

Supporting Information for

Photochemistry of 5-Allyloxy-tetrazoles: Steady-state and Laser Flash Photolysis Study

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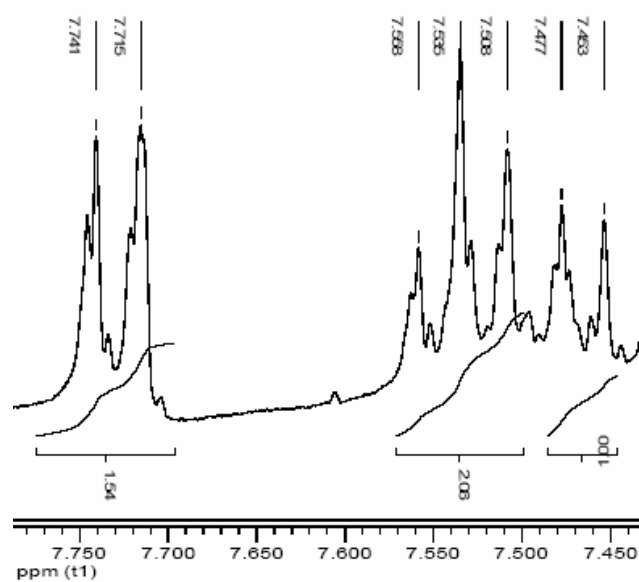
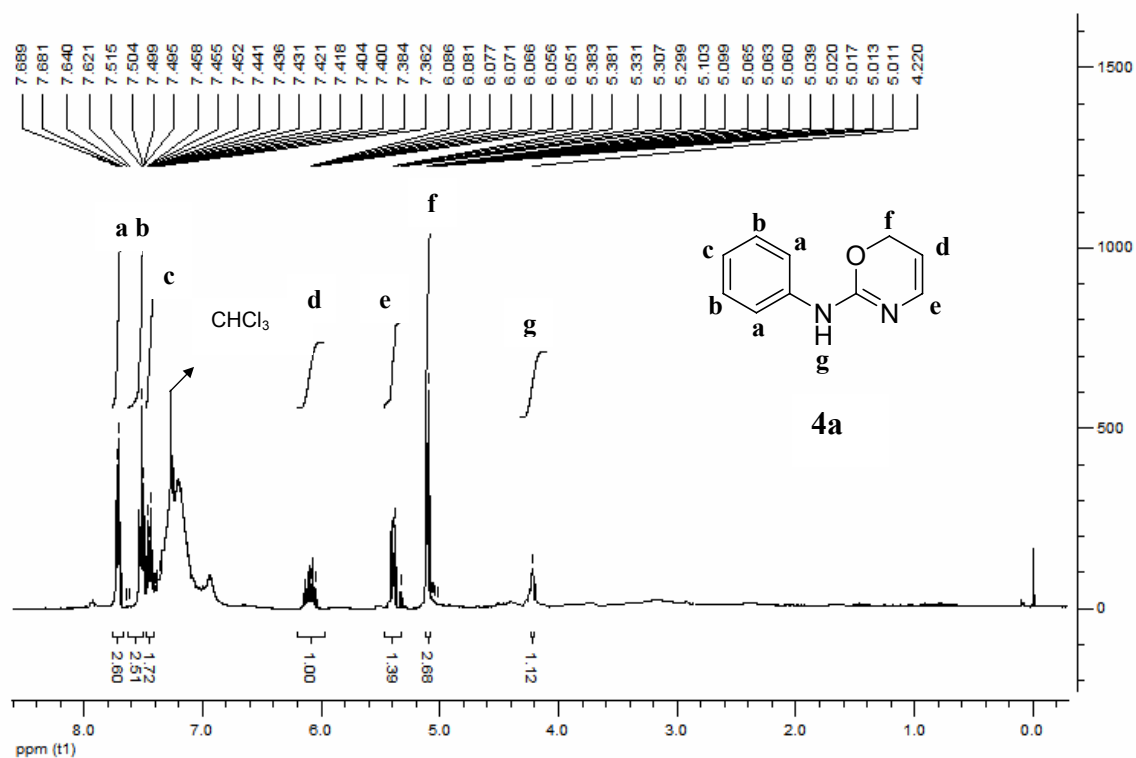
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Pages S2-S3: ¹H-NMR for compounds **4a-c** with structure.

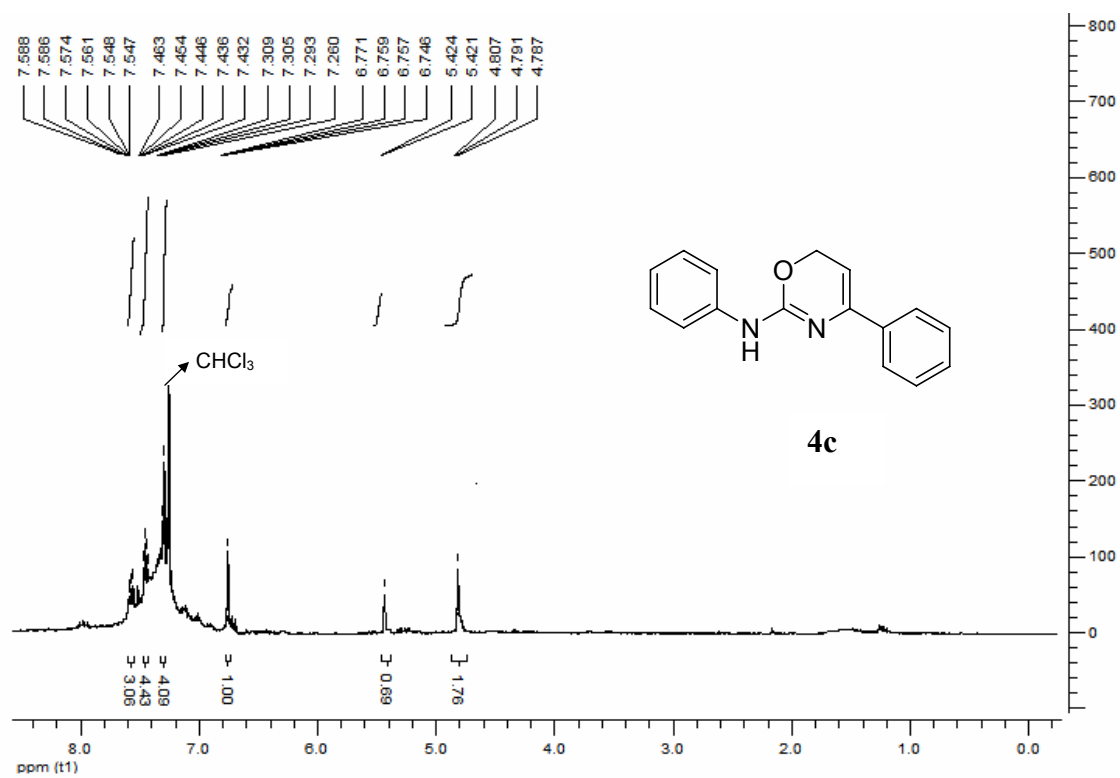
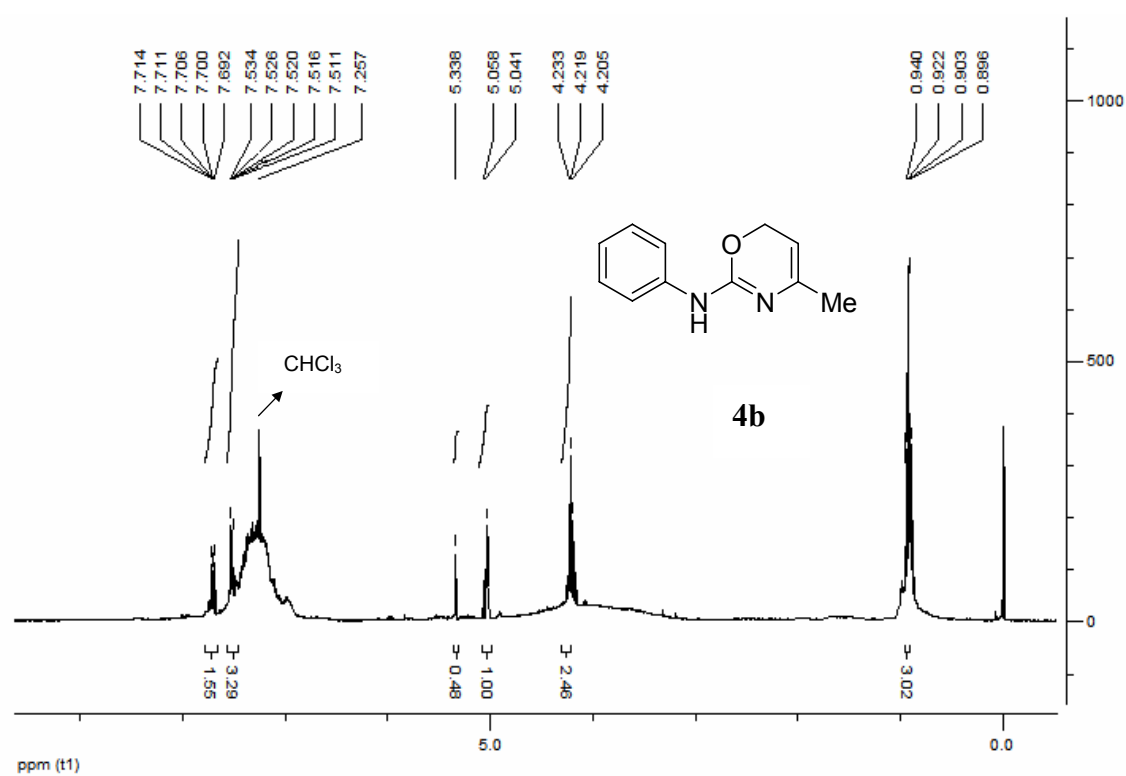
Pages S4-S15: Geometries and energies of compounds **4a-c**, **5a-c**, **6**, **7a-c**, **8**, **9**, **10** and **11a-c**.

Pages S16-S26: Cartesian coordinates of compounds **4a-c**, **5a-c**, **6**, **7a-c**, **8**, **9**, **10** and **11a-c**.

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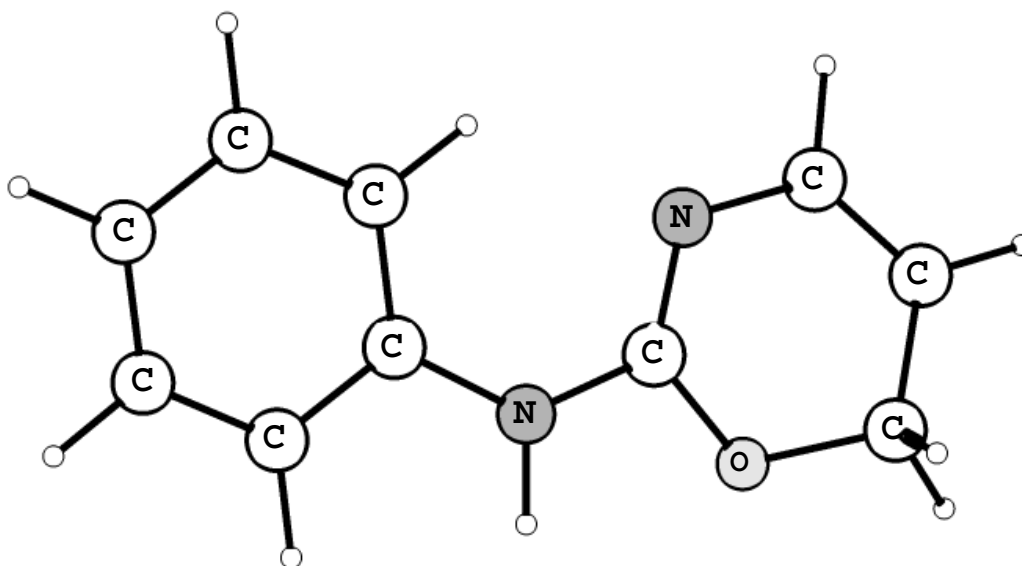
Signals corresponding to the hydrogen atoms of phenyl ring. Spectra expansion (7.440-7.790 ppm).



GEOMETRIES AND ENERGIES

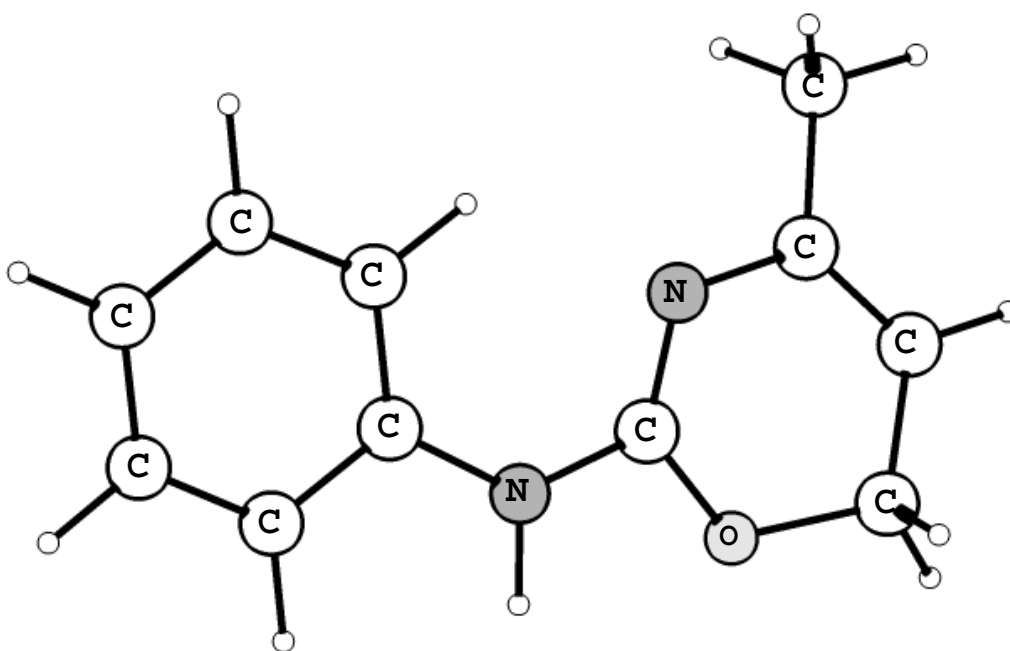
All energies are expressed in Hartrees ($1 \text{ Hartree} = 1 \text{ kJ mol}^{-1}$) and were calculated for the geometries fully optimized at the DFT(B3LYP)/6-31G(d,p) level of theory. The nature of the calculated structures as minima on the corresponding potential energy surfaces was confirmed by analysis of the corresponding Hessian matrices (no imaginary vibrational frequencies). For every compound, all possible conformers and tautomers were investigated and only the data for the most stable structure are included.

Note: CARTESIAN COORDINATES for these structures see starting from page S16.



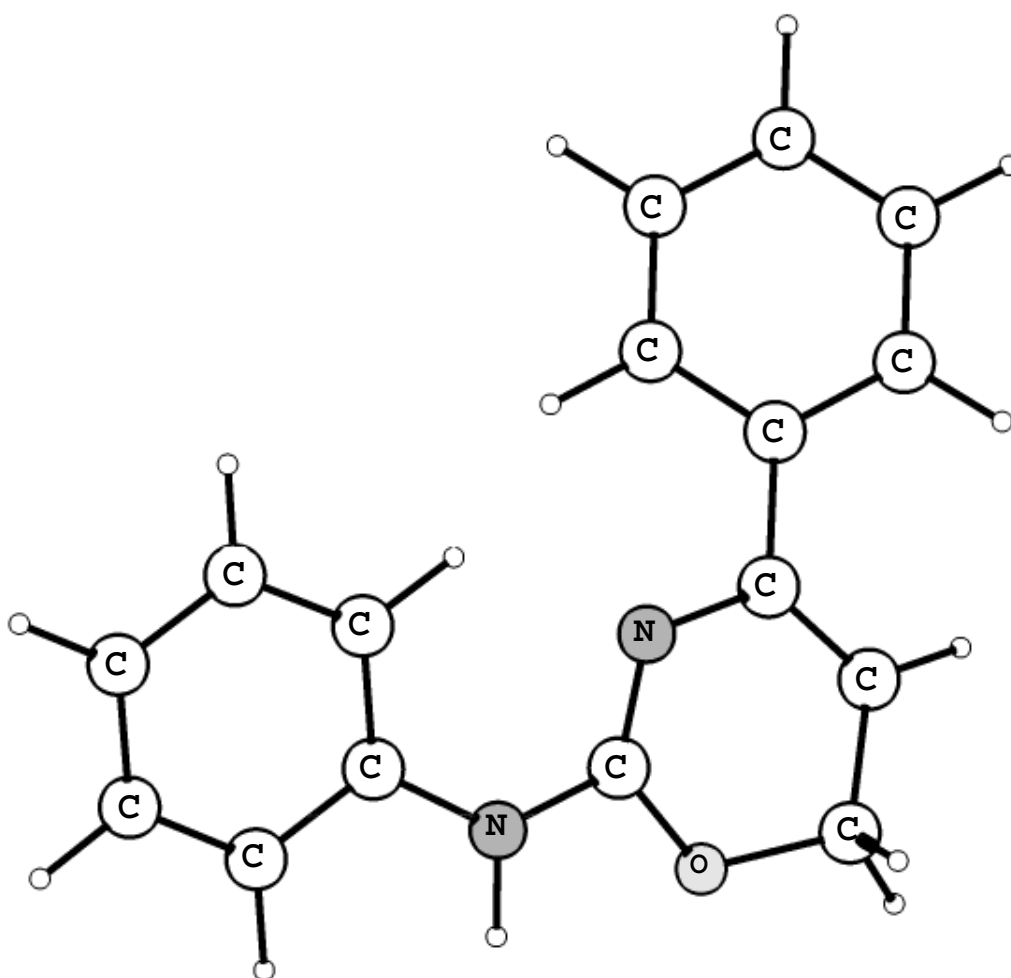
4a

Sum of electronic and zero-point Energies=	-571.618474
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Sum of electronic and thermal Free Energies=	-571.655856



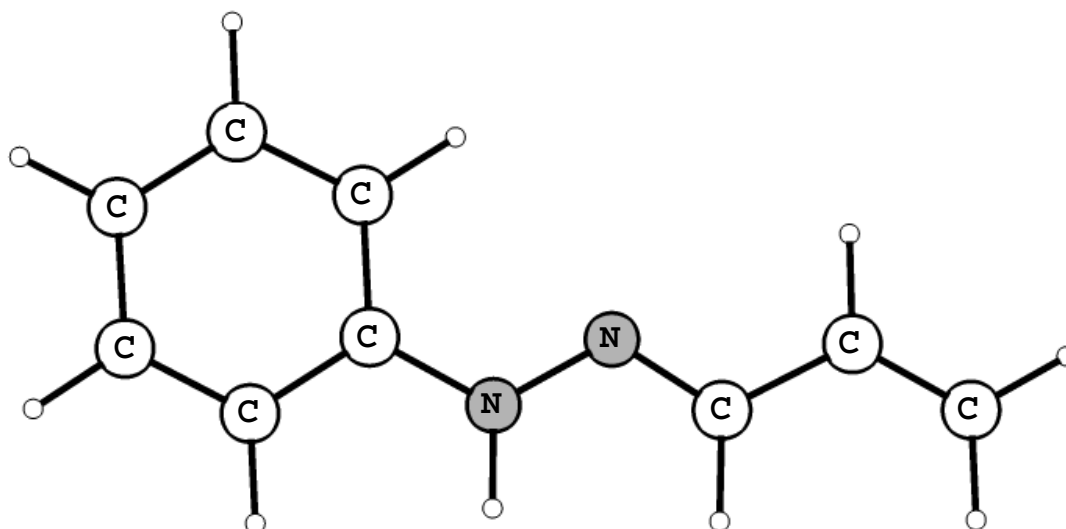
4b

Sum of electronic and zero-point Energies=	-610.915106
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Sum of electronic and thermal Free Energies=	-610.954186



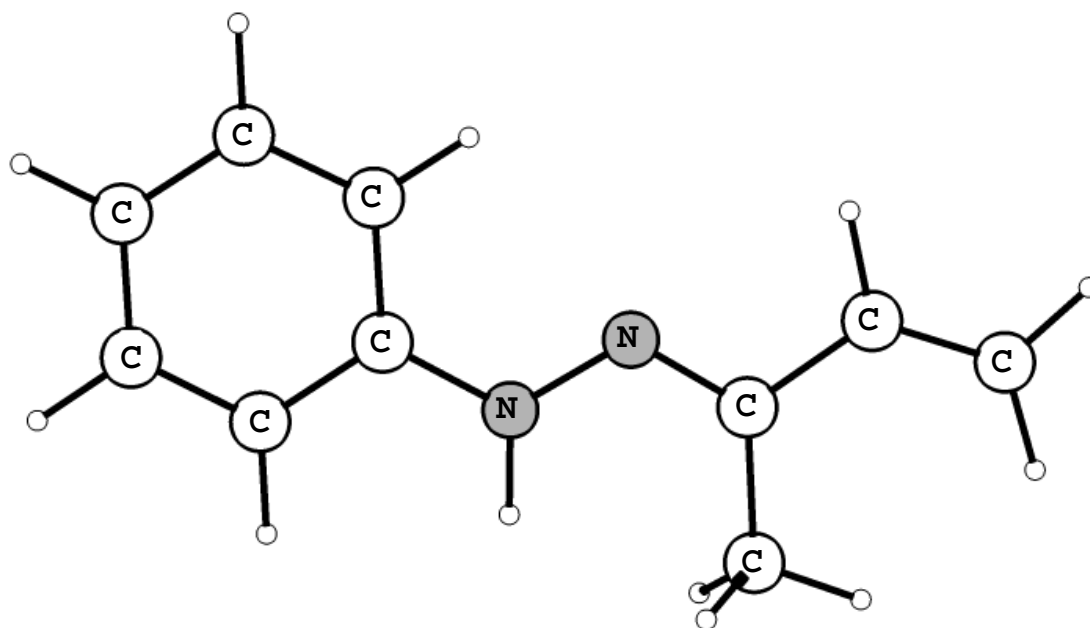
4c

Sum of electronic and zero-point Energies=	-802.603942
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Sum of electronic and thermal Free Energies=	-802.648096



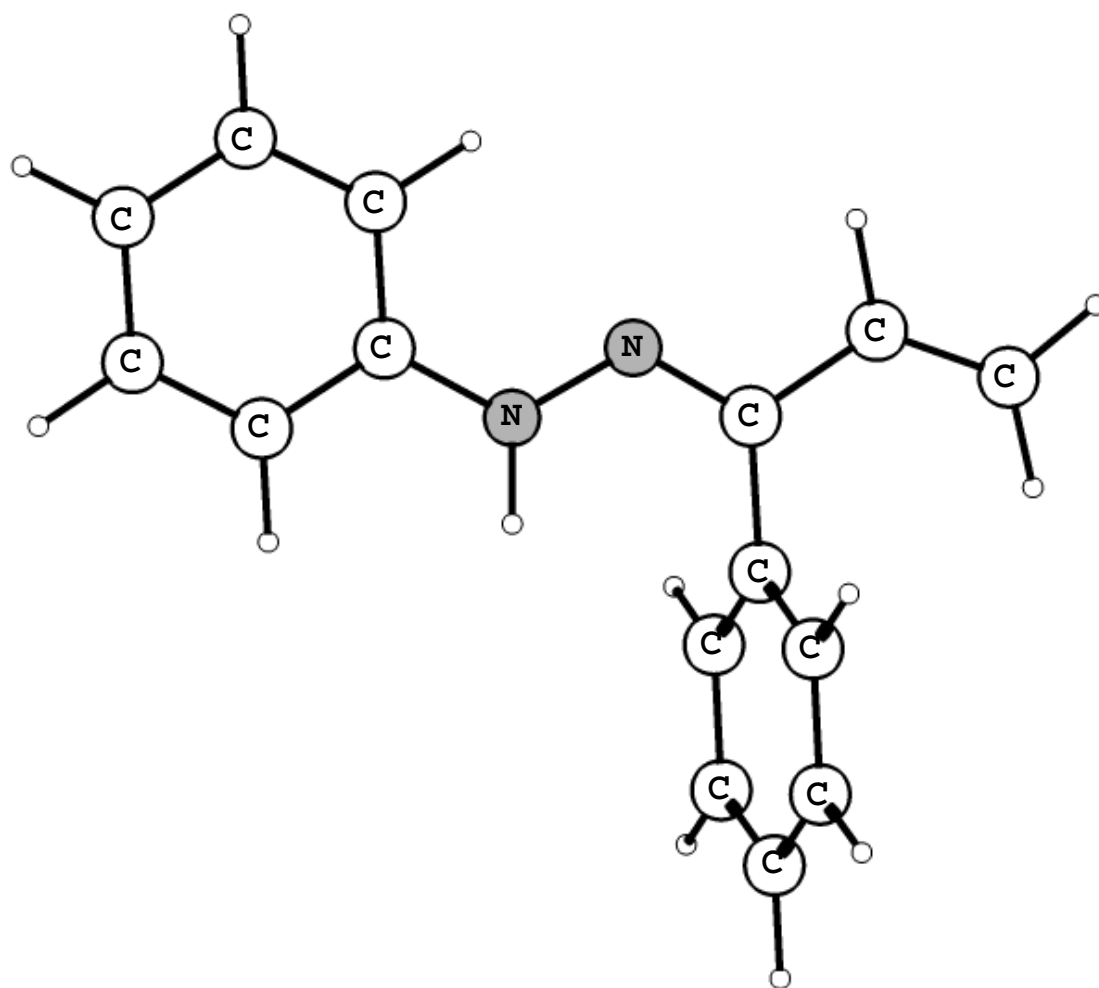
5a

Sum of electronic and zero-point Energies=	-458.270545
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Sum of electronic and thermal Free Energies=	-458.306670



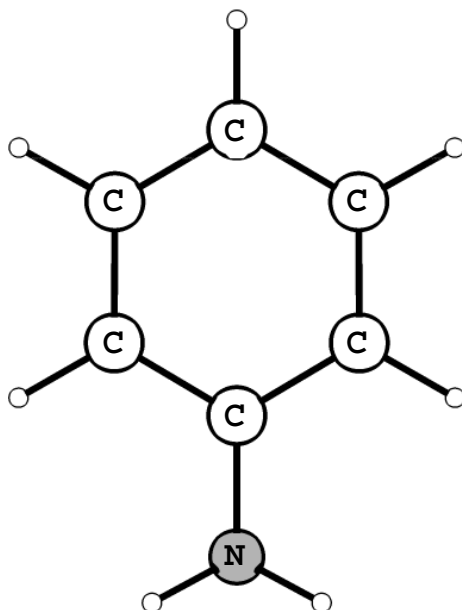
5b

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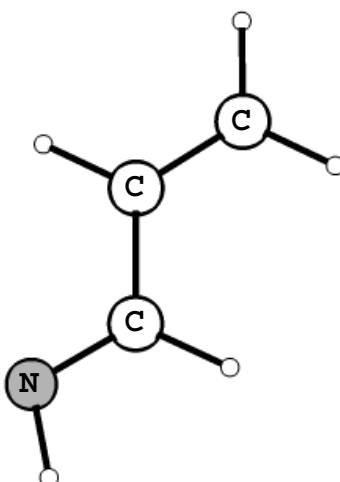
5c

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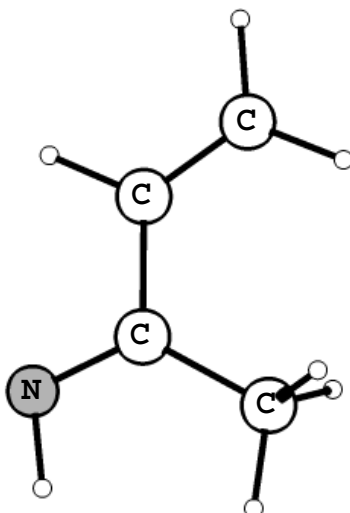
6

Sum of electronic and zero-point Energies=	-287.499273
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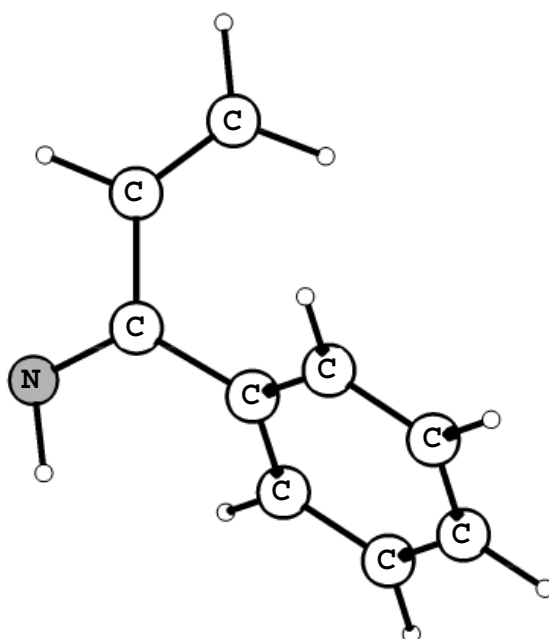
7a

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Sum of electronic and thermal Free Energies=	-171.996448



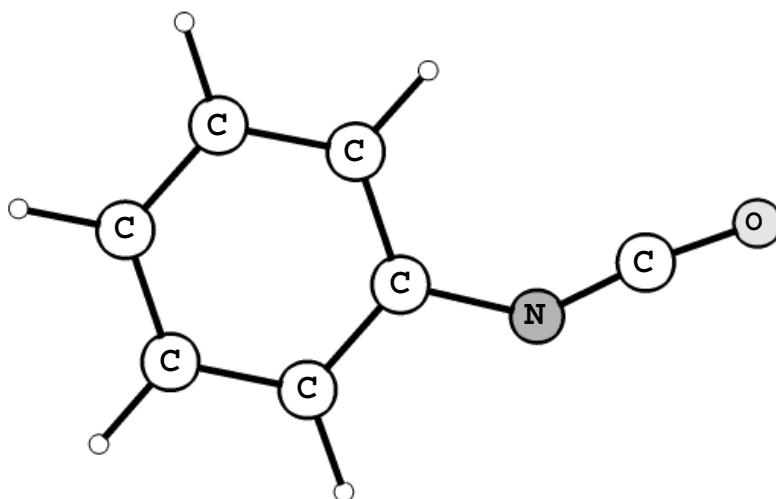
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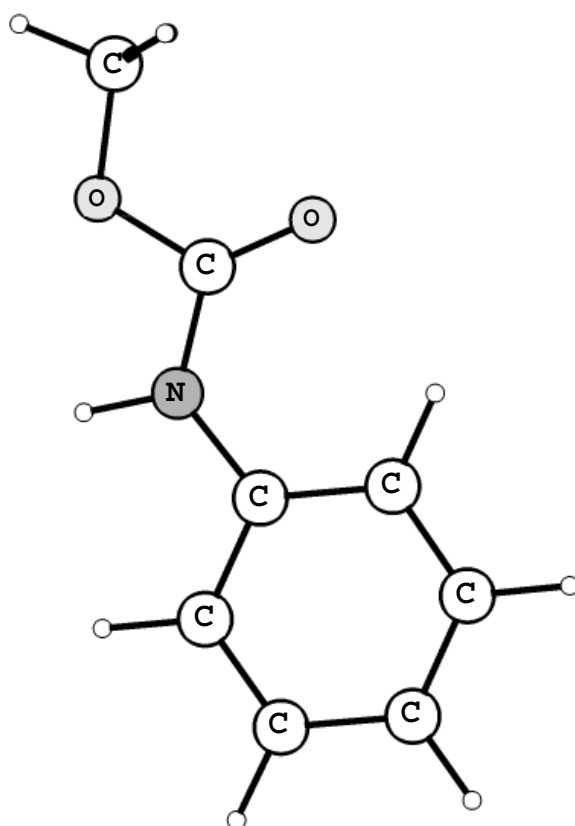
7c

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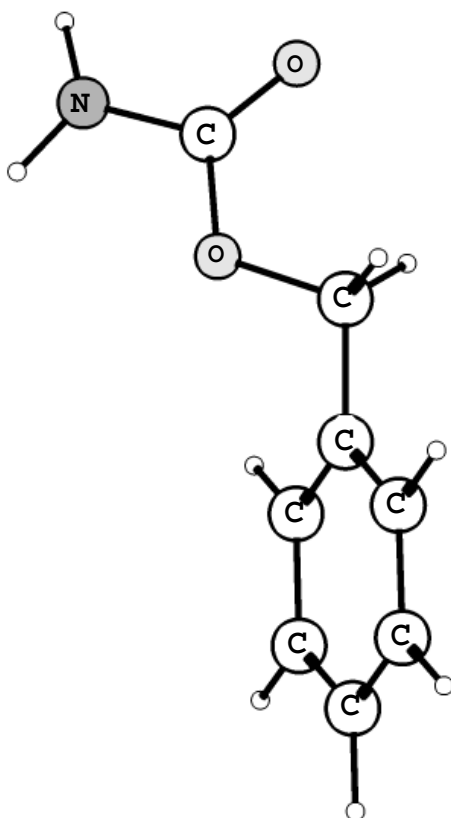
8

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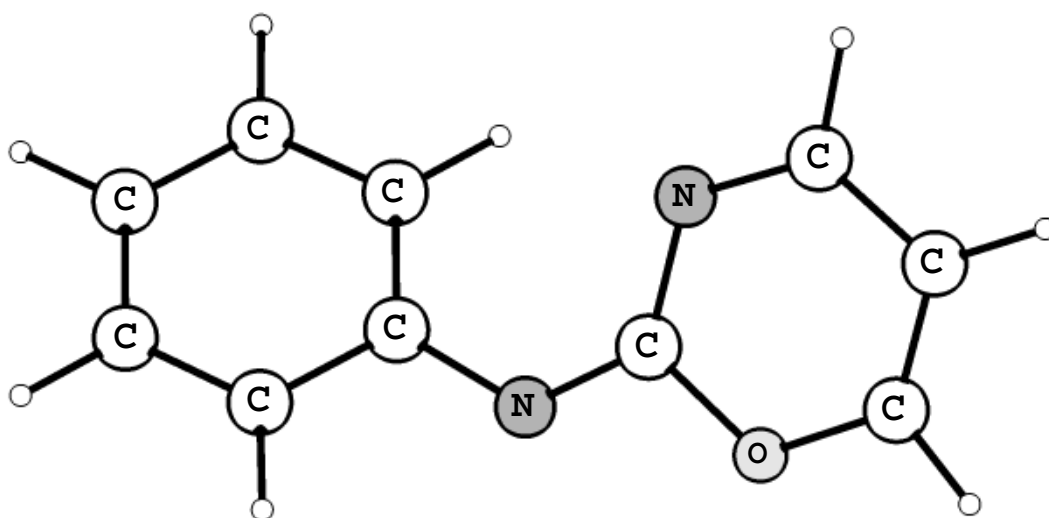
9

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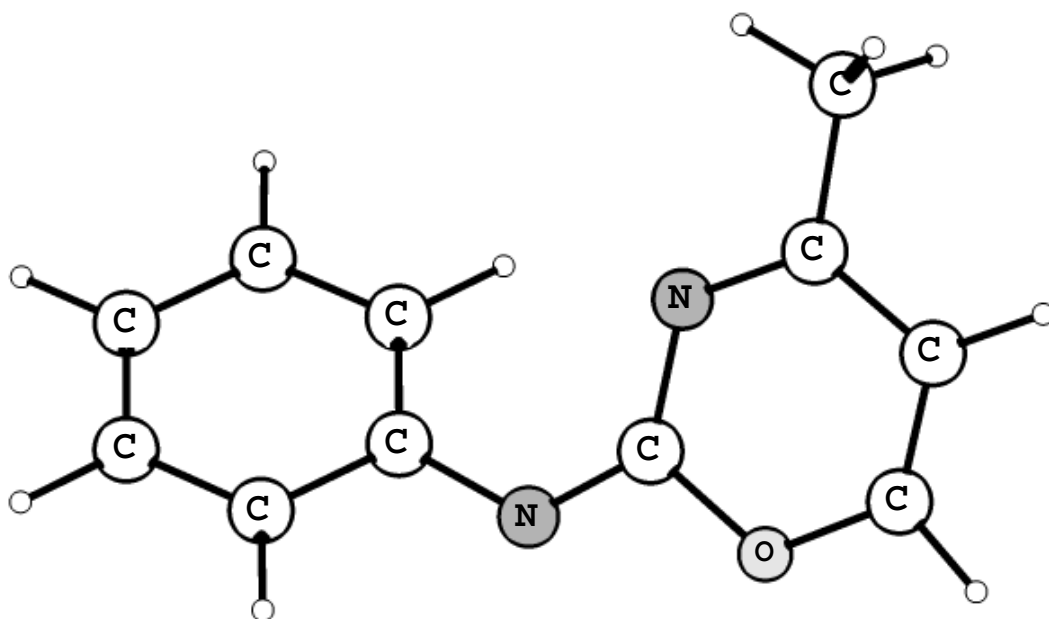
10

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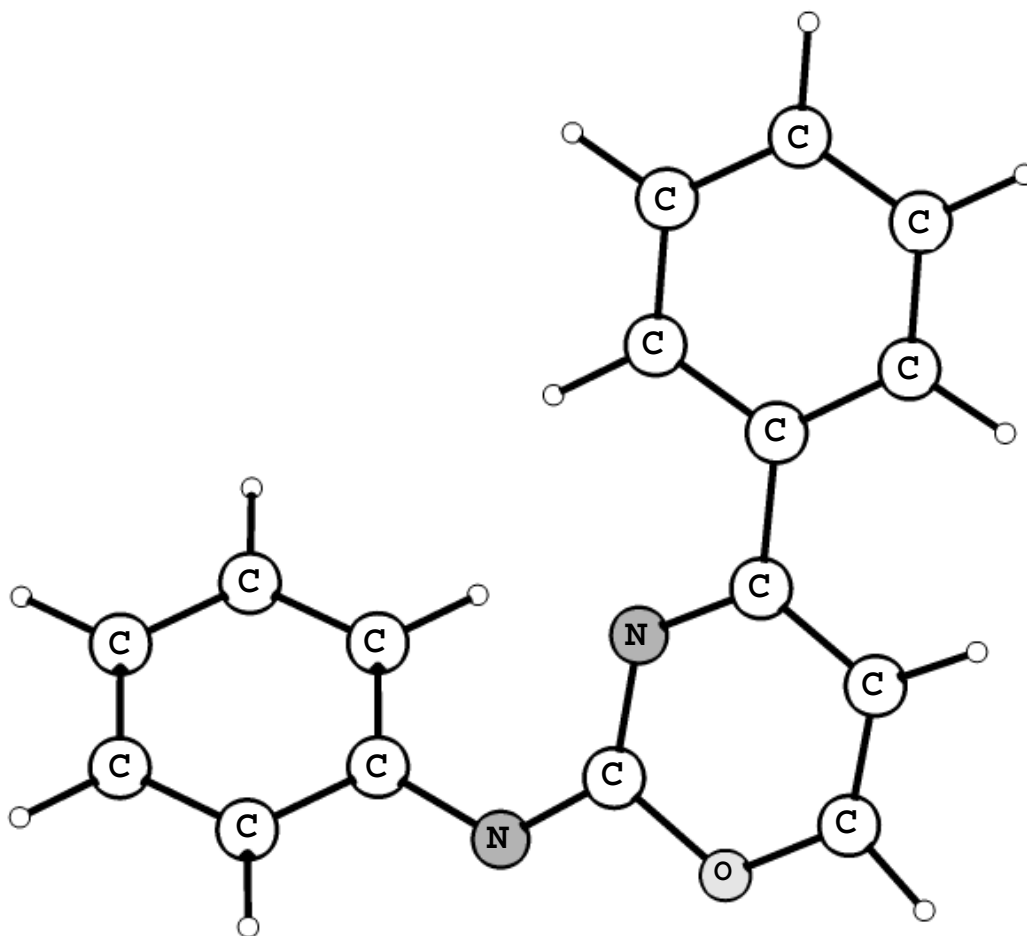
11a

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Sum of electronic and thermal Free Energies=	-570.452803



11b

Sum of electronic and zero-point Energies=	-609.715205
Sum of electronic and thermal Energies=	-609.703515
Sum of electronic and thermal Enthalpies=	-609.702570
Sum of electronic and thermal Free Energies=	-609.754733



11c

Sum of electronic and zero-point Energies=	-801.404997
Sum of electronic and thermal Energies=	-801.390371
Sum of electronic and thermal Enthalpies=	-801.389427
Sum of electronic and thermal Free Energies=	-801.449238

CARTESIAN COORDINATES

The first column corresponds to the atomic number
(1 – hydrogen, 6 – carbon, 7 – nitrogen, 8 – oxygen)

Columns 2, 3, 4 correspond to the Cartesian coordinates (Angstroms),
in the Standard Orientation

4a

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4b

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4c

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5a

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5b

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1	-1.932102000	2.453052000	-0.885925000
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5c

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6

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1	-0.008041000	0.762883000	-2.151200000
7	-0.062804000	2.336081000	0.000000000
1	0.297497000	2.776421000	0.835711000
1	0.297497000	2.776421000	-0.835711000

7a

7	-1.230076000	-1.318803000	0.000000000
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7b

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7c

7	-1.846912000	1.746896000	-0.639717000
6	-1.438765000	0.595901000	-0.232618000
6	-2.487317000	-0.381660000	0.128877000
6	-2.306961000	-1.538052000	0.776990000
1	-1.044322000	2.342180000	-0.868993000
1	-3.487034000	-0.053139000	-0.145062000
1	-3.150398000	-2.174306000	1.026142000
1	-1.326070000	-1.880797000	1.089680000
6	0.009812000	0.236136000	-0.100931000
6	0.887165000	1.121234000	0.544527000
6	0.529552000	-0.940145000	-0.663206000
6	2.248958000	0.836762000	0.630413000
1	0.491256000	2.027104000	0.995048000
6	1.894719000	-1.216675000	-0.589408000
1	-0.136104000	-1.627385000	-1.175369000
6	2.756963000	-0.332116000	0.060527000
1	2.912771000	1.526166000	1.143819000
1	2.285078000	-2.123698000	-1.041715000
1	3.818445000	-0.552705000	0.123434000

8

6	0.000000000	0.270954000	0.000000000
6	-1.235659000	0.928468000	0.000000000
6	-2.414631000	0.185661000	0.000000000
6	-2.371864000	-1.209525000	0.000000000
6	-1.136973000	-1.861944000	0.000000000
6	0.048506000	-1.130957000	0.000000000
1	-1.254618000	2.012848000	0.000000000
1	-3.370166000	0.701351000	0.000000000
1	-3.292433000	-1.784636000	0.000000000
1	-1.093401000	-2.946999000	0.000000000
1	1.009954000	-1.635620000	0.000000000
7	1.161712000	1.049343000	0.000000000
6	2.364696000	0.928598000	0.000000000
8	3.543029000	0.955016000	0.000000000

9

8	-1.716279000	-2.342254000	0.000000000
6	-0.557790000	-1.625501000	0.000000000
6	-1.537283000	-3.765069000	0.000000000
7	-0.873092000	-0.291427000	0.000000000
6	0.000000000	0.814173000	0.000000000
6	-0.582259000	2.091239000	0.000000000
6	0.217851000	3.230014000	0.000000000
6	1.608695000	3.114178000	0.000000000
6	2.183523000	1.842997000	0.000000000
6	1.397255000	0.691017000	0.000000000
1	-2.543177000	-4.184896000	0.000000000
1	-0.989308000	-4.087485000	0.888766000
1	-1.862394000	-0.089332000	0.000000000
1	-1.665604000	2.188429000	0.000000000
1	-0.250782000	4.209784000	0.000000000
1	2.233974000	4.001436000	0.000000000
1	3.264688000	1.737589000	0.000000000
1	1.845303000	-0.292680000	0.000000000
1	-0.989308000	-4.087485000	-0.888766000
8	0.552317000	-2.121954000	0.000000000

10

6	0.834768000	-0.352876000	0.146878000
6	1.816093000	-1.229700000	-0.324803000
6	3.144557000	-0.815320000	-0.442415000
6	3.502029000	0.487638000	-0.098346000
6	2.526148000	1.373279000	0.366873000
6	1.203450000	0.954432000	0.492261000
1	1.539781000	-2.243497000	-0.603179000
1	3.895770000	-1.508558000	-0.809487000
1	4.533615000	0.813885000	-0.193024000
1	2.798393000	2.390017000	0.635384000
1	0.445186000	1.644276000	0.851220000
6	-0.587831000	-0.818920000	0.317304000
1	-0.725280000	-1.824461000	-0.093916000
1	-0.884666000	-0.852061000	1.370149000
8	-1.462102000	0.099311000	-0.374478000
6	-2.775883000	0.022834000	-0.024259000
7	-3.509656000	0.884659000	-0.789142000
1	-3.037613000	1.589961000	-1.331561000
1	-4.459204000	1.048798000	-0.498637000
8	-3.227696000	-0.721708000	0.823989000

11a

8	2.292250000	-1.211124000	-0.292345000
6	1.162010000	-0.365618000	-0.078291000
7	1.390792000	0.954286000	0.267334000
6	2.612272000	1.378548000	0.396242000
6	3.772808000	0.560130000	0.189582000
6	3.527301000	-0.725018000	-0.151884000
7	0.061903000	-0.978955000	-0.219427000
6	-1.212478000	-0.403262000	-0.112222000
6	-2.246270000	-1.273779000	0.277370000
6	-3.557961000	-0.821242000	0.386276000
6	-3.871157000	0.504584000	0.078981000
6	-2.855853000	1.369505000	-0.334401000
6	-1.536753000	0.929865000	-0.427599000
1	2.736130000	2.423563000	0.682766000
1	4.779572000	0.939240000	0.299582000
1	4.285178000	-1.478676000	-0.342201000
1	-1.989346000	-2.305599000	0.494036000
1	-4.339213000	-1.507938000	0.699959000
1	-4.895528000	0.857808000	0.152272000
1	-3.091212000	2.399992000	-0.586648000
1	-0.755960000	1.611011000	-0.740687000

11b

8	1.875240000	-1.721349000	-0.251694000
6	0.852451000	-0.742748000	-0.100621000
7	1.223086000	0.569801000	0.115371000
6	2.482723000	0.898146000	0.185707000
6	3.540117000	-0.073672000	0.028688000
6	3.156481000	-1.350137000	-0.182396000
7	-0.312234000	-1.242540000	-0.162623000
6	-1.504391000	-0.507213000	-0.094072000
6	-2.604687000	-1.161068000	0.488488000
6	-3.845450000	-0.535348000	0.569898000
6	-4.022999000	0.745545000	0.042354000
6	-2.943209000	1.391345000	-0.563196000
6	-1.692653000	0.780108000	-0.630680000
1	4.586153000	0.198207000	0.080281000
1	3.830612000	-2.190733000	-0.313828000
1	-2.456533000	-2.164063000	0.875557000
1	-4.679165000	-1.054165000	1.034880000
1	-4.993099000	1.231089000	0.093798000
1	-3.073827000	2.383243000	-0.987704000
1	-0.859637000	1.291584000	-1.096391000
6	2.828959000	2.336789000	0.443965000
1	3.422265000	2.427776000	1.361350000
1	3.441266000	2.735914000	-0.373197000
1	1.920030000	2.930627000	0.540772000

11c

8	-0.399304000	2.975803000	0.073458000
6	-0.806261000	1.614465000	0.044034000
7	0.160103000	0.640825000	0.019869000
6	1.434374000	0.943694000	-0.005393000
6	1.872220000	2.322715000	0.007816000
6	0.905267000	3.263051000	0.043373000
7	-2.070533000	1.481041000	0.018191000
6	-2.727046000	0.243360000	0.054893000
6	-3.910504000	0.133457000	-0.696445000
6	-4.653886000	-1.043597000	-0.686903000
6	-4.250244000	-2.125991000	0.098141000
6	-3.092700000	-2.015191000	0.871179000
6	-2.331742000	-0.847752000	0.851602000
1	2.910615000	2.615436000	-0.036402000
1	1.084723000	4.333405000	0.047590000
1	-4.223648000	0.988514000	-1.286907000
1	-5.558514000	-1.111546000	-1.284893000
1	-4.836208000	-3.040177000	0.116159000
1	-2.777642000	-2.845167000	1.498138000
1	-1.435708000	-0.770181000	1.455614000
6	2.401811000	-0.177360000	-0.061992000
6	1.934088000	-1.477779000	-0.325335000
6	3.777025000	0.017139000	0.148302000
6	2.819865000	-2.547892000	-0.383133000
1	0.871512000	-1.621972000	-0.483659000
6	4.661442000	-1.058595000	0.095429000
1	4.166160000	1.003702000	0.375200000
6	4.186695000	-2.342649000	-0.173666000
1	2.445676000	-3.545248000	-0.593572000
1	5.720774000	-0.893126000	0.266543000
1	4.877272000	-3.179575000	-0.219311000