_600_28.txt	600.00	203.9655	268.0909	255.8849	254.3735	253.8557	0.7237	0.7642	0.7705	0.7698
THA_600_28.txt	680.00	198.6962	312.3735	295.9144	293.6151	292.7796	0.6978	0.7437	0.7521	0.7516
THA_600_28.txt	770.00	193.9016	360.3076	338.8641	335.5517	334.2869	0.6720	0.7227	0.7331	0.7331
THA_600_28.txt	870.00	189.6688	412.1822	385.1020	380.5735	378.7727	0.6463	0.7008	0.7133	0.7138
THA_600_28.txt	980.00	185.8967	467.9826	434.5894	428.6263	426.1738	0.6213	0.6788	0.6932	0.6945
THA_600_28.txt	1100.00	182.5431	527.7879	487.4353	479.8266	476.6083	0.5972	0.6571	0.6732	0.6752

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
THA_600_28.txt	0.0000	0.0000	0.0000	0.0000
THA_600_28.txt	184.0882	1.2511	-0.0617	184.0882
THA_600_28.txt	217.7106	1.9293	-0.0791	217.7106
THA_600_28.txt	253.8557	2.8458	-0.0984	253.8557
THA_600_28.txt	292.7796	4.0561	-0.1197	292.7796
THA_600_28.txt	334.2869	5.5653	-0.1413	334.2869
THA_600_28.txt	378.7727	7.4228	-0.1639	378.7727
THA_600_28.txt	426.1738	9.6380	-0.1866	426.1738
THA_600_28.txt	476.6083	12.2319	-0.2092	476.6083

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
MULTI STRUCTURE Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Teff	Ed (Td)	Ec (Td)	alpha (Td)	Kho (Td)
295	0.0000	0.0000	0.0000	0.8792
296	12.6402	0.0006	-0.0004	0.8788
297	17.8849	0.0018	-0.0009	0.8784
298.5	23.6759	0.0043	-0.0016	0.8778
300	28.3114	0.0067	-0.0020	0.8774
302	33.5198	0.0099	-0.0026	0.8769
305	40.1237	0.0167	-0.0041	0.8756
308	45.8551	0.0291	-0.0063	0.8736
312	52.5296	0.0464	-0.0080	0.8722
315	57.0461	0.0595	-0.0092	0.8711
320	63.9438	0.0857	-0.0116	0.8690
325	70.2019	0.1140	-0.0137	0.8671
330	76.0147	0.1449	-0.0161	0.8651
340	86.5628	0.2052	-0.0201	0.8615
350	96.1423	0.2683	-0.0245	0.8577
365	109.1575	0.3780	-0.0304	0.8525
380	121.0209	0.4962	-0.0360	0.8475
420	149.0913	0.8541	-0.0503	0.8350
460	173.9178	1.2622	-0.0638	0.8231

470	180.0322	1.3910	-0.0683	0.8191
530	215.1325	2.3289	-0.0949	0.7958
600	253.8557	3.7450	-0.1245	0.7698
680	292.7796	5.2649	-0.1451	0.7516
770	334.2869	7.0418	-0.1661	0.7331
870	378.7727	9.1206	-0.1881	0.7138
980	426.1738	11.3783	-0.2101	0.6945
1100	476.6083	13.8473	-0.2321	0.6752

Time taken is a mere 118.0042 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.070
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
THA_295_11.txt	295.00	239.4260	0.0000	0.0000	0.0000	0.0000	0.8792	0.8792	0.8792	0.8792
THA_295_11.txt	296.00	239.1768	12.6434	12.6397	12.6397	12.6397	0.8786	0.8789	0.8789	0.8789
THA_295_11.txt	297.00	238.9365	17.8927	17.8833	17.8833	17.8833	0.8780	0.8785	0.8785	0.8785
THA_295_11.txt	298.50	238.5663	23.6927	23.6724	23.6723	23.6723	0.8772	0.8780	0.8780	0.8780
THA_295_11.txt	300.00	238.1443	28.3391	28.3052	28.3051	28.3051	0.8765	0.8776	0.8776	0.8776
THA_295_11.txt	302.00	237.5882	33.5643	33.5092	33.5089	33.5089	0.8757	0.8772	0.8772	0.8772
THA_295_11.txt	305.00	236.8985	40.1987	40.1064	40.1056	40.1055	0.8739	0.8760	0.8760	0.8760
THA_295_11.txt	308.00	236.4286	45.9671	45.8325	45.8311	45.8309	0.8714	0.8741	0.8741	0.8741
THA_295_11.txt	312.00	235.4980	52.6974	52.4983	52.4956	52.4953	0.8692	0.8727	0.8728	0.8727
THA_295_11.txt	315.00	234.7817	57.2578	57.0052	57.0012	57.0006	0.8677	0.8718	0.8719	0.8718
THA_295_11.txt	320.00	233.7584	64.2410	63.8918	63.8851	63.8841	0.8646	0.8698	0.8698	0.8698
THA_295_11.txt	325.00	232.6763	70.5918	70.1364	70.1261	70.1245	0.8619	0.8680	0.8682	0.8681
THA_295_11.txt	330.00	231.7007	76.5100	75.9413	75.9267	75.9242	0.8590	0.8660	0.8662	0.8661
THA_295_11.txt	340.00	229.6358	87.2740	86.4553	86.4291	86.4243	0.8539	0.8628	0.8630	0.8629
THA_295_11.txt	350.00	227.7851	97.1048	96.0133	95.9723	95.9642	0.8484	0.8591	0.8595	0.8593
THA_295_11.txt	365.00	225.0796	110.5430	109.0017	108.9315	108.9164	0.8408	0.8540	0.8546	0.8544
THA_295_11.txt	380.00	222.5090	122.8708	120.8388	120.7314	120.7067	0.8336	0.8492	0.8501	0.8498
THA_295_11.txt	420.00	216.4968	152.4162	148.9189	148.6744	148.6105	0.8149	0.8366	0.8382	0.8377

THA_460_1.txt	295.00	241.1359	0.0000	0.0000	0.0000	0.0000	0.8730	0.8730	0.8730	0.8730
THA_460_1.txt	296.00	240.8824	12.7336	12.7299	12.7299	12.7299	0.8724	0.8726	0.8726	0.8726
THA_460_1.txt	297.00	240.6748	18.0229	18.0138	18.0137	18.0137	0.8717	0.8721	0.8721	0.8721
THA_460_1.txt	298.50	240.2677	23.8617	23.8418	23.8418	23.8418	0.8710	0.8717	0.8717	0.8717
THA_460_1.txt	300.00	239.8981	28.5478	28.5148	28.5146	28.5146	0.8701	0.8712	0.8712	0.8712
THA_460_1.txt	302.00	239.3984	33.8200	33.7664	33.7661	33.7660	0.8691	0.8705	0.8705	0.8705
THA_460_1.txt	305.00	238.6529	40.4964	40.4062	40.4055	40.4055	0.8675	0.8695	0.8695	0.8695
THA_460_1.txt	308.00	237.9950	46.2716	46.1396	46.1383	46.1381	0.8656	0.8683	0.8683	0.8683
THA_460_1.txt	312.00	236.9745	53.0278	52.8316	52.8292	52.8288	0.8638	0.8672	0.8672	0.8672
THA_460_1.txt	315.00	236.2994	57.6279	57.3794	57.3758	57.3753	0.8621	0.8661	0.8662	0.8661
THA_460_1.txt	320.00	235.1733	64.6298	64.2854	64.2793	64.2783	0.8594	0.8644	0.8645	0.8644
THA_460_1.txt	325.00	234.0593	71.0114	70.5615	70.5521	70.5505	0.8569	0.8628	0.8629	0.8628
THA_460_1.txt	330.00	232.9711	76.9295	76.3668	76.3533	76.3509	0.8543	0.8612	0.8613	0.8612
THA_460_1.txt	340.00	230.9447	87.7715	86.9608	86.9367	86.9322	0.8490	0.8577	0.8579	0.8578
THA_460_1.txt	350.00	229.0109	97.6273	96.5442	96.5061	96.4985	0.8439	0.8543	0.8547	0.8545
THA_460_1.txt	365.00	226.2130	111.0997	109.5647	109.4990	109.4847	0.8366	0.8496	0.8501	0.8499
THA_460_1.txt	380.00	223.5961	123.4711	121.4416	121.3401	121.3165	0.8295	0.8450	0.8458	0.8454
THA_460_1.txt	420.00	217.4094	153.0586	149.5439	149.3074	149.2451	0.8115	0.8330	0.8346	0.8341
THA_460_1.txt	460.00	212.2263	179.6469	174.4651	174.0397	173.9178	0.7943	0.8213	0.8238	0.8231
THA_460_1.txt	470.00	211.0396	185.9653	180.3415	179.8605	179.7202	0.7902	0.8184	0.8212	0.8205
THA_460_1.txt	530.00	204.8515	222.1318	213.7105	212.8332	212.5544	0.7667	0.8016	0.8061	0.8053

THA_600_28.txt	295.00	246.5516	0.0000	0.0000	0.0000	0.0000	0.8538	0.8538	0.8538	0.8538
THA_600_28.txt	470.00	216.2376	190.5457	184.7504	184.2378	184.0882	0.7712	0.7990	0.8018	0.8011
THA_600_28.txt	530.00	209.8664	227.5698	218.9245	218.0039	217.7106	0.7483	0.7827	0.7871	0.7863
THA_600_28.txt	600.00	203.9655	268.0909	255.8849	254.3735	253.8557	0.7237	0.7642	0.7705	0.7698
THA_600_28.txt	680.00	198.6962	312.3735	295.9144	293.6151	292.7796	0.6978	0.7437	0.7521	0.7516
THA_600_28.txt	770.00	193.9016	360.3076	338.8641	335.5517	334.2869	0.6720	0.7227	0.7331	0.7331
THA_600_28.txt	870.00	189.6688	412.1822	385.1020	380.5735	378.7727	0.6463	0.7008	0.7133	0.7138
THA_600_28.txt	980.00	185.8967	467.9826	434.5894	428.6263	426.1738	0.6213	0.6788	0.6932	0.6945
THA_600_28.txt	1100.00	182.5431	527.7879	487.4353	479.8266	476.6083	0.5972	0.6571	0.6732	0.6752

TAA_multiTemperature_candidate2.xlsx - Sheet #7

x	y	z	Radius	Charge	Atom	
8.167250	-1.147400	0.380760	1.55000	-0.4466500000		14
9.576010	-1.385500	1.008700	1.70000	-0.0721640000	1	12
9.628080	-1.907400	2.491800	1.70000	-0.2161900000		12
11.034600	-2.328800	2.794100	1.70000	-0.1968800000	410	12
11.250700	-2.685800	4.223500	1.70000	-0.1816200000		12
10.484700	-3.893700	4.676900	1.70000	-0.1794900000		12
10.790200	-5.313500	3.984600	1.70000	-0.1808300000		12
10.008700	-6.360900	4.696300	1.70000	-0.3215500000		12
2.288060	2.518000	-0.594710	1.70000	-0.3196800000		12
2.675800	1.689700	0.634210	1.70000	-0.1779000000		12
3.594550	2.414400	1.628600	1.70000	-0.1746400000		12
4.918910	2.943500	1.111500	1.70000	-0.1870200000		12
6.143420	2.088000	1.524500	1.70000	-0.1875700000		12
6.375490	0.893180	0.598550	1.70000	-0.2162500000		12
7.596920	0.081910	1.155700	1.70000	-0.0603870000		12
7.294830	-2.405800	0.574490	1.70000	-0.0548790000		12
5.752720	-2.249700	0.382760	1.70000	-0.2106000000		12
5.107000	-3.605300	0.644620	1.70000	-0.2030700000		12
4.914990	-3.834700	2.203900	1.70000	-0.1862200000		12
4.016610	-5.117900	2.529400	1.70000	-0.1806800000		12
3.801730	-5.355200	4.022500	1.70000	-0.1798900000		12
3.012140	-6.657100	4.294200	1.70000	-0.3220400000		12
8.496250	-0.863880	-1.090500	1.70000	-0.0531930000		12
7.316000	-1.042000	-2.092500	1.70000	-0.2183500000		12
7.658340	-0.659300	-3.519400	1.70000	-0.1924000000		12
6.527750	-0.802120	-4.430100	1.70000	-0.1895400000		12
5.535710	0.321630	-4.630400	1.70000	-0.1745600000		12
4.477490	0.118990	-5.720500	1.70000	-0.1789000000		12
3.443330	1.313600	-5.697600	1.70000	-0.3197700000		12
10.123500	-2.179100	0.487460	1.10000	0.1510800000		1
10.183700	-0.485920	0.752560	1.10000	0.1501400000		1
9.103560	-2.805100	2.681600	1.10000	0.1455200000		1
9.214420	-1.041800	3.105800	1.10000	0.1472600000		1
11.368200	-3.219900	2.191100	1.10000	0.1457500000		1
11.734200	-1.520100	2.500800	1.10000	0.1573400000		1
12.321300	-2.977400	4.354600	1.10000	0.1500500000		1
11.071500	-1.803000	4.904700	1.10000	0.1478500000		1
10.614400	-4.037600	5.784900	1.10000	0.1322400000		1
9.402470	-3.749400	4.492900	1.10000	0.1246200000		1
10.461800	-5.058100	2.954700	1.10000	0.1098300000		1
11.846900	-5.286900	3.801300	1.10000	0.1073300000		1

8.984160	-6.110700	4.804000	1.10000	0.1145800000	1
10.031800	-7.280400	4.113100	1.10000	0.1025100000	1
10.569100	-6.797400	5.638200	1.10000	0.0843780000	1
1.769090	3.500100	-0.279630	1.10000	0.0941700000	1
3.129290	2.792000	-1.212700	1.10000	0.1039900000	1
1.588170	2.005700	-1.238000	1.10000	0.1052400000	1
1.758960	1.306900	1.250100	1.10000	0.1204000000	1
3.202360	0.795080	0.245750	1.10000	0.1058200000	1
3.138750	3.275600	2.081400	1.10000	0.0996690000	1
3.909050	1.600500	2.305800	1.10000	0.1088100000	1
4.901270	3.189000	0.028309	1.10000	0.1133800000	1
5.024310	3.917900	1.608500	1.10000	0.1112700000	1
7.038360	2.781200	1.591000	1.10000	0.0881070000	1
5.923600	1.601900	2.519300	1.10000	0.0961400000	1
5.457180	0.256650	0.436690	1.10000	0.1067200000	1
6.757680	1.336300	-0.330510	1.10000	0.0956700000	1
7.403020	-0.262950	2.163300	1.10000	0.0989680000	1
8.332610	0.817690	1.258200	1.10000	0.0969550000	1
7.675530	-3.142800	-0.138140	1.10000	0.1065500000	1
7.448470	-2.803200	1.611900	1.10000	0.1099000000	1
5.318410	-1.613600	1.158600	1.10000	0.1271700000	1
5.352780	-1.928700	-0.622540	1.10000	0.1265100000	1
4.171280	-3.634700	0.060715	1.10000	0.1266000000	1
5.554620	-4.475400	0.179090	1.10000	0.1209000000	1
5.975230	-3.793600	2.653000	1.10000	0.1249100000	1
4.490260	-2.849600	2.624800	1.10000	0.1068400000	1
2.951100	-5.158900	2.058300	1.10000	0.1008200000	1
4.490860	-6.082800	2.159800	1.10000	0.1194100000	1
4.785300	-5.439800	4.475300	1.10000	0.0686190000	1
3.127660	-4.518900	4.496800	1.10000	0.1159600000	1
3.421670	-7.584900	3.795500	1.10000	0.1155700000	1
2.835180	-6.931900	5.353200	1.10000	0.0745290000	1
2.060360	-6.513300	3.857700	1.10000	0.1227700000	1
9.026630	0.092079	-1.050400	1.10000	0.1175900000	1
9.212210	-1.634800	-1.529500	1.10000	0.0902110000	1
6.984150	-2.108300	-2.044800	1.10000	0.1254900000	1
6.576020	-0.374110	-1.747600	1.10000	0.1215900000	1
8.094840	0.407340	-3.652600	1.10000	0.1102900000	1
8.385700	-1.407900	-3.866100	1.10000	0.1227700000	1
7.011110	-0.879300	-5.461800	1.10000	0.0959550000	1
6.270010	-1.837900	-4.371000	1.10000	0.0881460000	1
5.117130	0.523970	-3.604900	1.10000	0.1018500000	1
6.227050	1.162700	-4.897400	1.10000	0.1050900000	1
4.882740	-0.037622	-6.753700	1.10000	0.0910520000	1
3.914710	-0.850620	-5.655100	1.10000	0.0935530000	1
4.045500	2.267800	-5.901200	1.10000	0.1117100000	1
2.683660	1.210400	-6.544500	1.10000	0.1124100000	1
2.918420	1.558400	-4.730400	1.10000	0.1123700000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #8

x	y	z	Radius	Charge	Atom		
8.032490	-1.879600	0.913910	1.55000	-0.4466500000			14
9.230490	-2.091500	1.740600	1.70000	-0.0721640000		1	12
9.053280	-1.921500	3.287700	1.70000	-0.2161900000			12
9.901190	-3.010800	4.164600	1.70000	-0.1968800000		410	12
11.219400	-2.445100	4.709300	1.70000	-0.1816200000			12
10.779500	-1.615100	5.937000	1.70000	-0.1794900000			12
11.976300	-1.137300	6.787800	1.70000	-0.1808300000			12
11.374900	-0.512880	8.076700	1.70000	-0.3215500000			12
2.355350	2.342600	-2.018600	1.70000	-0.3196800000			12
3.540980	2.173600	-0.963540	1.70000	-0.1779000000			12
3.198620	1.246900	0.246450	1.70000	-0.1746400000			12
3.973450	1.501000	1.543100	1.70000	-0.1870200000			12
5.508960	1.189800	1.557500	1.70000	-0.1875700000			12
5.884400	-0.252320	1.123100	1.70000	-0.2162500000			12
7.335860	-0.510200	1.396200	1.70000	-0.0603870000			12
7.168040	-3.099700	1.147200	1.70000	-0.0548790000			12
6.109610	-3.371200	0.032800	1.70000	-0.2106000000			12
4.993680	-4.251300	0.735770	1.70000	-0.2030700000			12
3.807950	-4.552700	-0.262030	1.70000	-0.1862200000			12
2.749680	-5.461000	0.478760	1.70000	-0.1806800000			12
3.048900	-6.948600	0.663660	1.70000	-0.1798900000			12
1.753260	-7.718700	1.004000	1.70000	-0.3220400000			12
8.481180	-1.859500	-0.538030	1.70000	-0.0531930000			12
7.643960	-1.132400	-1.629200	1.70000	-0.2183500000			12
8.342000	-0.861230	-2.978000	1.70000	-0.1924000000			12
7.776090	0.350670	-3.861700	1.70000	-0.1895400000			12
6.436390	0.084724	-4.637000	1.70000	-0.1745600000			12

5.702360	1.337200	-5.053900	1.70000	-0.1789000000	12
4.504100	0.837500	-5.791000	1.70000	-0.3197700000	12
9.678710	-3.120400	1.511000	1.10000	0.1510800000	1
10.070000	-1.395000	1.448800	1.10000	0.1501400000	1
8.017890	-2.078100	3.535700	1.10000	0.1455200000	1
9.362520	-0.921120	3.539000	1.10000	0.1472600000	1
9.211350	-3.360800	4.981300	1.10000	0.1457500000	1
10.053400	-3.896300	3.539900	1.10000	0.1573400000	1
11.823100	-3.344500	5.091200	1.10000	0.1500500000	1
11.766400	-1.844200	3.889300	1.10000	0.1478500000	1
10.207200	-0.768000	5.651100	1.10000	0.1322400000	1
10.162300	-2.260500	6.590600	1.10000	0.1246200000	1
12.621100	-1.995100	7.093600	1.10000	0.1098300000	1
12.546500	-0.375510	6.194600	1.10000	0.1073300000	1
10.788400	-1.210800	8.717200	1.10000	0.1145800000	1
12.198900	-0.189490	8.738200	1.10000	0.1025100000	1
10.751100	0.373780	7.867200	1.10000	0.0843780000	1
2.121520	1.421400	-2.506800	1.10000	0.0941700000	1
1.378440	2.709600	-1.544400	1.10000	0.1039900000	1
2.649090	2.980800	-2.846600	1.10000	0.1052400000	1
4.535080	1.926100	-1.451600	1.10000	0.1204000000	1
3.727650	3.265000	-0.694580	1.10000	0.1058200000	1
2.054710	1.345300	0.394970	1.10000	0.0996690000	1
3.188210	0.150450	-0.061510	1.10000	0.1088100000	1
3.711740	2.511600	1.945900	1.10000	0.1133800000	1
3.615550	0.796480	2.337600	1.10000	0.1112700000	1
6.022710	1.904400	0.906250	1.10000	0.0881070000	1
5.882890	1.453600	2.616200	1.10000	0.0961400000	1
5.288960	-0.928850	1.793200	1.10000	0.1067200000	1
5.631830	-0.469010	-0.029130	1.10000	0.0956700000	1
7.502330	-0.494440	2.511700	1.10000	0.0989680000	1
7.995100	0.381210	1.133700	1.10000	0.0969550000	1
7.819990	-3.999500	1.087900	1.10000	0.1065500000	1
6.657380	-2.947200	2.085200	1.10000	0.1099000000	1
5.536180	-2.470700	-0.098929	1.10000	0.1271700000	1
6.417520	-3.855000	-0.923170	1.10000	0.1265100000	1
5.422070	-5.182600	1.076400	1.10000	0.1266000000	1
4.587960	-3.717000	1.609000	1.10000	0.1209000000	1
3.237830	-3.631800	-0.458940	1.10000	0.1249100000	1
4.142710	-5.039000	-1.240500	1.10000	0.1068400000	1
2.531120	-5.068600	1.567000	1.10000	0.1008200000	1
1.778040	-5.511300	-0.047999	1.10000	0.1194100000	1
3.428830	-7.304900	-0.331160	1.10000	0.0686190000	1
3.796810	-7.065300	1.420400	1.10000	0.1159600000	1
1.004920	-7.677900	0.152680	1.10000	0.1155700000	1
2.073410	-8.777300	1.055600	1.10000	0.0745290000	1
1.343950	-7.346400	1.993100	1.10000	0.1227700000	1
9.400210	-1.215000	-0.552380	1.10000	0.1175900000	1
8.950630	-2.769200	-0.922220	1.10000	0.0902110000	1
6.675210	-1.617400	-2.005000	1.10000	0.1254900000	1
7.365550	-0.163260	-1.222500	1.10000	0.1215900000	1
9.401020	-0.626050	-2.651500	1.10000	0.1102900000	1
8.466110	-1.811600	-3.545500	1.10000	0.1227700000	1
7.692800	1.185600	-3.162700	1.10000	0.0959550000	1
8.540680	0.624870	-4.618700	1.10000	0.0881460000	1
6.739560	-0.455570	-5.568700	1.10000	0.1018500000	1
5.732180	-0.613930	-4.044300	1.10000	0.1050900000	1
5.455190	2.102500	-4.216100	1.10000	0.0910520000	1
6.384120	1.889800	-5.721200	1.10000	0.0935530000	1
4.770880	0.176520	-6.667100	1.10000	0.1117100000	1
3.787160	0.215030	-5.153100	1.10000	0.1124100000	1
4.005980	1.735500	-6.266600	1.10000	0.1123700000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #9

x	y	z	Radius	Charge	Atom		
6.682130	-0.315510	1.467300	1.55000	-0.4466500000			14
7.585210	-0.333310	2.692400	1.70000	-0.0721640000		1	12
7.727350	-1.708800	3.439100	1.70000	-0.2161900000			12
8.912860	-1.685900	4.352800	1.70000	-0.1968800000		410	12
10.317100	-2.003100	3.772500	1.70000	-0.1816200000			12
11.225900	-2.541700	4.907900	1.70000	-0.1794900000			12
12.547500	-3.243200	4.416300	1.70000	-0.1808300000			12
13.244600	-2.702900	3.159300	1.70000	-0.3215500000			12
1.049500	-4.602800	0.672230	1.70000	-0.3196800000			12
1.871430	-3.852600	1.704000	1.70000	-0.1779000000			12
1.203680	-2.681000	2.468600	1.70000	-0.1746400000			12
2.098270	-1.841300	3.335700	1.70000	-0.1870200000			12
3.029480	-0.826830	2.637500	1.70000	-0.1875700000			12

4.518220	-1.180600	2.740100	1.70000	-0.2162500000	12
5.214940	-0.107210	1.833400	1.70000	-0.0603870000	12
7.058650	-1.661600	0.754750	1.70000	-0.0548790000	12
6.389540	-1.933100	-0.617430	1.70000	-0.2106000000	12
6.816640	-3.290200	-1.134900	1.70000	-0.2030700000	12
6.463750	-4.468200	-0.188590	1.70000	-0.1862200000	12
6.678710	-5.846600	-0.800210	1.70000	-0.1806800000	12
5.308320	-6.363300	-1.362600	1.70000	-0.1798900000	12
5.277700	-7.657700	-2.311900	1.70000	-0.3220400000	12
7.201490	0.899780	0.622890	1.70000	-0.0531930000	12
6.360740	1.216000	-0.618560	1.70000	-0.2183500000	12
7.345290	1.891100	-1.621200	1.70000	-0.1924000000	12
6.700140	2.534600	-2.847300	1.70000	-0.1895400000	12
7.671470	3.077600	-3.900500	1.70000	-0.1745600000	12
7.010370	3.667500	-5.174100	1.70000	-0.1789000000	12
7.909370	4.337500	-6.185700	1.70000	-0.3197700000	12
8.663290	-0.096624	2.436300	1.10000	0.1510800000	1
7.116980	0.370630	3.416300	1.10000	0.1501400000	1
7.641760	-2.626000	2.779000	1.10000	0.1455200000	1
6.712210	-1.763600	3.838100	1.10000	0.1472600000	1
8.988920	-0.737680	4.950100	1.10000	0.1457500000	1
8.552970	-2.523700	4.990500	1.10000	0.1573400000	1
10.371500	-2.743800	3.003100	1.10000	0.1500500000	1
10.810600	-1.020200	3.462800	1.10000	0.1478500000	1
11.618200	-1.631700	5.424000	1.10000	0.1322400000	1
10.616100	-3.265800	5.489200	1.10000	0.1246200000	1
13.281700	-3.305800	5.192000	1.10000	0.1098300000	1
12.186900	-4.320200	4.219700	1.10000	0.1073300000	1
13.998300	-3.430700	2.840800	1.10000	0.1145800000	1
12.474700	-2.564700	2.228600	1.10000	0.1025100000	1
13.759900	-1.728100	3.264500	1.10000	0.0843780000	1
0.692510	-4.031600	-0.230540	1.10000	0.0941700000	1
1.515700	-5.643900	0.520060	1.10000	0.1039900000	1
0.100234	-4.869300	1.148400	1.10000	0.1052400000	1
2.053590	-4.577600	2.470700	1.10000	0.1204000000	1
2.841750	-3.357500	1.301700	1.10000	0.1058200000	1
0.712967	-2.007500	1.824000	1.10000	0.0996690000	1
0.408006	-3.088800	3.120600	1.10000	0.1088100000	1
1.461010	-1.460100	4.164200	1.10000	0.1133800000	1
2.782050	-2.568200	3.841500	1.10000	0.1112700000	1
2.589750	-0.653120	1.589300	1.10000	0.0881070000	1
2.823150	0.118390	3.157300	1.10000	0.0961400000	1
4.802650	-0.973200	3.789500	1.10000	0.1067200000	1
4.789290	-2.263300	2.556500	1.10000	0.0956700000	1
4.959080	0.981130	2.299600	1.10000	0.0989680000	1
4.628910	-0.310300	0.866480	1.10000	0.0969550000	1
8.233770	-1.827900	0.719630	1.10000	0.1065500000	1
6.418110	-2.371900	1.355500	1.10000	0.1099000000	1
5.269940	-1.760300	-0.743850	1.10000	0.1271700000	1
6.765620	-1.134700	-1.316100	1.10000	0.1265100000	1
6.197510	-3.355400	-2.097500	1.10000	0.1266000000	1
7.937380	-3.265200	-1.383100	1.10000	0.1209000000	1
7.120190	-4.385700	0.687550	1.10000	0.1249100000	1
5.435420	-4.238500	0.188320	1.10000	0.1068400000	1
7.453810	-5.948700	-1.520700	1.10000	0.1008200000	1
6.864190	-6.585900	0.080820	1.10000	0.1194100000	1
4.532650	-6.402600	-0.503900	1.10000	0.0686190000	1
4.930470	-5.541500	-2.004100	1.10000	0.1159600000	1
6.133870	-7.566500	-3.047400	1.10000	0.1155700000	1
5.372990	-8.613000	-1.722200	1.10000	0.0745290000	1
4.355770	-7.600200	-2.925300	1.10000	0.1227700000	1
7.328150	1.802900	1.265800	1.10000	0.1175900000	1
8.114880	0.533680	0.095220	1.10000	0.0902110000	1
5.523030	0.561640	-0.914690	1.10000	0.1254900000	1
5.831680	2.129500	-0.193430	1.10000	0.1215900000	1
7.983720	2.636400	-1.075100	1.10000	0.1102900000	1
8.053070	1.045100	-1.900000	1.10000	0.1227700000	1
6.144660	1.767400	-3.370000	1.10000	0.0959550000	1
6.050730	3.369900	-2.545500	1.10000	0.0881460000	1
8.220610	3.954100	-3.481100	1.10000	0.1018500000	1
8.367680	2.272300	-4.085400	1.10000	0.1050900000	1
6.467840	2.843600	-5.689500	1.10000	0.0910520000	1
6.296860	4.463600	-4.742700	1.10000	0.0935530000	1
7.491720	4.841300	-6.993100	1.10000	0.1117100000	1
8.457860	5.316000	-5.825800	1.10000	0.1124100000	1
8.585350	3.567300	-6.613200	1.10000	0.1123700000	1

excelfile Savefile Gas
/filefolder/TAA_multiTemperature_candidate2.xlsx /savefolder/THA_SI2.txt N2

DNRCustomRange 0 0
interface 0
fromvalue 7
tovalue 9
red_coef 1.07
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 410
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0
qpol 0
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1
ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
MultiT 1
MultiTval 295
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

Independent Result for One Structure (295K) of TDA:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDA_295_25.txt

Number of atoms: 125
Molecular Weight: 578.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDA_295_25.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDA_295_25.txt	295.00	290.7105	0.0000	0.0000	0.0000	0.0000	0.7173	0.7173	0.7173	0.7173
TDA_295_25.txt	296.00	290.4167	15.4967	15.4920	15.4920	15.4920	0.7168	0.7171	0.7171	0.7171
TDA_295_25.txt	297.00	290.1149	21.9299	21.9172	21.9171	21.9171	0.7164	0.7168	0.7168	0.7168
TDA_295_25.txt	298.50	289.7624	29.0483	29.0197	29.0196	29.0196	0.7154	0.7162	0.7162	0.7162
TDA_295_25.txt	300.00	289.3211	34.7535	34.7051	34.7049	34.7049	0.7147	0.7158	0.7158	0.7158
TDA_295_25.txt	302.00	288.7962	41.1829	41.1035	41.1030	41.1029	0.7137	0.7151	0.7151	0.7151
TDA_295_25.txt	305.00	288.0854	49.3451	49.2111	49.2098	49.2097	0.7119	0.7139	0.7140	0.7140
TDA_295_25.txt	308.00	287.3031	56.3845	56.1874	56.1849	56.1847	0.7104	0.7130	0.7130	0.7130
TDA_295_25.txt	312.00	286.2142	64.6496	64.3570	64.3523	64.3517	0.7085	0.7119	0.7119	0.7119

TDA_295_25.txt	315.00	285.5184	70.2873	69.9166	69.9097	69.9088	0.7068	0.7108	0.7109	0.7108
TDA_295_25.txt	320.00	284.3413	78.8783	78.3655	78.3540	78.3523	0.7042	0.7091	0.7092	0.7091
TDA_295_25.txt	325.00	283.1958	86.7285	86.0609	86.0433	86.0406	0.7016	0.7074	0.7075	0.7075
TDA_295_25.txt	330.00	282.0605	94.0169	93.1826	93.1574	93.1534	0.6990	0.7058	0.7059	0.7059
TDA_295_25.txt	340.00	279.8931	107.3768	106.1813	106.1371	106.1292	0.6940	0.7025	0.7027	0.7026
TDA_295_25.txt	350.00	277.9259	119.5961	118.0078	117.9391	117.9258	0.6889	0.6989	0.6994	0.6992
TDA_295_25.txt	365.00	274.9236	136.2950	134.0601	133.9438	133.9191	0.6819	0.6944	0.6950	0.6948
TDA_295_25.txt	380.00	272.0497	151.6429	148.7034	148.5262	148.4859	0.6754	0.6901	0.6910	0.6907
TDA_295_25.txt	420.00	265.4318	188.6275	183.6152	183.2213	183.1180	0.6584	0.6786	0.6803	0.6798
TDA_295_25.txt	470.00	258.5709	229.9959	222.0867	221.3181	221.0924	0.6389	0.6648	0.6676	0.6670
TDA_295_25.txt	530.00	251.5769	275.3691	263.6385	262.2814	261.8453	0.6184	0.6500	0.6545	0.6538
TDA_295_25.txt	600.00	245.2578	325.4025	308.9760	306.8050	306.0558	0.5962	0.6330	0.6392	0.6387
TDA_295_25.txt	680.00	239.5333	380.1223	358.0880	354.8431	353.6577	0.5734	0.6147	0.6228	0.6226
TDA_295_25.txt	770.00	234.4510	439.7612	411.2468	406.6716	404.9214	0.5505	0.5955	0.6054	0.6057
TDA_295_25.txt	870.00	229.8945	504.3066	468.4165	462.2271	459.7665	0.5282	0.5762	0.5878	0.5887
TDA_295_25.txt	980.00	225.8393	573.8924	529.7777	521.7105	518.3993	0.5066	0.5568	0.5700	0.5716
TDA_295_25.txt	1100.00	222.2003	648.5024	595.2850	585.0624	580.7524	0.4860	0.5379	0.5526	0.5548

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDA_295_25.txt	0.0000	0.0000	0.0000	0.0000
TDA_295_25.txt	15.4920	0.0002	-0.0004	15.4920
TDA_295_25.txt	21.9171	0.0011	-0.0007	21.9171
TDA_295_25.txt	29.0196	0.0047	-0.0016	29.0196
TDA_295_25.txt	34.7049	0.0087	-0.0022	34.7049
TDA_295_25.txt	41.1029	0.0149	-0.0031	41.1029
TDA_295_25.txt	49.2097	0.0266	-0.0047	49.2097
TDA_295_25.txt	56.1847	0.0388	-0.0060	56.1847
TDA_295_25.txt	64.3517	0.0556	-0.0076	64.3517
TDA_295_25.txt	69.9088	0.0714	-0.0091	69.9088
TDA_295_25.txt	78.3523	0.1010	-0.0114	78.3523
TDA_295_25.txt	86.0406	0.1334	-0.0138	86.0406
TDA_295_25.txt	93.1534	0.1679	-0.0160	93.1534
TDA_295_25.txt	106.1292	0.2440	-0.0205	106.1292
TDA_295_25.txt	117.9258	0.3348	-0.0253	117.9258
TDA_295_25.txt	133.9191	0.4832	-0.0315	133.9191
TDA_295_25.txt	148.4859	0.6363	-0.0372	148.4859
TDA_295_25.txt	183.1180	1.1069	-0.0524	183.1180
TDA_295_25.txt	221.0924	1.7942	-0.0701	221.0924
TDA_295_25.txt	261.8453	2.6859	-0.0885	261.8453
TDA_295_25.txt	306.0558	3.9043	-0.1096	306.0558
TDA_295_25.txt	353.6577	5.4798	-0.1320	353.6577
TDA_295_25.txt	404.9214	7.4603	-0.1556	404.9214
TDA_295_25.txt	459.7665	9.8660	-0.1793	459.7665
TDA_295_25.txt	518.3993	12.7597	-0.2032	518.3993
TDA_295_25.txt	580.7524	16.1393	-0.2266	580.7524

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 519.5137 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.010
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)

H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDA_295_25.txt	295.00	290.7105	0.0000	0.0000	0.0000	0.0000	0.7173	0.7173	0.7173	0.7173
TDA_295_25.txt	296.00	290.4167	15.4967	15.4920	15.4920	15.4920	0.7168	0.7171	0.7171	0.7171
TDA_295_25.txt	297.00	290.1149	21.9299	21.9172	21.9171	21.9171	0.7164	0.7168	0.7168	0.7168
TDA_295_25.txt	298.50	289.7624	29.0483	29.0197	29.0196	29.0196	0.7154	0.7162	0.7162	0.7162
TDA_295_25.txt	300.00	289.3211	34.7535	34.7051	34.7049	34.7049	0.7147	0.7158	0.7158	0.7158
TDA_295_25.txt	302.00	288.7962	41.1829	41.1035	41.1030	41.1029	0.7137	0.7151	0.7151	0.7151
TDA_295_25.txt	305.00	288.0854	49.3451	49.2111	49.2098	49.2097	0.7119	0.7139	0.7140	0.7140
TDA_295_25.txt	308.00	287.3031	56.3845	56.1874	56.1849	56.1847	0.7104	0.7130	0.7130	0.7130
TDA_295_25.txt	312.00	286.2142	64.6496	64.3570	64.3523	64.3517	0.7085	0.7119	0.7119	0.7119
TDA_295_25.txt	315.00	285.5184	70.2873	69.9166	69.9097	69.9088	0.7068	0.7108	0.7109	0.7108
TDA_295_25.txt	320.00	284.3413	78.8783	78.3655	78.3540	78.3523	0.7042	0.7091	0.7092	0.7091
TDA_295_25.txt	325.00	283.1958	86.7285	86.0609	86.0433	86.0406	0.7016	0.7074	0.7075	0.7075
TDA_295_25.txt	330.00	282.0605	94.0169	93.1826	93.1574	93.1534	0.6990	0.7058	0.7059	0.7059
TDA_295_25.txt	340.00	279.8931	107.3768	106.1813	106.1371	106.1292	0.6940	0.7025	0.7027	0.7026
TDA_295_25.txt	350.00	277.9259	119.5961	118.0078	117.9391	117.9258	0.6889	0.6989	0.6994	0.6992
TDA_295_25.txt	365.00	274.9236	136.2950	134.0601	133.9438	133.9191	0.6819	0.6944	0.6950	0.6948
TDA_295_25.txt	380.00	272.0497	151.6429	148.7034	148.5262	148.4859	0.6754	0.6901	0.6910	0.6907
TDA_295_25.txt	420.00	265.4318	188.6275	183.6152	183.2213	183.1180	0.6584	0.6786	0.6803	0.6798
TDA_295_25.txt	470.00	258.5709	229.9959	222.0867	221.3181	221.0924	0.6389	0.6648	0.6676	0.6670
TDA_295_25.txt	530.00	251.5769	275.3691	263.6385	262.2814	261.8453	0.6184	0.6500	0.6545	0.6538
TDA_295_25.txt	600.00	245.2578	325.4025	308.9760	306.8050	306.0558	0.5962	0.6330	0.6392	0.6387
TDA_295_25.txt	680.00	239.5333	380.1223	358.0880	354.8431	353.6577	0.5734	0.6147	0.6228	0.6226
TDA_295_25.txt	770.00	234.4510	439.7612	411.2468	406.6716	404.9214	0.5505	0.5955	0.6054	0.6057
TDA_295_25.txt	870.00	229.8945	504.3066	468.4165	462.2271	459.7665	0.5282	0.5762	0.5878	0.5887
TDA_295_25.txt	980.00	225.8393	573.8924	529.7777	521.7105	518.3993	0.5066	0.5568	0.5700	0.5716
TDA_295_25.txt	1100.00	222.2003	648.5024	595.2850	585.0624	580.7524	0.4860	0.5379	0.5526	0.5548

TAA_multiTemperature_candidate2.xlsx - Sheet #4

x	y	z	Radius	Charge	Atom		
10.740700	-10.46140	0.716860	1.55000	-0.4542700000			14
9.365520	-11.15800	0.975750	1.70000	-0.0589730000		1	12
11.727500	-10.84750	1.883300	1.70000	-0.0552500000			12
11.273900	-10.83320	-0.633770	1.70000	-0.0556390000		578	12
10.503400	-8.953400	0.745960	1.70000	-0.0567740000			12
8.196120	-10.77580	0.063620	1.70000	-0.2182700000			12
13.241300	-10.57670	1.612300	1.70000	-0.2176800000			12

11.197800	-12.36740	-0.820460	1.70000	-0.2216600000	12
11.662000	-7.925480	0.596350	1.70000	-0.2160500000	12
6.998940	-11.63780	0.584240	1.70000	-0.1899600000	12
14.174800	-10.95570	2.812900	1.70000	-0.1972700000	12
11.727900	-12.75470	-2.165500	1.70000	-0.1854500000	12
11.081900	-6.468520	0.525130	1.70000	-0.2032200000	12
6.067200	-11.99930	-0.561490	1.70000	-0.1936200000	12
14.241000	-9.940030	3.934300	1.70000	-0.1970300000	12
11.254200	-14.17680	-2.633500	1.70000	-0.1868500000	12
10.386900	-6.236210	-0.792990	1.70000	-0.1978400000	12
5.549010	-10.78690	-1.332800	1.70000	-0.1839800000	12
14.995900	-8.651170	3.664500	1.70000	-0.1744700000	12
9.836450	-13.98310	-3.285700	1.70000	-0.1788700000	12
11.372000	-6.264820	-2.040900	1.70000	-0.1826500000	12
4.223920	-10.14590	-0.959340	1.70000	-0.1842200000	12
14.889000	-7.705570	4.901900	1.70000	-0.1865100000	12
9.289450	-15.33140	-3.823500	1.70000	-0.1801600000	12
10.683900	-5.950930	-3.350300	1.70000	-0.1812300000	12
4.005540	-8.699260	-1.623400	1.70000	-0.1815900000	12
15.736500	-6.421420	4.646000	1.70000	-0.1845900000	12
8.122270	-15.04860	-4.825300	1.70000	-0.1801500000	12
9.713750	-7.058420	-3.912500	1.70000	-0.1788200000	12
4.022020	-8.711810	-3.136300	1.70000	-0.1710600000	12
15.439100	-5.612840	3.407400	1.70000	-0.1771600000	12
6.973710	-14.29750	-4.223300	1.70000	-0.1657700000	12
10.321600	-8.456960	-3.953200	1.70000	-0.1743400000	12
4.004880	-7.258300	-3.707400	1.70000	-0.1773500000	12
14.018500	-5.002830	3.288400	1.70000	-0.1776300000	12
5.656620	-14.43660	-4.983300	1.70000	-0.1759200000	12
9.309950	-9.470410	-4.554400	1.70000	-0.1795700000	12
4.113970	-7.312350	-5.268700	1.70000	-0.3212300000	12
13.671700	-3.972390	4.371500	1.70000	-0.3203100000	12
4.540760	-13.59640	-4.333200	1.70000	-0.3193800000	12
8.037310	-9.560480	-3.724900	1.70000	-0.3167000000	12
9.476790	-12.26990	1.079800	1.10000	0.1479700000	1
9.027790	-10.93610	2.000500	1.10000	0.1495100000	1
11.318700	-10.26290	2.759100	1.10000	0.1505000000	1
11.552800	-11.92700	2.194300	1.10000	0.1472700000	1
10.701000	-10.29470	-1.461700	1.10000	0.1522800000	1
12.368100	-10.51870	-0.894080	1.10000	0.1546800000	1
9.788270	-8.685960	-0.057612	1.10000	0.1482100000	1
9.949270	-8.649610	1.712700	1.10000	0.1480000000	1
7.941130	-9.726880	0.190130	1.10000	0.1293200000	1
8.441070	-11.00880	-1.011800	1.10000	0.1239400000	1
13.456000	-11.33280	0.789190	1.10000	0.1189100000	1
13.550100	-9.550350	1.256100	1.10000	0.1336000000	1
11.725800	-12.88060	-0.003330	1.10000	0.1230800000	1
10.116400	-12.61390	-0.890780	1.10000	0.1218200000	1
12.191800	-8.023410	1.559200	1.10000	0.1207300000	1
12.357200	-8.076310	-0.254520	1.10000	0.1315300000	1
7.385240	-12.56190	1.087300	1.10000	0.1061000000	1
6.501810	-11.04980	1.376600	1.10000	0.1156300000	1
13.849600	-11.93540	3.180000	1.10000	0.1062500000	1
15.219500	-11.05430	2.486400	1.10000	0.1230300000	1
11.537600	-12.04470	-2.978700	1.10000	0.1108700000	1
12.828500	-12.87270	-2.070700	1.10000	0.1074700000	1
10.298500	-6.206510	1.352500	1.10000	0.1098800000	1
11.895700	-5.714050	0.720600	1.10000	0.1232900000	1
6.683430	-12.68900	-1.220600	1.10000	0.0959780000	1
5.161450	-12.64700	-0.274340	1.10000	0.1147200000	1
13.221300	-9.636520	4.295600	1.10000	0.0853470000	1
14.746800	-10.47440	4.802700	1.10000	0.1204800000	1
11.862300	-14.50300	-3.500800	1.10000	0.0965310000	1
11.143900	-14.80320	-1.724900	1.10000	0.0981120000	1
9.517720	-6.877500	-1.003400	1.10000	0.0870150000	1
9.928620	-5.227030	-0.818020	1.10000	0.1153900000	1
6.268940	-9.951830	-1.378100	1.10000	0.0896280000	1
5.471890	-11.12420	-2.434700	1.10000	0.1114300000	1
16.116600	-8.751150	3.428800	1.10000	0.1133100000	1
14.521800	-8.083460	2.840400	1.10000	0.1041400000	1
9.123390	-13.55270	-2.496500	1.10000	0.0995120000	1
10.002700	-13.27150	-4.151300	1.10000	0.1055000000	1
12.225600	-5.565500	-1.941500	1.10000	0.1108900000	1
11.901600	-7.228790	-2.125000	1.10000	0.1070500000	1
3.378360	-10.84320	-1.225400	1.10000	0.1103500000	1
4.114730	-9.997920	0.169100	1.10000	0.0977480000	1
13.842600	-7.568550	5.141500	1.10000	0.0717050000	1
15.358000	-8.180100	5.733700	1.10000	0.0835220000	1
10.205600	-15.79060	-4.313200	1.10000	0.0885920000	1
8.923840	-15.92940	-2.962300	1.10000	0.0835240000	1

10.044300	-5.057890	-3.241900	1.10000	0.0606510000	1
11.477200	-5.657910	-4.117500	1.10000	0.1094600000	1
3.081560	-8.349610	-1.193400	1.10000	0.1012300000	1
4.852850	-8.017090	-1.308000	1.10000	0.0558290000	1
15.595000	-5.821340	5.573700	1.10000	0.0943790000	1
16.797200	-6.735330	4.545600	1.10000	0.1046000000	1
8.543400	-14.51560	-5.659200	1.10000	0.0966740000	1
7.698230	-15.95470	-5.265700	1.10000	0.0952930000	1
8.831840	-7.016810	-3.217000	1.10000	0.0821630000	1
9.369240	-6.645240	-4.838200	1.10000	0.0878050000	1
4.940770	-9.270810	-3.599200	1.10000	0.1059900000	1
3.095530	-9.234420	-3.515000	1.10000	0.0880460000	1
16.124000	-4.707400	3.328400	1.10000	0.1052200000	1
15.689000	-6.149530	2.498200	1.10000	0.0978580000	1
6.937660	-14.61340	-3.104400	1.10000	0.0826530000	1
7.237950	-13.25270	-4.203200	1.10000	0.0901030000	1
11.172100	-8.411990	-4.628300	1.10000	0.0991210000	1
10.702600	-8.741500	-2.922900	1.10000	0.0953380000	1
3.024550	-6.797370	-3.476200	1.10000	0.0706920000	1
4.871240	-6.634150	-3.379900	1.10000	0.1052800000	1
13.875100	-4.526660	2.272000	1.10000	0.1086500000	1
13.341400	-5.910300	3.316200	1.10000	0.0725830000	1
5.760840	-14.12390	-6.034100	1.10000	0.0979530000	1
5.349820	-15.50810	-4.969600	1.10000	0.0964140000	1
8.982000	-9.188080	-5.631300	1.10000	0.0936640000	1
9.770160	-10.54180	-4.658100	1.10000	0.1067300000	1
5.065120	-7.877500	-5.507000	1.10000	0.1174000000	1
3.175510	-7.807480	-5.665000	1.10000	0.1035200000	1
4.219250	-6.269720	-5.652100	1.10000	0.1053800000	1
13.729100	-4.358380	5.412200	1.10000	0.0910840000	1
14.349000	-3.113640	4.228700	1.10000	0.1194800000	1
12.558500	-3.594780	4.242700	1.10000	0.1038000000	1
4.453570	-13.77350	-3.261400	1.10000	0.1010000000	1
4.806080	-12.54510	-4.442800	1.10000	0.1025200000	1
3.553490	-13.81550	-4.745300	1.10000	0.1101200000	1
7.387430	-8.610670	-3.642500	1.10000	0.0866880000	1
7.391480	-10.38940	-4.086700	1.10000	0.1143100000	1
8.289870	-9.738930	-2.699100	1.00000	0.1054300000	1

IMoS.cla

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excelfile Savefile Gas
/filefolder/TAA_multiTemperature_candidate2.xlsx /savefolder/TDA_SI.txt N2

DNRCustomRange 0 0
interface 0
fromvalue 4
tovalue 4
red_coef 1.01
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 578
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0
qpol 0
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1

ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

Result of Multistructures Calculation for TDA Salt:

IMoS v1.13 RESULTS FILE

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDA_295_25.txt

Number of atoms: 125
Molecular Weight: 578.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDA_295_25.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDA_295_25.txt	295.00	290.7105	0.0000	0.0000	0.0000	0.0000	0.7173	0.7173	0.7173	0.7173
TDA_295_25.txt	296.00	290.4167	15.4967	15.4920	15.4920	15.4920	0.7168	0.7171	0.7171	0.7171
TDA_295_25.txt	297.00	290.1149	21.9299	21.9172	21.9171	21.9171	0.7164	0.7168	0.7168	0.7168
TDA_295_25.txt	298.50	289.7624	29.0483	29.0197	29.0196	29.0196	0.7154	0.7162	0.7162	0.7162
TDA_295_25.txt	300.00	289.3211	34.7535	34.7051	34.7049	34.7049	0.7147	0.7158	0.7158	0.7158
TDA_295_25.txt	302.00	288.7962	41.1829	41.1035	41.1030	41.1029	0.7137	0.7151	0.7151	0.7151
TDA_295_25.txt	305.00	288.0854	49.3451	49.2111	49.2098	49.2097	0.7119	0.7139	0.7140	0.7140
TDA_295_25.txt	308.00	287.3031	56.3845	56.1874	56.1849	56.1847	0.7104	0.7130	0.7130	0.7130
TDA_295_25.txt	312.00	286.2142	64.6496	64.3570	64.3523	64.3517	0.7085	0.7119	0.7119	0.7119
TDA_295_25.txt	315.00	285.5184	70.2873	69.9166	69.9097	69.9088	0.7068	0.7108	0.7109	0.7108
TDA_295_25.txt	320.00	284.3413	78.8783	78.3655	78.3540	78.3523	0.7042	0.7091	0.7092	0.7091
TDA_295_25.txt	325.00	283.1958	86.7285	86.0609	86.0433	86.0406	0.7016	0.7074	0.7075	0.7075
TDA_295_25.txt	330.00	282.0605	94.0169	93.1826	93.1574	93.1534	0.6990	0.7058	0.7059	0.7059
TDA_295_25.txt	340.00	279.8931	107.3768	106.1813	106.1371	106.1292	0.6940	0.7025	0.7027	0.7026
TDA_295_25.txt	350.00	277.9259	119.5961	118.0078	117.9391	117.9258	0.6889	0.6989	0.6994	0.6992
TDA_295_25.txt	365.00	274.9236	136.2950	134.0601	133.9438	133.9191	0.6819	0.6944	0.6950	0.6948
TDA_295_25.txt	380.00	272.0497	151.6429	148.7034	148.5262	148.4859	0.6754	0.6901	0.6910	0.6907

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDA_295_25.txt	0.0000	0.0000	0.0000	0.0000
TDA_295_25.txt	15.4920	0.0002	-0.0004	15.4920
TDA_295_25.txt	21.9171	0.0011	-0.0007	21.9171
TDA_295_25.txt	29.0196	0.0047	-0.0016	29.0196
TDA_295_25.txt	34.7049	0.0087	-0.0022	34.7049
TDA_295_25.txt	41.1029	0.0149	-0.0031	41.1029
TDA_295_25.txt	49.2097	0.0266	-0.0047	49.2097
TDA_295_25.txt	56.1847	0.0388	-0.0060	56.1847
TDA_295_25.txt	64.3517	0.0556	-0.0076	64.3517
TDA_295_25.txt	69.9088	0.0714	-0.0091	69.9088
TDA_295_25.txt	78.3523	0.1010	-0.0114	78.3523
TDA_295_25.txt	86.0406	0.1334	-0.0138	86.0406
TDA_295_25.txt	93.1534	0.1679	-0.0160	93.1534
TDA_295_25.txt	106.1292	0.2440	-0.0205	106.1292
TDA_295_25.txt	117.9258	0.3348	-0.0253	117.9258
TDA_295_25.txt	133.9191	0.4832	-0.0315	133.9191
TDA_295_25.txt	148.4859	0.6363	-0.0372	148.4859

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 369.6057 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDA_400_23.txt

Number of atoms: 125
Molecular Weight: 578.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDA_400_23.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDA_400_23.txt	295.00	291.5065	0.0000	0.0000	0.0000	0.0000	0.7154	0.7154	0.7154	0.7154
TDA_400_23.txt	296.00	291.2570	15.5416	15.5368	15.5368	15.5368	0.7148	0.7150	0.7150	0.7150
TDA_400_23.txt	297.00	290.8832	21.9879	21.9752	21.9752	21.9752	0.7145	0.7149	0.7149	0.7149
TDA_400_23.txt	298.50	290.5242	29.1247	29.0960	29.0959	29.0959	0.7136	0.7143	0.7143	0.7143
TDA_400_23.txt	300.00	290.0654	34.8429	34.7944	34.7942	34.7942	0.7129	0.7139	0.7140	0.7140
TDA_400_23.txt	302.00	289.4278	41.2729	41.1933	41.1928	41.1927	0.7121	0.7136	0.7136	0.7136
TDA_400_23.txt	305.00	288.9386	49.4912	49.3572	49.3559	49.3558	0.7098	0.7118	0.7118	0.7118
TDA_400_23.txt	308.00	288.2065	56.5618	56.3651	56.3626	56.3623	0.7081	0.7107	0.7108	0.7108
TDA_400_23.txt	312.00	287.1133	64.8526	64.5605	64.5558	64.5552	0.7063	0.7096	0.7097	0.7097
TDA_400_23.txt	315.00	286.3106	70.4823	70.1114	70.1046	70.1036	0.7049	0.7088	0.7089	0.7089
TDA_400_23.txt	320.00	285.2323	79.1255	78.6130	78.6015	78.5998	0.7020	0.7069	0.7070	0.7069
TDA_400_23.txt	325.00	284.0578	86.9925	86.3244	86.3067	86.3040	0.6994	0.7052	0.7054	0.7053
TDA_400_23.txt	330.00	282.9044	94.2982	93.4633	93.4381	93.4340	0.6969	0.7036	0.7038	0.7037
TDA_400_23.txt	340.00	280.7813	107.7175	106.5201	106.4755	106.4676	0.6918	0.7002	0.7005	0.7004
TDA_400_23.txt	350.00	278.7153	119.9358	118.3415	118.2718	118.2584	0.6869	0.6970	0.6974	0.6972
TDA_400_23.txt	365.00	275.6194	136.6400	134.3943	134.2760	134.2511	0.6802	0.6927	0.6933	0.6930
TDA_400_23.txt	380.00	272.8906	152.1116	149.1610	148.9816	148.9409	0.6733	0.6880	0.6889	0.6886
TDA_400_23.txt	400.00	269.4816	171.2878	167.3328	167.0545	166.9862	0.6646	0.6820	0.6833	0.6829
TDA_400_23.txt	420.00	266.2871	189.2354	184.2076	183.8096	183.7055	0.6563	0.6764	0.6781	0.6776
TDA_400_23.txt	470.00	259.3981	230.7317	222.7769	221.9953	221.7661	0.6369	0.6627	0.6656	0.6650

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDA_400_23.txt	0.0000	0.0000	0.0000	0.0000
TDA_400_23.txt	15.5368	-0.0001	-0.0005	15.5368
TDA_400_23.txt	21.9752	-0.0002	-0.0006	21.9752
TDA_400_23.txt	29.0959	0.0029	-0.0015	29.0959
TDA_400_23.txt	34.7942	0.0071	-0.0020	34.7942
TDA_400_23.txt	41.1927	0.0121	-0.0025	41.1927
TDA_400_23.txt	49.3558	0.0263	-0.0049	49.3558
TDA_400_23.txt	56.3623	0.0416	-0.0065	56.3623
TDA_400_23.txt	64.5552	0.0606	-0.0080	64.5552
TDA_400_23.txt	70.1036	0.0758	-0.0091	70.1036
TDA_400_23.txt	78.5998	0.1093	-0.0118	78.5998
TDA_400_23.txt	86.3040	0.1449	-0.0141	86.3040
TDA_400_23.txt	93.4340	0.1787	-0.0163	93.4340
TDA_400_23.txt	106.4676	0.2527	-0.0210	106.4676
TDA_400_23.txt	118.2584	0.3388	-0.0254	118.2584
TDA_400_23.txt	134.2511	0.4771	-0.0312	134.2511
TDA_400_23.txt	148.9409	0.6350	-0.0375	148.9409
TDA_400_23.txt	166.9862	0.8638	-0.0454	166.9862
TDA_400_23.txt	183.7055	1.1131	-0.0528	183.7055
TDA_400_23.txt	221.7661	1.7966	-0.0704	221.7661

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5

Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
Time taken is a mere 428.7498 seconds

File: TAA_multiTemperature_candidate2.xlsx Molecule: TDA_500_2.txt

Number of atoms: 125
Molecular Weight: 578.00 Da
Total Charge: 1

The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDA_500_2.txt.

Results

Summary of ion calculations:
Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
TDA_500_2.txt	295.00	301.1197	0.0000	0.0000	0.0000	0.0000	0.6925	0.6925	0.6925	0.6925
TDA_500_2.txt	420.00	275.9746	196.1197	190.8643	190.4339	190.3210	0.6333	0.6529	0.6546	0.6541
TDA_500_2.txt	470.00	268.8040	239.0982	230.8018	229.9631	229.7157	0.6146	0.6398	0.6427	0.6421
TDA_500_2.txt	500.00	265.2330	263.3675	253.1431	252.0143	251.6643	0.6039	0.6319	0.6355	0.6349
TDA_500_2.txt	530.00	261.9253	286.6962	274.4627	273.0087	272.5386	0.5940	0.6245	0.6289	0.6283
TDA_500_2.txt	600.00	255.4167	338.8811	321.7585	319.4396	318.6331	0.5725	0.6079	0.6140	0.6136
TDA_500_2.txt	680.00	249.5313	395.9884	373.0522	369.6038	368.3322	0.5504	0.5902	0.5980	0.5979
TDA_500_2.txt	770.00	244.1778	458.0056	428.2939	423.4230	421.5392	0.5286	0.5720	0.5816	0.5820
TDA_500_2.txt	870.00	239.4405	525.2472	487.8673	481.2964	478.6540	0.5071	0.5533	0.5646	0.5656
TDA_500_2.txt	980.00	235.1920	597.6590	551.7257	543.1799	539.6319	0.4865	0.5348	0.5477	0.5492
TDA_500_2.txt	1100.00	231.4586	675.5230	620.1511	609.3473	604.7416	0.4666	0.5165	0.5307	0.5329

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Ion	Ed (Td)	Ec (Td)	alpha (Td)	E/n (Td)
TDA_500_2.txt	0.0000	0.0000	0.0000	0.0000
TDA_500_2.txt	190.3210	1.0726	-0.0555	190.3210
TDA_500_2.txt	229.7157	1.7483	-0.0729	229.7157
TDA_500_2.txt	251.6643	2.2259	-0.0833	251.6643
TDA_500_2.txt	272.5386	2.7358	-0.0928	272.5386
TDA_500_2.txt	318.6331	4.0576	-0.1140	318.6331
TDA_500_2.txt	368.3322	5.7780	-0.1366	368.3322
TDA_500_2.txt	421.5392	7.9034	-0.1596	421.5392
TDA_500_2.txt	478.6540	10.4730	-0.1833	478.6540
TDA_500_2.txt	539.6319	13.4817	-0.2069	539.6319
TDA_500_2.txt	604.7416	17.0094	-0.2305	604.7416

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
Maximum value of [1-cosX] at b_max (cmin) = 0.000100
Seed = 13
MULTI STRUCTURE Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)

Teff	Ed (Td)	Ec (Td)	alpha (Td)	Kho (Td)
295	0.0000	0.0000	0.0000	0.7173

296	15.4924	0.0003	-0.0004	0.7170
297	21.9182	0.0012	-0.0008	0.7168
298.5	29.0221	0.0049	-0.0017	0.7161
300	34.7091	0.0092	-0.0023	0.7157
302	41.1089	0.0156	-0.0032	0.7150
305	49.2236	0.0280	-0.0050	0.7138
308	56.2067	0.0412	-0.0064	0.7127
312	64.3847	0.0594	-0.0081	0.7116
315	69.9459	0.0759	-0.0096	0.7105
320	78.4112	0.1078	-0.0122	0.7086
325	86.1159	0.1426	-0.0146	0.7068
330	93.2469	0.1792	-0.0170	0.7051
340	106.2742	0.2607	-0.0219	0.7017
350	118.1000	0.3560	-0.0267	0.6981
365	134.1404	0.5095	-0.0331	0.6936
380	148.8542	0.6768	-0.0395	0.6890
400	166.9862	0.9212	-0.0480	0.6829
420	185.0286	1.2867	-0.0620	0.6729
470	227.3308	2.5369	-0.0953	0.6489
500	251.6643	3.4900	-0.1150	0.6349
530	272.5386	4.2715	-0.1242	0.6283
600	318.6331	6.0592	-0.1446	0.6136
680	368.3322	8.1478	-0.1665	0.5979
770	421.5392	10.2911	-0.1887	0.5820
870	478.6540	12.6021	-0.2115	0.5656
980	539.6319	14.9721	-0.2343	0.5492
1100	604.7416	18.0415	-0.2571	0.5329

Time taken is a mere 209.6883 seconds

PARAMETERS USED:

Gas: N2
Reduction Coef: 1.010
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 295 K
Pressure: 101325 Pa

Lennard Jones parameters for basic

Atom	eps(J*10^21)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000

SUMMARY OF HIGH FIELD CALCULATIONS

FAIMS/DMS Dispersion field curve used

ft (AU)	t (s)
0.33333000	0.0000
0.28885000	0.1000
0.90371000	0.2000
0.90371000	0.3000
0.28885000	0.4000
-0.33333000	0.5000
-0.49486000	0.6000
-0.36437000	0.7000
-0.36437000	0.8000
-0.49486000	0.9000
-0.33333000	1.0000

Ion	Teff	CCS	E/n1	E/n2	E/n3	E/n4	<Ko1>	<Ko2>	<Ko3>	<Ko4>

	(K)	(A2)	(Td)	(Td)	(Td)	(Td)	(cm2/Vs)	(cm2/Vs)	(cm2/Vs)	(cm2/Vs)
TDA_295_25.txt	295.00	290.7105	0.0000	0.0000	0.0000	0.0000	0.7173	0.7173	0.7173	0.7173
TDA_295_25.txt	296.00	290.4167	15.4967	15.4920	15.4920	15.4920	0.7168	0.7171	0.7171	0.7171
TDA_295_25.txt	297.00	290.1149	21.9299	21.9172	21.9171	21.9171	0.7164	0.7168	0.7168	0.7168
TDA_295_25.txt	298.50	289.7624	29.0483	29.0197	29.0196	29.0196	0.7154	0.7162	0.7162	0.7162
TDA_295_25.txt	300.00	289.3211	34.7535	34.7051	34.7049	34.7049	0.7147	0.7158	0.7158	0.7158
TDA_295_25.txt	302.00	288.7962	41.1829	41.1035	41.1030	41.1029	0.7137	0.7151	0.7151	0.7151
TDA_295_25.txt	305.00	288.0854	49.3451	49.2111	49.2098	49.2097	0.7119	0.7139	0.7140	0.7140
TDA_295_25.txt	308.00	287.3031	56.3845	56.1874	56.1849	56.1847	0.7104	0.7130	0.7130	0.7130
TDA_295_25.txt	312.00	286.2142	64.6496	64.3570	64.3523	64.3517	0.7085	0.7119	0.7119	0.7119
TDA_295_25.txt	315.00	285.5184	70.2873	69.9166	69.9097	69.9088	0.7068	0.7108	0.7109	0.7108
TDA_295_25.txt	320.00	284.3413	78.8783	78.3655	78.3540	78.3523	0.7042	0.7091	0.7092	0.7091
TDA_295_25.txt	325.00	283.1958	86.7285	86.0609	86.0433	86.0406	0.7016	0.7074	0.7075	0.7075
TDA_295_25.txt	330.00	282.0605	94.0169	93.1826	93.1574	93.1534	0.6990	0.7058	0.7059	0.7059
TDA_295_25.txt	340.00	279.8931	107.3768	106.1813	106.1371	106.1292	0.6940	0.7025	0.7027	0.7026
TDA_295_25.txt	350.00	277.9259	119.5961	118.0078	117.9391	117.9258	0.6889	0.6989	0.6994	0.6992
TDA_295_25.txt	365.00	274.9236	136.2950	134.0601	133.9438	133.9191	0.6819	0.6944	0.6950	0.6948
TDA_295_25.txt	380.00	272.0497	151.6429	148.7034	148.5262	148.4859	0.6754	0.6901	0.6910	0.6907
TDA_400_23.txt	295.00	291.5065	0.0000	0.0000	0.0000	0.0000	0.7154	0.7154	0.7154	0.7154
TDA_400_23.txt	296.00	291.2570	15.5416	15.5368	15.5368	15.5368	0.7148	0.7150	0.7150	0.7150
TDA_400_23.txt	297.00	290.8832	21.9879	21.9752	21.9752	21.9752	0.7145	0.7149	0.7149	0.7149
TDA_400_23.txt	298.50	290.5242	29.1247	29.0960	29.0959	29.0959	0.7136	0.7143	0.7143	0.7143
TDA_400_23.txt	300.00	290.0654	34.8429	34.7944	34.7942	34.7942	0.7129	0.7139	0.7140	0.7140
TDA_400_23.txt	302.00	289.4278	41.2729	41.1933	41.1928	41.1927	0.7121	0.7136	0.7136	0.7136
TDA_400_23.txt	305.00	288.9386	49.4912	49.3572	49.3559	49.3558	0.7098	0.7118	0.7118	0.7118
TDA_400_23.txt	308.00	288.2065	56.5618	56.3651	56.3626	56.3623	0.7081	0.7107	0.7108	0.7108
TDA_400_23.txt	312.00	287.1133	64.8526	64.5605	64.5558	64.5552	0.7063	0.7096	0.7097	0.7097
TDA_400_23.txt	315.00	286.3106	70.4823	70.1114	70.1046	70.1036	0.7049	0.7088	0.7089	0.7089
TDA_400_23.txt	320.00	285.2323	79.1255	78.6130	78.6015	78.5998	0.7020	0.7069	0.7070	0.7069
TDA_400_23.txt	325.00	284.0578	86.9925	86.3244	86.3067	86.3040	0.6994	0.7052	0.7054	0.7053
TDA_400_23.txt	330.00	282.9044	94.2982	93.4633	93.4381	93.4340	0.6969	0.7036	0.7038	0.7037
TDA_400_23.txt	340.00	280.7813	107.7175	106.5201	106.4755	106.4676	0.6918	0.7002	0.7005	0.7004
TDA_400_23.txt	350.00	278.7153	119.9358	118.3415	118.2718	118.2584	0.6869	0.6970	0.6974	0.6972
TDA_400_23.txt	365.00	275.6194	136.6400	134.3943	134.2760	134.2511	0.6802	0.6927	0.6933	0.6930
TDA_400_23.txt	380.00	272.8906	152.1116	149.1610	148.9816	148.9409	0.6733	0.6880	0.6889	0.6886
TDA_400_23.txt	400.00	269.4816	171.2878	167.3328	167.0545	166.9862	0.6646	0.6820	0.6833	0.6829
TDA_400_23.txt	420.00	266.2871	189.2354	184.2076	183.8096	183.7055	0.6563	0.6764	0.6781	0.6776
TDA_400_23.txt	470.00	259.3981	230.7317	222.7769	221.9953	221.7661	0.6369	0.6627	0.6656	0.6650
TDA_500_2.txt	295.00	301.1197	0.0000	0.0000	0.0000	0.0000	0.6925	0.6925	0.6925	0.6925
TDA_500_2.txt	420.00	275.9746	196.1197	190.8643	190.4339	190.3210	0.6333	0.6529	0.6546	0.6541
TDA_500_2.txt	470.00	268.8040	239.0982	230.8018	229.9631	229.7157	0.6146	0.6398	0.6427	0.6421
TDA_500_2.txt	500.00	265.2330	263.3675	253.1431	252.0143	251.6643	0.6039	0.6319	0.6355	0.6349
TDA_500_2.txt	530.00	261.9253	286.6962	274.4627	273.0087	272.5386	0.5940	0.6245	0.6289	0.6283
TDA_500_2.txt	600.00	255.4167	338.8811	321.7585	319.4396	318.6331	0.5725	0.6079	0.6140	0.6136
TDA_500_2.txt	680.00	249.5313	395.9884	373.0522	369.6038	368.3322	0.5504	0.5902	0.5980	0.5979
TDA_500_2.txt	770.00	244.1778	458.0056	428.2939	423.4230	421.5392	0.5286	0.5720	0.5816	0.5820
TDA_500_2.txt	870.00	239.4405	525.2472	487.8673	481.2964	478.6540	0.5071	0.5533	0.5646	0.5656
TDA_500_2.txt	980.00	235.1920	597.6590	551.7257	543.1799	539.6319	0.4865	0.5348	0.5477	0.5492
TDA_500_2.txt	1100.00	231.4586	675.5230	620.1511	609.3473	604.7416	0.4666	0.5165	0.5307	0.5329

TAA_multiTemperature_candidate2.xlsx - Sheet #4

x	y	z	Radius	Charge	Atom		
10.740700	-10.46140	0.716860	1.55000	-0.4542700000			14
9.365520	-11.15800	0.975750	1.70000	-0.0589730000		1	12
11.727500	-10.84750	1.883300	1.70000	-0.0552500000			12
11.273900	-10.83320	-0.633770	1.70000	-0.0556390000		578	12
10.503400	-8.953400	0.745960	1.70000	-0.0567740000			12
8.196120	-10.77580	0.063620	1.70000	-0.2182700000			12
13.241300	-10.57670	1.612300	1.70000	-0.2176800000			12
11.197800	-12.36740	-0.820460	1.70000	-0.2216600000			12
11.662000	-7.925480	0.596350	1.70000	-0.2160500000			12
6.998940	-11.63780	0.584240	1.70000	-0.1899600000			12
14.174800	-10.95570	2.812900	1.70000	-0.1972700000			12
11.727900	-12.75470	-2.165500	1.70000	-0.1854500000			12
11.081900	-6.468520	0.525130	1.70000	-0.2032200000			12
6.067200	-11.99930	-0.561490	1.70000	-0.1936200000			12
14.241000	-9.940030	3.934300	1.70000	-0.1970300000			12
11.254200	-14.17680	-2.633500	1.70000	-0.1868500000			12
10.386900	-6.236210	-0.792990	1.70000	-0.1978400000			12
5.549010	-10.78690	-1.332800	1.70000	-0.1839800000			12
14.995900	-8.651170	3.664500	1.70000	-0.1744700000			12
9.836450	-13.98310	-3.285700	1.70000	-0.1788700000			12
11.372000	-6.264820	-2.040900	1.70000	-0.1826500000			12

4.223920	-10.14590	-0.959340	1.70000	-0.1842200000	12
14.889000	-7.705570	4.901900	1.70000	-0.1865100000	12
9.289450	-15.33140	-3.823500	1.70000	-0.1801600000	12
10.683900	-5.950930	-3.350300	1.70000	-0.1812300000	12
4.005540	-8.699260	-1.623400	1.70000	-0.1815900000	12
15.736500	-6.421420	4.646000	1.70000	-0.1845900000	12
8.122270	-15.04860	-4.825300	1.70000	-0.1801500000	12
9.713750	-7.058420	-3.912500	1.70000	-0.1788200000	12
4.022020	-8.711810	-3.136300	1.70000	-0.1710600000	12
15.439100	-5.612840	3.407400	1.70000	-0.1771600000	12
6.973710	-14.29750	-4.223300	1.70000	-0.1657700000	12
10.321600	-8.456960	-3.953200	1.70000	-0.1743400000	12
4.004880	-7.258300	-3.707400	1.70000	-0.1773500000	12
14.018500	-5.002830	3.288400	1.70000	-0.1776300000	12
5.656620	-14.43660	-4.983300	1.70000	-0.1759200000	12
9.309950	-9.470410	-4.554400	1.70000	-0.1795700000	12
4.113970	-7.312350	-5.268700	1.70000	-0.3212300000	12
13.671700	-3.972390	4.371500	1.70000	-0.3203100000	12
4.540760	-13.59640	-4.333200	1.70000	-0.3193800000	12
8.037310	-9.560480	-3.724900	1.70000	-0.3167000000	12
9.476790	-12.26990	1.079800	1.10000	0.1479700000	1
9.027790	-10.93610	2.000500	1.10000	0.1495100000	1
11.318700	-10.26290	2.759100	1.10000	0.1505000000	1
11.552800	-11.92700	2.194300	1.10000	0.1472700000	1
10.701000	-10.29470	-1.461700	1.10000	0.1522800000	1
12.368100	-10.51870	-0.894080	1.10000	0.1546800000	1
9.788270	-8.685960	-0.057612	1.10000	0.1482100000	1
9.949270	-8.649610	1.712700	1.10000	0.1480000000	1
7.941130	-9.726880	0.190130	1.10000	0.1293200000	1
8.441070	-11.00880	-1.011800	1.10000	0.1239400000	1
13.456000	-11.33280	0.789190	1.10000	0.1189100000	1
13.550100	-9.550350	1.256100	1.10000	0.1336000000	1
11.725800	-12.88060	-0.003330	1.10000	0.1230800000	1
10.116400	-12.61390	-0.890780	1.10000	0.1218200000	1
12.191800	-8.023410	1.559200	1.10000	0.1207300000	1
12.357200	-8.076310	-0.254520	1.10000	0.1315300000	1
7.385240	-12.56190	1.087300	1.10000	0.1061000000	1
6.501810	-11.04980	1.376600	1.10000	0.1156300000	1
13.849600	-11.93540	3.180000	1.10000	0.1062500000	1
15.219500	-11.05430	2.486400	1.10000	0.1230300000	1
11.537600	-12.04470	-2.978700	1.10000	0.1108700000	1
12.828500	-12.87270	-2.070700	1.10000	0.1074700000	1
10.298500	-6.206510	1.352500	1.10000	0.1098800000	1
11.895700	-5.714050	0.720600	1.10000	0.1232900000	1
6.683430	-12.68900	-1.220600	1.10000	0.0959780000	1
5.161450	-12.64700	-0.274340	1.10000	0.1147200000	1
13.221300	-9.636520	4.295600	1.10000	0.0853470000	1
14.746800	-10.47440	4.802700	1.10000	0.1204800000	1
11.862300	-14.50300	-3.500800	1.10000	0.0965310000	1
11.143900	-14.80320	-1.724900	1.10000	0.0981120000	1
9.517720	-6.877500	-1.003400	1.10000	0.0870150000	1
9.928620	-5.227030	-0.818020	1.10000	0.1153900000	1
6.268940	-9.951830	-1.378100	1.10000	0.0896280000	1
5.471890	-11.12420	-2.434700	1.10000	0.1114300000	1
16.116600	-8.751150	3.428800	1.10000	0.1133100000	1
14.521800	-8.083460	2.840400	1.10000	0.1041400000	1
9.123390	-13.55270	-2.496500	1.10000	0.0995120000	1
10.002700	-13.27150	-4.151300	1.10000	0.1055000000	1
12.225600	-5.565500	-1.941500	1.10000	0.1108900000	1
11.901600	-7.228790	-2.125000	1.10000	0.1070500000	1
3.378360	-10.84320	-1.225400	1.10000	0.1103500000	1
4.114730	-9.997920	0.169100	1.10000	0.0977480000	1
13.842600	-7.568550	5.141500	1.10000	0.0717050000	1
15.358000	-8.180100	5.733700	1.10000	0.0835220000	1
10.205600	-15.79060	-4.313200	1.10000	0.0885920000	1
8.923840	-15.92940	-2.962300	1.10000	0.0835240000	1
10.044300	-5.057890	-3.241900	1.10000	0.0606510000	1
11.477200	-5.657910	-4.117500	1.10000	0.1094600000	1
3.081560	-8.349610	-1.193400	1.10000	0.1012300000	1
4.852850	-8.017090	-1.308000	1.10000	0.0558290000	1
15.595000	-5.821340	5.573700	1.10000	0.0943790000	1
16.797200	-6.735330	4.545600	1.10000	0.1046000000	1
8.543400	-14.51560	-5.659200	1.10000	0.0966740000	1
7.698230	-15.95470	-5.265700	1.10000	0.0952930000	1
8.831840	-7.016810	-3.217000	1.10000	0.0821630000	1
9.369240	-6.645240	-4.838200	1.10000	0.0878050000	1
4.940770	-9.270810	-3.599200	1.10000	0.1059900000	1
3.095530	-9.234420	-3.515000	1.10000	0.0880460000	1
16.124000	-4.707400	3.328400	1.10000	0.1052200000	1
15.689000	-6.149530	2.498200	1.10000	0.0978580000	1

6.937660	-14.61340	-3.104400	1.10000	0.0826530000	1
7.237950	-13.25270	-4.203200	1.10000	0.0901030000	1
11.172100	-8.411990	-4.628300	1.10000	0.0991210000	1
10.702600	-8.741500	-2.922900	1.10000	0.0953380000	1
3.024550	-6.797370	-3.476200	1.10000	0.0706920000	1
4.871240	-6.634150	-3.379900	1.10000	0.1052800000	1
13.875100	-4.526660	2.272000	1.10000	0.1086500000	1
13.341400	-5.910300	3.316200	1.10000	0.0725830000	1
5.760840	-14.12390	-6.034100	1.10000	0.0979530000	1
5.349820	-15.50810	-4.969600	1.10000	0.0964140000	1
8.982000	-9.188080	-5.631300	1.10000	0.0936640000	1
9.770160	-10.54180	-4.658100	1.10000	0.1067300000	1
5.065120	-7.877500	-5.507000	1.10000	0.1174000000	1
3.175510	-7.807480	-5.665000	1.10000	0.1035200000	1
4.219250	-6.269720	-5.652100	1.10000	0.1053800000	1
13.729100	-4.358380	5.412200	1.10000	0.0910840000	1
14.349000	-3.113640	4.228700	1.10000	0.1194800000	1
12.558500	-3.594780	4.242700	1.10000	0.1038000000	1
4.453570	-13.77350	-3.261400	1.10000	0.1010000000	1
4.806080	-12.54510	-4.442800	1.10000	0.1025200000	1
3.553490	-13.81550	-4.745300	1.10000	0.1101200000	1
7.387430	-8.610670	-3.642500	1.10000	0.0866880000	1
7.391480	-10.38940	-4.086700	1.10000	0.1143100000	1
8.289870	-9.738930	-2.699100	1.00000	0.1054300000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #5

x	y	z	Radius	Charge	Atom		
10.382200	-9.897360	0.184320	1.55000	-0.4542700000			14
9.252000	-10.14430	1.212100	1.70000	-0.0589730000	1		12
11.647400	-9.844170	1.101500	1.70000	-0.0552500000			12
10.460500	-11.00790	-0.841630	1.70000	-0.0556390000	578		12
10.185600	-8.606510	-0.575470	1.70000	-0.0567740000			12
7.865600	-10.21190	0.526100	1.70000	-0.2182700000			12
13.027900	-10.06060	0.410100	1.70000	-0.2176800000			12
10.570200	-12.42680	-0.284990	1.70000	-0.2216600000			12
11.355700	-8.073320	-1.378400	1.70000	-0.2160500000			12
6.889570	-10.18370	1.738400	1.70000	-0.1899600000			12
14.182600	-10.29990	1.422400	1.70000	-0.1972700000			12
10.570700	-13.54520	-1.344400	1.70000	-0.1854500000			12
11.078800	-6.721530	-2.180500	1.70000	-0.2032200000			12
5.464400	-9.827250	1.308200	1.70000	-0.1936200000			12
14.315500	-9.177440	2.480200	1.70000	-0.1970300000			12
10.328000	-14.97320	-0.918080	1.70000	-0.1868500000			12
10.131700	-6.970420	-3.439800	1.70000	-0.1978400000			12
5.379860	-8.376760	0.737330	1.70000	-0.1839800000			12
14.635200	-7.730270	1.988100	1.70000	-0.1744700000			12
10.043800	-15.94810	-2.083500	1.70000	-0.1788700000			12
10.605600	-8.030850	-4.418100	1.70000	-0.1826500000			12
5.579790	-7.137810	1.699400	1.70000	-0.1842200000			12
14.438900	-6.652040	3.053700	1.70000	-0.1865100000			12
9.752810	-17.36900	-1.725800	1.70000	-0.1801600000			12
9.742260	-8.131330	-5.702200	1.70000	-0.1812300000			12
7.018270	-6.457820	1.708000	1.70000	-0.1815900000			12
14.591600	-5.228400	2.479500	1.70000	-0.1845900000			12
9.309330	-18.18020	-2.989700	1.70000	-0.1801500000			12
8.244310	-8.444980	-5.478000	1.70000	-0.1788200000			12
7.097480	-5.559460	0.426430	1.70000	-0.1710600000			12
13.679100	-4.891790	1.290300	1.70000	-0.1771600000			12
7.828520	-17.89630	-3.390300	1.70000	-0.1657700000			12
8.047070	-9.674890	-4.576800	1.70000	-0.1743400000			12
8.319970	-4.595300	0.385650	1.70000	-0.1773500000			12
12.176600	-4.998900	1.610200	1.70000	-0.1776300000			12
7.298660	-18.66410	-4.622000	1.70000	-0.1759200000			12
6.556730	-10.06590	-4.435300	1.70000	-0.1795700000			12
8.504460	-3.861030	-0.968350	1.70000	-0.3212300000			12
11.715600	-4.261010	2.903800	1.70000	-0.3203100000			12
8.013930	-18.31300	-5.891700	1.70000	-0.3193800000			12
5.814650	-9.190270	-3.463600	1.70000	-0.3167000000			12
9.346040	-11.15660	1.796300	1.10000	0.1479700000			1
9.238440	-9.392800	1.992400	1.10000	0.1495100000			1
11.557800	-8.929020	1.715800	1.10000	0.1505000000			1
11.570700	-10.67060	1.832600	1.10000	0.1472700000			1
9.507330	-11.03330	-1.401900	1.10000	0.1522800000			1
11.356700	-10.85590	-1.558800	1.10000	0.1546800000			1
9.234980	-8.691090	-1.214400	1.10000	0.1482100000			1
9.863960	-7.814230	0.136140	1.10000	0.1480000000			1
7.753650	-9.302520	-0.106640	1.10000	0.1293200000			1
7.668350	-11.04930	-0.144920	1.10000	0.1239400000			1

13.099300	-10.96370	-0.262930	1.10000	0.1189100000	1
13.425600	-9.210870	-0.253030	1.10000	0.1336000000	1
11.459700	-12.45100	0.329370	1.10000	0.1230800000	1
9.667690	-12.53490	0.362860	1.10000	0.1218200000	1
12.059200	-7.782910	-0.549270	1.10000	0.1207300000	1
11.859000	-8.742270	-2.140600	1.10000	0.1315300000	1
6.841580	-11.20760	2.163800	1.10000	0.1061000000	1
7.052690	-9.419800	2.472400	1.10000	0.1156300000	1
14.106400	-11.31400	1.958300	1.10000	0.1062500000	1
15.145600	-10.24330	0.837810	1.10000	0.1230300000	1
9.880680	-13.25690	-2.160800	1.10000	0.1108700000	1
11.566000	-13.50140	-1.793700	1.10000	0.1074700000	1
10.646000	-5.928380	-1.571300	1.10000	0.1098800000	1
12.046100	-6.490300	-2.699800	1.10000	0.1232900000	1
5.138470	-10.65660	0.591570	1.10000	0.0959780000	1
4.729170	-9.943040	2.177200	1.10000	0.1147200000	1
13.474500	-9.156610	3.101500	1.10000	0.0853470000	1
15.217200	-9.471090	3.019800	1.10000	0.1204800000	1
11.247900	-15.35220	-0.263560	1.10000	0.0965310000	1
9.476510	-14.92940	-0.177870	1.10000	0.0981120000	1
9.185020	-7.367550	-3.026300	1.10000	0.0870150000	1
9.976890	-6.006570	-4.010700	1.10000	0.1153900000	1
5.960850	-8.236920	-0.174970	1.10000	0.0896280000	1
4.315100	-8.389310	0.313550	1.10000	0.1114300000	1
15.689100	-7.588820	1.582900	1.10000	0.1133100000	1
13.867100	-7.515980	1.154600	1.10000	0.1041400000	1
9.253610	-15.47600	-2.691500	1.10000	0.0995120000	1
10.748300	-15.99080	-2.864200	1.10000	0.1055000000	1
11.658900	-7.903130	-4.730500	1.10000	0.1108900000	1
10.559100	-9.024680	-3.881600	1.10000	0.1070500000	1
4.787590	-6.339830	1.512900	1.10000	0.1103500000	1
5.374520	-7.443480	2.832600	1.10000	0.0977480000	1
13.535200	-6.835280	3.637400	1.10000	0.0717050000	1
15.095600	-6.892080	3.878700	1.10000	0.0835220000	1
10.594600	-17.83720	-1.158600	1.10000	0.0885920000	1
8.917670	-17.40720	-1.013600	1.10000	0.0835240000	1
9.771050	-7.159980	-6.320500	1.10000	0.0606510000	1
10.182400	-8.931990	-6.363500	1.10000	0.1094600000	1
7.218700	-5.774560	2.595900	1.10000	0.1012300000	1
7.816910	-7.240860	1.668400	1.10000	0.0558290000	1
14.387700	-4.563370	3.357600	1.10000	0.0943790000	1
15.681000	-5.039710	2.135100	1.10000	0.1046000000	1
10.098800	-18.00420	-3.726100	1.10000	0.0966740000	1
9.404760	-19.29040	-2.735200	1.10000	0.0952930000	1
7.672670	-7.610700	-4.965200	1.10000	0.0821630000	1
7.748310	-8.559610	-6.476800	1.10000	0.0878050000	1
7.145160	-6.202380	-0.514980	1.10000	0.1059900000	1
6.222900	-4.902020	0.255130	1.10000	0.0880460000	1
14.061800	-3.882880	1.016000	1.10000	0.1052200000	1
13.967300	-5.516810	0.369700	1.10000	0.0978580000	1
7.201090	-18.15540	-2.506700	1.10000	0.0826530000	1
7.590290	-16.80640	-3.508200	1.10000	0.0901030000	1
8.654870	-10.52270	-5.002800	1.10000	0.0991210000	1
8.497800	-9.694130	-3.602800	1.10000	0.0953380000	1
8.225760	-3.848920	1.220300	1.10000	0.0706920000	1
9.260560	-5.116140	0.668860	1.10000	0.1052800000	1
11.560600	-4.666380	0.669830	1.10000	0.1086500000	1
11.877000	-6.050250	1.640300	1.10000	0.0725830000	1
7.531810	-19.73090	-4.442500	1.10000	0.0979530000	1
6.234290	-18.54130	-4.776900	1.10000	0.0964140000	1
6.040630	-10.08800	-5.409000	1.10000	0.0936640000	1
6.552840	-11.13800	-4.020100	1.10000	0.1067300000	1
8.377160	-4.533750	-1.824500	1.10000	0.1174000000	1
7.766300	-3.026190	-1.064600	1.10000	0.1035200000	1
9.556040	-3.382820	-1.009500	1.10000	0.1053800000	1
12.219900	-4.721550	3.814300	1.10000	0.0910840000	1
12.060700	-3.237940	2.832700	1.10000	0.1194800000	1
10.558200	-4.337370	3.105400	1.10000	0.1038000000	1
7.705150	-17.33640	-6.308200	1.10000	0.1010000000	1
9.124820	-18.26040	-5.793300	1.10000	0.1025200000	1
7.680180	-19.04050	-6.792700	1.10000	0.1101200000	1
5.838580	-8.091080	-3.693100	1.10000	0.0866880000	1
4.715000	-9.434660	-3.334000	1.10000	0.1143100000	1
6.262350	-9.207130	-2.421900	1.00000	0.1054300000	1

TAA_multiTemperature_candidate2.xlsx - Sheet #6

x	y	z	Radius	Charge	Atom
10.432000	-10.06510	0.967150	1.55000	-0.4542700000	14

9.449080	-10.60150	2.022100	1.70000	-0.0589730000	1	12
11.772600	-10.11660	1.689300	1.70000	-0.0552500000		12
10.427300	-10.87300	-0.328560	1.70000	-0.0556390000	578	12
9.980290	-8.622850	0.687640	1.70000	-0.0567740000		12
8.004600	-10.86870	1.484400	1.70000	-0.2182700000		12
12.984600	-9.825390	0.875900	1.70000	-0.2176800000		12
10.566500	-12.35450	-0.040873	1.70000	-0.2216600000		12
10.819700	-7.677840	-0.290050	1.70000	-0.2160500000		12
6.964540	-10.29950	2.469800	1.70000	-0.1899600000		12
14.280000	-9.845400	1.695300	1.70000	-0.1972700000		12
10.600100	-13.10030	-1.342900	1.70000	-0.1854500000		12
9.891280	-6.695500	-1.016500	1.70000	-0.2032200000		12
5.463660	-10.53210	2.115700	1.70000	-0.1936200000		12
14.509600	-8.794420	2.837800	1.70000	-0.1970300000		12
10.726100	-14.62100	-1.087500	1.70000	-0.1868500000		12
9.022000	-7.286150	-2.089100	1.70000	-0.1978400000		12
5.056360	-9.897250	0.764750	1.70000	-0.1839800000		12
15.264400	-7.559030	2.318100	1.70000	-0.1744700000		12
10.692800	-15.53420	-2.340200	1.70000	-0.1788700000		12
9.850540	-7.611710	-3.362800	1.70000	-0.1826500000		12
5.425020	-8.373680	0.648810	1.70000	-0.1842200000		12
15.239200	-6.417270	3.355000	1.70000	-0.1865100000		12
9.283270	-16.07180	-2.598800	1.70000	-0.1801600000		12
8.837870	-7.913930	-4.531700	1.70000	-0.1812300000		12
4.953910	-7.743030	-0.694050	1.70000	-0.1815900000		12
15.934500	-5.119440	3.022400	1.70000	-0.1845900000		12
9.068650	-16.85260	-3.928200	1.70000	-0.1801500000		12
7.840190	-9.082270	-4.337600	1.70000	-0.1788200000		12
5.342670	-6.268010	-0.912330	1.70000	-0.1710600000		12
15.419700	-4.629520	1.639100	1.70000	-0.1771600000		12
9.035790	-16.02610	-5.227100	1.70000	-0.1657700000		12
8.419360	-10.46570	-3.969100	1.70000	-0.1743400000		12
4.954270	-5.719640	-2.273300	1.70000	-0.1773500000		12
13.934400	-4.306670	1.530300	1.70000	-0.1776300000		12
9.227360	-16.95190	-6.423200	1.70000	-0.1759200000		12
7.487520	-11.66820	-4.196800	1.70000	-0.1795700000		12
5.432560	-4.260760	-2.405900	1.70000	-0.3212300000		12
13.643700	-3.137490	2.488400	1.70000	-0.3203100000		12
9.549710	-16.15050	-7.738600	1.70000	-0.3193800000		12
6.253840	-11.76700	-3.291000	1.70000	-0.3167000000		12
9.833730	-11.51570	2.549100	1.10000	0.1479700000		1
9.412770	-9.825570	2.877500	1.10000	0.1495100000		1
11.751600	-9.425800	2.551600	1.10000	0.1505000000		1
11.946100	-11.09240	2.175500	1.10000	0.1472700000		1
9.523230	-10.69540	-0.927980	1.10000	0.1522800000		1
11.197700	-10.50420	-1.046700	1.10000	0.1546800000		1
8.961100	-8.603300	0.241910	1.10000	0.1482100000		1
9.861490	-8.094620	1.652500	1.10000	0.1480000000		1
7.872960	-10.37530	0.491400	1.10000	0.1293200000		1
7.809230	-11.96590	1.297200	1.10000	0.1239400000		1
13.085800	-10.53770	0.028933	1.10000	0.1189100000		1
12.921600	-8.790240	0.444900	1.10000	0.1336000000		1
11.486700	-12.60290	0.509210	1.10000	0.1230800000		1
9.712240	-12.74690	0.588390	1.10000	0.1218200000		1
11.635000	-7.162350	0.241500	1.10000	0.1207300000		1
11.236900	-8.333380	-1.062200	1.10000	0.1315300000		1
7.125380	-10.80430	3.489800	1.10000	0.1061000000		1
7.156780	-9.172650	2.511700	1.10000	0.1156300000		1
14.352400	-10.84670	2.109000	1.10000	0.1062500000		1
15.144700	-9.767300	0.973080	1.10000	0.1230300000		1
9.703510	-12.84810	-1.967300	1.10000	0.1108700000		1
11.471900	-12.78300	-1.971700	1.10000	0.1074700000		1
9.236620	-6.193420	-0.263010	1.10000	0.1098800000		1
10.484700	-5.863770	-1.504600	1.10000	0.1232900000		1
5.237090	-11.64360	2.153600	1.10000	0.0959780000		1
4.844950	-10.03170	2.894700	1.10000	0.1147200000		1
13.562800	-8.505770	3.312300	1.10000	0.0853470000		1
15.071500	-9.271760	3.704900	1.10000	0.1204800000		1
11.682400	-14.75370	-0.508230	1.10000	0.0965310000		1
9.886230	-14.90430	-0.405300	1.10000	0.0981120000		1
8.591540	-8.184200	-1.659000	1.10000	0.0870150000		1
8.171270	-6.563810	-2.343100	1.10000	0.1153900000		1
5.586380	-10.38260	-0.093393	1.10000	0.0896280000		1
3.961490	-10.02060	0.558250	1.10000	0.1114300000		1
16.306900	-7.812090	1.954700	1.10000	0.1133100000		1
14.765100	-7.248830	1.398500	1.10000	0.1041400000		1
11.202800	-14.99320	-3.182900	1.10000	0.0995120000		1
11.388100	-16.38980	-2.135600	1.10000	0.1055000000		1
10.476200	-6.769550	-3.695100	1.10000	0.1108900000		1
10.605300	-8.460630	-3.194900	1.10000	0.1070500000		1

4.930770	-7.805990	1.486300	1.10000	0.1103500000	1
6.505160	-8.174070	0.636660	1.10000	0.0977480000	1
14.208200	-6.188150	3.687900	1.10000	0.0717050000	1
15.795800	-6.829330	4.221200	1.10000	0.0835220000	1
9.011900	-16.75970	-1.793000	1.10000	0.0885920000	1
8.546320	-15.23860	-2.556800	1.10000	0.0835240000	1
8.304630	-6.922980	-4.681800	1.10000	0.0606510000	1
9.455500	-8.047310	-5.450600	1.10000	0.1094600000	1
5.285360	-8.378100	-1.575300	1.10000	0.1012300000	1
3.880460	-7.814910	-0.616760	1.10000	0.0558290000	1
15.831600	-4.311690	3.770700	1.10000	0.0943790000	1
17.024400	-5.263690	2.910700	1.10000	0.1046000000	1
9.937070	-17.59240	-3.910600	1.10000	0.0966740000	1
8.127440	-17.44550	-3.821000	1.10000	0.0952930000	1
7.081660	-8.873770	-3.512000	1.10000	0.0821630000	1
7.188960	-9.189950	-5.258000	1.10000	0.0878050000	1
4.857030	-5.685330	-0.119020	1.10000	0.1059900000	1
6.456350	-6.291310	-0.730230	1.10000	0.0880460000	1
15.939100	-3.654150	1.307600	1.10000	0.1052200000	1
15.641800	-5.334030	0.831630	1.10000	0.0978580000	1
8.036260	-15.50240	-5.374400	1.10000	0.0826530000	1
9.848790	-15.21150	-5.161800	1.10000	0.0901030000	1
9.302920	-10.63130	-4.576600	1.10000	0.0991210000	1
8.755820	-10.40760	-2.869500	1.10000	0.0953380000	1
5.443860	-6.248000	-3.111900	1.10000	0.0706920000	1
3.852440	-5.813490	-2.427800	1.10000	0.1052800000	1
13.661800	-4.017570	0.484780	1.10000	0.1086500000	1
13.315000	-5.184830	1.810400	1.10000	0.0725830000	1
10.083000	-17.61620	-6.199500	1.10000	0.0979530000	1
8.285040	-17.50240	-6.520200	1.10000	0.0964140000	1
7.160880	-11.73290	-5.260300	1.10000	0.0936640000	1
8.087010	-12.59470	-3.985300	1.10000	0.1067300000	1
4.701860	-3.621690	-1.865900	1.10000	0.1174000000	1
6.447930	-4.082790	-1.968000	1.10000	0.1035200000	1
5.347790	-3.887460	-3.462400	1.10000	0.1053800000	1
13.691200	-3.506300	3.537200	1.10000	0.0910840000	1
14.401200	-2.377970	2.303600	1.10000	0.1194800000	1
12.630600	-2.709670	2.331200	1.10000	0.1038000000	1
8.757640	-15.33990	-7.820700	1.10000	0.1010000000	1
10.558600	-15.69390	-7.599400	1.10000	0.1025200000	1
9.551600	-16.77640	-8.678800	1.10000	0.1101200000	1
5.504490	-11.00190	-3.579700	1.10000	0.0866880000	1
5.750430	-12.76370	-3.372900	1.10000	0.1143100000	1
6.408590	-11.59640	-2.201500	1.00000	0.1054300000	1

IMoS.cla

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excelfile Savefile Gas
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DNRCustomRange 0 0
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fromvalue 4
tovalue 6
red_coef 1.01
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 578
Temperature 295
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0
Timestep 100
Boxdomain 16
Diffuse? 1
reemvel 1
Other 0
Simplify 0
PA 0
PATSA 0
EHSS/DHSS 0
TM 0
TDHSS 0

qpol 0
LennardJones 1
DTM 0
HEN 4
TeffRange 295 296 297 298.5 300 302 305 308 312 315 320 325 330 340 350 365 380 420 470 530 600 680 770 870 980 1100
EsEc 1
ft_vector 0.33333 0.28885 0.90371 0.90371 0.28885 -0.33333 -0.49486 -0.36437 -0.36437 -0.49486 -0.33333
t_vector 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
MultiT 1
MultiTval 295
seed 13
Numthreads 15
Repeatseed 1
DragRG 1

1. V. D. Gandhi, K. Short, L. Hua, I. Rodríguez, C. Larriba-Andaluz, A numerical tool to calculate ion mobility at arbitrary fields from all-atom models. *Journal of Aerosol Science*, 106122 (2022).
2. V. D. Gandhi, C. Larriba-Andaluz, Predicting ion mobility as a function of the electric field for small ions in light gases. *Analytica Chimica Acta* **1184**, 339019 (2021).