

**Table S1.** Cartesian coordinates (in Å) of GFN2-xTB/ALPB optimized structures of KR-12-Cu(II) (Cl<sup>-</sup> anions are omitted).

System	Coordinates			
1	Cu	4.604269000	-1.921542000	-3.130345000
	N	-5.039230000	-5.594747000	-0.908345000
	C	-4.715791000	-4.765547000	0.276911000
	C	-4.809626000	-3.288299000	-0.103599000
	O	-4.109216000	-2.435388000	0.432257000
	C	-3.318671000	-5.221587000	0.728188000
	C	-2.724664000	-4.596921000	1.994007000
	C	-1.615005000	-5.527835000	2.491614000
	C	-0.771891000	-4.924101000	3.607537000
	N	0.262011000	-5.907923000	4.005959000
	H	-5.454585000	-4.951086000	1.063946000
	H	-2.632459000	-5.073918000	-0.104620000
	H	-3.405481000	-6.294772000	0.906137000
	H	-2.310518000	-3.619899000	1.766660000
	H	-3.503004000	-4.481391000	2.747632000
	H	-0.973690000	-5.762477000	1.649465000
	H	-2.083928000	-6.448157000	2.839421000
	H	-1.420936000	-4.698086000	4.450302000
	H	-0.292633000	-4.019097000	3.251607000
	H	1.143922000	-5.844143000	3.464030000
	H	0.531767000	-5.807974000	4.982075000
	H	-0.104497000	-6.853183000	3.894286000
	H	-6.030567000	-5.537096000	-1.219905000
	H	-4.440999000	-5.266668000	-1.688714000
	H	-4.830457000	-6.578276000	-0.722681000
	N	-5.725203000	-2.981229000	-1.027095000
	C	-5.680441000	-1.726108000	-1.751834000
	C	-5.693221000	-0.509792000	-0.827607000
	O	-4.976215000	0.468090000	-1.016983000
	C	-6.863113000	-1.627822000	-2.718971000
	C	-6.665712000	-0.490865000	-3.719885000
	C	-7.851278000	-0.369726000	-4.679918000
	N	-9.053275000	0.096810000	-4.015876000
	C	-9.353265000	1.370529000	-3.763759000
	N	-8.507248000	2.359820000	-4.033156000
	N	-10.471269000	1.663817000	-3.098768000
	H	-6.381945000	-3.671800000	-1.381078000
	H	-4.751816000	-1.687821000	-2.337803000
	H	-6.951133000	-2.576643000	-3.251934000
	H	-7.786052000	-1.476691000	-2.157107000
	H	-6.532987000	0.452863000	-3.190128000
	H	-5.767230000	-0.678800000	-4.308468000
H	-8.072200000	-1.346016000	-5.113333000	
H	-7.604061000	0.307086000	-5.501132000	
H	-9.711267000	-0.603988000	-3.713703000	
H	-7.715506000	2.200934000	-4.633825000	
H	-8.908727000	3.292432000	-4.026604000	
H	-10.761844000	2.636027000	-3.134209000	
H	-11.198267000	0.974974000	-3.002393000	
N	-6.556743000	-0.597997000	0.185719000	

	C	-6.789467000	0.475918000	1.132364000
	C	-5.459863000	0.979786000	1.707340000
	O	-5.308242000	2.160924000	2.023802000
	C	-7.711755000	-0.036744000	2.259747000
	C	-7.737785000	0.934571000	3.437754000
	C	-9.129887000	-0.259153000	1.712814000
	C	-9.965034000	-1.181609000	2.595823000
	H	-7.140217000	-1.419889000	0.254338000
	H	-7.270608000	1.326983000	0.632295000
	H	-7.316490000	-0.996918000	2.606946000
	H	-9.087593000	-0.698800000	0.714584000
	H	-9.634826000	0.704651000	1.618896000
	H	-10.953801000	-1.321696000	2.163192000
	H	-9.497528000	-2.158840000	2.689539000
	H	-10.099496000	-0.767689000	3.591600000
	H	-8.450472000	0.598638000	4.185175000
	H	-6.764004000	1.007933000	3.912137000
	H	-8.037240000	1.926155000	3.106680000
	N	-4.544546000	0.044341000	1.895987000
	C	-3.244317000	0.253571000	2.501648000
	C	-2.204200000	0.555238000	1.412696000
	O	-1.545675000	1.599306000	1.437307000
	C	-2.943215000	-1.000330000	3.346602000
	C	-3.874063000	-1.024138000	4.559503000
	C	-1.488251000	-1.065503000	3.786556000
	H	-4.700318000	-0.892695000	1.534179000
	H	-3.299020000	1.145887000	3.133050000
	H	-3.169311000	-1.867489000	2.723612000
	H	-1.369646000	-1.915562000	4.445861000
	H	-0.845432000	-1.167636000	2.923513000
	H	-1.223282000	-0.160856000	4.326695000
	H	-3.759181000	-1.955463000	5.104367000
	H	-4.917367000	-0.933879000	4.265268000
	H	-3.648837000	-0.204702000	5.239327000
	N	-2.076229000	-0.388250000	0.482387000
	C	-1.234205000	-0.270854000	-0.696594000
	C	-1.211594000	1.155419000	-1.242182000
	O	-0.152881000	1.700016000	-1.584564000
	C	-1.741584000	-1.179788000	-1.824400000
	C	-1.566629000	-2.668781000	-1.505404000
	C	-2.175340000	-3.495429000	-2.618544000
	N	-1.502174000	-3.488958000	-3.768223000
	O	-3.209085000	-4.146793000	-2.463601000
	H	-2.732501000	-1.167884000	0.483503000
	H	-0.198472000	-0.537093000	-0.454282000
	H	-1.188574000	-0.935352000	-2.733758000
	H	-2.792051000	-0.949766000	-2.005550000
	H	-0.508724000	-2.901225000	-1.446178000
	H	-2.064189000	-2.915376000	-0.571373000
	H	-1.880789000	-3.968012000	-4.568687000
	H	-0.699742000	-2.890132000	-3.917851000
	N	-2.399400000	1.739370000	-1.323408000
	C	-2.637106000	3.129922000	-1.662540000
	C	-1.377720000	3.977793000	-1.445859000

	O	-0.929129000	4.685536000	-2.344152000
	C	-3.802536000	3.590230000	-0.778165000
	C	-4.144950000	5.070811000	-0.912185000
	C	-5.420713000	5.393435000	-0.115616000
	N	-5.360491000	4.868497000	1.229959000
	C	-4.730436000	5.407794000	2.269989000
	N	-4.345950000	6.681752000	2.284989000
	N	-4.503056000	4.633768000	3.323240000
	H	-3.248161000	1.201023000	-1.146581000
	H	-2.891653000	3.233424000	-2.726099000
	H	-4.672684000	2.989860000	-1.050048000
	H	-3.541570000	3.368974000	0.257201000
	H	-4.307522000	5.329487000	-1.959360000
	H	-3.309366000	5.677122000	-0.558371000
	H	-6.277274000	4.929479000	-0.606554000
	H	-5.594524000	6.470735000	-0.107717000
	H	-5.544180000	3.869740000	1.322257000
	H	-4.531890000	7.290272000	1.509062000
	H	-3.932811000	7.078425000	3.110263000
	H	-4.777798000	3.662589000	3.266449000
	H	-4.144675000	5.007300000	4.184171000
	N	-0.887894000	3.950431000	-0.197214000
	C	0.395016000	4.533527000	0.133885000
	C	1.485411000	3.464925000	0.272750000
	O	2.598105000	3.583876000	-0.255442000
	C	0.310325000	5.348788000	1.444859000
	C	1.674107000	5.954155000	1.771437000
	C	-0.767948000	6.429813000	1.308230000
	C	-0.948896000	7.262765000	2.572945000
	H	-1.263359000	3.261148000	0.452108000
	H	0.679492000	5.188366000	-0.697488000
	H	0.025791000	4.665057000	2.249764000
	H	-0.508183000	7.085264000	0.472543000
	H	-1.711909000	5.942488000	1.062859000
	H	-1.761523000	7.970250000	2.436149000
	H	-1.162244000	6.622407000	3.423148000
	H	-0.053895000	7.838649000	2.792094000
	H	1.675269000	6.399328000	2.761413000
	H	1.933225000	6.724311000	1.046163000
	H	2.458092000	5.201979000	1.739311000
	N	1.177731000	2.448366000	1.074851000
	C	2.169806000	1.489352000	1.515552000
	C	2.922738000	0.861663000	0.362382000
	O	4.062191000	0.405036000	0.549070000
	C	1.506039000	0.403520000	2.374002000
	C	2.511090000	-0.383516000	3.220933000
	C	1.833491000	-1.601509000	3.845889000
	C	2.774364000	-2.421889000	4.718604000
	N	2.070113000	-3.675527000	5.047508000
	H	0.212969000	2.273753000	1.357438000
	H	2.929474000	2.019149000	2.107601000
	H	0.962879000	-0.263013000	1.707728000
	H	0.794968000	0.904905000	3.028984000
	H	3.350685000	-0.693351000	2.600638000

	H	2.915964000	0.276585000	3.990877000
	H	1.005486000	-1.244246000	4.450818000
	H	1.478585000	-2.246028000	3.048254000
	H	3.048741000	-1.867175000	5.615178000
	H	3.686033000	-2.660929000	4.178186000
	H	2.591161000	-4.216761000	5.735408000
	H	1.135426000	-3.456700000	5.395610000
	H	2.060905000	-4.263719000	4.193547000
	N	2.288293000	0.710192000	-0.799805000
	C	2.987960000	0.132214000	-1.919075000
	C	4.351003000	0.746271000	-2.194051000
	O	5.206030000	0.075257000	-2.815911000
	C	2.160365000	0.123619000	-3.210905000
	C	1.817859000	-1.300321000	-3.699329000
	O	2.713694000	-2.201592000	-3.677717000
	O	0.664978000	-1.517912000	-4.073307000
	H	1.381494000	1.158954000	-0.996001000
	H	3.239680000	-0.915760000	-1.673270000
	H	2.724314000	0.587525000	-4.024194000
	H	1.236727000	0.688518000	-3.081578000
	N	4.620948000	1.968949000	-1.748355000
	C	5.972107000	2.491901000	-1.803402000
	C	6.989211000	1.466686000	-1.250836000
	O	8.073332000	1.265660000	-1.798596000
	C	6.045354000	3.775862000	-0.964086000
	C	7.471381000	4.227152000	-0.822640000
	C	8.114250000	4.870349000	-1.872124000
	C	8.184003000	3.965937000	0.339879000
	C	9.512470000	4.334873000	0.450666000
	C	10.146459000	4.970337000	-0.602949000
	C	9.442931000	5.239274000	-1.764766000
	H	3.906267000	2.538375000	-1.287003000
	H	6.273175000	2.685134000	-2.840966000
	H	5.621681000	3.571561000	0.019206000
	H	5.446173000	4.544666000	-1.453597000
	H	7.572907000	5.079030000	-2.783782000
	H	7.697837000	3.462622000	1.161968000
	H	10.059498000	4.120871000	1.357006000
	H	11.185873000	5.252048000	-0.522036000
	H	9.933806000	5.732685000	-2.590850000
	N	6.605304000	0.919319000	-0.097757000
	C	7.352240000	-0.035620000	0.695993000
	C	7.195231000	-1.482192000	0.209084000
	O	8.194426000	-2.223626000	0.073564000
	C	6.839397000	0.088600000	2.143366000
	C	7.241857000	-1.051207000	3.086362000
	C	8.753657000	-1.077934000	3.307520000
	C	6.497207000	-0.900742000	4.412948000
	H	5.619704000	1.001130000	0.172928000
	H	8.420376000	0.197565000	0.605549000
	H	7.205684000	1.032761000	2.549269000
	H	5.750905000	0.123896000	2.087949000
	H	6.970667000	-2.004840000	2.614617000
	H	9.028202000	-1.835830000	4.040386000

	H	9.117926000	-0.113135000	3.653870000
	H	9.271872000	-1.324599000	2.377380000
	H	6.722215000	-1.742145000	5.061450000
	H	6.823614000	0.010009000	4.907197000
	H	5.429085000	-0.849465000	4.234359000
	N	5.933567000	-1.904825000	0.068703000
	C	5.595559000	-3.276782000	-0.304076000
	C	6.315358000	-3.767014000	-1.545449000
	O	7.244162000	-4.692873000	-1.516927000
	C	4.072023000	-3.460724000	-0.454341000
	C	3.187580000	-2.756441000	0.577760000
	C	1.695140000	-2.921137000	0.239254000
	N	1.200247000	-4.223713000	0.613426000
	C	1.108522000	-5.292321000	-0.170703000
	N	0.869549000	-6.453877000	0.435275000
	N	1.011426000	-5.199275000	-1.505526000
	H	5.203360000	-1.194321000	0.048633000
	H	6.026331000	-3.893667000	0.496596000
	H	3.846857000	-3.106568000	-1.474624000
	H	3.900648000	-4.539385000	-0.459553000
	H	3.429217000	-1.700770000	0.569606000
	H	3.375902000	-3.154173000	1.570783000
	H	1.135082000	-2.192833000	0.823760000
	H	1.554240000	-2.699012000	-0.819098000
	H	1.389925000	-4.446857000	1.598653000
	H	0.798832000	-7.294347000	-0.111697000
	H	1.183266000	-6.533232000	1.399424000
	H	0.974706000	-6.035517000	-2.060836000
	H	1.329838000	-4.381021000	-1.995987000
	N	6.322927000	-2.797745000	-2.649242000
	H	6.748794000	-3.253912000	-3.453055000
	H	6.924716000	-1.992614000	-2.425061000
2	Cu	-3.931987000	-1.861599000	-1.726242000
	N	-6.230990000	-4.989718000	2.067550000
	C	-5.002890000	-4.216109000	1.800673000
	C	-5.193948000	-3.138126000	0.749400000
	O	-4.187223000	-2.505471000	0.376444000
	C	-3.879296000	-5.173117000	1.338969000
	C	-2.521140000	-4.882008000	1.978349000
	C	-1.492485000	-5.901907000	1.488440000
	C	-0.089340000	-5.564017000	1.987233000
	N	0.838530000	-6.638243000	1.586570000
	H	-4.699829000	-3.720316000	2.729982000
	H	-3.786466000	-5.129157000	0.254327000
	H	-4.166321000	-6.190576000	1.599773000
	H	-2.189091000	-3.882165000	1.717017000
	H	-2.612620000	-4.943320000	3.061601000
	H	-1.501484000	-5.915688000	0.401375000
	H	-1.784212000	-6.890957000	1.840108000
	H	-0.119548000	-5.487393000	3.069408000
	H	0.243646000	-4.631559000	1.545392000
	H	1.858975000	-6.394039000	1.572610000
	H	0.738676000	-7.459447000	2.180518000

	H	0.629226000	-6.919246000	0.629391000
	H	-7.088477000	-4.412411000	2.242486000
	H	-6.468712000	-5.583608000	1.266741000
	H	-6.091136000	-5.593629000	2.883162000
	N	-6.404853000	-2.911041000	0.259566000
	C	-6.561888000	-2.018271000	-0.872497000
	C	-5.965644000	-0.638043000	-0.553779000
	O	-5.013233000	-0.172993000	-1.196951000
	C	-8.020091000	-1.876724000	-1.309403000
	C	-8.081148000	-1.191857000	-2.683242000
	C	-9.311333000	-0.294414000	-2.850483000
	N	-9.171229000	0.947619000	-2.108040000
	C	-8.413217000	1.977118000	-2.492439000
	N	-7.586195000	1.888210000	-3.528224000
	N	-8.339349000	3.067946000	-1.726756000
	H	-7.261669000	-3.279734000	0.686129000
	H	-5.981532000	-2.427233000	-1.721086000
	H	-8.479032000	-2.863613000	-1.357377000
	H	-8.579037000	-1.301024000	-0.572870000
	H	-7.192781000	-0.575639000	-2.823220000
	H	-8.090769000	-1.944304000	-3.470940000
	H	-10.201319000	-0.806020000	-2.485526000
	H	-9.471607000	-0.075704000	-3.910610000
	H	-9.799665000	1.101992000	-1.335027000
	H	-7.708271000	1.168084000	-4.220265000
	H	-7.187710000	2.768116000	-3.845180000
	H	-7.938669000	3.884170000	-2.184575000
	H	-9.055067000	3.243734000	-1.040144000
	N	-6.527512000	-0.048459000	0.489300000
	C	-6.220571000	1.265418000	1.022605000
	C	-4.782601000	1.359314000	1.549726000
	O	-4.243105000	2.455281000	1.703777000
	C	-7.231782000	1.547984000	2.161171000
	C	-6.902621000	2.821819000	2.934523000
	C	-8.657213000	1.640400000	1.589918000
	C	-9.709026000	1.181940000	2.596702000
	H	-7.261716000	-0.557065000	0.968668000
	H	-6.332806000	2.023380000	0.237914000
	H	-7.190114000	0.703241000	2.856992000
	H	-8.749989000	1.026030000	0.695002000
	H	-8.858638000	2.675101000	1.311556000
	H	-10.713293000	1.327996000	2.202889000
	H	-9.594934000	0.125259000	2.833190000
	H	-9.640872000	1.742140000	3.526202000
	H	-7.686755000	3.019580000	3.660778000
	H	-5.968558000	2.728660000	3.477927000
	H	-6.840740000	3.672914000	2.262596000
	N	-4.192385000	0.215318000	1.863509000
	C	-2.861013000	0.130214000	2.437926000
	C	-1.814751000	0.341047000	1.334780000
	O	-1.107478000	1.348946000	1.324061000
	C	-2.729842000	-1.221277000	3.162119000
	C	-3.656702000	-1.244364000	4.378573000
	C	-1.289689000	-1.498275000	3.580929000

	H	-4.632018000	-0.665764000	1.635735000
	H	-2.735722000	0.963534000	3.137495000
	H	-3.049783000	-1.997932000	2.465026000
	H	-1.250972000	-2.439145000	4.117213000
	H	-0.639964000	-1.544055000	2.717136000
	H	-0.932957000	-0.715560000	4.245454000
	H	-3.601153000	-2.207385000	4.876703000
	H	-4.691674000	-1.054886000	4.106630000
	H	-3.362237000	-0.486373000	5.101879000
	N	-1.741463000	-0.639918000	0.434112000
	C	-0.793227000	-0.665876000	-0.669861000
	C	-0.720067000	0.689388000	-1.373386000
	O	0.348572000	1.208218000	-1.701481000
	C	-1.149845000	-1.728010000	-1.715887000
	C	-1.332580000	-3.141117000	-1.144360000
	C	-2.185281000	-3.972868000	-2.072144000
	N	-1.809144000	-5.227008000	-2.248887000
	O	-3.248798000	-3.541064000	-2.569243000
	H	-2.450176000	-1.368748000	0.458823000
	H	0.215431000	-0.864984000	-0.293408000
	H	-0.355443000	-1.718215000	-2.465878000
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	H	-0.370092000	-3.613652000	-0.986636000
	H	-1.877132000	-3.102270000	-0.199808000
	H	-2.333760000	-5.816146000	-2.877399000
	H	-0.896751000	-5.537184000	-1.948153000
	N	-1.906499000	1.273078000	-1.555739000
	C	-2.105114000	2.624869000	-2.043809000
	C	-0.879552000	3.497845000	-1.736887000
	O	-0.359192000	4.192152000	-2.607823000
	C	-3.365233000	3.145686000	-1.342579000
	C	-3.724339000	4.589550000	-1.678113000
	C	-5.030792000	4.990031000	-0.976919000
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	N	-4.690117000	7.090576000	1.077483000
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	C	1.849484000	3.164529000	0.218072000
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	H	1.938789000	-3.833686000	6.076770000
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	C	4.914861000	0.265162000	-2.456149000
	O	5.765516000	-0.538023000	-2.900448000
	C	2.817886000	0.359573000	-3.791997000
	C	1.578398000	-0.496613000	-4.211503000
	O	1.176334000	-1.365440000	-3.421003000
	O	1.081109000	-0.234290000	-5.320562000
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	H	3.550364000	0.268884000	-4.600189000
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	C	6.809981000	3.012869000	-0.897962000
	C	8.252998000	3.340237000	-0.649509000
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	C	8.895173000	2.882364000	0.493241000
	C	10.239542000	3.140268000	0.697240000
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	H	5.952149000	-2.143938000	-2.538399000
	Cu	7.317983000	-0.651502000	-2.320772000
	N	-4.938391000	-5.421549000	-1.353444000
	C	-4.693515000	-4.675396000	-0.095742000
	C	-4.814311000	-3.175060000	-0.369778000
	O	-4.122138000	-2.348680000	0.215033000
	C	-3.317714000	-5.139926000	0.407132000
	C	-2.810559000	-4.567038000	1.736674000
	C	-1.871373000	-5.597388000	2.372625000
	C	-1.005917000	-5.024444000	3.488335000
	N	-0.026080000	-6.055961000	3.900566000
	H	-5.470891000	-4.933274000	0.632095000
	H	-2.583843000	-4.948266000	-0.374829000
	H	-3.405435000	-6.220495000	0.527856000
	H	-2.270609000	-3.644361000	1.549417000
	H	-3.654090000	-4.354148000	2.391645000
	H	-1.223048000	-5.976795000	1.591874000
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	H	-1.642315000	-4.752396000	4.327375000
	H	-0.478385000	-4.150540000	3.122786000
	H	0.825070000	-6.091036000	3.307207000
	H	0.298755000	-5.917328000	4.854895000
	H	-0.465077000	-6.975917000	3.864989000
	H	-5.921258000	-5.385227000	-1.692870000
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	C	-5.785937000	-1.527396000	-1.888828000
	C	-5.707002000	-0.376250000	-0.885323000
	O	-4.960969000	0.586256000	-1.042934000
	C	-7.062547000	-1.379006000	-2.721841000
	C	-7.005465000	-0.140289000	-3.613276000
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	N	-6.534342000	-0.502777000	0.153296000
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	C	-7.593730000	-0.064477000	2.304007000
	C	-7.557668000	0.828851000	3.541876000
	C	-9.037792000	-0.249317000	1.814361000
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	C	-5.193934000	5.571386000	0.208907000
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	C	0.583702000	5.260418000	1.536341000
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	C	2.226445000	0.075203000	-3.286053000
	C	1.294062000	-1.142463000	-3.558776000
	O	1.380369000	-2.132671000	-2.817774000
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	H	1.479140000	1.053071000	-1.071363000
	H	3.142148000	-1.136943000	-1.804209000
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	H	1.618301000	0.981970000	-3.288090000
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	H	5.286524000	4.261207000	-1.349288000
	H	7.223333000	5.243422000	-2.572356000
	H	7.767259000	3.222685000	1.142878000
	H	10.052564000	4.127421000	1.300179000
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	N	6.678457000	0.782331000	0.175742000
	C	7.204057000	-0.501173000	0.708103000
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	O	7.337267000	-2.183056000	-1.066083000
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	H	6.415460000	-2.607433000	2.425020000
	H	8.650270000	-3.234099000	3.392074000
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	C	5.724956000	-3.816720000	-1.596631000
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	C	1.163897000	-3.087570000	0.353283000
	N	0.716001000	-4.446382000	0.534685000
	C	0.617819000	-5.372513000	-0.406260000
	N	0.391451000	-6.622820000	0.010786000
	N	0.527768000	-5.074071000	-1.708502000
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	H	2.894445000	-3.450181000	1.594941000
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	H	0.980762000	-2.714144000	-0.650964000
	H	0.952469000	-4.811728000	1.464880000
	H	0.338743000	-7.370119000	-0.658165000
	H	0.686573000	-6.843353000	0.956368000
	H	0.462194000	-5.806755000	-2.391476000
	H	0.830282000	-4.179751000	-2.061243000
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	O	-3.995782000	-2.427871000	0.288089000
	C	-3.090081000	-5.183392000	0.510341000
	C	-2.557956000	-4.559340000	1.805303000
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	C	-5.405857000	0.872941000	1.751919000
	O	-5.293063000	2.049233000	2.100696000
	C	-7.578014000	-0.272730000	2.355506000
	C	-7.589973000	0.643649000	3.577038000
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	C	-3.718296000	-1.150215000	4.487786000
	C	-1.329203000	-1.018756000	3.742391000
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	H	-1.152836000	-1.882020000	4.370107000
	H	-0.674572000	-1.035110000	2.883299000
	H	-1.133114000	-0.119381000	4.319028000
	H	-3.540991000	-2.080511000	5.017137000
	H	-4.762573000	-1.129731000	4.185180000
	H	-3.558232000	-0.329504000	5.184151000
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	C	-1.234407000	-0.167844000	-0.810639000
	C	-1.233447000	1.284252000	-1.280800000
	O	-0.187555000	1.854229000	-1.614650000
	C	-1.828871000	-0.996061000	-1.959088000
	C	-1.527353000	-2.490544000	-1.817622000
	C	-2.155345000	-3.247868000	-2.965758000
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	O	-3.128507000	-3.989344000	-2.812681000
	H	-2.625822000	-1.156504000	0.414791000
	H	-0.189016000	-0.460963000	-0.655602000
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	H	-1.919033000	-2.867319000	-0.876609000
	H	-1.972093000	-3.511334000	-4.968520000
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	O	-1.046128000	4.827140000	-2.327848000
	C	-3.838015000	3.660143000	-0.645023000
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	N	-5.320286000	4.812495000	1.479297000
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	C	0.374247000	5.468671000	1.387983000
	C	1.742599000	6.111631000	1.606803000
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	N	0.913310000	-4.938305000	-1.603654000
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