

Supplementary Materials

Ab Initio Calculations on the Ground and Excited Electronic States of Thorium–Ammonia, Thorium–Aza-Crown, and Thorium–Crown Ether Complexes

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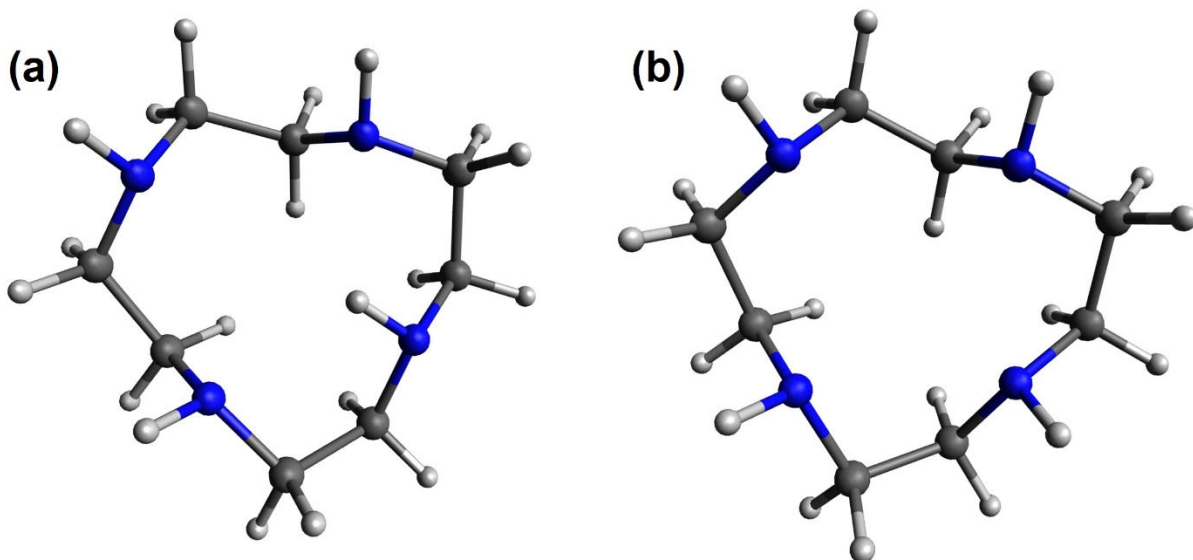


Figure S1. Structures of aza-crown ether 12C4N: (a) fully optimized, (b) fixed at the geometry in the $\text{Th}(\text{12C4N})_2^{4+}$ complex.

Table S1. Energies (hartrees) for the $\text{Th}(\text{NH}_3)_{n=0-10}^{4+,3+,0}$ species. The spin for the charged species is singlet (4+) and doublet (3+), while for the neutral species both the lowest singlet (S=0) and triplet (S=1) states are reported.

n	$\text{Th}(\text{NH}_3)_n^{4+} (\text{S}=0)$	$\text{Th}(\text{NH}_3)_n^{3+} (\text{S}=1/2)$	$\text{Th}(\text{NH}_3)_n^0 (\text{S}=0)$	$\text{Th}(\text{NH}_3)_n^0 (\text{S}=1)$
0	-404.214983	-405.278100	-406.593310	-406.598549
1	-461.053438	-461.978898	-463.157366	-463.164141
2	-517.825621	-518.654077	-519.723392	-519.729842
3	-574.558086	-575.312384	-576.278371	-576.279880
4	-631.262347	-631.956535	-632.834821	-632.835097
5	-687.925485	-688.574423	-689.390959	-689.386922
6	-744.569805	-745.180261	-745.945630	-745.942632
7	-801.199465	-801.773312	-802.496153	-802.495036
8	-857.813602	-858.362174	-859.051770	-859.048942
9	-914.408325	914.921105	-915.598359	-915.597735
10	-970.985977	-971.475997	-972.142435	-972.139865

Table S2. Cartesian coordinates (Å) for the $\text{Th}(\text{NH}_3)_{n=1-10}^{4+,3+,0}$ species. The spin for the charged species is singlet (4+) and doublet (3+), while for the neutral species both the lowest singlet (S=0) and triplet (S=1) states are reported.

n	$\text{Th}(\text{NH}_3)_n^{4+} (\text{S}=0)$	$\text{Th}(\text{NH}_3)_n^{3+} (\text{S}=1/2)$	$\text{Th}(\text{NH}_3)_n^0 (\text{S}=0)$	$\text{Th}(\text{NH}_3)_n^0 (\text{S}=1)$
1	Th -0.246876 0.000000 0.000001 N 2.075202 -0.000000 0.000013 H 2.564039 -0.831207 -0.476032 H 2.564038 0.827812 -0.481914 H 2.564381 0.003396 0.957757	Th -0.263568 -0.000000 0.000001 N 2.234263 -0.000002 0.000008 H 2.693713 -0.807113 -0.477132 H 2.693681 0.816750 -0.460468 H 2.693886 -0.009613 0.937493	Th -0.270210 -0.000102 -0.000002 N 2.316789 -0.001188 -0.000020 H 2.711028 -0.484307 0.815544 H 2.711161 -0.456442 -0.831385 H 2.679200 0.958214 0.016170	Th -0.269575 0.000000 -0.000002 N 2.311247 0.000001 -0.000032 H 2.694129 0.799161 0.517534 H 2.694136 -0.847677 0.433519 H 2.694720 0.048502 -0.950670
2	Th -0.000258 -0.258676 -0.000001 N 1.976349 1.085714 -0.000003 H 2.119755 1.740301 0.820415 H 2.891363 0.550187 -0.000765 H 2.119109 1.741447 -0.819603 N -1.973644 1.088013 0.000001 H -2.634481 0.943557 0.816886 H -2.630859 0.949442 -0.820825 H -1.860609 2.139776 0.003971	Th -0.000220 -0.290728 0.000000 N 2.033464 1.229136 -0.000001 H 2.142533 1.862525 0.817007 H 2.944615 0.727013 -0.013389 H 2.129078 1.881437 -0.803668 N -2.031416 1.230687 -0.000001 H -2.683498 1.096373 0.799392 H -2.664257 1.123763 -0.818739 H -1.862996 2.255631 0.019392	Th 0.000011 0.016628 -0.000934 N 2.626899 -0.067883 0.005247 H 3.054150 0.510270 0.736241 H 2.950778 -1.030919 0.151641 H 3.019055 0.245221 -0.888737 N -2.626935 -0.069011 0.001981 H -2.978038 -0.271478 0.944374 H -2.986305 -0.803364 -0.618322 H -3.060345 0.812034 -0.291771	Th 0.000000 0.000001 -0.000026 N -2.633334 0.000015 0.000115 H -3.016983 0.858923 -0.407924 H -3.016581 -0.782972 -0.539763 H -3.016810 -0.076204 0.948027 N 2.633331 -0.000029 0.000116 H 3.016829 0.076179 -0.947792 H 3.017000 -0.858911 0.408185 H 3.016549 0.782975 0.539987
3	Th 0.000388 -0.000652 -0.216373 N -1.754317 -1.488519 0.605929 H -2.479080 -1.073075 1.241774 H -2.354221 -1.924724 -0.140335 H -1.450637 -2.332881 1.150997 N -0.417611 2.262281 0.604266 H -1.253762 2.402139 1.223457 H -0.586744 2.983146 -0.143368 H 0.343379 2.717617 1.166088 N 2.168841 -0.768349 0.606863 H 2.183454 -1.661271 1.158879 H 2.882140 -0.970982 -0.139608 H 2.702195 -0.119154 1.236314	Th -0.000046 -0.000055 -0.145074 N 0.740449 2.348277 0.404796 H 1.213064 2.863917 -0.362487 H -0.010866 3.003473 0.691583 H 1.416784 2.422870 1.187928 N 1.663802 -1.814968 0.404870 H 2.609948 -1.491869 0.681389 H 1.866331 -2.488740 -0.358637 H 1.395038 -2.430994 1.195200 N -2.403864 -0.532897 0.405035 H -3.090464 -0.358132 -0.353891 H -2.600224 -1.516833 0.668484 H -2.798151 -0.001597 1.204175	Th 0.143217 -0.021051 -0.006042 N -1.944694 1.657573 0.009342 H -1.739230 2.398313 -0.665153 H -2.898946 1.338882 -0.187803 H -1.959938 2.098650 0.935136 N 2.759969 0.051462 0.029188 H 3.145357 0.656643 -0.702492 H 3.060989 -0.908646 -0.186575 H 3.194113 0.328509 0.913512 N -2.060324 -1.514364 0.014991 H -2.999702 -1.139093 0.181763 H -2.087020 -2.033416 -0.870189 H -1.889836 -2.207918 0.750944	Th 0.000260 -0.000010 -0.050023 N 2.612630 -0.022591 0.146594 H 3.008663 -0.847686 -0.320382 H 3.022858 0.795452 -0.320532 H 2.944048 -0.025369 1.116501 N -1.327005 -2.250171 0.146403 H -0.823355 -3.015565 -0.318571 H -2.238602 -2.180600 -0.322487 H -1.497268 -2.534212 1.116415 N -1.287795 2.272847 0.146395 H -0.771525 3.029122 -0.319662 H -2.200999 2.218737 -0.321399 H -1.452010 2.560427 1.116408
4	Th -0.000884 -0.000257 0.000055 N -0.031027 2.420062 -0.575221 H 0.270033 3.078913 0.177882 H 0.575971 2.715498 -1.372840 H -0.956216 2.819741 -0.851388 N 1.350047 -0.342651 2.061110 H 1.995345 0.434919 2.327395 H 1.994902 -1.164930 2.061318 H 0.815806 -0.489980 2.947015 N 1.016161 -1.283838 -1.872064 H 1.075105 -0.792695 -2.792568 H 2.002563 -1.600808 -1.735871 H 0.539674 -2.175597 -2.136010 N -2.327832 -0.791375 0.385741 H -2.473176 -1.423417 1.205172	Th 0.000057 -0.000014 -0.000001 N 1.689186 1.497461 -1.217624 H 1.269577 2.203276 -1.847069 H 2.322605 2.059714 -0.622800 H 2.340315 0.996193 -1.846282 N -1.497109 1.688906 1.218290 H -0.995692 2.339757 1.847115 H -2.202944 1.269211 1.847657 H -2.059297 2.322604 0.623702 N 1.496968 -1.689720 1.217518 H 2.058729 -2.323518 0.622635 H 2.203167 -1.270375 1.846709 H 0.995516 -2.340484 1.846402 N -1.689525 -1.496541 -1.218165 H -2.322966 -2.058998 -0.623559	Th 0.000017 -0.000050 0.000480 N 2.149776 -1.050478 -1.007585 H 2.739476 -0.352608 -1.490334 H 2.738891 -1.503048 -0.289186 H 1.928965 -1.772736 -1.699391 N 2.151692 1.049673 1.005631 H 2.743936 0.351434 1.484716 H 1.931170 1.769299 1.700282 H 2.738028 1.505661 0.287173 N -2.151957 -1.008407 1.046456 H -2.737731 -1.493942 0.347144 H -1.931522 -1.698561 1.770427 H -2.744774 -0.291218 1.495936 N -2.149644 1.009645 -1.048578 H -2.739039 1.491060 -0.349431	Th -0.000000 -0.000021 -0.000031 N 2.188170 -1.584823 -0.000107 H 3.114565 -1.137537 0.000243 H 2.163503 -2.198493 0.819451 H 2.163977 -2.198210 -0.819887 N 2.188058 1.584953 0.000408 H 3.114473 1.137710 0.000199 H 2.163678 2.198278 0.820231 H 2.163515 2.198682 -0.819108 N -2.188100 -1.584889 -0.000340 H -2.163993 -2.198074 -0.820273 H -2.163579 -2.198751 0.819074 H -3.114391 -1.137399 0.000092 N -2.188129 1.584897 0.000282 H -2.163712 2.197987 0.820283

	H -3.046973 -0.052596 0.555787 H -2.764921 -1.341320 -0.387830	H -2.340645 -0.994810 -1.846460 H -1.270122 -2.202090 -1.848047	H -1.928653 1.703194 -1.769120 H -2.739333 0.292897 -1.502874	H -2.163369 2.198859 -0.819052 H -3.114644 1.137853 -0.000165
5	Th -0.000026 0.001009 0.088091 N 2.368037 -0.039535 -0.838832 H 2.472083 -0.057923 -1.872911 H 2.973044 0.763583 -0.573993 H 2.953925 -0.847418 -0.546514 N -0.041099 -2.359945 -0.856474 H 0.752017 -2.972623 -0.579234 H -0.038654 -2.456235 -1.891461 H -0.859245 -2.941954 -0.586003 N 0.040291 2.375348 -0.822248 H -0.752406 2.984052 -0.535141 H 0.858372 2.953493 -0.543333 H 0.037193 2.486989 -1.855718 N -2.369891 0.041786 -0.834160 H -2.985261 -0.740645 -0.533261 H -2.943554 0.869590 -0.575678 H -2.476793 0.017940 -1.867836 N 0.002862 -0.025826 2.611311 H -0.786787 0.467185 3.078251 H -0.032800 -0.964152 3.061864 H 0.829832 0.404492 3.075635	Th -0.002553 -0.019804 0.004700 N 1.216075 -1.842972 -1.383392 H 1.877044 -1.456405 -2.076109 H 1.780096 -2.544991 -0.878001 H 0.591917 -2.419741 -1.969730 N -2.406450 0.561884 -0.871981 H -2.948728 -0.246077 -1.215126 H -2.403319 1.189077 -1.691043 H -3.060552 1.020627 -0.218569 N 2.492126 0.485075 0.654130 H 2.593884 1.094560 1.479728 H 3.051954 -0.339662 0.919005 H 3.079139 0.946196 -0.058623 N 0.068662 2.587139 0.040102 H -0.841607 3.069790 0.009374 H 0.512201 2.995318 0.877286 H 0.585518 3.018408 -0.742734 N -1.351975 -1.630036 1.522910 H -1.982163 -1.143768 2.180924 H -1.966388 -2.327560 1.073065 H -0.768290 -2.201054 2.155128	Th 0.126675 -0.064040 0.000075 N 2.121160 1.607237 -0.000600 H 2.716661 1.455387 0.832901 H 2.716225 1.455502 -0.834429 H 1.882997 2.602647 -0.000450 N -1.929135 -0.808488 1.475291 H -1.778724 -0.529928 2.451630 H -2.038967 -1.829813 1.496029 H -2.864891 -0.439359 1.210558 N 2.441197 -1.293390 0.000470 H 3.013345 -1.075562 -0.830715 H 3.013004 -1.074085 0.831539 H 2.314142 -2.309532 0.001383 N -1.928158 -0.806178 -1.477570 H -1.776700 -0.527099 -2.453596 H -2.038309 -1.827465 -1.499058 H -2.864100 -0.436949 -1.213602 N -1.774634 1.854982 0.001707 H -1.731255 2.472972 -0.815496 H -2.743359 1.479012 -0.000739 H -1.733799 2.468773 0.822216	Th -0.003024 0.008773 -0.017559 N -2.548425 -0.184727 0.863817 H -2.484227 -0.064508 1.881420 H -3.199016 0.524529 0.512398 H -3.010132 -1.084715 0.708822 N 2.159824 -1.500566 0.564431 H 1.985582 -2.509216 0.530566 H 2.434966 -1.300190 1.534159 H 2.981152 -1.334224 -0.029531 N -1.026916 2.479062 -0.405228 H -0.995354 2.688385 -1.409414 H -1.995628 2.637694 -0.112314 H -0.472134 3.195964 0.077037 N 2.179011 1.588976 -0.026326 H 2.804986 1.190851 -0.740507 H 2.035841 2.565854 -0.302277 H 2.695689 1.616089 0.861461 N -0.755175 -2.459152 -0.838276 H -0.712033 -2.387114 -1.860792 H -0.147303 -3.238623 -0.567832 H -1.708464 -2.755465 -0.611831
6	Th -0.000013 -0.000029 -0.000347 N 1.588979 -1.989948 -0.467301 N -1.574319 -1.742458 -1.089737 N 1.579645 1.410102 -1.489570 N 1.577220 0.592775 1.964733 N -1.585319 -0.077321 2.044736 N -1.586100 1.807102 -0.960019 H 1.686545 -2.283164 -1.456864 H -2.575032 1.751388 -0.655239 H 1.349661 -2.883252 0.002121 H 2.576978 -1.858521 -0.183434 H -1.680424 1.840869 -1.991862 H -1.347651 2.790035 -0.730673 H -1.328397 -2.038829 -2.052702 H -1.343303 -0.764928 2.782473 H -2.563125 -1.453262 -1.202192 H -1.670101 -2.651081 -0.599872 H -2.573047 -0.318859 1.844614 H -1.684104 0.799809 2.588442 H 1.338114 1.452025 -2.497305 H 1.332185 1.444001 2.504177 H 2.568846 1.102645 -1.520538 H 2.565653 0.777177 1.713757 H 1.673522 2.413420 -1.246108 H 1.674086 -0.118677 2.712521	Th 0.018040 0.001947 -0.000218 N 0.147328 -2.387804 1.132320 N -2.162865 0.898228 1.209868 N -1.923185 -1.335530 -1.209722 N 2.207131 -1.034388 -1.065734 N 1.937046 1.477237 1.067187 N -0.360437 2.365568 -1.132103 H -0.650021 -2.603299 1.747615 H -0.467734 3.193705 -0.529078 H 0.950358 -2.489082 1.769648 H 0.213825 -3.220324 0.529437 H -1.187280 2.409168 -1.744727 H 0.401540 2.632550 -1.771978 H -2.949929 1.234603 0.637078 H 2.559834 0.946952 1.693379 H -1.977447 1.685759 1.847502 H -2.601882 0.208078 1.835895 H 1.591993 2.226919 1.683518 H 2.590405 1.967242 0.439286 H -2.620440 -1.831834 -0.636821 H 2.704053 -0.384640 -1.691933 H -1.575085 -2.065238 -1.848112 H 2.029197 -1.840500 -1.681766 H -2.499072 -0.753963 -1.835056 H 2.948941 -1.374476 -0.436943	Th 0.000001 -0.000004 -0.009662 N -1.985326 0.825842 1.559190 N 1.985328 -0.826665 1.558777 N 2.022404 1.773215 -0.121628 N -2.079570 0.933777 -1.393579 N -2.022438 -1.773139 -0.122520 N 2.079597 -0.933013 -1.394038 H -1.822494 0.564327 2.537896 H 2.117853 -1.959130 -1.406790 H -2.938041 0.474358 1.329830 H -2.073257 1.849935 1.562000 H 3.021382 -0.628275 -1.075908 H 2.012690 -0.652487 -2.379555 H 2.937997 -0.474913 1.329651 H -2.198511 -2.101152 -1.078522 H 2.073396 -1.850746 1.560962 H 1.822434 -0.565765 2.537635 H -2.937717 -1.417062 0.211547 H -1.839151 -2.614884 0.430940 H 2.937681 1.417107 0.212414 H -3.021363 0.628807 -1.075698 H 1.838937 2.614708 0.432158 H -2.012598 0.653888 -2.379271 H 2.198572 2.101653 -1.077468 H -2.117866 1.959900 -1.405671	Th -0.000006 0.073224 -0.000679 N -1.990991 -0.323115 -1.779169 N 1.857540 -1.591112 -1.046226 N -1.857638 -1.578300 1.064708 N -2.137851 1.572532 0.721480 N 2.139132 1.563210 -0.738375 N 1.989845 -0.302435 1.783659 H -1.772101 -1.082053 -2.431828 H 2.960513 -0.453295 1.480483 H -1.951655 0.540745 -2.330933 H -2.962391 -0.463994 -1.473572 H 1.767387 -1.048783 2.449444 H 1.954663 0.570943 2.320547 H 1.996229 -2.434395 -0.479730 H 1.597442 2.164306 -1.371089 H 2.796604 -1.215763 -1.247894 H 1.490439 -1.918333 -1.946570 H 2.901049 1.173349 -1.303661 H 2.563437 2.171665 -0.034704 H -1.995675 -2.428531 0.508513 H -1.594575 2.182466 1.344317 H -2.796992 -1.200552 1.260595 H -2.897770 1.189984 1.294374 H -1.491621 -1.894462 1.969439 H -2.564668 2.171058 0.010829
7	Th -0.022171 0.000240 -0.000021 N -0.696122 -2.031413 -1.515128 N 1.649140 -1.883548 0.778437 N -0.656439 -0.317397 2.524758 N -0.704406 2.339776 -0.968981	Th 0.006280 0.059886 -0.023644 N 2.154809 -0.299844 -1.599381 N 1.823202 -1.066488 1.593875 N -0.171684 -2.611878 -0.404934 N -1.460263 2.285601 0.306976	Th 0.002895 0.087356 -0.059320 N 2.214017 -0.415994 -1.486839 N 1.862873 -1.043363 1.510779 N -0.216816 -2.583054 -0.325284 N -1.461799 2.301784 0.323442	Th -0.036544 0.011472 -0.006761 N -2.078715 -0.105188 1.749799 N -2.115291 -1.395324 -0.930772 N 0.947149 -2.521953 -0.077124 N 1.192289 2.433781 -0.014345

	N	1.593280	0.260856	-2.066210	N	1.626169	2.177575	0.310968	N	1.802522	2.009864	0.341291	N	-1.960619	1.667912	-0.811376
	N	1.645015	1.638020	1.218606	N	-1.890816	-0.875725	1.626712	N	-1.912665	-0.881968	1.565365	N	2.212601	-0.116139	-1.468177
	H	0.078118	-2.570565	-1.935561	H	3.087862	-0.384918	-1.175470	H	3.127898	-0.301632	-1.025543	H	-2.911622	0.470299	1.527570
	H	2.285729	2.177337	0.613251	H	-2.356110	-0.116739	2.141163	H	-2.495072	-0.166906	2.019838	H	2.537377	0.780009	-1.850857
	H	-1.276490	-1.805944	-2.341244	H	2.262805	0.474767	-2.267351	H	2.169557	0.292017	-2.232090	H	-1.741458	0.246125	2.651869
	H	-1.251701	-2.773013	-1.055231	H	2.100397	-1.115498	-2.221877	H	2.259702	-1.324526	-1.964845	H	-2.450072	-1.045386	1.933417
	H	2.301007	1.211598	1.893590	H	-1.538265	-1.471151	2.386729	H	-1.492935	-1.408881	2.346217	H	2.029280	-0.698822	-2.292650
	H	1.203715	2.382170	1.785291	H	-2.672096	-1.421728	1.240767	H	-2.584149	-1.543251	1.135200	H	3.050123	-0.519551	-1.004858
	H	2.299386	-1.637189	1.542778	H	1.433283	-1.541172	2.417909	H	1.499379	-1.348053	2.423052	H	-2.074204	-1.397846	-1.957150
	H	1.128868	0.371329	-2.983714	H	1.577678	2.895206	-0.425583	H	1.909369	2.497143	-0.558494	H	-1.837827	2.646382	-0.527260
	H	2.295865	-2.251102	0.061153	H	2.443861	-0.365806	2.019662	H	2.627693	-0.379371	1.729721	H	-3.045007	-1.011010	-0.684372
	H	1.209391	-2.747901	1.137816	H	2.473751	-1.759573	1.201562	H	2.349284	-1.861884	1.122838	H	-2.148519	-2.380564	-0.641462
	H	2.243161	-0.522431	-2.244972	H	2.630726	1.967554	0.360525	H	2.746012	1.661012	0.590172	H	-2.920121	1.420783	-0.504023
	H	2.236375	1.069542	-2.049900	H	1.454220	2.708026	1.174456	H	1.591272	2.735742	1.035574	H	-1.987402	1.666593	-1.839496
	H	-1.219424	-1.156374	2.746842	H	0.469063	-2.992404	-1.113003	H	0.430242	-3.015413	-0.998234	H	0.510744	-3.170650	0.582622
	H	0.067680	2.970630	-1.238810	H	-1.248552	2.806311	1.167599	H	-1.049838	2.958543	0.990686	H	1.172866	2.878688	-0.939857
	H	-1.219543	0.440346	2.947727	H	-1.091486	-2.934168	-0.730695	H	-1.160895	-2.868431	-0.633401	H	1.954016	-2.551537	0.133294
	H	-1.266775	2.941415	-0.342953	H	-2.476802	2.145625	0.360373	H	-2.435930	2.173899	0.614250	H	2.185963	2.382477	0.243671
	H	0.128325	-0.401187	3.191123	H	0.005466	-3.206555	0.414825	H	-0.075594	-3.103372	0.554374	H	0.851146	-2.942191	-1.010296
	H	-1.280066	2.322323	-1.828312	H	-1.363662	2.995462	-0.432334	H	-1.471934	2.779325	-0.586090	H	0.768895	3.094395	0.641877
	N	-2.641823	-0.008241	0.028775	N	-2.135555	-0.128877	-1.634242	N	-2.325002	-0.121823	-1.402930	N	2.101344	-0.063448	1.620482
	H	-3.106716	0.107545	-0.887477	H	-2.212655	0.685539	-2.257614	H	-2.296530	0.509674	-2.209503	H	1.920702	0.514009	2.450987
	H	-3.089661	-0.866088	0.392824	H	-2.087615	-0.908322	-2.302118	H	-2.443924	-1.065204	-1.792100	H	2.333039	-0.997268	1.984404
	H	-3.092411	0.729570	0.595873	H	-3.078079	-0.212772	-1.231338	H	-3.206066	0.059450	-0.903564	H	2.999730	0.285140	1.231658
8	Th	0.000099	-0.000061	0.000261	Th	0.000081	0.000197	-0.000600	Th	0.000086	-0.007166	-0.000266	Th	-0.001418	-0.001915	0.001915
	N	1.683751	1.443269	1.476705	N	2.103132	1.063317	1.359260	N	2.262682	0.867201	1.136073	N	-0.252036	-2.355750	-1.232081
	N	-1.443166	1.683161	1.477440	N	-1.066145	2.102296	1.358160	N	-0.724516	2.201809	1.342644	N	-2.355934	0.264797	-1.226419
	N	-1.683096	-1.444182	1.476661	N	-2.102646	-1.064088	1.359826	N	-2.155591	-0.870729	1.317104	N	0.254247	2.347701	-1.238883
	N	0.163437	2.211169	-1.477390	N	0.567987	2.288552	-1.356335	N	0.718985	2.205289	-1.340398	N	-1.980136	-1.313979	1.224737
	N	-0.164013	-2.209653	-1.480022	N	-0.564727	-2.287303	-1.360028	N	-0.994174	-2.180406	-1.228612	N	1.974287	1.303811	1.237190
	N	2.211875	-0.163497	-1.476731	N	2.287930	-0.569223	-1.359321	N	2.158233	-0.865258	-1.317242	N	1.326149	-1.967740	1.227476
	N	1.442754	-1.684226	1.476972	N	1.061366	-2.100317	1.364143	N	0.998186	-2.178812	1.228476	N	2.347193	-0.239712	-1.244823
	N	-2.212317	0.164542	-1.475903	N	-2.287578	0.564977	-1.360890	N	-2.264493	0.863373	-1.135977	N	-1.300908	1.976857	1.236615
	H	1.640947	2.465668	1.349181	H	2.638226	1.826245	0.927052	H	2.829284	1.512736	0.565578	H	-0.711454	-3.090758	-0.662621
	H	1.574625	1.348112	2.498613	H	1.843331	1.438119	2.278828	H	2.123751	1.357477	2.030004	H	-0.800247	-2.320402	-2.099505
	H	2.687613	1.246152	1.347301	H	2.829458	0.375333	1.588824	H	2.913908	0.089842	1.355613	H	0.653594	-2.769514	-1.500266
	H	-2.465226	1.643864	1.346269	H	-1.821077	2.644273	0.920503	H	-1.293837	2.869667	0.801205	H	-3.087003	0.729464	-0.655433
	H	-1.351999	1.570503	2.499342	H	-1.452340	1.840565	2.272428	H	-1.263359	2.030887	2.203560	H	-2.321031	0.809750	-2.095805
	H	-1.242601	2.686866	1.352137	H	-0.376249	2.823266	1.598653	H	0.093152	2.757657	1.642766	H	-2.774106	-0.639849	-1.491204
	H	-1.642698	-2.466160	1.345057	H	-2.629933	-1.835236	0.932688	H	-2.904022	-1.244359	0.698016	H	0.761083	3.070416	-0.693516
	H	-1.571295	-1.353244	2.498647	H	-1.844214	-1.428210	2.284059	H	-2.001765	-1.609119	2.015551	H	0.757346	2.298877	-2.132531
	H	-2.686868	-1.244439	1.350629	H	-2.835423	-0.379565	1.579182	H	-2.620273	-0.111665	1.837333	H	-0.651811	2.786022	-1.463211
	H	2.465494	-1.637168	1.353899	H	1.834931	-2.627561	0.941371	H	1.049906	-3.044280	0.672420	H	3.076840	-0.728469	-0.693271
	H	1.343054	-1.579450	2.498908	H	1.420959	-1.839773	2.289565	H	1.978687	-2.006148	1.506453	H	2.303147	-0.755857	-2.131205
	H	1.249815	-2.688316	1.343001	H	0.376704	-2.833412	1.581850	H	0.518585	-2.435199	2.098276	H	2.770904	0.669883	-1.482233
	H	1.011474	2.783695	-1.349220	H	1.177935	2.987626	-0.915377	H	1.284348	2.874894	-0.797031	H	-2.426824	-2.051257	0.648034
	H	0.152568	2.066684	-2.499276	H	1.007567	2.122141	-2.268822	H	1.260434	2.037172	-2.200189	H	-1.703031	-1.794486	2.088780
	H	-0.591281	2.902002	-1.348905	H	-0.266594	2.834085	-1.600310	H	-0.100285	2.757986	-1.641821	H	-2.759879	-0.696510	1.497072
	H	-1.009789	-2.784593	-1.347801	H	-1.190676	-2.978885	-0.929876	H	-1.970747	-2.004756	-1.517899	H	2.385429	2.083174	0.689797
	H	-0.159075	-2.064096	-2.501792	H	-0.985052	-2.117653	-2.280953	H	-0.506676	-2.444781	-2.091617	H	1.700992	1.730325	2.130168
	H	0.593300	-2.898514	-1.356388	H	0.268480	-2.842336	-1.586630	H	-1.056339	-3.042142	-0.667710	H	2.777602	0.698048	1.462658
	H	2.786789	-1.009359	-1.344944	H	2.973207	-1.204172	-0.932296	H	2.906183	-1.239935	-0.698154	H	2.076082	-2.403716	0.658230
	H	2.067496	-0.157379	-2.498655	H	2.117494	-0.980491	-2.284176	H	2.006467	-1.601378	-2.018496	H	1.793535	-1.683492	2.096355

	H 2.900565 0.593687 -1.351384 H -2.784155 1.012996 -1.347465 H -2.068622 0.153569 -2.497892 H -2.903648 -0.589638 -1.346901	H 2.850200 0.261450 -1.577239 H -2.973139 1.200445 -0.935108 H -2.116726 0.974752 -2.286347 H -2.849614 -0.266192 -1.577608	H 2.622818 -0.103857 -1.834143 H -2.829558 1.511539 -0.566925 H -2.127038 1.349917 -2.032156 H -2.916560 0.085489 -1.351186	H 0.716720 -2.755599 1.494273 H -2.062761 2.404218 0.677359 H -1.749796 1.701416 2.117894 H -0.687747 2.768786 1.481186
9	Th 0.000000 0.000020 0.000088 N -0.084406 -2.551244 0.906178 N 1.925334 -1.463030 -1.212184 N 1.972488 1.772780 -0.531337 N -1.904389 -1.381226 -1.334794 N -1.858736 1.852450 -0.654992 N -1.984415 -0.350570 1.804578 N -0.013639 2.059958 1.758723 N 0.096656 0.492198 -2.661124 H 0.704453 -3.159013 0.647417 H -0.107360 -2.645496 1.931075 H -0.894456 -3.115222 0.616019 H 2.437826 -0.999333 -1.974336 H 2.690349 -1.800935 -0.611784 H 1.600180 -2.329180 -1.666177 H 1.687213 2.598351 -1.078152 H 2.431610 2.201959 0.283243 H 2.774978 1.416791 -1.069125 H -0.831342 2.129987 2.379197 H 0.767309 2.100341 2.427295 H 0.016778 2.994937 1.328934 H -2.725437 -1.674469 -0.787194 H -2.338730 -0.902692 -2.135362 H -1.591183 -2.267548 -1.757084 H -1.505155 2.663757 -1.182943 H -2.640021 1.528968 -1.242242 H -2.349695 2.302797 0.129012 H -2.760219 0.325285 1.769589 H -2.480544 -1.251131 1.767133 H -1.694236 -0.304797 2.792341 H 0.099100 -0.347700 -3.256380 H -0.679817 1.039230 -3.056520 H 0.918698 1.006978 -3.004197 N 1.851227 -0.431546 1.924296 H 1.504393 -0.365294 2.892442 H 2.658281 0.207573 1.933464 H 2.306188 -1.354351 1.921052	Th -0.006306 0.006816 -0.077266 N 2.161089 0.353799 -1.743603 N 2.083001 -1.620808 0.778805 N -1.558289 -1.994029 1.073753 N 1.723287 1.930667 0.929656 N -1.953920 1.486378 1.237080 N -0.444245 2.424839 -1.341592 N -2.399699 -0.230021 -1.439332 N 0.290440 -0.128031 2.817868 H 3.116555 0.262909 -1.378786 H 2.132675 -0.297331 -2.534573 H 2.172764 1.266413 -2.210033 H 1.790621 -2.523377 1.169506 H 2.741999 -1.889136 0.040145 H 2.692467 -1.237990 1.509361 H -2.076302 -1.736684 1.920756 H -2.290733 -2.349974 0.450310 H -1.057395 -2.843517 1.357108 H -2.438506 0.434736 -2.218181 H -2.517279 -1.131216 -1.913723 H -3.296027 -0.101975 -0.954677 H 2.064484 2.589085 0.221452 H 1.351541 2.542177 1.664926 H 2.588432 1.565598 1.342733 H -2.516121 0.986022 1.934164 H -1.612750 2.305262 1.753066 H -2.661310 1.884279 0.610108 H -1.429113 2.640489 -1.524759 H -0.089236 3.298020 -0.935647 H -0.038077 2.399088 -2.282279 H 1.185573 0.206307 3.189859 H -0.394242 0.402479 3.367020 H 0.217826 -1.073388 3.208392 N 0.155746 -2.280186 -1.616123 H -0.218646 -2.049350 -2.542229 H -0.350312 -3.130139 -1.343532 H 1.096790 -2.630532 -1.822117	Th -0.013250 0.019830 -0.106458 N -2.538601 -0.039076 -1.079353 N -1.796535 1.142702 1.578772 N 1.517187 1.866574 1.156059 N -1.303974 -2.155494 0.855737 N 2.149801 -1.547527 0.264307 N 0.026038 -2.065814 -1.837401 N 2.124981 0.811350 -1.556665 N 0.591289 -0.630885 2.565376 H -3.198480 -0.700565 -0.645908 H -3.023353 0.873111 -0.994667 H -2.546224 -0.244677 -2.085810 H -1.426488 1.728134 2.339965 H -2.487528 1.749434 1.096262 H -2.386450 0.440871 2.053396 H 2.444306 1.455019 1.371682 H 1.749552 2.704281 0.604597 H 1.173218 2.225206 2.055996 H 2.310963 0.185132 -2.349479 H 2.029661 1.740805 -1.983095 H 3.012483 0.848151 -1.024123 H -1.953789 -2.614879 0.202690 H -0.647582 -2.906560 1.142478 H -1.874031 -1.977921 1.698008 H 2.887929 -1.059036 0.804753 H 1.953807 -2.416230 0.790903 H 2.635632 -1.860288 -0.587873 H 0.684621 -1.903301 -2.605092 H 0.267144 -2.981935 -1.438751 H -0.884577 -2.188219 -2.291864 H -0.073896 -0.304091 3.276289 H 0.636206 -1.651944 2.703761 H 1.511303 -0.290677 2.874407 N -0.664616 2.474457 -1.043086 H -1.623902 2.781613 -0.827211 H -0.649355 2.300054 -2.054911 H -0.067622 3.289804 -0.871398	Th -0.012230 0.012286 -0.117556 N 0.154774 -2.192815 -1.676122 N -1.401513 -2.065867 0.931703 N -1.873373 1.387994 1.284910 N 2.044568 -1.576015 0.637383 N 1.538744 1.905782 1.054547 N 2.275584 0.508074 -1.487940 N -0.463412 2.440799 -1.260503 N 0.320788 -0.326823 2.682014 H 0.316997 -3.082492 -1.181777 H -0.695343 -2.335506 -2.232119 H 0.909295 -2.117236 -2.366903 H -2.070277 -1.777110 1.663261 H -1.976755 -2.583054 0.251918 H -0.810301 -2.788448 1.374830 H -1.537910 2.047753 2.003280 H -2.512440 1.950822 0.695901 H -2.519480 0.757722 1.794321 H 0.175786 2.613257 -2.041036 H -1.401918 2.468714 -1.674357 H -0.416241 3.268739 -0.657092 H 2.583544 -1.996744 -0.132880 H 2.755304 -1.045038 1.175826 H 1.786969 -2.374356 1.239561 H 1.140317 2.392202 1.869574 H 2.415644 1.475445 1.406603 H 1.874191 2.655172 0.433593 H 2.288124 1.398414 -2.001180 H 3.121419 0.535849 -0.893844 H 2.474114 -0.203742 -2.202288 H 0.296994 -1.316887 2.959135 H 1.229442 0.013110 3.021875 H -0.381575 0.127731 3.276519 N -2.496829 -0.172086 -1.185611 H -2.540188 -0.757134 -2.028988 H -2.874728 0.741833 -1.482478 H -3.225615 -0.538015 -0.553874
10	Th 0.000165 -0.000397 -0.004258 N 1.217173 2.267658 -0.946978 N 1.071924 -1.133195 -2.254037 N -1.217160 -2.337474 -0.760423 N 1.225788 0.965975 2.242935 N -1.230431 -0.780125 2.311871 N -1.120087 2.316992 0.927890 N -2.786955 0.073464 -0.132498 N 1.119164 -2.232939 1.113304 H 1.900892 2.708007 -0.318022 H 1.761043 2.155007 -1.812203 H 0.593257 3.049949 -1.180934	Th 0.000262 0.000026 -0.043516 N 1.810341 -1.852360 1.095451 N 1.046711 -1.207810 -2.384248 N -1.045162 1.235960 -2.368104 N -1.160511 -1.015697 2.344757 N -1.813833 1.844261 1.100538 N 1.148505 0.994590 2.359711 N 0.702313 2.756875 -0.308114 N -2.776061 -0.554754 -0.549947 H 1.420024 -2.568128 1.716027 H 2.300049 -2.405935 0.385324 H 2.573703 -1.446180 1.644970	Th 0.000024 -0.000032 -0.009355 N -1.159529 -2.311986 -0.720063 N -1.001144 1.119569 -2.232892 N 1.161782 2.313247 -0.712778 N -1.246035 -0.849467 2.206085 N 1.245913 0.845098 2.208102 N 1.139262 -2.187666 1.015764 N 2.710010 -0.051956 -0.225528 N -1.139897 2.185128 1.020787 H -1.793271 -2.688910 0.015445 H -1.761352 -2.254934 -1.556082 H -0.505406 -3.084001 -0.921378	Th 0.000370 0.001124 0.000152 N -1.385421 -1.813482 -1.394948 N -1.438780 1.583682 -1.599389 N 0.971532 2.471015 -0.270975 N -0.827142 -1.755091 1.853683 N 1.539899 0.001841 2.200751 N 1.194114 -2.388636 -0.147241 N 2.692707 0.187791 -0.381814 N -0.809527 1.741399 1.863683 H -1.884128 -2.493673 -0.786845 H -2.118287 -1.427182 -2.009801 H -0.815866 -2.407815 -2.015263

H	1.686688	-1.942905	-2.100071	H	0.442073	-1.887232	-2.855600	H	-1.559604	1.964603	-1.991358	H	-1.919615	2.332349	-1.053141
H	0.398517	-1.493406	-2.941776	H	1.221330	-0.500115	-3.104173	H	-0.307698	1.455337	-2.913491	H	-0.902210	2.093941	-2.315538
H	1.663742	-0.518071	-2.827331	H	1.945260	-1.697277	-2.322448	H	-1.648807	0.530713	-2.774194	H	-2.198784	1.123324	-2.122747
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H	-1.762463	-2.295408	-1.631104	H	-0.449058	1.932993	-2.824377	H	1.761592	2.258558	-1.550482	H	1.457884	2.638632	-1.165412
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H	-3.295412	-0.371823	0.641004	H	-0.072894	3.369106	-0.578522	H	3.225995	0.440801	0.521684	H	3.123416	0.890136	0.245973
H	1.818094	1.796077	2.111247	H	-0.625761	-1.734319	2.842492	H	-1.834995	-1.683488	2.012472	H	-1.454740	-2.474669	1.446029
H	0.596886	1.263221	2.999494	H	-1.344768	-0.317055	3.071266	H	-0.632218	-1.145303	2.975819	H	-0.066294	-2.306287	2.275907
H	1.862278	0.317851	2.724636	H	-2.074108	-1.457302	2.204214	H	-1.904138	-0.179746	2.627451	H	-1.354995	-1.379331	2.653437
H	-1.826178	-1.615592	2.246416	H	-2.299696	2.402147	0.391091	H	1.837248	1.677694	2.016033	H	2.112721	0.867677	2.268085
H	-0.603158	-1.018591	3.090302	H	-2.580140	1.435367	1.643941	H	0.631714	1.141949	2.977157	H	1.062197	-0.061645	3.110055
H	-1.864345	-0.092945	2.739827	H	-1.426171	2.556087	1.727303	H	1.901630	0.173348	2.629970	H	2.241178	-0.757339	2.225871
H	-1.630952	2.877574	0.233594	H	2.068424	1.426486	2.230658	H	1.619562	-2.725813	0.259994	H	1.695045	-2.553246	-1.034744
H	-1.815261	2.213861	1.678302	H	0.616352	1.717856	2.853487	H	1.879435	-2.045183	1.717326	H	1.904807	-2.546800	0.586671
H	-0.464969	3.003040	1.323186	H	1.316977	0.291983	3.086257	H	0.495971	-2.871279	1.440380	H	0.548990	-3.191840	-0.058991
H	1.633201	-2.845875	0.467332	H	-2.897982	-0.924966	-1.497023	H	-1.620929	2.725402	0.267030	H	-1.422943	2.463809	1.436110
H	1.811422	-2.069404	1.855659	H	-3.242013	-1.253751	0.036736	H	-1.879402	2.040461	1.722676	H	-1.362771	1.371418	2.646867
H	0.463568	-2.886434	1.559686	H	-3.426563	0.236345	-0.524735	H	-0.496296	2.867755	1.446603	H	-0.044310	2.274478	2.299875
N	-1.068155	0.944741	-2.341103	N	2.776933	0.553850	-0.539438	N	0.999708	-1.108944	-2.238265	N	0.746356	-0.138078	-2.574133
H	-0.394479	1.243797	-3.057319	H	3.420243	-0.243457	-0.541945	H	0.305762	-1.440158	-2.920601	H	-0.034649	-0.263484	-3.235842
H	-1.679806	1.766696	-2.254603	H	3.250592	1.229320	0.068310	H	1.557138	-1.956072	-2.001195	H	1.397875	-0.909812	-2.793411
H	-1.662941	0.285889	-2.860108	H	2.899679	0.953397	-1.474361	H	1.648271	-0.518067	-2.776328	H	1.232712	0.711695	-2.909222
N	2.787530	-0.081665	-0.121261	N	-0.691529	-2.755008	-0.335296	N	-2.710280	0.047497	-0.225337	N	-2.691004	0.085993	0.454766
H	3.204812	0.302351	-0.977474	H	0.081317	-3.354686	-0.638638	H	-3.053805	-0.388618	-1.093625	H	-3.256940	-0.335171	-0.295520
H	3.217729	-1.012972	-0.071616	H	-1.401179	-2.907455	-1.057358	H	-3.124517	0.993567	-0.242390	H	-3.044965	1.056463	0.517145
H	3.293973	0.428947	0.612138	H	-1.068795	-3.254038	0.476720	H	-3.223806	-0.460375	0.513542	H	-3.038070	-0.376008	1.305791

Table S3. Energies (hartrees) for the $\text{Th}(\text{12C4X})_2^q$ and $\text{Th}(\text{15C5X})_2^q$ species ($q = 4+, 3+, 2+, 1+, 0$ and $X = \text{N}, \text{O}$). Different spin states are reported (spin is given in parenthesis).

q	$\text{Th}(\text{12C4N})_2$	$\text{Th}(\text{15C5N})_2$	$\text{Th}(\text{12C4O})_2$	$\text{Th}(\text{15C5O})_2$
4 (S=0)	-1476.839126	-1744.736150	-1635.730076	-1943.393506
3 (S=1/2)	-1477.326154	-1745.193644	-1636.233438	-1943.850463
2 (S=0)	-1477.664916	-1745.485247	-1636.564960	-1944.145241
2 (S=1)	-1477.667265	-1745.476753	-1636.566613	-1944.140814
1 (S=1/2)	-1477.849360	-1745.657442	-1636.749266	-1944.296001
1 (S=3/2)	-1477.851669	-1745.651736	-1636.737169	-1944.287642
0 (S=0)	-1477.943915	-1745.740132	-1636.813739	-1944.371739
0 (S=1)	-1477.944112	-1745.750461	-1636.813744	-1944.366650
0 (S=2)	-1477.942209	-1745.745896	-1636.804662	-1944.362478

Table S4. Cartesian coordinates (Å) for the Th(12C4X)₂^q and Th(15C5X)₂^q species ($q = 4+, 3+, 2+, 1+, 0$ and X = N, O). Different spin states are reported (spin is given in parenthesis).

q	Th(12C4O) ₂	Th(15C5O) ₂	Th(12C4N) ₂	Th(15C5N) ₂
4 (S=0)	O -1.940506 0.672850 1.411955	O 0.410822 1.304549 -2.113994	N 1.644022 0.484427 -1.980167	N -0.275437 1.368031 -2.427902
	O -1.275173 -1.850496 0.898317	O -0.629678 -1.093440 -2.218302	N 1.422423 -2.160739 -0.600453	N -1.433812 -1.214048 -1.907143
	O -1.275366 1.850461 -0.898025	O -1.511226 2.048634 -0.509600	N 1.852453 1.841190 0.564622	N -1.614511 2.297354 0.010570
	O -1.940587 -0.672862 -1.411474	O -1.309323 -2.198805 0.094962	N 1.560788 -0.676384 1.958933	N -1.273570 -2.453219 0.718064
	C -2.744791 1.851418 1.059500	O -2.638051 -0.056674 0.602913	C 2.138285 1.901109 -1.930272	N -2.395008 0.008350 1.542016
	C -1.901315 -1.601124 2.204288	C -1.596873 -2.187628 -2.294350	C 2.224210 -1.932799 -1.856478	C -2.561024 -2.041584 -1.398397
	C -1.941227 2.703123 0.099431	C -1.496577 2.726784 -1.797926	C 2.750466 2.232347 -0.582446	C -2.188338 2.557311 -1.338216
	C -1.941116 -2.703198 -0.099042	C -1.393454 -3.051555 -1.079707	C 2.232847 -2.626946 0.582435	C -2.057827 -3.063483 -0.402174
	C -1.901649 1.601084 -2.203922	C 0.689070 0.537628 -3.320155	C 2.654239 1.564942 1.812686	C -0.711138 0.462372 -3.532446
	C -2.744772 -1.851502 -1.059036	C -0.432663 -0.445234 -3.511409	C 2.718146 -1.486078 1.456959	C -1.854854 -0.419645 -3.095380
	C -2.724111 0.332095 -2.142378	C -2.732447 2.283270 0.253948	C 1.978900 0.550144 2.716436	C -2.686707 2.386247 1.043798
	C -2.723909 -0.332211 2.142843	C -2.355325 -2.342584 1.088538	C 2.760517 -0.518662 -1.975330	C -2.080569 -2.373164 1.965947
	H -2.981322 2.418850 1.971254	C -3.541171 1.022997 0.250191	H 1.287538 2.560144 -2.156682	C -3.385838 1.060290 1.198077
	H -3.682687 1.488978 0.615806	C -3.382808 -1.283473 0.816905	H 2.882551 2.080560 -2.721009	C -3.095558 -1.267375 1.851694
	H -1.066593 -1.528160 2.916054	C -0.077898 2.671232 -2.283926	H 1.569546 -2.161057 -2.711267	C -1.088821 2.622920 -2.369195
	H -2.513681 -2.465788 2.495020	H 0.001203 2.967551 -3.337167	H 3.056525 -2.649816 -1.908908	H -1.511325 2.854897 -3.357364
	H -2.578225 3.438659 -0.410426	H -1.413815 -2.768172 -3.209255	H 3.701731 1.704032 -0.453345	H -3.060253 -2.562426 -2.229387
	H -1.130387 3.243003 0.604771	H -2.603830 -1.749202 -2.348290	H 2.994717 3.303019 -0.541416	H -3.303625 -1.362903 -0.961001
	H -2.578048 -3.438743 0.410884	H -1.809273 3.771902 -1.666209	H 3.089527 -3.227422 0.242976	H -2.745759 3.506054 -1.341346
	H -1.130309 -3.243060 -0.604455	H -2.201651 2.223844 -2.475822	H 1.596763 -3.305964 1.170285	H -2.914504 1.768012 -1.566555
	H -1.067001 1.528196 -2.915783	H -2.223122 -3.761638 -0.970244	H 2.838954 2.491572 2.373560	H -2.902900 -3.648019 -0.010406
	H -2.514121 2.465702 -2.494569	H -0.455387 -3.614774 -1.138178	H 3.640018 1.202986 1.500385	H -1.420869 -3.795489 -0.922957
	H -2.981313 -2.418917 -1.970798	H 1.651404 0.037841 -3.153336	H 3.299034 -1.886704 2.301150	H 0.147766 -0.163301 -3.823784
	H -3.682671 -1.489144 -0.615280	H 0.793495 1.208073 -4.182071	H 3.392699 -0.824012 0.902679	H -0.986749 1.039180 -4.426829
	H -3.671082 0.471431 -1.602247	H -1.376218 0.034665 -3.810413	H 2.660912 0.286089 3.539037	H -2.744102 0.163437 -2.827713
	H -2.943749 -0.038868 -3.153939	H -0.166169 -1.203938 -4.261051	H 1.078140 0.971074 3.188462	H -2.155455 -1.086414 -3.916829
	H -2.943531 0.038694 3.154429	H -3.293516 3.117432 -0.184957	H 3.356875 -0.426658 -2.895165	H -3.411214 3.172514 0.786081
	H -3.670892 -0.471610 1.602749	H -2.431941 2.560175 1.268776	H 3.435400 -0.283618 -1.144524	H -2.236956 2.698987 1.997905
	Th -0.000022 -0.000003 0.000037	H -1.871467 -2.204356 2.063815	Th -0.000322 -0.001221 -0.013429	H -1.399273 -2.178719 2.810217
	H 2.980871 2.419003 -1.971409	H -2.779997 -3.353854 1.057509	H 1.193514 0.385670 -2.897306	H -2.573287 -3.332680 2.181357
	H 2.943088 0.038875 -3.154595	H -4.352675 1.085991 0.989756	H 1.303960 2.683078 0.775886	H -4.166860 1.135650 1.969749
	C 2.744518 1.851547 -1.059624	H -3.980705 0.803153 -0.734847	H 1.087334 -1.274927 2.646001	H -3.893493 0.763889 0.269609
	H 1.130127 3.243065 -0.604635	H -3.976639 -1.498594 -0.084832	H 0.826045 -2.961588 -0.826985	H -3.821219 -1.472601 1.055969
	C 2.723643 -0.332062 -2.142982	H -4.069880 -1.159046 1.666690	H -1.281441 -2.954797 -1.572983	H -3.676615 -1.178630 2.781272
	O 1.940263 0.672921 -1.411959	H 0.570178 3.319766 -1.683993	H -1.300555 -2.455564 1.326708	H -0.410860 3.457197 -2.130805
	H 1.066346 -1.528163 -2.915997	Th -0.000094 0.008249 -0.000056	H -1.194491 -0.983382 -2.751396	Th 0.000076 0.013505 0.000053
	C 1.941055 2.703199 -0.099422	O -0.412394 1.305644 2.113055	C -2.134394 -2.266018 -1.487743	N 0.275017 1.361992 2.431042
	H 3.682508 1.489169 -0.616078	O 0.631791 -1.090581 2.218823	N -1.851249 -1.680202 0.939574	N 1.434313 -1.218340 1.904236
	C 1.901160 -1.601053 -2.204331	O 1.507502 2.051946 0.507395	N -1.644765 -0.889746 -1.833590	N 1.613545 2.297641 -0.004886
	H 3.670717 -0.471387 -1.603029	O 1.312381 -2.197225 -0.093937	H -1.084333 -0.279656 3.324647	N 1.274484 -2.450883 -0.723932
	H 2.578092 3.438739 0.410381	O 2.638103 -0.053457 -0.601393	H -2.982879 -3.349422 0.165906	N 2.394891 0.012948 -1.542018
	H 2.513564 -2.465668 -2.495127	C 1.600703 -2.183282 2.295376	C -2.745259 -2.309883 -0.099660	C 2.561895 -2.044087 1.393406
	O 1.275354 1.850466 0.898078	C 1.492353 2.730896 1.795258	H -2.878634 -2.609250 -2.222391	C 2.187566 2.554490 1.344408
	O 1.275186 -1.850452 -0.898288	C 1.397696 -3.048538 1.081640	C -1.982469 0.034301 2.771199	C 2.058978 -3.063721 0.394748

	C 1.901808 1.601086 2.203904 H 2.514212 2.465772 2.494490 C 1.941308 -2.703115 0.099001 H 2.578190 -3.438624 -0.411039 O 1.940890 -0.672928 1.411669 H 1.067260 1.528097 2.915873 H 3.671276 0.471630 1.601908 C 2.724455 0.332207 2.142280 H 3.682872 -1.488926 0.614949 H 1.130609 -3.243030 0.604531 C 2.745123 -1.851436 1.058896 H 2.944387 -0.038651 3.153816 H 2.981946 -2.418909 1.970548	C -0.689477 0.539200 3.319770 C 0.433602 -0.442059 3.511657 C 2.728626 2.287095 -0.256066 C 2.359299 -2.339788 -1.086671 C 3.539373 1.028129 -0.249644 C 3.385016 -1.279058 -0.814791 C 0.074049 2.673260 2.282034 H -0.004948 2.969977 3.335169 H 1.419099 -2.763190 3.210971 H 2.607016 -1.743280 2.348243 H 1.803199 3.776467 1.662729 H 2.198585 2.229598 2.473174 H 2.227774 -3.758228 0.972656 H 0.460058 -3.612375 1.141043 H -1.651198 0.038068 3.153497 H -0.794605 1.210109 4.181237 H 1.376455 0.039227 3.810622 H 0.167983 -1.200866 4.261498 H 3.288121 3.123073 0.181406 H 2.428191 2.561433 -1.271618 H 1.875899 -2.202639 -2.062309 H 2.785519 -3.350395 -1.054945 H 4.351289 1.091156 -0.988745 H 3.978538 0.810479 0.736040 H 3.978851 -1.493000 0.087216 H 4.072194 -1.153712 -1.664353 H -0.575509 3.320411 1.682219	C -2.657096 -1.146790 2.098378 N -1.560288 1.073408 1.773772 H -1.086115 1.801956 2.320345 H -2.846070 -1.934749 2.840523 H -0.823900 2.715450 -1.436901 N -1.422554 1.984161 -1.043178 H -1.581027 1.543380 -3.106697 C -2.763833 0.089311 -2.037214 C -2.230534 1.497882 -2.219378 H -3.699900 -1.772237 -0.084394 H -2.666492 0.466459 3.517437 H -3.361368 -0.195162 -2.916013 H -1.584735 3.475927 0.448732 C -2.226393 2.692796 0.017094 H -3.640839 -0.857007 1.712841 C -2.715364 1.762765 1.111606 H -3.436977 0.032545 -1.174294 H -3.391674 1.000771 0.708348 H -3.064843 2.187128 -2.415439 H -3.295203 2.333417 1.852364 H -3.080771 3.214251 -0.438803	C 0.710678 0.453756 3.533494 C 1.854847 -0.426745 3.094523 C 2.685315 2.389765 -1.038231 C 2.081451 -2.367580 -1.971622 C 3.385247 1.064623 -1.195881 C 3.095992 -1.261690 -1.854749 C 1.088142 2.617217 2.375657 H 1.510668 2.846622 3.364414 H 3.061446 -2.566747 2.223059 H 3.304119 -1.363984 0.957590 H 2.744688 3.503398 1.349763 H 2.913999 1.764849 1.570733 H 2.904190 -3.647083 0.001522 H 1.422248 -3.797160 0.913821 H -0.148083 -0.172945 3.823028 H 0.985823 1.028460 4.429369 H 2.743927 0.157347 2.828489 H 2.155512 -1.095441 3.914378 H 3.409340 3.175955 -0.778938 H 2.234925 2.704337 -1.991419 H 1.400046 -2.171425 -2.815410 H 2.574564 -3.326389 -2.189289 H 4.165966 1.142257 -1.967631 H 3.893360 0.766304 -0.268282 H 3.821780 -1.468506 -1.059550 H 3.676955 -1.170503 -2.784153 H 0.410014 3.452000 2.139539 H 0.749212 -1.887842 2.271091 H -0.651421 1.684876 2.707719 H 1.002545 3.097311 -0.184806 H 0.543252 -3.128382 -0.936695 H 0.650807 1.691849 -2.704153 H -1.004204 3.097067 0.192744 H -0.748419 -1.882293 -2.275756 H -0.542155 -3.131034 0.929066 H -2.004070 0.294126 2.443342 H 2.003659 0.300557 -2.442627
3 (S=1/2)	O 2.081076 -0.821358 1.291993 O 1.359358 1.772330 1.096698 O 1.355626 -1.772012 -1.097246 O 2.082796 0.819869 -1.292224 C 2.888666 -1.917593 0.798177 C 2.006026 1.351988 2.329832 C 2.056574 -2.683973 -0.207666 C 2.061706 2.683014 0.206861 C 2.002957 -1.352884 -2.330468 C 2.892318 1.914902 -0.798891 C 2.839372 -0.107575 -2.109403 C 2.839712 0.104866 2.108792 H 3.176700 -2.574826 1.631717 H 3.804349 -1.503485 0.351304 H 1.184838 1.172690 3.034250 H 2.625901 2.169061 2.724460	O -0.034789 -1.320132 -2.209898 O 0.766351 1.248340 -2.276122 O 1.546775 -2.191184 -0.238599 O 1.371232 2.212433 0.187604 O 2.625861 -0.015767 0.953786 C 1.803323 2.242612 -2.191464 C 1.832775 -2.685661 -1.561388 C 1.544098 3.072016 -0.960467 C -0.256407 -0.551134 -3.416033 C 0.799739 0.518034 -3.513700 C 2.634844 -2.365117 0.695026 C 2.340331 2.309874 1.247552 C 3.496725 -1.132582 0.715984 C 3.357976 1.213488 1.085987 C 0.544574 -2.641765 -2.336973 H 0.720129 -2.876979 -3.394424	N -1.733434 0.675174 1.934545 N -1.507295 -2.095166 0.825000 N -1.892039 1.825027 -0.763803 N -1.597869 -0.870873 -1.901017 C -2.186015 2.079368 1.723634 C -2.338585 -1.729036 2.014829 C -2.781747 2.296206 0.343175 C -2.274827 -2.663442 -0.327720 C -2.686208 1.383303 -1.952711 C -2.745951 -1.619824 -1.324794 C -2.008792 0.282347 -2.751413 C -2.853824 -0.301408 1.985466 H -1.315897 2.733616 1.880802 H -2.934037 2.369599 2.477903 H -1.713126 -1.875256 2.908440 H -3.188175 -2.421142 2.116125	N 0.303037 -1.402595 -2.437083 N 1.316881 1.330248 -2.049942 N 1.619710 -2.362990 0.024030 N 1.324137 2.466556 0.668181 N 2.425428 -0.047270 1.597728 C 2.460966 2.115507 -1.538345 C 2.229446 -2.538634 -1.313649 C 2.024983 3.106262 -0.480033 C 0.655701 -0.491385 -3.555100 C 1.757939 0.464968 -3.167511 C 2.654721 -2.445468 1.082374 C 2.179724 2.372772 1.874194 C 3.372987 -1.128031 1.255013 C 3.155316 1.228620 1.759241 C 1.160695 -2.618007 -2.379549 H 1.626544 -2.813800 -3.356687

	H	2.676629	-3.377178	-0.791713	H	1.777289	2.884288	-3.085185	H	-3.731815	1.756675	0.260646	H	2.964741	2.659074	-2.353924
	H	1.269513	-3.266193	0.289344	H	2.781471	1.735771	-2.150834	H	-3.032757	3.360066	0.226101	H	3.188770	1.400338	-1.133515
	H	2.683026	3.375276	0.790682	H	2.195587	-3.721950	-1.498188	H	-3.140569	-3.238480	0.034307	H	2.841655	-3.454188	-1.348246
	H	1.275426	3.266459	-0.289970	H	2.611271	-2.063574	-2.030638	H	-1.616783	-3.384493	-0.835848	H	2.904576	-1.694620	-1.498160
	H	1.181975	-1.171589	-3.034615	H	2.375522	3.768428	-0.790611	H	-2.902152	2.227453	-2.622857	H	2.898774	3.678593	-0.134084
	H	2.620890	-2.171280	-2.725376	H	0.618310	3.650525	-1.070861	H	-3.660172	1.033903	-1.592853	H	1.353921	3.852176	-0.934878
	H	3.181378	2.571353	-1.632693	H	-1.259180	-0.114773	-3.322922	H	-3.329462	-2.114307	-2.117000	H	-0.244080	0.081537	-3.829861
	H	3.807354	1.499376	-0.351981	H	-0.241072	-1.209030	-4.293907	H	-3.416545	-0.903415	-0.839563	H	0.944605	-1.060547	-4.451333
	H	3.780018	-0.332773	-1.585874	H	1.803717	0.084276	-3.653604	H	-2.693228	-0.041724	-3.550945	H	2.652395	-0.082292	-2.843491
	H	3.084229	0.358213	-3.075284	H	0.590708	1.195529	-4.355745	H	-1.104859	0.662332	-3.250811	H	2.059287	1.066926	-4.038518
	H	3.083853	-0.361215	3.074711	H	3.220454	-3.255104	0.429035	H	-3.486149	-0.127461	2.869927	H	3.386521	-3.237069	0.857809
	H	3.780665	0.328002	1.584946	H	2.176365	-2.529452	1.675627	H	-3.488691	-0.142823	1.107599	H	2.173691	-2.745368	2.025414
	Th	0.000000	0.001571	0.000010	H	1.778157	2.195075	2.183039	Th	0.000002	-0.000422	0.035186	H	1.527381	2.216133	2.747813
	H	-3.176688	-2.574818	-1.631737	H	2.816237	3.299220	1.247197	H	-1.304040	0.662615	2.864105	H	2.719898	3.314951	2.053567
	H	-3.083817	-0.361204	-3.074730	H	4.243929	-1.207457	1.520869	H	-1.362254	2.645027	-1.067063	H	4.156773	-1.234464	2.021788
	C	-2.888661	-1.917585	-0.798194	H	4.029914	-0.979214	-0.236667	H	-1.123268	-1.522676	-2.532321	H	3.884177	-0.842909	0.325432
	H	-1.269519	-3.266189	-0.289338	H	3.978310	1.362767	0.186904	H	-0.926364	-2.869659	1.149945	H	3.810359	1.364127	0.889462
	C	-2.839685	0.104875	-2.108808	H	4.022788	1.163961	1.961999	H	1.317239	-2.733110	1.881432	H	3.814920	1.203982	2.640389
	O	-2.081061	-0.821354	-1.292003	H	-0.179560	-3.358870	-1.929182	H	1.363874	-2.645409	-1.066203	H	0.512201	-3.484895	-2.177189
	H	-1.184795	1.172693	-3.034245	Th	0.000059	-0.005371	-0.000094	H	1.304221	-0.661957	2.864494	Th	0.000365	-0.013099	0.000560
	C	-2.056585	-2.683967	0.207661	O	0.025045	-1.311819	2.214581	C	2.187032	-2.078438	1.724318	N	-0.304435	-1.393456	2.441867
	H	-3.804348	-1.503472	-0.351332	O	-0.757759	1.262469	2.271318	N	1.893234	-1.825029	-0.763230	N	-1.316095	1.338797	2.044477
	C	-2.005991	1.351993	-2.329838	O	-1.561210	-2.181362	0.246285	N	1.733661	-0.674442	1.934956	N	-1.621383	-2.362268	-0.015232
	H	-3.780641	0.328015	-1.584971	O	-1.356886	2.220658	-0.195474	H	1.105765	-0.663612	-3.250909	N	-1.323176	2.465221	-0.677909
	H	-2.676650	-3.377169	0.791700	O	-2.625887	-0.002377	-0.952801	H	3.034850	-3.358985	0.227288	N	-2.425221	-0.051983	-1.597581
	H	-2.625858	2.169069	-2.724474	C	-1.787776	2.263635	2.183407	C	2.783094	-2.295259	0.343999	C	-2.460017	2.122497	1.530149
	O	-1.355646	-1.772006	1.097249	C	-1.851071	-2.667966	1.571136	H	2.935088	-2.368149	2.478755	C	-2.232404	-2.530886	1.322712
	O	-1.359338	1.772334	-1.096696	C	-1.523995	3.086303	0.948820	C	2.009268	-0.282890	-2.751287	C	-2.023903	3.109140	0.468007
	C	-2.002992	-1.352877	2.330463	C	0.253475	-0.539545	3.417409	C	2.687217	-1.383253	-1.952202	C	-0.655095	-0.477243	3.556404
	H	-2.620933	-2.171271	2.725363	C	-0.795095	0.537353	3.511841	N	1.597467	0.870340	-1.901298	C	-1.757011	0.478239	3.165795
	C	-2.061695	2.683021	-0.206868	C	-2.650800	-2.350824	-0.686388	H	1.122710	1.521663	-2.532982	C	-2.655444	-2.448550	-1.074138
	H	-2.683004	3.375285	-0.790697	C	-2.324875	2.320246	-1.256270	H	2.903642	-2.227482	-2.622093	C	-2.179023	2.366831	-1.883430
	O	-2.082811	0.819873	1.292214	C	-3.504242	-1.112496	-0.711227	H	0.924281	2.869144	1.148964	C	-3.373254	-1.131594	-1.252516
	H	-1.182018	-1.171584	3.034621	C	-3.349781	1.231188	-1.090529	N	1.506160	2.095222	0.824380	C	-3.154850	1.223373	-1.763978
	H	-3.780041	-0.332761	1.585849	C	-0.563286	-2.628897	2.347698	H	1.711887	1.876360	2.907942	C	-1.164432	-2.607501	2.389594
	C	-2.839400	-0.107565	2.109387	H	-0.741581	-2.857485	3.406152	C	2.853518	0.302750	1.985714	H	-1.631215	-2.797711	3.367380
	H	-3.807355	1.499390	0.351952	H	-1.756542	2.908690	3.074523	C	2.337522	1.730120	2.014457	H	-2.963377	2.669347	2.343785
	H	-1.275419	3.266463	0.289974	H	-2.769478	1.763484	2.145625	H	3.732806	-1.755104	0.261427	H	-3.188128	1.405978	1.128295
	C	-2.892323	1.914912	0.798873	H	-2.220532	-3.702172	1.512388	H	2.693705	0.041419	-3.550729	H	-2.846376	-3.445119	1.360974
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	H	-3.181389	2.571363	1.632673	H	-2.351469	3.786789	0.776408	H	1.614873	3.384245	-0.836771	H	-2.897529	3.680551	0.120102
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					H	0.234766	-1.193820	4.297915	C	2.745098	1.620074	-1.325152	H	-0.943524	-1.042359	4.455346
					H	-1.801939	0.111165	3.654410	H	3.488583	0.144186	1.107987	H	-2.652024	-0.069793	2.844600
					H	-0.580608	1.216731	4.350990	H	3.415947	0.904138	-0.839577	H	-2.057395	1.083861	4.034585
					H	-3.242470	-3.235875	-0.417307	H	3.186705	2.422754	2.115549	H	-3.387706	-3.239061	-0.847210
					H	-2.193979	-2.521482	-1.666682	H	3.328484	2.114576	-2.117437	H	-2.173545	-2.752279	-2.015490
					H	-1.763152	2.197770	-2.191039	H	3.138719	3.239401	0.033469	H	-1.526804	2.206687	-2.756517
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					H	-4.036277	-0.952371	0.240946					H	-3.885825	-0.843210	-0.324708
					H	-3.969537	1.388350	-0.192393					H	-3.809863	1.362310	-0.894725

		H -4.014540 1.182231 -1.966612 H 0.156418 -3.353050 1.944514		H -3.814463 1.195519 -2.645036 H -0.517572 -3.476634 2.191711 H -0.665174 2.013590 2.457029 H 0.626205 -1.741295 2.661576 H -1.026499 -3.182712 -0.147202 H -0.574948 3.104060 -0.938639 H -0.628036 -1.749743 -2.656054 H 1.024066 -3.182170 0.160357 H 0.666537 2.003744 -2.465534 H 0.575454 3.105813 0.926434 H 2.069782 -0.266839 2.531476 H -2.068397 -0.274316 -2.530210
2 (S=0)	O -2.236502 1.088546 1.092190 O -1.516254 -1.471937 1.467033 O -1.516256 1.471937 -1.467032 O -2.236501 -1.088547 -1.092190 C -3.019964 2.044474 0.363914 C -2.190286 -0.805228 2.548438 C -2.190120 2.551162 -0.796643 C -2.190117 -2.551163 0.796644 C -2.190288 0.805227 -2.548437 C -3.019962 -2.044475 -0.363913 C -3.020067 -0.357030 -2.045555 C -3.020066 0.357029 2.045555 H -3.303696 2.881470 1.020891 H -3.943524 1.553639 0.018615 H -1.388795 -0.453297 3.209581 H -2.816946 -1.517292 3.104559 H -2.816688 3.109807 -1.506809 H -1.388521 3.210971 -0.442454 H -2.816685 -3.109808 1.506809 H -1.388517 -3.210971 0.442454 H -1.388796 0.453297 -3.209581 H -2.816948 1.517291 -3.104558 H -3.303694 -2.881472 -1.020890 H -3.943523 -1.553642 -0.018614 H -3.943560 -0.013372 -1.553443 H -3.303921 -1.011175 -2.884725 H -3.303921 1.011174 2.884726 H -3.943560 0.013370 1.553444 Th -0.000000 0.000001 0.000000 H 3.303860 2.884152 -1.012931 H 3.303757 1.019136 -2.882052 C 3.020027 2.045372 -0.358275 H 1.388658 3.209776 0.451276 C 3.020002 0.362670 -2.044662 O 2.236502 1.091531 -1.089211 H 1.388657 -0.444476 -3.210782 C 2.190202 2.548931 0.803655 H 3.943533 1.553506 -0.014297 C 2.190204 -0.798217 -2.550673 H 3.943550 0.017690 -1.553580 H 2.816804 3.105572 1.515363	O -0.416021 -1.677803 -1.984082 O -1.049997 1.045751 -2.337098 O 2.092315 -1.562359 -0.830466 O 0.267585 2.596406 -0.395158 O 2.603382 1.129160 -0.112481 C -0.465392 2.302576 -2.695103 C 1.983678 -1.952618 -2.204469 C -0.430745 3.210685 -1.491979 C -1.379346 -1.233646 -2.954144 C -1.033861 0.146453 -3.450658 C 3.399553 -1.100049 -0.465094 C 1.475125 3.210676 0.075305 C 3.593104 0.357582 -0.797610 C 2.675618 2.503436 -0.494982 C 0.627114 -2.577117 -2.408005 H 0.492633 -2.840630 -3.466010 H -1.064117 2.776818 -3.490163 H 0.554812 2.111957 -3.069091 H 2.762566 -2.695245 -2.440439 H 2.106634 -1.066869 -2.847512 H 0.057392 4.155678 -1.767372 H -1.447881 3.431868 -1.143759 H -2.348416 -1.233122 -2.438373 H -1.426620 -1.942751 -3.791541 H -0.026357 0.155821 -3.900038 H -1.765685 0.476593 -4.205359 H 4.164282 -1.705728 -0.972946 H 3.487476 -1.260101 0.613856 H 1.452100 3.122643 1.169204 H 1.491142 4.276322 -0.190821 H 4.599652 0.677218 -0.481553 H 3.491738 0.536943 -1.880937 H 2.681237 2.568746 -1.596509 H 3.605306 2.952677 -0.109587 H 0.532424 -3.488561 -1.801726 Th 0.006353 -0.009379 -0.000399 O 1.534579 -0.857432 1.960794 O -0.046399 1.439318 2.366390 O -0.261003 -2.604298 0.794627 O -2.090588 1.554839 0.428713 O -2.591616 -1.156655 0.110754	N 1.972667 -1.355481 -1.431762 N 1.796262 -1.608676 1.489947 N 1.979275 1.504635 -1.283615 N 1.710852 1.330580 1.567023 C 2.351104 -0.566769 -2.622150 C 2.666278 -2.470662 0.652169 C 2.878215 0.804743 -2.234738 C 2.509891 -0.800996 2.508309 C 2.714229 2.447879 -0.406509 C 2.902973 0.573902 2.000053 C 2.035705 2.629803 0.941212 C 3.128035 -1.784658 -0.620392 H 1.450912 -0.464604 -3.244333 H 3.115493 -1.082614 -3.227825 H 2.082481 -3.363482 0.385872 H 3.543942 -2.817925 1.220850 H 3.857170 0.700201 -1.751607 H 3.055053 1.396609 -3.145446 H 3.406712 -1.325971 2.874598 H 1.835345 -0.685657 3.369519 H 2.849180 3.432253 -0.879679 H 3.724169 2.047670 -0.257640 H 3.457041 1.112669 2.786234 H 3.582313 0.479154 1.145800 H 2.687835 3.241985 1.586621 H 1.091377 3.179782 0.819798 H 3.786533 -2.464899 -1.185276 H 3.727195 -0.899901 -0.376468 Th -0.000071 -0.131352 -0.005895 H 1.512781 -2.205269 -1.762261 H 1.327744 2.056945 -1.840722 H 1.176277 1.531409 2.413870 H 1.189448 -2.243480 2.005741 H -1.458282 -0.823752 3.173809 H -1.333148 1.837345 2.056615 H -1.516245 -2.389690 1.507983 C -2.356989 -0.856587 2.542052 N -1.983922 1.350122 1.440923 N -1.974946 -1.508061 1.272587 H -1.094322 3.253151 -0.460036 H -3.062852 1.036825 3.277562	N 0.270074 1.406979 2.442874 N 1.166873 -1.426225 2.140666 N 1.628660 2.396390 0.005738 N 1.307058 -2.493880 -0.622527 N 2.461513 0.044849 -1.577111 C 2.298559 -2.245573 1.667945 C 2.210210 2.561777 1.352041 C 1.899133 -3.186008 0.549071 C 0.573255 0.488886 3.563298 C 1.637395 -0.522999 3.208185 C 2.676026 2.449319 -1.033171 C 2.228162 -2.389454 -1.771561 C 3.386714 1.123623 -1.190268 C 3.189083 -1.235271 -1.619229 C 1.123117 2.619929 2.403603 H 1.577400 2.813148 3.387982 H 2.734333 -2.838423 2.491851 H 3.066130 -1.544097 1.318725 H 2.812536 3.485617 1.412022 H 2.878463 1.713889 1.537416 H 2.776577 -3.781412 0.250494 H 1.169874 -3.918360 0.931886 H -0.354170 -0.043305 3.828690 H 0.876206 1.050508 4.461380 H 2.539863 -0.015594 2.844802 H 1.926198 -1.089517 4.109513 H 3.420017 3.231986 -0.809014 H 2.211129 2.745645 -1.985741 H 1.624145 -2.241910 -2.680855 H 2.790426 -3.325933 -1.918019 H 4.204313 1.236543 -1.923337 H 3.847845 0.831637 -0.237910 H 3.757463 -1.333855 -0.686017 H 3.925683 -1.253655 -2.439872 H 0.472944 3.485125 2.196006 Th 0.001360 0.005153 -0.000491 N -0.222435 1.373841 -2.465420 N -1.216524 -1.423928 -2.121988 N -1.546744 2.447837 -0.041223 N -1.393871 -2.442778 0.659341 N -2.457425 0.149074 1.578965

	H 2.816831 -1.508741 -3.108797 O 1.516257 1.467908 1.471061 O 1.516255 -1.467908 -1.471061 C 2.190206 0.798217 2.550672 H 2.816834 1.508740 3.108796 C 2.190200 -2.548932 -0.803655 H 2.816801 -3.105573 -1.515364 O 2.236501 -1.091531 1.089210 H 1.388659 0.444477 3.210782 H 3.943551 -0.017692 1.553580 C 3.020003 -0.362672 2.044661 H 3.943531 -1.553508 0.014296 H 1.388655 -3.209776 -0.451276 C 3.020026 -2.045374 0.358274 H 3.303757 -1.019138 2.882051 H 3.303857 -2.884153 1.012930	C -1.370731 1.838355 2.734573 C 0.111956 -2.813216 2.161640 C -2.064766 2.457625 1.548078 C 1.862171 0.135447 2.947221 C 0.613364 0.801169 3.464466 C -1.485011 -3.253343 0.425326 C -3.362673 1.085876 -0.039307 C -2.691100 -2.418920 0.774298 C -3.650355 -0.285695 0.511477 C 1.491754 -2.240869 2.362653 H 1.786284 -2.337978 3.416557 H -1.321957 2.576159 3.552322 H -1.913959 0.941993 3.079054 H 0.134945 -3.893357 2.377650 H -0.618009 -2.318119 2.821425 H -3.089457 2.733921 1.832265 H -1.537463 3.362734 1.219999 H 2.510808 0.861331 2.439784 H 2.424334 -0.322715 3.772066 H -0.069625 0.055464 3.905509 H 0.867958 1.550491 4.231170 H -1.550585 -4.233939 0.918952 H -1.431907 -3.410395 -0.656417 H -3.289914 1.060377 -1.134145 H -4.157021 1.790100 0.243256 H -3.606463 -2.940117 0.449233 H -2.755933 -2.242275 1.860717 H -3.697565 -0.263392 1.613600 H -4.612103 -0.660061 0.124704 H 2.220898 -2.778259 1.740796	C -2.884083 0.549151 2.307424 H -3.122595 -1.436638 3.084848 C -2.037365 2.718378 -0.643447 C -2.718010 2.385654 0.674022 N -1.708777 1.497872 -1.409629 H -1.172226 1.793118 -2.226982 H -2.854574 3.310443 1.254747 H -1.182343 -2.006620 -2.239923 N -1.790320 -1.432611 -1.658411 H -2.078007 -3.300045 -0.758918 C -3.127816 -1.844799 0.415402 C -2.662060 -2.383409 -0.924750 H -3.862003 0.498277 1.813725 H -2.689760 3.397602 -1.217623 H -3.786463 -2.585085 0.898761 H -1.824930 -0.306769 -3.424222 C -2.501871 -0.517679 -2.583237 H -3.727460 2.004379 0.479075 C -2.898385 0.791843 -1.926703 H -3.728345 -0.939422 0.270495 H -3.579041 0.601693 -1.089561 H -3.537908 -2.665134 -1.531224 H -3.452056 1.413437 -2.649481 H -3.396753 -0.999707 -3.008497	C -2.377146 -2.192592 -1.634568 C -2.123676 2.606228 -1.390265 C -2.011144 -3.130058 -0.501820 C -0.556203 0.449586 -3.571808 C -1.654848 -0.519466 -3.202118 C -2.591397 2.551300 0.996495 C -2.308292 -2.289540 1.808273 C -3.345457 1.252384 1.174521 C -3.228462 -1.104576 1.641214 C -1.036375 2.613645 -2.443169 H -1.485621 2.806291 -3.429988 H -2.836802 -2.781439 -2.448298 H -3.117130 -1.457466 -1.295111 H -2.698309 3.546359 -1.466422 H -2.817147 1.775606 -1.560705 H -2.908838 -3.689796 -0.194546 H -1.307915 -3.892678 -0.873744 H 0.352559 -0.117858 -3.828540 H -0.839876 1.007529 -4.478461 H -2.538615 0.024742 -2.846042 H -1.964286 -1.087852 -4.095375 H -3.309588 3.354066 0.759622 H -2.116909 2.847749 1.944256 H -1.697534 -2.150544 2.714420 H -2.902934 -3.203393 1.969115 H -4.158788 1.404333 1.905286 H -3.816375 0.960661 0.226885 H -3.801936 -1.196908 0.710493 H -3.963637 -1.085526 2.463121 H -0.358898 3.460909 -2.249363 H -0.588443 -2.103124 -2.569011 H 0.729612 1.681822 -2.649621 H -0.941034 3.261251 0.096115 H -0.652123 -3.056526 0.989601 H -0.671766 1.747573 2.622674 H 1.048759 3.225834 -0.146473 H 0.513502 -2.074804 2.597037 H 0.545784 -3.086961 -0.946070 H 2.189764 0.232621 -2.547955 H -2.177409 0.343785 2.546072
2 (S=1)	O -2.256205 1.090762 -1.089243 O -1.528285 1.463426 1.465514 O -1.528288 -1.463425 -1.465515 O -2.256196 -1.090764 1.089246 C -3.036950 0.361378 -2.044649 C -2.201020 2.546434 0.799823 C -2.201104 -0.796273 -2.547580 C -2.201093 0.796272 2.547582 C -2.201017 -2.546434 -0.799821 C -3.036939 -0.361381 2.044655 C -3.036922 -2.045132 0.358488 C -3.036930 2.045129 -0.358481 H -3.320702 1.016867 -2.882980	O -1.550165 0.076371 2.138520 O 1.036077 -0.978682 2.417180 O -1.086881 2.410266 0.735226 O 2.631232 -0.157288 0.258697 O 1.586450 2.366983 -0.167093 C 2.401297 -0.618351 2.635014 C -1.387792 2.494807 2.131794 C 3.189961 -0.869068 1.374089 C -1.212928 -0.854544 3.179828 C 0.235919 -0.712255 3.570400 C -0.439475 3.575197 0.209643 C 3.418406 0.869601 -0.357967 C 1.050068 3.543680 0.439921	N 1.832825 0.088842 2.032797 N 1.643322 2.230170 0.007179 N 2.114337 -1.910876 -0.005547 N 1.833851 0.101432 -2.031657 C 2.285510 -1.269961 2.400160 C 2.429348 2.354952 1.260068 C 2.938714 -1.979157 1.225438 C 2.429738 2.362810 -1.244663 C 2.939468 -1.971433 -1.236445 C 2.946344 1.035192 -1.767837 C 2.286888 -1.255040 -2.407146 C 2.945566 1.024049 1.775214 H 1.399735 -1.828229 2.734463	N -0.896612 -0.952336 2.645689 N -1.780159 1.671302 1.447369 N -1.547172 -2.424179 0.142267 N -1.383251 2.236505 -1.414887 N -2.178812 -0.531385 -1.963197 C -2.781874 2.391008 0.639657 C -2.476174 -2.358786 1.286202 C -2.143262 3.131945 -0.516265 C -1.502885 0.162655 3.393146 C -2.461008 0.984113 2.559070 C -2.236679 -2.830642 -1.098393 C -2.133718 1.835213 -2.624102 C -3.035588 -1.692240 -1.690486

	H	-3.960708	0.013696	-1.555609	C	2.977096	2.226121	0.124221	H	2.999921	-1.248295	3.240911	C	-2.995404	0.615276	-2.392397
	H	-1.398610	3.204364	0.443011	C	-2.223364	1.295830	2.501759	H	1.767715	2.800575	2.017574	C	-1.727905	-2.173108	2.593086
	H	-2.820671	3.105397	1.515483	H	-2.434103	1.305637	3.579992	H	3.275584	3.048603	1.128428	H	-2.450986	-2.198471	3.425155
	H	-2.820826	-1.511169	-3.107440	H	2.822825	-1.224877	3.453930	H	3.906102	-1.511753	1.004661	H	-3.354225	3.104715	1.257327
	H	-1.398740	-0.438618	-3.205105	H	2.441533	0.447430	2.918578	H	3.166603	-3.017204	1.511895	H	-3.494180	1.643515	0.268271
	H	-2.820814	1.511167	3.107445	H	-1.962563	3.413261	2.332931	H	3.275822	3.055765	-1.108465	H	-3.080112	-3.281206	1.358399
	H	-1.398726	0.438620	3.205103	H	-0.451486	2.513165	2.712298	H	1.768277	2.812989	-1.999622	H	-3.165018	-1.524592	1.115566
	H	-1.398604	-3.204362	-0.443013	H	4.234357	-0.565822	1.530754	H	3.167671	-3.007661	-1.529171	H	-2.920145	3.684692	-1.067885
	H	-2.820669	-3.105399	-1.515477	H	3.171885	-1.936672	1.117367	H	3.906659	-1.505283	-1.012187	H	-1.463747	3.902360	-0.117538
	H	-3.320686	-1.016870	2.882988	H	-1.408679	-1.853625	2.768324	H	3.549779	1.210071	-2.674044	H	-0.689893	0.814540	3.752578
	H	-3.960699	-0.013701	1.555618	H	-1.864556	-0.700802	4.050701	H	3.614782	0.576164	-1.030773	H	-2.029244	-0.197079	4.293545
	H	-3.960655	-1.555596	0.011438	H	0.445195	0.311646	3.925386	H	3.001781	-1.228112	-3.247334	H	-3.239661	0.342350	2.127178
	H	-3.320719	-2.884381	1.012781	H	0.486365	-1.423986	4.373991	H	1.401369	-1.811330	-2.745398	H	-2.976274	1.708682	3.212884
	H	-3.320731	2.884378	-1.012774	H	-0.872133	4.480363	0.660814	H	3.548651	1.193239	2.682732	H	-2.902355	-3.692153	-0.923445
	H	-3.960661	1.555592	-0.011428	H	-0.655172	3.583163	-0.863531	H	3.614245	0.569498	1.035598	H	-1.475244	-3.165180	-1.819021
	Th	0.000000	0.000004	-0.000006	H	3.254831	0.769472	-1.439122	Th	0.000023	0.000145	-0.000184	H	-1.389352	1.604159	-3.399021
	H	3.320825	-1.010096	-2.885257	H	4.485778	0.713087	-0.149900	H	1.319875	0.458125	2.835225	H	-2.759504	2.664042	-2.993766
	H	3.320596	-2.882096	-1.019547	H	1.511184	4.440495	-0.005911	H	1.509034	-2.731458	-0.008275	H	-3.554326	-2.041146	-2.599152
	C	3.036992	-0.356582	-2.045412	H	1.290357	3.529495	1.516233	H	1.321201	0.475580	-2.832019	H	-3.819441	-1.373730	-0.989490
	H	1.398815	0.446090	-3.204068	H	3.128258	2.323499	1.213051	H	0.997341	3.017321	0.009567	H	-3.745987	0.802876	-1.612665
	C	3.036880	-2.044363	-0.363279	H	3.551985	3.018784	-0.382155	H	-1.401828	1.811435	2.745800	H	-3.554158	0.386102	-3.315835
	O	2.256202	-1.088227	-1.091774	H	-3.176923	1.314439	1.955845	H	-1.509083	2.730689	0.008060	H	-1.067391	-3.042060	2.747465
	H	1.398526	-3.205391	0.435538	Th	-0.032182	-0.023406	-0.027633	H	-1.322361	-0.475548	2.833405	Th	-0.082527	0.034953	-0.165245
	C	2.201152	0.802222	-2.545685	O	-0.744083	1.474027	-2.061901	C	-2.287185	1.255042	2.407277	N	1.138924	-1.880968	-1.951975
	H	3.960705	-0.010015	-1.555496	O	1.241827	-0.481326	-2.436697	N	-2.114702	1.910369	0.005452	N	2.286209	0.791190	-1.653139
	C	2.200965	-2.548325	0.793872	O	-2.674174	0.148203	-0.615002	N	-1.834006	-0.101539	2.032326	N	1.557627	-2.229262	0.971364
	H	3.960657	-1.555706	-0.015113	O	1.127361	-2.371051	-0.356580	H	-1.399997	1.828231	-2.734691	N	1.188116	2.716075	0.208092
	H	2.820887	1.518424	-3.103858	O	-1.586457	-2.344545	0.202040	H	-3.167858	3.007537	1.528876	N	1.986406	0.508465	1.938746
	H	2.820602	-3.108977	1.508220	C	1.430552	-1.874755	-2.716530	C	-2.939711	1.971226	1.236378	C	3.082961	1.948058	-1.265008
	O	1.528295	1.466848	-1.462091	C	-2.949789	0.459414	-1.986640	H	-3.002354	1.228235	3.247240	C	2.351705	-2.933672	-0.051952
	O	1.528274	-1.466850	1.462092	C	1.977601	-2.574888	-1.497258	C	-2.285504	1.269677	-2.400142	C	2.183925	3.091977	-0.822766
	C	2.200987	2.548319	-0.793866	C	0.217770	1.561444	-3.127079	C	-2.939025	1.978743	-1.225502	C	2.171199	-1.325685	-2.862568
	H	2.820633	3.108967	-1.508210	C	0.653084	0.184843	-3.560454	N	-1.832331	-0.088959	-2.032733	C	3.080326	-0.295782	-2.216721
	C	2.201129	-0.802228	2.545691	C	-3.485992	-0.906032	-0.079729	H	-1.319835	-0.458103	-2.835519	C	2.383757	-1.912923	2.152438
	H	2.820855	-1.518434	3.103869	C	0.493250	-3.505666	0.250889	H	-3.167068	3.016789	-1.511870	C	1.660643	2.928587	1.588349
	O	2.256201	1.088220	1.091781	C	-2.901252	-2.266368	-0.363278	H	-0.996344	-3.016544	-0.008838	C	3.011111	-0.540555	2.050476
	H	1.398549	3.205390	-0.435537	C	-0.952759	-3.574262	-0.164688	N	-1.643194	-2.230092	-0.006648	C	2.602282	1.840210	2.054887
	H	3.960668	1.555689	0.015132	C	-2.138500	1.674744	-2.363842	H	-1.768836	-2.813071	2.000196	C	1.551769	-3.149203	-1.319444
	C	3.036891	2.044352	0.363291	H	-2.266567	1.888227	-3.433907	C	-2.946548	-1.035071	1.767826	H	2.140086	-3.769198	-2.015391
	H	3.960694	0.009996	1.555514	H	2.141919	-1.989822	-3.550873	C	-2.429961	-2.362822	1.244976	H	3.715579	2.309177	-2.095283
	H	1.398789	-0.446091	3.204069	H	0.454500	-2.300894	-3.003369	H	-3.906949	1.505078	1.012317	H	3.774528	1.643945	-0.467731
	C	3.036980	0.356570	2.045424	H	-4.020522	0.692941	-2.104071	H	-3.000040	1.247671	-3.240783	H	2.708680	-3.907449	0.323023
	H	3.320607	2.882083	1.019562	H	-2.684350	-0.402135	-2.619217	H	-3.550499	-1.209877	2.673703	H	3.245959	-2.336003	-0.263997
	H	3.320812	1.010081	2.885271	H	2.070818	-3.648600	-1.711315	H	-1.766972	-2.800634	-2.017135	H	2.803782	3.939004	-0.484717
					H	2.969546	-2.183360	-1.236220	C	-2.428825	-2.355106	-1.259759	H	1.627280	3.447825	-1.703411
					H	1.065918	2.131480	-2.724410	H	-3.906344	1.511115	-1.004889	H	1.639659	-0.837970	-3.691602
					H	-0.204922	2.115208	-3.976176	C	-2.945011	-1.024186	-1.774880	H	2.781395	-2.134237	-3.296609
					H	-0.213533	-0.404059	-3.905266	H	-3.614537	-0.575932	1.030393	H	3.696781	-0.735409	-1.418428
					H	1.390304	0.257192	-4.376576	H	-3.613692	-0.569616	-1.035240	H	3.784954	0.068459	-2.985282
					H	-4.502466	-0.842436	-0.494911	H	-3.276057	-3.055670	1.108410	H	3.173921	-2.666472	2.302116
					H	-3.539447	-0.729124	0.999462	H	-3.548163	-1.193495	-2.682331	H	1.754621	-1.962296	3.053795
					H	0.583949	-3.359662	1.335648	H	-3.274990	-3.048846	-1.128242	H	0.779199	2.953079	2.247999
					H	1.016970	-4.431849	-0.023050					H	2.158148	3.907128	1.696520

		H -3.542203 -3.043849 0.083503 H -2.825750 -2.448841 -1.447639 H -1.036977 -3.703675 -1.257069 H -1.456241 -4.417967 0.334567 H -2.471899 2.548996 -1.787441		H 3.665285 -0.380339 2.924838 H 3.652441 -0.477290 1.159211 H 3.517271 1.845889 1.452643 H 2.920223 2.051015 3.089498 H 0.646570 -3.729728 -1.085147 H 1.590166 1.070876 -2.359929 H 0.343084 -2.097643 -2.550415 H 0.845046 -2.886971 1.285238 H 0.408992 3.359151 0.089623 H -0.056194 -1.208159 3.157096 H -0.898563 -3.184338 0.353215 H -1.190897 2.389331 1.879972 H -0.575370 2.749139 -1.765126 H -1.564331 -0.751535 -2.754830 H 1.360336 0.406324 2.739065
1 (S=1/2)	O -2.433437 1.079302 -1.066243 O -1.673498 1.442515 1.460364 O -1.673501 -1.442505 -1.460372 O -2.433372 -1.079340 1.066282 C -3.197863 0.367681 -2.030815 C -2.344930 2.522985 0.808434 C -2.345249 -0.777682 -2.532725 C -2.345207 0.777679 2.532732 C -2.344896 -2.522989 -0.808428 C -3.197804 -0.367706 2.030843 C -3.197693 -2.035194 0.342868 C -3.197749 2.035170 -0.342838 H -3.470578 1.032263 -2.869140 H -4.131626 0.011707 -1.562214 H -1.536583 3.164040 0.430868 H -2.949417 3.087969 1.534401 H -2.950027 -1.496799 -3.106097 H -1.537105 -0.392572 -3.169540 H -2.949995 1.496782 3.106111 H -1.537042 0.392594 3.169534 H -1.536528 -3.164033 -0.430890 H -2.949396 -3.087979 -1.534381 H -3.470512 -1.032274 2.869181 H -4.131570 -0.011750 1.562236 H -4.131443 -1.562323 -0.007438 H -3.470406 -2.881594 0.997134 H -3.470468 2.881557 -0.997118 H -4.131495 1.562306 0.007488 Th -0.000000 0.000018 -0.000020 H 3.470418 -0.996520 -2.881786 H 3.470575 -2.868932 -1.032866 C 3.197716 -0.342427 -2.035248 H 1.536540 0.431566 -3.163913 C 3.197844 -2.030750 -0.368111 O 2.433407 -1.066040 -1.079534 H 1.537092 -3.169652 0.391890 C 2.344917 0.808970 -2.522801 H 4.131472 0.007777 -1.562313	O 1.584463 0.914115 1.879626 O -1.193617 0.990376 2.248120 O 1.973274 -1.643649 0.918300 O -2.481234 -0.757354 0.486567 O -0.550015 -2.732871 0.341814 C -2.299706 0.205671 2.715105 C 2.325434 -1.357390 2.281857 C -3.206111 -0.130758 1.562328 C 0.961436 1.844293 2.784551 C -0.311340 1.268472 3.341445 C 1.792197 -3.044631 0.677666 C -2.829415 -2.105072 0.142240 C 0.413997 -3.505923 1.066173 C -1.868761 -3.071988 0.775858 C 2.665880 0.103120 2.384747 H 2.860998 0.352522 3.437808 H -2.868605 0.781956 3.466796 H -1.898120 -0.712495 3.186143 H 3.205469 -1.957798 2.568069 H 1.478079 -1.609037 2.947799 H -3.996005 -0.806165 1.922987 H -3.675487 0.771451 1.147849 H 0.765994 2.749159 2.194857 H 1.655143 2.092314 3.599869 H -0.112274 0.326789 3.887607 H -0.790460 1.988637 4.027848 H 2.547943 -3.616086 1.238650 H 1.963546 -3.195293 -0.392910 H -2.781322 -2.157159 -0.953181 H -3.857880 -2.324012 0.462706 H 0.295055 -4.574675 0.812544 H 0.229503 -3.370517 2.147988 H -1.907843 -3.005066 1.879413 H -2.106352 -4.105889 0.470126 H 3.555861 0.344593 1.786471 Th 0.010930 0.011882 -0.015200 O 1.120061 -1.477167 -1.860152 O -1.482188 -0.463983 -2.284675	N -2.097418 -1.442856 1.300071 N -1.846722 -1.469222 -1.581328 N -2.011356 1.431843 1.308278 N -1.710208 1.404309 -1.439048 C -2.632052 -0.681405 2.440726 C -2.557767 -2.533147 -0.854747 C -3.081564 0.704562 2.019756 C -2.695530 -0.604441 -2.424053 C -2.515453 2.602680 0.562819 C -2.975198 0.744988 -1.785345 C -1.869270 2.722519 -0.817533 C -3.147748 -2.015907 0.443514 H -1.818968 -0.590702 3.174598 H -3.476250 -1.207918 2.920619 H -1.824749 -3.322505 -0.632634 H -3.354630 -2.982627 -1.471319 H -3.945464 0.637471 1.343986 H -3.427905 1.256038 2.910344 H -3.646689 -1.104361 -2.669417 H -2.157067 -0.436580 -3.369027 H -2.366207 3.540124 1.119445 H -3.601746 2.494788 0.446977 H -3.577543 1.362427 -2.474946 H -3.564786 0.619689 -0.868371 H -2.472634 3.406489 -1.439488 H -0.866789 3.166819 -0.733991 H -3.694145 -2.824403 0.957621 H -3.885361 -1.231021 0.228768 Th -0.000024 -0.155558 -0.000149 H -1.540938 -2.212911 1.678149 H -1.340665 1.731727 2.022543 H -1.155579 1.489619 -2.300523 H -1.153408 -1.900259 -2.198066 H 1.819486 -0.587794 -3.174943 H 1.341070 1.734185 -2.021582 H 1.540832 -2.210768 -1.679609 C 2.632507 -0.678979 -2.441056 N 2.011330 1.433489 -1.307313	N 0.089258 2.569826 -1.185248 N 1.160932 2.027050 1.480944 N 1.567017 0.330847 -2.294275 N 1.420377 -0.736716 2.353773 N 2.514764 -1.465886 -0.215844 C 2.405781 1.555538 2.117884 C 2.123350 1.695183 -2.347628 C 2.123091 0.378434 3.019884 C 0.268560 3.615735 -0.161191 C 1.419649 3.284411 0.757714 C 2.634221 -0.653708 -2.527360 C 2.291399 -1.907646 2.174357 C 3.408334 -0.953922 -1.266872 C 3.256149 -1.692855 1.035456 C 1.006233 2.710641 -2.340190 H 1.419814 3.730171 -2.389907 H 2.857613 2.361061 2.726497 H 3.115927 1.306897 1.316967 H 2.703033 1.831447 -3.279197 H 2.814238 1.840554 -1.507085 H 3.057096 0.033746 3.490803 H 1.473274 0.726382 3.848226 H -0.656755 3.692438 0.431906 H 0.426707 4.602347 -0.625517 H 2.342351 3.161087 0.175500 H 1.596736 4.114522 1.460784 H 3.323343 -0.308252 -3.315815 H 2.179264 -1.572940 -2.931491 H 1.655651 -2.788022 1.976177 H 2.843019 -2.136261 3.100089 H 4.219243 -1.669960 -1.489599 H 3.887410 -0.043260 -0.881978 H 3.879948 -0.810214 1.227521 H 3.943662 -2.550897 0.946461 H 0.414295 2.555935 -3.258434 Th -0.000266 0.000329 -0.006598 N -0.106680 -2.393900 -1.508310 N -1.142375 -2.209065 1.218986

	C	2.345225	-2.532907	0.777139	O	2.504528	0.700281	-0.876441	N	2.097911	-1.441355	-1.301082	N	-1.588085	-0.029394	-2.298701
	H	4.131598	-1.562214	-0.012030	O	-1.958263	1.685340	-0.529151	H	0.866358	3.165729	0.736852	N	-1.397900	0.422014	2.437818
	H	2.949416	1.535044	-3.087637	O	0.612276	2.747485	-0.312509	H	3.428630	1.258836	-2.908866	N	-2.517151	1.487553	-0.002752
	H	2.949999	-3.106431	1.496137	C	-2.162560	0.707329	-2.746826	C	3.081818	0.706684	-2.018883	C	-2.381412	-1.826454	1.922963
	O	1.673525	1.460691	-1.442177	C	2.769177	0.268040	-2.214900	H	3.476818	-1.204973	-2.921326	C	-2.158468	-1.373106	-2.508232
	O	1.673470	-1.460698	1.442184	C	-2.868800	1.382420	-1.597202	C	1.868973	2.721646	0.820002	C	-2.091196	-0.771543	2.963570
	C	2.345282	2.532892	-0.777123	C	0.192631	-2.091788	-2.767886	C	2.515257	2.603525	-0.560449	C	-0.262239	-3.564721	-0.625421
	H	2.950077	3.106404	-1.496113	C	-0.741198	-1.062350	-3.351429	N	1.710162	1.402716	1.439980	C	-1.403107	-3.364769	0.343068
	C	2.344856	-0.808986	2.522817	C	2.884287	2.057669	-0.623968	H	1.155044	1.486836	2.301318	C	-2.648852	0.984351	-2.400483
	H	2.949335	-1.535067	3.087666	C	-1.742863	3.053681	-0.168469	H	2.365900	3.541597	-1.115981	C	-2.272670	1.603933	2.421877
	O	2.433404	1.066027	1.079552	C	1.810947	3.034034	-1.035443	H	1.153110	-1.902283	2.196207	C	-3.417217	1.124546	-1.108558
	H	1.537151	3.169651	-0.391892	C	-0.462835	3.561261	-0.779406	N	1.846590	-1.470746	1.579994	C	-3.248113	1.539297	1.273672
	H	4.131625	1.562173	0.012082	C	2.461305	-1.205966	-2.303797	H	1.824816	-3.323146	0.629580	C	-1.050729	-2.388826	-2.650093
	C	3.197871	2.030724	0.368145	H	2.591322	-1.546735	-3.340699	C	3.148019	-2.015510	-0.445099	H	-1.474501	-3.392296	-2.812264
	H	4.131439	-0.007827	1.562354	H	-2.905962	0.423444	-3.511663	C	2.557776	-2.533987	0.852578	H	-2.824971	-2.703755	2.429986
	H	1.536476	-0.431564	3.163913	H	-1.403456	1.382035	-3.182410	H	3.945381	0.639013	-1.342743	H	-3.100703	-1.481917	1.166969
	C	3.197683	0.342396	2.035276	H	3.835179	0.427321	-2.449236	H	2.472074	3.405077	1.442799	H	-2.758191	-1.389313	-3.437010
	H	3.470601	2.868902	1.032905	H	2.132677	0.838906	-2.912143	H	3.694284	-2.823619	-0.959965	H	-2.833010	-1.616246	-1.676957
	H	3.470387	0.996481	2.881820	H	-3.340875	2.305818	-1.962310	H	2.156555	-0.439542	3.368567	H	-3.020655	-0.492573	3.484208
					H	-3.646498	0.730728	-1.178308	C	2.695259	-0.606680	2.423602	H	-1.432258	-1.219318	3.734934
					H	-0.359287	-2.832883	-2.174342	H	3.601564	2.495656	-0.444686	H	0.672063	-3.707896	-0.059431
					H	0.737875	-2.611049	-3.568026	C	2.975124	0.743302	1.786110	H	-0.419268	-4.484869	-1.210760
					H	-0.169079	-0.270448	-3.866729	H	3.885801	-1.231024	-0.229436	H	-2.334194	-3.174758	-0.207040
					H	-1.437338	-1.538057	-4.062425	H	3.565088	0.618874	0.869250	H	-1.565681	-4.280093	0.935026
					H	3.819705	2.285854	-1.156808	H	3.354533	-2.984011	1.468887	H	-3.342978	0.746158	-3.223498
					H	3.068168	2.124093	0.452799	H	3.577120	1.360202	2.476495	H	-2.189254	1.944451	-2.686515
					H	-1.690704	3.069388	0.928219	H	3.646310	-1.106885	2.668788	H	-1.639484	2.504175	2.335843
					H	-2.592604	3.671388	-0.491783					H	-2.815095	1.707308	3.375040
					H	2.142774	4.061547	-0.807059					H	-4.223671	1.868773	-1.232924
					H	1.591923	2.952525	-2.114209					H	-3.901780	0.174483	-0.845017
					H	-0.504189	3.490081	-1.880928					H	-3.866296	0.635350	1.350116
					H	-0.289121	4.610955	-0.488837					H	-3.939786	2.398028	1.307827
					H	3.136059	-1.778835	-1.652418					H	-0.478124	-2.127855	-3.556532
													H	-0.505040	-2.539381	1.961041
													H	0.817762	-2.475981	-1.934452
													H	-0.977619	0.131777	-3.145106
													H	-0.677377	0.641229	3.161117
													H	-0.844095	2.706735	-1.574791
													H	0.948585	0.265325	-3.148075
													H	0.531860	2.262061	2.265768
													H	0.707404	-1.044940	3.050903
													H	2.211855	-2.392533	-0.525329
													H	-2.215123	2.448071	-0.182438
1 (S=3/2)	O	-2.389433	1.548474	-0.017064	O	0.445342	-1.385384	2.116475	N	2.129874	-1.389791	-1.328842	N	0.303049	2.547772	-1.214808
	O	-1.660942	0.022687	2.082564	O	-0.101761	1.356800	2.351838	N	1.896602	-1.497264	1.533626	N	1.384610	1.950888	1.411748
	O	-1.660943	-0.022687	-2.082563	O	-1.561005	-2.219713	0.426378	N	1.924926	1.484858	-1.287896	N	1.620729	0.206736	-2.286902
	O	-2.389434	-1.548474	0.017064	O	-1.515269	2.191696	0.093192	N	1.657880	1.372710	1.474103	N	1.437639	-0.783455	2.337488
	C	-3.166081	1.682070	-1.204286	O	-3.218924	-0.065652	-0.671082	C	2.621378	-0.587883	-2.458336	N	2.414454	-1.650008	-0.227721
	C	-2.332993	1.253318	2.347261	C	-1.174497	2.295380	2.496849	C	2.636403	-2.524574	0.785290	C	2.627292	1.385821	1.969616
	C	-2.333062	1.201740	-2.374458	C	-1.634836	-2.585968	1.806738	C	3.021218	0.805351	-2.012871	C	2.303445	1.510720	-2.285248
	C	-2.333061	-1.201740	2.374459	C	-1.322710	3.069797	1.212200	C	2.714546	-0.629118	2.399128	C	2.293520	0.267946	2.926705
	C	-2.332995	-1.253318	-2.347261	C	0.938347	-0.614241	3.224897	C	2.397811	2.648944	-0.508166	C	0.510967	3.589085	-0.191388
	C	-3.166081	-1.682069	1.204287	C	0.015111	0.541122	3.522085	C	2.947110	0.745298	1.794903	C	1.659180	3.221161	0.718891

	C	-3.166215	-1.707616	-1.166909	C	-2.810942	-2.366801	-0.264265	C	1.768469	2.709991	0.884476	C	2.581723	-0.873220	-2.543789
	C	-3.166213	1.707616	1.166910	C	-2.769303	2.266197	-0.607658	C	3.204617	-1.962226	-0.504202	C	2.166761	-2.048343	2.171827
	H	-3.454027	2.736326	-1.356640	C	-3.766584	-1.214299	-0.046859	H	1.797081	-0.516479	-3.182701	C	3.343316	-1.249811	-1.296202
	H	-4.090801	1.091001	-1.093891	C	-3.729318	1.170114	-0.205135	H	3.480150	-1.070068	-2.958322	C	3.135247	-1.960743	1.017364
	H	-1.524363	1.973068	2.537917	C	-0.234867	-2.628122	2.366351	H	1.923171	-3.327394	0.547753	C	1.284141	2.623515	-2.324286
	H	-2.959414	1.162169	3.248815	H	-0.278698	-2.823112	3.447329	H	3.446886	-2.964828	1.390585	H	1.786975	3.602800	-2.332568
	H	-2.959698	1.090511	-3.273613	H	-0.945220	2.990417	3.323153	H	3.884425	0.754827	-1.335214	H	3.197258	2.159092	2.515150
	H	-1.524463	1.917035	-2.581316	H	-2.095924	1.729100	2.724663	H	3.349872	1.386895	-2.890784	H	3.251803	1.048332	1.128035
	H	-2.959696	-1.090510	3.273614	H	-2.091025	-3.586689	1.900815	H	3.682883	-1.101164	2.631600	H	2.955688	1.604969	-3.171389
	H	-1.524463	-1.917035	2.581316	H	-2.241781	-1.839312	2.350807	H	2.172081	-0.504464	3.348974	H	2.948298	1.583327	-1.397321
	H	-1.524366	-1.973068	-2.537917	H	-2.172611	3.761263	1.302663	H	2.210817	3.597352	-1.033880	H	3.215147	-0.160607	3.349040
	H	-2.959416	-1.162168	-3.248814	H	-0.414517	3.655739	1.012820	H	3.488392	2.575158	-0.408704	H	1.730464	0.699355	3.779225
	H	-3.454027	-2.736325	1.356641	H	1.934498	-0.263343	2.924159	H	3.533769	1.365880	2.495070	H	-0.407635	3.687708	0.407828
	H	-4.090800	-1.091000	1.093893	H	1.033218	-1.254921	4.114132	H	3.532810	0.661971	0.870667	H	0.694766	4.571627	-0.655052
	H	-4.090693	-1.113904	-1.069434	H	-0.991419	0.170879	3.789976	H	2.361904	3.396180	1.513699	H	2.578814	3.100109	0.130675
	H	-3.454600	-2.764822	-1.296254	H	0.419367	1.144820	4.353433	H	0.752964	3.128081	0.829308	H	1.850982	4.032504	1.439095
	H	-3.454598	2.764822	1.296255	H	-3.281517	-3.311639	0.050435	H	3.760378	-2.745666	-1.046359	H	3.286848	-0.592696	-3.343812
	H	-4.090692	1.113905	1.069435	H	-2.553965	-2.441289	-1.327249	H	3.929379	-1.168016	-0.277404	H	2.027443	-1.740406	-2.942088
	Th	-0.002652	-0.000001	-0.000001	H	-2.520524	2.185049	-1.674290	Th	0.000051	-0.213165	-0.000213	H	1.434948	-2.854766	1.995145
	H	3.449879	1.282398	-2.753308	H	-3.226644	3.251098	-0.430037	H	1.570552	-2.158142	-1.711555	H	2.703348	-2.321014	3.094993
	H	3.449820	-1.339811	-2.726074	H	-4.744780	-1.469205	-0.493920	H	1.258753	1.794075	-2.000468	H	4.066748	-2.051560	-1.525292
	C	3.171579	1.166796	-1.691544	H	-3.911551	-1.021282	1.030219	H	1.112843	1.417267	2.344175	H	3.927819	-0.395085	-0.926792
	H	1.530134	2.528499	-1.979182	H	-3.833010	1.137624	0.895030	H	1.199929	-1.957389	2.128221	H	3.863290	-1.158304	1.196099
	C	3.171639	-1.202100	-1.666923	H	-4.719882	1.373881	-0.650648	H	-1.796296	-0.521230	3.181669	H	3.714742	-2.894810	0.927490
	O	2.401639	-0.015912	-1.509078	H	0.356340	-3.417758	1.881235	H	-1.259132	1.789760	2.002965	H	0.727027	2.532268	-3.271635
	H	1.530597	-2.570193	-1.925941	Th	-0.000035	0.030524	-0.000006	H	-1.570652	-2.161689	1.708449	Th	-0.005605	0.003780	-0.005931
	C	2.333455	2.349984	-1.252242	O	-0.445381	-1.383871	-2.117382	C	-2.620966	-0.592280	2.457682	N	-0.346832	-2.399575	-1.489261
	H	4.102112	1.082675	-1.105009	O	0.102151	1.358155	-2.350850	N	-1.925536	1.481996	1.289901	N	-1.329932	-2.109111	1.240071
	C	2.333687	-2.375928	-1.202804	O	1.560597	-2.219566	-0.427695	N	-2.129543	-1.392499	1.326919	N	-1.664407	0.053020	-2.272121
	H	4.102246	-1.105688	-1.082398	O	1.515701	2.191576	-0.092127	H	-0.753535	3.130067	-0.823381	N	-1.367211	0.534491	2.439596
	H	2.956860	3.253990	-1.168098	O	3.218503	-0.066633	0.671217	H	-3.350398	1.381606	2.892698	N	-2.430922	1.652657	-0.001749
	H	2.957297	-3.277785	-1.099366	C	1.174916	2.296746	-2.495693	C	-3.021620	0.801284	2.014032	C	-2.535611	-1.619999	1.933685
	O	1.652039	2.096729	-0.021822	C	1.634538	-2.584954	-1.808321	H	-3.479187	-1.075577	2.957525	C	-2.359717	-1.238616	-2.394734
	O	1.652042	-2.096728	0.021822	C	1.323762	3.070382	-1.210659	C	-1.768843	2.711681	-0.879804	C	-2.151372	-0.596692	2.974305
	C	2.333683	2.375929	1.202804	C	-0.938516	-0.612043	-3.225298	C	-2.398530	2.647607	0.512567	C	-0.538182	-3.547561	-0.584354
	H	2.957292	3.277787	1.099366	C	-0.015255	0.543469	-3.521790	N	-1.657622	1.375589	-1.472166	C	-1.652214	-3.274731	0.399778
	C	2.333456	-2.349983	1.252242	C	2.810470	-2.367462	0.262914	H	-1.113021	1.422403	-2.342295	C	-2.622099	1.159396	-2.394246
	H	2.956863	-3.253988	1.168099	C	2.769548	2.265443	0.609134	H	-2.211721	3.594947	1.040272	C	-2.146673	1.779965	2.420217
	O	2.401636	0.015913	1.509080	C	3.766298	-1.214957	0.046469	H	-1.199091	-1.953248	-2.130136	C	-3.370250	1.388445	-1.102886
	H	1.530591	2.570194	1.925940	C	3.729439	1.169344	0.206438	N	-1.896722	-1.494438	-1.535534	C	-3.137664	1.784218	1.282729
	H	4.102242	1.105691	1.082400	C	0.234691	-2.626509	-2.368243	H	-1.923917	-3.326758	-0.553820	C	-1.353090	-2.347871	-2.577158
	C	3.171635	1.202103	1.666924	H	0.278874	-2.820398	-3.449409	C	-3.204563	-1.963223	0.501377	H	-1.865757	-3.316741	-2.679473
	H	4.102111	-1.082671	1.105012	H	0.945334	2.992359	-3.321445	C	-2.636840	-2.523091	-0.789413	H	-3.065321	-2.451969	2.431650
	H	1.530135	-2.528499	1.979181	H	2.096195	1.730531	-2.724325	H	-3.884850	0.751290	1.336365	H	-3.214002	-1.207341	1.171679
	C	3.171578	-1.166794	1.691545	H	2.090578	-3.585693	-1.902954	H	-2.362326	3.398921	-1.507836	H	-3.033073	-1.232041	-3.270163
	H	3.449815	1.339814	2.726076	H	2.241691	-1.838028	-2.351831	H	-3.760324	-2.747595	1.042184	H	-2.983438	-1.400704	-1.503571
	H	3.449877	-1.282395	2.753309	H	2.174251	3.761174	-1.300883	H	-2.170759	-0.498971	-3.349562	H	-3.048040	-0.242221	3.505416
					H	0.416162	3.657201	-1.011040	C	-2.713990	-0.624994	-2.400311	H	-1.519450	-1.092626	3.740310
					H	-1.934698	-0.261418	-2.924361	H	-3.489086	2.573862	0.412793	H	0.397846	-3.725693	-0.031847
					H	-1.033326	-1.252154	-4.114950	C	-2.946761	0.748513	-1.794177	H	-0.751375	-4.468923	-1.149800
					H	0.991151	0.173296	-3.790291	H	-3.929211	-1.168432	0.276307	H	-2.583511	-3.058231	-0.140821
					H	-0.419670	1.147991	-4.352470	H	-3.532611	0.663864	-0.870173	H	-1.846105	-4.168103	1.014856
					H	3.280891	-3.312103	-0.052600	H	-3.447584	-2.961646	-1.395569	H	-3.336690	0.975158	-3.213624

		H 2.553465 -2.442814 1.325829 H 2.520470 2.184114 1.675684 H 3.227303 3.250229 0.431893 H 4.744297 -1.470232 0.493762 H 3.911665 -1.021290 -1.030438 H 3.833833 1.137615 -0.893687 H 4.719755 1.372616 0.652751 H -0.356773 -3.416547 -1.884101	H -3.533355 1.370048 -2.493571 H -3.682187 -1.096611 -2.634189	H -2.069239 2.065276 -2.695451 H -1.443294 2.624970 2.320045 H -2.667879 1.934324 3.378681 H -4.092043 2.214285 -1.226488 H -3.955639 0.497791 -0.834007 H -3.830542 0.937254 1.376562 H -3.753928 2.698675 1.312599 H -0.815377 -2.158983 -3.521550 H -0.699036 -2.437307 1.982026 H 0.547634 -2.537003 -1.963281 H -1.040872 0.123762 -3.118509 H -0.622995 0.696564 3.162399 H -0.602714 2.731403 -1.648117 H 0.982706 0.218553 -3.126552 H 0.794895 2.172362 2.228228 H 0.719686 -0.968581 3.073626 H 1.988225 -2.526777 -0.530837 H -2.021542 2.569813 -0.186414
0 (S=0)	O 2.248350 0.972519 1.154791 O 1.105665 1.731180 -1.153073 O 2.013860 -1.690922 1.071086 O 2.340729 -0.650385 -1.344469 C 3.219051 0.252579 1.905083 C 1.736751 2.738773 -0.345586 C 2.649441 -1.114735 2.214078 C 1.718725 1.405167 -2.410216 C 2.807689 -2.433074 0.145294 C 2.795969 0.350489 -2.255570 C 3.374406 -1.542279 -0.941345 C 2.785323 2.157842 0.569961 H 3.446796 0.788300 2.843463 H 4.150183 0.190363 1.315391 H 0.933020 3.188361 0.250111 H 2.167367 3.526872 -0.983334 H 3.434957 -1.791183 2.588141 H 1.839956 -1.030144 2.952580 H 2.139945 2.314407 -2.869253 H 0.896511 1.026991 -3.028079 H 2.105359 -3.159841 -0.288428 H 3.612957 -2.965377 0.676432 H 3.009445 -0.103511 -3.239436 H 3.734409 0.781905 -1.867809 H 4.243806 -0.956703 -0.595596 H 3.697301 -2.156965 -1.800047 H 3.035480 2.895641 1.353659 H 3.716513 1.914083 0.030599 Th 0.022872 -0.354471 0.055610 H -3.187009 -0.175306 3.139491 H -3.702754 -2.243307 1.704144 C -2.953964 0.302446 2.170843 H -1.110069 0.995939 3.032342 C -3.385676 -1.624747 0.845371 O -2.429439 -0.662172 1.268261	O 1.748600 -0.433324 1.936559 O -0.315140 1.460993 2.307392 O 0.382746 -2.584504 0.848072 O -2.386739 1.051547 0.444930 O -2.236604 -1.717048 0.178876 C -1.682509 1.551643 2.722281 C 0.770578 -2.635594 2.227031 C -2.548453 1.948440 1.556491 C 1.847153 0.642313 2.882422 C 0.488759 1.022807 3.406156 C -0.672695 -3.493924 0.526943 C -3.516950 0.278974 0.028258 C -2.026990 -2.941964 0.885531 C -3.452260 -1.106596 0.610065 C 1.990431 -1.772927 2.405681 H 2.263499 -1.755809 3.471485 H -1.777393 2.313898 3.517087 H -1.990890 0.571929 3.131233 H 1.020181 -3.675107 2.502264 H -0.057598 -2.281673 2.865861 H -3.598470 1.951515 1.886414 H -2.286499 2.952187 1.195964 H 2.309080 1.475884 2.337386 H 2.503535 0.350057 3.714849 H -0.001388 0.158986 3.891281 H 0.577880 1.837448 4.147043 H -0.513329 -4.447495 1.055448 H -0.601284 -3.669335 -0.551324 H -3.471168 0.250993 -1.068518 H -4.449612 0.775066 0.334385 H -2.808290 -3.670477 0.601951 H -2.109786 -2.746107 1.969416 H -3.466375 -1.071567 1.714757 H -4.313604 -1.706793 0.266714 H 2.834590 -2.167264 1.821816	N -1.738004 -1.302047 -1.493486 N -1.570495 1.611319 -1.482230 N -2.283040 -1.380968 1.203307 N -2.026198 1.388640 1.372654 C -2.141125 -2.605393 -0.942624 C -2.422867 0.860036 -2.424990 C -2.882963 -2.435052 0.380189 C -2.272545 2.652808 -0.709180 C -3.237801 -0.645373 2.035946 C -2.976519 2.093975 0.514875 C -2.637312 0.674986 2.493489 C -2.889618 -0.474846 -1.882437 H -1.222900 -3.186643 -0.785557 H -2.780038 -3.165442 -1.650160 H -1.819027 0.672304 -3.329045 H -3.294163 1.462681 -2.735111 H -3.928109 -2.156882 0.185136 H -2.917148 -3.406336 0.902757 H -2.999259 3.193869 -1.339759 H -1.514084 3.376631 -0.375970 H -3.566240 -1.225553 2.917690 H -4.140840 -0.463745 1.432058 H -3.474058 2.920679 1.054258 H -3.771922 1.397758 0.211177 H -3.413007 1.282720 2.996003 H -1.833157 0.483999 3.219062 H -3.494106 -0.983262 -2.657153 H -3.535550 -0.338795 -1.006835 Th 0.001073 -0.012805 0.169806 H -1.200355 -1.475926 -2.359457 H -1.542163 -1.782101 1.799180 H -1.327286 2.058875 1.742366 H -0.875478 2.092971 -2.064945 H 1.168656 3.181488 -0.734051 H 1.512829 1.772935 1.818733	N -0.278400 1.827019 -2.152847 N -1.358888 -0.934897 -2.299797 N -1.498866 2.410223 0.440901 N -1.461197 -2.488063 0.194966 N -2.373431 -0.114219 1.679612 C -2.568126 -1.672401 -1.901693 C -2.156884 2.805029 -0.812998 C -2.230580 -2.845752 -1.013998 C -0.586416 1.115599 -3.404398 C -1.727156 0.140763 -3.228155 C -2.470945 2.349614 1.535879 C -2.261802 -2.552213 1.423314 C -3.251793 1.056666 1.540079 C -3.162106 -1.348721 1.563780 C -1.130830 3.011142 -1.902994 H -1.631663 3.333299 -2.831011 H -3.104858 -2.056066 -2.791642 H -3.222790 -0.951162 -1.391195 H -2.707664 3.756401 -0.677038 H -2.880122 2.028004 -1.090816 H -3.154122 -3.387430 -0.748424 H -1.619573 -3.563894 -1.595582 H 0.311335 0.560077 -3.720594 H -0.821534 1.825792 -4.215664 H -2.599481 0.662059 -2.810858 H -2.029717 -0.265129 -4.209635 H -3.173959 3.200892 1.491605 H -1.931285 2.480061 2.488413 H -1.573230 -2.606600 2.284127 H -2.865810 -3.474853 1.456173 H -4.005607 1.088951 2.350378 H -3.797083 0.939857 0.593876 H -3.803247 -1.255224 0.677660 H -3.834003 -1.479579 2.431214 H -0.475152 3.841963 -1.591258

	H	-2.002312	-3.182460	0.291352	Th	0.008076	-0.011154	-0.000561	H	1.198011	1.490691	-2.352494	Th	0.001186	-0.000956	-0.000794
	C	-1.908458	1.381977	2.385076	O	-0.061228	-1.797433	-1.940576	C	2.099491	2.623454	-0.907624	N	0.397316	0.864715	2.678853
	H	-3.890568	0.707141	1.750223	O	-1.326115	0.706416	-2.304817	N	2.253985	1.364787	1.214088	N	1.207944	-1.842292	1.754612
	C	-2.713429	-2.497969	-0.195957	O	2.382947	-1.075103	-0.849280	N	1.728373	1.321152	-1.484153	N	1.691563	2.288496	0.480592
	H	-4.274428	-1.102769	0.449728	O	-0.359506	2.582231	-0.439899	H	1.832386	-0.508933	3.217004	N	1.269021	-2.320526	-1.156149
	H	-2.365161	2.278700	2.833841	O	2.263063	1.682461	-0.182274	H	2.839431	3.405619	0.957201	N	2.399796	0.365710	-1.628871
	H	-3.455891	-3.079261	-0.765053	C	-1.041662	2.048489	-2.715177	C	2.840527	2.444782	0.413865	C	2.348771	-2.509181	1.103777
	O	-1.235722	1.733421	1.170056	C	2.322202	-1.456538	-2.229763	H	2.723769	3.213964	-1.602713	C	2.379718	2.083772	1.762505
	O	-1.900931	-1.728121	-1.080666	C	-1.183492	2.986241	-1.546077	C	2.640755	-0.689921	2.494137	C	1.935918	-3.198149	-0.175764
	C	-1.851459	2.709980	0.320176	C	-1.122701	-1.596246	-2.886270	C	3.220665	0.642279	2.044143	C	0.608492	-0.293070	3.562368
	H	-2.336779	3.491372	0.925085	C	-1.117704	-0.183711	-3.404841	N	2.039691	-1.408231	1.368892	C	1.658213	-1.230535	3.012270
	C	-2.493652	-1.178683	-2.256789	C	3.545452	-0.306780	-0.528840	H	1.353304	-2.084557	1.727913	C	2.653303	2.592236	-0.582316
	H	-3.238049	-1.880362	-2.667489	C	0.693013	3.458282	-0.024163	H	3.530563	1.223929	2.931454	C	2.126950	-1.977761	-2.296889
	O	-2.222732	0.934547	-1.203381	C	3.383654	1.146351	-0.889828	H	0.900214	-2.054891	-2.086935	C	3.348887	1.349465	-1.088329
	H	-1.032555	3.176679	-0.240652	C	2.006759	3.019264	-0.610894	N	1.598183	-1.582564	-1.495591	C	3.105408	-0.879253	-1.963993
	H	-3.777178	1.806029	-0.152333	C	1.161241	-2.396753	-2.408354	H	1.855656	-0.636542	-3.335919	C	1.372628	1.960233	2.880863
	C	-2.832937	2.091293	-0.646570	H	1.070518	-2.655804	-3.473884	C	2.897265	0.516257	-1.868415	H	1.895572	1.843105	3.844406
	H	-4.080406	0.071553	-1.444453	H	-1.751092	2.350390	-3.507183	C	2.452622	-0.819896	-2.425498	H	2.792288	-3.269664	1.778185
	H	-1.656765	-1.073201	-2.959207	H	-0.015834	2.080605	-3.125726	H	3.893781	2.197238	0.221943	H	3.103252	-1.732542	0.919125
	C	-3.125569	0.170787	-1.989943	H	3.254993	-1.975471	-2.510972	H	3.424602	-1.288664	2.994893	H	3.045413	2.939084	1.988833
	H	-3.072111	2.822218	-1.440171	H	2.200578	-0.560636	-2.863672	H	3.502782	1.041583	-2.630775	H	2.994649	1.177189	1.685539
	H	-3.331987	0.686611	-2.944463	H	-0.900636	3.997942	-1.874514	H	1.543317	-3.365908	-0.423032	H	2.811948	-3.697490	-0.622740
					H	-2.218445	3.007074	-1.179809	C	2.300482	-2.632245	-0.737501	H	1.230669	-4.016462	0.070265
					H	-2.050724	-1.816822	-2.342397	H	4.131215	0.481016	1.445664	H	-0.344527	-0.838445	3.658842
					H	-1.018415	-2.303261	-3.721985	C	2.997492	-2.087119	0.497018	H	0.890206	0.030255	4.579013
					H	-0.150620	0.053972	-3.884618	H	3.534157	0.383120	-0.985962	H	2.581388	-0.673722	2.803504
					H	-1.922533	-0.046370	-4.149023	H	3.778154	-1.370564	0.204114	H	1.905537	-2.002086	3.763335
					H	4.419028	-0.720842	-1.057407	H	3.333504	-1.410939	-2.730500	H	3.411506	3.318662	-0.238423
					H	3.695902	-0.420838	0.549787	H	3.513178	-2.913087	1.020402	H	2.119892	3.103896	-1.400048
					H	0.710065	3.405859	1.072544	H	3.034024	-3.159867	-1.371903	H	1.475508	-1.661308	-3.130894
					H	0.469553	4.491116	-0.329082					H	2.670868	-2.865251	-2.662409
					H	4.297418	1.700095	-0.607186					H	4.106570	1.632644	-1.843057
					H	3.217189	1.278285	-1.973815					H	3.884088	0.859321	-0.263519
					H	1.973220	3.044370	-1.715553					H	3.714142	-1.162330	-1.095488
					H	2.820502	3.683119	-0.268658					H	3.801724	-0.730086	-2.809954
					H	1.310243	-3.315744	-1.823602					H	0.811178	2.909038	2.936059
													H	0.558665	-2.599027	2.014150
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													H	1.126273	3.154519	0.603854
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													H	2.068570	0.742791	-2.523050
0 (S=1)	O	2.248017	0.951291	1.206819	O	-1.357391	1.387484	1.768744	N	-1.741249	-1.311581	-1.485848	N	-0.452497	2.175318	-1.754282
	O	1.215112	1.726978	-1.162628	O	-0.903990	-1.343725	2.217862	N	-1.569003	1.600422	-1.492360	N	-1.504879	-0.533766	-2.276992
	O	1.924169	-1.718190	1.087017	O	1.124094	2.305815	0.984381	N	-2.288374	-1.369772	1.213819	N	-1.564460	2.184164	0.996168
	O	2.412241	-0.656443	-1.266720	O	1.214263	-2.249551	0.617042	N	-2.022191	1.398731	1.366114	N	-1.227768	-2.590371	-0.184405
	C	3.170471	0.181538	1.962837	O	2.734289	0.042323	0.551985	C	-2.150532	-2.608314	-0.923352	N	-2.348919	-0.555229	1.558268
	C	1.840650	2.709289	-0.326707	C	0.072389	-2.229446	2.760609	C	-2.417330	0.844974	-2.434778	C	-2.515756	-1.584579	-2.070802
	C	2.537618	-1.163291	2.249170	C	0.674983	2.582545	2.312588	C	-2.895415	-2.423071	0.395646	C	-2.081696	3.041524	-0.084507

	C	1.867384	1.379013	-2.390322	C	0.669387	-3.069165	1.659035	C	-2.273970	2.644512	-0.725841	C	-1.929837	-2.832498	-1.453511
	C	2.721745	-2.492023	0.192065	C	-2.235511	0.598058	2.595576	C	-3.235673	-0.628237	2.049345	C	-1.186865	1.798602	-2.975717
	C	2.914362	0.296410	-2.195152	C	-1.474943	-0.524348	3.244858	C	-2.975785	2.093432	0.502770	C	-2.174919	0.680132	-2.773933
	C	3.373102	-1.624140	-0.867566	C	2.543463	2.407243	0.817913	C	-2.630709	0.694463	2.494512	C	-2.648102	1.836956	1.925832
	C	2.847062	2.098400	0.618508	C	2.624660	-2.318590	0.352079	C	-2.889886	-0.484396	-1.884699	C	-2.042859	-2.921256	0.992076
	H	3.412138	0.694363	2.910528	C	3.260514	1.158777	1.262384	H	-1.234571	-3.190753	-0.757900	C	-3.325475	0.544341	1.557375
	H	4.106701	0.075029	1.387292	C	3.335388	-1.169003	1.007995	H	-2.789254	-3.172693	-1.627729	C	-3.033594	-1.835870	1.324240
	H	1.030016	3.169823	0.250955	C	-0.832665	2.611303	2.303868	H	-1.808634	0.649636	-3.334271	C	-0.999204	3.367159	-1.083831
	H	2.305722	3.494339	-0.942756	H	-1.210132	2.768464	3.323989	H	-3.285127	1.447591	-2.754517	H	-1.379135	4.090899	-1.822999
	H	3.285410	-1.865322	2.652926	H	-0.402543	-2.891596	3.504891	H	-3.937131	-2.135908	0.195541	H	-3.003147	-1.847477	-3.027819
	H	1.711955	-1.049065	2.963524	H	0.853620	-1.617728	3.245771	H	-2.940962	-3.391205	0.923291	H	-3.292598	-1.155508	-1.425202
	H	2.317666	2.276831	-2.843055	H	1.055835	3.566961	2.632962	H	-3.001553	3.179641	-1.360529	H	-2.478231	3.982693	0.336180
	H	1.058674	0.998929	-3.027783	H	1.042151	1.795784	2.991572	H	-1.517251	3.372767	-0.397594	H	-2.922457	2.528175	-0.569551
	H	2.002700	-3.180556	-0.277579	H	1.456338	-3.711085	2.079894	H	-3.557923	-1.202491	2.937269	H	-2.723735	-3.588157	-1.330503
	H	3.475391	-3.068763	0.751105	H	-0.099173	-3.706796	1.201593	H	-4.143186	-0.449606	1.451379	H	-1.209826	-3.290477	-2.159023
	H	3.116585	-0.193158	-3.164795	H	-3.028362	0.214552	1.937389	H	-3.475271	2.923226	1.035665	H	-0.427940	1.493098	-3.722713
	H	3.864410	0.700925	-1.805960	H	-2.717117	1.232930	3.352898	H	-3.769194	1.392015	0.206098	H	-1.695711	2.673708	-3.412368
	H	4.275143	-1.106855	-0.496590	H	-0.659104	-0.133772	3.877358	H	-3.403719	1.307310	2.994985	H	-2.946510	0.949678	-2.040147
	H	3.663619	-2.245977	-1.733340	H	-2.161061	-1.130174	3.861650	H	-1.824321	0.507681	3.218619	H	-2.691342	0.475142	-3.730101
	H	3.113084	2.838010	1.395071	H	2.922162	3.277319	1.376434	H	-3.493402	-0.997263	-2.657014	H	-3.388428	2.652111	1.994483
	H	3.775003	1.803713	0.099681	H	2.713843	2.576278	-0.249946	H	-3.537966	-0.339797	-1.012113	H	-2.216882	1.747774	2.939879
	Th	-0.022607	-0.358518	-0.034028	H	2.739940	-2.274487	-0.739559	Th	0.001016	-0.011420	0.166533	H	-1.352670	-3.086898	1.838413
	H	-3.084085	-0.047426	3.215183	H	3.033926	-3.277495	0.701184	H	-1.203620	-1.496996	-2.349357	H	-2.566327	-3.881311	0.849977
	H	-3.742441	-2.130414	1.795026	H	4.338143	1.261017	1.043106	H	-1.545517	-1.771497	1.806186	H	-4.141570	0.347876	2.278707
	C	-2.837378	0.383922	2.229093	H	3.130202	0.980096	2.343962	H	-1.326506	2.075438	1.729459	H	-3.779537	0.593600	0.556642
	H	-0.945578	1.047949	3.025249	H	3.242042	-1.217964	2.107768	H	-0.872416	2.081272	-2.074763	H	-3.745642	-1.695724	0.500808
	C	-3.394235	-1.529241	0.936678	H	4.404133	-1.181191	0.729297	H	1.179631	3.177792	-0.737765	H	-3.631124	-2.130387	2.204877
	O	-2.364419	-0.638831	1.353455	H	-1.198689	3.430053	1.666861	H	1.515020	1.782782	1.817425	H	-0.173446	3.875020	-0.559802
	H	-2.110317	-3.154286	0.334244	Th	-0.003095	0.013585	-0.002873	H	1.200881	1.487069	-2.352639	Th	0.000133	0.015913	-0.010147
	C	-1.754940	1.431191	2.393365	O	1.352069	1.363878	-1.789095	C	2.108333	2.616041	-0.910593	N	0.423158	0.281021	2.772859
	H	-3.760113	0.816120	1.805628	O	0.898584	-1.367056	-2.185787	N	2.254140	1.366440	1.216578	N	1.452323	-1.979604	1.253330
	C	-2.807503	-2.437370	-0.123842	O	-1.131439	2.280413	-1.019755	N	1.732761	1.314418	-1.485394	N	1.619639	2.113250	0.888312
	H	-4.250834	-0.942892	0.561296	O	-1.201087	-2.272956	-0.575717	H	1.821994	-0.505451	3.221259	N	1.340137	-1.937619	-1.627680
	H	-2.177246	2.346013	2.839198	O	-2.719677	0.017921	-0.554207	H	2.854438	3.401836	0.949376	N	2.263660	0.766615	-1.575950
	H	-3.602587	-2.981068	-0.658541	C	-0.055875	-2.281674	-2.720488	C	2.848588	2.438280	0.410775	C	2.656526	-2.308185	0.471112
	O	-1.119481	1.744898	1.145321	C	-0.686108	2.541283	-2.352818	H	2.733774	3.203036	-1.607935	C	2.378948	1.660049	2.066552
	O	-2.000884	-1.709347	-1.049516	C	-0.651109	-3.105366	-1.606517	C	2.633289	-0.687304	2.501929	C	2.259051	-2.832429	-0.889232
	C	-1.738498	2.742447	0.314565	C	2.231814	0.562984	-2.605004	C	3.215808	0.644075	2.053057	C	0.677809	-1.038789	3.374130
	H	-2.184432	3.536242	0.934631	C	1.478723	-0.576687	-3.230515	N	2.036495	-1.406197	1.374744	C	1.805300	-1.746227	2.662980
	C	-2.621015	-1.148501	-2.209227	C	-2.552158	2.380966	-0.853109	H	1.351457	-2.084453	1.731597	C	2.519469	2.707496	-0.115186
	H	-3.408938	-1.825151	-2.578055	C	-2.613261	-2.339560	-0.318924	H	3.521740	1.226787	2.940951	C	1.994756	-1.317595	-2.790887
	O	-2.225198	0.947097	-1.160596	C	-3.263887	1.122643	-1.273347	H	0.901148	-2.066228	-2.078216	C	3.237112	1.644374	-0.910278
	H	-0.925121	3.188669	-0.270063	C	-3.322783	-1.199394	-0.991902	N	1.599617	-1.588093	-1.492140	C	2.975186	-0.268045	-2.338619
	H	-3.715241	1.923890	-0.098205	C	0.820998	2.575894	-2.346151	H	1.848865	-0.645535	-3.335251	C	1.426720	1.286745	3.175486
	C	-2.767257	2.149497	-0.615868	H	1.196410	2.715779	-3.369608	C	2.899053	0.508280	-1.875175	H	1.987096	0.951102	4.062848
	H	-4.130277	0.184545	-1.366054	H	0.441917	-2.953794	-3.441019	C	2.450221	-0.828313	-2.427613	H	3.246492	-3.092987	0.981483
	H	-1.805013	-1.084603	-2.942125	H	-0.839071	-1.696639	-3.234356	H	3.899948	2.181968	0.220051	H	3.282096	-1.405723	0.407825
	C	-3.182636	0.229000	-1.930473	H	-1.071548	3.519811	-2.685709	H	3.415102	-1.285930	3.006086	H	3.042033	2.468379	2.429285
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	H	-3.377846	0.757857	-2.880133	H	-1.435092	-3.757116	-2.018083	H	1.549432	-3.367837	-0.414389	H	3.157816	-3.050681	-1.487537
					H	0.119999	-3.733119	-1.139682	C	2.304877	-2.632564	-0.729544	H	1.739162	-3.795975	-0.734484
					H	3.028194	0.196028	-1.942271	H	4.129168	0.481406	1.459397	H	-0.240322	-1.644054	3.300772
					H	2.705517	1.185434	-3.377677	C	2.998151	-2.081968	0.504731	H	0.903554	-0.944793	4.448695

		H 0.669891 -0.207069 -3.884020 H 2.173808 -1.199620 -3.821488 H -2.934508 3.238492 -1.428505 H -2.723873 2.572569 0.210730 H -2.732779 -2.280585 0.771002 H -3.019671 -3.302757 -0.660064 H -4.339910 1.218842 -1.039719 H -3.146449 0.929272 -2.353690 H -3.230640 -1.264801 -2.091020 H -4.391798 -1.204752 -0.712368 H 1.183307 3.407137 -1.723511	H 3.541707 0.376423 -0.996798 H 3.775320 -1.361880 0.211400 H 3.328591 -1.420683 -2.736853 H 3.517571 -2.904702 1.029597 H 3.041033 -3.159560 -1.361465	H 2.719870 -1.139274 2.700690 H 2.033134 -2.701258 3.166323 H 3.251543 3.380020 0.363006 H 1.929260 3.325205 -0.807265 H 1.230640 -0.841353 -3.427684 H 2.501286 -2.074607 -3.412699 H 3.884917 2.137278 -1.658364 H 3.885202 1.030724 -0.268170 H 3.755875 -0.711343 -1.705489 H 3.476319 0.179844 -3.215613 H 0.876069 2.198061 3.478269 H 0.892042 -2.856477 1.246076 H -0.460227 0.617672 3.194921 H 1.021567 2.879870 1.237805 H 0.611741 -2.554432 -2.004767 H 0.469135 2.490781 -2.140050 H -0.931900 2.797853 1.555694 H -0.884847 -0.853008 -3.031440 H -0.469528 -3.313723 -0.155992 H -1.988996 -0.597773 2.519880 H 1.856303 1.378772 -2.329747
0 (S=2)	O 2.657466 -0.982888 -0.840740 O 1.224117 -1.663262 1.299744 O 1.935659 1.488582 -1.390702 O 1.921192 0.980010 1.257963 C 3.622235 -0.252517 -1.574498 C 2.084103 -2.654222 0.738104 C 2.894183 0.888541 -2.258373 C 1.624469 -1.048463 2.527324 C 2.344011 2.530153 -0.507370 C 2.474503 0.185675 2.313912 C 2.832218 1.985681 0.819507 C 3.207237 -2.041866 -0.075478 H 4.099045 -0.897531 -2.333754 H 4.409867 0.106032 -0.887593 H 1.432930 -3.240583 0.076562 H 2.488640 -3.300607 1.533517 H 3.603398 1.645885 -2.627877 H 2.297138 0.505939 -3.097336 H 2.169238 -1.765244 3.163830 H 0.693494 -0.799171 3.052666 H 1.439734 3.140572 -0.368450 H 3.124032 3.149288 -0.978894 H 2.506116 0.769247 3.252714 H 3.508859 -0.081800 2.044102 H 3.835556 1.537207 0.725733 H 2.890087 2.796367 1.565877 H 3.638354 -2.811642 -0.740803 H 4.017354 -1.646625 0.562415 Th -0.000104 -0.002185 -0.433167 H -4.100252 0.895444 -2.333051 H -3.636163 2.812329 -0.745529 C -3.623632 0.251480 -1.572772	O -0.700725 -1.755021 1.816631 O 1.592908 -0.229121 2.220593 O -2.567490 0.080811 0.981552 O 1.536658 2.047028 0.619893 O -1.166865 2.466438 0.514907 C 2.050482 1.013248 2.752475 C -2.668357 -0.437431 2.310615 C 2.538557 1.898191 1.632333 C 0.378277 -2.237132 2.643895 C 1.111556 -1.082482 3.266789 C -3.250154 1.325421 0.784587 C 1.027416 3.358133 0.325874 C -2.414584 2.505422 1.206234 C -0.326857 3.537103 0.951538 C -2.039246 -1.808849 2.330175 H -2.032509 -2.200252 3.357058 H 2.879898 0.828559 3.457120 H 1.206755 1.489242 3.283110 H -3.731557 -0.521810 2.593422 H -2.144566 0.238807 3.006176 H 2.807630 2.882581 2.041089 H 3.425848 1.460769 1.154106 H 1.040892 -2.825505 1.992083 H -0.007301 -2.916002 3.417883 H 0.442702 -0.493822 3.917895 H 1.965539 -1.461971 3.855826 H -4.200510 1.321335 1.340703 H -3.474697 1.386453 -0.285367 H 0.963589 3.433634 -0.768804 H 1.723460 4.130567 0.683751 H -2.947219 3.438208 0.948438 H -2.212262 2.491588 2.291064	N -1.702846 -1.288070 -1.520622 N -1.553582 1.635070 -1.457565 N -2.240204 -1.375222 1.190968 N -1.994459 1.380295 1.404233 C -2.136319 -2.580907 -0.962989 C -2.345470 0.888582 -2.454900 C -2.884123 -2.390909 0.350735 C -2.317561 2.627205 -0.676933 C -3.159568 -0.673134 2.091211 C -2.987706 2.025715 0.545846 C -2.558578 0.650873 2.543092 C -2.835320 -0.454071 -1.954805 H -1.231938 -3.179593 -0.788129 H -2.775972 -3.134348 -1.674950 H -1.689155 0.716030 -3.325910 H -3.200492 1.489307 -2.810439 H -3.914901 -2.065503 0.153811 H -2.956553 -3.365929 0.863775 H -3.074213 3.126941 -1.306642 H -1.601524 3.392302 -0.340824 H -3.427614 -1.276440 2.976263 H -4.097110 -0.495768 1.543135 H -3.534471 2.820611 1.085255 H -3.736974 1.280214 0.244289 H -3.324983 1.243360 3.076226 H -1.727819 0.466275 3.238580 H -3.396029 -0.954835 -2.766374 H -3.527785 -0.333581 -1.113483 Th -0.000198 -0.000358 0.168691 H -1.152798 -1.483281 -2.374314 H -1.495852 -1.839384 1.748312 H -1.328244 2.089176 1.752306	N -0.627803 2.220386 -1.662523 N -1.624925 -0.502399 -2.214679 N -1.636492 2.097009 1.121705 N -1.152614 -2.630877 -0.233526 N -2.310690 -0.682476 1.580823 C -2.566214 -1.616523 -2.024494 C -2.202201 2.990904 0.097476 C -1.884046 -2.854405 -1.490119 C -1.433759 1.862928 -2.844688 C -2.367204 0.700764 -2.624378 C -2.684499 1.675573 2.060779 C -1.923090 -3.023231 0.954174 C -3.326322 0.377558 1.649401 C -2.945689 -1.987917 1.347966 C -1.159329 3.376921 -0.922308 H -1.573681 4.127419 -1.614638 H -3.078009 -1.863154 -2.972512 H -3.339978 -1.263403 -1.330355 H -2.603682 3.904464 0.569778 H -3.048941 2.482866 -0.384347 H -2.624572 -3.664107 -1.379357 H -1.161388 -3.230968 -2.239523 H -0.716728 1.610959 -3.650708 H -2.001358 2.734812 -3.209455 H -3.105718 0.913737 -1.838058 H -2.933263 0.511779 -3.555188 H -3.448762 2.461676 2.182582 H -2.221701 1.556998 3.058778 H -1.202270 -3.183806 1.775411 H -2.413384 -3.999162 0.799274 H -4.120761 0.120535 2.374720 H -3.802610 0.454242 0.659592

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