Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Oxidation Pathways, Kinetics and Branching ratios of Chloromethyl ethyl ether (CMEE) Initiated by OH Radical and Fate of Its Product Radical: An Insight from Computational Study

Subrata Paul, Nand Kishor Gour* and Ramesh Ch. Deka*

Department of Chemical Sciences, Tezpur University Tezpur, Assam - 784028, India

Email-addresses: nkgour1@tezu.ernet.in & ramesh@tezu.ernet.in

Table S1: T1 diagnostic value of all species of CMEE + OH radical reaction.

Species	T1 Diagnostic
R	0.01026976
IM1a	0.01061523
IM1b	0.01050101
IM2	0.01161228
IM3	0.01223772
TS1a	0.01633129
TS1b	0.01659291
TS2	0.01857304
TS3	0.01923135
$CH_2ClOCH_2CH_2$(P1)	0.01132827
$CH_2ClOCHCH_3$(P2)	0.01415136
$CHClOCH_2CH_3$(P3)	0.01473525

Table S2: Vibrational frequencies (in cm^{-1}) of all the species involved in the all reaction channels at M06-2X/6-311++G (d, p) level of theory.

CMEE	34	120	170	228	373	442	816	819	919	1023	1079
	1163	1184	1193	1266	1316	1382	1408	1448	1485	1503	1518
	1541	3022	3058	3061	3069	3125	3140	3151			
$^{\bullet}$OH	3767										
TS1a	***986i***	33	62	89	124	157	190	335	376	428	766
	820	828	893	1019	1037	1081	1185	1189	1215	1260	1295
	1309	1378	1387	1427	1482	1513	1534	3024	3063	3065	3104
	3121	3181	3802								
TS1b	***1309i***	31	78	139	154	186	362	372	419	438	697
	823	874	921	964	1019	1082	1160	1188	1195	1252	1281
	1311	1375	1425	1458	1500	1506	1531	3014	3064	3066	3108
	3125	3188	3761								
TS2	***825i***	21	99	116	134	210	237	299	358	524	664
	722	785	889	1013	1079	1119	1143	1164	1255	1311	1368
	1377	1404	1421	1483	1491	1509	1532	3050	3060	3095	3139
	3157	3210	3784								
TS3	***782i***	44	73	95	127	164	198	252	378	444	678
	823	831	921	973	1083	1146	1163	1185	1214	1320	1349
	1406	1443	1457	1489	1505	1528	1706	3032	3066	3086	3092
	3148	3153	3772								
IM1a	26	64	104	117	139	161	178	291	334	374	446
	818	837	922	1022	1079	1164	1187	1195	1257	1320	1377
	1400	1447	1493	1515	1521	1543	3031	3053	3066	3070	3124
	3131	3143	3775								
IM1b	18	66	76	99	143	206	288	363	403	447	455
	827	828	927	1013	1073	1164	1186	1191	1243	1317	1368

	1411	1446	1496	1506	1512	1538	3038	3068	3073	3078	3130
	3155	3156	3700								
IM2	42	85	104	113	144	231	299	359	369	488	520
	666	822	872	1009	1069	1147	1184	1220	1302	1319	1369
	1400	1439	1488	1498	1507	1528	3036	3058	3096	3099	3136
	3155	3194	3736								
IM3	70	87	103	112	143	190	263	282	371	404	450
	810	830	921	1021	1075	1160	1182	1190	1261	1319	1377
	1406	1444	1490	1505	1513	1533	3027	3066	3072	3075	3139
	3148	3153	3789								
P1	56	105	172	199	374	417	476	823	864	982	1023
	1106	1150	1196	1247	1269	1377	1421	1462	1497	1528	2947
	3008	3055	3113	3181	3300						
P2	73	102	180	201	377	448	620	828	937	1009	1027
	1115	1170	1240	1273	1365	1400	1448	1477	1496	1519	3016
	3078	3103	3148	3148	3164						
P3	61	82	173	233	386	443	723	816	875	92	1089
	1153	1183	1278	1315	1329	1406	1446	1487	1504	1528	3050
	3062	3095	3133	3139	3154						
H_2O	1594	3899	4005								
$CH_2ClOCH(O^{\bullet})CH_3$	51	118	190	277	333	387	527	594	697	844	
	932	1013	1034	1076	1152	1187	1218	1305	1335	1379	
	1392	1480	1494	1509	2943	3072	3122	3164	3172	3221	
TS4	***671i***	64	72	149	227	276	407	427	536	725	
	887	910	968	1021	1117	1165	1228	1330	1375	1397	
	1419	1461	1476	1535	3053	3057	3078	3135	3136	3165	
TS5	570i	65	89	143	209	323	376	472	663	673	
	737	751	932	1008	1035	1088	1161	1313	1361	1386	
	1426	1433	1488	1612	3068	3098	3144	3224	3262	3270	

TS6	***1058i***	71	125	167	303	341	464	574	617	670
	694	737	843	1008	1042	1074	1135	1213	1303	1385
	1401	1474	1479	1481	1721	3063	3139	3150	3188	3222
$CH_2ClO^{\bullet}$	407	697	707	1098	1130	1309	1344	2997	3049	
CH_3CHO	148	512	777	901	1137	1143	1379	1432	1467	1474
	1873	2962	3046	3116	3166					
$CH_2ClOCHO$	85	233	337	443	764	781	999	1036	1060	1190
	1313	1394	1406	1489	1873	3144	3146	3231		
$^{\bullet}CH_3$	493	1412	1412	3135	3316	3316				
$CH_2ClOCOCH_3$	57	85	99	306	355	469	605	661	762	851
	1003	1046	1071	1125	1251	1310	1390	1410	1474	1480
	1483	1891	3073	3139	3147	3196	3221			

Table S3: Total energy with zero point correction and Relative Energy (R.E.) of all species at 298 K calculated at M06-2X and CCSD(T)//M06-2X along with 6-311++G(d,p) basis set**.**

H-abstraction Channels	**M06-2X/6-311++G(d,p)**		**CCSD(T)//M06-2X/6-311++G(d,p)**	
	E_0 (Hartree)	**RE (kcal mol^{-1})**	**E_0 (Hartree)**	**RE (kcal mol^{-1})**
R+OH	-729.5267890	0.0	-728.4548000	0.0
IM1a	-729.5284988	-1.1	-728.4529033	1.2
IM1b	-729.5354347	-5.4	-728.4585542	-2.4
IM2	-729.5406965	-8.7	-728.4612375	-4.0
IM3	-729.5355213	-5.5	-728.4561601	-0.9
TS1a	-729.5213236	3.4	-728.4464974	5.2
TS1b	-729.525898	0.6	-728.4500189	3.0
TS2	-729.5354173	-5.4	-728.459651	-3.0
TS3	-729.5282095	-0.9	-728.4538568	0.6
$CH_2ClOCH_2CH_2$(P1) + H_2O	-729.5503437	-14.8	-728.4702418	-9.7
$CH_2ClOCHCH_3$(P2) + H_2O	-729.5610804	-21.5	-728.4807697	-16.3
$CHClOCH_2CH_3$(P3) + H_2O	-729.5631832	-22.8	-728.4837661	-18.2
Decomposition Channels	**E_0 (Hartree)**	**RE (kcal mol^{-1})**	**E_0 (Hartree)**	**RE (kcal mol^{-1})**
$CH_2ClOCH(O)CH_3$	-728.3810837	0.0	-727.3037122	0.0
TS4	-728.340001	25.8	-727.2670274	23.0
TS5	-728.3599655	13.3	-727.2832771	12.8
TS6	-728.3579915	14.5	-727.2791662	15.4
CH_2ClO + CH_3CHO	-728.3601316	13.2	-727.2883217	9.7
$CH_2ClOCHO$ + CH_3	-728.378199	1.8	-727.3064878	-1.7
$CH_2ClOCOCH_3$ + H	-728.3742599	4.3	-727.3003555	2.1

Table S4: Without corrected and with BSSE corrected HF energy (in **Hartree)** of intermediates along with BSSE energy at M06-2X and CCSD(T) methods.

Intermediates	Without Corrected HF Energy	BSSE Energy	With BSSE corrected HF energy
	M06-2X/6-311++G(d,p) level of theory		
IM1a	-729.6343752	0.0005545	-729.6338207
IM1b	-729.6426408	0.0012594	-729.6413814
IM2	-729.6479819	0.0011449	-729.6468370
IM3	-729.6425259	0.0011247	-729.6414012
	CCSD(T)/6-311++G(d,p) level of theory		
IM1a	-728.5602222	0.0019971	-728.5582251
IM1b	-728.5679504	0.0034495	-728.5645009
IM2	-728.5718059	0.0044278	-728.5673781
IM3	-728.5665526	0.0045126	-728.5620400

Table S5: Rate constant for reaction channels in the temperature range of 250 K–450 K at M06-2X and CCSD(T)//M06-2X along with 6-311++G(d,p) basis set.

Temp. (in K)	**Rate Constant(unit cm^3 $molecule^{-1}$ s^{-1})**										**Exp.**
	M06-2X level					**CCSD(T)//M06-2X level**					**kOH [Ref. 27]**
	k1a	**k1b**	**k2**	**k3**	**kOH**	**k1a**	**k1b**	**k2**	**k3**	**kOH**	
250	1.17×10^{-16}	3.48×10^{-14}	2.80×10^{-09}	3.79×10^{-13}	2.81×10^{-09}	3.14×10^{-18}	2.43×10^{-16}	1.88×10^{-11}	1.62×10^{-14}	1.88×10^{-11}	
298	**3.41×10^{-16}**	**3.56×10^{-14}**	**4.44×10^{-10}**	**2.78×10^{-13}**	**4.44×10^{-10}**	**1.63×10^{-17}**	**5.53×10^{-16}**	**6.43×10^{-12}**	**1.92×10^{-14}**	**6.45×10^{-12}**	**2.33×10^{-12}**
300	3.51×10^{-16}	3.57×10^{-14}	4.12×10^{-10}	2.66×10^{-13}	4.12×10^{-10}	1.70×10^{-17}	5.65×10^{-16}	6.11×10^{-12}	1.86×10^{-14}	6.12×10^{-12}	
350	7.83×10^{-16}	3.69×10^{-14}	1.07×10^{-10}	2.11×10^{-13}	1.07×10^{-10}	5.83×10^{-17}	1.05×10^{-15}	2.79×10^{-12}	2.10×10^{-14}	2.82×10^{-12}	
400	1.46×10^{-15}	3.85×10^{-14}	3.96×10^{-11}	1.97×10^{-13}	3.99×10^{-11}	1.50×10^{-16}	1.70×10^{-15}	1.59×10^{-12}	2.35×10^{-14}	1.61×10^{-12}	
450	2.42×10^{-15}	4.05×10^{-14}	1.87×10^{-11}	1.63×10^{-13}	1.89×10^{-11}	3.18×10^{-16}	2.51×10^{-15}	1.04×10^{-12}	2.61×10^{-14}	1.07×10^{-12}	

Table S6: Percentage branching ratios of the H-abstraction reactions at M06-2X and CCSD(T)//M06-2X levels along with 6-311++G(d, p) basis set.

Reaction Channels	Branching Ratios	
	M06-2X	**CCSD(T)//M06-2X**
R1a	0.00008	0.00032
R1b	0.00803	0.00857
R2	99.93	99.69
R3	0.06	0.30

Cartesian coordinates of all the species at M06-2X/6-311++G(d,p) level of theory. All values are given in Angstroms.

CMEE

At. No.	X	Y	Z
6	-0.671642000	0.667871000	-0.000029000
1	-0.690716000	1.291484000	-0.898538000
1	-0.690680000	1.291500000	0.898471000
6	1.644511000	0.506746000	0.000036000
1	1.699311000	1.150810000	0.888225000
1	1.699362000	1.150931000	-0.888061000
6	2.764585000	-0.509477000	-0.000001000
1	2.700408000	-1.142784000	-0.885507000
1	3.731565000	-0.003389000	0.000057000
1	2.700362000	-1.142900000	0.885419000
17	-2.168485000	-0.294341000	0.000015000
8	0.411240000	-0.197838000	-0.000045000

TS1a

At. No.	X	Y	Z
6	-1.354442000	-0.665549000	0.021782000
1	-1.329856000	-1.253660000	0.943511000
1	-1.290052000	-1.319595000	-0.852453000
6	0.934775000	-0.268911000	0.081060000
1	1.095481000	-0.945447000	-0.768036000
1	1.034979000	-0.852507000	1.005016000
6	1.935124000	0.857959000	0.056162000
1	1.865816000	1.513887000	0.923258000
1	3.000149000	0.342123000	0.140440000
1	1.911041000	1.423521000	-0.874275000
17	-2.936052000	0.144001000	-0.043320000
8	-0.362309000	0.306726000	0.008350000
1	4.469712000	-0.003083000	-0.803913000
8	4.120167000	-0.418509000	0.000259000

TS1b

At. No.	X	Y	Z
6	-1.128544000	-0.742722000	0.327800000
1	-1.086874000	-0.751601000	1.420173000
1	-1.430388000	-1.720256000	-0.056434000
6	1.179928000	-1.099455000	0.241617000
1	1.035649000	-2.153115000	-0.036733000
1	1.238613000	-1.035017000	1.335544000
6	2.422825000	-0.537934000	-0.391200000

1	2.457538000	0.627543000	-0.094401000
1	3.339995000	-0.966067000	0.011074000
1	2.398348000	-0.565867000	-1.479464000
17	-2.386280000	0.421184000	-0.143465000
8	0.079129000	-0.325960000	-0.222640000
1	1.077086000	1.678677000	0.010826000
8	2.007313000	1.826739000	0.255018000

TS2

At. No.	**X**	**Y**	**Z**
6	-0.946316000	-1.223825000	0.147221000
1	-0.938732000	-1.416829000	1.221366000
1	-1.454384000	-2.004482000	-0.409220000
6	1.194137000	-0.284216000	0.391157000
1	1.099215000	-0.521972000	1.458388000
1	0.919045000	0.839174000	0.293095000
6	2.591802000	-0.437540000	-0.145400000
1	2.616892000	-0.154259000	-1.198150000
1	3.269117000	0.215674000	0.405798000
1	2.931517000	-1.470710000	-0.046666000
17	-1.986266000	0.267672000	-0.052732000
8	0.307295000	-1.067019000	-0.370943000
1	-0.189750000	2.179761000	-0.227868000
8	0.752188000	2.249108000	0.001172000

TS3

At. No.	**X**	**Y**	**Z**

6	-0.577516000	-0.102014000	0.558948000
1	-0.696524000	1.037664000	0.464279000
1	-0.569274000	-0.343053000	1.627810000
6	1.733650000	0.059372000	0.422889000
1	1.830326000	-0.214936000	1.481174000
1	1.649429000	1.149755000	0.351549000
6	2.899281000	-0.463357000	-0.385121000
1	2.788393000	-0.182858000	-1.433029000
1	3.832974000	-0.043242000	-0.007404000
1	2.952155000	-1.550689000	-0.318496000
17	-2.013789000	-0.829901000	-0.173250000
8	0.541296000	-0.526886000	-0.103961000
1	-1.072442000	2.176552000	-0.964000000
8	-0.642935000	2.416276000	-0.125654000

IM1a

At. No.	**X**	**Y**	**Z**
6	-1.244694000	-0.319309000	0.580190000
1	-1.431666000	0.091713000	1.576658000
1	-0.972926000	-1.376637000	0.646400000
6	0.962125000	0.407707000	0.567118000
1	1.314271000	-0.623864000	0.690764000
1	0.845260000	0.853727000	1.563965000
6	1.937170000	1.207805000	-0.268601000
1	1.575896000	2.228536000	-0.401206000
1	2.912455000	1.240880000	0.222079000

1	2.042568000	0.752565000	-1.255709000
17	-2.779309000	-0.228495000	-0.318326000
8	-0.290036000	0.414647000	-0.106054000
1	4.029424000	-0.947543000	-1.003097000
8	3.665706000	-1.178670000	-0.131515000

IM1b

At. No.	X	Y	Z
6	-0.984559000	-0.979515000	0.000304000
1	-1.108314000	-1.586655000	0.900669000
1	-1.108391000	-1.587438000	-0.899523000
6	1.355589000	-1.195101000	0.000117000
1	1.308640000	-1.835794000	-0.889165000
1	1.308862000	-1.835204000	0.889832000
6	2.611211000	-0.350121000	-0.000291000
1	2.642944000	0.286411000	0.885705000
1	3.493660000	-0.991939000	-0.000192000
1	2.642751000	0.285871000	-0.886668000
17	-2.273027000	0.245242000	-0.000173000
8	0.235571000	-0.311457000	-0.000029000
1	0.540173000	1.619690000	0.000041000
8	1.142889000	2.389503000	0.000210000

IM2

At. No.	X	Y	Z
6	-0.891082000	-0.988115000	-0.616425000
1	-0.978675000	-1.958384000	-0.123904000

1	-1.315175000	-0.990338000	-1.615623000
6	1.154503000	-0.705538000	0.517830000
1	1.072561000	-1.753273000	0.832608000
1	0.737715000	-0.068469000	1.304075000
6	2.584366000	-0.328030000	0.209332000
1	2.632852000	0.712500000	-0.112833000
1	3.198411000	-0.444427000	1.104107000
1	2.987621000	-0.965946000	-0.578281000
17	-1.982789000	0.124701000	0.365453000
8	0.386143000	-0.527367000	-0.677691000
1	-0.224825000	1.862750000	-0.233634000
8	0.677633000	2.229339000	-0.254013000

IM3

At. No.	**X**	**Y**	**Z**
6	-0.743113000	-0.690112000	0.557790000
1	-0.685688000	-0.148607000	1.505303000
1	-0.871572000	-1.763441000	0.717970000
6	1.587552000	-0.645897000	0.417074000
1	1.669404000	-1.712918000	0.660910000
1	1.603677000	-0.069992000	1.350191000
6	2.699534000	-0.204549000	-0.507158000
1	2.596111000	0.859271000	-0.724366000
1	3.668850000	-0.375172000	-0.035533000
1	2.661460000	-0.764700000	-1.442332000
17	-2.208412000	-0.110351000	-0.283160000

8	0.348792000	-0.411419000	-0.252220000
1	-0.284812000	1.906764000	-0.385458000
8	0.391426000	2.059933000	0.297320000

P1

At. No.	**X**	**Y**	**Z**
6	0.604213000	0.660459000	0.020765000
1	0.598293000	1.232663000	0.953215000
1	0.627925000	1.333300000	-0.841378000
6	-1.709268000	0.459445000	0.028379000
1	-1.797334000	1.182485000	-0.796657000
1	-1.745617000	1.041223000	0.967796000
6	-2.801994000	-0.537281000	-0.024979000
1	-2.624513000	-1.533711000	0.353239000
1	-3.805787000	-0.226379000	-0.275103000
17	2.112654000	-0.279994000	-0.007853000
8	-0.465723000	-0.220677000	-0.046575000

P2

6	-0.654669000	0.680213000	0.128305000
1	-0.629367000	1.396980000	-0.695506000
1	-0.713014000	1.190032000	1.090497000
6	1.644149000	0.475229000	-0.042759000
1	1.632564000	1.373149000	-0.657843000
6	2.825097000	-0.420479000	-0.000276000
1	2.847243000	-1.103354000	-0.859833000
1	3.743010000	0.167838000	-0.008898000

1	2.808987000	-1.031964000	0.904811000
17	-2.127171000	-0.294160000	-0.055088000
8	0.448127000	-0.175219000	0.081456000

P3

At. No.	**X**	**Y**	**Z**
6	0.687850000	0.616112000	-0.099647000
1	0.658173000	1.552482000	0.453814000
6	-1.632458000	0.529565000	-0.023029000
1	-1.705491000	1.147512000	-0.923509000
1	-1.642830000	1.187942000	0.853492000
6	-2.746216000	-0.489589000	0.042194000
1	-2.650067000	-1.102404000	0.939184000
1	-3.712522000	0.017012000	0.066257000
1	-2.715183000	-1.141835000	-0.831132000
17	2.178866000	-0.244534000	0.019643000
8	-0.390981000	-0.180021000	-0.051143000

$CH_2ClOCH(O)CH_3$

At. No.	X	Y	Z
6	0.925395000	0.442990000	-0.807871000
1	0.806721000	1.488023000	-0.524247000
1	1.403124000	0.331706000	-1.775196000
6	-1.122079000	0.008345000	0.272216000
1	-0.598740000	-0.298257000	1.200715000
6	-2.372654000	-0.844581000	0.067886000
1	-2.072853000	-1.885326000	-0.042635000
1	-3.036881000	-0.732501000	0.922553000
1	-2.879695000	-0.518148000	-0.839939000
17	2.080183000	-0.269078000	0.410854000
8	-0.268459000	-0.234716000	-0.837900000
8	-1.427636000	1.303253000	0.448005000

TS4

At. No.	X	Y	Z
6	0.738181000	0.832182000	0.241271000
1	0.330839000	0.650886000	1.237009000
1	1.099494000	1.863370000	0.155873000
6	-1.581610000	-0.429497000	-0.394748000
1	-1.844011000	-0.532642000	-1.455731000
6	-2.495909000	0.441064000	0.425579000
1	-2.731968000	1.359529000	-0.111604000
1	-3.422475000	-0.112469000	0.599760000
1	-2.044222000	0.663806000	1.392642000

17	2.187727000	-0.220859000	0.078196000
8	-0.176150000	0.674329000	-0.748061000
8	-0.891723000	-1.324375000	0.150574000

TS5

At. No.	**X**	**Y**	**Z**
6	-0.717289000	-0.782115000	0.422950000
1	-0.375936000	-0.384653000	1.376144000
1	-1.026473000	-1.819800000	0.485357000
6	1.090226000	0.417495000	-0.488356000
1	1.567260000	0.549549000	-1.468155000
6	2.759691000	-0.419166000	0.244242000
1	2.420457000	-0.702870000	1.233303000
1	2.907617000	-1.228452000	-0.461157000
1	3.464451000	0.401977000	0.206227000
17	-2.179162000	0.167662000	-0.024917000
8	0.263907000	-0.698234000	-0.556128000
8	0.897670000	1.327823000	0.303483000

TS6

At. No.	**X**	**Y**	**Z**
6	-0.914742000	0.407825000	-0.847315000
1	-0.799146000	-0.440939000	-1.515636000
1	-1.369871000	1.268460000	-1.324392000
6	1.202900000	-0.181943000	-0.006986000
1	0.602079000	-0.518512000	1.466761000
6	2.489614000	0.422040000	0.505553000

1	2.290640000	1.240789000	1.193811000
1	3.083196000	-0.353461000	0.983675000
1	3.033481000	0.811769000	-0.358805000
17	-2.036526000	-0.118391000	0.462319000
8	0.303170000	0.822567000	-0.321491000
8	1.086071000	-1.307939000	-0.455053000

CH_2ClO

At. No.	**X**	**Y**	**Z**
6	0.000000000	0.816683000	0.000000000
1	0.434795000	1.293057000	0.890903000
1	0.434795000	1.293057000	-0.890903000
17	0.565788000	-0.905329000	0.000000000
8	-1.310998000	0.988048000	0.000000000

CH_3CHO

At. No.	**X**	**Y**	**Z**
6	-0.234715000	0.398725000	0.000039000
1	-0.317538000	1.504644000	-0.000097000
6	1.164729000	-0.147194000	-0.000030000
1	1.698877000	0.223756000	-0.879068000
1	1.698314000	0.223272000	0.879531000
1	1.149071000	-1.235586000	-0.000241000
8	-1.226101000	-0.278159000	-0.000022000

$CH_2ClOCHO$

At. No.	**X**	**Y**	**Z**
6	0.405380000	0.695439000	0.584147000

1	0.065849000	0.196897000	1.487950000
1	0.883230000	1.648591000	0.779145000
6	-1.639352000	0.015355000	-0.329484000
1	-2.393200000	0.318260000	-1.064355000
17	1.618728000	-0.368993000	-0.183219000
8	-0.664495000	0.951224000	-0.287629000
8	-1.669308000	-0.970678000	0.335629000

CH_3

At. No.	**X**	**Y**	**Z**
6	0.000000000	0.000000000	0.000000000
1	0.000000000	1.078647000	0.000000000
1	0.934135000	-0.539323000	0.000000000
1	-0.934135000	-0.539323000	0.000000000

$CH_2ClOCOCH_3$

At. No.	**X**	**Y**	**Z**
6	-0.903122000	-0.397415000	0.830661000
1	-0.794052000	0.450555000	1.501048000
1	-1.351047000	-1.262017000	1.307331000
6	1.247249000	0.179976000	0.080227000
6	2.481151000	-0.394901000	-0.545316000
1	2.226681000	-0.783202000	-1.533078000
1	3.236679000	0.381020000	-0.632358000
1	2.848398000	-1.227572000	0.054893000
17	-2.008256000	0.114899000	-0.484006000
8	0.331649000	-0.806102000	0.319463000

8	1.046103000	1.326349000	0.347640000