Direct MD simulations of Terahertz Absorption ans 2-D Spectroscopy Applied to Explosive Crystals

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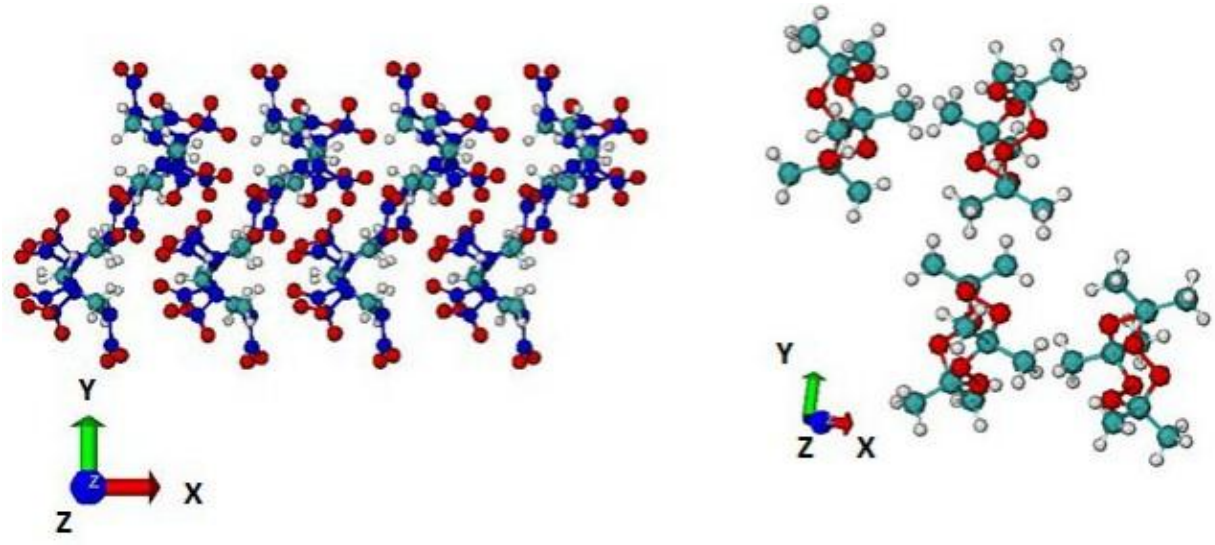

Figure S1: RDX two unit cells crystal(left) and TATP two unit cells(right).

RDX two unit cells :

1	C	0.200082943756700D	0.414542999677426D	0.480922006476816D
2	C	0.437149437566998D	0.290239999677426D	0.320694006476816D
3	C	0.231134943756700D	0.433621999677426D	0.225238006476816D
4	H	0.272439943756700D	0.346466999677426D	0.530547006476816D
5	H	0.185866943756700D	0.492424999677426D	0.558771006476816D
6	H	-0.642760562433002D	0.268813999677426D	0.307454006476816D
7	H	0.894889437566998D	0.189295999677426D	0.312856006476816D
8	H	0.307325943756700D	0.360535999677426D	0.190446006476816D
9	H	0.245537943756700D	0.517268999677426D	0.153980006476816D
10	N	0.275553943756700D	0.469198999677426D	0.363817006476816D
11	N	0.748739437566998D	0.335032999677426D	0.460154006476816D
12	N	0.985569437566998D	0.367170999677426D	0.204369006476816D
13	N	0.300144943756700D	0.618884999677427D	0.379105006476816D
14	N	-0.451780562433002D	0.404335999677426D	0.523591006476816D

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15 N    -0.484605624330024D-01 0.466202999677426D 0.152174006476816D
16 O     0.299983943756700D 0.695439999677427D 0.274596006476816D
17 O     0.338674943756700D 0.664650999677427D 0.494167006476816D
18 O    -0.164434056243300D 0.377490999677427D 0.480654006476816D
19 O    -0.276620562433002D 0.478186999677426D 0.628648006476816D
20 O    -0.129770056243300D 0.431721999677426D 0.150999006476816D
21 O     0.328399437566998D 0.579479999677427D 0.101956006476816D
22 C     0.412014943756700D 0.742202999677427D 0.104671300647682D
23 C     0.599162943756700D 0.898857999677427D 0.971573006476816D
24 C     0.491882943756700D 0.742544999677426D 0.800879006476816D
25 H     0.319649943756700D 0.800232999677426D 0.106838700647682D
26 H     0.403073943756700D 0.658127999677427D 0.111841100647682D
27 H     0.698771943756700D 0.935839999677426D 0.100354700647682D
28 H     0.543415943756700D 0.992992999677427D 0.952078006476816D
29 H     0.428686943756700D 0.802326999677426D 0.731889006476816D
30 H     0.524719943756700D 0.659649999677426D 0.734776006476816D
31 N     0.396042943756700D 0.695103999677426D 0.905472006476816D
32 N     0.526296943756700D 0.831490999677427D 0.108394400647682D
33 N     0.607165943756700D 0.830570999677427D 0.838524006476816D
34 N     0.373150943756700D 0.544496999677426D 0.897676006476816D
35 N     0.624320943756700D 0.758988999677427D 0.117529500647682D
36 N     0.739427943756700D 0.756521999677426D 0.822459006476816D
37 O     0.400337943756700D 0.480948999677427D 0.788034006476816D
38 O     0.309508943756700D 0.484689999677426D 0.993473006476816D
39 O     0.744679943756700D 0.805322999677426D 0.118867300647682D
40 O     0.582125943756700D 0.663049999677426D 0.125151300647682D
41 O     0.835489943756700D 0.775354999677426D 0.907306006476816D
42 O     0.757897943756700D 0.682644999677427D 0.717610006476816D
43 C     0.106937894375670D 0.102171899967743D 0.695680064768158D
44 C     0.127692594375670D 0.879313999677426D 0.105930006476816D
45 C     0.118931094375670D 0.102334599967743D 0.297720006476816D
46 H     0.985465943756700D 0.948644999677427D 0.717910064768158D
47 H     0.103082594375670D 0.109892799967743D 0.322006476815795D-02
48 H     0.137189194375670D 0.848722999677426D 0.573590064768158D
49 H     0.122893294375670D 0.781794999677426D 0.129098006476816D
50 H     0.113646194375670D 0.956384999677427D 0.368628006476816D
51 H     0.122724294375670D 0.110265099967743D 0.365439006476816D
52 N     0.107834894375670D 0.107251499967743D 0.210051006476816D
53 N     0.118447594375670D 0.947132999677427D 0.941000647681580D-01
54 N     0.130114894375670D 0.942099999677426D 0.239764006476816D
55 N     0.106497394375670D 0.122428299967743D 0.217060006476816D
56 N     0.126232394375670D 0.103637999967743D0.864759935231842D
57 N     0.143267494375670D 0.101917799967743D 0.240148006476816D
58 O     0.110063094375670D 0.128614499967743D 0.325255006476816D
59 O     0.100122294375670D 0.128753399967743D 0.123656006476816D
60 O     0.138987894375670D 0.101877799967743D0.100667993523184D
61 O     0.119856694375670D 0.111874199967743D0.163597993523184D
62 O     0.153521294375670D 0.970322999677427D 0.177629006476816D
63 O     0.144459694375670D 0.112583599967743D 0.312586006476816D
64 C     0.875768943756700D 0.144587999677426D 0.614526006476816D
65 C     0.723527943756700D 0.265443999677426D 0.784760006476816D
66 C     0.925845943756700D 0.133629999677426D 0.866318006476816D
67 H     0.947132943756700D 0.205486999677426D 0.554994006476816D
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 85 C     0.109012894375670D 0.738835999677426D 0.599740006476816D
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127 C     0.196521943756700D 0.155803999677426D 0.101944600647682D
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166 O     0.499992943756700D 0.114650199967743D 0.702234006476816D
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168 O     0.765231943756700D 0.113295199967743D 0.245370006476816D
169 C     0.154012294375670D 0.414542941102413D 0.480921947901805D
170 C     0.138375494375670D 0.290239941102413D 0.320693947901805D
171 C     0.157117494375670D 0.433621941102413D 0.225237947901805D
172 H     0.161247994375670D 0.346466941102413D 0.530546947901805D
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174 H     0.127576394375670D 0.268813941102413D 0.307453947901805D
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210 O     0.209793794375670D 0.682644941102413D 0.717609947901805D
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212 C     0.261696594375670D 0.879313941102413D 0.105929947901805D
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214 H     0.232550594375670D 0.948644941102413D 0.717909479018050D
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224 N     0.260236394375670D 0.103637994110241D0.864760520981950D
225 N     0.277271494375670D 0.101917794110241D 0.240147947901805D
226 O     0.244067094375670D 0.128614494110241D 0.325254947901805D
227 O     0.234126294375670D 0.128753394110241D 0.123655947901805D
228 O     0.272991894375670D 0.101877794110241D0.100668052098195D
229 O     0.253860694375670D 0.111874194110241D0.163598052098195D
230 O     0.287525294375670D 0.970322941102413D 0.177628947901805D
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231 O     0.278463694375670D 0.112583594110241D 0.312585947901805D
232 C     0.221580894375670D 0.144587941102413D 0.614525947901805D
233 C     0.206356794375670D 0.265443941102413D 0.784759947901805D
234 C     0.226588594375670D 0.133629941102413D 0.866317947901805D
235 H     0.228717294375670D 0.205486941102413D 0.554993947901805D
236 H     0.218954694375670D 0.647839411024132D 0.541925947901805D
237 H     0.195382794375670D 0.269649941102413D 0.800846947901805D
238 H     0.209228994375670D 0.372350941102413D 0.795214947901805D
239 H     0.233834694375670D 0.216297941102413D 0.882386947901805D
240 H     0.229653094375670D 0.595029411024132D 0.942531947901805D
241 N     0.229655694375670D 0.878869411024132D 0.727095947901805D
242 N     0.209856994375670D 0.233334941102413D 0.642682947901805D
243 N     0.213207194375670D 0.193613941102413D 0.896885947901805D
244 N     0.230622294375670D0.640580588975868D 0.717067947901805D
245 N     0.197518394375670D 0.188954941102413D 0.565086947901805D
246 N     0.203968394375670D 0.919679411024132D 0.963233947901805D
247 O     0.228358994375670D0.138062058897587D 0.820852947901805D
248 O     0.235086294375670D0.116399058897587D 0.607202947901805D
249 O     0.185884494375670D 0.234653941102413D 0.599586947901805D
250 O     0.198951494375670D 0.120146941102413D 0.456224947901805D
251 O     0.191158094375670D 0.111389941102413D 0.962260947901805D
252 O     0.209052494375670D0.604605889758685D-01 0.103099994790180D
253 C     0.243016894375670D 0.738835941102413D 0.599739947901805D
254 C     0.262692694375670D 0.887817941102413D 0.664901947901805D
255 C     0.251990194375670D 0.738425941102413D 0.842044947901805D
256 H     0.234012594375670D 0.802151941102413D 0.583810947901805D
257 H     0.241203894375670D 0.656062941102413D 0.528269947901805D
258 H     0.272631094375670D 0.921302941102413D 0.628787947901805D
259 H     0.257482394375670D 0.983868941102413D 0.685253947901805D
260 H     0.245967694375670D 0.802270941102413D 0.910003947901805D
261 H     0.255132694375670D 0.656630941102413D 0.910139947901805D
262 N     0.241933694375670D 0.691917941102413D 0.741539947901805D
263 N     0.254690594375670D 0.821976941102413D 0.556550947901805D
264 N     0.263691094375670D 0.821589941102413D 0.798887947901805D
265 N     0.239655794375670D 0.541337941102413D 0.749795947901805D
266 N     0.263750994375670D 0.743564941102413D 0.462427947901805D
267 N     0.276742494375670D 0.744037941102413D 0.812612947901805D
268 O     0.243109994375670D 0.476868941102413D 0.856771947901805D
269 O     0.232570294375670D 0.482794941102413D 0.658355947901805D
270 O     0.276140094375670D 0.779292941102413D 0.449283947901805D
271 O     0.258633794375670D 0.654189941102413D 0.383713947901805D
272 O     0.286522394375670D 0.766216941102413D 0.730596947901805D
273 O     0.278279294375670D 0.663654941102413D 0.913049947901805D
274 C     0.223632994375670D 0.416165941102413D 0.467599479018050D
275 C     0.207230894375670D 0.296179941102413D 0.203481947901805D
276 C     0.226287394375670D 0.431457941102413D 0.302874947901805D
277 H     0.230880394375670D 0.342189941102413D 0.670694790180503D-01
278 H     0.223002894375670D 0.489673941102413D0.361580520981950D
279 H     0.196336994375670D 0.278141941102413D 0.214565947901805D
280 H     0.211427894375670D 0.193544941102413D 0.210720947901805D
281 H     0.233503294375670D 0.351285941102413D 0.329512947901805D
282 H     0.228383194375670D 0.508615941102413D 0.379586947901805D
283 N     0.230607794375670D 0.474281941102413D 0.165800947901805D
284 N     0.210764894375670D 0.341768941102413D 0.650789479018050D
```

```
285 N     0.212797994375670D 0.369299941102413D 0.321773947901805D
286 N     0.232111694375670D 0.625703941102413D 0.153663947901805D
287 N     0.199154194375670D 0.417051941102413D 0.106194790180503D-01
288 N     0.202787794375670D 0.471570941102413D 0.374337947901805D
289 O     0.231541894375670D 0.699916941102413D 0.259630947901805D
290 O     0.235763894375670D 0.676136941102413D 0.399509479018050D
291 O     0.187040494375670D 0.390920941102413D 0.389039479018050D
292 O     0.201389994375670D 0.494487941102413D0.100414052098195D
293 O     0.190090394375670D 0.447448941102413D 0.364764947901805D
294 O     0.207041294375670D 0.576662941102413D 0.437030947901805D
295 C     0.153656194375670D 0.155803941102413D 0.1019445947901805D
296 C     0.138213494375670D 0.282790941102413D 0.858154947901805D
297 C     0.156893294375670D 0.137924941102413D 0.764716947901805D
298 H     0.161141794375670D 0.223044941102413D 0.106653294790181D
299 H     0.152079694375670D 0.803919411024131D 0.109939694790180D
300 H     0.127400094375670D 0.303846941102413D 0.845044947901805D
301 H     0.142718194375670D 0.384114941102413D 0.849701947901805D
302 H     0.164563794375670D 0.213369941102413D 0.736920947901805D
303 H     0.158673194375670D 0.581729411024132D 0.690129947901805D
304 N     0.160860794375670D 0.957389411024132D 0.902841947901805D
305 N     0.141424894375670D 0.239463941102413D 0.997963947901805D
306 N     0.143698594375670D 0.205171941102413D 0.742378947901805D
307 N     0.161710994375670D0.559760588975868D 0.915736947901805D
308 N     0.129232594375670D 0.176713941102413D 0.1064433947901805D
309 N     0.133381194375670D 0.106953941102413D 0.687961947901805D
310 O     0.159721694375670D0.131224058897587D 0.812186947901805D
311 O     0.166114294375670D0.106717058897587D 0.102664994790181D
312 O     0.117385794375670D 0.209997941102413D 0.1023832947901805D
313 O     0.130816194375670D 0.102302941102413D 0.1169344947901805D
314 O     0.120776494375670D 0.135770941102413D 0.696439947901805D
315 O     0.137300694375670D 0.190194110241316D-01 0.623055947901805D
316 C     0.172052594375670D 0.103148894110241D 0.474479947901805D
317 C     0.193137494375670D 0.892150941102413D 0.451849947901805D
318 C     0.185027094375670D 0.103014794110241D 0.2522989479018050D
319 H     0.164115194375670D 0.953870941102413D 0.467351947901805D
320 H     0.167370694375670D 0.110705794110241D 0.5402749479018050D
321 H     0.202502894375670D 0.865104941102413D 0.5048929479018050D
322 H     0.188609594375670D 0.792804941102413D 0.4308679479018050D
323 H     0.180000694375670D 0.961254941102413D 0.1814639479018050D
324 H     0.189084794375670D 0.110759194110241D 0.1839829479018050D
325 N     0.173605894375670D 0.108150194110241D 0.3342769479018050D
326 N     0.183483694375670D 0.962419941102413D 0.5423449479018050D
327 N     0.195954894375670D 0.950218941102413D 0.3166529479018050D
328 N     0.172436594375670D 0.123335294110241D 0.3252409479018050D
329 N     0.190773494375670D 0.105825294110241D 0.6357709479018050D
330 N     0.209163094375670D 0.102629694110241D 0.3174809479018050D
331 O     0.175936194375670D 0.129317294110241D 0.2156729479018050D
332 O     0.166294094375670D 0.129873194110241D 0.4187079479018050D
333 O     0.203474694375670D 0.104362694110241D 0.6567599479018050D
334 O     0.184003294375670D 0.114650194110241D 0.7022339479018050D
335 O     0.219251594375670D 0.977708941102413D 0.3828459479018050D
336 O     0.210527194375670D 0.113295194110241D 0.2453699479018050D
```

TATP unitcell:

```
TATP  132

 O     8.587875    -0.480200    11.639984
 O     7.468651     0.475700    11.647903
 O     8.451699     1.545100     9.790223
 O     7.378213     0.975300     8.947859
 O     8.559075    -1.058400     8.952428
 O     7.526053    -1.596500     9.853982
 C     8.116574    -1.707200    11.170802
 C     7.942044     1.693100    11.118547
 C     7.943129    -0.045800     8.161812
 C     6.968553    -2.276400    11.973399
 H     7.241011    -2.398300    12.884806
 H     6.710065    -3.122800    11.599417
 H     6.223914    -1.670900    11.940004
 C     9.346456    -2.587300    11.163764
 H     9.712400    -2.656700    12.048789
 H     9.993292    -2.182000    10.579829
 H     9.127252    -3.462600    10.838173
 C     6.698316     2.575800    11.146763
 H     6.386623     2.659500    12.049731
 H     6.011078     2.179200    10.606478
 H     6.914308     3.445800    10.800185
 C     9.119861     2.272200    11.854393
 H     8.870885     2.415100    12.770196
 H     9.378368     3.108800    11.459295
 H     9.857096     1.659700    11.815240
 C     9.125121     0.421500     7.318351
 H     9.458142    -0.317300     6.802273
 H     9.821988     0.749800     7.891130
 H     8.838913     1.120500     6.726075
 C     6.774972    -0.548500     7.363420
 H     7.069651    -1.258100     6.787446
 H     6.404721     0.160100     6.833153
 H     6.103672    -0.881800     7.962975
 O     2.220352     6.593000    10.341662
 O     3.362979     7.517500    10.338797
 O     2.328914     8.622000     8.519964
 O     3.360903     8.097700     7.629737
 O     2.179975     6.039800     7.635097
 O     3.230064     5.503400     8.500404
 C     2.673566     5.343400     9.788161
 C     2.892746     8.772300     9.798670
 C     2.775730     7.057000     6.835548
 C     1.451188     4.507300     9.841269
 H     1.640547     3.633900     9.492759
 H     0.773481     4.925800     9.305303
 H     1.141531     4.431500    10.746226
 C     3.841768     4.764800    10.578771
 H     4.120559     3.931600    10.193593
 H     3.571522     4.622500    11.488421
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H	4.571630	5.389100	10.555892
C	4.159867	9.607200	9.841075
H	3.980083	10.486200	9.501391
H	4.815257	9.177500	9.285576
H	4.493985	9.671800	10.739433
C	1.761807	9.357800	10.604963
H	1.488433	10.191300	10.212099
H	2.049070	9.508900	11.508643
H	1.022405	8.745000	10.603173
C	1.579893	7.553500	6.013948
H	1.208574	6.843800	5.484230
H	1.875638	8.262000	5.437426
H	0.910744	7.888500	6.613971
C	3.927922	6.581300	6.010453
H	3.626828	5.877800	5.430556
H	4.609949	6.242900	6.595700
H	4.286483	7.298800	5.482811
O	3.157714	-1.648200	8.086905
O	2.110784	-1.095800	8.969074
O	3.297069	0.941100	9.009763
O	2.240590	1.502400	8.144931
O	3.250198	0.430500	6.306314
O	2.126770	-0.512800	6.290756
C	2.587446	-1.745400	6.765516
C	2.723569	-0.087300	9.776498
C	2.775740	1.654400	6.824636
C	3.744927	-2.311000	5.976720
H	4.013055	-3.153700	6.348892
H	4.481217	-1.696200	6.011373
H	3.475805	-2.434800	5.063709
C	1.354408	-2.627200	6.743027
H	1.578858	-3.504800	7.058048
H	1.004355	-2.687500	5.851291
H	0.693646	-2.241000	7.321531
C	1.522459	0.378800	10.606402
H	1.175584	-0.362300	11.107791
H	0.839446	0.718900	10.024923
H	1.804353	1.070000	11.208657
C	3.877950	-0.595900	10.594458
H	3.570475	-1.308700	11.158234
H	4.234312	0.109500	11.138167
H	4.563086	-0.923900	10.008027
C	4.024776	2.524700	6.834285
H	4.358869	2.614500	5.938574
H	4.693979	2.114600	7.385420
H	3.810883	3.392400	7.184506
C	1.623517	2.240200	6.066403
H	1.890615	2.381400	5.155223
H	1.367081	3.077900	6.458749
H	0.879906	1.634400	6.091630
O	-1.982064	6.547300	4.998458
O	-3.098066	7.492800	5.006519
O	-2.018231	8.637500	6.772010
O	-3.065147	8.125800	7.659232

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 O    -1.911884     6.051000     7.686882
 O    -2.985308     5.480700     6.857755
 C    -2.451303     5.306600     5.558627
 C    -2.578951     8.761300     5.491703
 C    -2.488489     7.099700     8.463760
 C    -3.649162     4.754700     4.798903
 H    -3.938624     3.926000     5.189569
 H    -3.399235     4.608400     3.884073
 H    -4.366255     5.391900     4.835456
 C    -1.246940     4.437700     5.494544
 H    -1.461828     3.572200     5.851575
 H    -0.546842     4.835900     6.017418
 H    -0.953298     4.344400     4.585342
 C    -3.809879     9.630200     5.430682
 H    -3.583223    10.514300     5.727475
 H    -4.474785     9.259000     6.014466
 H    -4.156704     9.671800     4.535823
 C    -1.439457     9.271300     4.651322
 H    -1.130929    10.112700     4.993379
 H    -1.728791     9.382500     3.742522
 H    -0.724536     8.632700     4.682909
 C    -3.635417     6.647000     9.311113
 H    -3.343838     5.950800     9.903775
 H    -4.318340     6.307400     8.729588
 H    -3.988633     7.377400     9.825097
 C    -1.283063     7.580400     9.271207
 H    -0.921322     6.874700     9.812037
 H    -1.546894     8.312600     9.834350
 H    -0.617044     7.880100     8.647830
```

ReaxFF-lg force field parameters:

```
Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN)
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.4514 !Overcoordination parameter
   30.0000 !Valency angle conjugation parameter
  216.4305 !Triple bond stabilisation parameter
   12.4838 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0701 !Undercoordination parameter
    7.5000 !Triple bond stabilisation parameter
   11.9083 !Undercoordination parameter
   13.3822 !Undercoordination parameter
  -10.4637 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    3.5895 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
```

```
    0.0283 !Double bond/angle parameter: overcoord
    0.0570 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.8374 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.8820 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1861 !Conjugation
    1.5591 !vdWaals shielding
    0.0100 !Cutoff for bond order (*100)
    5.2216 !Valency angle conjugation parameter
    3.4021 !Overcoordination parameter
   38.5241 !Overcoordination parameter
    2.1533 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    6.5560 !Valency angle conjugation parameter
  7    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
           alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
           cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
           ov/un;val1;n.u.;val3,vval4
 C    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712   1.2385
4.0000
      9.4606   2.1346   4.0000  31.0823  79.5548   5.7254   6.9235
0.0000
      1.2104   0.0000 183.7012   5.7419  33.3951  11.9957   0.8563
0.0000
     -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000   0.0000
0.0000
 H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910  -0.1000
1.0000
      9.3858   5.0013   1.0000   0.0000 121.1250   3.8446  10.0839
1.0000
     -0.1000   0.0000  58.4228   3.8461   3.2540   1.0000   1.0698
0.0000
    -15.7683   2.1504   1.0338   1.0000   2.8793   0.0000   0.0000
0.0000
 O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712   1.1139
6.0000
     10.2186   7.7719   4.0000  29.5271 116.0768   8.5000   7.1412
2.0000
      0.9909  14.9473  69.2812   9.1371   1.6258   0.1863   0.9745
0.0000
     -3.5965   2.5000   1.0493   4.0000   2.9225   0.0000   0.0000
0.0000
 N    1.2450   3.0000  14.0000   1.9951   0.1088   1.0512   1.1911
5.0000
      9.9303   7.8431   4.0000  32.4758 100.0000   6.7768   6.8035
2.0000
      1.0636   0.1045 128.0119   2.1604   2.9464   2.5181   0.9745
0.0000
```

```
     -4.0959   2.0047   1.0183   4.0000   2.8793   0.0000   0.0000
0.0000
 S    1.9647   2.0000  32.0600   2.0783   0.2176   1.0336   1.5386
6.0000
      9.9676   5.0812   4.0000  35.1648 112.1416   6.5000   8.2545
2.0000
      1.4703   9.4922  70.0338   8.5146  28.0801   8.5010   0.9745
0.0000
    -10.0773   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000
0.0000
 Si   2.0276   4.0000  28.0600   2.2042   0.1322   0.8218   1.5758
4.0000
     11.9413   2.0618   4.0000  11.8211 136.4845   1.8038   7.3852
0.0000
     -1.0000   0.0000 126.5331   6.4918   8.5961   0.2368   0.8563
0.0000
     -3.8112   3.1873   1.0338   4.0000   2.5791   0.0000   0.0000
0.0000
 X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000
6.0000
     10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000
0.0000
     -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745
0.0000
    -11.0000   2.7466   1.0338   4.0000   2.8793   0.0000   0.0000
0.0000
 18      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                        pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
  1  1 141.9346 113.4487  67.6027   0.1554  -0.3045   1.0000  30.4515
0.4283
         0.0801  -0.2113   8.5395   1.0000  -0.0933   6.6967   1.0000
0.0000
  1  2 163.6889   0.0000   0.0000  -0.4525   0.0000   1.0000   6.0000
0.5921
        12.1053   1.0000   0.0000   1.0000  -0.0097   8.6351   0.0000
0.0000
  2  2 169.8421   0.0000   0.0000  -0.3591   0.0000   1.0000   6.0000
0.7503
         9.3119   1.0000   0.0000   1.0000  -0.0169   5.9406   0.0000
0.0000
  1  3 164.0476 117.4881  72.1261  -0.6031  -0.1795   1.0000  14.9755
0.5413
         1.2626  -0.3063   7.0000   1.0000  -0.1588   4.5000   0.0000
0.0000
  3  3 110.4748 155.6441  40.0000   0.1150  -0.1054   1.0000  28.5221
0.2000
         0.9590  -0.2635   8.5715   1.0000  -0.1007   6.8548   1.0000
0.0000
  1  4 130.7147 175.2276  97.2523  -0.0368  -0.4942   1.0000  26.7545
0.5133
         0.3296  -0.3653   7.0000   1.0000  -0.1171   5.1025   1.0000
0.0000
  3  4  85.4950 114.0081  70.1453   0.5778  -0.1070   1.0000  16.6611
0.2339
```

```
         0.3474  -0.1948   8.3762   1.0000  -0.1089   5.8148   1.0000
0.0000
  4  4 157.7518  67.1322 160.9732  -0.5869  -0.1824   1.0000  12.0000
0.7136
         0.8204  -0.1657  10.6490   1.0000  -0.0967   4.5976   1.0000
0.0000
  2  3 224.3076   0.0000   0.0000  -0.6280   0.0000   1.0000   6.0000
1.0000
         5.0050   1.0000   0.0000   1.0000  -0.0512   5.1982   0.0000
0.0000
  2  4 212.1772   0.0000   0.0000  -0.3585   0.0000   1.0000   6.0000
0.3316
        10.4316   1.0000   0.0000   1.0000  -0.0658   6.4545   0.0000
0.0000
  1  5 128.7959  56.4134  39.0716   0.0688  -0.4463   1.0000  31.1766
0.4530
         0.1955  -0.3587   6.2148   1.0000  -0.0770   6.6386   1.0000
0.0000
  2  5 128.6090   0.0000   0.0000  -0.5555   0.0000   1.0000   6.0000
0.4721
        10.8735   1.0000   0.0000   1.0000  -0.0242   9.1937   1.0000
0.0000
  3  5   0.0000   0.0000   0.0000   0.5563  -0.4038   1.0000  49.5611
0.6000
         0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145   1.0000
0.0000
  4  5   0.0000   0.0000   0.0000   0.4438  -0.2034   1.0000  40.3399
0.6000
         0.3296  -0.3153   9.1227   1.0000  -0.1805   5.6864   1.0000
0.0000
  5  5  96.1871  93.7006  68.6860   0.0955  -0.4781   1.0000  17.8574
0.6000
         0.2723  -0.2373   9.7875   1.0000  -0.0950   6.4757   1.0000
0.0000
  6  6 109.1904  70.8314  30.0000   0.2765  -0.3000   1.0000  16.0000
0.1583
         0.2804  -0.1994   8.1117   1.0000  -0.0675   8.2993   0.0000
0.0000
  2  6 137.1002   0.0000   0.0000  -0.1902   0.0000   1.0000   6.0000
0.4256
        17.7186   1.0000   0.0000   1.0000  -0.0377   6.4281   0.0000
0.0000
  3  6 191.1743  52.0733  43.3991  -0.2584  -0.3000   1.0000  36.0000
0.8764
         1.0248  -0.3658   4.2151   1.0000  -0.5004   4.2605   1.0000
0.0000
 10    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.0464   1.8296  10.1311   1.0029  -1.0000  -1.0000
  2  3   0.0375   1.7275  10.8037   0.8813  -1.0000  -1.0000
  2  4   0.0509   1.7672  10.4261   0.9990  -1.0000  -1.0000
  1  3   0.1036   1.8869   9.5668   1.3590   1.1099   1.1534
  1  4   0.1971   1.7356  10.0734   1.2754   1.2113   1.1172
  3  4   0.0535   1.6709  10.8180   1.2968   1.1416   1.0167
  2  6   0.0470   1.6738  11.6877   1.1931  -1.0000  -1.0000
```

```
 3  6   0.1263   1.8163  10.6833   1.6266   1.2052  -1.0000
 1  5   0.1408   1.8161   9.9393   1.7986   1.3021   1.4031
 2  5   0.0895   1.6239  10.0104   1.4640  -1.0000  -1.0000
62    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  74.0317  32.2712   0.9501   0.0000   0.1780  10.5736   1.0400
 1  1  2  70.6558  14.3658   5.3224   0.0000   0.0058   0.0000   1.0400
 2  1  2  76.7339  14.4217   3.3631   0.0000   0.0127   0.0000   1.0400
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  65.3104   6.3897   7.5000   0.0000   0.2000  10.0000   1.8525
 3  1  3  71.9855  28.5708   6.4252   0.0000   0.2000   0.0000   1.8525
 1  1  4  65.8892  45.0000   1.6598   0.0000   0.2000  10.0000   1.8525
 3  1  4  73.1057  25.8227   4.2145   0.0000   0.2000   0.0000   1.8525
 4  1  4  65.8759  40.9838   2.4369   0.0000   0.2000   0.0000   1.8525
 2  1  3  56.3039  17.3681   5.3095   0.0000   0.9110   0.0000   1.0400
 2  1  4  71.5505  11.1820   3.7129   0.0000   0.9110   0.0000   1.0400
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  72.3642  37.8942   1.1566   0.0000   0.7472   0.0000   1.2639
 1  3  3  90.0000  45.0000   0.5719   0.0000   0.7472   0.0000   1.2639
 1  3  4  70.4313  14.4055   7.1593   0.0000   0.7472   0.0000   1.2639
 3  3  3  83.8833  23.3345   2.3433 -10.0000   0.7472   0.0000   1.2639
 3  3  4  84.0407  45.0000   1.0695   0.0000   0.7472   0.0000   1.2639
 4  3  4  73.9966  24.4410   5.2760   0.0000   0.7472   0.0000   1.2639
 1  3  2  89.1394  37.0874   0.3849   0.0000   3.0000   0.0000   1.2618
 2  3  3  80.7068   5.0854   5.7151   0.0000   3.0000   0.0000   1.2618
 2  3  4  76.0238  45.0000   0.8637   0.0000   3.0000   0.0000   1.2618
 2  3  2  82.3474  13.5165   3.4896   0.0000   0.3596   0.0000   1.3307
 1  4  1  68.4330  19.3525   2.1625   0.0000   1.7325   0.0000   1.0440
 1  4  3  86.2893  37.5587   1.2660   0.0000   1.7325   0.0000   1.0440
 1  4  4  74.2404  12.0547   7.5000   0.0000   1.7325   0.0000   1.0440
 3  4  3  78.5566  43.8492   1.3351 -26.1471   1.7325  40.0000   1.0440
 3  4  4  77.4239  33.7297   1.7944  -0.9193   1.7325   0.0000   1.0440
 4  4  4  64.9107  17.5558   7.5000   0.0000   1.7325   0.0000   1.0440
 1  4  2  90.0000  32.0540   0.7195   0.0000   0.5355   0.0000   2.5279
 2  4  3  84.1185  45.0000   1.3826   0.0000   0.5355   0.0000   2.5279
 2  4  4  78.7133  24.6250   3.8202   0.0000   0.5355   0.0000   2.5279
 2  4  2  56.3036  14.1532   3.3914   0.0000   0.2000   0.0000   2.1689
 1  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 3  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 3  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 4  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 1  1  5  74.4180  33.4273   1.7018   0.1463   0.5000   0.0000   1.6178
 1  5  1  79.7037  28.2036   1.7073   0.1463   0.5000   0.0000   1.6453
 2  1  5  63.3289  29.4225   2.1326   0.0000   0.5000   0.0000   3.0000
 1  5  2  85.9449  38.3109   1.2492   0.0000   0.5000   0.0000   1.1000
 1  5  5  85.6645  40.0000   2.9274   0.1463   0.5000   0.0000   1.3830
 2  5  2  83.8555   5.1317   0.4377   0.0000   0.5000   0.0000   3.0000
 2  5  5  97.0064  32.1121   2.0242   0.0000   0.5000   0.0000   2.8568
 6  6  6  69.3456  21.7361   1.4283   0.0000  -0.2101   0.0000   1.3241
```

```
  2  6  6  75.6168  21.5317   1.0435   0.0000   2.5179   0.0000   1.0400
  2  6  2  78.3939  20.9772   0.8630   0.0000   2.8421   0.0000   1.0400
  3  6  6  70.3016  15.4081   1.3267   0.0000   2.1459   0.0000   1.0400
  2  6  3  73.8232  16.6592   3.7425   0.0000   0.8613   0.0000   1.0400
  3  6  3  90.0344   7.7656   1.7264   0.0000   0.7689   0.0000   1.0400
  6  3  6  22.1715   3.6615   0.3160   0.0000   4.1125   0.0000   1.0400
  2  3  6  83.7634   5.6693   2.7780   0.0000   1.6982   0.0000   1.0400
  3  3  6  73.4663  25.0761   0.9143   0.0000   2.2466   0.0000   1.0400
  2  2  6   0.0000  47.1300   6.0000   0.0000   1.6371   0.0000   1.0400
  6  2  6   0.0000  31.5209   6.0000   0.0000   1.6371   0.0000   1.0400
  3  2  6   0.0000  31.0427   4.5625   0.0000   1.6371   0.0000   1.0400
  2  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 23    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255   0.0000
0.0000
  1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081   0.0000
0.0000
  2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359   0.0000
0.0000
  0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  1  3  0  -0.0002  85.8794   0.3236  -3.8134  -2.0000   0.0000
0.0000
  0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000
0.0000
  0  3  3  0  -0.9667 116.4743   0.0002  -4.9422   0.0000   0.0000
0.0000
  0  1  4  0  -0.0069 150.0000   0.4891  -7.4921  -2.0000   0.0000
0.0000
  0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000
0.0000
  0  3  4  0   1.6745  56.6301  -0.0008  -4.5064  -2.0000   0.0000
0.0000
  0  4  4  0   1.1253  75.3447   0.0080  -9.0000  -2.0000   0.0000
0.0000
  0  1  1  0   0.0930  18.5962   0.0002  -9.0000  -1.0000   0.0000
0.0000
  4  1  4  4  -2.0000  20.8732  -1.5000  -9.0000  -2.0000   0.0000
0.0000
  0  1  5  0   4.0885  78.7058   0.1174  -2.1639   0.0000   0.0000
0.0000
  0  5  5  0  -0.0170 -56.0786   0.6132  -2.2092   0.0000   0.0000
0.0000
  0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  6  6  0   0.0000   0.0000   0.1200  -2.4426   0.0000   0.0000
0.0000
  0  2  6  0   0.0000   0.0000   0.1200  -2.4847   0.0000   0.0000
0.0000
  0  3  6  0   0.0000   0.0000   0.1200  -2.4703   0.0000   0.0000
0.0000
```

```
  1  1  3  3  -0.0002  21.5452   0.1727  -9.0000  -2.0000   0.0000
0.0000
  1  3  3  1   0.0002  79.3777  -1.5000  -5.2139  -2.0000   0.0000
0.0000
  3  1  3  3  -1.3476  22.4932   1.5000  -9.0000  -2.0000   0.0000
0.0000
  9    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
  3  2  3   2.0000  -5.0000   3.0000   3.0000
  3  2  4   1.7753  -5.0000   3.0000   3.0000
  4  2  3   1.3884  -5.0000   3.0000   3.0000
  4  2  4   1.6953  -4.0695   3.0000   3.0000
  3  2  5   2.6644  -3.0000   3.0000   3.0000
  4  2  5   4.0476  -3.0000   3.0000   3.0000
  5  2  3   2.1126  -4.5790   3.0000   3.0000
  5  2  4   2.2066  -5.7038   3.0000   3.0000
  5  2  5   1.9461  -4.0000   3.0000   3.0000
```

Electric field:

$$A^{\frac{-(t-t_0)^2}{\sigma^2}} \cos(\omega t)$$

Where :

A=0.004 volt/cm^2, $t_0 = 5psec$, σ=$\sqrt{\frac{t_0}{2\log 2}}$