Polymer-oxide interfaces in XHNBR/PA6 blends: Computational insights toward sustainable crosslinking

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1 Figures

XHNBR dimer

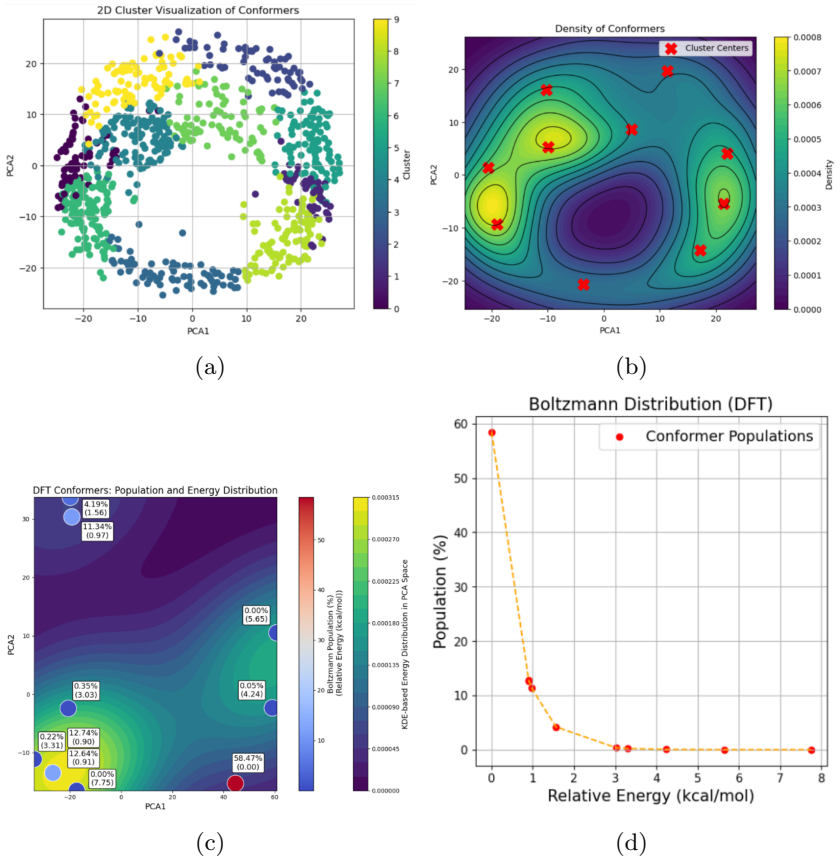

Figure 1: Clustering and Boltzmann-weighted analysis of XHNBR dimer conformers. (a) PCA projection of all sampled conformers colored by cluster. (b) Kernel density map highlighting the most populated regions. (c) Relative DFT energies and cluster centroids. (d) Boltzmann populations of the ten DFT-refined conformers.

PA6 dimer

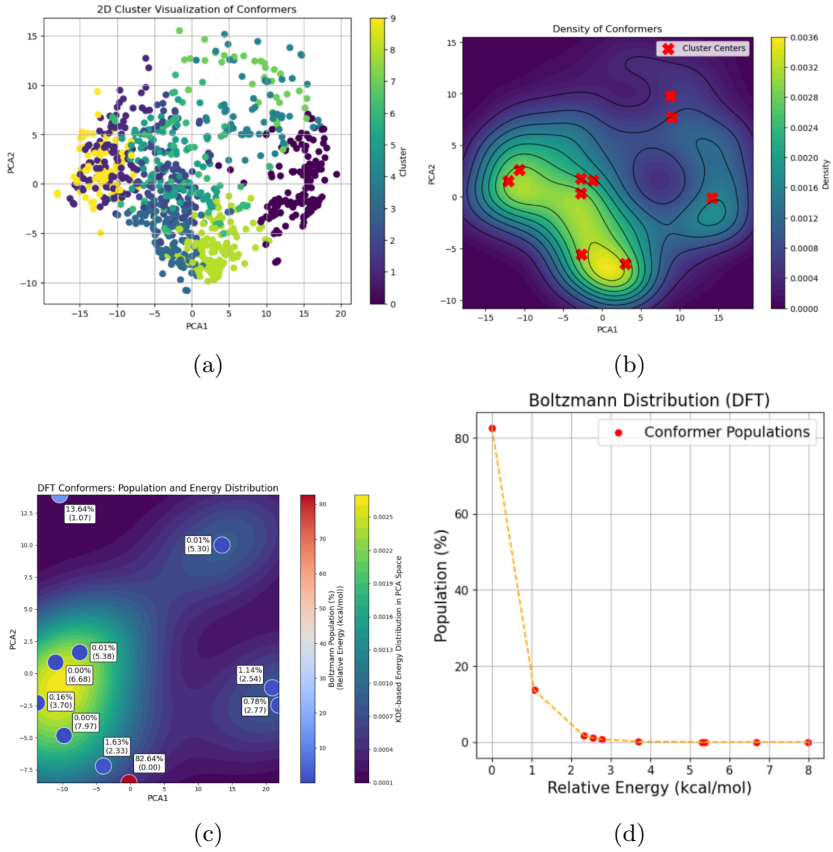

Figure 2: Clustering and Boltzmann-weighted analysis of PA6 dimer conformers. (a) PCA projection of all sampled conformers colored by cluster. (b) Kernel density map highlighting the most populated regions. (c) Relative DFT energies and cluster centroids. (d) Boltzmann populations of the ten DFT-refined conformers.

XHNBR-PA6

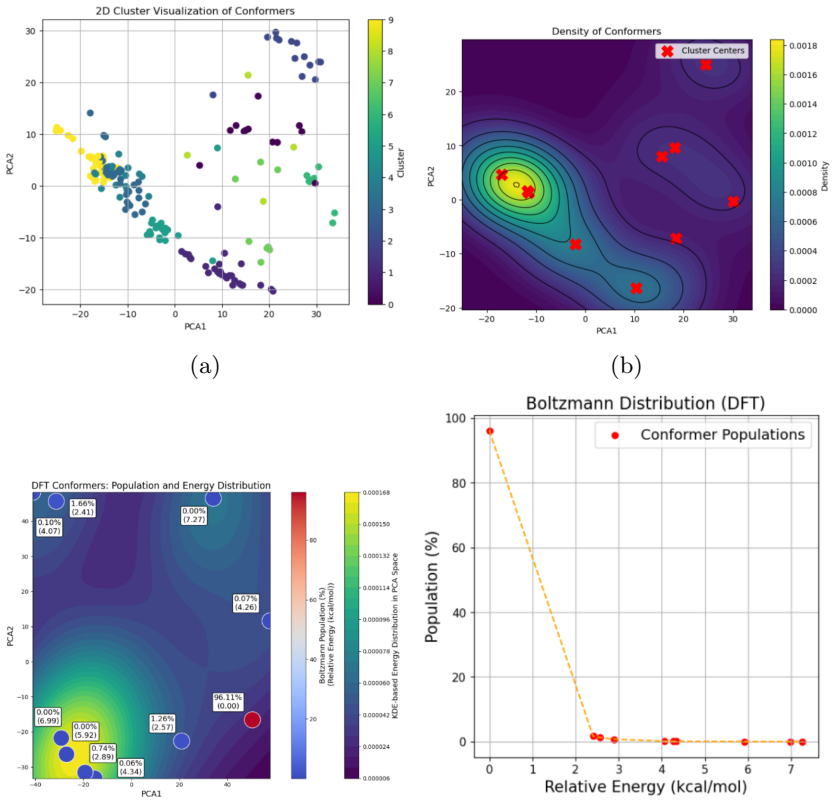

Figure 3: Clustering and Boltzmann-weighted analysis of PA6–XHNBR conformers. (a) PCA projection of all sampled conformers colored by cluster. (b) Kernel density map highlighting the most populated regions. (c) Relative DFT energies and cluster centroids. (d) Boltzmann populations of the ten DFT-refined conformers.

2 Tables

Table 1: Bond distances (R_i), in Å, of the optimized XHNBR monomer/MO structures and interaction energies (ΔH), in kcal/mol.

	Nitrile		Carboxyl					
	R_1	R_2	R_1	R_2	R_3	R_4	R_5	ΔH
$(ZnO)_{12}$	1.157	2.118	1.568	1.013	1.927	1.250	1.284	-58.74
$(MgO)_{12}$	1.156	2.231	2.324	0.962	2.085	1.270	1.267	-72.44
$(CaO)_{12}$	1.158	2.606	2.360	0.964	2.393	1.265	1.266	-81.45
$(MgO_2)_6$	1.153	2.148	0.994	1.790	—	1.362	1.209	-42.91

Table 2: Bond distances (R_i), in Å, of the optimized XHNBR dimer/MO and interaction energies (ΔH), in kcal/mol.

	Nitrile		Carboxyl					
	R_1	R_2	R_1	R_2	R_3	R_4	R_5	ΔH
$(MgO)_{12}$	1.156	2.253	2.538	0.969	2.054	1.263	1.263	-79.15
	1.158	—	0.968	—	—	1.349	1.210	
$(ZnO)_{12}$	1.157	2.118	1.568	1.013	1.927	1.250	1.284	-60.67
	1.158	—	0.950	—	—	1.400	1.220	
$(CaO)_{12}$	1.158	2.589	2.942	0.961	2.408	1.262	1.263	-86.98
	1.159	2.715	0.968	—	—	1.349	1.210	
$(MgO_2)_6$	1.158	—	0.969	—	2.036	1.319	1.228	-35.15
	1.159	—	0.968	—	—	1.350	1.210	

3 Coordinates (xyz coordinates)

3.1 MO Models

$(MgO)_{12}$

```
24

Mg      2.647321      0.000000      1.337261
Mg      2.647321      0.000000     -1.337261
Mg     -2.647321      0.000000      1.337261
Mg     -2.647321      0.000000     -1.337261
Mg      1.336508      2.646581      0.000000
Mg     -1.336508      2.646581      0.000000
Mg      1.336508     -2.646581      0.000000
Mg     -1.336508     -2.646581      0.000000
Mg      0.000000     -1.337426     -2.653076
```

Mg	0.000000	-1.337426	2.653076
Mg	0.000000	1.337426	2.653076
Mg	0.000000	1.337426	-2.653076
O	0.000000	-2.759957	-1.410529
O	0.000000	-2.759957	1.410529
O	0.000000	2.759957	1.410529
O	0.000000	2.759957	-1.410529
O	1.410266	0.000000	-2.764591
O	-1.410266	0.000000	-2.764591
O	1.410266	0.000000	2.764591
O	-1.410266	0.000000	2.764591
O	2.762910	-1.409566	0.000000
O	2.762910	1.409566	0.000000
O	-2.762910	-1.409566	0.000000
O	-2.762910	1.409566	0.000000

$(ZnO)_{12}$

24

Zn	1.685651	1.095923	2.086858
Zn	-0.762823	0.259925	2.782841
Zn	0.762435	-0.260189	-2.782981
Zn	-1.685979	-1.095622	-2.086632
Zn	1.176790	-1.991638	1.745585
Zn	0.695649	-2.699002	-0.793448
Zn	-0.695793	2.699321	0.794235
Zn	-1.176263	1.992424	-1.745117
Zn	-2.837002	0.421159	0.420445
Zn	1.860777	2.024756	-0.915644
Zn	2.837120	-0.421519	-0.421525
Zn	-1.860350	-2.025132	0.914850
O	-2.290031	2.104074	-0.151522
O	0.262824	2.975446	-0.877575
O	2.290027	-2.103795	0.152163
O	-0.262310	-2.975775	0.878648
O	-2.291837	-0.500468	2.046348
O	-2.794644	-1.236772	-0.600096
O	2.793963	1.235875	0.599884
O	2.291975	0.499905	-2.047318
O	-0.009126	2.008676	2.378619
O	1.008465	-0.540093	2.896127
O	-1.008748	0.540244	-2.895219
O	0.008649	-2.008840	-2.378061

$(CaO)_{12}$

24

Ca	3.161890	-0.000000	1.619218
Ca	3.161890	-0.000000	-1.619218
Ca	-3.161890	0.000000	1.619218
Ca	-3.161890	0.000000	-1.619218
Ca	1.618437	3.161043	-0.000000
Ca	-1.618437	3.161043	0.000000
Ca	1.618437	-3.161043	-0.000000
Ca	-1.618437	-3.161043	0.000000
Ca	-0.000000	-1.619594	-3.167840
Ca	0.000000	-1.619594	3.167840
Ca	0.000000	1.619594	3.167840
Ca	-0.000000	1.619594	-3.167840
O	-0.000000	-3.189987	-1.594993
O	-0.000000	-3.189987	1.594993
O	0.000000	3.189987	1.594993
O	0.000000	3.189987	-1.594993
O	1.593692	-0.000000	-3.194797
O	-1.593692	0.000000	-3.194797
O	1.593692	-0.000000	3.194797
O	-1.593692	0.000000	3.194797
O	3.193336	-1.593947	-0.000000
O	3.193336	1.593947	-0.000000
O	-3.193336	-1.593947	0.000000
O	-3.193336	1.593947	0.000000

$(\mathbf{MgO}_2)_6$

18

O	-0.201779	0.238546	0.389966
Mg	-0.728047	2.226111	-0.096709
Mg	-1.273652	-1.057505	1.668526
O	-0.449278	1.370957	-2.086520
Mg	-1.274775	-0.433945	-1.416333
O	-2.164429	-1.618852	-0.050178
Mg	0.760766	-2.166803	-0.052143
O	1.492390	-1.586200	1.721013
Mg	1.269139	0.395429	1.774788
O	0.347751	-1.529372	-1.876493
Mg	1.393415	1.014466	-1.209731
O	1.205366	2.660894	-0.043008
O	0.445066	-1.148498	2.715426
O	1.625730	-0.913613	-1.379935
O	2.149141	1.673653	0.566314

```
O    -0.918878     1.000589     1.483466
O    -1.128076    -2.584679     0.470377
O    -1.842977     1.494513    -1.501638
```

3.2 XHNBR Models

Carboxyl fragment

```
      16

C     1.248157    -0.316495     0.024403
C     1.247803    -1.645630     0.192790
C     2.543998     0.421721    -0.210327
H     2.179155    -2.202145     0.147554
H     0.344335    -2.214941     0.370764
C     0.019568     0.513210     0.120746
C     0.049694     1.847807     0.257646
C    -1.363372    -0.072736     0.064905
H    -0.873586     2.408306     0.351723
H     0.979962     2.403030     0.284534
H     2.486874     1.046637    -1.108124
H     2.789375     1.077031     0.633176
H     3.369285    -0.282549    -0.333873
O    -1.463847    -1.182534    -0.690200
O    -2.334054     0.418294     0.598305
H    -2.398240    -1.433746    -0.680206
```

Nitrile fragment

```
      6

N     4.411328     2.532256    -1.266477
C     4.606513     3.392771    -0.517241
C     4.852487     4.478515     0.427994
H     4.318250     4.287376     1.361230
H     5.921509     4.553477     0.638691
H     4.505558     5.424494     0.006548
```

XHNBR monomer

```
      42

N     6.614393     2.086251     1.155237
C     7.610908     2.244464     1.724740
C     8.874911     2.428178     2.456441
C     9.892859     1.359663     2.030250
```

```
H      9.255391      3.416826      2.168523
C      8.627290      2.424305      3.976397
H     10.843775      1.538133      2.540152
H      9.538482      0.360680      2.299933
H     10.067183      1.383679      0.951909
H      9.603973      2.536441      4.463901
C      7.681708      3.522263      4.460274
H      8.239331      1.440362      4.268946
C      7.498942      3.515225      5.977942
H      8.069497      4.501008      4.144879
H      6.703954      3.404678      3.975954
C      6.548052      4.605500      6.472136
H      7.120066      2.533260      6.292981
H      8.476789      3.638982      6.464849
C      6.395971      4.611144      7.993263
H      6.918082      5.580139      6.127696
H      5.562536      4.466665      6.006401
C      5.310246      5.554578      8.536235
H      6.156258      3.592439      8.327086
H      7.364722      4.856788      8.451790
C      5.248154      5.410779     10.067377
C      5.482013      7.011211      8.066907
H      4.349311      5.203447      8.136728
H      4.623922      7.602570      8.409283
C      6.775051      7.692660      8.517872
H      5.424741      7.035718      6.972844
H      6.821985      8.720080      8.144631
H      6.853369      7.735866      9.609694
H      7.659552      7.165670      8.144373
C      4.217542      6.292096     10.771811
H      5.034810      4.363316     10.306829
H      6.232166      5.634888     10.497645
H      4.269042      6.130383     11.856148
H      4.406592      7.358476     10.619780
C      2.793798      5.990312     10.374740
O      1.968948      7.029969     10.616481
O      2.389789      4.944703      9.919019
H      1.076302      6.745994     10.373863
```

XHNBR dimer

```
     82

C     12.185935     -0.364526     -0.771129
C     10.930567     -0.164373      0.091133
```

C	10.985912	1.139235	0.772536
N	11.027850	2.172923	1.294139
C	9.633293	-0.291006	-0.729082
C	8.355098	-0.185128	0.100866
C	7.090472	-0.346203	-0.742590
C	5.805530	-0.245298	0.079587
C	4.547467	-0.430503	-0.768647
C	3.222079	-0.158611	-0.037723
C	2.064487	-0.334553	-1.034579
C	0.653059	-0.095138	-0.466967
C	-0.393774	-0.270206	-1.577532
C	-1.886817	-0.218895	-1.169808
C	-2.296908	1.160696	-0.863398
N	-2.596566	2.264366	-0.679697
C	3.048301	-0.991477	1.246508
C	2.981987	-2.504492	1.033028
C	0.576921	1.266423	0.195065
O	0.399620	1.456869	1.377244
C	-2.292766	-1.264173	-0.097443
C	-2.182090	-0.898800	1.391731
C	-3.274392	0.009598	1.982071
C	-4.721947	-0.454809	1.739113
C	-5.386647	0.179979	0.513220
C	-6.878853	-0.144490	0.343186
C	-7.166811	-1.654427	0.248985
C	-6.525939	-2.366982	-0.943251
C	-7.423287	0.655447	-0.854223
C	-8.892370	0.416148	-1.199894
C	-9.847141	0.802699	-0.098070
O	-9.622683	1.583790	0.798077
O	-11.043783	0.191670	-0.228442
H	10.917718	-0.924885	0.882623
H	12.158465	-1.356697	-1.230382
H	12.229763	0.383820	-1.567586
H	13.096506	-0.284071	-0.172715
H	9.664356	-1.262928	-1.237516
H	9.635161	0.476256	-1.513653
H	8.368277	-0.952031	0.887799
H	8.328790	0.785176	0.612937
H	7.079897	0.420555	-1.529424
H	7.115300	-1.316733	-1.258345
H	5.835557	-0.999361	0.876595
H	5.769533	0.732142	0.580366
H	4.603731	0.243764	-1.634266
H	4.538400	-1.448987	-1.182512
H	3.238746	0.896694	0.273236

```
H     2.146502    -0.655073     1.769830
H     3.875435    -0.759638     1.926357
H     2.872759    -3.023152     1.989986
H     2.129251    -2.791665     0.407381
H     3.888350    -2.887639     0.551839
H     2.221739     0.343892    -1.881916
H     2.087242    -1.352970    -1.443911
H     0.462671    -0.822652     0.325691
H    -0.213571     0.470588    -2.363557
H    -0.229551    -1.257389    -2.024996
H    -2.442363    -0.468372    -2.082868
H    -1.664723    -2.142669    -0.290841
H    -3.317546    -1.587867    -0.302950
H    -2.208101    -1.849408     1.940490
H    -1.210349    -0.445262     1.609691
H    -3.085914     0.050046     3.060730
H    -3.152736     1.035846     1.623779
H    -5.332424    -0.204856     2.616083
H    -4.742977    -1.551223     1.663515
H    -5.277220     1.269002     0.587828
H    -4.849917    -0.098308    -0.403644
H    -7.395369     0.221350     1.240737
H    -8.251943    -1.813008     0.220800
H    -6.833618    -2.134758     1.175775
H    -6.789758    -3.428885    -0.949395
H    -6.853394    -1.940024    -1.897565
H    -5.432936    -2.301200    -0.910915
H    -7.278056     1.721358    -0.649486
H    -6.828548     0.428884    -1.748078
H    -9.173207     1.023962    -2.069574
H    -9.090254    -0.621171    -1.485265
H   -11.607310     0.519232     0.486633
O     0.753890     2.270425    -0.680961
H     0.614110     3.100473    -0.203950
```

3.3 PA6 Models

Amide fragment

```
      12

C    -0.005894    -0.020664    -0.095634
N     1.231235     0.729069    -0.197517
H    -0.184012    -0.335124     0.936678
H     0.032831    -0.917687    -0.720205
```

H	-0.830410	0.612898	-0.426303
C	2.421552	0.170241	0.153049
H	1.207864	1.677464	-0.532351
O	2.495824	-0.979942	0.565522
C	3.646598	1.049809	0.004325
H	3.427003	2.051400	-0.375171
H	4.347980	0.556934	-0.672945
H	4.133019	1.135632	0.978794

PA6 dimer

50

C	-0.357837	-0.132784	-1.102229
C	0.624191	0.655105	-0.234386
C	2.026143	0.048001	-0.250101
H	0.237433	0.675619	0.791078
H	0.666201	1.695087	-0.585446
C	3.022760	0.823806	0.611226
H	2.399491	0.006360	-1.283073
H	1.973930	-0.991027	0.102768
C	4.424721	0.216686	0.595481
H	2.649440	0.864801	1.644168
H	3.074865	1.863086	0.258965
C	5.405608	1.001328	1.467522
H	4.812772	0.199056	-0.429637
H	4.381939	-0.824352	0.943140
N	-1.705853	0.408886	-1.077080
H	-0.414541	-1.166904	-0.750091
H	-0.020091	-0.151545	-2.144070
N	6.752982	0.458223	1.443709
H	5.065672	1.017197	2.508641
H	5.464154	2.036513	1.118826
C	7.634440	0.759563	0.450355
H	6.999719	-0.258070	2.107832
O	7.369317	1.565806	-0.434021
C	8.966005	0.027176	0.501265
C	10.143736	0.954155	0.199574
H	8.920955	-0.765997	-0.256326
H	9.108931	-0.466149	1.470341
C	11.470214	0.200642	0.131851
H	10.199679	1.730329	0.974054
H	9.943607	1.470924	-0.745139
C	12.649109	1.127772	-0.165768
H	11.414833	-0.574227	-0.644079

```
 H    11.669181    -0.317955     1.075826
 C    13.978803     0.392138    -0.116831
 H    12.694424     1.917703     0.594908
 H    12.507272     1.625533    -1.132870
 O    14.251685    -0.408399     0.769709
 C    -2.583856     0.104234    -0.080441
 H    -1.955457     1.120519    -1.744590
 C    -3.929622     0.798219    -0.141969
 H    -4.041987     1.418610     0.750740
 H    -4.712991     0.037619    -0.116438
 H    -4.063842     1.422019    -1.029738
 O    -2.309161    -0.688082     0.812049
 N    14.861603     0.685752    -1.108916
 C    16.182220     0.087600    -1.140850
 H    16.702469     0.428605    -2.037285
 H    16.107766    -1.003042    -1.160263
 H    16.761732     0.371087    -0.257085
 H    14.605377     1.356263    -1.814296
```

3.4 MO-XHNBR Models

MgO-Nitrile

```
       30

 O    -1.867917     1.412303     1.305610
Mg    -2.554044    -0.002967     0.099233
 O    -1.977305    -0.000548    -1.730493
Mg    -0.689999    -1.327186    -2.297338
 O    -0.083018    -2.780937    -1.253427
Mg     1.756997    -2.651653    -0.644459
 O     3.015126    -1.407713    -1.312456
Mg     3.545062     0.002850    -0.080478
 O     3.138007     0.000510     1.764219
Mg     1.835153    -1.336767     2.321696
 O     1.250388    -2.762209     1.230508
Mg    -0.599882    -2.633539     0.620163
 O    -1.865824    -1.420229     1.302100
Mg    -1.113728    -0.004703     2.383995
 O     0.645520    -0.003699     3.086462
Mg     1.832161     1.333735     2.324767
 O     1.245168     2.760856     1.237006
Mg     1.751918     2.655169    -0.638158
 O     3.012556     1.415412    -1.309082
Mg     2.267697     0.004533    -2.425949
```

O	0.500581	0.003685	-3.083857
Mg	-0.692995	1.330253	-2.294411
O	-0.088378	2.782462	-1.246898
Mg	-0.604826	2.630030	0.626422
N	-4.763313	-0.001766	0.089017
C	-5.913574	-0.002691	0.025611
C	-7.367155	-0.003932	-0.059834
H	-7.780041	-0.650036	0.717576
H	-7.742979	1.012163	0.077149
H	-7.675421	-0.374077	-1.039858

ZnO-Nitrile

30

O	0.223586	-2.742935	-1.316932
Zn	0.230778	-1.300459	-2.487701
O	-1.210897	-0.028041	-2.811124
Zn	0.108695	1.371801	-2.493038
O	1.574109	0.099607	-2.602311
Zn	2.611564	0.150090	-1.051081
O	2.729137	1.567024	0.259425
Zn	1.226484	2.638069	0.161032
O	-0.030268	2.812198	-1.327943
Zn	-1.445555	2.540024	-0.020007
O	-0.215817	2.833363	1.455568
Zn	-0.166363	1.358600	2.590896
Zn	-0.045304	-1.292377	2.596254
Zn	-1.210898	-2.595727	-0.009884
Zn	-2.467790	-0.082757	-1.441400
O	-2.832891	1.302953	-0.123931
Zn	-2.623013	-0.084554	1.229319
O	-2.705261	-1.490767	-0.118402
Zn	1.458925	-2.449042	0.171166
O	0.040163	-2.769899	1.466656
O	2.857614	-1.245032	0.264992
Zn	2.720852	0.160448	1.673445
O	1.253536	0.095811	2.893617
O	-1.535796	-0.031923	2.729430
N	4.537662	0.245800	2.709072
C	5.543810	0.293721	3.265342
C	6.817633	0.354580	3.966528
H	6.640253	0.413910	5.042290
H	7.399975	-0.541725	3.743233
H	7.371390	1.237371	3.640376

CaO-Nitrile

30

C	3.005908	-7.486381	-0.747103
C	2.502397	-6.128967	-0.583421
N	2.103346	-5.053520	-0.454162
Ca	1.169786	-2.647793	-0.176017
O	-0.481749	-2.218962	-1.719553
O	2.855639	-1.172471	-0.042045
Ca	-0.320052	-0.488645	-3.095778
Ca	3.032999	0.229349	1.726936
O	1.526174	0.269983	3.361399
Ca	2.988417	0.570199	-1.481388
O	1.441577	0.948322	-3.033057
O	3.236520	1.980592	0.287459
Ca	1.858636	3.710166	0.489088
Ca	-0.237566	-1.152953	3.168024
O	-0.440535	-2.556648	1.464326
Ca	0.123351	2.046210	3.524545
O	0.276233	3.765132	2.121019
Ca	0.039989	2.715502	-2.783186
O	0.234213	4.100772	-1.053685
O	-1.726954	1.295281	-2.930825
Ca	-3.263967	1.299103	-1.326300
O	-3.452370	-0.442176	0.118641
Ca	-2.042197	-2.155085	-0.082481
Ca	-3.222159	0.957466	1.891675
O	-1.643199	0.621939	3.418428
O	-3.101559	2.711147	0.448893
Ca	-1.355056	4.080565	0.570879
H	2.709169	-8.094120	0.110249
H	2.593183	-7.923560	-1.658703
H	4.095526	-7.468452	-0.816778

MgO_2-Nitrile

24

O	-0.201907	0.259097	0.401925
O	-0.751929	1.031400	1.581356
Mg	-1.217760	-1.033559	1.684371
O	-1.366747	-2.507382	0.427488
Mg	0.536250	-2.364956	-0.283365
O	1.360898	-0.987770	-1.566278
Mg	1.303470	0.935121	-1.311651

O	2.290089	1.462039	0.395205
O	1.386715	2.552375	-0.088587
Mg	-0.581816	2.285976	0.024304
O	-1.890636	1.704785	-1.288639
Mg	-1.463311	-0.265798	-1.296986
O	-0.004993	-1.449564	-1.980131
Mg	1.411304	0.180839	1.605159
O	0.541641	-1.300631	2.598959
O	1.423088	-1.793165	1.474765
O	-2.359632	-1.426597	0.073574
O	-0.562469	1.520047	-1.996059
N	1.255450	-4.354206	-0.651826
C	1.601558	-5.435550	-0.840636
C	2.038431	-6.802345	-1.079649
H	1.175583	-7.470760	-1.045603
H	2.510137	-6.867734	-2.062267
H	2.755967	-7.095630	-0.310582

MgO-Carboxyl

40

O	-0.420925	-2.996428	-1.044152
Mg	-0.441049	-1.738075	-2.458659
O	-1.754164	-0.307918	-2.601243
Mg	-0.228676	0.884678	-2.834613
O	1.040509	-0.574636	-2.854374
Mg	2.686869	-0.470096	-1.907235
O	2.819388	1.003112	-0.611996
Mg	1.520326	2.376327	-0.632996
O	0.023578	2.483868	-1.863758
Mg	-1.114359	2.693332	-0.304062
O	-2.621514	1.609251	0.054449
Mg	-2.803042	0.029304	-1.069976
O	-2.860993	-1.169927	0.466399
Mg	-1.567144	-2.539490	0.466565
O	-0.057975	-2.594512	1.709993
Mg	0.192781	-1.035530	2.745050
O	-1.062507	0.441868	2.825188
Mg	0.425089	1.596133	2.335937
O	1.715325	0.134645	2.456325
Mg	2.779247	-0.104187	0.929260
O	2.677062	-1.825136	-0.108881
Mg	1.060776	-2.863165	0.167075
O	0.408655	2.821289	0.905217

Mg	-2.468016	0.390981	1.560229
O	4.406879	-1.202787	-2.564386
C	5.202290	-2.037674	-2.024905
O	4.962245	-2.652880	-0.957705
H	3.559908	-2.244554	-0.363227
C	6.500793	-2.338414	-2.746690
C	7.221931	-1.288711	-3.511188
C	6.945257	-3.601417	-2.662557
C	8.387561	-1.740051	-4.358703
C	6.912263	0.013121	-3.432758
H	6.406943	-4.327192	-2.063565
H	7.841150	-3.937700	-3.172749
H	7.494352	0.747559	-3.982647
H	6.079508	0.376263	-2.844073
H	8.818242	-0.895186	-4.900951
H	9.180445	-2.184717	-3.746287
H	8.076021	-2.493997	-5.090225

ZnO-Carboxyl

40

O	-0.424708	-3.030734	-1.000647
Zn	-0.383722	-1.725008	-2.334072
O	-1.718755	-0.318681	-2.581334
Zn	-0.204046	0.897734	-2.751228
O	1.041656	-0.565754	-2.874820
Zn	2.701242	-0.466526	-1.988393
O	2.867596	0.985045	-0.663170
Zn	1.537662	2.288504	-0.650269
O	0.039709	2.513740	-1.858086
Zn	-1.096518	2.609374	-0.284628
O	-2.614590	1.598412	0.089981
Zn	-2.702239	0.017626	-1.046387
O	-2.865834	-1.153740	0.505490
Zn	-1.558550	-2.468269	0.485612
O	-0.062877	-2.642501	1.733396
Zn	0.223429	-1.056542	2.660535
O	-0.997792	0.441320	2.860636
Zn	0.451918	1.584419	2.255920
O	1.746476	0.131446	2.446767
Zn	2.702439	-0.084406	0.881453
O	2.647656	-1.836897	-0.092369
Zn	1.070574	-2.833963	0.183255
O	0.451776	2.828416	0.880612

Zn	-2.354915	0.384637	1.584740
O	4.376219	-1.154068	-2.652840
C	5.138175	-2.006447	-2.080246
O	4.859029	-2.614585	-1.022267
H	3.532560	-2.250199	-0.388541
C	6.443820	-2.324715	-2.772384
C	7.205802	-1.279681	-3.502428
C	6.856115	-3.598596	-2.690490
C	8.381267	-1.746451	-4.326962
C	6.923615	0.027270	-3.410064
H	6.286342	-4.320667	-2.116809
H	7.757467	-3.948099	-3.181289
H	7.535252	0.756521	-3.933599
H	6.087808	0.403600	-2.834083
H	8.842752	-0.904906	-4.848230
H	9.149452	-2.214462	-3.700716
H	8.071769	-2.484812	-5.074920

CaO-Carboxyl

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C	6.551070	-2.760228	-2.635150
C	5.876273	-1.691857	-2.192953
C	6.418785	-0.312772	-2.193057
C	5.651786	0.738728	-1.864137
C	4.477115	-1.880674	-1.648383
O	4.346834	-1.898578	-0.392368
O	3.532349	-2.003332	-2.476938
Ca	1.510193	-0.738444	-2.296627
C	7.858757	-0.134389	-2.605162
O	-0.534842	-0.199834	-3.017010
O	1.357135	-2.277107	-0.343435
Ca	-0.664561	-2.882515	0.501263
Ca	2.766777	-0.584535	0.822819
O	1.776783	0.080840	2.711111
O	2.460839	0.797263	-0.937501
Ca	1.782603	2.894953	-0.771802
Ca	-2.528911	-0.949627	-2.240791
O	-2.587160	-2.285692	-0.460593
Ca	-0.173580	-0.662953	3.596278
O	-1.401964	-2.141199	2.472453
Ca	1.046308	2.237194	2.897673
O	1.031423	3.684429	1.215346
Ca	-1.266958	1.955979	-2.832061

O	-0.162937	3.539837	-1.737609
O	-3.264626	1.184259	-2.068523
Ca	-4.023159	1.969672	-0.130437
O	-4.066270	0.624305	1.702779
Ca	-3.368317	-1.467546	1.523958
Ca	-2.812023	2.117496	2.873550
O	-0.895432	1.472877	3.800429
O	-2.851190	3.497964	1.071875
Ca	-0.939769	4.290319	0.261167
H	2.120167	-2.800590	-0.617071
H	6.099078	-3.747088	-2.629541
H	7.565028	-2.688215	-3.014981
H	6.080527	1.739153	-1.888783
H	4.598084	0.664760	-1.575690
H	8.150751	0.916744	-2.542962
H	8.529008	-0.716380	-1.962656
H	8.020889	-0.470421	-3.635797

MgO_2-Carboxyl

34

C	6.191983	-3.313561	-3.582726
C	6.138044	-2.066054	-3.088281
C	7.171249	-1.037733	-3.374303
C	7.246197	0.129076	-2.719841
C	4.939014	-1.742607	-2.252231
O	4.404946	-2.736503	-1.621913
O	4.477475	-0.583254	-2.198767
C	8.197932	-1.391745	-4.422634
O	2.419771	-1.796974	-0.503793
Mg	2.827041	0.104242	-1.288523
O	3.025982	1.215363	0.422043
O	2.467606	2.037182	-0.694428
Mg	0.586263	1.733122	-1.180582
O	-0.218388	0.658748	-2.573871
Mg	-0.137884	-1.103243	-1.590108
O	1.238533	-2.503622	-1.080929
Mg	0.995162	-2.374990	0.870273
O	-0.990216	-2.354552	0.873424
O	-1.601256	-1.593201	-0.275561
Mg	-1.101973	-0.462532	1.336121
O	-0.360431	1.294297	0.546045
O	0.482548	0.117587	0.097722
Mg	1.641159	0.600892	1.657611

O	0.286154	-0.308957	2.808094
O	1.421623	-1.224942	2.426490
O	1.194132	0.112407	-2.566447
H	3.523859	-2.421325	-1.116204
H	5.425011	-4.039668	-3.340982
H	6.992623	-3.633708	-4.239189
H	8.043259	0.829810	-2.949780
H	6.533247	0.427312	-1.962416
H	8.878068	-0.554051	-4.588893
H	8.800724	-2.255472	-4.119160
H	7.721249	-1.640121	-5.377337

MgO-XHNBR monomer

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C	4.162207	6.079684	-0.605590
C	3.954526	4.783323	0.190687
C	4.343591	3.518421	-0.606322
C	4.246365	2.226927	0.203969
C	4.355694	0.979195	-0.669326
C	4.210265	-0.314968	0.134963
C	3.968297	-1.552141	-0.737733
C	3.428336	-2.767759	0.031854
C	4.319173	-3.181887	1.217777
C	5.778175	-3.484375	0.869679
C	2.550879	4.643908	0.595068
N	1.440909	4.457842	0.857225
Mg	-0.048797	2.818246	0.589180
O	-0.695334	2.032078	2.285144
Mg	-0.454867	0.190903	2.596490
O	-1.831728	-1.187313	2.728882
Mg	-3.534173	-0.555393	2.199224
O	-4.585143	-1.115690	0.639999
Mg	-3.593512	-2.089737	-0.600765
O	-1.979721	-2.922826	0.131458
Mg	-0.672379	-2.335481	1.611214
O	0.700131	-0.949761	1.559419
Mg	1.153154	-0.175484	-0.090331
O	0.368597	-0.836891	-1.731108
Mg	-0.920145	-2.226879	-1.697069
O	-2.732006	-1.637293	-2.242698
Mg	-2.985205	0.214189	-2.627682
O	-4.122156	1.353997	-1.522769
Mg	-4.706218	0.764766	0.173916

O	-3.949727	1.324553	1.863342
Mg	-2.475336	2.500736	1.716937
O	-1.891325	3.336230	0.073291
Mg	-2.627301	2.617136	-1.501356
O	-1.641330	1.590561	-2.828147
Mg	0.026875	1.015180	-2.161724
O	0.961465	1.688941	-0.607026
C	3.141612	-3.925881	-0.939528
C	2.117982	-4.945793	-0.407129
C	0.780249	-4.256528	-0.224629
O	0.157017	-3.930936	-1.282398
O	0.388630	-4.005616	0.953703
H	4.544007	4.822886	1.115396
H	5.219956	6.174204	-0.864132
H	3.581208	6.060243	-1.531702
H	3.867187	6.958815	-0.027785
H	5.365254	3.666901	-0.976221
H	3.686508	3.448089	-1.481400
H	5.015538	2.217285	0.988399
H	3.267232	2.189755	0.697171
H	3.553880	1.032956	-1.418203
H	5.306303	0.968116	-1.219553
H	5.097431	-0.461120	0.763599
H	3.388115	-0.207424	0.864938
H	3.237079	-1.305648	-1.523498
H	4.892197	-1.812881	-1.271839
H	2.472369	-2.462195	0.482659
H	3.871146	-4.058127	1.700636
H	4.286280	-2.387894	1.973159
H	6.327629	-3.805238	1.760065
H	5.865607	-4.283162	0.125759
H	6.290753	-2.603070	0.468366
H	2.747148	-3.519151	-1.877731
H	4.071102	-4.450428	-1.191591
H	2.000330	-5.751825	-1.137580
H	2.438134	-5.374287	0.545515
H	-1.746981	-3.852903	0.047394

ZnO-XHNBR monomer

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O	-3.667120	0.085210	1.753738
Zn	-3.682426	-1.423280	0.672507
Zn	-2.111429	-2.684006	-1.109653

Zn	1.180446	-2.343239	-1.005773
O	0.881295	-2.256213	1.092490
Zn	0.897488	-0.458835	2.011884
O	-0.681579	-0.978984	2.971022
Zn	-0.975625	-2.469106	1.803743
O	-2.439701	-2.934190	0.798815
Zn	-1.983756	0.342798	2.695547
O	-1.732700	2.096930	1.967005
Zn	-0.050276	2.518092	1.194103
O	1.402408	1.140786	1.287298
Zn	1.326376	0.989107	-0.648759
O	1.402265	-0.510872	-1.721032
Zn	-0.280770	-0.722785	-2.639968
O	-0.502979	-2.535853	-1.994305
Zn	-3.163785	1.688857	0.741141
Zn	-3.213982	0.142323	-1.995405
O	-3.665874	-1.509129	-1.259815
O	-3.197746	1.875161	-1.106714
Zn	-1.363946	2.063643	-1.741203
O	0.158058	2.534641	-0.799316
O	-1.586428	0.563624	-2.963937
N	0.739475	4.439718	1.608306
C	1.449965	5.037973	0.918008
C	2.356793	5.674125	-0.040857
C	1.609236	6.728600	-0.869605
H	3.151319	6.153698	0.544490
C	2.964936	4.549952	-0.911896
H	2.309707	7.193668	-1.567718
H	0.806198	6.260684	-1.445074
H	1.180294	7.509803	-0.237595
H	3.620110	5.030633	-1.647980
C	3.732544	3.505225	-0.104595
H	2.144240	4.064459	-1.454519
C	4.228759	2.329118	-0.946808
H	4.583322	3.974133	0.407856
H	3.081619	3.098455	0.680666
C	4.714183	1.173323	-0.071838
H	3.411973	1.973325	-1.599349
H	5.019065	2.651822	-1.637400
C	5.090401	-0.087038	-0.852146
H	5.559915	1.516096	0.538628
H	3.911573	0.927461	0.639120
C	5.082980	-1.348645	0.022927
H	4.354529	-0.240738	-1.652805
H	6.065337	0.041537	-1.342344
C	5.396218	-2.603436	-0.810468

C	5.960701	-1.234914	1.283357
H	4.046562	-1.440189	0.382520
H	5.874487	-2.166435	1.854826
C	7.437537	-0.931100	1.023685
H	5.547362	-0.453932	1.933034
H	7.991646	-0.881141	1.966034
H	7.911632	-1.700647	0.405959
H	7.568486	0.029341	0.513192
C	4.880395	-3.910386	-0.176843
H	4.924160	-2.502174	-1.793208
H	6.475422	-2.686446	-0.984400
H	5.044502	-4.739909	-0.871529
H	5.384150	-4.137949	0.765280
C	3.395224	-3.753893	0.079180
O	2.956195	-3.738270	1.249642
O	2.684105	-3.548420	-0.969625
H	1.625793	-2.909386	1.304501

CaO-XHNBR monomer

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C	3.781096	6.500086	-0.951849
C	3.850288	5.332292	0.046403
C	4.115999	3.985313	-0.654229
C	4.496312	2.839118	0.280778
C	4.815253	1.581807	-0.530448
C	4.926344	0.284412	0.280096
C	4.970187	-0.958306	-0.624930
C	4.478463	-2.262074	0.024895
C	5.195187	-2.587288	1.346326
C	6.709537	-2.776955	1.243492
C	2.587807	5.259102	0.791504
N	1.564022	5.205119	1.329988
C	4.542916	-3.394975	-1.012387
C	3.783149	-4.670878	-0.618234
C	2.301705	-4.367326	-0.448363
O	1.653822	-4.051829	-1.488895
O	1.811154	-4.405120	0.717040
O	-0.717059	2.154514	2.646534
Ca	0.089848	0.144915	3.083672
Ca	-0.164132	3.338996	0.764000
O	1.188653	2.362658	-0.774737
Ca	-2.913884	2.372235	2.207537
O	-4.219645	0.569057	2.258604

O	-2.413040	3.464209	0.287025
Ca	-3.239345	2.689252	-1.620242
Ca	-5.103991	-0.143029	0.302388
O	-4.509598	0.792225	-1.621018
Ca	0.250984	1.550210	-2.685246
O	-1.900895	1.732297	-3.179740
Ca	1.899039	0.249604	-0.257613
O	1.488555	-0.853442	1.619966
Ca	-3.330691	-1.484598	2.671187
O	-1.162032	-1.762102	3.093004
O	-4.326489	-2.226783	0.756901
Ca	-3.083593	-3.209324	-0.764208
O	-2.264512	-2.247259	-2.604527
Ca	-3.063558	-0.205402	-3.070582
Ca	-0.022220	-2.484538	-2.168569
O	1.004124	-0.517684	-2.181556
O	-0.933496	-3.654923	-0.126476
Ca	0.338394	-2.804258	1.722172
H	4.640191	5.531407	0.782038
H	4.745511	6.596345	-1.457420
H	3.012700	6.309859	-1.706274
H	3.554554	7.445524	-0.452852
H	4.923023	4.156296	-1.378295
H	3.205700	3.681497	-1.192243
H	5.353597	3.109535	0.912289
H	3.650097	2.637794	0.951814
H	4.033908	1.478907	-1.301020
H	5.742951	1.730439	-1.098584
H	5.817643	0.322888	0.917274
H	4.096550	0.196220	1.002942
H	4.348134	-0.782336	-1.517470
H	5.988012	-1.088868	-1.016246
H	3.423717	-2.110702	0.305458
H	4.741387	-3.488356	1.773983
H	4.974747	-1.787109	2.062675
H	7.138658	-2.990973	2.227305
H	6.973094	-3.610006	0.583435
H	7.206469	-1.879312	0.857833
H	4.116283	-3.031340	-1.954818
H	5.589870	-3.649528	-1.221191
H	3.895056	-5.409978	-1.418152
H	4.173860	-5.100073	0.307696
H	-0.352666	-4.417796	-0.225289

MgO_2-XHNBR monomer

60

C	2.720872	6.218324	-0.045460
C	2.933421	4.839633	0.597112
C	1.741448	4.003175	0.422264
N	0.818554	3.323515	0.296588
C	4.195400	4.119991	0.069044
C	4.358657	2.669990	0.558123
C	3.862686	1.626405	-0.448932
C	3.761012	0.222564	0.142375
C	3.359093	-0.814794	-0.904541
C	2.973494	-2.177577	-0.314427
C	2.319261	-3.036891	-1.408030
C	1.866354	-4.433668	-0.959036
C	1.003747	-4.431644	0.276275
O	1.182194	-5.085134	1.270856
Mg	-0.804285	-1.658939	-0.388537
O	-1.446460	-2.081497	1.560063
O	-2.814480	-1.651361	1.999143
Mg	-3.740214	-1.076264	0.299139
O	-5.044241	0.453601	0.430806
O	-4.589916	0.305034	-1.009783
Mg	-2.753141	0.706623	-1.916028
O	-1.492227	2.228323	-1.639967
O	-2.901550	2.667694	-1.376961
Mg	-3.805783	1.931053	0.215809
O	-2.277730	1.582845	1.479692
Mg	-1.395256	-0.213236	2.112571
O	0.351494	0.420439	1.407707
Mg	-0.511527	1.660259	0.018548
O	0.425253	-0.124216	0.010385
O	-2.244113	0.536568	0.385941
O	-2.632639	-1.969407	-1.106145
O	-1.867954	-1.027044	-1.990894
C	4.136338	-2.890773	0.400544
C	5.311426	-3.286173	-0.495727
O	-0.070527	-3.601366	0.163044
H	3.037551	4.957222	1.683571
H	3.607616	6.832349	0.131642
H	2.576704	6.124104	-1.124957
H	1.854273	6.731228	0.378099
H	5.040789	4.739799	0.385614
H	4.182226	4.146377	-1.027444
H	5.414711	2.476411	0.776294
H	3.828567	2.535775	1.511447
H	2.874300	1.908742	-0.832047

H	4.537814	1.624114	-1.316532
H	4.720692	-0.047633	0.604596
H	3.000120	0.229184	0.933820
H	2.485296	-0.424434	-1.439169
H	4.160945	-0.934683	-1.647431
H	2.208594	-1.966993	0.446525
H	3.754102	-3.783335	0.909647
H	4.499490	-2.237260	1.201757
H	6.091651	-3.782227	0.089368
H	5.006586	-3.980381	-1.286941
H	5.765068	-2.414271	-0.978438
H	1.463714	-2.487383	-1.824936
H	3.009914	-3.164500	-2.250342
H	1.288563	-4.907044	-1.761566
H	2.719464	-5.079010	-0.741400
H	-0.612224	-3.561912	0.996080

MgO-XHNBR dimer

106

C	9.496916	2.077874	0.158990
C	8.165955	2.097452	-0.610501
C	7.818098	0.732973	-1.022221
N	7.521130	-0.355821	-1.275004
C	7.008872	2.677824	0.232200
C	5.760789	3.045444	-0.568090
C	4.631792	3.518315	0.351422
C	3.337215	3.915925	-0.371000
C	2.169417	4.066550	0.606302
C	0.864449	4.598577	-0.007741
C	-0.276109	4.510367	1.037888
C	-1.310482	3.381443	0.810959
C	-0.588665	2.036797	0.696452
O	-0.216841	1.683655	-0.457753
Mg	0.674393	0.032301	-1.321421
O	2.477053	0.769779	-1.513489
Mg	3.382444	0.816407	0.127831
O	5.045526	-0.086266	0.573866
Mg	4.114677	-0.727466	2.140906
O	4.051521	-2.489531	2.805448
Mg	4.554885	-3.762004	1.423062
O	5.419186	-3.320449	-0.192780
Mg	4.324716	-3.527185	-1.777892
O	2.660081	-4.423004	-1.844091

Mg	1.942837	-4.939556	-0.123907
O	2.821185	-4.665798	1.524404
Mg	2.254958	-3.197640	2.684288
O	0.625130	-2.243231	2.424219
Mg	0.719310	-0.324785	1.908021
O	-0.392925	1.396861	1.767876
C	0.996720	6.019034	-0.588119
C	1.498263	7.077178	0.396253
O	1.145986	-1.463510	-2.536470
Mg	1.078665	-3.290252	-2.054639
O	0.236214	-4.085804	-0.474490
Mg	-0.217708	-2.809444	0.807237
O	-0.379329	-0.967842	0.151426
Mg	2.959528	-0.750876	-2.580059
O	4.563032	-1.708604	-2.355895
Mg	5.615092	-1.414270	-0.708142
O	2.513103	0.284448	1.766967
H	8.284665	2.688253	-1.527520
H	9.781254	3.103522	0.407756
H	9.392306	1.512524	1.089101
H	10.298438	1.629572	-0.433056
H	7.397598	3.569106	0.740160
H	6.732286	1.941856	0.996236
H	5.993964	3.833418	-1.297018
H	5.427313	2.172630	-1.145826
H	4.434077	2.734299	1.103225
H	4.980947	4.369718	0.951426
H	3.516944	4.854623	-0.909644
H	3.068947	3.166583	-1.131573
H	1.960589	3.087941	1.063880
H	2.468225	4.716216	1.441851
H	0.619058	3.936823	-0.846866
H	0.012910	6.318946	-0.972830
H	1.661568	5.996572	-1.459878
H	1.462002	8.075035	-0.051546
H	0.892066	7.100090	1.308942
H	2.534835	6.888031	0.694239
H	0.150180	4.376653	2.038794
H	-0.836613	5.453588	1.070976
C	-2.199498	3.656566	-0.407191
H	-1.258360	-0.563610	0.097967
C	-3.530704	2.865110	-0.435982
H	-2.478294	4.716636	-0.420576
H	-1.634489	3.453668	-1.320901
H	-4.033432	3.100722	-1.383198
C	-3.284249	1.415101	-0.449334

C	-4.481382	3.241187	0.727521
N	-3.073478	0.276641	-0.412737
C	-5.969640	3.033251	0.433116
H	-4.197979	2.685382	1.628283
H	-4.311828	4.301293	0.947959
H	-6.537846	3.418923	1.289215
H	-6.255853	3.655029	-0.427078
C	-6.390597	1.585913	0.172849
C	-7.905096	1.429525	0.034854
H	-5.912967	1.209470	-0.740781
H	-6.027802	0.946463	0.988830
C	-8.320858	-0.010041	-0.267527
H	-8.393420	1.764353	0.960997
H	-8.259275	2.098895	-0.760549
H	-7.848592	-0.673828	0.469038
C	-9.835477	-0.270491	-0.239944
H	-7.909762	-0.306534	-1.242929
C	-10.085160	-1.767266	-0.497951
H	-10.182732	-0.053800	0.779224
C	-10.627101	0.651571	-1.185840
H	-11.700554	0.475966	-1.043316
H	-10.466545	1.691093	-0.877947
C	-10.286460	0.508822	-2.670207
H	-10.890873	1.192256	-3.274178
H	-9.233750	0.738779	-2.865918
H	-10.475044	-0.506695	-3.035130
C	-11.550624	-2.198691	-0.525346
H	-9.632841	-2.055280	-1.455017
H	-9.565028	-2.341401	0.276467
H	-11.618184	-3.274212	-0.733356
C	-12.270933	-1.982695	0.782176
H	-12.115789	-1.706098	-1.321813
O	-13.610376	-1.952409	0.622738
O	-11.753639	-1.874069	1.870739
H	-13.998231	-1.851779	1.503444
H	-1.925187	3.334276	1.715543

ZnO-XHNBR dimer

106

C	-7.839302	3.000815	0.408014
C	-6.501063	3.297124	1.102937
C	-5.397558	3.718872	0.105951
C	-4.088994	4.151043	0.768752

C	-2.999031	4.497537	-0.248403
C	-1.678700	4.911713	0.403782
C	-0.532505	5.029812	-0.603303
C	0.759885	5.644571	-0.032439
C	0.618422	7.138932	0.316827
C	0.220709	8.043218	-0.851240
C	-6.043372	2.107646	1.826188
N	-5.639549	1.143438	2.322281
Zn	-4.075619	-0.065675	1.561885
O	-4.374073	0.269634	-0.383888
Zn	-4.197674	-1.200274	-1.496511
O	-2.932744	-1.460601	-2.954966
Zn	-2.503562	-3.172092	-2.149495
O	-4.075094	-3.082849	-0.999631
Zn	-3.616305	-3.187518	0.795449
O	-3.696589	-1.826164	2.163609
Zn	-1.882671	-2.299052	2.591118
Zn	0.867291	-1.460626	1.337831
O	1.018886	-2.875939	0.179817
Zn	0.536545	-2.356067	-1.635743
O	-0.803040	-3.789899	-1.711266
Zn	-0.611777	-3.957612	0.204045
O	-1.936864	-3.909595	1.506757
Zn	-1.490953	-0.298399	-2.759130
O	0.371924	-0.685834	-2.400493
Zn	0.455818	0.920346	-1.287557
O	1.593537	2.486738	-1.265826
C	2.114364	3.008574	-0.224569
O	2.019558	2.565435	0.941585
O	0.658393	0.431754	0.754835
Zn	-0.948785	0.511483	1.968945
Zn	-2.713897	1.277980	-0.415256
O	-1.431674	1.331640	-1.734362
O	-0.405634	-1.150569	2.748207
O	-2.552819	1.245161	1.518087
C	1.965514	5.393351	-0.976692
C	2.907031	4.282008	-0.474501
H	-6.636824	4.089778	1.849339
H	-8.183268	3.904296	-0.101660
H	-7.713732	2.208903	-0.335097
H	-8.605957	2.693273	1.123130
H	-5.808132	4.541136	-0.492413
H	-5.222645	2.877719	-0.577569
H	-4.273844	5.023190	1.410853
H	-3.714270	3.348460	1.418668
H	-2.811208	3.640648	-0.917153

H	-3.347742	5.299273	-0.914149
H	-1.833517	5.861491	0.932529
H	-1.407713	4.170024	1.167838
H	-0.316734	4.029622	-0.995419
H	-0.859808	5.618985	-1.471234
H	0.970486	5.130373	0.916522
H	1.577765	7.480009	0.727411
H	-0.110092	7.259707	1.127563
H	0.261478	9.096751	-0.558019
H	0.889207	7.911177	-1.709420
H	-0.798749	7.836880	-1.192413
H	1.613326	5.133038	-1.982102
H	2.565079	6.306961	-1.079585
C	4.039361	4.013596	-1.473625
H	3.322318	4.601815	0.485640
H	1.294863	1.192126	0.950558
C	5.101990	2.952440	-1.082599
H	3.594606	3.723859	-2.431437
H	4.585445	4.950294	-1.637863
C	5.903164	3.279788	0.205451
H	5.826296	2.957615	-1.907494
C	4.549444	1.586320	-1.098765
N	4.118354	0.511786	-1.138551
H	6.049459	4.366736	0.187779
C	5.330509	2.888094	1.578071
H	6.904115	2.847179	0.106121
H	5.880534	3.483864	2.318750
H	4.281281	3.183988	1.657345
C	5.433712	1.413442	2.002599
H	5.056915	1.367530	3.031101
H	4.751484	0.798575	1.408297
C	6.848974	0.808638	1.957255
H	6.969488	0.106990	2.792714
C	7.168637	0.052582	0.664007
H	7.586684	1.605472	2.127405
C	8.511193	-0.694034	0.665180
H	6.368732	-0.675856	0.482537
H	7.133015	0.732474	-0.197122
C	8.633065	-1.487606	-0.648463
C	9.717425	0.223923	0.936984
H	8.477744	-1.424452	1.484765
H	10.626757	-0.386261	1.004186
C	9.934860	1.335213	-0.091475
H	9.601570	0.671909	1.930297
H	10.818042	1.930408	0.159811
H	10.083220	0.933747	-1.099986

H	9.079565	2.018402	-0.131625
C	9.939393	-2.256305	-0.841473
H	7.796830	-2.192537	-0.702667
H	8.517548	-0.806122	-1.500518
H	9.925766	-2.776463	-1.807911
H	10.810994	-1.595864	-0.872073
C	10.180220	-3.320864	0.199125
O	11.481358	-3.675485	0.267547
O	9.338554	-3.845634	0.891862
H	11.546160	-4.383530	0.923714

CaO-XHNBR dimer

106

Ca	-4.689296	1.078583	-1.108191
Ca	-1.966163	1.560715	0.604584
Ca	-3.209831	-5.086654	-1.157963
Ca	-0.599129	-4.438971	0.641147
Ca	-1.079123	0.440659	-2.872956
Ca	-0.493462	-2.960153	-2.868672
Ca	-4.778303	-0.475354	2.488137
Ca	-4.032145	-3.647290	2.322557
Ca	-0.995992	-1.371903	2.873024
Ca	-6.060545	-2.449244	-0.712595
Ca	-4.146303	-1.933599	-3.280717
Ca	0.934531	-0.638299	0.304571
O	-3.119555	-1.841717	3.300377
O	-5.677479	-2.343263	1.470996
O	-1.978342	-1.509858	-3.671759
O	0.738879	-1.166357	-2.071299
O	-0.427476	0.461849	1.746696
O	0.291091	-2.556128	1.396913
O	-5.604567	-0.696614	-2.070176
O	-4.740451	-3.752510	-2.046664
O	-4.205177	1.223200	1.101162
O	-2.545249	1.494694	-1.592214
O	-2.767455	-4.985818	1.060299
O	-1.016039	-4.664971	-1.585805
C	-6.450105	4.355454	2.717603
C	-5.321881	3.814426	3.610139
C	-3.957698	3.716333	2.890440
C	-3.428566	4.961469	2.166692
C	-2.348463	4.479194	1.192906
C	-1.507291	5.487875	0.417503

C	-0.607232	4.735844	-0.575191
C	0.504629	5.576905	-1.213172
C	-0.027712	6.869646	-1.865253
C	-1.095543	6.668061	-2.943278
C	-5.644618	2.432657	4.006063
N	-5.849330	1.313462	4.227856
C	1.358828	4.790126	-2.225954
C	2.039818	3.473524	-1.764447
C	2.699833	3.600187	-0.386664
C	3.966253	2.739448	-0.151090
C	5.085096	2.989389	-1.191007
C	6.505179	2.745500	-0.673252
C	6.807161	1.307425	-0.248410
C	8.278114	1.095838	0.110342
C	8.567448	-0.328491	0.583803
C	10.055021	-0.657415	0.788061
C	10.763540	0.311249	1.753115
C	10.220317	0.319701	3.183005
C	1.092244	2.267676	-1.918711
O	0.745044	1.995963	-3.101154
O	0.721169	1.620674	-0.899272
C	3.635191	1.313803	-0.059030
N	3.371377	0.188941	0.021538
C	10.182944	-2.133906	1.203643
C	11.605465	-2.626650	1.464057
C	12.499144	-2.568289	0.250315
O	12.133046	-2.533775	-0.902627
O	13.806243	-2.591449	0.583406
H	-5.256677	4.414812	4.526048
H	-6.277902	5.412049	2.500564
H	-6.473820	3.800220	1.775354
H	-7.423577	4.263469	3.205945
H	-4.069216	2.888510	2.159355
H	-3.207407	3.388275	3.621895
H	-4.219307	5.460418	1.594520
H	-3.022514	5.701977	2.868140
H	-1.649013	3.850025	1.769732
H	-2.868100	3.856841	0.449135
H	-2.162926	6.191558	-0.110279
H	-0.895947	6.082571	1.110146
H	-0.131717	3.903846	-0.039203
H	-1.228324	4.262463	-1.348985
H	1.166108	5.902348	-0.395502
H	0.821106	7.416184	-2.296617
H	-0.433722	7.519595	-1.080646
H	-1.414194	7.632593	-3.350600

H	-0.727027	6.063643	-3.777467
H	-1.983586	6.167725	-2.543613
H	0.761507	4.542854	-3.109147
H	2.153874	5.466446	-2.568022
H	1.532048	-0.757905	-2.429750
H	3.035070	4.634241	-0.244954
H	1.971072	3.381336	0.399282
H	4.353224	3.006886	0.841576
H	4.904312	2.381308	-2.084402
H	4.997199	4.035954	-1.504091
H	7.206107	3.036354	-1.465909
H	6.701258	3.422276	0.170328
H	6.191745	1.029239	0.616953
H	6.524072	0.618913	-1.056282
H	8.904249	1.325853	-0.763264
H	8.558673	1.816414	0.890067
H	8.162059	-1.033379	-0.154427
H	8.012956	-0.518665	1.513641
H	10.547065	-0.550286	-0.187973
H	11.834854	0.076411	1.775344
H	10.704162	1.324399	1.339356
H	10.774310	1.030165	3.803847
H	9.164695	0.610018	3.211515
H	10.303945	-0.664781	3.655996
H	9.594512	-2.311855	2.112239
H	9.735838	-2.752738	0.418100
H	11.584318	-3.679416	1.773492
H	12.090778	-2.086569	2.282157
H	14.309495	-2.591788	-0.243001
H	2.813076	3.289365	-2.519263

MgO_2-XHNBR dimer

100

O	-0.881176	3.251231	0.529647
Mg	-0.356316	2.941873	2.491348
Mg	-1.497497	5.010856	-0.404996
O	1.445006	2.067943	1.499050
Mg	1.223650	3.523425	0.067519
O	0.484603	5.195750	-0.810468
Mg	-0.679609	2.817254	-2.089742
O	-2.630508	2.743183	-1.698093
Mg	-2.641984	2.351096	0.254273
O	1.083791	2.214676	-1.464647

Mg	0.011148	0.706391	0.871846
O	-1.209031	1.172032	2.476713
O	-3.135376	3.914999	-0.896051
O	0.025877	1.220251	-1.077964
O	-2.018625	0.807130	1.279918
O	-1.560163	4.210571	1.487066
O	-0.369337	4.777771	-1.980878
O	1.461344	3.465973	2.077948
C	-11.496322	-3.054959	0.846657
C	-10.250802	-2.156058	0.837739
C	-10.027452	-1.585039	2.175989
N	-9.847899	-1.149745	3.234599
C	-8.995230	-2.904036	0.352176
C	-7.745693	-2.030699	0.254700
C	-6.531148	-2.795254	-0.271482
C	-5.274518	-1.929424	-0.357206
C	-4.071161	-2.686031	-0.920192
C	-2.736766	-1.928892	-0.820505
C	-1.622477	-2.791900	-1.431491
C	-0.175087	-2.330729	-1.146207
C	0.797584	-3.286745	-1.872815
C	2.332878	-3.151643	-1.707330
C	2.745188	-3.386088	-0.314017
N	3.038707	-3.628251	0.780138
C	-2.799694	-0.516939	-1.425215
C	-3.149358	-0.425893	-2.909447
C	0.053263	-2.302714	0.342699
O	0.331945	-1.300219	0.994845
C	3.002962	-1.921599	-2.365098
C	2.705840	-0.520396	-1.821695
C	3.207942	-0.151834	-0.418998
C	4.729484	0.016888	-0.278668
C	5.498079	-1.260939	0.064836
C	7.004533	-1.066330	0.295773
C	7.721692	-0.419241	-0.903825
C	7.626114	-1.201567	-2.214947
C	7.613974	-2.416622	0.715089
C	9.125696	-2.421748	0.940344
C	9.575632	-1.503632	2.049170
O	8.905966	-1.142845	2.989814
O	10.865310	-1.129795	1.907387
H	-10.430518	-1.305872	0.166983
H	-11.681472	-3.431590	-0.163257
H	-11.349802	-3.909882	1.512917
H	-12.380361	-2.506282	1.180000
H	-9.229788	-3.325727	-0.633328

H	-8.807776	-3.752275	1.022704
H	-7.950406	-1.175359	-0.404144
H	-7.511609	-1.613621	1.242462
H	-6.334845	-3.657487	0.380525
H	-6.758763	-3.205286	-1.265721
H	-5.492171	-1.053468	-0.982191
H	-5.027169	-1.544570	0.641849
H	-3.965864	-3.635375	-0.377710
H	-4.268378	-2.956849	-1.967452
H	-2.527906	-1.788835	0.250707
H	-1.843738	-0.010514	-1.261328
H	-3.547327	0.050836	-0.857027
H	-3.238499	0.625621	-3.199084
H	-2.381208	-0.889006	-3.538897
H	-4.103819	-0.912471	-3.137118
H	-1.728480	-3.821438	-1.068781
H	-1.744618	-2.835431	-2.520576
H	-0.034514	-1.304196	-1.492543
H	0.525026	-4.311808	-1.598295
H	0.592087	-3.182318	-2.943782
H	2.736392	-4.020412	-2.244733
H	2.692164	-1.954340	-3.417251
H	4.083673	-2.099636	-2.368131
H	3.149753	0.192810	-2.527287
H	1.634288	-0.311399	-1.865823
H	2.737511	0.806529	-0.179061
H	2.850546	-0.863262	0.334195
H	4.928394	0.750334	0.513248
H	5.116387	0.458790	-1.207127
H	5.062743	-1.696028	0.972403
H	5.354323	-2.018802	-0.716078
H	7.119693	-0.378704	1.144570
H	8.777986	-0.262724	-0.652748
H	7.314111	0.586227	-1.056397
H	8.182577	-0.696928	-3.010595
H	8.035047	-2.213333	-2.116433
H	6.587074	-1.295655	-2.549587
H	7.118457	-2.745888	1.634408
H	7.387570	-3.173837	-0.046087
H	9.453201	-3.428187	1.231315
H	9.683138	-2.175570	0.032282
H	11.084120	-0.578521	2.671887
O	-0.083049	-3.472672	0.936199
H	0.160859	-3.380474	1.869926

3.5 MO-PA6 Models

MgO-Amide(-N)

36

C	4.684798	3.445666	1.922101
Mg	2.873681	1.228200	0.623285
N	4.653602	2.692096	0.666958
Mg	2.225686	1.094001	-2.010590
Mg	-2.198339	-0.280634	1.635001
H	5.318221	4.334637	1.841914
Mg	-2.722431	-0.410649	-0.983645
H	5.073978	2.812546	2.719535
Mg	0.525310	3.314375	-0.448612
H	3.663182	3.740718	2.170616
C	5.862045	2.179576	0.185263
Mg	-1.983933	2.566812	0.091193
Mg	2.043796	-1.737429	-0.484670
H	4.021616	3.074035	-0.053168
O	6.851112	2.121933	0.889645
Mg	-0.462056	-2.508754	0.045836
C	5.806108	1.652342	-1.229278
Mg	-0.113220	-1.003048	-2.806192
Mg	0.927550	-0.738543	2.380727
H	5.402428	2.410193	-1.909753
Mg	0.161188	1.814642	2.394494
H	5.145045	0.774844	-1.258394
Mg	-0.887377	1.556217	-2.790377
H	6.811195	1.374169	-1.544281
O	0.551182	-2.296220	-1.603274
O	1.096706	-2.168202	1.157902
O	-0.484463	3.129009	1.200939
O	-1.034898	2.979175	-1.558047
O	0.802558	0.675405	-3.174314
O	-1.844478	-0.129569	-2.633394
O	1.883190	0.943924	2.214299
O	-0.760908	0.145169	2.781281
O	3.034491	-0.150720	-0.762450
O	2.241659	2.572251	-0.746365
O	-2.157802	-1.726491	0.333726
O	-2.965711	0.976340	0.360322

MgO-Amide(-O)

36

C	4.377677	3.432713	3.097050
Mg	3.186293	1.103620	0.392763
N	4.754703	4.016222	1.814313
Mg	2.422970	0.533641	-2.142944
Mg	-2.110948	0.369228	1.598623
H	5.247751	2.989305	3.590082
Mg	-2.660254	-0.198819	-0.952577
H	3.619954	2.654564	2.937074
Mg	0.970727	3.162543	-1.070480
H	3.973116	4.225275	3.728746
C	5.016250	3.259098	0.742160
Mg	-1.609139	2.837148	-0.452038
Mg	1.921254	-1.926244	-0.129061
H	4.812363	5.017892	1.722653
O	4.987665	2.014543	0.825620
Mg	-0.651912	-2.302250	0.497172
C	5.284297	3.928088	-0.573148
Mg	-0.134657	-1.407588	-2.578394
Mg	0.967032	-0.269151	2.435794
H	5.336273	5.017721	-0.509272
Mg	0.473555	2.294305	1.953461
H	4.455653	3.616225	-1.224947
Mg	-0.623570	1.173204	-3.061009
H	6.214901	3.536366	-0.989207
O	0.365653	-2.528857	-1.144678
O	0.939247	-1.937261	1.552169
O	-0.058547	3.448661	0.557133
O	-0.627457	2.815351	-2.129417
O	0.956240	0.059998	-3.243324
O	-1.763781	-0.337573	-2.609435
O	2.096843	1.244106	1.986704
O	-0.620047	0.845695	2.651372
O	3.070315	-0.543887	-0.678818
O	2.593480	2.215107	-1.187846
O	-2.249174	-1.295557	0.601758
O	-2.751427	1.436867	0.100549

ZnO-Amide(-N)

36

C	3.608123	4.032748	2.832058
Zn	-0.838391	1.527291	2.723734
N	4.010489	2.676200	2.437719

Zn	-2.205631	-0.776935	2.647271
Zn	2.674612	-0.428921	-0.434070
H	4.393316	4.760651	2.609548
Zn	1.331490	-2.747260	-0.524205
H	3.416597	4.045241	3.904582
Zn	0.659225	-0.930615	3.936416
H	2.688176	4.283628	2.302015
C	5.082166	2.084589	3.145956
Zn	2.481415	-1.941772	2.277429
Zn	-2.016810	0.755111	-0.092935
H	4.072223	2.541055	1.425750
O	5.504831	2.578822	4.167187
Zn	-0.179154	-0.275101	-1.747811
C	5.556941	0.765814	2.588606
Zn	-1.764356	-2.374529	-0.036902
Zn	0.861752	2.002059	0.155083
H	5.418705	0.690432	1.506560
Zn	2.328142	1.290212	2.341053
H	4.957745	-0.019901	3.063546
Zn	-0.372015	-3.261758	2.071557
H	6.604428	0.620011	2.851723
O	-1.924118	-0.884888	-1.140387
O	-0.485439	1.506753	-1.028533
O	2.391667	-0.318404	3.325391
O	0.973054	-2.722131	3.231679
O	-2.138203	-2.466861	1.870831
O	-0.212722	-3.536200	0.148902
O	0.693151	2.340416	2.059554
O	2.645877	1.263336	0.319846
O	-2.395438	0.923853	1.718614
O	-0.953558	-0.003561	3.919298
O	1.427926	-1.208727	-1.712570
O	2.888683	-2.136957	0.474104

ZnO-Amide(-O)

36

C	5.658608	2.803436	1.533612
Zn	1.450416	0.968482	2.562417
N	5.708747	3.052519	0.096873
Zn	-0.841759	-0.388970	2.845412
Zn	0.943771	0.894356	-2.493155
H	6.389964	2.039600	1.808834
Zn	-1.352211	-0.469677	-2.271543

H	4.653823	2.462966	1.807608
Zn	1.509521	-1.875436	1.385718
H	5.894936	3.733433	2.051504
C	5.412199	2.105849	-0.795797
Zn	1.246386	-1.915017	-1.258220
Zn	-1.138259	2.478925	1.588941
H	5.927430	3.977575	-0.237663
O	5.156044	0.939376	-0.418521
Zn	-1.405149	2.437368	-1.072633
C	5.350067	2.472912	-2.248356
Zn	-2.840540	0.102728	0.452476
Zn	1.544377	2.642010	-0.026286
H	5.733813	3.473057	-2.462221
Zn	3.199470	0.447439	-0.159153
H	4.290003	2.408341	-2.525470
Zn	-1.458121	-2.187023	0.351319
H	5.902662	1.730766	-2.827472
O	-2.584350	1.945424	0.398046
O	-0.175717	3.341611	0.134558
O	2.655874	-1.364228	-0.071366
O	0.279172	-2.810599	0.186916
O	-2.200867	-1.132143	1.813544
O	-2.477790	-1.175985	-0.968389
O	2.587658	1.707737	1.302809
O	2.307174	1.672211	-1.512215
O	-0.385648	1.500146	2.975730
O	1.032450	-0.898930	2.898683
O	-0.940383	1.413866	-2.550741
O	0.477194	-0.983411	-2.676090

CaO-Amide(-N)

36

C	5.574891	2.263975	4.021272
Ca	3.657859	1.748543	1.212548
N	4.459074	2.831674	3.271935
Ca	3.279363	1.064428	-1.940985
Ca	-2.637766	-0.047965	1.547205
H	5.334600	2.120849	5.084234
Ca	-2.733185	-0.633724	-1.628923
H	6.464280	2.907895	3.990283
Ca	1.004105	3.972641	-0.846477
H	5.845002	1.287517	3.596197
C	4.052929	4.016370	3.759581

Ca	-2.105847	3.073099	-0.662238
Ca	2.786544	-2.061531	0.191131
H	2.686660	1.828533	3.486590
O	4.514285	4.607919	4.749730
Ca	-0.331050	-2.957823	0.348539
C	2.881609	4.682200	3.025164
Ca	0.729964	-1.583334	-3.099660
Ca	0.804923	-0.589336	3.171879
H	2.578426	4.176560	2.099302
Ca	-0.049642	2.633827	2.623640
H	3.158354	5.709078	2.773196
Ca	-0.169117	1.492183	-3.605906
H	2.026777	4.754762	3.711337
O	1.220174	-2.783018	-1.291300
O	1.241101	-2.288919	1.852377
O	-0.536196	3.786282	0.818884
O	-0.574867	3.262966	-2.321437
O	1.801866	0.379755	-3.448607
O	-1.252196	-0.482982	-3.274546
O	1.952971	1.421047	2.990425
O	-1.052456	0.646917	2.963060
O	3.830942	-0.123352	-0.079962
O	2.900225	2.858375	-0.616466
O	-2.256760	-1.854838	0.235168
O	-3.164843	1.155029	-0.292468

CaO-Amide(-O)

36

C	6.929549	1.252622	-0.047444
Ca	3.186284	1.886023	1.302142
N	6.584663	2.670528	-0.118329
Ca	3.456977	1.442596	-1.929339
Ca	-2.680884	-0.400811	1.468877
H	7.571756	0.976067	-0.888891
Ca	-2.553328	-0.890027	-1.730038
H	6.002152	0.651934	-0.061458
Ca	0.702090	3.969454	-0.736905
H	7.471339	1.081510	0.885227
C	5.934266	3.193946	-1.176162
Ca	-2.326894	2.824624	-0.660639
Ca	2.966702	-1.797193	0.232755
H	6.915202	3.300388	0.595012
O	5.629626	2.481186	-2.148300

Ca	-0.038459	-3.001020	0.322719
C	5.496027	4.625169	-1.095366
Ca	1.039796	-1.456286	-3.062715
Ca	0.789135	-0.505644	3.176031
H	6.009659	5.197756	-0.317747
Ca	-0.383805	2.470193	2.677700
H	4.414194	4.547312	-0.868733
Ca	-0.125219	1.510507	-3.566026
H	5.632680	5.105074	-2.065856
O	1.534255	-2.691580	-1.282510
O	1.422326	-2.176955	1.858725
O	-0.874116	3.667458	0.873112
O	-0.776328	3.198217	-2.274486
O	1.935085	0.603438	-3.339586
O	-1.036173	-0.559459	-3.318137
O	1.687782	1.565389	2.911667
O	-1.283507	0.408928	2.998139
O	3.919571	0.198916	-0.019254
O	2.774514	3.179556	-0.514851
O	-2.070592	-2.123014	0.119818
O	-3.222398	0.810145	-0.375052

MgO_2-Amide(-N)

30

C	4.546852	2.385619	-0.680274
O	-0.302943	0.189706	0.357817
N	3.669890	1.525581	-1.496004
Mg	-0.019925	2.250569	0.261265
Mg	-2.112641	-0.839256	0.701583
H	5.147389	3.049737	-1.308206
O	0.904335	1.733887	-1.583255
H	5.220533	1.755216	-0.100555
Mg	-0.540489	0.194921	-1.797237
H	3.922688	2.965472	0.002091
C	4.316379	0.582564	-2.346323
O	-2.219115	-0.813471	-1.317164
Mg	0.146050	-2.311485	-0.330555
H	2.943987	2.050506	-1.992873
O	5.466626	0.265395	-2.142744
O	0.104704	-2.288943	1.670753
C	3.444720	0.010513	-3.430166
Mg	0.397579	-0.380175	2.162335
O	0.801879	-1.295940	-1.919069

H	2.981468	0.808724	-4.018980
Mg	2.141023	0.613642	-0.204752
H	2.636803	-0.587390	-2.988317
O	1.689834	2.025517	1.227107
H	4.056615	-0.619190	-4.074798
O	-1.128766	-1.651342	2.260421
O	1.772301	-1.237972	-0.773764
O	2.007304	0.693114	1.824909
O	-1.259942	0.986011	1.220337
O	-1.803045	-2.135521	-0.722979
O	-0.541193	2.189889	-1.617103

MgO_2-Amide(-O)

30

C	5.048103	3.037563	-0.005503
O	-0.176818	0.294104	0.341492
N	4.544670	3.425951	-1.320262
Mg	0.204207	2.289443	0.136982
Mg	-1.908600	-0.669283	0.981024
H	5.799393	2.251335	-0.109513
O	0.785174	1.750850	-1.830801
H	4.220618	2.673502	0.612445
Mg	-0.723419	0.268530	-1.760930
H	5.503967	3.912719	0.458091
C	3.911590	2.567139	-2.117248
O	-2.354853	-0.663863	-0.998737
Mg	0.052345	-2.268103	-0.420301
H	4.630640	4.384125	-1.620151
O	3.796262	1.365276	-1.781864
O	0.368302	-2.245411	1.557967
C	3.315754	3.053699	-3.403187
Mg	0.887839	-0.359490	1.897111
O	0.494277	-1.287695	-2.084165
H	3.540268	4.100816	-3.617510
Mg	2.264942	0.622079	-0.759406
H	2.232181	2.906569	-3.314357
O	2.041652	2.036056	0.809045
H	3.674765	2.423127	-4.219338
O	-0.680498	-1.508459	2.353952
O	1.612207	-1.215563	-1.080594
O	2.438580	0.681568	1.292444
O	-0.984521	1.148014	1.299893
O	-1.921013	-1.999126	-0.447986

O	-0.625611	2.271828	-1.626692

3.6 XHNBR dimer-PA6 dimer (conformer 1)

132

C	-0.9868432613	5.7898668303	-0.6675853584
C	-1.3784412625	4.8533434340	-1.8177100613
C	-0.9179653556	3.4107694395	-1.6054298999
H	-0.9519923785	5.2481148374	-2.7416742177
H	-2.4667690926	4.8646436886	-1.9157322961
C	0.6026248522	3.2699329739	-1.5962986343
H	-1.3307435141	2.7857726690	-2.4005549492
H	-1.3305036171	3.0501133384	-0.6621243626
C	1.0714807320	1.8253420386	-1.4214908148
H	1.0231240336	3.8848188952	-0.8011115224
H	0.9994245203	3.6455768179	-2.5430335597
C	0.6419098502	1.1629703578	-0.1134219137
H	2.1613890103	1.8012818874	-1.4863421910
H	0.6753782199	1.2146140769	-2.2351440992
N	-1.4768229177	5.3210380005	0.6070377226
H	-1.3976446711	6.7866569934	-0.8571244876
H	0.0983222872	5.8710032933	-0.5873965347
N	1.1510782743	1.8659885174	1.0452137815
H	1.0423242018	0.1468828249	-0.0934287821
H	-0.4503084689	1.1018480717	-0.0622850268
C	1.5488983314	1.2838183314	2.1693287721
H	1.1150305067	2.8820398484	1.0212982484
O	1.4904159422	0.0585386165	2.3606103647
C	2.0961090852	2.2221203119	3.2203426468
C	3.5809073902	1.9822388615	3.5251734916
H	1.5294726070	2.0494743522	4.1391762412
H	1.9467474218	3.2544238996	2.9025728065
C	4.5028043984	2.1981348954	2.3239649172
H	3.7164339305	0.9755185077	3.9209015581
H	3.8682623183	2.6846933325	4.3108676613
C	4.5414310995	1.0389741520	1.3185995934
H	5.5207953107	2.3468269473	2.6914054305
H	4.2011179331	3.1093537106	1.8013754102
C	5.1287508716	-0.2136417961	1.9519276628
H	5.1978657361	1.3268072581	0.4955620829
H	3.5517120717	0.8286618422	0.9185741917
O	6.3204222318	-0.4639866683	1.9116628088
C	-0.6969295105	4.7140158906	1.5119956542
H	-2.4803017090	5.2063787444	0.6949807284

C	-1.4428296342	4.1860517655	2.7145564363
H	-1.7097129966	5.0186068621	3.3624459308
H	-0.8105821668	3.4995768928	3.2706264368
H	-2.3548498801	3.6833560785	2.4041832597
O	0.5199253079	4.6192109389	1.3941240436
N	4.2289762443	-1.0067658855	2.5631155823
C	4.6094563507	-2.2137991174	3.2563602456
H	4.1335906895	-3.0823386956	2.7996790293
H	4.3193518779	-2.1577377207	4.3076066881
H	5.6919645169	-2.3087662134	3.1837821987
H	3.2424040379	-0.7765577604	2.5353387774
C	-5.6333039626	3.1451630021	-2.3437531589
C	-4.9792834305	2.3057356921	-1.2403352285
C	-4.4255392819	3.1867143196	-0.2503605735
N	-4.0044453612	3.9149807652	0.5270752449
C	-5.9787126055	1.3414779035	-0.5796140113
C	-5.2647179063	0.2909091631	0.2662966242
C	-6.2399126833	-0.6940327691	0.9099449427
C	-5.5290730114	-1.9164462921	1.4985728542
C	-5.1638949091	-2.9270371419	0.4107126765
C	-4.2553557271	-4.0820820317	0.8587684585
C	-2.8907786540	-3.6172107013	1.3851710985
C	-2.1552659345	-2.5900500856	0.5128312834
C	-1.8568380681	-3.1114450675	-0.8986516434
C	-1.1464817794	-2.0633798681	-1.7754394753
C	-1.9054136311	-0.8415391342	-1.7949627535
N	-2.5375111361	0.1130344750	-1.8372505818
C	-4.9585302042	-4.9532746584	1.9089404098
C	-4.2779802169	-6.2993716992	2.1317508346
C	-0.8335116410	-2.2635205343	1.1933207609
O	0.0212788565	-3.0998905831	1.3992286153
C	-0.9844832951	-2.5616380411	-3.2240784448
C	-0.0892409884	-1.6476207845	-4.0647428283
C	1.3931433463	-1.8673618934	-3.7676921699
C	2.2822771808	-0.8189490775	-4.4300055457
C	3.7745482546	-1.0462121462	-4.1784375362
C	4.1733012648	-0.9983216119	-2.6899573185
C	5.4535505527	-0.1765049945	-2.4883818589
C	5.2235570416	1.3231228582	-2.6373923358
C	4.3664749460	-2.4209892612	-2.1402923892
C	4.2728362978	-2.5265944356	-0.6147023594
C	2.8567723214	-2.4521048457	-0.0986917142
O	1.9879398603	-1.7337331074	-0.5458055347
O	2.6444797687	-3.2735027025	0.9097990513
H	-4.1508499013	1.7232198388	-1.6623331378
H	-6.4645393787	3.7235254216	-1.9441903765

H	-4.9133406209	3.8318424259	-2.7844970693
H	-6.0092519751	2.4911083127	-3.1265334247
H	-6.5449415099	0.8423840593	-1.3692123845
H	-6.6868061091	1.9040531475	0.0348974329
H	-4.5652351766	-0.2443136500	-0.3782501987
H	-4.6793801652	0.7834972660	1.0470612968
H	-6.7939080891	-0.1786696203	1.6976853178
H	-6.9655676054	-1.0290949426	0.1645503875
H	-4.6340675804	-1.5823721053	2.0240844856
H	-6.1847430044	-2.3956722219	2.2269782852
H	-6.0888534359	-3.3579790066	0.0172437019
H	-4.6847931370	-2.4023448625	-0.4166975286
H	-4.0860346194	-4.7115348893	-0.0228610805
H	-5.9840379195	-5.1334469690	1.5775468723
H	-5.0064359563	-4.4151559300	2.8570995203
H	-4.8675345402	-6.9079161282	2.8136495212
H	-4.1798019655	-6.8385293830	1.1917981347
H	-3.2884577275	-6.1745550860	2.5625762235
H	-3.0216690467	-3.1834734862	2.3793618613
H	-2.2386756722	-4.4856673395	1.4920770786
H	-2.7274046468	-1.6612838032	0.4571481768
H	-1.2155069802	-3.9915691463	-0.8202396499
H	-2.7883079540	-3.4070759101	-1.3849285092
H	-0.1610015284	-1.8403794921	-1.3510420861
H	-1.9750810776	-2.6318113513	-3.6824924817
H	-0.5560654253	-3.5656185049	-3.2000641246
H	-0.2766534720	-1.8392928309	-5.1242086833
H	-0.3560143176	-0.6052578407	-3.8709323832
H	1.5539142269	-1.8314119021	-2.6923281910
H	1.6795745854	-2.8609685605	-4.1223039796
H	2.0074128718	0.1697022249	-4.0549406403
H	2.1027377098	-0.8234546348	-5.5090937671
H	4.0685604576	-2.0091178470	-4.6025920833
H	4.3233238579	-0.2790850726	-4.7272329258
H	3.3697925782	-0.5186423044	-2.1262325383
H	6.2069037540	-0.5048297005	-3.2087963339
H	5.8543290032	-0.3654370323	-1.4906603159
H	6.1552930073	1.8651695994	-2.4918453797
H	4.8377604002	1.5693353316	-3.6240255467
H	4.5065481842	1.6721608946	-1.8971628563
H	3.6171951204	-3.0844127692	-2.5744046391
H	5.3484709787	-2.7845264095	-2.4519557432
H	4.6960837595	-3.4710883776	-0.2706715233
H	4.8414558716	-1.7226153409	-0.1428736850
H	1.7033763682	-3.2194642429	1.2249684080
O	-0.7361124916	-1.0030540221	1.5200376326

H	0.1697783930	-0.7250867418	1.8811644207