

Electronic Supplementary Information belonging to the manuscript:

π -Conjugation in Donor-Substituted Cyanoethynylethenes: an EDA Study

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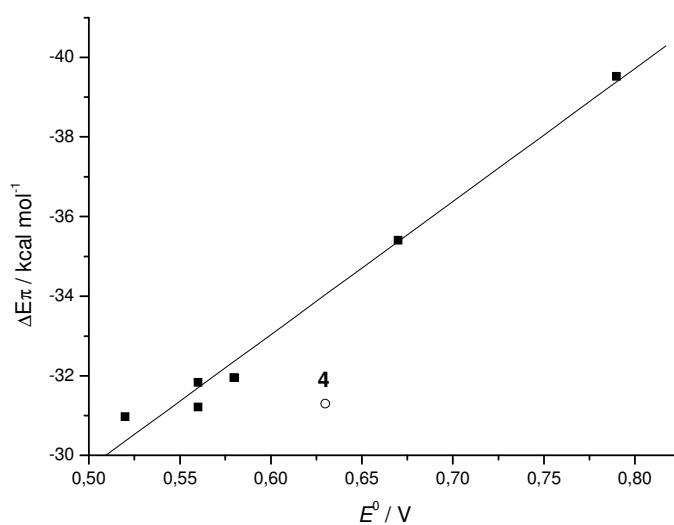


Figure 1S. Plot of the ΔE_π values versus the first oxidation potentials E^0 .

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Cartesian coordinates (in Å) and total energies (in a.u.) of all species discussed in the text. All calculations have been performed at the BP86/TZ2P level of theory. See text for computational details.

1, E = -7.246656

C	1.549840000	1.713620000	0.000000000
C	0.337210000	0.980310000	0.000000000
C	-0.879230000	1.708870000	0.000000000
C	-0.885320000	3.087200000	0.000000000
C	0.331200000	3.826320000	0.000000000
C	1.550890000	3.092280000	0.000000000
C	0.333740000	-0.416260000	0.000000000
C	0.306680000	-1.642380000	0.000000000
C	0.275620000	-3.031850000	0.000000000
C	1.537100000	-3.708650000	0.000000000
N	2.578370000	-4.227710000	0.000000000
N	0.328350000	5.194210000	0.000000000
C	-0.908290000	-3.777400000	0.000000000
C	-0.907490000	-5.195610000	0.000000000
N	-0.924820000	-6.361210000	0.000000000
C	-2.164140000	-3.115210000	0.000000000
N	-3.188980000	-2.559810000	0.000000000
C	-0.931380000	5.929230000	0.000000000
C	1.584770000	5.934430000	0.000000000
H	2.493690000	1.171920000	0.000000000
H	-1.820150000	1.162150000	0.000000000
H	-1.840090000	3.606090000	0.000000000
H	2.503270000	3.615340000	0.000000000
H	-0.718260000	7.001250000	0.000000000
H	-1.532420000	5.698500000	-0.892690000
H	-1.532420000	5.698500000	0.892690000
H	1.367290000	7.005570000	0.000000000
H	2.186840000	5.706320000	0.892750000
H	2.186840000	5.706320000	-0.892750000

2, E = -7.366271

C	1.547470000	1.699530000	0.000000000
C	0.336120000	0.967560000	0.000000000
C	-0.876800000	1.698080000	0.000000000
C	-0.881250000	3.078170000	0.000000000
C	0.334570000	3.815610000	0.000000000
C	1.551500000	3.079960000	0.000000000
C	0.331640000	-0.433260000	0.000000000
C	0.305440000	-1.658020000	0.000000000
C	0.292130000	-3.054310000	0.000000000
C	1.543230000	-3.726070000	0.000000000
C	2.616690000	-4.286720000	0.000000000
N	0.333570000	5.186420000	0.000000000
C	-0.901060000	-3.787500000	0.000000000
C	-0.900450000	-5.206380000	0.000000000
N	-0.910600000	-6.372400000	0.000000000
C	-2.156810000	-3.125280000	0.000000000

N	-3.184390000	-2.574360000	0.000000000
C	-0.924960000	5.920700000	0.000000000
C	1.590370000	5.922930000	0.000000000
H	2.490990000	1.156990000	0.000000000
H	-1.818570000	1.152860000	0.000000000
H	-1.835770000	3.597630000	0.000000000
H	2.505200000	3.601010000	0.000000000
H	3.556800000	-4.794050000	0.000000000
H	-0.712270000	6.993040000	0.000000000
H	-1.527470000	5.690640000	-0.892400000
H	-1.527470000	5.690640000	0.892400000
H	1.375840000	6.994950000	0.000000000
H	2.193540000	5.694340000	0.892490000
H	2.193540000	5.694340000	-0.892490000

3, E = -7.958079

C	1.160650000	2.170910000	0.000000000
C	-0.045410000	1.430420000	0.000000000
C	-1.263890000	2.151910000	0.000000000
C	-1.278540000	3.531770000	0.000000000
C	-0.068090000	4.278090000	0.000000000
C	1.154280000	3.551320000	0.000000000
C	-0.042610000	0.029450000	0.000000000
C	-0.069740000	-1.195040000	0.000000000
C	-0.095960000	-2.592550000	0.000000000
C	1.141360000	-3.268700000	0.000000000
C	2.229890000	-3.827060000	0.000000000
N	-0.079320000	5.648690000	0.000000000
C	-1.301660000	-3.311840000	0.000000000
C	-1.318360000	-4.729390000	0.000000000
N	-1.342270000	-5.895360000	0.000000000
C	-2.546260000	-2.631770000	0.000000000
N	-3.564610000	-2.063350000	0.000000000
C	-1.343250000	6.373910000	0.000000000
C	1.171990000	6.394720000	0.000000000
C	3.428440000	-4.453120000	0.000000000
C	4.507390000	-5.016770000	0.000000000
H	2.108160000	1.635470000	0.000000000
H	-2.201640000	1.599820000	0.000000000
H	-2.236880000	4.044150000	0.000000000
H	2.104090000	4.079380000	0.000000000
H	-1.138280000	7.447750000	0.000000000
H	-1.943990000	6.139490000	-0.892420000
H	-1.943990000	6.139490000	0.892420000
H	0.949280000	7.465010000	0.000000000
H	1.776710000	6.170590000	0.892520000
H	1.776710000	6.170590000	-0.892520000
H	5.450670000	-5.517250000	0.000000000

4, E = -11.489572

C	0.000000000	-3.407970000	1.475940000
C	0.000000000	-3.424230000	0.062480000
C	0.000000000	-4.683670000	-0.580280000
C	0.000000000	-5.859820000	0.145320000
C	0.000000000	-5.845370000	1.565770000
C	0.000000000	-4.579250000	2.209710000
C	0.000000000	-2.231350000	-0.679770000

C	0.000000000	-1.199490000	-1.336450000
C	0.000000000	0.000000000	-2.064250000
C	0.000000000	1.199490000	-1.336450000
C	0.000000000	2.231350000	-0.679770000
N	0.000000000	-7.012570000	2.290420000
C	0.000000000	0.000000000	-3.471690000
C	0.000000000	-1.215670000	-4.200210000
N	0.000000000	-2.219340000	-4.795560000
C	0.000000000	1.215670000	-4.200210000
N	0.000000000	2.219340000	-4.795560000
C	0.000000000	-8.298790000	1.608870000
C	0.000000000	-6.972450000	3.744990000
C	0.000000000	3.424220000	0.062480000
C	0.000000000	4.683670000	-0.580280000
C	0.000000000	3.407970000	1.475940000
C	0.000000000	5.859820000	0.145320000
C	0.000000000	4.579250000	2.209710000
C	0.000000000	5.845370000	1.565770000
N	0.000000000	7.012570000	2.290420000
C	0.000000000	8.298790000	1.608870000
C	0.000000000	6.972450000	3.744990000
H	0.000000000	-2.449300000	1.991450000
H	0.000000000	-4.718290000	-1.668000000
H	0.000000000	-6.804570000	-0.391950000
H	0.000000000	-4.517400000	3.294840000
H	0.000000000	-9.098260000	2.354930000
H	-0.892150000	-8.422350000	0.974710000
H	0.892150000	-8.422350000	0.974710000
H	0.000000000	-7.995610000	4.130820000
H	0.892230000	-6.459040000	4.137600000
H	-0.892230000	-6.459040000	4.137600000
H	0.000000000	4.718290000	-1.668000000
H	0.000000000	2.449300000	1.991450000
H	0.000000000	6.804570000	-0.391950000
H	0.000000000	4.517400000	3.294840000
H	0.000000000	9.098260000	2.354930000
H	0.892150000	8.422350000	0.974710000
H	-0.892150000	8.422350000	0.974710000
H	0.000000000	7.995610000	4.130820000
H	-0.892230000	6.459040000	4.137600000
H	0.892230000	6.459040000	4.137600000

5, E = -14.011915

C	-5.031920000	-0.909300000	0.000000000
C	-4.514280000	0.408250000	0.000000000
C	-5.444060000	1.475100000	0.000000000
C	-6.805640000	1.243910000	0.000000000
C	-7.324380000	-0.078590000	0.000000000
C	-6.391800000	-1.150080000	0.000000000
C	-3.131310000	0.642870000	0.000000000
C	-1.922700000	0.842850000	0.000000000
C	-0.531560000	1.004160000	0.000000000
C	0.251230000	-0.151270000	0.000000000
C	0.909260000	-1.186060000	0.000000000
N	-8.678300000	-0.312930000	0.000000000
C	0.061130000	2.302060000	0.000000000
C	-0.734780000	3.473710000	0.000000000
C	-1.382830000	4.498650000	0.000000000
C	1.440280000	2.444760000	0.000000000

C	2.661420000	2.595530000	0.000000000
C	-9.615360000	0.800950000	0.000000000
C	-9.186710000	-1.676730000	0.000000000
C	4.041520000	2.707730000	0.000000000
C	4.745650000	3.923510000	0.000000000
C	4.772180000	1.476020000	0.000000000
C	4.052800000	5.160160000	0.000000000
C	6.162060000	3.964260000	0.000000000
N	7.327980000	4.009800000	0.000000000
C	1.669120000	-2.363350000	0.000000000
C	1.053160000	-3.635680000	0.000000000
C	3.082940000	-2.328140000	0.000000000
C	1.796760000	-4.798220000	0.000000000
C	3.831080000	-3.486430000	0.000000000
C	3.221460000	-4.773080000	0.000000000
N	3.967270000	-5.928160000	0.000000000
C	5.423180000	-5.953200000	0.000000000
C	3.393150000	-7.264980000	0.000000000
N	3.488580000	6.180910000	0.000000000
N	5.326220000	0.452580000	0.000000000
H	-4.335930000	-1.746120000	0.000000000
H	-5.068700000	2.496450000	0.000000000
H	-7.480800000	2.095790000	0.000000000
H	-6.741240000	-2.179380000	0.000000000
H	-1.944110000	5.406770000	0.000000000
H	-10.636050000	0.408620000	0.000000000
H	-9.492330000	1.434700000	0.892370000
H	-9.492330000	1.434700000	-0.892370000
H	-10.279870000	-1.650070000	0.000000000
H	-8.858150000	-2.232580000	-0.892390000
H	-8.858150000	-2.232580000	0.892390000
H	-0.033710000	-3.696510000	0.000000000
H	3.597470000	-1.369360000	0.000000000
H	1.257970000	-5.740500000	0.000000000
H	4.910960000	-3.379580000	0.000000000
H	5.849810000	-4.951380000	0.000000000
H	5.793550000	-6.484060000	0.891530000
H	5.793550000	-6.484060000	-0.891530000
H	2.304250000	-7.242970000	0.000000000
H	3.724800000	-7.821560000	-0.891310000
H	3.724800000	-7.821560000	0.891310000

6, E = -11.486780

C	4.849360000	-2.287070000	0.000000000
C	4.270760000	-0.997280000	0.000000000
C	5.145300000	0.114690000	0.000000000
C	6.517510000	-0.050490000	0.000000000
C	7.100470000	-1.345410000	0.000000000
C	6.221030000	-2.460410000	0.000000000
C	2.877960000	-0.818260000	0.000000000
C	1.667500000	-0.634360000	0.000000000
C	0.289020000	-0.412220000	0.000000000
C	-0.568470000	-1.553310000	0.000000000
N	8.465230000	-1.513230000	0.000000000
C	-0.291780000	0.867250000	0.000000000
C	-1.668770000	1.096200000	0.000000000
C	-2.875960000	1.301560000	0.000000000
C	0.567160000	2.007670000	0.000000000
N	1.258470000	2.945660000	0.000000000

C	9.345980000	-0.355000000	0.000000000
C	9.038730000	-2.850190000	0.000000000
C	-4.262590000	1.518350000	0.000000000
C	-5.173750000	0.437870000	0.000000000
C	-4.803540000	2.824930000	0.000000000
C	-6.539790000	0.649250000	0.000000000
C	-6.167580000	3.043020000	0.000000000
C	-7.088330000	1.961130000	0.000000000
N	-8.453280000	2.140320000	0.000000000
C	-9.343210000	0.987870000	0.000000000
C	-9.103980000	3.440370000	0.000000000
N	-1.259480000	-2.491540000	0.000000000
H	4.196170000	-3.157630000	0.000000000
H	4.721480000	1.117130000	0.000000000
H	7.149320000	0.834000000	0.000000000
H	6.619710000	-3.471500000	0.000000000
H	10.384980000	-0.696180000	0.000000000
H	9.192210000	0.273040000	-0.892060000
H	9.192210000	0.273040000	0.892060000
H	10.129440000	-2.771410000	0.000000000
H	8.737230000	-3.422270000	0.892120000
H	8.737230000	-3.422270000	-0.892120000
H	-4.785880000	-0.579020000	0.000000000
H	-4.124700000	3.675700000	0.000000000
H	-7.196380000	-0.216480000	0.000000000
H	-6.516890000	4.071680000	0.000000000
H	-10.378170000	1.344040000	0.000000000
H	-9.197790000	0.360010000	-0.892990000
H	-9.197790000	0.360010000	0.892990000
H	-8.373800000	4.249920000	0.000000000
H	-9.738440000	3.558540000	-0.892750000
H	-9.738440000	3.558540000	0.892750000

(E)-7, E = -7.482135

C	1.538900000	1.676900000	0.000000000
C	0.327300000	0.948200000	0.000000000
C	-0.881800000	1.681800000	0.000000000
C	-0.882400000	3.063500000	0.000000000
C	0.334000000	3.797100000	0.000000000
C	1.547300000	3.059100000	0.000000000
C	0.320200000	-0.456200000	0.000000000
C	0.292900000	-1.679700000	0.000000000
C	0.287800000	-3.080200000	0.000000000
C	1.548900000	-3.735500000	0.000000000
C	2.639900000	-4.263100000	0.000000000
N	0.335200000	5.170500000	0.000000000
C	-0.896400000	-3.824500000	0.000000000
C	-0.915400000	-5.236500000	0.000000000
C	-0.957500000	-6.449300000	0.000000000
C	-2.150600000	-3.149400000	0.000000000
N	-3.181700000	-2.604800000	0.000000000
H	-1.825500000	1.139700000	0.000000000
H	-1.835700000	3.585400000	0.000000000
H	2.502700000	3.577500000	0.000000000
H	2.480900000	1.131800000	0.000000000
C	-0.917900000	5.904500000	0.000000000
C	1.586100000	5.909700000	0.000000000
H	3.597000000	-4.736600000	0.000000000
H	-0.985900000	-7.516600000	0.000000000

H	1.369400000	6.984100000	0.000000000
H	2.194500000	5.683500000	0.893500000
H	2.194500000	5.683500000	-0.893500000
H	-0.704400000	6.979200000	0.000000000
H	-1.524900000	5.676000000	-0.893200000
H	-1.524900000	5.676000000	0.893200000

(Z)-7, E = -7.481372

C	1.036380000	2.027320000	0.000000000
C	0.048310000	1.016020000	0.000000000
C	-1.305190000	1.424740000	0.000000000
C	-1.655010000	2.761820000	0.000000000
C	-0.663050000	3.778440000	0.000000000
C	0.696530000	3.367360000	0.000000000
C	0.395530000	-0.346090000	0.000000000
C	0.683040000	-1.535800000	0.000000000
C	1.051250000	-2.888390000	0.000000000
C	2.439590000	-3.189680000	0.000000000
C	3.625730000	-3.436510000	0.000000000
N	-1.006360000	5.108920000	0.000000000
C	0.104470000	-3.917140000	0.000000000
C	-1.286490000	-3.669830000	0.000000000
C	-2.486020000	-3.487150000	0.000000000
C	0.522590000	-5.278770000	0.000000000
N	0.838260000	-6.400860000	0.000000000
H	-2.082810000	0.663530000	0.000000000
H	-2.709110000	3.026730000	0.000000000
H	1.491570000	4.108450000	0.000000000
H	2.085580000	1.737880000	0.000000000
C	-2.406960000	5.504480000	0.000000000
C	0.027580000	6.133190000	0.000000000
H	-3.541320000	-3.326140000	0.000000000
H	4.667350000	-3.671730000	0.000000000
H	-0.445940000	7.118840000	0.000000000
H	0.669810000	6.062430000	0.892260000
H	0.669810000	6.062430000	-0.892260000
H	-2.470090000	6.596130000	0.000000000
H	-2.934680000	5.131550000	-0.892240000
H	-2.934680000	5.131550000	0.892240000

8, E = -7.480958

C	1.671890000	1.531610000	0.000000000
C	0.391850000	0.931460000	0.000000000
C	-0.732880000	1.787910000	0.000000000
C	-0.591550000	3.162740000	0.000000000
C	0.693830000	3.766550000	0.000000000
C	1.823150000	2.906000000	0.000000000
C	0.239510000	-0.465760000	0.000000000
C	0.090000000	-1.680320000	0.000000000
C	-0.048800000	-3.072920000	0.000000000
C	1.158380000	-3.840050000	0.000000000
N	2.158250000	-4.437150000	0.000000000
N	0.836460000	5.133120000	0.000000000
C	-1.281090000	-3.731160000	0.000000000
C	-2.494410000	-3.000710000	0.000000000
C	-3.550520000	-2.403560000	0.000000000
C	-1.366570000	-5.143800000	0.000000000

C	-1.463860000	-6.352840000	0.000000000
H	-1.728300000	1.348070000	0.000000000
H	-1.485640000	3.780730000	0.000000000
H	2.827290000	3.322020000	0.000000000
H	2.552620000	0.892260000	0.000000000
C	-0.333920000	5.991480000	0.000000000
C	2.156220000	5.740640000	0.000000000
H	-4.479550000	-1.877470000	0.000000000
H	-1.534080000	-7.418290000	0.000000000
H	-0.011600000	7.038790000	0.000000000
H	-0.961710000	5.827010000	-0.893290000
H	-0.961710000	5.827010000	0.893290000
H	2.050790000	6.831940000	0.000000000
H	2.738690000	5.453550000	0.893560000
H	2.738690000	5.453550000	-0.893560000

9a, E = -10.660920

C	0.373320000	5.451430000	0.000000000
C	-0.618180000	4.443070000	0.000000000
C	-1.970060000	4.857520000	0.000000000
C	-2.314670000	6.196210000	0.000000000
C	-1.319080000	7.209100000	0.000000000
C	0.038710000	6.792750000	0.000000000
C	-0.271930000	3.081100000	0.000000000
C	0.023500000	1.892600000	0.000000000
C	0.409760000	0.546360000	0.000000000
C	1.803460000	0.272960000	0.000000000
C	2.999840000	0.074850000	0.000000000
N	-1.656880000	8.541450000	0.000000000
C	-0.523550000	-0.503450000	0.000000000
C	-1.916980000	-0.238350000	0.000000000
C	-3.114120000	-0.041880000	0.000000000
C	-0.117380000	-1.848190000	0.000000000
C	0.200250000	-3.028950000	0.000000000
C	-3.055490000	8.943040000	0.000000000
C	-0.618450000	9.560870000	0.000000000
C	0.581990000	-4.385090000	0.000000000
C	-0.393780000	-5.410510000	0.000000000
C	1.950290000	-4.747730000	0.000000000
C	-0.017790000	-6.744260000	0.000000000
C	2.328640000	-6.080360000	0.000000000
C	1.340910000	-7.068240000	0.000000000
N	1.741840000	-8.481970000	0.000000000
O	0.843890000	-9.336250000	0.000000000
O	2.954900000	-8.736850000	0.000000000
H	1.421350000	5.157850000	0.000000000
H	-2.750900000	4.099540000	0.000000000
H	-3.367790000	6.465230000	0.000000000
H	0.836760000	7.530650000	0.000000000
H	4.052180000	-0.104990000	0.000000000
H	-4.166900000	0.134400000	0.000000000
H	-3.113900000	10.034980000	0.000000000
H	-3.584990000	8.572440000	-0.892240000
H	-3.584990000	8.572440000	0.892240000
H	-1.087330000	10.548740000	0.000000000
H	0.023640000	9.487210000	0.892210000
H	0.023640000	9.487210000	-0.892210000
H	-1.446720000	-5.136750000	0.000000000

H	2.702830000	-3.962380000	0.000000000
H	-0.753480000	-7.544040000	0.000000000
H	3.374200000	-6.376680000	0.000000000

9b, E = -10.660063

C	4.353400000	-0.414120000	0.000000000
C	2.941150000	-0.340010000	0.000000000
C	2.357650000	0.947370000	0.000000000
C	3.129640000	2.093320000	0.000000000
C	4.547820000	2.019000000	0.000000000
C	5.135620000	0.725870000	0.000000000
C	2.146530000	-1.499080000	0.000000000
C	1.443230000	-2.501330000	0.000000000
C	0.685810000	-3.679790000	0.000000000
C	1.398470000	-4.907560000	0.000000000
C	2.030220000	-5.942680000	0.000000000
N	5.319940000	3.155410000	0.000000000
C	-0.719040000	-3.673040000	0.000000000
C	-1.446050000	-2.470850000	0.000000000
C	-2.118410000	-1.449750000	0.000000000
C	-1.457960000	-4.883540000	0.000000000
C	4.690790000	4.467840000	0.000000000
C	6.771680000	3.055720000	0.000000000
C	-2.116440000	-5.902470000	0.000000000
C	-2.893870000	-0.273660000	0.000000000
C	-4.307860000	-0.342580000	0.000000000
C	-2.276760000	0.999800000	0.000000000
C	-5.072240000	0.813210000	0.000000000
C	-3.037840000	2.157060000	0.000000000
C	-4.430810000	2.054140000	0.000000000
N	-5.239470000	3.280950000	0.000000000
O	-6.472570000	3.158750000	0.000000000
O	-4.639890000	4.366230000	0.000000000
H	4.828500000	-1.393360000	0.000000000
H	1.273130000	1.029940000	0.000000000
H	2.632550000	3.059820000	0.000000000
H	6.217180000	0.617560000	0.000000000
H	2.576470000	-6.860000000	0.000000000
H	5.467870000	5.237070000	0.000000000
H	4.062080000	4.616990000	-0.892270000
H	4.062080000	4.616990000	0.892270000
H	7.198840000	4.062300000	0.000000000
H	7.142690000	2.526730000	0.892300000
H	7.142690000	2.526730000	-0.892300000
H	-2.684820000	-6.806090000	0.000000000
H	-4.788040000	-1.318720000	0.000000000
H	-1.191120000	1.056830000	0.000000000
H	-6.158460000	0.778070000	0.000000000
H	-2.579960000	3.142550000	0.000000000

10, E = -10.659548

C	-0.230790000	3.699910000	0.000000000
C	-1.510400000	3.100730000	0.000000000
C	-2.632090000	3.959950000	0.000000000
C	-2.488430000	5.335590000	0.000000000
C	-1.202880000	5.937950000	0.000000000
C	-0.076180000	5.074400000	0.000000000

C	-1.661950000	1.701030000	0.000000000
C	-1.802840000	0.486110000	0.000000000
C	-1.920330000	-0.914510000	0.000000000
C	-0.723850000	-1.664220000	0.000000000
C	0.326360000	-2.285790000	0.000000000
N	-1.054630000	7.305360000	0.000000000
C	-3.165030000	-1.561560000	0.000000000
C	-4.373230000	-0.825280000	0.000000000
C	-5.427610000	-0.223590000	0.000000000
C	-3.265440000	-2.973290000	0.000000000
C	-3.393000000	-4.180670000	0.000000000
C	-2.225270000	8.168760000	0.000000000
C	0.274040000	7.897500000	0.000000000
C	1.534590000	-3.015990000	0.000000000
C	1.519740000	-4.429800000	0.000000000
C	2.779590000	-2.346050000	0.000000000
C	2.705200000	-5.148430000	0.000000000
C	3.966950000	-3.061700000	0.000000000
C	3.917760000	-4.456670000	0.000000000
N	5.178210000	-5.218430000	0.000000000
O	5.102770000	-6.454390000	0.000000000
O	6.237470000	-4.576940000	0.000000000
H	0.649740000	3.060090000	0.000000000
H	-3.628450000	3.522220000	0.000000000
H	-3.381990000	5.954510000	0.000000000
H	0.929270000	5.487290000	0.000000000
h	-6.353830000	0.307060000	0.000000000
H	-3.502270000	-5.242590000	0.000000000
H	-1.899640000	9.212720000	0.000000000
H	-2.851210000	8.006200000	-0.892170000
H	-2.851210000	8.006200000	0.892170000
H	0.180070000	8.987010000	0.000000000
H	0.850490000	7.604340000	0.892140000
H	0.850490000	7.604340000	-0.892140000
H	0.562640000	-4.946450000	0.000000000
H	2.793570000	-1.258310000	0.000000000
H	2.713990000	-6.235070000	0.000000000
H	4.933280000	-2.564630000	0.000000000