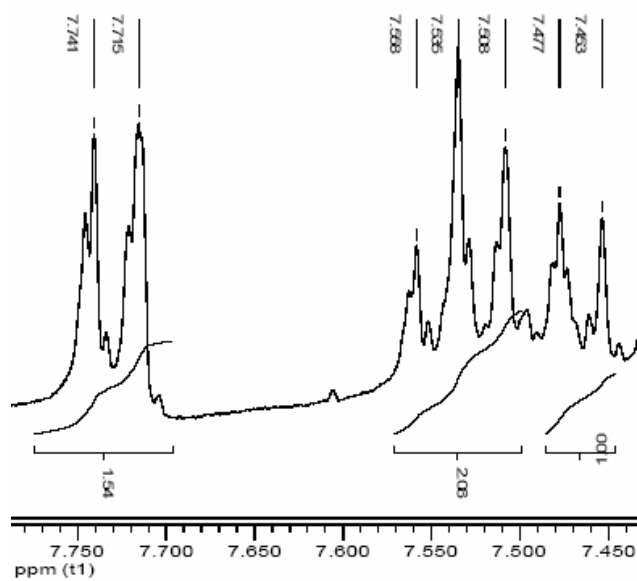
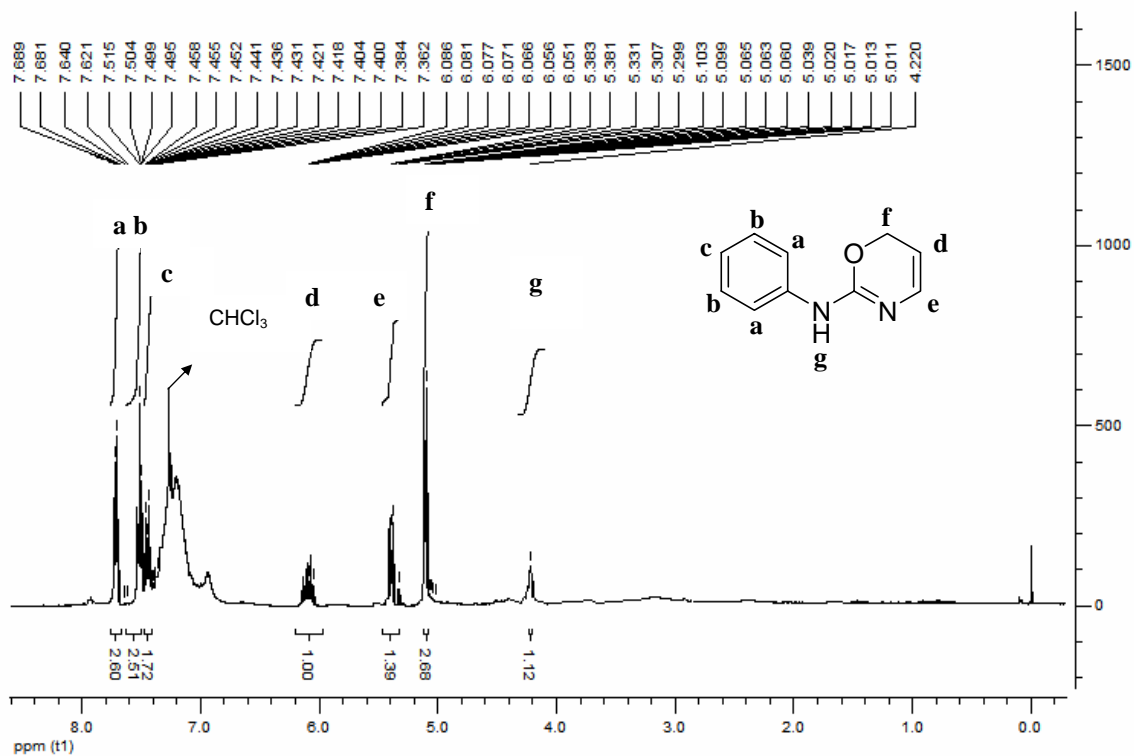
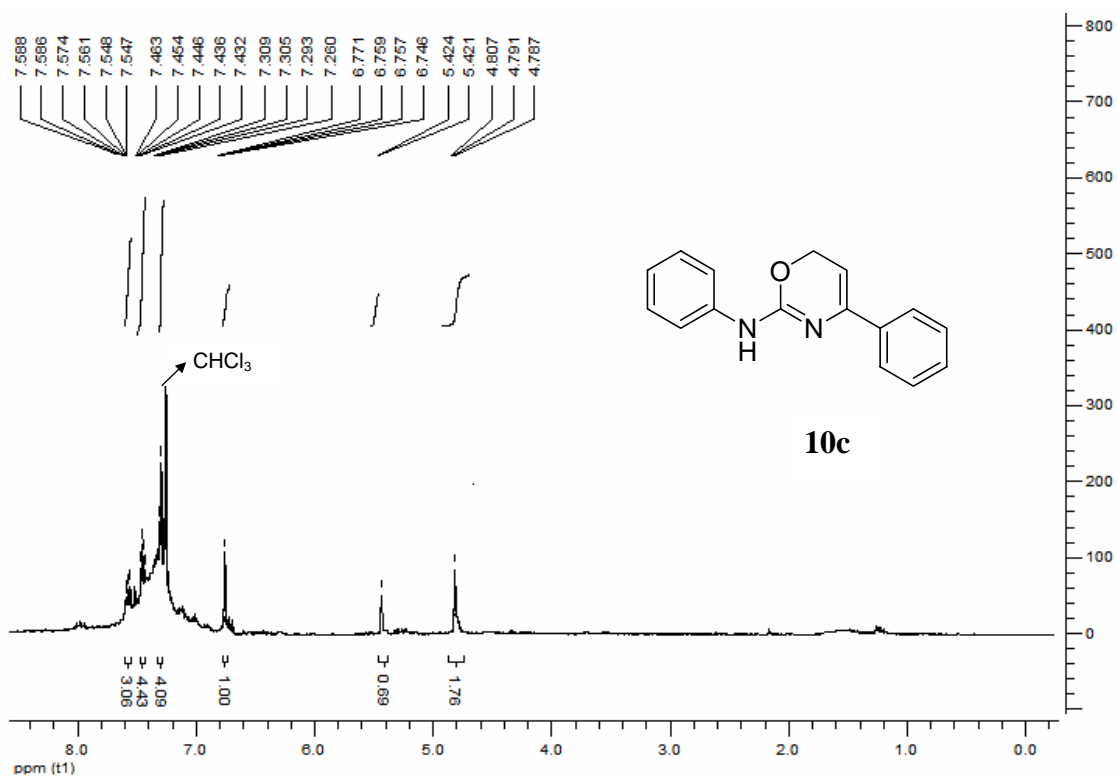
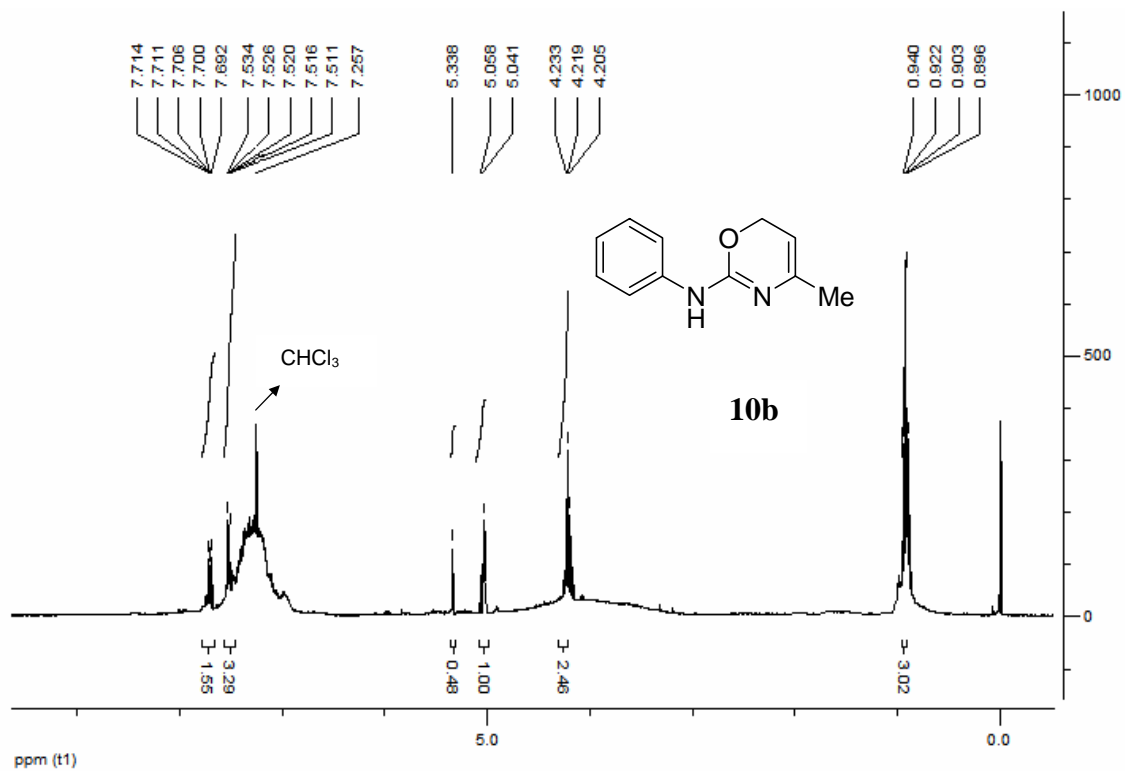


Appendix A

¹H-NMR spectra for compounds **10a-c** with structure.

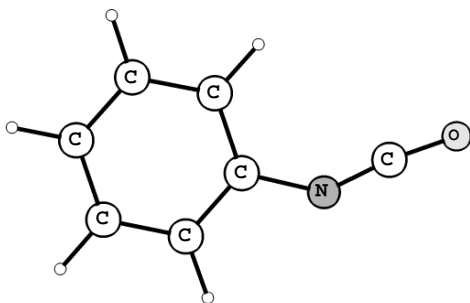




GEOMETRIES AND ENERGIES

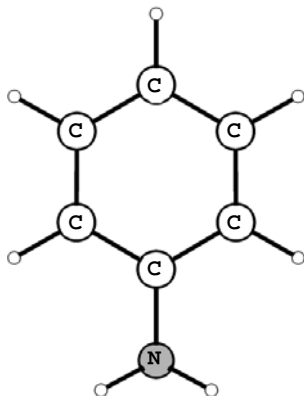
All energies are expressed in Hartrees ($1 \text{ Hartree} = 1 \text{ kJ mol}^{-1}$) and were calculated for the geometries fully optimized at the DFT(B3LYP)/6-31G(d,p) level of theory. The nature of the calculated structures as minima on the corresponding potential energy surfaces was confirmed by analysis 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 S10.



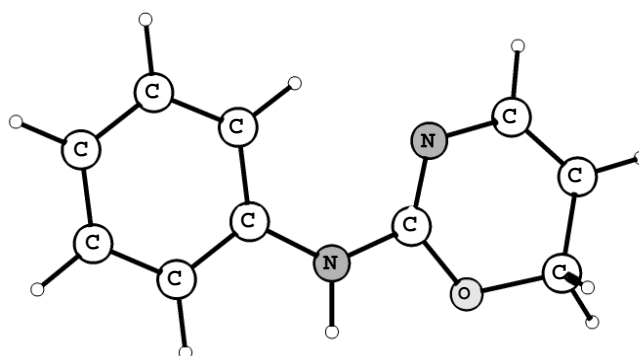
6

Sum of electronic and zero-point Energies=	-399.636495
Sum of electronic and thermal Energies=	-399.629390
Sum of electronic and thermal Enthalpies=	-399.628446
Sum of electronic and thermal Free Energies=	-399.668890



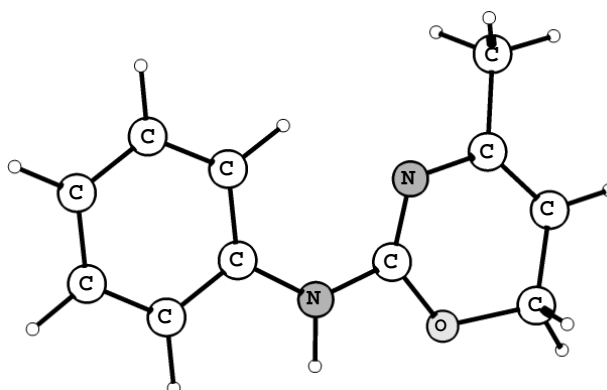
8

Sum of electronic and zero-point Energies=	-287.499273
Sum of electronic and thermal Energies=	-287.493476
Sum of electronic and thermal Enthalpies=	-287.492532
Sum of electronic and thermal Free Energies=	-287.528423



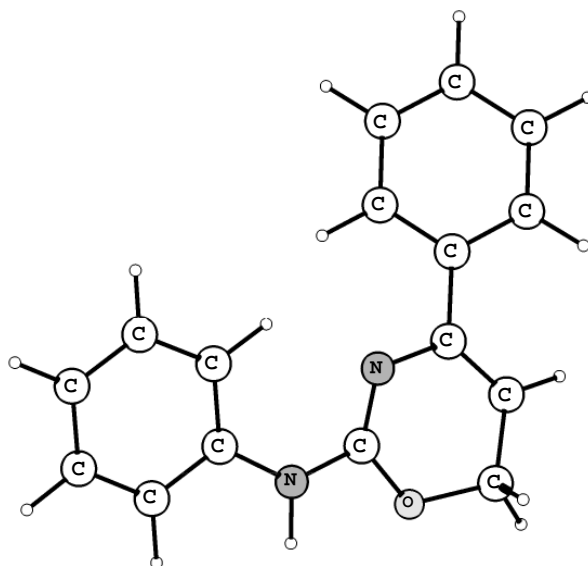
10a

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



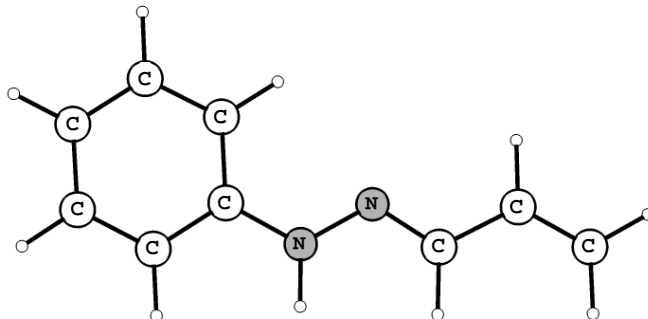
10b

Sum of electronic and zero-point Energies=	-610.915106
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Sum of electronic and thermal Enthalpies=	-610.902080
Sum of electronic and thermal Free Energies=	-610.954186



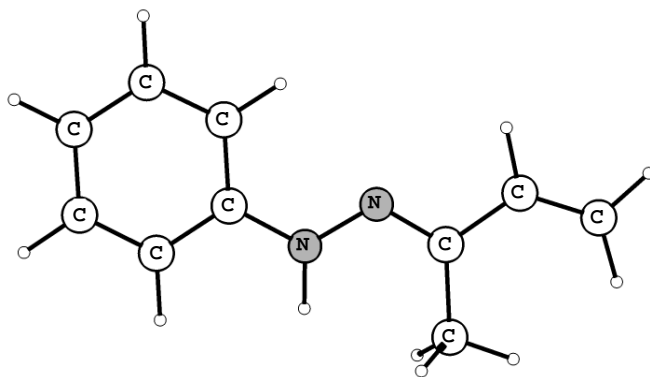
10c

Sum of electronic and zero-point Energies=	-802.603942
Sum of electronic and thermal Energies=	-802.588814
Sum of electronic and thermal Enthalpies=	-802.587870
Sum of electronic and thermal Free Energies=	-802.648096



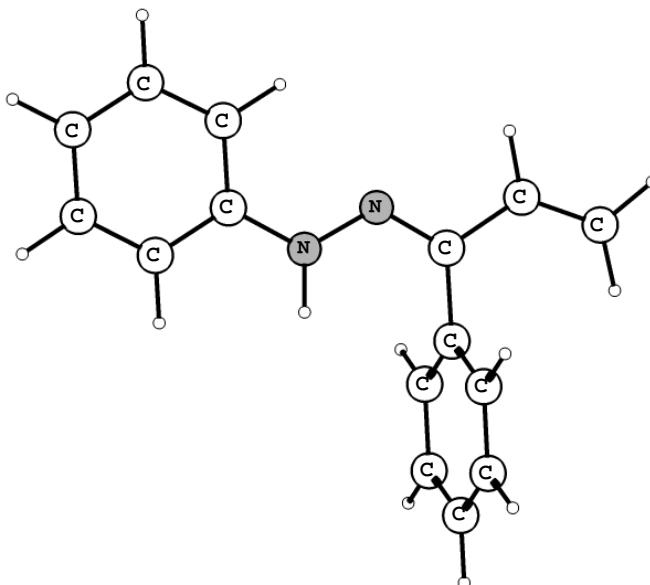
11a

Sum of electronic and zero-point Energies=	-458.270545
Sum of electronic and thermal Energies=	-458.260499
Sum of electronic and thermal Enthalpies=	-458.259555
Sum of electronic and thermal Free Energies=	-458.306670



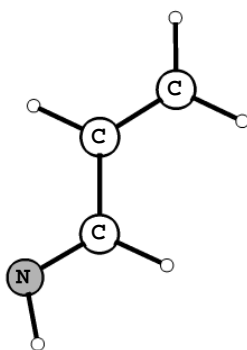
11b

Sum of electronic and zero-point Energies=	-497.562757
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Sum of electronic and thermal Free Energies=	-497.601061



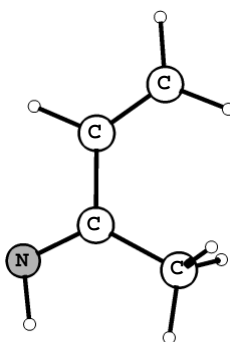
11c

Sum of electronic and zero-point Energies=	-689.250244
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Sum of electronic and thermal Enthalpies=	-689.234725
Sum of electronic and thermal Free Energies=	-689.293710



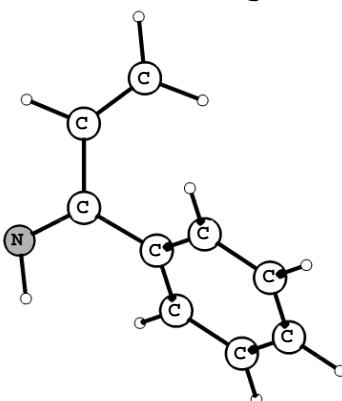
12a

Sum of electronic and zero-point Energies=	-171.970154
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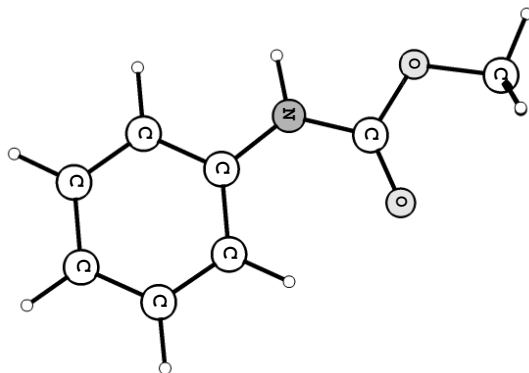
12b

Sum of electronic and zero-point Energies=	-211.264957
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Sum of electronic and thermal Free Energies=	-211.293548



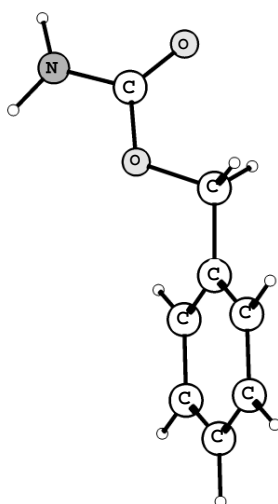
12c

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Sum of electronic and thermal Free Energies=	-402.984767



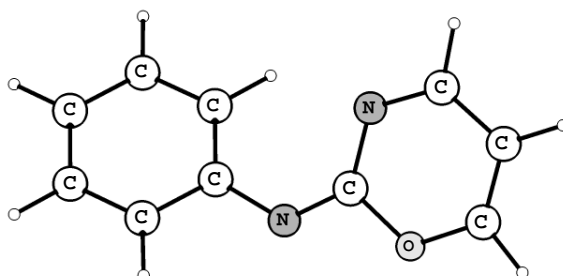
13

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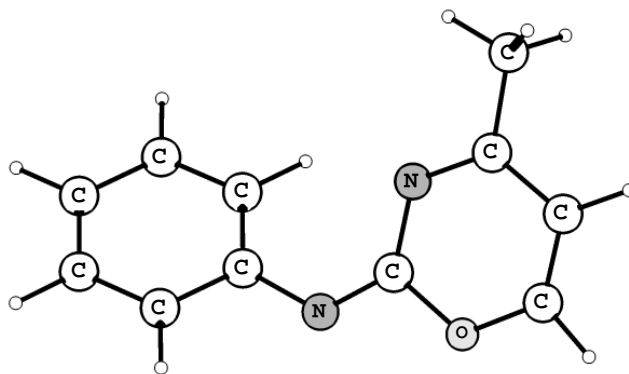
14

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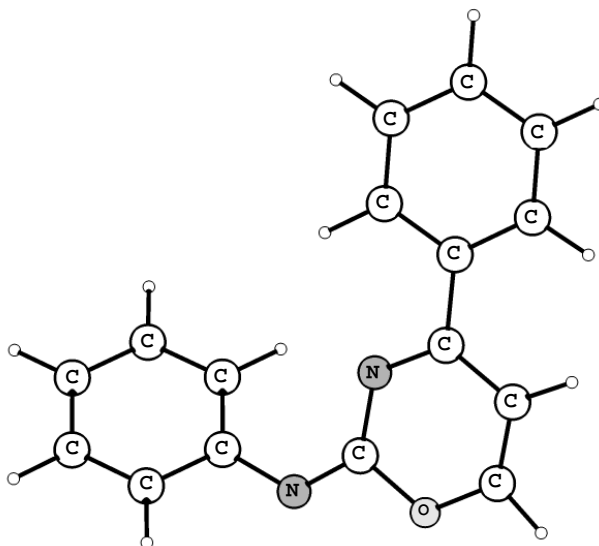
15a

Sum of electronic and zero-point Energies=	-570.415294
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Sum of electronic and thermal Free Energies=	-570.452803



15b

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



15c

Sum of electronic and zero-point Energies=	-801.404997
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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

6

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8

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1	0.297497000	2.776421000	-0.835711000

10a

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10b

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10c

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11a

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11b

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11c

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12a

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1	2.115288000	0.844198000	0.000000000

12b

7	-0.583502000	1.696651000	0.000000000
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1	1.815769000	-0.225703000	-0.881558000
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12c

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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

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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

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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

15a

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

15b

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

15c

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