ARTICLE

Supporting Information for

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Deciphering the Atomic-Scale Evolution Pathway of Keggin-Type Aluminum Nanoclusters in Aqueous Media

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COMPUTATIONAL METHODS AND EXPERIMENTAL SECTION

Computational Methods. AIMD simulations were conducted using the Quickstep module of the CP2K-7.1 package.[1, 2] The Becke-Lee-Yang-Parr (BLYP) density functional, coupled with Grimme's D3 empirical dispersion correction, was employed, as previous studies indicate its effectiveness in examining the behavior of aluminum polyoxocations in aqueous environments.[3-7] To accurately depict the potential near the nucleus, the Goedecker-Teter-Hutter (GTH) pseudopotential was utilized.[8] A hybrid Gaussian and Plane Wave (PW) approach was adopted, featuring a double ζ-valence enhanced polarization Gaussian basis set and the PW expansion of the charge density with a cutoff energy of 300 Ry. [9, 10] The self-consistent field method achieved convergence with an accuracy of 10^{-6} au. Additionally, AIMD simulations were performed in a canonical ensemble (NVT) at 363 K, with the temperature regulated by a Nose-Hoover thermostat. The time step for nuclear motion in the AIMD was set to 0.5 fs. [11, 12]

Model Setup and Details for AIMD Simulation. The Al_{10} cubic box measures 25 Å × 25 Å × 13 Å and contains 1 Al_{10} molecule and 247 H_2O molecules, totaling 830 atoms, with a density of approximately 1 g cm^{-3}. The system has a net charge of +7, and a compensation gel background is included to prevent divergence. All starting reactants are pre-equilibrated for at least 2 ps. [13]

Well-Tempered Metadynamics. For the well-tempered ab initio metadynamics simulations, a Gaussian hill with a width of 0.2 and an initial height of 15.1 kJ mol^{-1} was incorporated into the two-dimensional path (*pp*) variables defined in PLUMED-2.9.0.[14] The reference path connecting the reactants and products consisted of nine equally spaced points within the two critical distances. Then, two collective variables (CVs) were used in pMtD to measure the following: (i) the progress of the system along the reference path (S) and (ii) the distance of the sampled configurations from the path (Z).[15] Wall constraints were implemented to ensure the plausibility of the metadynamic structure. The results from the well-tempered metadynamics were analyzed using the metadynminer package.

Static Calculations and Topological Analysis. All static calculations were conducted with Gaussian 16.[16] The geometry optimization and frequency calculations were carried out at the B3LYP/6-31g(d) level, incorporating the D3 empirical dispersion correction and a polarizable continuum model (PCM) to account for solvent effects.[17] The absence of imaginary frequencies in the vibrational frequency analysis post-geometry optimization confirmed the stability of the conformation. Single-point energies were determined at the PBE/def-TZVP level. The interaction between O and Al was investigated via topological analysis of the electron density, as per the quantum theory of atoms in molecules. The characteristics of the Al-O ligand bond were described using various electron densities at bond critical points (BCPs), with the topological analysis descriptors being computed by Multiwfn software.[18, 19]

Synthesis. The ε-Al_{13} solution was prepared by gradually adding aluminum powder to the $AlCl_3$ (or $Al(NO_3)_3$) solution. The temperature of synthesis was 70 °C to ensure a complete reaction of the aluminum powder. Subsequently, the solution was placed at room temperature and subjected to filtration. The obtained Al^{3+}/Al molar ratio of the ε-Al_{13} solution was 4.5 (while the molar ratio of Al^{3+}/Al was 2.0 in the $Al(NO_3)_3$ solution). The target sample was prepared using 5 mL of a stock solution of 0.5 M ε-Al_{13} and various HCl/HNO_3. The specific solution composition, aging duration, and aging temperature are shown in **Tables S1** and **S2**. The concentrated system was prepared by rotary evaporation of 15g of solution at 40 °C until half of its original mass was obtained.

Characterization. The liquid sample ^{27}Al NMR spectra were acquired on a Bruker Avance 500 MHz spectrometer, and the solid-state ^{27}Al (150.03 MHz) CP MAS NMR spectra were performed on a Bruker WB 600 spectrometer at 300 K with a 4.0 mm double channel probe head. Samples were carefully packed into a 4.0 mm cylindrical zirconia rotor with Kel-F caps. ^{27}Al spectra were originally calibrated with an aluminum nitrate solution as the standard sample. The ^{27}Al CP/TOSS (total suppression of sidebands) and ^{27}Al CP/TOSSNQS (non-quarternary suppression) experiments were performed with a spinning speed of 15 kHz, and recycle delays of 5 s were applied. Wide-angle X-ray scattering (WAXS) data were obtained from Xenocs' in-house X-ray scattering beamline, Xeuss 3.0, France. Mass spectrum (MS) was recorded on a Bruker Impact II high-definition mass spectrometer, quadrupole, and time-of-flight (Q/TOF) modules in positive ion mode. Typical measurement conditions are as follows: end plate offset = −500 V; dry gas = 4 L min^{-1}, nebulizer = 0.4 bar, capillary voltage = 2600 V.

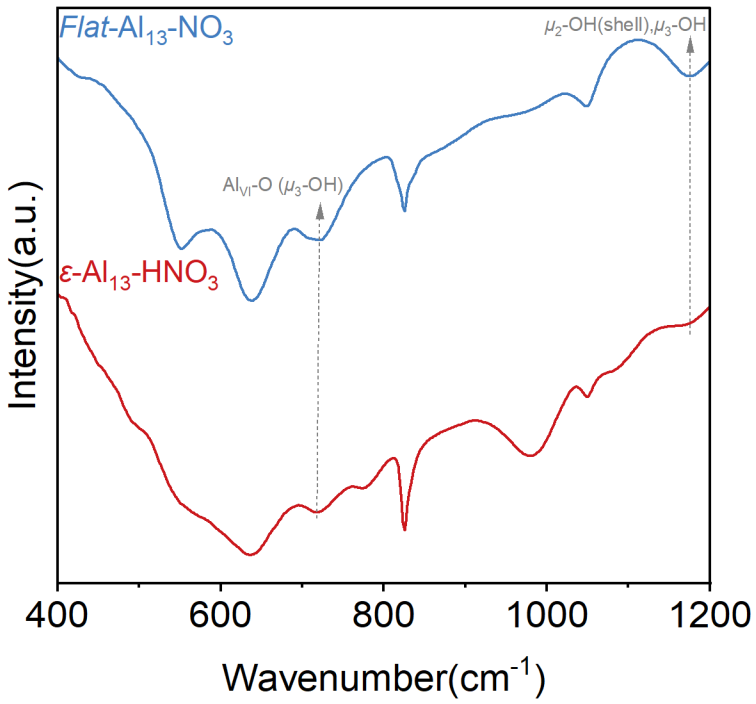

Fig. S1. IR spectra of the titration process of ε-Al_{13}-NO_3 solution and *Flat*-Al_{13} crystal.

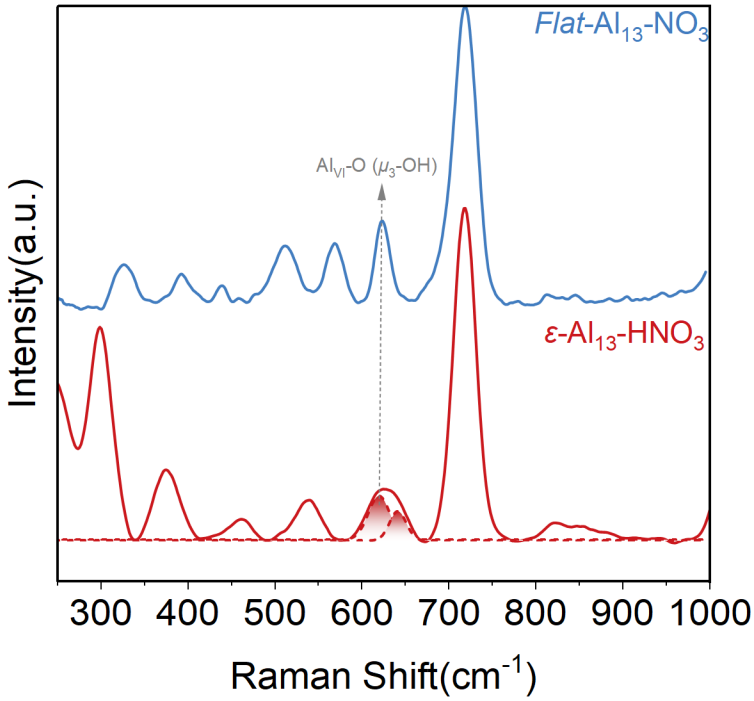

Fig. S2. Raman spectra of the titration process of ε-Al_{13}-NO_3 solution and *Flat*-Al_{13} crystal.

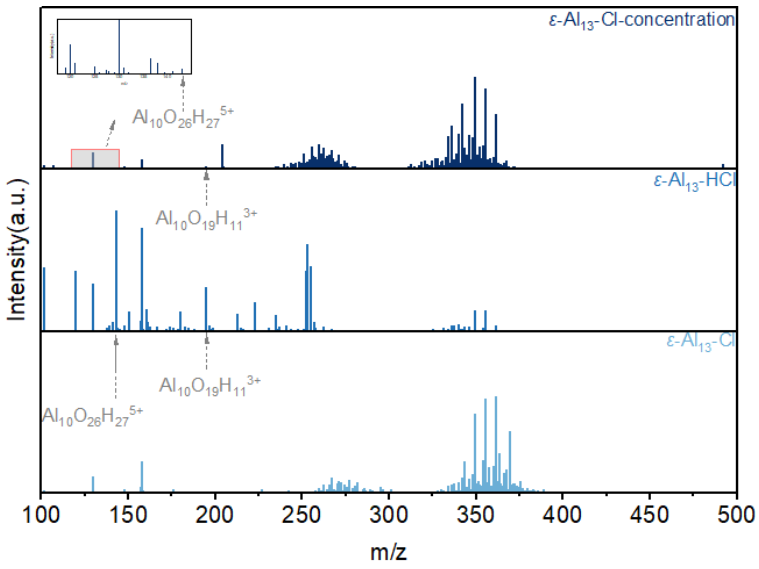

Fig. S3. ESI-MS spectra of the titration and concentration process of ε-Al_{13}-Cl solution.

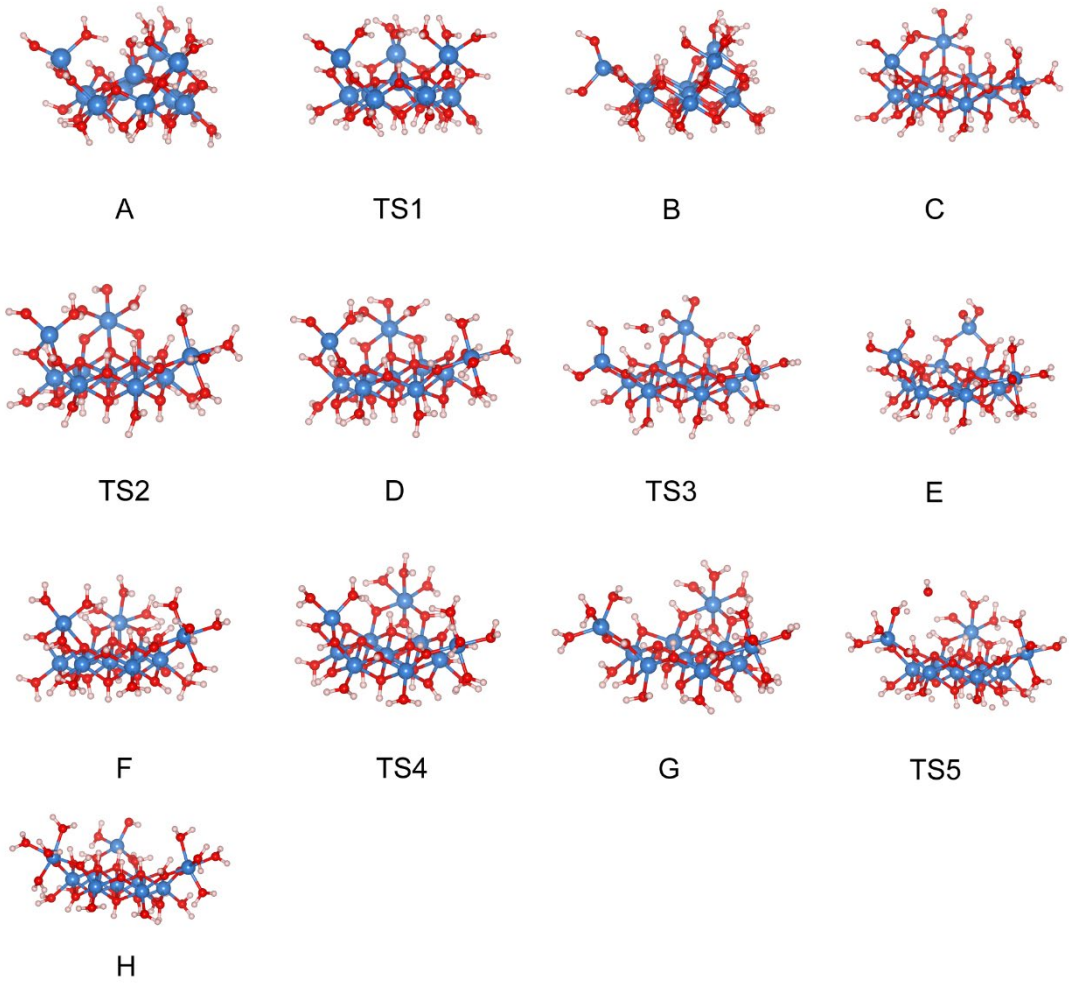

Fig. S4. The structure of each intermediate of the *Cage*-to-*Flat*-Al_{10} transformation

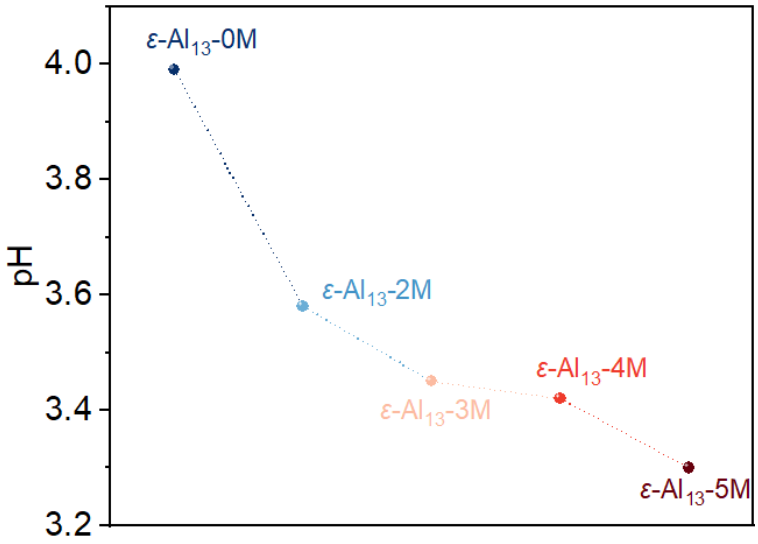

Fig. S5. The pH of the acid titration process of ε-Al_{13}-Cl solution.

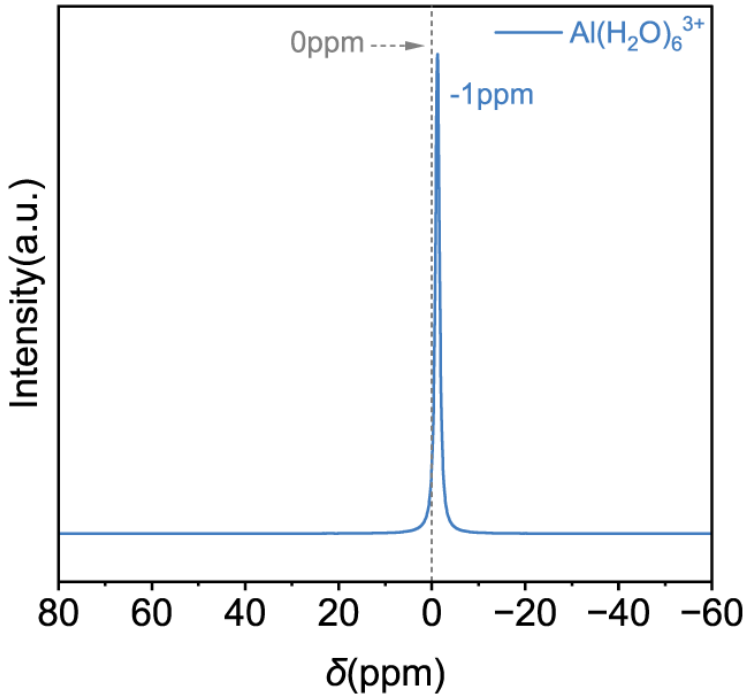

Fig. S6. The solid ^{27}Al NMR spectra of $Al(H_2O)_6^{3+}$.

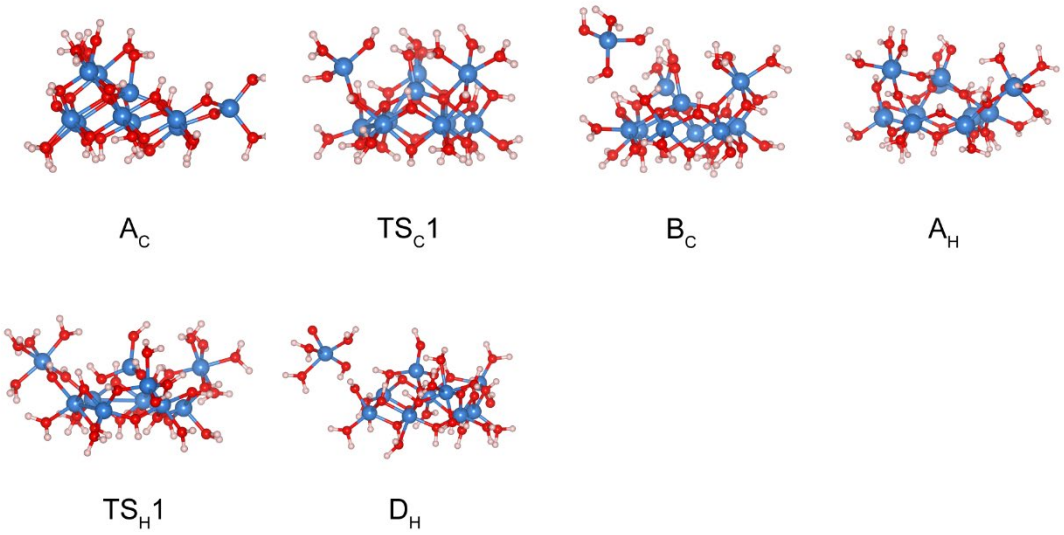

Fig. S7. The structure of each intermediate of on the dissociation of *Cage*-Al_{10} before and after protonation.

Table S1. Sample composition of ε-Al_{13}-Cl with different HCl concentrations.

sample	ε-Al_{13}-Cl	ε-Al_{13}-Cl-0M	ε-Al_{13}-Cl-2M	ε-Al_{13}-Cl-3M	ε-Al_{13}-Cl-4M	ε-Al_{13}-Cl-5M
concentration	5ml 0.5 M ε-Al_{13}-Cl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml H_2O	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 2M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 3M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 4M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 5M HCl
aging duration	3 h	3 h	3 h	3 h	3 h	3 h
aging temperature	40 ℃	40 ℃	40 ℃	40 ℃	40 ℃	40 ℃

Table S2. Sample composition of ε-Al_{13}-Cl under different titration rates.

sample	ε-Al_{13}-Cl-10uL	ε-Al_{13}-Cl-50uL	ε-Al_{13}-Cl-200uL	ε-Al_{13}-Cl-600uL
concentration	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 2M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 2M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 2M HCl	5ml 0.5 M ε-Al_{13}-Cl 0.5ml 2M HCl
titration speed	10ul min^{-1}	50ul min^{-1}	200ul min^{-1}	600ul min^{-1}
aging duration	3 h	3 h	3 h	3 h
aging temperature	40 ℃	40 ℃	40 ℃	40 ℃

Table S3. Aluminum species identified from ESI-MS

Identified	Assignments	Sim.	Exp.(ε-Al_{13})	Exp.(ε-Al_{13}-HCl)	Exp.(ε-Al_{13}-Cl-concentration)
Al_{13}	$Al_{13}O_{23}H_9^{2+}$	362.9	361.6113		361.6166
Al_{13}	$Al_{13}O_{22}H_7^{2+}$	355.0	355.6168	355.6129	355.61
Al_4	$Al_4O_{14}H_{17}^{+}$	349.0	349.6048	349.6092	349.6156
Al_{13}	$Al_{13}O_{20}H_3^{2+}$	337.0			335.9371
Al_{13}	$Al_{13}O_{25}H_{14}^{3+}$	255.0	255.4682	254.9433	255.4683
Al_3	$Al_3O_{10}H_{12}^{+}$	253.0		252.9365	
Al_{13}	$Al_{13}O_{32}H_{29}^{4+}$	223.0		222.9612	
Al_{13}	$Al_{13}O_{18}^{3+}$	213.0		212.9327	
Al_{10}	$Al_{10}O_{19}H_{11}^{3+}$	195.0		194.9611	194.9689
Al_{13}	$Al_{13}O_{35}H_{37}^{6+}$	157.6	158.0053	158.0026	158.0075
Al_{10}	$Al_{10}O_{26}H_{27}^{5+}$	142.6		143.0398	143.0416
Al_{13}	$Al_{13}O_{33}H_{34}^{7+}$	130.4	130.0054	130.0377	130.0051
Al_2	$Al_2O_4H_3^{+}$	121.0		120.0234	
Al_2	$Al_2O_3H^{+}$	103.0		102.0128	

Atomic coordinates

Al_1

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H	1.06021800	1.96980600	1.29852600
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O	3.46928200	1.19904100	-1.28798400
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H	3.94393800	0.54769900	0.32455400
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H	0.28524900	-3.65198800	-1.28294500
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H	-1.73307500	-3.99510600	1.84516900
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Al_2

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O	1.45950300	1.96630100	0.14578000
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Al_3

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O	1.91946600	1.84297500	3.94976900
H	1.93955900	2.60229000	4.54617700
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O	0.06700900	3.38861100	-3.17322100
H	-0.88262500	3.54021300	-2.97633400
H	0.35035800	4.09808200	-3.76135300
O	0.17525100	0.72223100	-3.59692300
H	0.07491700	0.34236600	-4.47673200
H	0.24685700	1.69691900	-3.69542100
O	-3.64802100	-1.23096000	-2.97517900
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H	-6.62987500	0.97773700	0.57422800
H	-5.52797200	1.94479100	1.13512300
O	-3.09010900	-2.67772400	0.60909300
H	-2.94677300	-3.20604700	-0.20386800
H	-3.46978700	-3.24581400	1.28677000
O	5.34802900	1.53945500	1.59545200
H	5.07054100	1.74132700	2.49632000
H	5.89635800	2.28403200	1.32230700
O	4.13409100	-1.01040100	-1.97085200
H	5.02950200	-1.27118800	-2.21917400
H	3.65948700	-0.83005400	-2.79216300
O	3.11467100	-4.87537100	0.32323000
H	2.39435300	-5.29268400	0.82953400
H	3.94975900	-5.19179600	0.68467900
O	0.55480400	-2.23413100	3.82711800
H	0.04599000	-2.80594400	4.41624000
H	1.45226200	-2.22231400	4.18414700
O	1.45932500	-5.13034000	-1.83522500

H	1.51862100	-5.61052600	-2.66832900
H	2.32843300	-5.18701600	-1.39658900
O	-2.34164200	-3.38260400	-1.89050000
H	-2.48498800	-4.21951500	-2.34764600
H	-2.82730900	-2.69437800	-2.39592800
O	-0.49035400	0.40183200	3.77554200
H	0.30428500	0.95823800	3.85271300
H	-0.15121000	-0.51081200	3.75559000
O	0.46477500	-5.46740300	0.69809900
H	-0.12910000	-6.12095700	1.08324500
H	0.48688600	-5.61766800	-0.26602500
O	3.48182200	4.63879200	0.91758100
H	4.12678500	4.80019300	1.61840800
H	2.98494400	5.46241800	0.82810300

Al_7

Al	0.02550900	0.03545200	0.01258200
Al	-1.01714200	-2.83689900	0.01501500

Al	1.98860800	-2.29834100	-0.04099800
Al	3.04223300	0.56358200	0.01764700
Al	1.06172700	2.89698600	-0.00311300
Al	-1.94029900	2.37625400	-0.00906500
Al	-2.99957500	-0.50074600	0.02708400
O	1.57792700	-0.52258300	0.96190700
O	-1.53311200	0.60460300	-0.93303700
O	-1.23315600	-1.03606100	0.95991600
O	0.30425700	-1.57693700	-0.96438300
O	1.28435800	1.10826400	-0.93742700
O	-0.25706600	1.66056100	0.96574300
O	0.61408000	-3.24073100	0.72625800
O	3.11752400	-1.08122500	-0.79889000
O	2.58949200	2.19324500	0.75922800
O	-0.55907800	3.31748400	-0.74527600
O	-3.06753000	1.17049300	0.82382000
O	-2.50821200	-2.09172500	-0.78467900
H	1.60845400	-0.56163400	1.92722600

H	-1.57294100	0.59612600	-1.89796800
H	-1.26172600	-1.04579600	1.92549500
H	0.29511300	-1.60058700	-1.93025800
H	1.32582200	1.13348700	-1.90253400
H	-0.27137100	1.70344400	1.93086800
H	0.82172200	-3.89960300	1.42587300
H	3.51713500	-1.13149300	-1.69636800
H	3.02342600	2.62337500	1.50898600
H	-0.59900300	3.99053600	-1.46091800
H	-3.56113900	1.40398900	1.62105600
H	-2.92280700	-2.49782400	-1.55839900
O	4.11897600	1.29881000	-1.34047700
H	4.44544100	2.23198900	-1.36077100
H	4.51329600	0.74087300	-2.04423000
O	1.94656200	3.83146400	-1.37124100
H	1.44461800	4.30158800	-2.07485400
H	2.91578800	4.02032700	-1.39213400
O	-3.13380900	2.92605700	-1.33906800

H	-4.10754500	2.77423100	-1.26381100
H	-2.87528900	3.14638900	-2.27360000
O	-4.29049300	-0.12640400	-1.24690100
H	-4.50726700	-0.68427100	-2.06236300
H	-4.92014400	0.62506900	-1.14862000
O	-4.04923000	-1.27919200	1.33962000
H	-4.36005200	-0.82989700	2.19145200
H	-4.39341900	-2.19969300	1.27153000
O	-1.92852300	-3.78364200	1.34509500
H	-2.90132400	-3.95495700	1.30478100
H	-1.58127200	-3.92410700	2.26606500
O	-0.95608100	-4.16733500	-1.30069100
H	-0.32783600	-4.93095900	-1.27604600
H	-1.70750000	-4.31712700	-1.91674300
O	2.38574400	-3.58502200	-1.34252100
H	3.24763000	-3.60524800	-1.84086700
H	2.00121900	-4.49417400	-1.29530200
O	-2.33429100	3.65963400	1.29334600

H	-1.98198600	4.58372200	1.28766100
H	-3.05670000	3.53681200	1.94924800
O	0.98847700	4.22254500	1.31717400
H	1.70133600	4.33622600	1.98459700
H	0.34645000	4.97554200	1.31694900
O	3.14992400	-2.85421800	1.32981000
H	2.84981700	-3.50038100	2.00877800
H	4.13125800	-2.73384500	1.32250200
O	4.33669600	0.22201200	1.30135900
H	4.92622200	-0.56746600	1.24812600
H	4.80073400	0.97061500	1.79767400
O	4.47912100	-0.76712900	-3.04971400
H	4.02022900	-0.68049600	-3.89429000
H	4.91780300	-1.63820900	-3.06559600
O	5.42651100	2.19519800	2.51635300
H	6.11399700	2.65825400	2.02281800
H	4.81271700	2.87839700	2.83033700
O	-5.65650600	2.15944600	-0.98040800

H	-6.04450300	2.35570700	-0.11695000
H	-6.32991800	2.37823800	-1.63842800
O	-4.58059300	-3.89124500	1.13302300
H	-5.09330600	-4.31605500	1.83376600
H	-4.93913100	-4.21675600	0.29646600
O	-0.83072700	-4.03888400	3.75845200
H	-1.22266500	-4.73956500	4.29749400
H	-0.94198200	-3.22497400	4.26866500
O	1.05353600	-5.89748900	-1.15808900
H	1.16377000	-6.39391900	-0.33544000
H	1.16993800	-6.53376900	-1.87677800
O	4.60070400	3.90385000	-1.25360200
H	5.11093800	4.32121000	-1.96099700
H	4.97040200	4.22913900	-0.42150300
O	-0.06463400	4.88762700	-2.80727800
H	-0.23004800	5.83769600	-2.83237400
H	-0.67420400	4.47395600	-3.44871100
O	5.67550200	-2.09356400	1.17826200

H	6.15453000	-2.29081300	0.36241700
H	6.28326500	-2.28453000	1.90549100
O	1.66748400	-4.61213400	2.71406400
H	0.97298700	-4.45558600	3.38276200
H	1.83691600	-5.56151100	2.69625200
O	3.17945100	4.02909100	2.91518400
H	3.65094300	4.87441200	2.91123100
H	2.90664700	3.88389400	3.83241900
O	-1.01453000	5.96226600	1.21342000
H	-1.12733800	6.58556300	1.94424200
H	-1.08865500	6.48021000	0.40010600
O	-4.29400100	2.75123800	2.93642200
H	-4.04736500	2.99292000	3.84063500
H	-5.13641500	3.19659500	2.76686100
O	-4.76782900	-0.07941100	3.47349600
H	-4.20328600	-0.26064800	4.23444300
H	-4.82464400	0.88773700	3.40999100
O	4.69281500	-3.50958000	-2.66523900

H	4.63328300	-3.98522300	-3.50501200
H	5.42648600	-3.91984400	-2.18787300
O	-3.19703000	-4.01373200	-2.82570800
H	-3.81794400	-4.72846600	-2.62500300
H	-2.93732800	-4.14144900	-3.74929100
O	-2.24873500	3.48090900	-3.79085800
H	-2.08362400	2.67064800	-4.29185800
H	-2.86487600	3.99792500	-4.32746700
O	-4.77866300	-1.57364600	-3.29534900
H	-4.47081700	-2.49152000	-3.23231500
H	-4.40927200	-1.22946800	-4.11749800

Al_{10}

Al	-2.77318500	1.18329400	-1.52043200
Al	-0.24508500	2.65424500	-1.44860100
Al	2.30532000	1.26674900	-0.84764900
Al	4.62042700	-0.03180400	0.58435200
Al	-1.91654000	2.56634400	0.90808000

Al	2.31490900	-1.61994800	-0.36855500
Al	-2.80031900	-1.77648100	-0.84672900
Al	-1.83603700	-2.35302600	1.82872300
Al	-0.24659000	-3.20071500	-0.39558900
Al	-0.24836100	-0.24248100	-0.78124000
O	-3.42836800	-2.32741000	0.86410400
O	-1.79675000	-3.23281800	-1.42326700
O	1.38462900	-2.95414900	0.49734200
O	0.68384200	-1.85046900	-1.54571900
O	-2.61704500	1.28235300	2.11965900
O	3.57783400	-1.44420100	1.01341600
O	3.66985000	1.49171000	0.44511400
O	6.07832500	-0.55293000	-0.26702400
O	3.34922400	-0.26764900	-1.28367500
O	1.29423600	2.75539400	-0.35870500
O	0.71671400	1.02397500	-2.05362400
O	-1.12646800	3.87335300	-0.30823100
O	-3.36289100	2.45391200	-0.28903400

O	-1.70834000	2.33137600	-2.54938300
O	-3.67988500	-0.17410400	-0.67592400
O	-1.75934800	-0.48875800	-2.04533200
O	1.34906500	-0.07344400	0.10948200
O	-2.73490200	-3.29981800	3.28457000
O	0.39426700	-4.74463700	-1.23505900
O	3.26601600	-2.88297400	-1.45646500
O	0.43324800	3.85286800	-2.75227200
O	-4.22504200	-2.41219500	-1.93552900
O	-1.02925200	-3.85636500	1.18698700
O	0.88594900	0.43542200	2.61139500
O	-1.15751200	-1.54802600	0.21911700
O	-1.16992400	1.31867000	-0.34512400
O	5.30701000	0.42804200	2.28538800
O	-4.03128000	1.28533600	-2.92070500
O	-2.69319100	3.99490500	1.91613100
O	-0.26652100	2.58700700	1.90948800
O	-1.04917300	-1.28685900	2.98983000

H	-3.11712200	-2.70576300	3.98520200
H	-0.22443300	-5.44211900	-1.62923300
H	4.09085000	-2.59650800	-1.93215000
H	-0.26426900	4.37770000	-3.23922000
H	1.27524100	-5.12641800	-0.98298500
H	3.31116500	-3.83502600	-1.17172600
H	-3.44030300	-3.92526500	2.97690400
H	4.61754800	0.88469200	2.85052200
H	-0.76965900	-4.64066300	1.68815900
H	-3.96367300	-3.15100700	0.96633600
H	-2.15246200	-3.95901800	-1.95887300
H	-4.11657600	-3.20388900	-2.51582500
H	-1.65851100	2.26053800	-3.51199300
H	-4.27044100	2.73625900	-0.11884500
H	-1.85354100	4.31233800	-0.78068500
H	0.84808400	0.88349500	-3.00521600
H	0.99418600	2.84245600	0.57268100
H	1.19149400	4.43443400	-2.47671300

H	-3.50615600	0.84454300	2.02813700
H	-4.30009500	-0.00012000	0.06126400
H	-1.60681200	-0.72403900	-2.97464600
H	1.43543100	-3.02713000	1.46061400
H	0.77548000	-2.05085700	-2.49113400
H	6.41843400	-1.35111600	0.19278000
H	3.46655500	1.92894500	1.30653100
H	3.82884700	-0.46039000	-2.11131900
H	4.17141600	-2.21145500	1.21722200
H	-4.92521700	-1.78883100	-2.27511700
H	-4.85327000	0.73305100	-2.88105900
H	-4.20352800	2.22119300	-3.27309600
H	-2.82247000	3.85067800	2.89489200
H	-2.28583500	1.11432400	3.04664600
H	0.12871800	1.69337400	2.24851200
H	-0.13002500	3.27724800	2.63220200
H	-1.10543400	-1.58556500	3.90785700
H	1.14731800	0.16146300	1.67947400

H	0.20235700	-0.25522000	2.86724900
H	-2.19203400	4.87131200	1.81166900
H	5.80525900	-0.24580100	2.83508900
O	-2.54383900	3.69545700	4.57029900
H	-3.15101500	4.15977000	5.16865400
H	-2.54460100	2.74188700	4.83305500
O	-0.09399800	4.46541600	3.73091100
H	0.67764900	4.45473900	4.32027300
H	-0.89385300	4.28645200	4.28830300
O	-3.54679100	-1.37377100	5.03807600
H	-3.56829800	-1.68779500	5.95970300
H	-4.47262600	-1.15605700	4.82868900
O	-3.48435100	-4.76306700	-3.15416500
H	-3.40409900	-4.67113400	-4.12052300
H	-4.22992900	-5.37437900	-3.01465300
O	-4.24882600	3.77600500	-3.68110600
H	-3.34161000	4.15191500	-3.73938000
H	-4.66594300	4.26047000	-2.95009000

O	5.83229500	-2.84452800	1.31214800
H	6.19144300	-2.68862800	2.21406000
H	6.03369900	-3.76420900	1.07876200
O	7.10308400	1.82458400	-0.99162800
H	8.04027300	1.95075600	-1.20929700
H	7.02761900	0.89852700	-0.66168000
O	-1.65701500	5.01989700	-3.97492000
H	-1.78778700	5.93325700	-3.66456300
H	-1.51708400	5.10262600	-4.93480700
O	2.62213900	4.79510900	-1.61673100
H	2.34103400	4.55867400	-0.71238700
H	3.10201900	5.63822000	-1.56969300
O	-1.02294800	5.98249000	1.60511900
H	-0.46893300	5.71911600	2.37230600
H	-0.62525300	5.52008100	0.84083100
O	2.92321000	-5.38039500	-0.59829000
H	3.06731500	-5.46771900	0.35974700
H	3.37118300	-6.13972400	-1.00945500

O	-1.30348900	-6.45699500	-2.21835700
H	-1.72682700	-6.94738200	-1.49445300
H	-2.04031300	-6.01695900	-2.68958300
O	-5.98766900	-0.56136600	-2.74093400
H	-6.49223600	-0.74825700	-3.55175000
H	-6.65303500	-0.39966100	-2.04942100
O	5.29124700	-1.50268300	-2.62514300
H	5.80095300	-1.24454700	-1.80614500
H	5.90393200	-1.94655100	-3.23454100
O	6.55897600	-1.53173600	3.58147500
H	7.50327100	-1.37222800	3.75214200
H	6.16851500	-1.74103400	4.44745500
O	-4.50497900	-4.63325200	1.75899200
H	-5.44934000	-4.74081300	1.96167700
H	-4.21623600	-5.47691500	1.37240200
O	3.18376400	1.74962100	3.08131100
H	3.12588200	2.47617400	3.72192700
H	2.35279500	1.21352300	3.16580600

O	-2.15366700	1.02454100	4.72203800
H	-2.67783100	0.22189200	4.96400300
H	-1.25958700	0.87576000	5.07096000
O	-4.82719300	-0.13003900	1.73777600
H	-5.70498500	-0.06036900	2.14625100
H	-4.58035600	-1.07954600	1.69222000
O	3.17428100	2.23868600	-2.23034500
H	4.08472400	1.92206500	-2.58219800
H	3.19601000	3.22057500	-2.10893300
O	5.45980200	1.43489100	-3.08993400
H	5.50484900	0.46852900	-3.22056600
H	6.13627900	1.63570400	-2.38426600

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Al	-0.13685700	3.37198600	0.17938500
Al	-2.94200000	-1.87018800	-0.08500300
Al	1.93900600	2.27822500	-1.54886200
Al	-0.73797700	-2.80117700	-1.81802000
Al	-0.90195700	2.13110500	-2.35169800

Al	2.03981000	-2.66511800	-1.00407400
Al	3.40408600	-0.10211500	-0.79165000
Al	-2.26131700	-0.44178600	-2.53887200
Al	2.63663300	-1.55956000	1.60950000
Al	-2.25534900	-0.62334100	2.44290600
Al	-0.84041000	1.95956000	2.61293700
Al	0.50360200	-0.56573300	3.28777600
Al	0.05047700	-0.08386700	-0.01827000
O	-1.61770100	2.80556400	1.15805900
O	-2.44912400	1.12315800	3.14950500
O	0.64650200	2.70200300	1.76443200
O	-1.15423100	-1.23833500	3.79617500
O	2.18220000	-0.01469500	2.60133800
O	-1.18995200	3.64786700	-1.31847100
O	1.03046700	-2.13745200	2.40399000
O	-0.89404100	0.53002700	-3.30373200
O	2.57667000	0.67376600	-2.26025000
O	-2.45510300	1.24844000	-1.64222700

O	4.09317800	-0.68214900	0.83080700
O	3.51853900	-1.75289700	-1.66072000
O	2.92182600	1.56671400	-0.09630700
O	2.82988400	-3.13393200	0.63860300
O	0.93053000	-2.16138700	-2.42582300
O	0.79727600	2.59750800	-2.99998800
O	0.40989500	-3.43654700	-0.44300400
O	-1.65050000	-2.04292100	-3.25256400
O	-3.67759200	-1.21259800	-1.63846900
O	1.45227800	3.80184700	-0.63480800
O	-2.25165100	-3.40074200	-0.88273400
O	-3.19508400	-0.21332000	0.83356400
O	-2.22081000	-2.25884200	1.57135600
O	1.69295100	-0.93977200	-0.03032500
O	-0.27514600	5.22267200	0.75864800
O	3.42980800	3.26188300	-2.30282700
O	-1.87401700	3.01283200	-3.78237600
O	-1.11594600	3.45363700	3.83867200

O	5.18639300	0.46724400	-1.32347500
O	-3.49275000	-0.07014200	-3.99230600
O	1.25463700	-1.11620400	5.00602000
O	3.75969800	-2.31658800	3.02278000
O	2.65568200	-4.30145300	-1.87436200
O	-0.58487400	-4.46898800	-2.82174200
O	-4.63533800	-2.66269200	0.35699500
O	-3.89513600	-1.07248300	3.41451400
O	0.10787800	1.13046100	3.96860500
O	0.19615700	1.56322900	-0.80294500
O	-0.53050900	0.12862000	1.72462300
O	-1.18998900	-1.10892100	-0.91507000
H	-0.89418100	5.52289400	1.45746200
H	4.05715400	2.84053900	-2.92679000
H	-2.02381900	2.59635300	-4.65835800
H	-1.55818300	4.27492100	3.52487800
H	5.34348100	0.82458000	-2.22662000
H	-4.45508300	-0.05038700	-3.80481700

H	0.63893400	-0.89874800	5.74591800
H	4.53789100	-2.80242100	2.68293400
H	2.18105000	-5.13457900	-1.66138300
H	-0.25352000	-5.28033200	-2.38335600
H	-5.41031200	-2.65852600	-0.24868400
H	-4.27431800	-1.97330000	3.30950200
H	2.16794300	-0.83253500	5.22331700
H	4.02950000	-1.71520400	3.75373500
H	-1.49152600	3.17384000	4.70065200
H	0.51683100	5.79882600	0.69342000
H	-1.87374600	3.99198600	-3.83143000
H	-3.25189100	0.49511400	-4.75744600
H	0.95117500	3.31553000	-3.61613700
H	-1.21384900	4.51527900	-1.74860300
H	2.03367500	4.46374500	-0.23371100
H	1.36307500	3.15301400	2.21342900
H	-2.49311900	2.77932900	0.77255400
H	0.70908400	1.62240600	4.53091200

H	-3.30289100	1.52121100	2.91045200
H	-1.37840300	-1.11603400	4.73338400
H	-4.60576300	-0.41461700	3.25281300
H	-4.84801300	-3.06761000	1.22486300
H	-2.83866800	-4.08847400	-1.20158000
H	-4.53139900	-0.75712300	-1.69329600
H	-2.23954800	-2.60392700	-3.77756800
H	0.18765600	-3.28724900	0.48298900
H	1.19322000	-2.33969900	-3.33136400
H	-1.29347400	-4.66651000	-3.47280200
H	3.62841100	-4.43514500	-1.82057900
H	3.66431600	-3.60789600	0.70231600
H	4.34632300	-2.25195700	-1.72085400
H	5.00294900	-0.98794400	0.87528500
H	-0.16120800	0.13468000	-3.77538700
H	-3.26877100	1.74953800	-1.75010500
H	-2.91406900	0.50255900	0.24259900
H	-1.84325400	-3.07258400	1.90452500

H	2.21974600	0.81643900	2.10873200
H	0.99903400	-2.97155200	2.87916400
H	2.16455700	0.13672500	-2.93777300
H	3.55122900	2.10807400	0.38335900
H	3.38548700	4.23632000	-2.42107800
H	5.96833400	0.00581600	-0.97202600
H	-3.00417700	2.03716800	6.26229800
O	-2.19503800	1.84165200	5.77480300
H	-2.47344800	1.42914100	4.92754000
H	3.52530400	0.28691400	4.06217500
O	3.81187900	-0.31222100	4.77365500
H	4.47387700	0.14235000	5.30678000
H	-1.24787700	-0.90302900	7.25970700
O	-0.90817500	-0.50905600	6.44922400
H	-1.28024700	0.39758400	6.38858300
O	5.66683000	-3.53203900	1.35997500
H	6.29283000	-2.81482000	1.14220300
H	6.18546100	-4.23050300	1.77978100

H	-4.38651800	-4.28522800	3.13089100
O	-4.93971400	-3.52982600	2.89328200
H	-5.81728900	-3.71654300	3.25139500
H	-4.84179500	0.68470200	1.46944700
O	-5.10857200	1.04089600	2.33524900
H	-5.97213200	1.45499100	2.23504600
H	-7.53599200	-2.56148600	-1.08958200
O	-6.65226600	-2.55965800	-1.48075700
H	-6.61932100	-3.34704700	-2.04038700
H	0.71466600	-6.93050200	-0.75428000
O	0.76081500	-6.04822200	-1.13923800
H	0.51979900	-5.40035800	-0.45257300
H	-2.57926100	-4.42898800	-5.44537000
O	-2.68679400	-4.31468100	-4.49320300
H	-3.52825600	-4.73071200	-4.26970000
H	5.55710000	-4.01979500	-0.54801000
O	5.28306300	-3.91795800	-1.47660300
H	6.00974700	-4.24246700	-2.02062500

H	4.60777100	1.12844200	-4.34340900
O	5.11437100	1.66989900	-3.72412600
H	5.88803000	1.98560400	-4.20840800
O	6.91019000	-1.25605300	0.16172800
H	7.56314800	-0.77356200	0.68695100
H	7.41959600	-1.71676800	-0.51950600
H	2.26758900	6.12859900	-3.00213600
O	3.00993500	5.96391800	-2.40573900
H	3.73212700	6.51295200	-2.73820000
O	-2.48114100	1.52363800	-5.94004300
H	-1.73682700	1.08771600	-6.37474400
H	-3.03459400	1.88224600	-6.64573200
H	-0.80622200	6.10637100	-3.64197400
O	-1.54391100	5.63313200	-3.23849700
H	-2.26908300	6.26732600	-3.18486200
H	-6.38774400	-1.01557100	-2.51247000
O	-5.92585400	-0.19876000	-2.78281200
H	-6.51004500	0.53762000	-2.57237100

H	-2.09133900	6.50169000	3.21952600
O	-2.10944800	5.68489400	2.70376300
H	-3.00625500	5.60906300	2.35216000
H	2.49356800	6.41999200	-0.65749600
O	2.18875900	6.24617800	0.25398600
H	2.84197500	6.62648100	0.85070800

F-Al_{13}

O	4.10234600	-1.23131600	1.47957400
Al	2.74098000	-1.35543100	0.24900800
O	0.98053500	-1.31808200	-0.79369200
Al	0.14524700	-2.98316600	0.00948800
O	-0.75556000	-1.42194800	0.99782500
O	3.26661300	0.18924900	-0.63155200
O	1.63847100	0.12237300	1.16072600
O	-0.76180200	-4.37210300	0.83708000
O	-1.36557100	-2.56509200	-1.05925000
O	1.15149600	-4.08152800	-1.10445100

O	1.64417500	-2.63726600	1.10647800
O	3.45639800	-2.58742600	-0.92204500
Al	-2.52648600	-1.50928400	0.00857100
O	-4.11061600	-1.37692800	-0.96649000
O	-3.08313500	-2.98887200	0.97991900
O	-2.99543000	-0.02293000	1.09642100
O	-1.58742600	0.04562100	-0.86034900
Al	2.66906100	1.67293200	0.29163500
Al	-2.62847600	1.53926100	0.08992800
O	1.49977200	2.90569900	1.08345700
O	3.41056200	2.92377800	-0.83864200
O	3.93228300	1.53067000	1.64560400
O	0.90037200	1.52062100	-0.80249000
O	-1.57933900	2.69328000	-0.98129100
O	-3.26461800	2.95673800	1.10502000
O	-4.16627300	1.33823900	-0.90725700
O	-0.83021800	1.52743000	1.00161400
Al	-0.02196600	3.11391600	-0.00349000

O	0.87331300	4.14343800	-1.28061300
O	-0.86964800	4.35849800	1.06013400
H	-1.77656800	-3.31952300	-1.48830400
H	-0.84878200	-1.47345300	1.95541400
H	-0.16281300	-5.13773200	0.98278200
H	0.59776400	-4.76623600	-1.53007500
H	1.82997700	-3.03336100	1.95800000
H	1.07206900	-1.35964500	-1.75005400
H	3.71978000	0.26269700	-1.49302300
H	1.66364300	0.10920600	2.12388900
H	4.38932300	2.88482000	-0.90573000
H	3.96391200	2.24340700	2.29057300
H	1.02904300	1.61893500	-1.75714300
H	1.67119300	3.49392500	1.82003000
H	-2.00644900	3.30736800	-1.57895800
H	-0.85016800	1.63651900	1.95827200
H	-4.16436200	2.79600800	1.45599500
H	-3.85631000	-0.06211300	1.51822800

H	-1.61184900	0.05864000	-1.82184700
H	4.45702600	-2.10847800	1.73532000
H	4.37960400	-2.36446300	-1.16022500
H	0.34218700	4.75956800	-1.79627300
H	-0.30265700	5.14085300	1.20568900
H	-4.49687500	2.21261300	-1.21550200
H	-3.98816500	-2.85727900	1.33240400
H	-4.46423400	-2.24824300	-1.23826200
Al	2.67152200	4.23493500	-1.94613500
O	3.04616700	5.63158800	-0.66993500
H	3.86865200	5.70954100	-0.11786100
O	2.31040900	2.81186800	-3.21756400
H	1.76626900	2.89255100	-4.10797100
O	1.99945900	5.67539800	-3.09387000
H	1.91068300	5.63163200	-4.09043100
O	4.42316100	4.48543700	-2.78417100
H	5.00791700	5.24756900	-2.50859700
H	2.97461700	2.10130100	-3.29918300

H	2.43486800	6.54512400	-2.91922100
H	4.50026400	4.41844000	-3.76617800
H	2.27397600	5.96410400	-0.14166900
Al	5.21036500	0.17174800	2.10117800
O	6.25141900	1.60443800	2.86081300
H	6.77069100	1.48404900	3.70285700
O	6.57504900	-1.14645500	2.48677100
H	7.14150900	-1.52463800	1.78192000
O	4.51777000	-0.11206600	3.87680000
H	4.45806000	-1.04313400	4.21067000
O	6.05190600	0.35672300	0.39711600
H	6.16938700	1.21702800	-0.07904800
H	6.99794500	-1.32396500	3.37598800
H	6.54676100	2.42015100	2.39267800
H	4.52674400	0.49581500	4.65671900
H	5.97831800	-0.35066100	-0.28465500
Al	2.99533400	-4.33815100	-1.39791200
O	2.65538200	-6.15454700	-2.02810500

H	3.16432200	-6.42864400	-2.83017200
O	3.26687500	-5.06006700	0.38220600
H	3.84092500	-4.62537200	1.05619800
O	4.89891600	-4.64516300	-1.70015400
H	5.54198800	-4.95136800	-1.02518200
O	2.78675200	-3.87214100	-3.26972100
H	2.03196900	-4.20643900	-3.80540000
H	5.34523800	-4.56315800	-2.58585400
H	2.63989200	-6.91418400	-1.39137800
H	2.49566400	-5.46451000	0.86028500
H	3.22873700	-3.11512300	-3.73397300
Al	-2.59235000	-4.80231100	0.99684800
O	-2.20961000	-6.73150700	0.86464000
H	-2.15568800	-7.34987100	1.63288200
O	-4.50697200	-5.25194300	1.19476900
H	-5.03056300	-5.65294400	0.44150900
O	-2.49246500	-4.95464900	2.88985700
H	-3.06791500	-4.42241800	3.49689500

O	-2.80018800	-4.96712500	-0.94717800
H	-2.12365300	-5.39869000	-1.52120900
H	-4.86152100	-5.62390500	2.03476300
H	-1.70540600	-5.34994900	3.34713100
H	-2.66053400	-7.22186800	0.13658200
H	-3.56313800	-4.58973600	-1.48618100
Al	-5.42913900	-0.02939200	-1.07503800
O	-6.82707800	1.34193300	-1.26278800
H	-7.35797000	1.64841700	-0.48041900
O	-5.75779300	-0.07167600	0.86138200
H	-5.83922000	-0.92027900	1.36222600
O	-6.83904000	-1.38405200	-1.07668000
H	-7.30411900	-1.67385700	-1.91134700
O	-5.42478500	-0.00633100	-2.98858700
H	-5.36950100	0.82629800	-3.51031400
H	-7.44015700	1.24972000	-2.02800500
H	-7.53129200	-1.27177800	-0.38557500
H	-5.31006100	-0.81495700	-3.55760500

H	-5.77129000	0.71998000	1.47282400
Al	-2.68137300	4.71370600	1.48768300
O	-4.53573300	5.19761000	1.90610000
H	-4.72591500	5.73519400	2.71058600
O	-2.16260300	6.56970600	1.85820100
H	-2.08532400	6.91956800	2.79600600
O	-2.49860600	4.31424300	3.32753300
H	-3.19427400	3.86084700	3.84680700
O	-3.00550400	5.31203100	-0.34066200
H	-2.38943400	5.93908900	-0.79161900
H	-1.69685900	4.57927600	3.90991700
H	-2.45375900	7.33312400	1.31489400
H	-5.21850600	5.37208800	1.21774200
H	-3.60630900	4.85984000	-0.98235700
Al	0.05420100	0.07610000	0.11789900
O	5.38712000	5.98890600	0.60913500
H	5.39558000	6.68865500	1.27806800
H	5.77360700	6.38145200	-0.20302100

O	4.28600600	0.55785600	-3.11248600
H	5.14821800	0.95584300	-3.27932700
H	4.28283100	-0.26914500	-3.63925300
O	0.86595000	6.48099300	0.64529600
H	1.00712300	7.17330100	1.30336100
H	0.24156800	6.84224800	-0.02089000
O	0.98621600	3.16663400	-5.26690000
H	1.19395500	3.99510400	-5.73816500
H	0.56995800	2.54349400	-5.87289900
O	3.47091700	8.02489000	-2.88778300
H	3.19670700	8.74249500	-2.29948200
H	3.56895400	8.45650200	-3.74910700
O	5.72498000	6.65711200	-2.02768800
H	5.06704000	7.33450400	-2.29554100
H	6.58321400	6.94841300	-2.36568300
O	4.61106700	4.58137000	-5.54600000
H	5.36074900	5.12271800	-5.83383300
H	4.67125800	3.78686400	-6.09516700

O	-4.74842100	3.83758200	-1.73621500
H	-4.93330600	3.67222100	-2.68238000
H	-5.53293500	4.27579000	-1.34943700
O	-1.15872700	7.11009500	-1.16455200
H	-1.01415100	7.33767600	-2.09262100
H	-1.59232400	7.90539700	-0.76869700
O	-0.53518000	5.24480400	4.56709300
H	-0.07510400	4.87497400	5.33038600
H	-0.88203100	6.11577100	4.83043700
O	-4.63167300	2.98313800	4.60872600
H	-5.28957700	3.49062600	5.10335900
H	-4.33000400	2.31861300	5.24571800
O	-2.52264000	8.86201300	0.33326000
H	-3.33182300	9.21325400	-0.06425900
H	-2.07172700	9.63876600	0.69525800
O	-4.85863100	6.73400900	4.20259300
H	-5.40850500	7.52056100	4.07274000
H	-5.21166100	6.33777800	5.01086400

O	-6.33962200	5.46088300	-0.15180100
H	-6.35890800	6.31917000	-0.59951700
H	-7.26298400	5.30945700	0.09240100
O	-2.15635300	7.43805300	4.31845200
H	-1.90122900	8.31676900	4.62884900
H	-3.09535500	7.30852400	4.55445700
O	7.36405300	-1.59824600	4.92212000
H	7.46592100	-0.68344300	5.26777000
H	8.14005200	-2.10041600	5.20497200
O	7.31154500	1.09962000	5.24891000
H	6.57318100	1.34577900	5.84310500
H	8.10780900	1.54334700	5.57211900
O	6.95205800	3.81973100	1.39966100
H	7.87436900	4.07415700	1.54556400
H	6.43601200	4.65322500	1.34466100
O	7.82172300	-2.56300600	0.46045400
H	7.76324300	-3.53222000	0.53935000
H	8.75912700	-2.35333000	0.33559700

O	6.03572900	-1.68748600	-1.33514500
H	6.77534900	-2.10417500	-0.82755300
H	6.37476900	-1.52171900	-2.22218200
O	6.14958000	2.68743500	-0.82760400
H	6.57897000	3.19028200	-0.08503000
H	6.71513600	2.80866300	-1.59942800
O	4.86723400	-2.65777900	4.66054500
H	5.78350900	-2.47519900	4.96688700
H	4.41085600	-3.07273500	5.40496600
O	4.75768500	1.34564600	6.15823800
H	4.39635700	2.23602800	6.26810000
H	4.47961400	0.86803400	6.95279200
O	1.10765600	-6.25115200	1.40212700
H	1.29120400	-7.11958600	0.99586500
H	0.82175000	-6.39643800	2.33075000
O	6.90252400	-5.26705700	0.15648100
H	7.64739300	-5.62012200	-0.35398000
H	6.74911200	-5.95511300	0.82061700

O	4.15728100	-6.71379400	-4.30026700
H	3.68661700	-6.93764000	-5.11557400
H	4.76914600	-7.45526400	-4.18039900
O	5.73264500	-4.38464800	-4.18354800
H	5.22000100	-5.15043200	-4.51613600
H	6.62674200	-4.48491900	-4.53945300
O	0.58798100	-4.93030400	-4.62507900
H	0.10309600	-4.30558400	-5.18503600
H	0.77582300	-5.67002300	-5.22025200
O	4.30615400	-2.01132300	-4.44375400
H	5.01576200	-2.68735000	-4.50166800
H	4.10855000	-1.78244900	-5.36382900
O	2.40877200	-8.13130700	-0.19744800
H	3.19194800	-8.34678200	0.32916500
H	2.12445700	-8.98422400	-0.55650500
O	4.87884400	-3.75264400	2.13938900
H	4.84569600	-3.61201700	3.11653000
H	5.79380100	-3.98612600	1.94388400

O	-5.57095800	-2.47223500	1.98258600
H	-5.33841300	-2.74946800	2.90191700
H	-6.14848100	-3.16036300	1.63292200
O	-5.68030300	2.14737900	2.18840400
H	-6.62008500	2.35727300	2.02607200
H	-5.47435800	2.31886800	3.13338500
O	-8.79216300	-0.84233000	0.86412800
H	-9.69752300	-0.99012100	0.55260800
H	-8.76541800	-1.29746600	1.71768000
O	-8.06056300	-1.87731600	-3.36572200
H	-8.40901800	-0.98440600	-3.56200400
H	-8.78173300	-2.50278500	-3.51875700
O	-5.40264300	2.51498600	-4.16113700
H	-4.81259200	2.60204500	-4.92451500
H	-6.24574600	2.85736100	-4.48802800
O	-8.61871300	0.85671800	-3.35075000
H	-8.51463600	1.23639600	-4.23377600
H	-9.53130300	1.07543900	-3.11149400

O	-5.52335700	-2.35770300	-4.18520300
H	-5.18733300	-2.55112500	-5.07169900
H	-6.50215000	-2.35737000	-4.23026900
O	-8.14789000	1.88012500	0.97923200
H	-8.48311100	0.97187000	1.13676100
H	-8.90653500	2.46599800	1.10252600
O	-3.62113000	-8.07027100	-1.12279000
H	-3.26937900	-8.19873800	-2.01459500
H	-3.89339800	-8.95911300	-0.84886600
O	-0.39678900	-6.40025800	3.71673100
H	-0.03278700	-6.31579100	4.60904800
H	-0.81169000	-7.28718900	3.67396600
O	-5.72981500	-6.00394000	3.58406800
H	-5.48022700	-6.78204100	4.10066800
H	-6.69697200	-6.03992900	3.55971700
O	-0.63587400	-5.81093100	-2.30537700
H	-0.41127600	-6.74605400	-2.23133800
H	-0.40495600	-5.56031700	-3.22865800

O	-5.70667800	-6.23848900	-0.91434700
H	-6.60191900	-6.60370400	-0.92932500
H	-5.10766500	-6.96607200	-1.18233300
O	-4.85692500	-3.85378800	-2.00005100
H	-5.48031600	-4.58186300	-1.80894000
H	-5.03998500	-3.51769600	-2.90746400
O	-4.47469100	-3.68321800	4.16639700
H	-4.37494500	-3.24833000	5.02510400
H	-5.04243500	-4.47023100	4.30353300
O	-1.93297200	-8.50821100	2.93519500
H	-1.52132500	-9.35652000	2.71667800
H	-2.64561000	-8.73761200	3.54749300
O	2.06017600	5.57778300	-5.71760000
H	1.71243200	6.23561900	-6.33415700
H	2.99096600	5.39108300	-5.94947300

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