Understanding the Atmospheric Oxidation of HFE-7500 ($C_3F_7CF(OC_2H_5)CF(CF_3)_2$) Initiated by Cl atom and NO_3 Radical From Theory

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Supporting Information

Table S1: Zero-point corrected total energy E_0 (in Hartree) obtained at M06-2X/6-31+G(d,p) level of theory of all the species involved in titled reaction.

Table S2: Frequencies obtained at M06-2x/6-31+G(d,p) level of theory of all the species involved in titled reaction.

Table S3: Rate Constants and branching ratios (at 298 K) for the reaction of HFE-7500 with Cl atom and NO_3 radical computed from TST.

Table S4. Rate Constants and branching ratios (at 298 K) for the reaction of HFE-7500 with Cl atom and NO_3 radical computed from CVT.

Figure S1. Rate constants vs $10^3/T$ for the HFE-7500 + Cl reactions in the temperature range of 250–450 K computed by TST method.

Figure S2. Rate constants vs $10^3/T$ for the HFE-7500 + NO_3 reactions in the temperature range of 250–450 K computed from TST.

Cartesian coordinates of all species (in Å).

Table S1: Zero-point corrected total energy E_0 (in Hartree) obtained at M06-2X/6-31+G(d,p) level of theory of all the species involved in titled reaction.

Species	E_0
HFE-7500 + Cl	-2378.185675
IM-Cl	-2378.193351
TS2a	-2378.180171
TS2b	-2378.182379
TS1	-2378.188316
PC1_Cl	-2378.196354
PC2_Cl	-2378.190046
P1+ HCl	-2378.191052
P2 + HCl	-2378.181587
HFE-7500 + NO_3	-2198.174168
TS3	-2198.173991
IM-NO_3	-2198.178856
TS4b	-2198.163715
TS4a	-2198.166148
P1 + HNO_3	-2198.191463
P2 + HNO_3	-2198.181999

Table S2: Frequencies (in cm^{-1}) obtained at M06-2X/6-31+G(d,p) level of theory of all the species involved in titled reaction.

	HFE-7500											
	41	50	63	67	71	84	89	111	134	149	153	164
	182	201	201	219	240	252	260	271	281	301	304	312
	316	330	340	353	359	374	389	411	478	512	526	544
	545	557	578	592	611	629	660	692	719	748	772	815
	822	928	992	1018	1077	1133	1140	1177	1188	1207	1224	1236
	1246	1257	1264	1277	1284	1310	1315	1323	1328	1331	1342	1354
	1370	1406	1424	1447	1488	1507	1529	3079	3104	3156	3162	
	IM-Cl											
	31	47	53	70	71	78	85	98	112	126	137	145
	166	170	180	195	205	215	221	238	267	276	280	297
	307	311	317	318	333	351	354	356	374	384	424	471
	499	530	545	546	561	582	597	603	651	668	674	726
	756	772	775	838	934	1009	1018	1056	1101	1114	1140	
1163	1192	1219	1236	1242	1249	1253	1269	1276	1296	1297	1309	
1316	1323	1331	1344	1355	1377	1391	1412	1432	1485	1493	1669	
3086	3159	3175	3182									
	IM-NO3											
	25	37	49	51	53	60	63	72	80	83	90	92
	109	123	145	152	162	181	186	205	218	221	247	256
	268	273	283	301	305	311	315	320	330	344	353	361
	372	389	410	481	513	528	544	547	559	579	595	614
	630	662	682	692	719	748	772	804	814	825	863	928
	992	1017	1078	1132	1139	1177	1189	1207	1226	1232	1245	

1258	1268	1280	1284	1309	1314	1319	1321	1330	1343	1355	1372	
1390	1404	1425	1443	1486	1507	1532	1696	3078	3112	3163	3163	
3183												
	TS1											
	898*i*	37	48	58	65	72	81	90	112	116	127	140
	155	171	181	187	205	211	220	224	240	267	277	286
	300	311	316	320	333	350	354	356	373	380	419	460
	480	500	532	545	547	563	584	598	604	651	669	675
	728	756	772	813	839	947	1014	1017	1031	1056	1097	
1142	1168	1196	1203	1221	1237	1245	1248	1255	1270	1278	1297	
1299	1315	1323	1333	1344	1356	1374	1392	1412	1436	1482	1488	
3077	3158	3172	3186									
	TS2a											
	671 *i*	17	35	44	54	56	61	72	77	91	106	143
	148	162	182	197	200	211	224	246	262	278	282	299
	303	312	323	328	339	354	360	372	389	401	416	482
	511	526	543	544	556	575	587	598	616	632	663	692
	719	747	771	799	814	867	895	952	993	1020	1091	
1135	1149	1189	1206	1222	1226	1236	1248	1259	1266	1280	1286	
1300	1305	1317	1320	1331	1342	1354	1371	1417	1426	1463	1498	
3069	3142	3153	3265									
	TS2b											
	752 *i*	20	38	45	48	56	65	68	84	94	115	148
	151	162	184	190	204	212	228	253	257	272	279	300
	305	313	318	332	341	354	359	375	388	397	415	479
	513	526	543	545	557	578	593	606	618	630	663	691
	719	748	772	789	815	858	911	947	993	1021	1092	
1132	1148	1185	1189	1215	1228	1241	1248	1261	1266	1277	1282	
1295	1311	1316	1325	1331	1342	1358	1370	1418	1426	1465	1495	
3063	3137	3166	3275									
	TS3											
	444 *i*	32	47	52	54	68	72	79	89	90	99	121
	139	146	153	157	169	184	203	208	218	229	252	257
	267	275	295	302	308	318	326	334	347	359	359	378
	391	416	481	512	523	529	544	546	560	580	595	614
	631	664	686	693	720	748	772	808	815	857	945	960
	989	1022	1101	1102	1137	1162	1168	1190	1218	1236	1248	
1250	1265	1271	1282	1287	1309	1316	1323	1333	1341	1355	1368	
1373	1398	1418	1423	1433	1479	1491	1681	1779	3078	3130	3164	
3181												
	TS4a											
	819 *i*	13	27	32	39	50	58	65	69	74	86	106
	108	119	150	154	165	172	185	200	215	226	247	254
	257	277	299	300	306	315	328	339	355	356	371	388
	396	407	472	499	518	529	543	544	560	580	593	613
	630	661	690	700	720	747	771	800	814	823	915	971
	992	993	1037	1085	1133	1160	1180	1189	1210	1223	1227	
1237	1247	1258	1265	1276	1283	1309	1315	1322	1326	1330	1342	
1351	1356	1371	1421	1424	1428	1481	1529	1775	3110	3130	3171	
3221												

	TS4b										
	726 *i*	17	30	35	41	45	54	56	64	70	83	87
	117	122	132	150	158	180	185	205	221	226	251	260
	273	280	300	305	312	317	331	344	355	359	373	388
	398	424	479	512	522	532	543	545	560	578	595	614
	630	663	691	698	718	748	771	801	814	817	924	966
	992	1021	1028	1090	1137	1143	1187	1205	1225	1233	1237	
1245	1257	1265	1275	1284	1289	1305	1311	1316	1321	1330	1343	
1356	1370	1374	1423	1424	1426	1463	1504	1764	3086	3122	3148	
3210												
	PC1_Cl											
	30	36	43	48	53	61	63	67	86	93	104	143
	151	163	166	184	197	203	220	248	251	265	267	282
	300	305	313	319	329	340	353	355	362	374	389	412
	434	480	513	527	541	544	558	579	595	614	630	664
	691	719	729	747	771	815	951	992	1022	1048	1118	
	1150	1178	1193	1217	1235	1243	1252	1261	1268	1282	1285	
	1309	1315	1319	1334	1340	1354	1368	1385	1425	1441	1476	
	PC2_Cl											
	21	34	41	53	58	67	77	85	89	103	112	143
	152	155	159	177	194	202	218	235	249	257	274	276
	296	300	312	318	329	340	353	362	365	381	388	408
	443	478	494	513	529	542	542	564	581	594	617	636
	660	691	718	747	770	814	832	974	992	1026	1103	
	1126	1155	1186	1201	1218	1233	1246	1254	1265	1277	1283	
	1303	1311	1316	1322	1330	1340	1355	1368	1415	1423	1475	
	1511	2886	3091	3166	3213	3331						
	P1											
	38	49	52	64	66	75	87	105	112	146	149	159
	182	185	203	214	224	247	256	274	284	301	305	316
	321	329	339	353	356	374	388	411	479	512	527	543
	544	557	578	593	607	626	638	662	694	721	749	772
	815	948	992	1021	1031	1120	1151	1177	1193	1214	1233	
1243	1251	1263	1266	1282	1286	1310	1316	1323	1333	1342	1354	
1369	1387	1424	1444	1470	1492	3031	3111	3164	3235			
	P2											
	38	48	58	66	70	73	88	94	114	141	153	154
	167	182	202	208	225	252	257	271	279	300	304	311
	317	330	340	353	358	374	388	410	476	507	520	538
	544	545	571	586	597	622	648	659	695	721	750	773
	814	815	970	993	1027	1120	1127	1164	1187	1203	1218	
1232	1244	1252	1264	1276	1284	1309	1315	1319	1323	1329	1341	
1355	1369	1415	1423	1484	1517	3108	3173	3207	3323			
	HCl											
	3033											
	NO_3											
	342	690	808	845	1385	1683						
	HNO_3											

537	621	704	812	990	1368	1444	1848	3778	

Table S3: Rate Constants and branching ratios (at 298 K) for the reaction of HFE-7500 with Cl and NO_3 computed from TST.

Rate Constant	**250 K**	**298 K**	**300 K**	**350 K**	**400 K**	**450 K**	**Branching Ratios**
k_1	2.66E-12	3.46E-12	3.51E-12	4.10E-12	4.73E-12	5.33E-12	98.2%
k_{2a}	1.85E-15	6.81E-15	7.06E-15	1.89E-14	4.01E-14	7.31E-14	0.2%
k_{2b}	2.40E-14	5.62E-14	5.77E-14	1.10E-13	1.83E-13	2.74E-13	1.6%
$k_{overall}$	2.69E-12	3.52E-12	3.57E-12	4.23E-12	4.95E-12	5.66E-12	
k_3	6.82E-17	8.44E-17	8.49E-17	1.02E-16	1.19E-16	1.36E-16	98.5%
k_{4b}	9.95E-21	1.01E-19	1.08E-19	6.09E-19	2.25E-18	6.33E-18	0.1%
k_{4a}	1.88E-19	1.16E-18	1.22E-18	4.75E-18	1.34E-17	3.05E-17	1.4%
$k_{overall}$	6.84E-17	8.56E-17	8.63E-17	1.07E-16	1.34E-16	1.72E-16	

Table 4. Rate Constants, branching ratios (at 298 K) and for the reaction of HFE-7500 with Cl and NO_3 computed from CVT.

Rate Constant	250 K	298 K	300 K	350 K	400 K	450 K	Branching Ratios
k_1	2.54E-12	3.18E-12	3.21E-12	3.87E-12	4.39E-12	5.10E-12	98.3%
k_{2a}	1.76E-15	5.30E-15	6.10E-15	1.01E-14	2.90E-14	5.90E-14	0.2%
k_{2b}	2.17E-14	4.90E-14	5.10E-14	9.80E-14	1.41E-13	2.54E-13	1.5%
$k_{overall}$	2.56E-12	3.23E-12	3.27E-12	3.98E-12	4.56E-12	5.41E-12	
k_3	6.77E-17	8.23E-17	8.27E-17	9.97E-17	1.16E-16	1.31E-16	98.7%
k_{4a}	9.86E-21	9.92E-20	9.98E-20	5.20E-19	1.17E-18	5.90E-18	0.1%
k_{4b}	1.73E-19	1.01E-18	1.09E-18	4.57E-18	1.21E-17	2.89E-17	1.2%
$k_{overall}$	6.79E-17	8.34E-17	8.39E-17	1.05E-16	1.29E-16	1.66E-16	

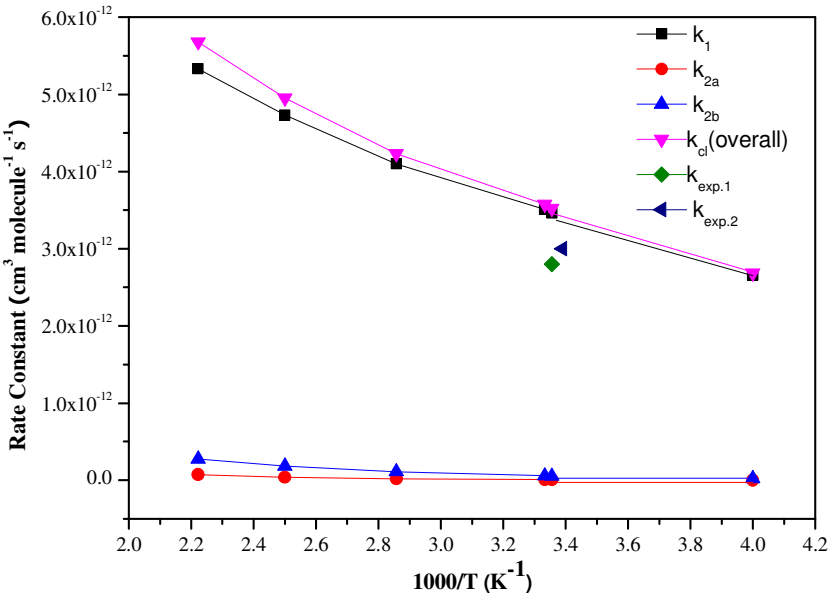


Figure S1. Rate constants vs 10^3/T for the HFE-7500 + Cl reactions in the temperature range of 250–450 K computed by TST method.

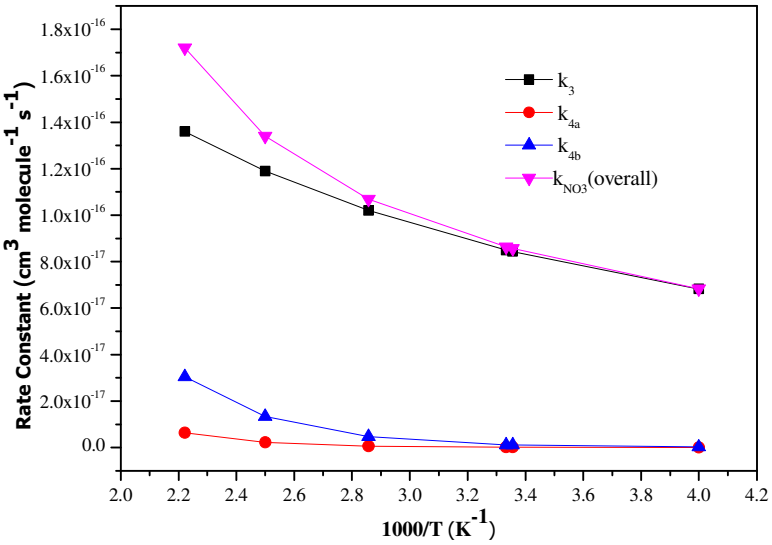


Figure S2. Rate constants vs 10^3/T for the HFE-7500 + NO_3 reactions in the temperature range of 250–450 K computed by TST method.

Cartesian coordinates of all species (in Å).

HFE-7500

At. No.	X	Y	Z
6	2.917723000	0.494930000	0.478597000
6	1.696003000	-0.118500000	-0.275705000
6	0.342330000	0.356663000	0.366606000
6	-0.919413000	-0.368836000	-0.191446000
6	-2.247462000	0.305133000	0.247979000
6	-3.484249000	-0.615111000	0.084389000
6	1.876154000	-1.663110000	-0.344792000
6	0.270654000	2.499629000	-0.868495000
1	1.331024000	2.605359000	-1.110894000
1	-0.239947000	2.004578000	-1.699324000
6	-0.349688000	3.841581000	-0.551302000
1	-0.253694000	4.500798000	-1.417954000
1	-1.408117000	3.729680000	-0.308923000
1	0.160318000	4.303266000	0.297320000
8	0.140256000	1.707781000	0.335904000
9	2.707591000	1.760450000	0.836928000
9	3.982444000	0.478167000	-0.322341000
9	3.191213000	-0.214511000	1.572457000
9	3.139748000	-1.958989000	-0.659034000
9	1.095415000	-2.164259000	-1.299909000
9	1.582878000	-2.246935000	0.811990000
9	0.431634000	0.015374000	1.682539000
9	-0.879983000	-0.358765000	-1.541041000
9	-0.953109000	-1.647025000	0.232324000
9	-2.460900000	1.395564000	-0.512129000
9	-2.180764000	0.667607000	1.536967000
9	-3.491068000	-1.168533000	-1.128114000
9	-4.586703000	0.117039000	0.229205000
9	-3.486684000	-1.573955000	1.003153000
9	1.761185000	0.320971000	-1.567711000

IM_Cl

At. No.	X	Y	Z

6	2.356805000	-0.354673000	1.076085000
6	1.379888000	-0.607299000	-0.119611000
6	-0.062990000	-0.102202000	0.228483000
6	-1.179936000	-0.545369000	-0.759746000
6	-2.572120000	0.127170000	-0.568990000
6	-3.215439000	0.078225000	0.837673000
6	1.477224000	-2.103166000	-0.535571000
6	0.255966000	2.222334000	-0.522849000
1	1.439983000	2.366594000	-0.468190000
1	0.079465000	1.899817000	-1.552599000
6	-0.335543000	3.551144000	-0.139792000
1	0.040166000	4.319448000	-0.818297000
1	-1.426092000	3.510560000	-0.203070000
1	-0.045920000	3.808109000	0.881516000
8	-0.125211000	1.262137000	0.428902000
9	2.088612000	0.781609000	1.711565000
9	3.600776000	-0.292663000	0.617898000
9	2.266527000	-1.358098000	1.951883000
9	2.757630000	-2.471298000	-0.580323000
9	0.964128000	-2.265927000	-1.753519000
9	0.838102000	-2.894127000	0.320250000
9	-0.384102000	-0.658087000	1.426067000
9	-0.796516000	-0.241611000	-2.019400000
9	-1.370839000	-1.870027000	-0.668906000
9	-3.405006000	-0.509009000	-1.409975000
9	-2.493952000	1.417393000	-0.947472000
9	-3.189130000	-1.162586000	1.315524000
9	-4.481381000	0.475900000	0.732453000
9	-2.583006000	0.890074000	1.677395000
9	1.836994000	0.109904000	-1.185071000
17	3.026553000	2.990492000	-0.525882000

IM_NO_3

At. No.	**X**	**Y**	**Z**
6	-2.169033000	0.959330000	0.689966000
6	-0.874631000	1.001090000	-0.178769000
6	0.245478000	0.090770000	0.450744000

6	1.643796000	0.219973000	-0.225736000
6	2.644757000	-0.867802000	0.253061000
6	4.123723000	-0.518603000	-0.055338000
6	-0.453128000	2.483587000	-0.399223000
6	-0.560820000	-2.021725000	-0.555592000
1	-1.571471000	-1.703749000	-0.819682000
1	0.096460000	-1.878724000	-1.417864000
6	-0.558386000	-3.453447000	-0.071860000
1	-0.949885000	-4.103759000	-0.858221000
1	0.453763000	-3.773427000	0.184033000
1	-1.197482000	-3.551535000	0.808716000
8	-0.091255000	-1.227878000	0.559931000
9	-2.460233000	-0.284575000	1.085742000
9	-3.206389000	1.391573000	-0.025636000
9	-2.038115000	1.727163000	1.766832000
9	-1.523992000	3.230917000	-0.676469000
9	0.373298000	2.560319000	-1.440299000
9	0.143377000	2.990808000	0.674320000
9	0.394903000	0.546481000	1.725936000
9	1.507072000	0.098592000	-1.563298000
9	2.191887000	1.419453000	0.047151000
9	2.372508000	-2.026326000	-0.376996000
9	2.540395000	-1.047171000	1.577388000
9	4.251863000	-0.130956000	-1.324182000
9	4.870693000	-1.602839000	0.140186000
9	4.559932000	0.448041000	0.744339000
9	-1.215597000	0.523373000	-1.412291000
7	-4.394127000	-1.684909000	-0.264456000
8	-5.289034000	-1.123621000	0.300803000
8	-3.936286000	-1.073928000	-1.344328000
8	-3.830605000	-2.719220000	-0.013133000

TS1

At. No.	**X**	**Y**	**Z**
6	2.361605000	-0.338812000	1.075994000
6	1.391683000	-0.594925000	-0.126333000
6	-0.053891000	-0.098639000	0.218078000

6	-1.175210000	-0.559409000	-0.757078000
6	-2.574223000	0.097607000	-0.558968000
6	-3.200805000	0.059487000	0.855634000
6	1.500589000	-2.089075000	-0.544984000
6	0.206229000	2.213151000	-0.570392000
1	1.543320000	2.469207000	-0.504797000
1	0.119594000	1.859704000	-1.599398000
6	-0.374654000	3.547730000	-0.218082000
1	0.001543000	4.300676000	-0.912830000
1	-1.467294000	3.511131000	-0.278586000
1	-0.085034000	3.825725000	0.798085000
8	-0.118440000	1.273019000	0.397757000
9	2.070503000	0.782938000	1.725568000
9	3.604462000	-0.252826000	0.621601000
9	2.284815000	-1.355067000	1.939115000
9	2.784355000	-2.442639000	-0.595547000
9	0.983390000	-2.254643000	-1.761021000
9	0.872392000	-2.888023000	0.311560000
9	-0.366716000	-0.634925000	1.424973000
9	-0.805808000	-0.262355000	-2.022005000
9	-1.349258000	-1.884772000	-0.651994000
9	-3.407559000	-0.558492000	-1.383161000
9	-2.515635000	1.384288000	-0.952971000
9	-3.156141000	-1.174249000	1.349416000
9	-4.471244000	0.443632000	0.760380000
9	-2.565310000	0.889227000	1.675961000
9	1.845557000	0.126304000	-1.189354000
17	2.945719000	3.009478000	-0.482379000

TS2a

At. No.	**X**	**Y**	**Z**
6	2.908526000	1.082915000	0.405514000
6	1.947480000	0.051450000	-0.264885000
6	0.485157000	0.183907000	0.301887000
6	-0.501689000	-0.899011000	-0.226712000
6	-1.983179000	-0.603799000	0.137693000
6	-2.894098000	-1.854470000	0.049744000

6	2.563623000	-1.376114000	-0.137600000
6	-0.164339000	2.121963000	-1.095749000
1	0.833009000	2.265757000	-1.530297000
1	-0.777731000	1.557368000	-1.805272000
6	-0.738452000	3.462830000	-0.791661000
1	-2.103604000	3.244392000	-0.219077000
1	-0.316587000	3.984492000	0.065965000
1	-1.002036000	4.077456000	-1.649046000
8	-0.071674000	1.430186000	0.157970000
9	2.341938000	2.284603000	0.533188000
9	3.990971000	1.239562000	-0.353256000
9	3.280447000	0.657328000	1.610120000
9	3.879404000	-1.327934000	-0.357484000
9	2.030540000	-2.172942000	-1.060789000
9	2.359977000	-1.896394000	1.067151000
9	0.597740000	-0.009328000	1.641806000
9	-0.406576000	-0.955203000	-1.572679000
9	-0.183612000	-2.101966000	0.285399000
9	-2.466496000	0.306283000	-0.726344000
9	-2.064647000	-0.127245000	1.386888000
9	-2.690462000	-2.489321000	-1.105902000
9	-4.164893000	-1.470364000	0.113485000
9	-2.648387000	-2.688034000	1.054871000
9	1.941051000	0.333568000	-1.603351000
17	-3.410047000	3.186324000	0.316863000

TS2b

At. No.	**X**	**Y**	**Z**
6	-2.733739000	-0.679722000	-0.333873000
6	-1.349875000	-1.003185000	0.311812000
6	-0.227355000	-0.070058000	-0.268841000
6	1.220549000	-0.452745000	0.163892000
6	2.265634000	0.637511000	-0.199245000
6	3.727773000	0.124005000	-0.171619000
6	-1.063398000	-2.525575000	0.164894000
6	-0.693469000	1.806230000	1.266307000
1	-1.730668000	1.601305000	1.550348000

1	-0.028642000	1.356951000	2.017924000
6	-0.443556000	3.272468000	1.172997000
1	-0.675777000	3.856296000	2.060564000
1	0.413841000	3.593640000	0.585638000
1	-1.537944000	3.736890000	0.284705000
8	-0.426959000	1.267740000	-0.037725000
9	-2.922376000	0.629189000	-0.468414000
9	-3.704012000	-1.147758000	0.449990000
9	-2.830358000	-1.255045000	-1.530864000
9	-2.166250000	-3.227193000	0.430021000
9	-0.130032000	-2.891212000	1.041411000
9	-0.655531000	-2.828689000	-1.063016000
9	-0.282148000	-0.225194000	-1.616940000
9	1.252052000	-0.621475000	1.504044000
9	1.602337000	-1.598817000	-0.427475000
9	2.180039000	1.641852000	0.696884000
9	2.027565000	1.119641000	-1.426550000
9	3.965568000	-0.531085000	0.964581000
9	4.549397000	1.168401000	-0.247292000
9	3.964445000	-0.680842000	-1.200399000
9	-1.472220000	-0.768427000	1.653395000
17	-2.685106000	4.118194000	-0.451159000

TS3

At. No.	**X**	**Y**	**Z**
6	3.290295000	0.511603000	0.692238000
6	1.801371000	0.102626000	0.444310000
6	0.851883000	0.821495000	1.466140000
6	-0.617680000	0.302564000	1.473878000
6	-1.572755000	1.205493000	2.302975000
6	-2.890448000	0.496597000	2.707087000
6	1.704318000	-1.449986000	0.445257000
6	0.586896000	2.877037000	0.136860000
1	1.546697000	2.853173000	-0.511808000
1	-0.170749000	2.370021000	-0.469175000
6	0.284969000	4.316338000	0.455344000
1	0.191491000	4.880777000	-0.475329000

1	-0.652856000	4.386467000	1.013241000
1	1.093104000	4.747918000	1.048235000
8	0.847431000	2.195311000	1.347807000
9	3.407734000	1.791207000	1.047451000
9	3.988328000	0.330777000	-0.422662000
9	3.814833000	-0.240141000	1.659422000
9	2.709238000	-1.960809000	-0.266662000
9	0.564166000	-1.828622000	-0.128986000
9	1.760556000	-1.945773000	1.676596000
9	1.362919000	0.557371000	2.695068000
9	-1.081054000	0.263786000	0.207094000
9	-0.667002000	-0.936386000	1.995008000
9	-1.906262000	2.280301000	1.562092000
9	-0.968186000	1.613884000	3.427207000
9	-3.434958000	-0.098912000	1.646403000
9	-3.740336000	1.406991000	3.175647000
9	-2.666788000	-0.407611000	3.652800000
9	1.467833000	0.495214000	-0.819010000
7	3.644355000	3.743135000	-1.069527000
8	4.669227000	3.686982000	-1.702512000
8	2.745356000	2.836721000	-1.472244000
8	3.349395000	4.483531000	-0.166233000

TS4a

At. No.	**X**	**Y**	**Z**
6	2.938464000	1.020400000	0.939344000
6	1.703350000	0.358108000	0.252162000
6	0.361461000	0.904740000	0.859590000
6	-0.918756000	0.154398000	0.381768000
6	-2.231309000	0.880627000	0.784319000
6	-3.483906000	-0.030239000	0.718855000
6	1.860343000	-1.189459000	0.313377000
6	0.287228000	2.911418000	-0.580605000
1	1.341044000	3.023635000	-0.846012000
1	-0.222566000	2.330211000	-1.353254000
6	-0.365561000	4.257115000	-0.381597000
1	-0.306636000	4.810483000	-1.450538000

1	-1.433188000	4.216183000	-0.165205000
1	0.174300000	4.926966000	0.289380000
8	0.182835000	2.256474000	0.700873000
9	2.749943000	2.321890000	1.157903000
9	4.000622000	0.899944000	0.146179000
9	3.198267000	0.426442000	2.101861000
9	3.116145000	-1.533005000	0.022989000
9	1.066030000	-1.756080000	-0.592174000
9	1.561742000	-1.663290000	1.518255000
9	0.454710000	0.696575000	2.199414000
9	-0.897845000	0.057187000	-0.964860000
9	-0.959491000	-1.082769000	0.908601000
9	-2.441017000	1.907367000	-0.063439000
9	-2.137170000	1.352607000	2.035419000
9	-3.516524000	-0.683687000	-0.442147000
9	-4.571714000	0.729498000	0.817799000
9	-3.482457000	-0.906233000	1.716498000
9	1.761164000	0.691591000	-1.072003000
7	-0.850123000	6.581366000	-2.621728000
8	-0.847647000	7.150492000	-3.681432000
8	-0.242134000	5.367619000	-2.691396000
8	-1.300384000	6.937907000	-1.563605000

TS4b

At. No.	**X**	**Y**	**Z**
6	2.693145000	0.876375000	0.445742000
6	1.502942000	0.474437000	-0.479648000
6	0.131763000	0.898324000	0.160160000
6	-1.130938000	0.363962000	-0.580688000
6	-2.446638000	1.012623000	-0.065962000
6	-3.714086000	0.197978000	-0.429107000
6	1.610486000	-1.038426000	-0.828198000
6	0.210096000	3.219848000	-0.680709000
1	1.281739000	3.327322000	-0.869905000
1	-0.284375000	2.911585000	-1.610232000
6	-0.377260000	4.503482000	-0.171974000

1	-0.260243000	5.338583000	-0.863960000
1	-1.394654000	4.411435000	0.211840000
1	0.266874000	4.814909000	0.777654000
8	-0.006421000	2.248804000	0.357117000
9	2.526030000	2.091394000	0.965094000
9	3.817945000	0.898618000	-0.266640000
9	2.826346000	-0.000839000	1.437714000
9	2.872755000	-1.354870000	-1.119591000
9	0.868861000	-1.300108000	-1.903146000
9	1.207030000	-1.802750000	0.181137000
9	0.119483000	0.338909000	1.397959000
9	-1.022815000	0.641341000	-1.898554000
9	-1.242678000	-0.967010000	-0.422526000
9	-2.580851000	2.232071000	-0.625229000
9	-2.414371000	1.140360000	1.267566000
9	-3.694677000	-0.131567000	-1.720228000
9	-4.788629000	0.946003000	-0.190944000
9	-3.790439000	-0.905302000	0.305322000
9	1.675225000	1.145611000	-1.658229000
7	0.973332000	6.436875000	2.114157000
8	0.079200000	7.032337000	1.568454000
8	1.203258000	5.149637000	1.761645000
8	1.735087000	6.819149000	2.964253000

PC1_Cl

At. No.	**X**	**Y**	**Z**
6	2.856194000	0.541209000	0.708479000
6	1.690052000	-0.016040000	-0.169202000
6	0.294415000	0.327412000	0.465899000
6	-0.932981000	-0.337567000	-0.227776000
6	-2.289135000	0.247760000	0.256856000
6	-3.498889000	-0.668975000	-0.057571000
6	1.919248000	-1.535423000	-0.419793000
6	0.141890000	2.564912000	-0.474971000
1	-0.092235000	2.163051000	-1.456218000
6	-0.231357000	3.943240000	-0.072208000

1	-0.041572000	4.635931000	-0.894751000
1	-1.295760000	4.002946000	0.194731000
1	0.352331000	4.257808000	0.798225000
8	0.065952000	1.681360000	0.589928000
9	2.594628000	1.767219000	1.160713000
9	3.962795000	0.608974000	-0.022851000
9	3.072325000	-0.259911000	1.750614000
9	3.196854000	-1.758930000	-0.725943000
9	1.178044000	-1.933304000	-1.452087000
9	1.606787000	-2.260809000	0.649586000
9	0.335349000	-0.154583000	1.732562000
9	-0.849820000	-0.148436000	-1.560630000
9	-0.943922000	-1.657969000	0.027909000
9	-2.506093000	1.424438000	-0.360006000
9	-2.258881000	0.442792000	1.583339000
9	-3.462152000	-1.056733000	-1.331682000
9	-4.621001000	0.013873000	0.154676000
9	-3.494677000	-1.739676000	0.728080000
9	1.792015000	0.584715000	-1.390054000
1	2.159392000	3.130263000	-1.074503000
17	3.163276000	3.739653000	-1.62506100

PC2_Cl

At. No.	**X**	**Y**	**Z**
6	3.030774000	0.515902000	0.097415000
6	1.739779000	-0.180802000	-0.437678000
6	0.454794000	0.475066000	0.181841000
6	-0.875614000	-0.275447000	-0.124675000
6	-2.136232000	0.546742000	0.263851000
6	-3.417943000	-0.316200000	0.387015000
6	1.861741000	-1.716111000	-0.211643000
6	0.339964000	2.341461000	-1.484823000
1	1.381627000	2.385165000	-1.806342000
1	-0.214834000	1.658624000	-2.137156000
6	-0.274828000	3.686837000	-1.435186000
1	0.303680000	4.567405000	-1.675004000
1	-1.304027000	3.794886000	-1.119373000

8	0.302027000	1.806923000	-0.118099000
9	2.882522000	1.836902000	0.189216000
9	4.035348000	0.283448000	-0.744259000
9	3.352322000	0.039874000	1.297822000
9	3.085975000	-2.126857000	-0.546630000
9	0.992240000	-2.354392000	-0.991694000
9	1.638933000	-2.046398000	1.055866000
9	0.632769000	0.420262000	1.530611000
9	-0.946380000	-0.529995000	-1.448418000
9	-0.918826000	-1.441027000	0.545861000
9	-2.366752000	1.466911000	-0.692388000
9	-1.948190000	1.166760000	1.437908000
9	-3.539723000	-1.109789000	-0.676682000
9	-4.474055000	0.490697000	0.447013000
9	-3.384946000	-1.058543000	1.487338000
9	1.723235000	-0.001022000	-1.791794000
1	0.639041000	3.221755000	1.263287000
17	0.950237000	4.329785000	1.846772000

P1

At. No.	**X**	**Y**	**Z**
6	2.918422000	0.523558000	0.482130000
6	1.699989000	-0.091857000	-0.274801000
6	0.344511000	0.378606000	0.366255000
6	-0.915646000	-0.352139000	-0.186990000
6	-2.243971000	0.320165000	0.254415000
6	-3.479943000	-0.601035000	0.090202000
6	1.883764000	-1.635134000	-0.349688000
6	0.247911000	2.517545000	-0.902515000
1	1.310146000	2.674829000	-1.105279000
1	-0.204560000	1.967483000	-1.731061000
6	-0.448450000	3.801410000	-0.651966000
1	-1.502939000	3.903799000	-0.870826000
1	0.049857000	4.584226000	-0.095164000
8	0.137667000	1.730204000	0.328298000
9	2.705204000	1.790061000	0.834992000
9	3.986023000	0.505739000	-0.315179000

9	3.189078000	-0.182463000	1.578701000
9	3.147405000	-1.928903000	-0.665132000
9	1.102874000	-2.134858000	-1.305523000
9	1.591676000	-2.221745000	0.806170000
9	0.436260000	0.043658000	1.683737000
9	-0.879271000	-0.342880000	-1.537285000
9	-0.945719000	-1.630018000	0.237217000
9	-2.459089000	1.411056000	-0.504985000
9	-2.176855000	0.681087000	1.543364000
9	-3.487079000	-1.152623000	-1.123237000
9	-4.583115000	0.129698000	0.236795000
9	-3.480714000	-1.561393000	1.007362000
9	1.765168000	0.355952000	-1.564365000

P2

At. No.	**X**	**Y**	**Z**
6	2.909915000	0.471167000	0.468239000
6	1.683430000	-0.139781000	-0.283366000
6	0.332915000	0.348824000	0.357130000
6	-0.945110000	-0.343721000	-0.203496000
6	-2.258767000	0.357207000	0.241358000
6	-3.514248000	-0.537620000	0.077116000
6	1.841550000	-1.688410000	-0.326492000
6	0.307331000	2.450573000	-0.853018000
1	-0.007907000	1.964670000	-1.770035000
6	0.116044000	3.899257000	-0.610928000
1	0.332694000	4.457821000	-1.523491000
1	-0.915400000	4.125757000	-0.304113000
1	0.784471000	4.245418000	0.183229000
8	0.159592000	1.711195000	0.317954000
9	2.714942000	1.739473000	0.818798000
9	3.974884000	0.430615000	-0.329296000
9	3.170515000	-0.235285000	1.569352000
9	3.101710000	-2.007001000	-0.628290000
9	1.057812000	-2.190391000	-1.279402000
9	1.530975000	-2.252251000	0.835863000
9	0.410972000	0.018679000	1.672364000

9	-0.902874000	-0.328954000	-1.551778000
9	-1.003014000	-1.620411000	0.218976000
9	-2.450459000	1.456609000	-0.508732000
9	-2.177662000	0.709479000	1.533221000
9	-3.530182000	-1.090039000	-1.135749000
9	-4.601379000	0.216100000	0.221809000
9	-3.535356000	-1.496670000	0.995389000
9	1.760343000	0.273579000	-1.580134000

HCl

At. No.	**X**	**Y**	**Z**
1	0.000000000	0.000000000	-1.209002000
17	0.000000000	0.000000000	0.071118000

NO_3

At. No.	**X**	**Y**	**Z**
7	0.000000000	0.000000000	-0.083609000
8	0.000000000	1.085139000	-0.582999000
8	0.000000000	-1.085139000	-0.582999000
8	0.000000000	0.000000000	1.239156000

HNO_3

At. No.	**X**	**Y**	**Z**
1	-1.729298000	0.144014000	0.000231000
7	0.137832000	0.037328000	0.000000000
8	1.070495000	-0.707676000	0.000015000
8	0.114407000	1.246026000	-0.000011000
8	-1.089343000	-0.589014000	-0.000033000