

## Supporting Information

# Aggregation of coronene: the effect of carboxyl and amine functional groups

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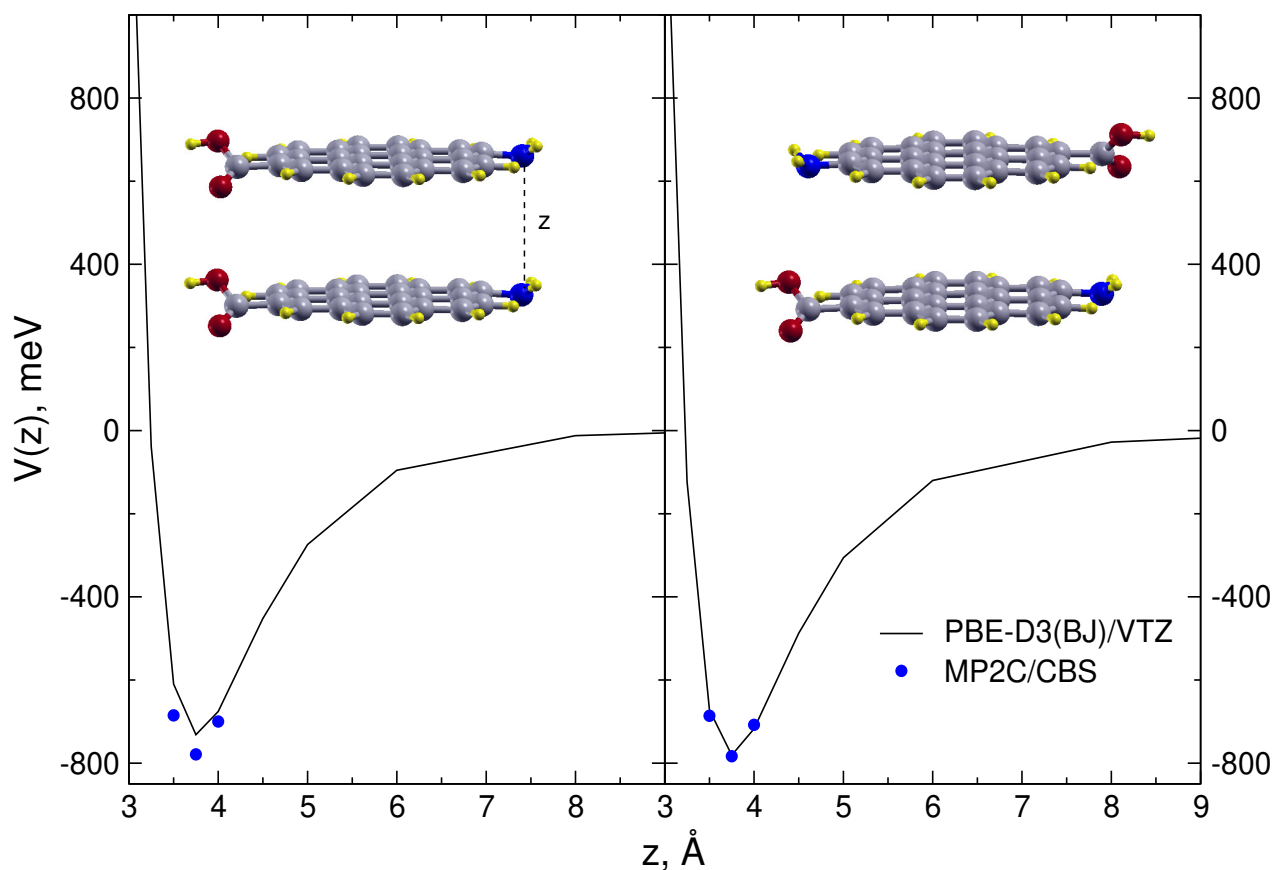


Figure S1: Interaction energy for two different parallel approaches of the R-Cor-R' dimer obtained at the PBE-D3(BJ) level of theory, together with the cc-pVTZ basis set, as a function of the distance  $z$  between the aromatic planes of the monomers. A comparison is provided in the well region with benchmark estimations (blue circles) computed at the MP2C level and exploiting a complete basis set (CBS) extrapolation scheme. In all calculations monomers are considered as rigid bodies.

## Cartesian coordinates and energies of the structures displayed in Fig. 2

All coordinates are in Å, while the energies are in  $\text{kJ mol}^{-1}$ .

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(R-Cor-R')<sub>2</sub> Energy=-112.28 (M1)

C 4.460989 -0.556509 0.728118

C 4.328785 0.801247 0.985401

C 3.107471 1.377709 1.394105  
C 1.957879 0.538178 1.495766  
C 2.083635 -0.869421 1.281641  
C 3.348341 -1.451183 0.931399  
C 3.410755 -2.863909 0.751711  
C 2.292533 -3.655636 0.911502  
C 1.024187 -3.105579 1.228714  
C 0.920059 -1.694051 1.407938  
C -0.350494 -1.111178 1.696480  
C -1.514864 -1.932185 1.800205  
C -1.372798 -3.341846 1.628190  
C -0.147651 -3.906382 1.357188  
C -2.771558 -1.330446 2.045618  
C -2.920556 0.043484 2.208045  
C -1.750672 0.887501 2.155102  
C -0.477965 0.296615 1.885534  
C 0.687396 1.120509 1.797293  
C 0.587175 2.530677 2.001662  
C 1.760786 3.336091 1.921728  
C 2.982827 2.777572 1.632291  
C -0.688605 3.087744 2.279860  
C -1.813604 2.294355 2.353074  
N -4.171743 0.591895 2.462145  
C 5.761166 -0.928457 0.114584  
D 6.218931 -2.179790 0.408145  
D 6.404997 -0.177234 -0.613317  
H 5.197329 1.448120 0.834414

H 4.364141 -3.325949 0.500618  
H 2.375115 -4.739337 0.775669  
H -2.264448 -3.971701 1.707942  
H -0.058640 -4.989526 1.222444  
H -3.658785 -1.971057 2.097377  
H 1.668366 4.414278 2.086208  
H 3.878960 3.403826 1.567002  
H -0.770645 4.167944 2.435420  
H -2.767725 2.775170 2.584097  
H -4.278969 1.565226 2.188560  
H -4.960931 0.046565 2.109267  
H 7.064960 -2.273425 -0.077906  
C 2.843297 -0.080138 -2.170948  
C 2.864196 1.293806 -1.964585  
C 1.621007 1.994654 -1.752155  
C 0.408354 1.243270 -1.665786  
C 0.413316 -0.172034 -1.841714  
C 1.647396 -0.833265 -2.122285  
C 1.641691 -2.247955 -2.302414  
C 0.476660 -2.972105 -2.197047  
C -0.764545 -2.337825 -1.906835  
C -0.794494 -0.922381 -1.730452  
C -2.029717 -0.264589 -1.432226  
C -3.233459 -1.029222 -1.279887  
C -3.165394 -2.441239 -1.461782  
C -1.975111 -3.064427 -1.767991  
C -4.425406 -0.326887 -0.882529

C -4.417266 1.053388 -0.733480  
C -3.256373 1.828556 -0.955030  
C -2.035803 1.154873 -1.265102  
C -0.828393 1.909926 -1.398825  
C -0.860616 3.330142 -1.249191  
C 0.353763 4.054859 -1.383301  
C 1.549718 3.408814 -1.619962  
C -2.102710 3.974969 -0.973708  
C -3.261178 3.248836 -0.825930  
N 4.070072 1.987941 -2.004512  
C -5.687329 -0.990940 -0.469516  
O -6.375740 -0.618214 0.477338  
O -6.056993 -2.063920 -1.224740  
H 2.589440 -2.754568 -2.508004  
H 0.491613 -4.059621 -2.322544  
H -4.072834 -3.035320 -1.363250  
H -1.951286 -4.151363 -1.898343  
H 0.330310 5.145526 -1.291939  
H 2.454784 4.012364 -1.730876  
H -2.116106 5.064796 -0.870188  
H -4.207208 3.753125 -0.602484  
H 3.787900 -0.605501 -2.347038  
H -5.340896 1.553750 -0.427229  
H 4.106035 2.823493 -1.425134  
H 4.892025 1.403447 -1.840355  
H -6.891290 -2.393771 -0.829362

(R-Cor-R')<sup>2</sup> Energy=-111.83 (M2)

C 2.578621 -2.392299 1.134653

C 1.929139 -3.513999 0.639898

C 0.525480 -3.591358 0.511762

C -0.257270 -2.459485 0.883213

C 0.382597 -1.308044 1.439083

C 1.810101 -1.260643 1.599781

C 2.373554 -0.079689 2.169577

C 1.588390 0.990142 2.539406

C 0.181442 0.981723 2.360842

C -0.424591 -0.183054 1.805068

C -1.836845 -0.204533 1.590549

C -2.631946 0.929415 1.934271

C -1.994640 2.075270 2.492120

C -0.634800 2.098851 2.698365

C -4.028719 0.892490 1.691956

C -4.647401 -0.201760 1.111813

C -3.870887 -1.355099 0.751188

C -2.466259 -1.346511 1.011903

C -1.669567 -2.478918 0.660481

C -2.277177 -3.624313 0.059731

C -1.467020 -4.745624 -0.285266

C -0.110082 -4.731613 -0.060807

C -3.674015 -3.597927 -0.200324

C -4.441367 -2.499710 0.126268

N -6.016734 -0.151969 0.768437

C 4.064470 -2.439789 0.953158

O 4.766425 -1.464408 1.587476  
O 4.624174 -3.266767 0.245110  
H 2.544932 -4.342582 0.280246  
H 3.449933 -0.024315 2.306766  
H 2.059014 1.884605 2.959517  
H -2.604331 2.950451 2.737347  
H -0.154718 2.993652 3.105910  
H -4.625350 1.774585 1.952637  
H -1.944819 -5.619598 -0.739734  
H 0.508503 -5.590642 -0.339021  
H -4.137197 -4.465967 -0.680474  
H -5.505050 -2.514564 -0.128233  
H -6.518654 0.579908 1.271075  
H -6.509188 -1.037277 0.886321  
H 5.651069 -1.447435 1.160324  
C 3.868781 0.824414 -0.959556  
C 3.418410 -0.375723 -1.495125  
C 2.053890 -0.609227 -1.784972  
C 1.103585 0.414232 -1.491398  
C 1.544479 1.647691 -0.918027  
C 2.933663 1.875897 -0.640484  
C 3.297830 3.103495 -0.012644  
C 2.355272 4.062851 0.290473  
C 0.980445 3.881991 -0.012367  
C 0.572036 2.654570 -0.614160  
C -0.808295 2.438673 -0.906239  
C -1.771209 3.455724 -0.629343

C -1.327252 4.677205 -0.041495  
C -0.000347 4.877644 0.265204  
C -3.139920 3.205830 -0.895355  
C -3.587307 1.994359 -1.405394  
C -2.629678 0.970134 -1.733856  
C -1.246582 1.202129 -1.466464  
C -0.282379 0.189590 -1.764603  
C -0.701669 -1.053357 -2.330005  
C 0.273297 -2.056045 -2.607311  
C 1.605926 -1.843115 -2.341696  
C -2.083671 -1.247232 -2.602448  
C -3.012825 -0.268992 -2.318073  
N -4.946846 1.769791 -1.651853  
C 5.339612 0.894277 -0.747549  
O 5.871238 2.150347 -0.833393  
O 6.066851 -0.073786 -0.547729  
H 4.148565 -1.161873 -1.706116  
H 4.343768 3.291317 0.222551  
H 2.669732 4.997027 0.768240  
H -2.065992 5.456614 0.173355  
H 0.322922 5.817918 0.724307  
H -3.870683 3.983811 -0.643284  
H -0.061344 -3.011357 -3.022942  
H 2.345343 -2.624540 -2.541137  
H -2.404688 -2.195174 -3.044576  
H -4.063222 -0.444195 -2.562762  
H -5.537296 2.525073 -1.305869



H -5.304420 0.878771 -1.298970

H 6.834941 2.034750 -0.698091

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(R-Cor-R')<sup>2</sup> Energy= -108.03 (M3)

C 4.227426 -0.613194 0.786786

C 3.834674 0.601449 1.337950

C 2.506311 0.849293 1.749935

C 1.527439 -0.171690 1.558240

C 1.915688 -1.435105 1.013424

C 3.275974 -1.688259 0.640089

C 3.602629 -2.963944 0.095440

C 2.637673 -3.936204 -0.069493

C 1.281195 -3.713199 0.282970

C 0.917303 -2.443648 0.823645

C -0.445018 -2.181624 1.155381

C -1.443590 -3.180362 0.942777

C -1.043400 -4.445857 0.417471

C 0.271435 -4.702179 0.101533

C -2.797915 -2.878177 1.217566

C -3.194687 -1.637670 1.705149

C -2.199113 -0.634413 1.985680

C -0.832102 -0.914657 1.684386

C 0.164206 0.087715 1.899863

C -0.201514 1.360939 2.434059

C 0.803439 2.352410 2.630489

C 2.114079 2.105043 2.298390

C -1.565917 1.602145 2.745034

C -2.527573 0.638448 2.528985  
N -4.538147 -1.376650 1.951984  
C 5.626212 -0.753420 0.324497  
O 6.203710 0.477111 0.034016  
O 6.271602 -1.777305 0.167390  
H 4.572097 1.398837 1.453476  
H 4.636084 -3.171947 -0.177920  
H 2.919013 -4.910469 -0.483679  
H -1.807497 -5.214676 0.262122  
H 0.559905 -5.676924 -0.305729  
H -3.559824 -3.637867 1.011170  
H 0.507139 3.326644 3.030464  
H 2.875675 2.879524 2.431307  
H -1.849440 2.576670 3.153309  
H -3.560971 0.872100 2.797794  
H -5.178232 -1.948629 1.402291  
H -4.805839 -0.396596 1.897112  
H 7.126702 0.270587 -0.218788  
C 2.992970 2.591076 -1.275100  
C 2.274208 3.678214 -0.793423  
C 0.869965 3.638256 -0.614302  
C 0.157915 2.441446 -0.929679  
C 0.876813 1.325639 -1.452913  
C 2.288398 1.393168 -1.655259  
C 2.950522 0.268134 -2.219132  
C 2.267216 -0.889433 -2.527740  
C 0.869682 -1.001463 -2.298246

C 0.168145 0.126462 -1.771785  
C -1.242966 0.047935 -1.555529  
C -1.930203 -1.166773 -1.850999  
C -1.201828 -2.283456 -2.356062  
C 0.152136 -2.201302 -2.577247  
C -3.321764 -1.230479 -1.622281  
C -4.056717 -0.142069 -1.166505  
C -3.390772 1.098292 -0.844855  
C -1.969938 1.167264 -1.041329  
C -1.251854 2.363770 -0.717729  
C -1.945705 3.488237 -0.178363  
C -1.211380 4.666730 0.140995  
C 0.146837 4.741913 -0.072897  
C -3.346062 3.386103 0.023810  
C -4.045458 2.241888 -0.297753  
N 4.377791 2.656717 -1.435595  
C -5.509161 -0.415576 -1.024901  
O -5.997888 -1.533945 -0.889408  
O -6.318965 0.687258 -1.082777  
H 2.810889 4.589553 -0.503909  
H 4.021980 0.322980 -2.427786  
H 2.802416 -1.746322 -2.947097  
H -1.741397 -3.213343 -2.557751  
H 0.704390 -3.065379 -2.958224  
H -3.852489 -2.163750 -1.827282  
H -1.751259 5.523735 0.557521  
H 0.693454 5.657493 0.176307

H -3.880709 4.245871 0.441913  
H -5.122731 2.215125 -0.144129  
H 4.898444 1.825501 -1.150082  
H 4.794282 3.488392 -1.020736  
H -7.232393 0.340579 -1.006306

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(R-Cor-R')<sup>2</sup> Energy= -94.85 (M4)

C 4.551831 -0.690428 0.636688  
C 4.427735 0.663771 0.926781  
C 3.202762 1.243243 1.325013  
C 2.045596 0.413237 1.411683  
C 2.156541 -0.987338 1.149991  
C 3.413955 -1.569362 0.777539  
C 3.463490 -2.975946 0.549941  
C 2.337709 -3.761127 0.689366  
C 1.078141 -3.211529 1.041294  
C 0.988612 -1.806450 1.269296  
C -0.271109 -1.224816 1.604347  
C -1.437444 -2.042072 1.708808  
C -1.311942 -3.445025 1.481625  
C -0.097272 -4.008038 1.164275  
C -2.683805 -1.439909 2.005045  
C -2.816205 -0.073202 2.218994  
C -1.644225 0.765619 2.167624  
C -0.383278 0.176412 1.844829  
C 0.785155 0.995328 1.754752  
C 0.699532 2.397958 2.011163

C 1.877963 3.196675 1.931516  
C 3.091053 2.637020 1.605931  
C -0.564385 2.952646 2.344075  
C -1.692759 2.163980 2.422639  
N -4.058519 0.479911 2.525394  
C 5.871525 -1.181715 0.169848  
O 6.255009 -2.339980 0.087762  
O 6.706664 -0.150407 -0.213115  
H 5.306555 1.306713 0.843125  
H 4.415103 -3.430261 0.279148  
H 2.409102 -4.840359 0.516394  
H -2.207240 -4.070233 1.555583  
H -0.019572 -5.086222 0.989388  
H -3.574617 -2.076601 2.047508  
H 1.798299 4.269131 2.135248  
H 3.993554 3.256260 1.558451  
H -0.633369 4.026637 2.542745  
H -2.636852 2.637957 2.702918  
H -4.182372 1.441057 2.214546  
H -4.850576 -0.083282 2.215370  
H 7.547779 -0.584639 -0.461474  
C 2.762495 0.335983 -2.175415  
C 2.686230 1.695442 -1.906344  
C 1.403753 2.297229 -1.647186  
C 0.248243 1.460236 -1.585374  
C 0.348008 0.060110 -1.837577  
C 1.620998 -0.500941 -2.158139

C 1.710830 -1.902781 -2.405249  
C 0.597620 -2.707836 -2.332202  
C -0.682484 -2.174249 -2.007191  
C -0.805082 -0.775752 -1.755207  
C -2.077549 -0.220531 -1.410229  
C -3.223807 -1.071747 -1.286169  
C -3.068601 -2.462261 -1.554533  
C -1.841787 -2.985639 -1.904500  
C -4.460700 -0.475598 -0.845061  
C -4.546003 0.896042 -0.638079  
C -3.438057 1.755947 -0.816627  
C -2.177388 1.184313 -1.167200  
C -1.026500 2.026454 -1.271456  
C -1.151788 3.431224 -1.044622  
C 0.008135 4.244517 -1.155655  
C 1.240408 3.695435 -1.444176  
C -2.430150 3.973881 -0.720364  
C -3.535615 3.163339 -0.605475  
N 3.834155 2.491582 -1.930961  
C -5.652082 -1.302282 -0.543441  
O -6.463173 -0.701390 0.406607  
O -5.949093 -2.393778 -1.002815  
H 2.689398 -2.334816 -2.634805  
H 0.685775 -3.784352 -2.509966  
H -3.939399 -3.112924 -1.485764  
H -1.748312 -4.059121 -2.098810  
H -0.089220 5.325167 -1.010099

H 2.101559 4.361690 -1.543422  
H -2.515814 5.052789 -0.555509  
H -4.511562 3.589986 -0.350353  
H 3.740275 -0.117435 -2.371053  
H 3.844708 3.235083 -1.234498  
H 4.698128 1.952903 -1.880752  
H -5.499711 1.327583 -0.323966  
H -7.236132 -1.295534 0.497957

## Cartesian coordinates and energies of the structures displayed in Fig. 3

All coordinates are in Å, while the energies are in kJ mol<sup>-1</sup>.

82

(R-Cor-R')<sub>2</sub>      Energy=-114.41542785

C	5.21827360	-1.55015898	-1.80329237
C	6.23150132	-0.80477215	-2.42298502
C	6.33598132	-0.75263134	-3.81319775
C	5.41046839	-1.46439117	-4.60815854
C	4.38682428	-2.22767788	-3.99200869
C	4.28127193	-2.28649320	-2.57455178
C	3.26256046	-3.10043130	-2.03052019
C	2.36935858	-3.80426037	-2.83853713
C	2.46795413	-3.73684126	-4.22705136
C	3.48167438	-2.94719630	-4.81454928
C	3.59057447	-2.89246538	-6.22773946
C	2.68959671	-3.62530351	-7.03018179

C	1.69376170	-4.40058246	-6.42564750
C	1.58186192	-4.45337410	-5.03834179
C	2.80444163	-3.57194322	-8.42311965
C	3.76355355	-2.76675974	-9.04899296
C	4.71963148	-2.08110716	-8.25616998
C	4.60931597	-2.12700836	-6.83977409
C	5.52501617	-1.41971475	-6.02129799
C	6.56659572	-0.67119879	-6.61584764
C	7.46894511	0.02934918	-5.80899723
C	7.35326236	-0.00896771	-4.42157685
C	6.69029386	-0.64756686	-8.00536868
C	5.78598234	-1.34283964	-8.80868596
N	3.86409273	-2.83937859	-10.45615447
C	5.25291267	-1.52634307	-0.32083196
O	4.03922857	-1.41243532	0.24204931
O	6.26357372	-1.49777151	0.35855744
H	6.94684439	-0.26277406	-1.80478176
H	3.14349473	-3.20851956	-0.95539409
H	1.60049355	-4.41096662	-2.36480171
H	0.99373519	-4.97278910	-7.03058469
H	0.79827200	-5.06584657	-4.59763012
H	2.12564418	-4.16000169	-9.03693413
H	8.27501131	0.60927673	-6.25333462
H	8.07268541	0.54355412	-3.82047729
H	7.49517484	-0.09219128	-8.48182668
H	5.93863545	-1.30597799	-9.88356657
H	2.99608449	-3.11192970	-10.90720617



H	4.24443661	-1.99798887	-10.87529161
H	4.23093760	-1.34314498	1.20095613
C	3.33178381	1.10875782	-10.19073121
C	4.30987388	1.87430381	-9.53993933
C	4.36063990	1.93995752	-8.14730206
C	3.41049322	1.22854138	-7.38163421
C	2.41229411	0.45773380	-8.02936003
C	2.35535252	0.39325516	-9.44935468
C	1.30827817	-0.36024294	-10.02564850
C	0.37420322	-1.04287892	-9.24616890
C	0.43813133	-0.98698151	-7.85511647
C	1.45960894	-0.23239921	-7.23583402
C	1.51360293	-0.16353257	-5.82009986
C	0.54961290	-0.84575788	-5.04678350
C	-0.45288144	-1.58673184	-5.68252653
C	-0.50632820	-1.65939859	-7.07241452
C	0.60428803	-0.77049308	-3.65119817
C	1.62527407	-0.07325690	-2.99440085
C	2.55846329	0.67459135	-3.75771837
C	2.51265429	0.60203146	-5.17655252
C	3.45632616	1.30555548	-5.96599003
C	4.44555619	2.09793714	-5.33972440
C	5.37890988	2.79024772	-6.11790587
C	5.33838552	2.71004085	-7.50776579
C	4.47405518	2.18978636	-3.94782643
C	3.54532314	1.49421854	-3.17313654
N	1.55451057	0.02195456	-1.58677432

C	3.39341848	1.15799060	-11.67168807
O	3.18769608	-0.03290641	-12.25673680
O	3.70633117	2.13369419	-12.33040668
H	5.03650100	2.42641540	-10.13562274
H	1.19346995	-0.42960895	-11.10442710
H	-0.40749178	-1.61267601	-9.74412006
H	-1.20421280	-2.11575787	-5.10025580
H	-1.29819210	-2.24231787	-7.53773070
H	-0.15677124	-1.27494067	-3.05987053
H	6.14541147	3.40352212	-5.64900904
H	6.07590493	3.26298906	-8.08611168
H	5.21595973	2.80805017	-3.44721164
H	3.60058813	1.61511688	-2.09500879
H	1.04957439	-0.74722999	-1.15716446
H	2.45873033	0.15524069	-1.14757562
H	3.32500462	0.14744870	-13.21050521

123

(R-Cor-R')3      Energy=-230.44488434

C	-2.92760113	2.07466445	6.66404650
C	-2.43601264	0.95764364	5.97349876
C	-2.43193918	0.92077668	4.57888397
C	-2.93420286	2.02268181	3.85178345
C	-3.44099414	3.15398769	4.53982713
C	-3.45087482	3.19187378	5.96188608
C	-4.00936746	4.33350552	6.57913933
C	-4.51128352	5.40291348	5.83716681
C	-4.49098083	5.36831524	4.44410223

C	-3.95580466	4.23928820	3.78440071
C	-3.95057586	4.19880804	2.36655192
C	-4.47895643	5.28187804	1.63136507
C	-5.00380192	6.38938434	2.30677125
C	-5.00691440	6.43378021	3.69887217
C	-4.47603805	5.23479811	0.23347826
C	-3.91425770	4.15763346	-0.46226067
C	-3.44426001	3.03183626	0.26193238
C	-3.44051188	3.07157195	1.68279859
C	-2.94002806	1.97891568	2.43399261
C	-2.45124722	0.83221340	1.76704393
C	-1.95457783	-0.24531531	2.50749032
C	-1.94273726	-0.20043306	3.89947859
C	-2.47921776	0.78287849	0.37298075
C	-2.97024904	1.86096086	-0.36399205
N	-4.03123521	4.15304192	-1.87001787
C	-2.88689424	1.95423655	8.14164454
O	-2.49722205	3.08013772	8.76079039
O	-3.07155673	0.92638650	8.76873791
H	-2.05566984	0.10755034	6.53947902
H	-4.07010340	4.41422215	7.66152181
H	-4.92431288	6.25940606	6.36584287
H	-5.41676745	7.23049314	1.75413935
H	-5.42286192	7.30769811	4.19547827
H	-4.90931558	6.05921578	-0.32861876
H	-1.57540491	-1.13374704	2.00707912
H	-1.55332898	-1.05588020	4.44787805

H	-2.12426479	-0.09722122	-0.15873394
H	-2.98639865	1.76322566	-1.44575779
H	-4.11219366	5.08321758	-2.26925342
H	-3.30233895	3.62016665	-2.33156770
H	-2.45588744	2.82548536	9.70657018
C	3.22165258	5.00155712	7.32024607
C	2.65824610	6.24963269	7.01836623
C	2.46795028	6.65000020	5.69555879
C	2.85227473	5.78764339	4.64495214
C	3.43020295	4.52676189	4.93867197
C	3.62991414	4.11835404	6.28667164
C	4.24944105	2.86712865	6.50314352
C	4.63190019	2.04001308	5.44688542
C	4.42569783	2.43744098	4.12712414
C	3.82340660	3.68810509	3.86367347
C	3.62890640	4.09801337	2.51975902
C	4.03829960	3.25650184	1.46288538
C	4.63276976	2.02227539	1.74836185
C	4.82166752	1.61528028	3.06692102
C	3.84885812	3.66760480	0.13947355
C	3.21462663	4.87708849	-0.16847632
C	2.86223092	5.76394588	0.88132078
C	3.04825098	5.35377574	2.22950873
C	2.66878315	6.20094214	3.30048375
C	2.11174983	7.47154366	3.02856643
C	1.73440284	8.30700600	4.08479623
C	1.90846174	7.89925329	5.40510953

C	1.95346048	7.88447851	1.70529105
C	2.32567798	7.04745332	0.65298635
N	3.14205008	5.25232318	-1.52840894
C	3.38097113	4.73030572	8.76955494
O	3.06145870	3.47361604	9.11809800
O	3.66284209	5.56196659	9.61377707
H	2.36950049	6.91375342	7.83275099
H	4.45342694	2.50734408	7.50847962
H	5.09955926	1.08401173	5.67277827
H	4.95575881	1.36402492	0.94475066
H	5.28767013	0.65091729	3.25720517
H	4.19094819	3.02836818	-0.67151220
H	1.30454031	9.28715085	3.88978676
H	1.60845613	8.57294722	6.20529931
H	1.54328355	8.86528828	1.47495493
H	2.19820602	7.42513210	-0.35752823
H	3.15531352	4.46094032	-2.16457503
H	2.36570349	5.87178093	-1.73293801
H	3.15086948	3.47101113	10.09434320
C	-0.75203215	5.46230405	-0.79047282
C	-1.19619285	6.42830600	0.12375496
C	-1.09039156	6.21729901	1.49874889
C	-0.53177814	5.01138727	1.97714916
C	-0.08675642	4.02442476	1.06175025
C	-0.19819810	4.23510840	-0.34073961
C	0.22705404	3.19075964	-1.19205327
C	0.76305339	2.00339413	-0.69311023

C	0.88110568	1.80334778	0.68103798
C	0.45385078	2.81493079	1.57012445
C	0.55989533	2.60314402	2.96864585
C	1.08799324	1.38836924	3.45666342
C	1.50454107	0.40098480	2.55679321
C	1.40522404	0.60745914	1.18295547
C	1.18572235	1.18248318	4.83665347
C	0.81806817	2.17461412	5.75340866
C	0.22062708	3.37118181	5.28005609
C	0.11966557	3.59068035	3.87931310
C	-0.43548048	4.79344010	3.37547175
C	-0.90583934	5.78037850	4.27178001
C	-1.45121267	6.96875888	3.77546412
C	-1.54029394	7.18609697	2.40265144
C	-0.83052323	5.55346387	5.64635837
C	-0.28134361	4.36954173	6.13954426
N	0.86933037	1.85006422	7.12728081
C	-0.95337895	5.82175503	-2.21515186
O	0.08533809	5.49764969	-3.00182972
O	-1.90046740	6.44891045	-2.65506278
H	-1.63233195	7.35415026	-0.25074203
H	0.14582451	3.27804032	-2.27258078
H	1.07988848	1.23553562	-1.39573389
H	1.91121276	-0.54125129	2.91764753
H	1.73613355	-0.17921375	0.50841330
H	1.56743532	0.23412124	5.20847575
H	-1.81684526	7.73655085	4.45392025

H	-1.97280015	8.11916203	2.04698511
H	-1.20298477	6.29245050	6.35237453
H	-0.26357500	4.23570947	7.21741405
H	1.54704085	1.12546335	7.34368816
H	0.99589404	2.65849855	7.72618785
H	-0.16589198	5.85293158	-3.88030227

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(R-Cor-R')4      Energy=-348.71155124

C	-11.42281157	8.61750045	-11.17372721
C	-12.03840454	8.82546393	-9.93113016
C	-11.27894184	8.98419612	-8.77167052
C	-9.86963009	8.93036593	-8.84965498
C	-9.23693737	8.71266372	-10.09961506
C	-10.00931299	8.54548283	-11.28252296
C	-9.31238564	8.29046730	-12.48481160
C	-7.91952786	8.22887431	-12.53203296
C	-7.16433889	8.40345300	-11.37382309
C	-7.82029072	8.64530596	-10.14599735
C	-7.05080356	8.80680051	-8.96541689
C	-5.64301875	8.72352705	-9.02813686
C	-5.01560681	8.48303907	-10.25562466
C	-5.76821558	8.32779961	-11.41726418
C	-4.88912072	8.87845743	-7.86025548
C	-5.49358178	9.16549180	-6.63055161
C	-6.90926025	9.18191417	-6.53913218
C	-7.68385619	9.02832085	-7.72102218
C	-9.09918809	9.08040627	-7.66813592

C	-9.74985395	9.27389747	-6.42803574
C	-11.14637796	9.32824765	-6.37534596
C	-11.90327468	9.18730531	-7.53596157
C	-8.99008177	9.39848685	-5.26448421
C	-7.59688126	9.34922115	-5.31986899
N	-4.66387004	9.22114652	-5.48863825
C	-12.36318034	8.44348407	-12.30725303
O	-11.97873833	9.07983238	-13.42533379
O	-13.44257834	7.88230062	-12.24564828
H	-13.12624995	8.85964112	-9.87565758
H	-9.84394218	8.12865638	-13.41916738
H	-7.43565415	8.03538747	-13.48707235
H	-3.93185369	8.41370528	-10.31948826
H	-5.25200607	8.14066121	-12.35634321
H	-3.80631456	8.78598297	-7.90848667
H	-11.65987833	9.47666897	-5.42783190
H	-12.98811730	9.23052142	-7.46234477
H	-9.47187999	9.53026767	-4.29815511
H	-7.05435773	9.43310874	-4.38249971
H	-3.70387964	9.47444510	-5.70177742
H	-5.03893281	9.80346260	-4.74802366
H	-12.72074536	8.92900304	-14.04801498
C	-9.66638184	2.87968193	-2.90699724
C	-8.30210336	2.77927823	-3.21507881
C	-7.87623027	2.56944535	-4.52692043
C	-8.83313505	2.45208608	-5.55924738
C	-10.21545769	2.54408665	-5.25789292



C	-10.65239627	2.75298164	-3.92027107
C	-12.04564206	2.79222058	-3.68882965
C	-12.97025058	2.66005159	-4.72502789
C	-12.53987360	2.46603964	-6.03627661
C	-11.15543221	2.40468690	-6.31173909
C	-10.71942168	2.19114258	-7.64450119
C	-11.66893488	2.04145010	-8.67830154
C	-13.03488931	2.10578114	-8.38125519
C	-13.46612558	2.31913863	-7.07418231
C	-11.23384335	1.82601815	-9.99001684
C	-9.87259106	1.80436794	-10.31629428
C	-8.90801186	1.88254174	-9.27887027
C	-9.34041846	2.10434487	-7.94310021
C	-8.39900771	2.22722801	-6.89080759
C	-7.01702093	2.11576805	-7.16710923
C	-6.08722324	2.23972001	-6.12974641
C	-6.51249600	2.46679285	-4.82308387
C	-6.59418296	1.87201540	-8.47417508
C	-7.52304005	1.75388416	-9.50847278
N	-9.52220167	1.49599233	-11.64956728
C	-9.96123453	3.07893442	-1.46726941
O	-10.93880458	3.97050757	-1.23859160
O	-9.33164196	2.58981162	-0.54629484
H	-7.56832533	2.86407123	-2.41380927
H	-12.44545525	2.92380478	-2.68653685
H	-14.03143291	2.70424435	-4.48920972
H	-13.77854653	1.98976231	-9.16669781

H	-14.53451788	2.36309215	-6.87426120
H	-11.96910070	1.68358266	-10.77897547
H	-5.02088870	2.15612450	-6.32833357
H	-5.76531409	2.55514449	-4.03690086
H	-5.53649579	1.76536671	-8.70485137
H	-7.14140805	1.54597398	-10.50404320
H	-10.24466549	1.73804028	-12.32085624
H	-8.62423711	1.87682210	-11.92688010
H	-10.96824616	4.04081692	-0.26122496
C	-7.52364713	4.94438777	-11.44368660
C	-6.46088070	5.05312540	-10.53541651
C	-6.69683684	5.26515653	-9.17685342
C	-8.02528699	5.37625619	-8.70993161
C	-9.10719993	5.27580772	-9.62068351
C	-8.86902058	5.06465450	-11.00721499
C	-9.99348489	5.01687611	-11.86134372
C	-11.29525117	5.14298365	-11.37598017
C	-11.52685745	5.33922222	-10.01580108
C	-10.43082774	5.40904506	-9.12688864
C	-10.66758881	5.62484338	-7.74510122
C	-11.99036849	5.76832085	-7.27351405
C	-13.05996474	5.69564119	-8.17289608
C	-12.83095649	5.48005078	-9.52973124
C	-12.21814189	5.98600800	-5.91077997
C	-11.16609201	6.01596895	-4.98761861
C	-9.82869680	5.94410315	-5.45557383
C	-9.58729874	5.72006946	-6.83832096

C	-8.26321743	5.60335678	-7.33011471
C	-7.17003228	5.72327043	-6.44173397
C	-5.86317858	5.60541222	-6.92573014
C	-5.62900868	5.37614347	-8.27938678
C	-7.40663802	5.96920349	-5.08889877
C	-8.71119800	6.08124790	-4.60716074
N	-11.47937187	6.32606705	-3.64553812
C	-7.11222320	4.74378916	-12.85434122
O	-7.86544218	3.84626268	-13.51004451
O	-6.12865930	5.23709911	-13.37690165
H	-5.43772056	4.97313550	-10.90201966
H	-9.87921557	4.88315151	-12.93410469
H	-12.12387776	5.09230658	-12.07917357
H	-14.08466245	5.80680043	-7.82498118
H	-13.68269694	5.42955654	-10.20452824
H	-13.23719603	6.12363418	-5.55590726
H	-5.01285971	5.69553541	-6.25317527
H	-4.60100322	5.29267293	-8.62638535
H	-6.57905785	6.08231537	-4.39204556
H	-8.83884739	6.29118679	-3.54902021
H	-12.43009159	6.07933499	-3.38780699
H	-10.81209346	5.95070672	-2.98061841
H	-7.43547726	3.77609406	-14.38825993
C	-6.23950628	12.83567570	-5.08512615
C	-7.61909411	12.92523807	-4.85067590
C	-8.53471803	12.78824530	-5.89431950
C	-8.06536779	12.56033402	-7.20691453

C	-6.67231084	12.47593487	-7.45664163
C	-5.73650681	12.62032020	-6.39494095
C	-4.36374764	12.56657303	-6.72491390
C	-3.92643472	12.35365484	-8.03239223
C	-4.84505567	12.20190825	-9.06938148
C	-6.22818660	12.26418928	-8.78761632
C	-7.16150757	12.12555450	-9.84669779
C	-6.70138317	11.92867745	-11.16664146
C	-5.32663867	11.87057098	-11.42141139
C	-4.40774652	12.00255557	-10.38307478
C	-7.62574967	11.79762073	-12.20812275
C	-9.00513430	11.80643047	-11.96905387
C	-9.48179854	12.07378247	-10.65982247
C	-8.55013947	12.20553374	-9.59440859
C	-8.99713963	12.43277640	-8.26880462
C	-10.38122391	12.54275123	-8.00259116
C	-10.82332238	12.76417228	-6.69433617
C	-9.90928120	12.88322938	-5.65023842
C	-11.29414450	12.43944327	-9.05260635
C	-10.85137869	12.21334019	-10.35619296
N	-9.86543773	11.75370147	-13.08824232
C	-5.39493496	13.02571614	-3.88095015
O	-4.35617547	12.17747531	-3.81533291
O	-5.64190046	13.78580311	-2.96165809
H	-7.97553184	13.10766542	-3.83710532
H	-3.59744303	12.69452614	-5.96454484
H	-2.85678461	12.31545848	-8.22748413

H	-4.95673894	11.72190669	-12.43357722
H	-3.34550309	11.95424741	-10.61256918
H	-7.26645966	11.67380815	-13.22740097
H	-11.88543350	12.85075888	-6.47543632
H	-10.28372110	13.05884173	-4.64369700
H	-12.36216635	12.53877346	-8.87163541
H	-11.60274168	12.15941887	-11.13886544
H	-9.44984707	11.29433577	-13.89287739
H	-10.77688785	11.36332191	-12.87578870
H	-3.94342826	12.37861060	-2.94916889

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(R-Cor-R')5      Energy=-464.66823544

C	-3.89670528	-1.62671476	5.00647103
C	-4.42243864	-1.65547090	3.70684476
C	-3.58629782	-1.57925066	2.59267011
C	-2.19027086	-1.46713198	2.77618313
C	-1.64854772	-1.42914119	4.08583471
C	-2.49948601	-1.50161961	5.22356734
C	-1.89321626	-1.41563969	6.49686349
C	-0.51221441	-1.29158219	6.65022566
C	0.32057579	-1.23139229	5.53439599
C	-0.24415272	-1.29804971	4.24096636
C	0.60341556	-1.22050892	3.10625203
C	1.99701349	-1.07692853	3.27944502
C	2.53341360	-1.01301957	4.57033506
C	1.70418661	-1.09269207	5.68656109
C	2.82788084	-0.99584327	2.15721635

C	2.31736432	-1.10403811	0.85813966
C	0.91348300	-1.17740625	0.66707130
C	0.06123609	-1.26320701	1.80142890
C	-1.34240490	-1.37810744	1.64248201
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C	1.78176496	1.73860490	-6.39225566
C	0.98701709	2.34579024	-5.42291185
C	2.54433335	-0.26010354	-7.54715910
C	2.56029928	-1.65004276	-7.71373505
C	1.66169758	-2.45035662	-6.96221296
C	0.85051522	-1.83828702	-5.96832779
C	-0.02773313	-2.61666029	-5.17366489
C	-0.10943847	-4.01319515	-5.37779232
C	-0.97374843	-4.78244210	-4.59214808
C	-1.76056570	-4.18216407	-3.61216296

C	0.66764586	-4.60995946	-6.37109023
C	1.53310531	-3.84158768	-7.15024807
N	3.32865138	-2.17476976	-8.77664698
C	-3.38309024	-0.31882748	-1.16838514
O	-2.84228417	0.61685673	-0.37160207
O	-4.49362408	-0.76645254	-0.94440199
H	-3.18089842	-2.80593081	-1.83288030
H	-2.14871083	1.95797679	-2.15555314
H	-0.65416645	3.26566568	-3.52283083
H	2.42870987	2.36170809	-7.00594226
H	1.03422156	3.42633769	-5.30650129
H	3.17608329	0.35604562	-8.18324022
H	-1.04643608	-5.85797018	-4.73860717
H	-2.42595065	-4.80668460	-3.01936658
H	0.60642817	-5.68017417	-6.55596996
H	2.10147415	-4.35330161	-7.92169852
H	4.10901564	-1.58055656	-9.03953921
H	3.63372260	-3.12881344	-8.61851323
H	-3.53963395	0.78822356	0.29577524
C	10.75939778	1.35842141	7.19885407
C	10.11617734	2.34382386	6.43629234
C	9.87528226	2.15446335	5.07524924
C	10.28907110	0.95466175	4.45525421
C	10.94738497	-0.04508488	5.21500683
C	11.19867234	0.14777142	6.60189030
C	11.89634671	-0.87308666	7.28551147
C	12.30604701	-2.04323162	6.64599387

C	12.04951560	-2.23474760	5.28961949
C	11.36811741	-1.23295613	4.56268618
C	11.12202403	-1.42252329	3.17868346
C	11.55945442	-2.60477789	2.54334494
C	12.23251172	-3.58289864	3.28393944
C	12.47232197	-3.40138414	4.64389134
C	11.31875638	-2.78457821	1.17731095
C	10.60704153	-1.84006963	0.42811205
C	10.22363282	-0.61682941	1.03593921
C	10.46136595	-0.42613206	2.42430920
C	10.05374981	0.76846065	3.06888005
C	9.41615137	1.78699986	2.32409855
C	9.01105225	2.96496531	2.95994568
C	9.23613459	3.14582716	4.32244813
C	9.20643601	1.61036257	0.95609009
C	9.60658966	0.43235470	0.32468155
N	10.48437808	-2.06215472	-0.96153432
C	10.96422229	1.71596176	8.62351815
O	10.72776267	0.70113714	9.47031048
O	11.21292107	2.83360027	9.03927668
H	9.80483394	3.27033130	6.91826968
H	12.14199489	-0.77694014	8.34010555
H	12.83466063	-2.79856231	7.22367401
H	12.57789796	-4.49804325	2.80788774
H	12.99905689	-4.17906941	5.19263391
H	11.68191558	-3.68457458	0.68591609
H	8.51934287	3.75673640	2.39886206

H	8.91269052	4.07467873	4.78805446
H	8.73361210	2.38909615	0.36170031
H	9.43612410	0.35389559	-0.74527907
H	10.53205367	-3.04379225	-1.21704328
H	9.66829743	-1.61855761	-1.36836113
H	10.83706989	1.10505207	10.35685458

## Cartesian coordinates and energies of the structures displayed in Fig. 7

All coordinates are in Å, while the energies are in kJ mol<sup>-1</sup>.

123

```
(R-Cor-R')3   Energy=-230.44488434   (GM)
C -4.0495668200  1.1227645900 -3.0510722700
C -5.1102835800  0.2081401900 -2.9833001800
C -5.2390170900  -0.6625139100 -1.9008421900
C -4.2847768200  -0.6253224700 -0.8600822800
C -3.2038316500  0.2899870800 -0.9222151600
C -3.0675768600  1.1753220000 -2.0273854400
C -1.9428891700  2.0303651600 -2.0421316700
C -1.0073395000  2.0376858000 -1.0073517200
C -1.1484424700  1.1769268400  0.0795807300
C -2.2499767900  0.2934317200  0.1283681000
C -2.3833662500  -0.5931617900  1.2275133900
C -1.4177136300  -0.5851000800  2.2571620600
C -0.3351418400  0.2988244500  2.1870032200
C -0.2034085400  1.1732527000  1.1109236700
```

C -1.5511481100 -1.4648719000 3.3362864100  
C -2.6502984400 -2.3245425800 3.4492835800  
C -3.5902332600 -2.3938135800 2.3888606500  
C -3.4645845800 -1.5017230500 1.2893877500  
C -4.4105818700 -1.5191016900 0.2341809700  
C -5.4829148700 -2.4398220500 0.2662642500  
C -6.4184692300 -2.4557347100 -0.7732040200  
C -6.2991019100 -1.5741627200 -1.8448234700  
C -5.5911968700 -3.3329726700 1.3326532000  
C -4.6598418900 -3.3119875900 2.3712290300  
N -2.6607448700 -3.2382019700 4.5265962300  
C -4.0359167100 1.9630283000 -4.2730487400  
O -3.7194139800 3.2464835400 -4.0376595700  
O -4.3788205700 1.5958861100 -5.3827539300  
H -5.8400496800 0.1792203300 -3.7921623500  
H -1.7667117600 2.7131711700 -2.8694727900  
H -0.1636257700 2.7218414500 -1.0685836900  
H 0.4183851800 0.3150175500 2.9714401900  
H 0.6495969200 1.8477949700 1.0837781500  
H -0.7900714400 -1.4745854900 4.1134703800  
H -7.2484494300 -3.1589281000 -0.7611068200  
H -7.0406943000 -1.6130561700 -2.6402469900  
H -6.3986873700 -4.0610108400 1.3673974300  
H -4.7801483000 -4.0408751300 3.1676456300  
H -2.1283731400 -2.9179885100 5.3298482100  
H -3.5938871500 -3.5268578900 4.7989880600  
H -3.8179339000 3.6767277500 -4.9130106600

C -2.1356041000 -5.6805335800 1.6212622500  
C -0.9889505600 -4.8896614600 1.7823767600  
C -0.6363578800 -3.9343055300 0.8288047400  
C -1.4435655400 -3.7640475800 -0.3177409200  
C -2.6008081200 -4.5637801300 -0.4946928300  
C -2.9596632500 -5.5420994900 0.4737589600  
C -4.1020271200 -6.3307348600 0.2105144300  
C -4.8747313800 -6.1512057900 -0.9369932000  
C -4.5273823100 -5.1850021400 -1.8793505300  
C -3.3835332600 -4.3838842900 -1.6645453700  
C -3.0223716800 -3.4119261400 -2.6324404300  
C -3.8053016800 -3.2558394700 -3.7966499900  
C -4.9338155900 -4.0609312000 -3.9876739800  
C -5.2932176700 -5.0136007600 -3.0373179800  
C -3.4419736600 -2.2994499100 -4.7503922700  
C -2.3441053000 -1.4524609700 -4.5574458800  
C -1.5079216000 -1.6450922800 -3.4276393800  
C -1.8705581700 -2.6125981700 -2.4514832200  
C -1.0774166600 -2.8003013900 -1.2920142600  
C 0.0927974000 -2.0286658500 -1.1080821100  
C 0.8745164100 -2.2112628500 0.0371616100  
C 0.5121728300 -3.1529408100 0.9972323000  
C 0.4625824400 -1.0974818900 -2.0790527000  
C -0.3214023400 -0.9131317500 -3.2183003100  
N -1.9992316300 -0.5751915200 -5.6095607000  
C -2.3637245000 -6.6655796500 2.7062052100  
D -3.6499957400 -6.7650737800 3.0782894000

O -1.4898764600 -7.2654333700 3.3065277600  
H -0.3661638100 -5.0296622700 2.6656600400  
H -4.4160293600 -7.1123126400 0.8977513800  
H -5.7477237000 -6.7833697400 -1.0850618200  
H -5.5455716300 -3.9541515700 -4.8808476500  
H -6.1751258500 -5.6253427600 -3.2144398500  
H -4.0321650500 -2.2015922300 -5.6589322800  
H 1.7773636200 -1.6242335900 0.1912978700  
H 1.1425866000 -3.2745023300 1.8758515800  
H 1.3686237700 -0.5064013400 -1.9650328100  
H 0.0216413900 -0.1886109900 -3.9513901600  
H -2.7869110900 -0.3281959300 -6.2009356300  
H -1.5047790700 0.2527376000 -5.2959939400  
H -3.6282414700 -7.3907426500 3.8326904800  
C -6.1210607800 -1.5441260700 5.3383689000  
C -7.1551803600 -1.7040237400 4.4049449000  
C -7.2058443700 -0.9239167800 3.2494396200  
C -6.2034474100 0.0440364500 3.0183427200  
C -5.1576127400 0.2196431500 3.9593457100  
C -5.1065537700 -0.5711148100 5.1408191400  
C -4.0593286200 -0.3120245100 6.0531953400  
C -3.0891348800 0.6596836900 5.8070579400  
C -3.1350135000 1.4260111500 4.6439261600  
C -4.1738734300 1.2115878300 3.7105910800  
C -4.2281743200 2.0034029600 2.5349885100  
C -3.2485359200 2.9946502900 2.3103473100  
C -2.2291560400 3.1888945700 3.2491446000



C -2.1709326000 2.4104388800 4.4026360000  
C -3.3095024900 3.7761738500 1.1519792500  
C -4.2933766400 3.5674436800 0.1781430900  
C -5.3244296100 2.6241814700 0.4230082300  
C -5.2694335600 1.8232546100 1.5960152100  
C -6.2627151800 0.8443733400 1.8487152200  
C -7.3263377200 0.6694293500 0.9339720400  
C -8.3053861600 -0.2982379500 1.1811432400  
C -8.2443543300 -1.0887341400 2.3262095600  
C -7.3943022200 1.4736272400 -0.2041294500  
C -6.4137916300 2.4348167700 -0.4515478900  
N -4.3311568200 4.4578372000 -0.9178756900  
C -6.2179018000 -2.4287368300 6.5247674500  
O -5.0385031600 -2.9444978000 6.9066691300  
O -7.2552182600 -2.7711423100 7.0637990900  
H -7.9295641100 -2.4478131600 4.5913853000  
H -3.9775109500 -0.8636152500 6.9863670200  
H -2.3018393000 0.8121237800 6.5423122300  
H -1.4685856300 3.9504802400 3.0912634000  
H -1.3672222000 2.5857260100 5.1144551300  
H -2.5686834300 4.5573969900 0.9963370800  
H -9.1292012000 -0.4433963500 0.4856202500  
H -9.0228018100 -1.8306828800 2.4926492200  
H -8.2139941300 1.3669965000 -0.9112522900  
H -6.5243886700 3.0463442000 -1.3425207200  
H -3.4292596400 4.8744779300 -1.1280233000  
H -4.7488863600 4.0538923100 -1.7489019400

H -5.2735005000 -3.5470280400 7.6434115100

123

(R-Cor-R')<sup>3</sup> Energy=-230.3363244 (M1)

C 4.8237352400 2.7369881100 -1.7817098600

C 5.4045201200 3.8868668200 -2.3355318700

C 5.4083921500 4.0956220700 -3.7149275400

C 4.8226978300 3.1328247000 -4.5664686600

C 4.2396901200 1.9627039400 -4.0178212800

C 4.2389713000 1.7451503200 -2.6119569400

C 3.6778373000 0.5373806200 -2.1400887000

C 3.1175639000 -0.4036476600 -3.0041696200

C 3.1098409800 -0.1836692600 -4.3803193400

C 3.6743372700 1.0037262000 -4.8977724000

C 3.6800042200 1.2186195800 -6.2998244400

C 3.1249675300 0.2476264200 -7.1611216500

C 2.5716197800 -0.9207521000 -6.6254870600

C 2.5611300600 -1.1329463100 -5.2489736300

C 3.1376163600 0.4620422800 -8.5432137000

C 3.6441332800 1.6439610800 -9.0967858000

C 4.2683158500 2.5960758600 -8.2502361600

C 4.2578630500 2.3883085300 -6.8441148200

C 4.8376667600 3.3409739800 -5.9695118100

C 5.4441735600 4.5033834000 -6.4982908000

C 6.0140608300 5.4453599400 -5.6357839100

C 5.9941396800 5.2446733600 -4.2577004500

C 5.4773599900 4.6943071900 -7.8799836800

C 4.9036797600 3.7559847000 -8.7384381700

N 3.6952893500 1.7396315800 -10.5052301100  
C 4.9194034000 2.6471919600 -0.3044691300  
O 3.7974594800 2.1959297700 0.2790064100  
O 5.8598716000 3.0372098400 0.3642816900  
H 5.8607709600 4.6233505300 -1.6744117400  
H 3.6681594600 0.2986565700 -1.0795826800  
H 2.6940529000 -1.3136772700 -2.5844605500  
H 2.1424707500 -1.6793005400 -7.2765184900  
H 2.1249790200 -2.0515363500 -4.8625450100  
H 2.7338847000 -0.3012346400 -9.2048450500  
H 6.4839440900 6.3441930700 -6.0292342000  
H 6.4488814200 5.9938328600 -3.6126108700  
H 5.9547380700 5.5731576100 -8.3077917500  
H 4.9734128500 3.9442629200 -9.8060142500  
H 2.9969821200 1.1690318100 -10.9720844400  
H 3.6712121000 2.6952042200 -10.8437198400  
H 3.9908486400 2.2572623500 1.2381178300  
C -1.4894615600 5.4224111900 -2.1360648800  
C -2.1135597700 4.3818178500 -2.8388577700  
C -2.2120564600 4.4135411100 -4.2301227300  
C -1.6793153000 5.5117250500 -4.9409798200  
C -1.0532230500 6.5731608800 -4.2399398900  
C -0.9560264600 6.5455322100 -2.8209352700  
C -0.3567169800 7.6571474100 -2.1873909100  
C 0.1496775700 8.7359054800 -2.9125956500  
C 0.0628985200 8.7560784100 -4.3033870200  
C -0.5427224200 7.6723594300 -4.9779966600

C -0.6445811500 7.7019253300 -6.3924618700  
C -0.1430356600 8.8096929200 -7.1094203200  
C 0.4525738600 9.8714887400 -6.4194598500  
C 0.5574994100 9.8436854900 -5.0308838700  
C -0.2505066600 8.8362558400 -8.5037147600  
C -0.8006918200 7.7644665200 -9.2168048100  
C -1.3721032600 6.6774528700 -8.5064084200  
C -1.2652389300 6.6401933900 -7.0894943500  
C -1.7904794400 5.5480537100 -6.3546286600  
C -2.4386240100 4.4906655900 -7.0332245200  
C -2.9547226300 3.4111913900 -6.3090787300  
C -2.8403531000 3.3718340700 -4.9215786100  
C -2.5664113700 4.5401880500 -8.4216935900  
C -2.0462772100 5.6153862600 -9.1427424700  
N -0.9476221600 7.9123245500 -10.6139571400  
C -1.4843980900 5.2561194500 -0.6623697500  
D -0.3227499900 5.6064039500 -0.0872924800  
D -2.3798821300 4.7516656300 -0.0085679900  
H -2.5286264600 3.5400497200 -2.2849633900  
H -0.2738166000 7.7098554900 -1.1047528200  
H 0.6062928200 9.5624461200 -2.3722214700  
H 0.8414218200 10.7331067800 -6.9578074700  
H 1.0245272400 10.6844555300 -4.5225992900  
H 0.1122950200 9.7042160700 -9.0499445200  
H -3.4557563500 2.5909059700 -6.8185799100  
H -3.2550779900 2.5203464900 -4.3857216000  
H -3.0771223800 3.7454583600 -8.9610141000

H -2.1892572300 5.6132569000 -10.2195814800  
H -0.2789509700 8.5585863900 -11.0218719900  
H -0.9524728600 7.0294064600 -11.1126616500  
H -0.4511823100 5.3798684700 0.8578226400  
C 1.5899753500 5.0599768800 -9.8908838400  
C 2.1984558700 6.1096374200 -9.1878794900  
C 2.2934665200 6.0811845400 -7.7963014000  
C 1.7653082800 4.9812662600 -7.0847063300  
C 1.1408874000 3.9182286700 -7.7848093000  
C 1.0382847900 3.9473177200 -9.2034040800  
C 0.3661800000 2.8740213500 -9.8299411600  
C -0.1585011100 1.8057825000 -9.1021693500  
C -0.0475818700 1.7740947100 -7.7133097400  
C 0.6031508100 2.8343517800 -7.0434413800  
C 0.7010290100 2.8083443200 -5.6286252600  
C 0.1486467200 1.7285075800 -4.9064391700  
C -0.4913472000 0.6897689100 -5.5917393000  
C -0.5857483100 0.7105377400 -6.9811934100  
C 0.2434022900 1.7101574000 -3.5110907400  
C 0.9194201800 2.7153241400 -2.8092552000  
C 1.4172434900 3.8410022000 -3.5148001000  
C 1.3281624200 3.8673139400 -4.9331886300  
C 1.8523973900 4.9592492100 -5.6690753700  
C 2.4585831800 6.0397770900 -4.9881556500  
C 2.9786835800 7.1163779400 -5.7137144900  
C 2.8991458100 7.1356933600 -7.1040693500  
C 2.5224915000 6.0258427700 -3.5944734800

C 2.0077474100 4.9484885400 -2.8727750700  
N 0.8925599500 2.6618845500 -1.3979055300  
C 1.5448769400 5.2462061100 -11.3615098000  
O 1.8178109500 4.1275943400 -12.0522008800  
O 1.3904132700 6.3119011400 -11.9309456100  
H 2.5984866000 6.9588926700 -9.7414080300  
H 0.2316057700 2.8478745300 -10.9083483000  
H -0.6609529500 1.0032270900 -9.6380034000  
H -0.9241028200 -0.1478070300 -5.0489726100  
H -1.0902442900 -0.1106932100 -7.4856000000  
H -0.2078542300 0.8900876100 -2.9568344400  
H 3.4477810100 7.9542687600 -5.2024601500  
H 3.3096788600 7.9888828100 -7.6404469500  
H 2.9688978000 6.8555306200 -3.0507574400  
H 2.0668721800 4.9965820600 -1.7891601200  
H 0.7746612500 1.7212774200 -1.0338613400  
H 1.6834819400 3.1246231300 -0.9636366400  
H 1.8161108700 4.4228185400 -12.9870246900

123

(R-Cor-R')3 Energy=-229.678374730507 (M2)

C -0.7561921000 -0.3230241500 -1.8917043200  
C -1.2434326700 -1.4379070400 -2.5887579100  
C -1.2472854100 -1.4666996100 -3.9835633900  
C -0.7573431900 -0.3550909000 -4.7042724800  
C -0.2696899000 0.7806479400 -4.0097322900  
C -0.2693893100 0.8144478300 -2.5875360600  
C 0.1922507600 1.9953781300 -1.9642137300

C 0.6585706500 3.0848950800 -2.7001314600  
C 0.6672730800 3.0456019400 -4.0931923000  
C 0.1999463800 1.8903819700 -4.7590708600  
C 0.1945377300 1.8582899800 -6.1771336400  
C 0.6531088400 2.9765957600 -6.9064011100  
C 1.1111943700 4.1097203700 -6.2249373900  
C 1.1213078200 4.1428550500 -4.8325561800  
C 0.6409624700 2.9417982100 -8.3045978700  
C 0.2304593200 1.8016672700 -9.0056842400  
C -0.2988064900 0.6979197000 -8.2884731600  
C -0.2879665700 0.7228623800 -6.8673066900  
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D 0.2465739000 0.0348309800 0.2199153500  
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H 0.8101616100 2.5685858400 -10.8048197400  
H 0.2709191900 0.9859623400 -10.8740023000  
H 0.0716038200 -0.1661179200 1.1633456800  
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C 2.0514148000 -2.4843514400 -9.6532384700  
C 1.9788576700 -2.6282560900 -8.2674704200  
C 2.4208529800 -1.5768609200 -7.4341954200  
C 2.9370373200 -0.3874199300 -8.0076746200  
C 3.0167347300 -0.2402910600 -9.4203975400

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C 3.3905070300 0.6454655300 -7.1468093700  
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C 2.7963933300 -0.6889565000 -5.1688897300  
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C 1.4240859900 -3.9580795100 -6.3175693700  
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C 2.2508780100 -2.0611482700 -3.2465003100  
N 3.1867947600 0.1266419800 -1.5187634400  
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D 2.8255397300 -2.2898303400 -12.4066268100  
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H 3.6935049300 1.1195380400 -10.9885774000  
H 4.4428930500 2.8743715700 -9.5147598600  
H 4.6849182500 3.4969166600 -4.8235774600  
H 4.8106289100 3.7614388100 -7.2485224700

H 4.0996457100 2.1605278600 -2.8642917600  
H 1.0394919800 -4.8887730900 -5.9059976000  
H 1.1370325000 -4.6241226900 -8.3317956200  
H 1.4579413600 -4.0122107700 -3.6426112400  
H 2.2153478200 -2.2413592300 -2.1758501800  
H 3.2280355400 1.0246849000 -1.0465472200  
H 2.4473620200 -0.4526994400 -1.1368252000  
H 2.2169927800 -0.3353289900 -13.2280582300

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(R-Cor-R')<sup>3</sup> Energy=-177.792477532461 (M3)

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C 5.97090934 6.22992888 0.06087391  
C 5.51972422 6.84657253 1.24886443  
C 4.35257561 7.65125718 1.23039115  
C 3.62736552 7.84706219 0.02228711  
C 2.49836387 8.69515795 0.07053133  
C 2.08166087 9.30311078 1.25494185  
C 2.78746886 9.10147608 2.43960075  
C 3.93214848 8.27322208 2.43454099  
C 4.65857334 8.08194904 3.63773786  
C 4.23331522 8.71919879 4.82339996  
C 3.09658880 9.53509185 4.80395552  
C 2.37897398 9.72185511 3.62494149  
C 4.95606029 8.53136173 6.00605349  
C 6.06855186 7.68307566 6.05807991  
C 6.54882578 7.09265530 4.86078566

C 5.81943425 7.27543506 3.65453804  
C 6.25148504 6.66539336 2.45043860  
C 7.42548609 5.87778899 2.44307135  
C 7.85099125 5.27312269 1.25591784  
C 7.12949919 5.44543745 0.07712914  
C 8.15553349 5.72000019 3.62152879  
C 7.72653530 6.31973420 4.80591972  
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O 2.12711638 7.24960946 -2.45725047  
O 4.06709896 7.37897071 -3.54734268  
H 5.60590907 5.94828698 -2.04490416  
H 1.91535626 8.90625990 -0.82238185  
H 1.20114701 9.94181874 1.23448092  
H 2.75799482 10.03483118 5.70895346  
H 1.50020551 10.36284742 3.64098227  
H 4.64089952 9.04632058 6.91095018  
H 8.75247521 4.66449380 1.23611993  
H 7.48775549 4.96519823 -0.83127236  
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H 8.34165115 6.18003127 5.69030971  
H 6.22202925 7.83312950 8.08663504  
H 7.29019384 6.74633387 7.39513997  
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C 3.81064537 3.67689133 5.08882616

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C 0.16737030 1.55807576 5.51699387  
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C -1.60266832 0.20075700 4.55572480  
C -1.03559335 0.31066769 3.28046831  
C 0.20790496 0.97641289 3.12792971  
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C 2.66553067 2.38432640 2.86786941  
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C -2.72334509 3.71223256 4.72128969  
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C -3.92877019 2.17136420 1.54496706  
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C 0.21720167 4.54277740 0.60843842

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C 0.58740731 5.97179217 6.07347168  
C -0.41699126 5.59912074 6.96346353  
C 1.52367863 5.96758017 3.83473568  
C 1.44275111 5.60963196 2.48869480  
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O -4.27911316 3.09412219 9.21349435  
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H -5.58332767 2.15267341 5.77827687  
H -5.69435616 1.53619125 3.45001919  
H -2.99952763 2.24435833 -0.38269911  
H -4.75319554 1.56512851 1.17596352  
H -0.89283845 3.39613517 -0.83275490  
H 1.43362220 6.54501581 6.44606991  
H -0.32733282 5.89287830 8.00741680  
H 2.39237321 6.52545825 4.17741543  
H 2.26712794 5.89776072 1.84261839  
H 0.90981019 4.77064220 -1.29668060  
H 1.72424422 5.68421542 -0.15547645  
H -6.36156080 3.27172067 8.50849426

## Cartesian coordinates and energies of the structures displayed in Fig. 8

All coordinates are in Å, while the energies are in kJ mol<sup>-1</sup>.

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(R-Cor-R')<sub>4</sub> Energy=-348.711551740240 (GM)

C -7.99920237 0.39598589 -1.96073509  
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C -7.18545396 -1.47836919 -0.63204192  
C -7.21272101 -0.78242869 -1.87248861  
C -6.47288423 -1.33141883 -2.94369821  
C -5.71774240 -2.49547447 -2.79943586  
C -5.68398366 -3.16989212 -1.58031348  
C -6.42145270 -2.66518109 -0.48590593  
C -6.39876891 -3.36165117 0.74955999  
C -5.64369955 -4.54798120 0.87291989  
C -4.92135358 -5.02869734 -0.22495753  
C -4.93856744 -4.34503547 -1.43831476  
C -5.62873465 -5.23371367 2.09187830  
C -6.30652923 -4.74581729 3.21548193  
C -7.12564288 -3.59455973 3.08729610  
C -7.14504821 -2.88929975 1.85332465  
C -7.92191664 -1.71303575 1.70651631  
C -8.69583634 -1.24151445 2.79158282  
C -9.46052614 -0.07928594 2.64846107



C -9.47053657 0.61577995 1.44157699  
C -8.69700842 -1.94852583 3.99439701  
C -7.92941248 -3.10481781 4.13683138  
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O -9.17102936 1.77439450 -3.54054602  
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H -5.06795090 -6.16218449 2.17440396  
H -10.06056871 0.29464651 3.47527293  
H -10.07826876 1.51475175 1.35983447  
H -9.29934175 -1.61235756 4.83551121  
H -7.98077451 -3.62695056 5.08802505  
H -5.49962994 -6.15711903 4.44765413  
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C -0.13648588 5.43209348 2.64376391  
C -0.14988678 4.75531042 3.88349130  
C -0.91798240 5.26492815 4.96071617  
C -1.67844960 6.45735202 4.80709458  
C -2.38586544 6.92861865 5.93568185

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C -0.11857525 2.72227710 7.59895582  
C -0.85473234 3.23609785 8.67239305  
C -1.60755203 4.39836806 8.52300726  
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C 0.62506812 2.87998155 5.27762230  
C 0.62116704 3.57538957 4.04268639  
C 1.39832879 3.09609999 2.96335581  
C 1.39284760 3.78013661 1.74348971  
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C 2.17336686 1.94799207 3.13006705  
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H -2.93993695 6.65397667 7.98733726  
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H 2.79196596 1.57283405 2.31773753  
H 2.80858612 0.38669639 4.42813299  
H 1.82831342 -0.68105012 7.72462941  
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C -4.16900710 -2.59547825 4.92441981  
C -3.29593639 -3.70119965 4.81780655  
C -2.62364808 -3.99952985 3.63243579  
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C -3.63506142 -2.06805174 2.57278273  
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C -3.22891848 -0.72314816 -0.87642230  
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C -4.75379348 0.73591091 0.33366833  
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C -5.28890605 0.21604833 2.68401611  
C -6.10057188 1.37126817 2.75694814

C -6.76989443 1.67817227 3.94599256  
C -6.63868254 0.85665884 5.06299082  
C -6.21747384 2.20151486 1.64175632  
C -5.55313463 1.89080141 0.45490638  
N -4.11850269 1.20025881 -2.01742514  
C -4.80562410 -2.98925264 7.38222929  
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O -4.81561977 -2.48621546 8.49158754  
H -6.20534272 -0.84281708 7.06329279  
H -3.11530831 -4.35846824 5.66464027  
H -1.96819551 -4.86748824 3.60595324  
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H -1.43952702 -4.34636517 1.25927681  
H -2.66494298 -0.94703857 -1.77927981  
H -7.39766720 2.56389938 4.01587293  
H -7.16906186 1.12373143 5.97487929  
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C -0.79066789 -1.15418165 4.96776481

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C -2.31507418 0.69273883 5.56655013  
C -3.00726840 1.88117115 5.21948103  
C -3.84325632 2.50912722 6.16791221  
C -3.98277488 1.95510175 7.44533025  
C -3.30145285 0.79034495 7.79039189  
C -4.52755707 3.67802186 5.81901339  
C -4.36628590 4.27425462 4.56265691  
C -3.58596474 3.61722133 3.57666558  
C -2.88446126 2.43037406 3.92270054  
C -2.06476079 1.77321093 2.97143717  
C -1.95195953 2.29332273 1.66169942  
C -1.14106688 1.64704619 0.72319572  
C -0.44678843 0.48968033 1.06709641  
C -2.66124207 3.44361938 1.31476380  
C -3.46552521 4.08980700 2.25395091  
N -5.16038906 5.40417817 4.26574263  
C 0.78879838 -3.02061923 4.17854747  
O 1.41755633 -3.08372591 5.36325014  
O 0.95010841 -3.88638814 3.33697435  
H 0.74912038 -1.71650623 1.95013250  
H -0.51017910 -2.58953034 6.58870322  
H -1.91562598 -1.46123059 8.19020881  
H -4.62528180 2.42606663 8.18612948  
H -3.43098682 0.38296001 8.79070230

H -5.19218056 4.14318598 6.54375122  
H -1.04522743 2.03647993 -0.28806615  
H 0.17331865 0.00751226 0.31400165  
H -2.60199447 3.84983739 0.30740870  
H -4.01028705 4.97072068 1.92645176  
H -5.43959331 5.92668078 5.09048869  
H -4.74569715 6.01461509 3.57027771  
H 1.92205807 -3.92298898 5.31665331

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(R-Cor-R')<sup>4</sup> Energy=-343.397413530418 (M1)

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C 2.2115561000 -7.1671995500 0.6583565800  
C 2.2759247900 -5.8481185600 0.1426274400  
C 2.7491896500 -5.6093101700 -1.1775148100  
C 2.8252007000 -4.2661185500 -1.6091364500  
C 2.4296979300 -3.2052066800 -0.7942009500  
C 1.9563896900 -3.4421665700 0.4950110200  
C 1.8780260000 -4.7691303600 0.9739138800  
C 1.4111946000 -5.0073053000 2.2919815300  
C 1.0320772400 -3.9207467300 3.1095308300  
C 1.1184810800 -2.6151355900 2.6134255700  
C 1.5728817300 -2.3782677000 1.3183042200  
C 0.5772155300 -4.1606505000 4.4102458500  
C 0.4392678900 -5.4610446800 4.9101247800  
C 0.8825166800 -6.5574501900 4.1264168000

C 1.3436364800 -6.3238719000 2.8023082400  
C 1.7551680200 -7.4027990900 1.9805831300  
C 1.7200470400 -8.7233584700 2.4841134800  
C 2.1232935900 -9.7889180500 1.6729510700  
C 2.5655565600 -9.5589477900 0.3724499600  
C 1.2921140900 -8.9495817900 3.7926717900  
C 0.8853019600 -7.8858062800 4.5985177900  
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O 3.0034529200 -5.7748190900 -4.1209415300  
O 4.5500773500 -7.3479910700 -3.8021146300  
H 3.3990155700 -8.8647753500 -2.0566816700  
H 3.2013815500 -4.0136945300 -2.5973297200  
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H 0.8323820100 -1.7674421800 3.2322710700  
H 1.6301022200 -1.3522962700 0.9612735400  
H 0.3124293800 -3.3187539700 5.0462061300  
H 2.1012643000 -10.8099723700 2.0477272600  
H 2.8761349400 -10.4080866000 -0.2330869200  
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C -3.9512851800 -7.8747153700 -2.3684890900  
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C 4.6997407700 -7.5572634100 4.0433901700  
C 4.1696952700 -7.1223965200 5.2787772300  
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C 5.0392022000 -4.2007259000 2.3675419300  
C 4.7974370700 -2.8404857100 2.6574084400  
C 4.2846759400 -2.4774154300 3.9077933800  
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C 6.2185813700 -6.3261046500 -0.4667455700  
C 6.4291016500 -7.6793342300 -0.7504009500  
C 6.1722635400 -8.6515463000 0.2132503700  
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C 6.2539513500 -4.0018756500 -1.1491729600  
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O 5.0644931700 -9.8544030000 5.8725728500  
O 4.2493977700 -11.1500753200 4.2522579100  
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H 4.8557476100 -0.8246376900 1.9064382600  
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C -2.5284495300 -8.9351232100 4.1501419000

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C -1.9039855800 -7.7046338400 2.1551190100  
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C -2.7581530400 -6.4920627500 4.1265556000  
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C -2.1252419800 -5.2743804400 2.0746913100  
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C -0.7886436800 -6.4805588900 -1.2247086000  
C -1.2748572500 -6.4853506400 0.1109661900  
C -1.4219012500 -7.7030522800 0.8210753600  
C -1.0950151500 -8.9269325400 0.1934481000  
C -1.2371384100 -10.1287897100 0.8944115500  
C -1.7044499500 -10.1305503400 2.2064339600  
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C -0.4965416000 -7.7235849000 -1.8221864100  
N -0.2225601800 -5.1675554900 -3.2501531000  
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D -2.9333602400 -6.9920725600 7.0377575000  
D -4.0877888700 -8.8363951800 6.5536744600  
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H 0.1239023200 -4.2513724900 -3.5180010000  
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R-Cor-R')4 Energy=-339.145613962141 (M2)  
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C -4.3859732900 -6.7003657100 0.1903133500  
C -4.2200721500 -7.0127239000 -1.1876176400  
C -5.3549432800 -7.4727193300 -1.8923944700  
C -6.5911243600 -7.6452939700 -1.2693770900  
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C -7.0729837800 -6.7179228800 2.8064366100  
C -8.1523586100 -7.1924701100 2.0528044500

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C -3.7974105600 -5.1886431800 5.0182788400  
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D -3.1350045000 -8.2189820100 -3.6621627400  
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C -6.7670263200 -0.0764169300 -0.1169282400  
C -7.2427046700 0.1231938700 1.2036701700  
C -8.5933978300 -0.1718239900 1.5388970800  
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C -6.8064767700 0.8741113000 3.4972939500  
C -6.3523302400 0.6407295500 2.1798701000  
C -5.0070954100 0.9397033000 1.8438356600  
C -4.1389674200 1.4664108600 2.8244779300  
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C -5.9307788500 1.3931538600 4.4567306800  
C -2.8147794100 1.7642707000 2.4866640500  
C -2.3091439100 1.5059927700 1.2069927100  
C -3.1872495400 1.0437018400 0.1930941300  
C -4.5339660200 0.7354905200 0.5274805400  
C -5.4245753200 0.2336805300 -0.4541894900  
C -4.9758882900 0.0490679800 -1.7820643100  
C -5.8532879900 -0.4487392200 -2.7507578700  
C -7.1697743700 -0.7593719600 -2.4188589500  
C -3.6613200400 0.3763432200 -2.1158751200  
C -2.7861141300 0.8678837600 -1.1469041600  
N -0.9864462900 1.9166041900 0.9288661000

C -10.8717324800 -1.0174503200 0.7050660000  
O -11.1253396700 -1.6712341300 1.8500941900  
O -11.7487632500 -0.8376341100 -0.1209516800  
H -9.6370990200 -1.2461723200 -1.5513658700  
H -10.0331068600 -0.0882384300 3.1779799100  
H -8.5048052500 0.7736467000 4.8316454300  
H -3.9552037900 2.0969844500 4.8885205100  
H -6.2692063800 1.5784034200 5.4738402500  
H -2.1570644200 2.1958324700 3.2380044400  
H -5.5211602200 -0.5956760500 -3.7762309900  
H -7.8295374900 -1.1415242100 -3.1952885100  
H -3.3015637600 0.2583923800 -3.1356548300  
H -1.7792714400 1.1241560700 -1.4641144900  
H -0.3970490600 1.9587809300 1.7547002700  
H -0.5449591200 1.3765954400 0.1928269100  
H -12.0821374200 -1.8776378800 1.7954011900

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(R-Cor-R')4 Energy=-336.873064547841 (M3)

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C 1.8545737600 -0.9097647500 9.1012668100  
C 1.9432296300 0.2576938400 8.3426452200  
C 2.3390554200 0.1800359200 6.9889724100  
C 2.6463766000 -1.0778710900 6.4116352600  
C 2.5616016100 -2.2691942000 7.1845175800  
C 2.9231408800 -3.4812048800 6.5547889800  
C 3.3238860300 -3.5285559400 5.2194098100  
C 3.3960900000 -2.3615693200 4.4610121600

C 3.0586062000 -1.1246208000 5.0546321800  
C 3.1480627700 0.0640901000 4.2859156400  
C 3.5727375800 0.0002161100 2.9411860200  
C 3.9018805000 -1.2363859400 2.3748938500  
C 3.8114298400 -2.4058346200 3.1259824700  
C 3.6641017800 1.1758863000 2.1890126600  
C 3.2956663800 2.4170548300 2.7216378000  
C 2.9351190300 2.5062648900 4.0908784400  
C 2.8366926500 1.3166269900 4.8625828300  
C 2.4398793400 1.3691187800 6.2221629300  
C 2.1510946000 2.6159416300 6.8227372600  
C 1.7567162800 2.6683880300 8.1635297800  
C 1.6514179700 1.5006614900 8.9152697400  
C 2.2730704700 3.7857962500 6.0722770700  
C 2.6615798200 3.7309032200 4.7334158200  
N 3.5005826800 3.5620266000 1.9200555700  
C 2.0313762000 -3.3025562700 9.4762834500  
D 1.4570660600 -4.3869461400 8.9312092500  
D 2.3114191000 -3.2710479500 10.6613595000  
H 1.5559501500 -0.8549037500 10.1479124700  
H 2.9043424400 -4.4235204700 7.0964935200  
H 3.5850908900 -4.4910113300 4.7845272700  
H 4.2331272700 -1.3013777600 1.3407477300  
H 4.0752192300 -3.3519682900 2.6584263700  
H 4.0182572700 1.1253593100 1.1617016700  
H 1.5314725200 3.6210338500 8.6381091900  
H 1.3456471500 1.5740983700 9.9570383300

H 2.0726433100 4.7564747500 6.5204956000  
H 2.7586526500 4.6723907500 4.2003040500  
H 3.4819286800 3.3636718800 0.9243259500  
H 2.8796395300 4.3298075800 2.1507415900  
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C 6.2348842600 4.1077946300 4.4205273600  
C 6.5894139600 2.9664373700 3.6871357700  
C 6.5641726600 1.7005474500 4.2729785300  
C 6.1801319000 1.5668911100 5.6256749400  
C 5.8273320600 2.7150804700 6.3788601700  
C 5.8571420400 4.0075325500 5.7851736900  
C 5.5336164700 5.1097471300 6.6077871200  
C 5.1704627800 4.9513439600 7.9453611100  
C 5.1316691200 3.6832451700 8.5221268400  
C 5.4627503600 2.5536142800 7.7406916500  
C 5.4382756900 1.2652977400 8.3336526000  
C 5.0859700200 1.1248954700 9.6933931100  
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C 4.7814776200 3.5243376600 9.8670748600  
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C 5.3437878400 -1.2983122200 9.5270389600  
C 5.7676875200 -1.1668482700 8.1795230800  
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C 6.1660847100 0.2804735700 6.2231804700  
C 6.5432671700 -0.8492618200 5.4615475500  
C 6.9156880900 -0.6936338900 4.1224836800  
C 6.9236443600 0.5683815000 3.5333828100

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C 6.1733518400 -2.2641678100 7.3929207100  
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H 5.5614048000 6.1259172000 6.2225832200  
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H 6.2142109200 -3.2649077700 7.8134919400  
H 4.8142065100 -2.5450371200 11.0522694500  
H 5.1831173300 -3.3288452200 9.6205518100  
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C -1.6091676200 0.0371989300 8.4137332200  
C -1.2122222300 -0.7607603800 7.3404105900  
C -0.9131340800 -0.1584786100 6.0982584800  
C -1.0208430400 1.2472106400 5.9481551600  
C -1.4302649800 2.0625058600 7.0396917000  
C -1.5557292900 3.4501065800 6.8050396300  
C -1.2668970400 4.0181723900 5.5640910000

C -0.8557637600 3.2189140200 4.4990118100  
C -0.7315596200 1.8237100700 4.6842170100  
C -0.3284670400 1.0097968900 3.5947112000  
C -0.0575383700 1.5989684900 2.3408368800  
C -0.1875896600 2.9831100500 2.1813209000  
C -0.5795320800 3.7854623300 3.2502164100  
C 0.3347116100 0.7913363400 1.2683711100  
C 0.5156379300 -0.5887906000 1.4182002700  
C 0.1793899100 -1.2038680900 2.6516465400  
C -0.2174088100 -0.3910810600 3.7481782400  
C -0.5208323500 -0.9722837900 5.0046860100  
C -0.4414980000 -2.3742574600 5.1684824200  
C -0.7380079400 -2.9483655300 6.4088417300  
C -1.1171612300 -2.1493388300 7.4847530200  
C -0.0772979500 -3.1740418000 4.0848165300  
C 0.2231694000 -2.5989569700 2.8497055900  
N 0.8298172900 -1.3386499000 0.2630000700  
C -2.1675070900 2.1362542300 9.4998140900  
D -1.5060659600 3.2807705800 9.7352230300  
D -2.9788857300 1.7058251600 10.2999500700  
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H -1.8881311900 4.1250768000 7.5896924300  
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H 0.5156190200 1.2460298600 0.2968397000  
H -0.6809436400 -4.0257088200 6.5487328800

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C -3.6621611900 -0.1424863900 2.9895675300  
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C -3.7367424900 2.2470623600 2.3804802600  
C -3.9607033600 3.5741239200 2.8105823500  
C -4.3622888400 3.8702306000 4.1133203400  
C -4.5409665500 2.8511892500 5.0470586300  
C -4.3130390600 1.5101854400 4.6648550800  
C -4.4798353800 0.4756872000 5.6208642700  
C -4.8691919700 0.7946819800 6.9397160800  
C -5.0891094500 2.1301904300 7.2950469200  
C -4.9298448900 3.1479051900 6.3575944600  
C -5.0273648100 -0.2286695200 7.8799530900  
C -4.8575238500 -1.5744993900 7.5337890900  
C -4.3980953200 -1.9047504900 6.2327770300  
C -4.2372241200 -0.8719221400 5.2695326200  
C -3.8184744400 -1.1747406700 3.9498266300  
C -3.5450638600 -2.5139607500 3.5887316200  
C -3.1345180400 -2.8140046400 2.2858750500

C -2.9869098800 -1.8017010900 1.3407616500  
C -3.6778811700 -3.5243226200 4.5417042800  
C -4.0925906800 -3.2235982200 5.8394265500  
N -4.9533017900 -2.5345718600 8.5655703600  
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O -2.2033652200 2.7552849700 -0.8668564800  
H -2.7467397200 0.3014633400 -0.2705196600  
H -3.8221960600 4.4147734500 2.1353935300  
H -4.5261080700 4.9102482600 4.3875422800  
H -5.3870550600 2.3919329800 8.3080255900  
H -5.1068526900 4.1765593300 6.6640277600  
H -5.3005158700 0.0240604700 8.9021385000  
H -2.9208788000 -3.8401648300 1.9945883200  
H -2.6625172800 -2.0661170700 0.3362596900  
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H -4.1618838200 -4.0450209900 6.5468819600  
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(R-Cor-R')4 Energy=-315.234011228039 (M4)

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C 1.4699249000 3.7815127400 3.2256019200



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C 0.2495167100 5.0520283900 4.9318480000  
C 1.4067558600 4.3518054300 4.5234278200  
C 2.5026967300 4.2370281900 5.4165688900  
C 2.4273890900 4.8220400000 6.6990728000  
C 1.2708396500 5.5108869800 7.0812896700  
C 0.1915537700 5.6220725500 6.2079596000  
C 3.5127951600 4.7103305600 7.5741312200  
C 4.6605239900 3.9865944600 7.2293732000  
C 4.7789748600 3.4540885000 5.9197245700  
C 3.6801047800 3.5601096100 5.0243487700  
C 3.7530060100 3.0029217900 3.7232333300  
C 4.9329304500 2.3462735300 3.3046108800  
C 5.0046927600 1.7936858700 2.0218379100  
C 3.9232968000 1.8900890800 1.1494416800  
C 6.0207885100 2.2652334700 4.1744532800  
C 5.9453375400 2.8125479900 5.4555684900  
N 5.7411342700 3.9975682100 8.1391238000  
C -0.5473829500 3.3713682600 -0.0119540600  
D -1.7884008900 3.1512579100 0.4509339600  
D -0.3362395600 3.4912133400 -1.2056364600  
H 1.7459934100 2.2309712700 -0.3406452600  
H -1.6188544900 4.7716784700 2.1265292600  
H -1.7203441200 5.7195539400 4.3411157600  
H 1.1988601200 5.9691694000 8.0652626000

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H 3.4612592200 5.1862664800 8.5509505500  
H 5.9064802000 1.2856699900 1.6868846700  
H 4.0106634800 1.4533176800 0.1565829900  
H 6.9438989800 1.7797976900 3.8654115200  
H 6.8270505200 2.7378033600 6.0856681200  
H 5.4542305000 4.1475692500 9.1015976800  
H 6.3407700000 3.1836710400 8.0598617700  
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C 5.9467979500 4.7417021100 0.4764234500  
C 6.6638374800 4.9433325900 1.6644682300  
C 6.0931462600 5.6238056300 2.7403837100  
C 4.7755535600 6.1207101300 2.6300466000  
C 4.0442624700 5.9294614700 1.4305751300  
C 4.6258087100 5.2403267100 0.3302652200  
C 3.8535535500 5.1240928700 -0.8471685600  
C 2.5588112900 5.6360408300 -0.9345075200  
C 1.9870610400 6.3015860100 0.1482618200  
C 2.7291225000 6.4547498900 1.3408251600  
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C 0.8470202400 7.6738346000 2.3245768300  
C 0.1313534700 7.5098012500 1.1333083300  
C 0.6941899300 6.8278524400 0.0571640100  
C 0.2840929400 8.3594175100 3.4059655300  
C 0.9643263200 8.4947132500 4.6220704200  
C 2.3015656600 8.0322580800 4.7255059900  
C 2.8811922900 7.3318080400 3.6328686000

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C 6.2561013500 6.5176522000 4.9882271300  
C 6.8187400700 5.8230966000 3.9201371600  
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C 3.0947834200 8.2308575000 5.8738878300  
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D 5.9571271700 3.1146071400 -1.2396747000  
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H 4.2484091000 4.6311963200 -1.7319837700  
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C 3.2145445200 0.3425905700 6.3974869400

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C 0.9748598800 2.2573991000 8.6963961000  
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C 4.1210663700 -1.0412208900 4.1228695900  
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C 0.7514302600 -0.0044333500 2.9897224800  
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D 5.9265865600 1.6864431800 10.4281695800  
D 6.5800393800 -0.4145690300 10.0713574300  
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H 3.6199344100 1.8535705900 10.7651453600  
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C -4.3511997100 5.9263255600 4.0049707600  
C -4.1883432100 6.3858317600 5.3414274500  
C -4.4067398600 5.4547577100 6.3814479600  
C -4.7939951800 4.1392399400 6.1254740100  
C -4.9632372000 3.6940719700 4.8157332700  
C -4.7403648600 4.5869829000 3.7436513200  
C -4.8974954200 4.1277924500 2.4108290200  
C -5.2723326600 2.7884235000 2.1693457100  
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C -5.3377012600 2.3713028500 4.5572194700  
C -5.4210035400 2.3392564200 0.8531168200  
C -5.2558273000 3.2005465200 -0.2381346000  
C -4.8107366500 4.5288456500 -0.0138836500

C -4.6596103300 4.9952695000 1.3203065100  
C -4.2553800900 6.3291947700 1.5770467000  
C -3.9867975600 7.2025350900 0.4982540900  
C -3.5905863800 8.5198406100 0.7507067400  
C -3.4525398000 8.9778180500 2.0587532900  
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C -4.5103975300 5.4238093900 -1.0609048300  
N -5.3410730300 2.6427293600 -1.5331474700  
C -3.5607049400 8.3546995400 6.8681221800  
D -4.4930519100 8.0343998400 7.7797013700  
D -2.6898789400 9.1677542000 7.1219454300  
H -3.2284160000 9.6062937600 4.6340196000  
H -4.2749862100 5.7348972600 7.4235221700  
H -4.9541350000 3.4671830800 6.9659298200  
H -5.7742726000 0.8869249600 3.0771030900  
H -5.5106877200 1.6742218100 5.3742361100  
H -5.6828992600 1.2992458000 0.6710852500  
H -3.3808049400 9.2024296200 -0.0699993000  
H -3.1392219300 10.0068834700 2.2231517400  
H -3.8909104200 7.3874078200 -1.6548864900  
H -4.5725787300 5.1070958400 -2.0981396600  
H -5.9184687000 1.8083823100 -1.5737590200  
H -5.6185895700 3.3132100100 -2.2414654300  
H -4.2441557100 8.5643501700 8.5659959100

## Cartesian coordinates and energies of the structures displayed in Fig. 9

All coordinates are in Å, while the energies are in kJ mol<sup>-1</sup>.

205

(R-Cor-R')<sub>5</sub> Energy== -464.668235435591 (GM)

C -3.89670528 -1.62671476 5.00647103

C -4.42243864 -1.65547090 3.70684476

C -3.58629782 -1.57925066 2.59267011

C -2.19027086 -1.46713198 2.77618313

C -1.64854772 -1.42914119 4.08583471

C -2.49948601 -1.50161961 5.22356734

C -1.89321626 -1.41563969 6.49686349

C -0.51221441 -1.29158219 6.65022566

C 0.32057579 -1.23139229 5.53439599

C -0.24415272 -1.29804971 4.24096636

C 0.60341556 -1.22050892 3.10625203

C 1.99701349 -1.07692853 3.27944502

C 2.53341360 -1.01301957 4.57033506

C 1.70418661 -1.09269207 5.68656109

C 2.82788084 -0.99584327 2.15721635

C 2.31736432 -1.10403811 0.85813966

C 0.91348300 -1.17740625 0.66707130

C 0.06123609 -1.26320701 1.80142890

C -1.34240490 -1.37810744 1.64248201

C -1.90412732 -1.39482612 0.34523809

C -3.28890205 -1.51102656 0.18742224

C -4.12145323 -1.60482488 1.30000770  
C -1.06954864 -1.28428874 -0.76736622  
C 0.31206822 -1.17371481 -0.60795954  
N 3.21604818 -0.92565951 -0.21705034  
C -4.91246571 -1.69281491 6.08504296  
O -4.55720260 -2.48642748 7.10817864  
O -6.01891701 -1.18522290 6.04102102  
H -5.50077048 -1.73554310 3.57104413  
H -2.48896569 -1.43956877 7.40585517  
H -0.09953119 -1.23579871 7.65533855  
H 3.60498498 -0.89994210 4.71985030  
H 2.15043751 -1.03883876 6.67717828  
H 3.89801381 -0.85741865 2.29506056  
H -3.73434695 -1.52521065 -0.80498497  
H -5.19514288 -1.69061312 1.14508357  
H -1.48331059 -1.27732316 -1.77336829  
H 0.91409465 -1.07199572 -1.50642907  
H 4.17534720 -1.16151940 0.01807842  
H 2.92298620 -1.39453485 -1.06707662  
H -5.34320683 -2.47989035 7.69402026  
C -0.75017600 8.98294718 9.75228366  
C -2.13827366 8.84537666 9.60906991  
C -2.72634255 8.77998600 8.34565184  
C -1.91235154 8.85780899 7.19391354  
C -0.50852617 9.00496022 7.32701260  
C 0.09296769 9.07695003 8.61418285  
C 1.49206949 9.26583224 8.66964717



C 2.27164074 9.35310409 7.51607505  
C 1.68164931 9.27173343 6.25610398  
C 0.28317946 9.09853345 6.15312062  
C -0.31761115 9.03200118 4.86992723  
C 0.48397630 9.14017984 3.71299972  
C 1.86700149 9.31144702 3.83994615  
C 2.46038413 9.37335095 5.09851302  
C -0.11399988 9.07902644 2.45006768  
C -1.48888116 8.86195100 2.30002363  
C -2.31592291 8.82220642 3.45206315  
C -1.71708436 8.88066328 4.73986319  
C -2.51291130 8.80278538 5.91002077  
C -3.91678630 8.67875625 5.79864245  
C -4.70260136 8.59899724 6.95282729  
C -4.11300508 8.64661779 8.21373747  
C -4.50660549 8.64770406 4.53461020  
C -3.72049593 8.72214249 3.38439591  
N -2.02023225 8.89968047 0.99169353  
C -0.27907901 9.06154785 11.15632977  
D 0.84281376 8.36033952 11.38546488  
D -0.87669672 9.60301396 12.06928627  
H -2.76225357 8.79234719 10.50097229  
H 2.01006904 9.35401453 9.62130687  
H 3.34572113 9.49262956 7.61881323  
H 2.49752734 9.39890402 2.95779255  
H 3.53775433 9.50827812 5.16507562  
H 0.50383063 9.19058839 1.56170607

H -5.78392494 8.50331060 6.88156868  
H -4.75118396 8.58584130 9.09305795  
H -5.58634752 8.57052891 4.42742443  
H -4.23170251 8.71212255 2.42596098  
H -1.34335035 8.65278216 0.27612231  
H -2.87273939 8.36026591 0.88904086  
H 0.98487276 8.45393063 12.35092628  
C -2.41676742 1.98829742 0.09383651  
C -3.64530225 1.85782451 0.75710863  
C -3.71120125 1.85029268 2.15063895  
C -2.52288674 1.97148858 2.90453489  
C -1.27443588 2.09597386 2.24425586  
C -1.20411827 2.09884451 0.82339984  
C 0.07753402 2.18413392 0.23490026  
C 1.23721396 2.28942975 1.00310047  
C 1.16518706 2.29707184 2.39485904  
C -0.09485577 2.19814329 3.02638648  
C -0.16499218 2.18992474 4.44306376  
C 1.01991668 2.27912499 5.20514029  
C 2.25652462 2.37612962 4.55737689  
C 2.32839954 2.38827822 3.16647357  
C 0.94568385 2.26549453 6.60178494  
C -0.28363007 2.21576338 7.26980259  
C -1.47652822 2.05468921 6.51892186  
C -1.41146190 2.07028785 5.09907088  
C -2.59033004 1.95205688 4.32127554  
C -3.84260149 1.80415927 4.96049061

C -5.00671606 1.69026260 4.19376102  
C -4.94191037 1.71559658 2.80273824  
C -3.90323075 1.76264599 6.35377061  
C -2.74138070 1.88168107 7.11694644  
N -0.26128790 2.11970658 8.67897223  
C -2.50749670 1.95534416 -1.38607504  
O -1.71419239 2.85333326 -1.99198201  
O -3.29005501 1.27727781 -2.02767505  
H -4.55836679 1.75811734 0.17057257  
H 0.20259393 2.16625371 -0.84482016  
H 2.19726777 2.35823642 0.49591856  
H 3.17845614 2.44303155 5.13093854  
H 3.30425776 2.46345929 2.69169888  
H 1.86312662 2.30650605 7.18484907  
H -5.97680590 1.57600421 4.67268182  
H -5.86454984 1.62114649 2.23354043  
H -4.85470047 1.63176684 6.86451875  
H -2.84265327 1.82449161 8.19699427  
H 0.57498036 2.51774855 9.09537113  
H -1.09794414 2.48603154 9.11952464  
H -1.93356693 2.75650788 -2.94253734  
C -2.49929653 5.35450794 8.54464136  
C -3.75990983 5.23974163 7.94137218  
C -3.89235840 5.22687116 6.55262530  
C -2.74050289 5.33535262 5.74231700  
C -1.46168661 5.45985374 6.34166907  
C -1.32451439 5.47830209 7.75751797

C -0.02422500 5.64733037 8.28374565  
C 1.09579918 5.76575576 7.46058249  
C 0.96038652 5.73681830 6.07383658  
C -0.32343910 5.58514612 5.50365323  
C -0.46127605 5.57200080 4.09199132  
C 0.68062227 5.71115839 3.27380447  
C 1.94188801 5.86024121 3.86133282  
C 2.08096503 5.86973289 5.24715140  
C 0.53867299 5.70263048 1.88236986  
C -0.70720625 5.50849187 1.27407010  
C -1.87146189 5.43821635 2.08174757  
C -1.73700364 5.44315266 3.49679187  
C -2.87788806 5.33372971 4.33050860  
C -4.16400265 5.23156086 3.75247386  
C -5.29011644 5.12070029 4.57441493  
C -5.15539173 5.11588334 5.96063714  
C -4.29789404 5.25304838 2.36386311  
C -3.17282878 5.35844698 1.54555908  
N -0.77118990 5.59954873 -0.13415569  
C -2.52406287 5.37705173 10.02731945  
O -1.54311272 4.65395374 10.59097318  
O -3.39219698 5.89318026 10.70833087  
H -4.64589624 5.16288435 8.57127213  
H 0.14627726 5.69497276 9.35631967  
H 2.07393396 5.88789997 7.92102174  
H 2.83079134 5.97107101 3.24410177  
H 3.07428002 5.98852932 5.67443959

H 1.41768393 5.83793018 1.25596687  
H -6.28558765 5.04133377 4.14286835  
H -6.05056133 5.03191295 6.57365503  
H -5.27987690 5.19344015 1.89970347  
H -3.33466122 5.38906628 0.47182597  
H 0.10576607 5.36973921 -0.59165525  
H -1.54051988 5.07498861 -0.53570537  
H -1.73158181 4.71127678 11.55131127  
C 1.89996868 -4.49932822 -1.31495470  
C 0.54533995 -4.61893609 -1.65689896  
C -0.43863060 -4.70449274 -0.67160297  
C -0.06478329 -4.67457361 0.69019068  
C 1.30265675 -4.56190518 1.04727339  
C 2.30828453 -4.47959237 0.04441646  
C 3.65253270 -4.41150063 0.47406635  
C 3.99570182 -4.39712968 1.82614059  
C 3.00823584 -4.46720325 2.80707831  
C 1.65125876 -4.55225201 2.42275861  
C 0.64861960 -4.63966481 3.42227594  
C 1.01475120 -4.64200015 4.78560588  
C 2.36526949 -4.55699717 5.14209064  
C 3.35186398 -4.46722528 4.16306156  
C 0.02256963 -4.73348865 5.76719549  
C -1.33657559 -4.77279803 5.43386004  
C -1.71547178 -4.84248881 4.06844669  
C -0.71453024 -4.74732848 3.06370080  
C -1.06536380 -4.77328280 1.69077822

C -2.42128151 -4.90793416 1.31393667  
C -2.76864467 -4.93079318 -0.04062073  
C -1.78733370 -4.82757999 -1.02355602  
C -3.40086010 -5.02758368 2.30021157  
C -3.05283876 -4.99930303 3.65098304  
N -2.26480022 -4.95108118 6.48366921  
C 2.82617658 -4.44291697 -2.47185254  
O 3.81249576 -3.54367377 -2.32564869  
O 2.68296291 -5.05099360 -3.51758420  
H 0.26302442 -4.64807212 -2.70908808  
H 4.47000166 -4.37181563 -0.24142331  
H 5.04712677 -4.33737656 2.09928214  
H 2.66317173 -4.56018743 6.18834617  
H 4.39319714 -4.40361907 4.47118809  
H 0.31100911 -4.76287661 6.81566388  
H -3.80811904 -5.03384990 -0.34453973  
H -2.08843196 -4.85209419 -2.06897912  
H -4.44773497 -5.14980422 2.03113390  
H -3.85219230 -5.11483865 4.37742334  
H -1.92802380 -4.61143982 7.37943449  
H -3.18409899 -4.57783671 6.27425953  
H 4.28868630 -3.57649555 -3.18193198

205

(R-Cor-R')5 Energy== -458.560026861149 (M1)

C 0.4637670900 5.8971529900 -1.4892685500  
C -0.6331432100 6.2405409100 -2.2924643300  
C -0.8471654800 5.6143933000 -3.5206580500

C 0.0564191300 4.6232348900 -3.9636916200  
C 1.1732732600 4.2738502400 -3.1632781500  
C 1.3964601900 4.9144696900 -1.9128466400  
C 2.5523834000 4.5453537200 -1.1890831600  
C 3.4364608000 3.5724259600 -1.6558754400  
C 3.2102543800 2.9384935700 -2.8762026700  
C 2.0747098200 3.2875847100 -3.6410527500  
C 1.8546257000 2.6528924300 -4.8903284900  
C 2.7690250600 1.6834830400 -5.3559953100  
C 3.8866916400 1.3542376400 -4.5809950500  
C 4.1035440900 1.9729377000 -3.3521293600  
C 2.5501235000 1.0642466200 -6.5908803000  
C 1.4147672300 1.3449657400 -7.3603583100  
C 0.5251853500 2.3667965200 -6.9393135400  
C 0.7377691500 2.9997535200 -5.6844720000  
C -0.1561336400 3.9957240100 -5.2179370900  
C -1.2631473000 4.3744765700 -6.0114864800  
C -2.1473311100 5.3552014600 -5.5506100100  
C -1.9427637200 5.9672578900 -4.3163794400  
C -1.4568400200 3.7716209200 -7.2547389200  
C -0.5766107700 2.7897491300 -7.7103994100  
N 1.3174135600 0.7377802300 -8.6321024500  
C 0.5685019100 6.6662216200 -0.2255359900  
D 0.9220556300 5.9163836800 0.8306752800  
D 0.2658214700 7.8381465900 -0.0884285300  
H -1.3235635900 7.0105229100 -1.9488070400  
H 2.7942635400 5.0146041300 -0.2387916700

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H 4.9820054100 1.6968577900 -2.7729505700  
H 3.2718494400 0.3380943300 -6.9585234500  
H -3.0031783700 5.6560932300 -6.1510132300  
H -2.6460179500 6.7294144200 -3.9866500300  
H -2.2922829400 4.0614148900 -7.8882546800  
H -0.7629924000 2.3659972200 -8.6931131400  
H 1.8222107100 -0.1409159500 -8.6972400600  
H 0.3618613200 0.6343392900 -8.9553577200  
H 0.8824321000 6.5407666800 1.5854147200  
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C 6.4118586300 3.6442636200 -5.5627298200  
C 5.8992827300 4.5874327500 -4.6716495300  
C 4.7055400400 5.2711856300 -4.9919607800  
C 4.0392273900 4.9994008400 -6.2135396700  
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C 3.8682172800 3.8534696000 -8.3420842300  
C 2.6979806500 4.5519938500 -8.6398869300  
C 2.1811576500 5.4820473600 -7.7398132500  
C 2.8515892800 5.7138685700 -6.5178877000  
C 2.3329975400 6.6724261200 -5.6100379200  
C 1.1576312400 7.3833892600 -5.9352637300  
C 0.5110119800 7.1368233300 -7.1515265700  
C 1.0156324800 6.1934984000 -8.0433908500  
C 0.6532089600 8.3311684800 -5.0388345500  
C 1.2580712600 8.5601068400 -3.7971976000



C 2.4778484600 7.9052901900 -3.4871468000  
C 2.9967429800 6.9383286500 -4.3905778300  
C 4.1918502300 6.2381928300 -4.0902401300  
C 4.8834387900 6.5111263900 -2.8877984800  
C 6.0613264500 5.8186685700 -2.5893152000  
C 6.5628815100 4.8645449700 -3.4712883600  
C 4.3878830100 7.4789833400 -2.0135526200  
C 3.2098793000 8.1649415500 -2.3106566700  
N 0.7320776800 9.5946084700 -2.9918267100  
C 6.4363076600 2.3547046400 -7.6203468200  
O 5.5931703800 1.4827363000 -8.1962201900  
O 7.6426016400 2.2231465800 -7.7269740800  
H 7.3360055900 3.1185242700 -5.3235574100  
H 4.2288700200 3.1550381600 -9.0930029900  
H 2.2016307800 4.3621861200 -9.5892451300  
H -0.3941615400 7.6785038300 -7.4173266200  
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H -0.2370677700 8.8964669700 -5.3056526900  
H 6.6034469900 6.0187769900 -1.6676013900  
H 7.4834306400 4.3449361800 -3.2128960800  
H 4.9144147400 7.7164136400 -1.0917723700  
H 2.8781282900 8.9211031600 -1.6048302400  
H -0.2509732400 9.7793675700 -3.1668839100  
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C 0.4027871200 -2.9332766500 -0.1935003500  
C 0.7675030900 -3.8613542000 -1.1793529000

C 0.0131706000 -4.0046889400 -2.3441549500  
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C -1.5195357700 -2.2705966500 -1.5375051400  
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C -3.1086034900 -0.5728301600 -0.7581884100  
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C -3.4546006700 -1.6427204800 -2.9288151800  
C -4.6230713100 -0.8718863100 -3.1110715200  
C -5.0184552700 0.0345674200 -2.1210110800  
C -4.2672648500 0.1850730900 -0.9578315400  
C -5.3767155500 -1.0254253800 -4.2793003900  
C -4.9743144900 -1.8923203200 -5.3022862300  
C -3.8424712100 -2.7242047400 -5.1031082900  
C -3.0686126700 -2.5734001600 -3.9203764100  
C -1.9094928300 -3.3616028000 -3.7109676700  
C -1.5240845900 -4.3165278600 -4.6795914500  
C -0.3788199500 -5.0927652900 -4.4750583600  
C 0.3835943300 -4.9366279500 -3.3200122200  
C -2.2985189700 -4.4825848900 -5.8282014300  
C -3.4377336900 -3.7035999000 -6.0328338800  
N -5.8392432000 -2.0485128900 -6.4081738200  
C 1.2892256300 -2.9148550600 0.9953408100  
D 1.5567931900 -1.6784864700 1.4454960300  
D 1.8339262100 -3.8899267700 1.4815079600  
H 1.6522038300 -4.4791741700 -1.0268537500

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H -5.9177910400 0.6337320000 -2.2459251800  
H -4.6006933100 0.8968446800 -0.2057882400  
H -6.2913030800 -0.4496533300 -4.4032486100  
H -0.0708423600 -5.8311564500 -5.2122304600  
H 1.2673035300 -5.5576978500 -3.1877216300  
H -2.0291138100 -5.2240645800 -6.5771449400  
H -4.0147616300 -3.8860939500 -6.9349229800  
H -6.4292264100 -1.2388294400 -6.5740127600  
H -5.3597081300 -2.3302397200 -7.2560831200  
H 2.1946163800 -1.8273506500 2.1749319900  
C -2.2676307900 -0.4528639800 -7.1950865900  
C -3.2338127200 0.5020005200 -6.8472688200  
C -3.1457478100 1.2077116400 -5.6470427800  
C -2.0702155800 0.9537717300 -4.7673361000  
C -1.0919916700 -0.0152200200 -5.1053116300  
C -1.1823482800 -0.7397329800 -6.3262544300  
C -0.1953254200 -1.7190911900 -6.5770172700  
C 0.8495688600 -1.9597055700 -5.6846176900  
C 0.9421336900 -1.2413769500 -4.4939565600  
C -0.0321584600 -0.2628150000 -4.1948027500  
C 0.0545806300 0.4560943300 -2.9751278400  
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(R-Cor-R')5 Energy=-447.475158434948 (M2)

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(R-Cor-R')5 Energy=-438.635582872376 (M3)

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205

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D -9.9452397500 -8.3374402600 8.0412446800

H -7.3829084600 -8.2149967200 7.7386228300  
H -10.8903242500 -5.3729516300 5.8717648200  
H -10.9813479300 -3.7862112500 4.0587201200  
H -7.9356776100 -2.1591628200 0.8137337300  
H -9.9028692200 -2.5947586600 2.1945113700  
H -5.5923299100 -2.5820969300 0.2686394900  
H -3.0842540600 -8.2072203000 5.7801458000  
H -5.0380035300 -8.6310762700 7.1827359500  
H -2.0285218700 -7.0469642700 3.8813001800  
H -2.1360528600 -5.4514220500 2.0637056500  
H -3.3008280000 -2.7456886400 -0.0075768900  
H -2.3028192700 -3.7276359600 0.9089512100  
H -11.1344362200 -6.5862265700 8.6610969700