

Electronic Supplementary Information

Theoretical investigation on the dimerization of the deprotonated aquo ion of Al(III) in water

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1. Species in Reaction 1, 3 and 4 for gas-phase reaction system at B3LYP/6-311+G(d,p) level

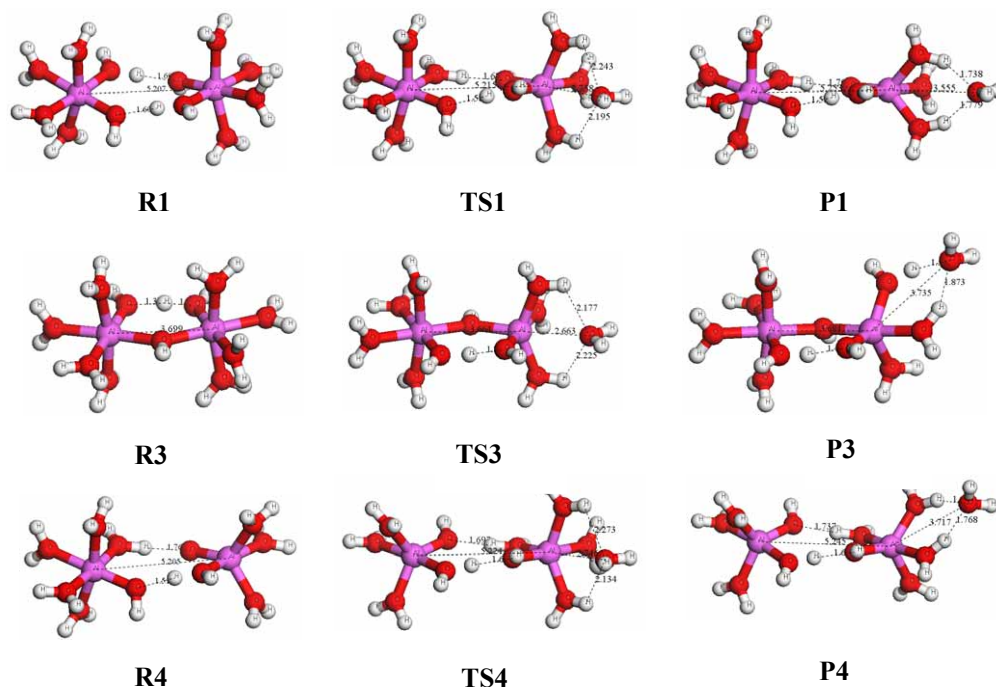


Figure S1. Species in Reaction 1, 3 and 4 for gas-phase reaction system at B3LYP/6-311+G(d,p) level

2. Species in Reaction 2, 5 and 6 for gas-phase reaction system at B3LYP/6-311+G(d,p) level

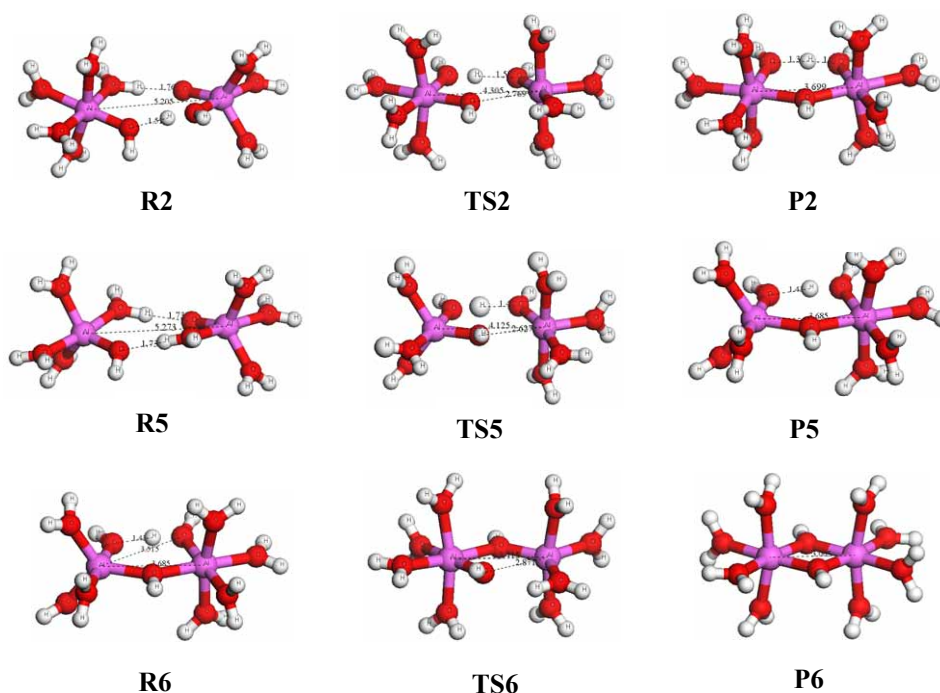


Figure S2. Species in Reaction 2, 5 and 6 for gas-phase reaction system at B3LYP/6-311+G(d,p)level

3. Selected structural parameters(\AA) for the complexes of Reaction 1, 3 and 4 in gas-phase reaction system

Table S1. Selected structural parameters(\AA) for the complexes of Reaction 1, 3 and 4 in gas-phase reaction system

complex	R1	TS1	P1	R3	TS3	P3	R4	TS4	P4
$r(\text{Al}-\text{Al})$	5.207	5.215	5.253	3.699	3.664	3.684	5.205	5.224	5.245
$r(\text{Al}-\text{O}_\text{I})$	1.991	2.758	3.555	1.994	2.663	3.735	1.972	2.746	3.717
$r(\text{HOH}\cdots\text{O}_\text{I})$	-	2.195,2.243	1.738,1.779	-	2.177,2.225	1.872,1.518	-	2.134,2.273	1.768,1.619
$r(\text{Al}-\text{O}_\text{I})$	1.946	1.899	1.895	1.952	1.911	1.900	1.960	1.900	1.886

4. Selected structural parameters(\AA) for the complexes of Reaction 2, 5 and 6 in gas-phase reaction system

Table S2. Selected structural parameters(\AA) for the complexes of Reaction 2, 5 and 6 in gas-phase reaction system

complex	R2	TS2	P2	R5	TS5	P5	R6	TS6	P6
$r(\text{Al}-\text{Al})$	5.205	4.305	3.699	5.273	4.125	3.685	3.685	3.415	3.005
$r(\text{Al}_\text{A}-\text{O}_\text{A})$	4.165	2.769	1.994	4.138	2.627	1.979	3.515	2.871	1.908
$r(\text{HOH}\cdots\text{OH})$	1.511,1.763	1.563	1.347	1.732,1.732	1.446	1.436	1.436	-	-
$\square\text{Al}-\text{O}-\text{Al}$	117.3°	137.7°	140.4°	121.6°	136.8°	141.8°	80.3°	91.2°	104.8°

5. The calculated energies of each reaction for the gas-phase reaction system, and supermolecular reaction system in gas phase and in aqueous solution

Table S3. The energies of each reaction for the gas-phase reaction system, and supermolecular reaction system in gas phase and in aqueous solution

complex	E (g) ^a	H (g) ^a	G (g) ^a	E _s (g) ^b	H _s (g) ^b	G _s (g) ^b	E _s (aq) ^c	H _s (aq) ^c	G _s (aq) ^c
R1/R _s 1	-1399.857351	-1399.856407	-1399.938337	-1705.789062	-1705.788118	-1705.892300	-1706.672445	-1706.671501	-1706.760988
TS1/TS _s 1	-1399.847986	-1399.847041	-1399.928983	-1705.783081	-1705.782137	-1705.885567	-1706.658152	-1706.657208	-1706.748045
P1/P _s 1	-1399.861697	-1399.860753	-1399.944752	-1705.800928	-1705.799984	-1705.903640	-1706.663266	-1706.662322	-1706.750636
R2/R _s 2	-1323.373313	-1323.372369	-1323.450311	-1629.324034	-1629.323090	-1629.421263	-1630.208639	-1630.207694	-1630.292029
TS2/TS _s 2	-1323.340139	-1323.339194	-1323.416300	-1629.291963	-1629.291019	-1629.387293	-1630.192480	-1630.191536	-1630.276115
P2/P _s 2	-1323.349114	-1323.348170	-1323.424819	-1629.338614	-1629.304731	-1629.303787	-1630.217959	-1630.217015	-1630.301801
R3/R _s 3	-1323.349114	-1323.348170	-1323.424819	-1629.299256	-1629.298312	-1629.394722	-1630.219067	-1630.218123	-1630.301974
TS3/TS _s 3	-1323.339760	-1323.338816	-1323.414889	-1629.293350	-1629.292405	-1629.388243	-1630.203491	-1630.202547	-1630.289599
P3/P _s 3	-1323.360856	-1323.359912	-1323.436498	-1629.311369	-1629.310425	-1629.407768	-1630.209320	-1630.208376	-1630.290848
R4/R _s 4	-1323.373313	-1323.372369	-1323.450311	-1629.316890	-1629.315946	-1629.416110	-1630.201729	-1630.200784	-1630.287708
TS4/TS _s 4	-1323.358907	-1323.357962	-1323.436738	-1629.309731	-1629.308787	-1629.408532	-1630.184462	-1630.183518	-1630.272188
P4/P _s 4	-1323.383138	-1323.382194	-1323.460707	-1629.323720	-1629.322776	-1629.424039	-1630.192734	-1630.191789	-1630.279770
R5/R _s 5	-1246.884250	-1246.883306	-1246.958466	-1552.850655	-1552.849711	-1552.943345	-1553.738778	-1553.737834	-1553.818729
TS5/TS _s 5	-1246.855674	-1246.855674	-1246.926864	-1552.821185	-1552.820241	-1552.912238	-1553.724927	-1553.723982	-1553.807810
P5/P _s 5	-1246.860755	-1246.859810	-1246.931838	-1552.831988	-1552.831044	-1552.922039	-1553.748495	-1553.747551	-1553.828145
R6/R _s 6	-1246.860755	-1246.859810	-1246.931838	-1552.833305	-1552.832361	-1552.922571	-1553.752350	-1553.751406	-1553.831098
TS6/TS _s 6	-1246.837986	-1246.837042	-1246.908377	-1552.812847	-1552.811903	-1552.901610	-1553.741315	-1553.740371	-1553.818832
P6/P _s 6	-1246.869982	-1246.869038	-1246.938974	-1552.835656	-1552.834712	-1552.925278	-1553.772759	-1553.771815	-1553.852743

^a The relative energies for the gas-phase reaction system. ^b The relative energies for supermolecular reaction system in gas phase.

^c The relative energies for the supermolecular reaction system in aqueous solution.

6. Cartesian coordinates of all supermolecular geometries optimized at B3LYP/6-311+G(d,p)

R_s1

O	3.24698400	-0.09103100	1.66741400
O	4.48718400	-0.63629300	-0.54559400
O	4.17339500	1.98617100	-0.02135200
O	2.97089400	0.93538200	-2.12335800
O	-0.87438700	0.91472200	0.89578400
O	1.69120500	-0.92541200	-0.62622800
Al	2.85238400	0.42905100	-0.18725800
O	-2.28364500	1.27201400	-1.40932900
O	-3.66762900	0.78086600	0.79540900
O	-3.39940500	-1.22106400	-1.07066300
O	-2.34194800	-1.34934600	1.49878400
Al	-2.17124900	-0.12282700	-0.02421000
O	-0.77340300	-1.07423100	-0.83945600
H	3.36240000	1.73526900	-2.50543000
H	2.44981300	0.48673300	-2.80359100
H	5.12410500	1.91437400	-0.19815000

H	5.03334000	-1.09194400	0.14867600
H	4.81837600	-0.87226200	-1.42383900
H	4.01112400	-0.63455200	1.97579800
H	2.81157700	0.32125000	2.42464700
H	2.03755500	-1.82403000	-0.65770100
H	0.31183300	-0.97596300	-0.72234800
H	-0.96013000	-1.81119500	-1.45046700
H	-3.11174500	-1.36094800	2.12315900
H	-1.74675700	-2.08287300	1.70153300
H	-4.35665100	-1.10010500	-1.13093800
H	-4.02158100	1.65286500	0.48687200
H	-4.17722300	0.44134900	1.57203500
H	-2.85128100	2.07509400	-1.29984200
H	-2.14691500	1.11781200	-2.35365200
H	-1.03661700	1.22935100	1.79334700
H	-3.12677500	-2.01773200	-1.61171400
H	4.04669100	2.78112000	0.51831300
H	1.51140100	2.47211800	0.17197400
O	1.48765100	1.52152500	0.32037400
H	0.12204600	1.16171100	0.62458400
O	5.53365300	-1.59505900	1.73895100
H	5.54116900	-2.54275300	1.94993300
H	6.36811500	-1.25420300	2.10090500
H	-4.54462000	-0.42223200	3.79869700
O	-4.58490400	-0.72200200	2.87577000
H	-5.40863400	-1.23358500	2.81917900
H	-3.95001900	3.95293200	-0.19758800
O	-4.15516400	3.07584700	-0.55967200
H	-4.97729100	3.20250000	-1.06147200
H	-2.25340400	-4.06095400	-2.13706500
O	-2.19560600	-3.13231800	-2.41256100
H	-2.25366600	-3.15821900	-3.38095300

TS₁

O	3.31408400	-0.01246200	1.62751400
O	4.42293500	-0.83067700	-0.49869800
O	4.51829500	2.21796400	-0.26918900
O	3.14192700	0.83154500	-2.00614500
O	-0.87911900	0.91524300	0.82376900
O	1.60495000	-1.13424700	-0.57744700
Al	2.77418100	0.16449700	-0.20925300

O	-2.21906300	1.19484700	-1.48432600
O	-3.67424900	0.92146400	0.72292900
O	-3.50937300	-1.18713000	-1.00847500
O	-2.45352000	-1.20282800	1.57905700
Al	-2.23084800	-0.10736900	-0.02207100
O	-0.90419100	-1.21144700	-0.76284000
H	3.69862900	1.63193500	-2.05277700
H	2.57695100	0.76294600	-2.78911800
H	5.47966000	2.09245300	-0.28300700
H	5.00860800	-1.20400500	0.21331400
H	4.78986900	-1.03270200	-1.37223900
H	4.10733200	-0.49954400	1.96791000
H	2.98217500	0.59782000	2.30053500
H	1.93864200	-2.03208500	-0.69154700
H	0.15278800	-1.14923200	-0.66428300
H	-1.12889500	-1.97406800	-1.33119500
H	-3.22638100	-1.12373200	2.19995100
H	-1.95178100	-2.00411800	1.78369500
H	-4.46349800	-1.03061800	-1.04542000
H	-3.94476100	1.81091000	0.37705200
H	-4.19478600	0.67040400	1.52592200
H	-2.72127900	2.04602000	-1.40117900
H	-2.22369100	0.93530800	-2.41701800
H	-0.97459700	1.14843200	1.75642200
H	-3.28371400	-2.03176500	-1.50245400
H	4.40745600	3.13715600	0.01906900
H	1.66165800	2.32263300	0.12055700
O	1.52550200	1.37742200	0.24356200
H	0.12201700	1.10993100	0.53977900
O	5.56999100	-1.49942000	1.82860700
H	5.56395200	-2.40888000	2.17106300
H	6.42732500	-1.13365000	2.10453600
H	-4.57218600	-0.02115200	3.81332900
O	-4.63903000	-0.38022500	2.91242500
H	-5.48766700	-0.85438700	2.89874300
H	-3.66188500	4.05353400	-0.39953100
O	-3.93729600	3.18110000	-0.72671800
H	-4.74280400	3.35419700	-1.24316900
H	-2.55499900	-4.14431300	-1.89168100
O	-2.42771400	-3.23831500	-2.21834700
H	-2.48049300	-3.31476500	-3.18546700

P₅I

O	3.36042300	1.94969700	-0.53315900
O	4.33687000	-0.07578800	0.71157400
O	5.58400200	-2.33610400	-0.34505100
O	3.41057900	-1.26525000	-1.38263500
O	-1.08776100	0.88482700	-0.95803700
O	1.59078800	-0.21775100	0.99857400
Al	2.68902200	0.17195800	-0.35604100
O	-2.25940700	-1.56102600	-1.14508100
O	-3.87974000	0.50786400	-0.86880000
O	-3.47708300	-1.11572200	1.30185600
O	-2.65672900	1.54318600	1.18864800
Al	-2.33112200	-0.07003500	0.11952200
O	-0.89285300	-0.67616500	1.17827100
H	4.23814300	-1.78574700	-1.15773200
H	2.97554900	-1.65221200	-2.15494400
H	5.58983500	-3.22083600	0.05466100
H	4.89616700	0.67398900	1.01827300
H	4.90641400	-0.87364000	0.63910700
H	4.16878500	2.32843800	-0.07959000
H	2.91732800	2.63104400	-1.05747500
H	1.99269400	-0.35815500	1.86364200
H	0.13435900	-0.46707200	1.07564000
H	-1.03177000	-1.24149300	1.96461800
H	-3.48832800	2.08173700	1.13726000
H	-2.11381700	1.85325500	1.92595600
H	-4.41730800	-1.29519700	1.16547500
H	-4.17057200	0.10051100	-1.72315900
H	-4.46540800	1.26234800	-0.61153100
H	-2.82055200	-1.59129200	-1.96096100
H	-1.92851400	-2.44859300	-0.95324400
H	-1.27156500	1.79763600	-1.21253600
H	-3.16491700	-1.57189500	2.13340700
H	6.44957400	-2.24822300	-0.77682600
H	1.47278900	0.59650500	-2.46923400
O	1.33272000	0.47714600	-1.52330500
H	-0.08279300	0.67374000	-1.19946800
O	5.51203200	2.43309300	0.92014800
H	5.48997300	2.99269400	1.71330300
H	6.37647100	2.60658900	0.51266300

H	-5.04712600	3.51550700	0.03077800
O	-5.00880500	2.62558200	0.41816400
H	-5.83298300	2.54228200	0.92549500
H	-3.94842900	-0.78333000	-3.94596800
O	-4.14730100	-1.08543500	-3.04495600
H	-4.91138200	-1.67702400	-3.14509100
H	-2.21111400	-1.84701900	4.20896900
O	-2.12729300	-2.18448900	3.30278100
H	-2.07773800	-3.14886800	3.40131000

R₂

O	-2.47177700	-1.70312500	-1.13360900
O	-3.76377200	-1.06454600	1.00855800
O	-3.73165000	0.71292800	-1.20957100
O	-2.83259600	1.42957800	1.13905800
O	-0.95297600	0.57940500	-0.92477200
O	-1.12595500	-0.74041800	1.28796500
Al	-2.38306800	-0.09288200	-0.02240200
O	3.68485500	1.51819400	0.78133100
O	1.57302200	0.96437300	-0.71657500
O	4.28416000	-1.03241300	1.20537900
O	3.63236000	-0.72962300	-1.29552800
Al	2.82701700	-0.06491300	0.27576600
O	1.51799200	-0.91826100	1.09035100
H	-3.48674600	2.13806900	0.90433800
H	-2.28855600	1.72620000	1.88149100
H	-4.24518700	1.53615800	-1.00699700
H	-4.16559000	-1.93044400	0.73647500
H	-4.31632100	-0.65878500	1.69171600
H	-3.08317400	-2.47393300	-1.01267500
H	-1.80916000	-1.90538400	-1.80782200
H	-1.38340500	-1.29318900	2.03789500
H	-0.12128400	-0.76153000	1.18561100
H	1.72258800	-1.71181100	1.59744900
H	4.46876500	-1.28557200	-1.32072100
H	3.30724700	-0.56692200	-2.19326100
H	5.01365700	-1.50338300	0.72634100
H	1.73113300	1.89204300	-0.96057800
H	0.54780400	0.76823600	-0.76790600
H	3.48926200	2.44649700	0.39576100
H	4.47650600	1.55271300	1.33905400

H	-1.17510800	1.08487000	-1.71526600
H	4.34798500	-1.23762800	2.15108100
H	-4.08408400	0.30543400	-2.01338000
H	6.70644600	-1.75832900	-0.97952300
O	5.82254100	-2.09901000	-0.75968700
H	5.88326700	-3.06073000	-0.88931500
O	3.01406600	3.67698100	-0.40373900
H	2.66503000	4.43490900	0.09165300
H	3.61001600	4.06071200	-1.06764400
H	-4.58268700	3.82289000	-0.41534600
O	-4.74174400	2.93804200	-0.04807700
H	-5.64812600	2.97362300	0.30018300
O	-4.39648000	-3.38139500	-0.22858500
H	-5.23504400	-3.50621900	-0.70312400
H	-4.21292900	-4.24284000	0.18078600

TS₂

O	-2.41392900	-1.75390400	-0.83665600
O	-3.77471300	-0.44976200	0.90304600
O	-2.88650900	0.85513700	-1.46141600
O	-2.22532000	1.73096400	0.89503300
O	-0.30515400	0.08034600	-0.61617000
O	-1.21001700	-0.71279900	1.64116300
Al	-2.01116300	-0.04720100	0.05831000
O	2.66325900	1.48753400	1.32180300
O	2.64168000	1.06829900	-1.18175800
O	4.07439900	-0.79213300	0.57628800
O	2.12715200	-1.49171500	-1.05295000
Al	2.30530600	-0.11317200	0.28631500
O	1.32884700	-0.80773100	1.58821200
H	-2.70617200	2.50060400	0.49803700
H	-1.85492900	1.98002400	1.75232100
H	-3.27860600	1.76501000	-1.42719200
H	-4.34617800	-1.23371200	0.70492000
H	-4.25219900	0.14429600	1.49852600
H	-3.22572700	-2.31155100	-0.69122100
H	-1.80846500	-2.22155200	-1.42441500
H	-1.63745300	-1.18312600	2.36820200
H	-0.18708900	-0.79609500	1.68104100
H	1.72795500	-1.37061500	2.26217600
H	2.78959800	-2.22150400	-1.18042200

H	1.23366400	-1.77842400	-1.28676200
H	4.41964300	-1.61917300	0.13637600
H	2.74888300	0.75284400	-2.09141100
H	3.05447500	1.97415600	-1.08547200
H	3.10200300	2.31845000	1.01023900
H	2.42018300	1.55675500	2.25700200
H	-0.25660100	0.65554900	-1.38759600
H	4.73088000	-0.45938600	1.20713000
H	-3.21904100	0.39929200	-2.24738000
H	5.01762500	-3.01516000	-1.64768900
O	4.38138700	-2.98487400	-0.91281200
H	4.43541100	-3.86421900	-0.50149700
O	3.74794300	3.34440100	-0.33034200
H	3.36298700	4.22447300	-0.47572400
H	4.70850000	3.48233100	-0.39157400
H	-3.33740700	4.13807500	-1.17409000
O	-3.68032400	3.34205400	-0.73643700
H	-4.61034300	3.54833300	-0.54526100
O	-4.77549800	-2.77825700	-0.06426700
H	-5.54570400	-2.81287400	-0.65565800
H	-4.85536900	-3.56841700	0.49537900

P₂

O	-2.11607900	-1.60367100	-1.09598500
O	-3.72724900	-0.58268600	0.63579700
O	-2.46020100	1.07460300	-1.30229800
O	-2.10363200	1.51542000	1.22719500
O	-0.02573200	0.13770500	-0.38374300
O	-1.22094800	-1.00987600	1.62961100
Al	-1.86394200	-0.11035000	0.15391400
O	2.07004900	1.71720300	0.95391200
O	2.41528800	0.76917800	-1.43929800
O	3.72935700	-0.40784700	0.75509100
O	2.07675700	-1.79812900	-0.73747000
Al	1.83092900	-0.09343400	0.23194600
O	1.15826000	-0.75045700	1.77530000
H	-2.53901700	2.35434900	0.92883900
H	-1.90763900	1.56101200	2.17395000
H	-2.83994000	1.98063900	-1.14137300
H	-4.24496000	-1.33937300	0.25934900
H	-4.26672700	-0.13811300	1.30536400

H	-2.92665600	-2.18859300	-1.11833800
H	-1.47256600	-1.93329500	-1.73585200
H	-1.70652000	-1.58245500	2.23565700
H	-0.11928300	-0.96626400	1.82214400
H	1.67524200	-1.16003400	2.47795900
H	2.95910600	-2.26742100	-0.75744200
H	1.39637400	-2.48402400	-0.72615900
H	4.27580800	-1.18139800	0.46802800
H	2.62104400	0.28114000	-2.25005400
H	2.89492000	1.64119800	-1.45483900
H	2.56817200	2.45177500	0.51614200
H	1.86361800	1.95257000	1.86948700
H	0.00008100	0.71822700	-1.15592500
H	4.23691100	0.10991800	1.39600100
H	-2.80579200	0.74649300	-2.14561600
H	5.25646500	-2.70294200	-1.13705300
O	4.59365600	-2.69410400	-0.42623400
H	4.78330300	-3.48952600	0.09947500
O	3.47985000	3.17704500	-0.86356700
H	3.15326900	3.99168700	-1.27989500
H	4.43728200	3.31754900	-0.77295200
H	-2.95917600	4.26750000	-0.49309400
O	-3.34441800	3.40541600	-0.26494400
H	-4.29529000	3.58182000	-0.16549200
O	-4.49975200	-2.76432200	-0.76915200
H	-5.19178200	-2.73006800	-1.45125800
H	-4.61871200	-3.62699200	-0.33695500

R₃

O	1.69364800	-0.82324600	2.08158300
O	3.84837200	-1.48236800	0.63507400
O	3.03180900	1.10127600	0.76764900
O	2.81639700	0.04683800	-1.56754500
O	0.40241700	0.37133500	0.05701300
O	1.39993500	-2.02275000	-0.51558300
Al	2.12144600	-0.52682100	0.16325500
O	-1.58226900	0.75718100	-1.90447300
O	-2.10054100	1.68988000	0.47753200
O	-3.33587200	-0.67396800	-0.23408100
O	-1.49703200	-0.55054100	1.85070400
Al	-1.47662300	-0.03312900	-0.11805900

O	-1.01877300	-1.72965900	-0.69297700
H	2.73019000	-0.51614100	-2.35064700
H	3.49591400	0.74491000	-1.73131400
H	3.66088000	1.63839800	0.20662900
H	4.66039100	-1.07689400	0.97771600
H	4.07403200	-2.39686200	0.40052100
H	2.16547400	-1.43880600	2.66488700
H	0.76926000	-0.76492400	2.36964800
H	1.79351000	-2.88854800	-0.66142800
H	0.01179700	-1.99863500	-0.68238400
H	-1.62531700	-2.43702000	-0.99533700
H	-1.86519900	0.09944800	2.50807200
H	-1.88289500	-1.41330600	2.07234800
H	-4.15103100	-0.17381400	-0.09068000
H	-2.34306500	1.90287400	1.41355900
H	-2.42473400	2.39777700	-0.13924300
H	-2.04164800	1.60941000	-2.11447800
H	-1.37052400	0.29226300	-2.72609600
H	0.53702700	1.32569600	0.00222400
H	-3.56723000	-1.56109500	-0.63882400
H	3.05961300	1.41611700	1.68319100
H	5.52347900	1.99691500	-1.19564400
O	4.55926700	2.11968500	-1.17382500
H	4.41814300	3.00414600	-1.55047700
H	-3.73707600	-3.85962000	-0.80479000
O	-3.40854800	-3.09459000	-1.30524200
H	-3.71367200	-3.24826600	-2.21453500
H	-3.48950300	1.54818900	3.50062700
O	-2.58229800	1.59201700	3.15350600
H	-2.10403800	2.13843100	3.79898300
O	-2.82858700	3.15662300	-1.68286300
H	-2.39101300	3.98804200	-1.93028700
H	-3.75886400	3.28896400	-1.93155300

TS₃

O	2.30786200	-0.82623100	2.04166000
O	4.42720000	-1.49819500	0.69295300
O	2.96193300	1.27644900	0.68991600
O	2.75586400	0.10412800	-1.55625600
O	0.30268800	0.40716000	0.24712500
O	1.45172300	-1.91209000	-0.42169900

Al	2.03012500	-0.34055900	0.17238600
O	-1.56814700	0.86851900	-1.78427400
O	-2.27289800	1.56772900	0.63221000
O	-3.38727700	-0.75453000	-0.45182700
O	-1.74101400	-0.75389300	1.78069100
Al	-1.57349300	-0.08031500	-0.06820800
O	-0.98936400	-1.70119300	-0.76045200
H	2.75088900	-0.55428300	-2.26714200
H	3.39084800	0.83327900	-1.77077500
H	3.54127200	1.81934700	0.08207600
H	5.28230000	-1.06562700	0.84286600
H	4.66893400	-2.40859800	0.45955000
H	3.16415400	-1.29326800	2.15457700
H	1.65882400	-1.18905300	2.66176900
H	1.91035300	-2.75767400	-0.44194000
H	0.02244800	-1.94986000	-0.68797000
H	-1.55003100	-2.40331200	-1.15898800
H	-2.14948100	-0.20931700	2.50176700
H	-1.92276200	-1.68650400	1.96810000
H	-4.23909600	-0.33460800	-0.26980300
H	-2.58623200	1.68133000	1.56720800
H	-2.58919700	2.31681300	0.06209500
H	-2.05127100	1.71896100	-1.94168200
H	-1.33593000	0.47113200	-2.63505700
H	0.34571000	1.35384200	0.43690400
H	-3.54665500	-1.62009300	-0.92273600
H	3.13895400	1.51847000	1.61181400
H	5.33089300	2.21388700	-1.38680000
O	4.36193400	2.28340300	-1.34631300
H	4.15937000	3.13718300	-1.76374900
H	-3.53338600	-3.93171200	-1.23952100
O	-3.20740100	-3.12154300	-1.66523900
H	-3.42159800	-3.23687500	-2.60571400
H	-3.85682500	1.13785300	3.52120500
O	-2.93129300	1.22148300	3.23571000
H	-2.49619000	1.69872400	3.96149300
O	-2.92916900	3.19356200	-1.43320900
H	-2.51546100	4.06102600	-1.57519500
H	-3.84816600	3.31223100	-1.72660900

O	2.78397000	0.84238800	-1.75361600
O	4.44559500	-1.12444800	-2.28451000
O	3.00562300	-0.94912600	0.09333700
O	2.78421900	1.15167900	1.57839000
O	0.33407000	-0.25532200	0.03063200
O	1.11104800	2.26672400	-0.20460700
Al	1.93816400	0.69459300	-0.05986200
O	-1.68586500	-0.01288300	1.96105300
O	-2.03111500	-1.84586000	0.12042500
O	-3.53679400	0.50651000	-0.04033300
O	-1.66586900	-0.26338500	-1.93933400
Al	-1.62399700	0.02787100	0.00087500
O	-1.31125500	1.84881600	-0.11634600
H	2.64359900	2.00452600	2.01744200
H	3.46532000	0.60957000	2.07737800
H	3.52067500	-1.15161000	0.91159900
H	4.29878000	-1.75359400	-3.01015600
H	5.40711100	-0.98079100	-2.27243000
H	3.46874300	0.21969400	-2.14176900
H	2.64334100	1.59945500	-2.34258800
H	1.49593000	3.14592400	-0.29089800
H	-0.32312400	2.19662800	-0.16400300
H	-1.99283700	2.55577300	-0.16096000
H	-2.00509400	-1.09354300	-2.35870300
H	-1.67913500	0.44958400	-2.59322900
H	-4.31000900	-0.07288500	-0.00995600
H	-2.27889900	-2.40220400	-0.66381700
H	-2.29531900	-2.29531600	0.96570300
H	-2.03961300	-0.77714100	2.48130300
H	-1.67324400	0.77468700	2.52281200
H	0.50806800	-1.20197100	0.12245100
H	-3.84492100	1.45379900	-0.09418600
H	3.52693800	-1.29504700	-0.67105900
H	5.39633400	-0.55973300	2.43471200
O	4.43386200	-0.69300200	2.46903400
H	4.28077700	-1.17610300	3.29798000
H	-4.11115800	3.59609600	-0.98989000
O	-3.76265500	3.16077300	-0.19450400
H	-4.10860900	3.68790600	0.54442800
H	-3.51717400	-2.94752500	-2.64596000
O	-2.60412900	-2.78420900	-2.35569700

H	-2.08245500	-3.47619900	-2.79432000
O	-2.64794900	-2.45374800	2.68562200
H	-2.13473500	-3.08421300	3.21722000
H	-3.56551100	-2.57706300	2.98136900

R₄

O	-3.31397700	1.55156900	0.91603500
O	-4.06192400	0.06036600	-1.06455700
O	-3.27662400	-1.70163200	0.67221000
O	1.27431300	0.09308800	1.55169100
O	-1.24857200	0.07139900	-0.97407800
Al	-2.57800600	-0.02182600	0.18878800
O	3.30523800	-1.60208500	0.92895500
O	4.01539500	-0.05129100	-0.99561600
O	3.26818900	1.74684800	0.69293000
Al	2.57666200	0.02952600	0.31496400
O	1.33148500	-0.06801500	-1.06415800
H	-4.05372300	-2.14154500	0.18911100
H	-2.87308500	-2.33617700	1.28271000
H	-4.61265100	0.86660300	-1.19566300
H	-4.58967800	-0.72850200	-1.32567700
H	-4.09733800	2.04685400	0.50514700
H	-2.93310000	2.07962300	1.63321500
H	-1.50251200	0.18736700	-1.89855800
H	0.30362900	-0.01524600	-0.98421000
H	1.58822700	-0.15941500	-1.99318700
H	2.87750800	2.36529200	1.32836400
H	4.04251100	2.18170300	0.21630700
H	4.55254900	0.74070000	-1.24076700
H	2.93470500	-2.11470800	1.66294900
H	4.08907300	-2.08719200	0.52307400
H	1.51009700	0.22405500	2.47846400
H	4.57567100	-0.85582600	-1.11967800
H	-1.54543900	-0.23085200	2.58177100
O	-1.32671400	-0.11260600	1.64585400
H	-0.30517600	-0.03284300	1.55591500
O	-5.22234400	-2.46546700	-0.86913000
H	-6.13249500	-2.55705900	-0.53922700
H	-5.11103400	-3.18958000	-1.50813900
H	-5.18261900	3.30648200	-1.03228700
O	-5.27830400	2.49567700	-0.50453800

H	-6.18999300	2.52000900	-0.16713600
O	5.23362600	2.42819700	-0.89712700
H	5.13437300	3.12967800	-1.56270600
H	6.14852700	2.51166300	-0.57849000
H	6.20977600	-2.47216400	-0.21331200
O	5.29539200	-2.45746100	-0.54375400
H	5.21823200	-3.24771200	-1.10450900

TS₄

O	-2.23907600	-1.95185500	-0.25219700
O	-3.93553200	0.04987700	0.11324900
O	-1.88483600	-0.07327300	-2.00082700
O	-2.10678400	1.90800300	-0.33098700
O	0.65185900	0.01291700	-0.50041700
O	-1.29541800	-0.02586900	1.53221800
O	3.00713700	-1.63240000	0.90801100
O	3.43281100	0.00081400	-1.06542800
O	3.02294400	1.60309300	0.93789700
Al	-2.05368800	-0.01797300	-0.07300100
Al	2.17444400	-0.00610100	0.42922900
H	-1.60446600	-2.57061800	0.13811100
H	-3.14668500	-2.37531100	-0.22029100
H	-4.46410400	0.88860300	0.12111500
H	-4.52319900	-0.74912900	0.12508900
H	-1.94884400	0.70364700	-2.57971200
H	-1.96182300	-0.88127500	-2.53384600
H	-2.97748000	2.40156100	-0.27321200
H	-1.40154000	2.49236600	-0.01761900
H	2.81214900	2.12953900	1.72363400
H	3.75204800	2.05906500	0.40466600
H	3.95371100	-0.79530400	-1.32025000
H	3.95938200	0.79693000	-1.30798400
H	3.73163100	-2.08624800	0.36695600
H	2.79005200	-2.17059800	1.68396400
H	0.76371300	0.01237500	-1.45747600
H	-1.85352700	-0.03816500	2.32040800
O	1.15867900	-0.01680700	2.01702700
H	0.11722000	-0.01974700	1.88713200
H	1.40142900	-0.02122500	2.95329600
H	5.72144000	-2.45130300	-0.62125800
O	4.77150300	-2.44384300	-0.82902600

H	4.62952100	-3.23459300	-1.37605500
O	4.79452500	2.42866300	-0.78503300
H	5.74461700	2.42196600	-0.57794700
H	4.66076000	3.23135700	-1.31652600
H	-4.95663100	3.15362100	0.72815100
O	-4.65349000	2.65705800	-0.05123900
H	-5.18435700	3.00408700	-0.78855500
H	-5.19970800	-2.95522400	0.75310300
O	-4.84834000	-2.49414100	-0.02790800
H	-5.39299500	-2.81133300	-0.76859100

P₄

O	1.82667500	1.93119200	-0.33532800
O	3.55661300	-0.00018300	0.03573500
O	1.71482300	-0.00199200	-2.15331300
O	1.82675000	-1.93178000	-0.33485500
O	-0.31425800	-0.00120100	-0.35063700
O	1.35707700	-0.00080100	1.69043000
O	-2.75436900	1.68132100	0.93714300
O	-2.98694800	-0.00007600	-1.00950900
O	-2.75634000	-1.67995900	0.93896900
Al	1.63625100	0.00030500	-0.15237800
Al	-1.93001300	-0.00012300	0.64154000
H	1.13545800	2.58563300	-0.16418300
H	2.71938900	2.38264800	-0.24319500
H	4.11947500	-0.81313800	0.04493200
H	4.11943500	0.81261400	0.04562000
H	1.90807700	-0.78789200	-2.68959700
H	1.91177600	0.78138000	-2.69197100
H	2.71980600	-2.38242700	-0.24460300
H	1.13689000	-2.58606500	-0.15761700
H	-2.63699900	-2.18561000	1.75849600
H	-3.44714200	-2.12016000	0.35410500
H	-3.50616300	0.79543200	-1.28589700
H	-3.50673700	-0.79521000	-1.28561400
H	-3.44471000	2.12168000	0.35207900
H	-2.63429100	2.18756100	1.75619000
H	-0.51911700	-0.00214200	-1.29719200
H	2.02520500	-0.00216000	2.38863200
O	-1.05497400	0.00108300	2.18769700
H	0.37971600	0.00019000	2.06981100

H	-1.40237500	0.00134900	3.08714400
H	-5.37442600	2.36098000	-0.82921600
O	-4.41203800	2.38295800	-0.96925900
H	-4.26331400	3.15970700	-1.53463600
O	-4.41443400	-2.38273000	-0.96584300
H	-5.37681000	-2.35962800	-0.82591700
H	-4.26635900	-3.16058000	-1.52987700
H	4.71220500	-3.05501900	0.74534300
O	4.38110400	-2.59971400	-0.04769900
H	4.90913800	-2.96237200	-0.77952600
H	4.70831000	3.05676500	0.74839200
O	4.37851500	2.60170200	-0.04533800
H	4.90688700	2.96553100	-0.77635100

R₅

O	3.10655700	1.62704300	0.87897700
O	3.73207300	-0.93752300	0.70421700
O	3.31673200	-0.07426800	-1.68481300
O	-1.46475100	0.63495000	-1.45586500
O	1.12924900	-0.92802300	0.77889400
Al	2.36088200	0.20508800	-0.06394400
O	-2.62691100	-2.01316400	-1.40982100
O	-4.05574700	0.16350600	-1.91842100
O	-4.31542900	-1.07761100	0.51358400
O	-3.35613000	1.36069700	0.44531900
Al	-2.77921600	-0.29524200	-0.41954000
O	-1.48049600	-0.82625300	0.71296400
H	3.02561300	0.26152900	-2.54480600
H	4.22570400	-0.49075900	-1.75791700
H	4.57661600	-1.15126000	0.24309100
H	3.54581600	-1.61736900	1.40586800
H	3.84820900	1.47372600	1.48271400
H	2.94800600	2.66160000	0.81629800
H	1.39440200	-1.64643200	1.39402100
H	0.10856000	-0.84592700	0.73348200
H	-1.74371200	-1.02489200	1.61860500
H	-2.81151300	2.15338300	0.54494100
H	-4.16367100	1.43912000	1.01740800
H	-4.94871500	-0.55814000	1.07781100
H	-4.20950100	1.06691000	-2.23857900
H	-4.85746600	-0.34200100	-2.12925800

H	-2.91102500	-2.27154900	-2.30047600
H	-2.03581100	-2.69946600	-1.06573100
H	-1.53387300	0.79851100	-2.40603400
H	-4.52616100	-2.02073400	0.57810100
H	1.13922900	1.99309000	-1.12983000
O	1.00592100	1.07375100	-0.86977500
H	-0.47914800	0.77407000	-1.17631800
H	2.43327500	4.63235900	1.44151100
O	2.76399600	4.10258300	0.70122100
H	3.39608900	4.66394900	0.22740700
O	5.65357700	-1.22819700	-1.26951400
H	6.48440000	-0.72506500	-1.29694000
H	5.87590100	-2.09816200	-1.64042300
O	2.62687300	-2.64087900	2.43349800
H	2.70449100	-2.50234700	3.39127600
H	2.72242000	-3.59914000	2.31150900
H	-6.48839600	1.18518300	1.57269500
O	-5.61545800	0.86085200	1.85111000
H	-5.64184100	0.88211000	2.82226900

TS₅

O	-3.15088900	1.66081000	-0.79891600
O	-3.83060700	-0.89645900	-0.63840400
O	-3.27861100	-0.08591900	1.74007400
O	1.47277300	0.55047900	1.32569900
O	-1.23967500	-0.92871600	-0.85397700
Al	-2.40030400	0.20414200	0.07986200
O	2.84039900	-1.88766800	1.34068100
O	4.43430700	-0.09321700	2.29770400
O	4.26906700	-1.02696900	-0.71046200
O	3.40123600	1.33424300	-0.33827200
Al	2.68566500	-0.35838700	0.18059700
O	1.38727700	-0.85977700	-0.91547500
H	-2.94052800	0.23010600	2.59032200
H	-4.19034000	-0.48994000	1.85058900
H	-4.65519200	-1.10383100	-0.13957500
H	-3.69174700	-1.56717100	-1.35905800
H	-3.92268900	1.53582000	-1.37078300
H	-2.95466000	2.69110400	-0.73854900
H	-1.54904900	-1.63374100	-1.46668900
H	-0.22373200	-0.85966600	-0.86442200

H	1.61928100	-1.15489800	-1.80341000
H	3.06478100	2.18531600	-0.02467300
H	4.19585800	1.47162200	-0.92289900
H	4.89568100	-0.47721200	-1.25419800
H	4.38131400	0.35764700	3.15471300
H	5.38776100	-0.17935800	2.14501100
H	3.45842200	-1.83153500	2.09554200
H	2.29468600	-2.68710900	1.37763300
H	1.59990500	0.69305700	2.27276500
H	4.53761100	-1.95768400	-0.74186400
H	-1.08729000	1.95679800	1.09282700
O	-0.98605300	1.03023100	0.84260900
H	0.46510200	0.71412300	1.09420700
H	-2.38638400	4.63604400	-1.37235400
O	-2.71164200	4.11710000	-0.62184900
H	-3.31108600	4.69810700	-0.12935100
O	-5.65032900	-1.19313300	1.42735000
H	-6.47019100	-0.67783400	1.50852800
H	-5.86712900	-2.06724200	1.79194900
O	-2.82341600	-2.58907600	-2.44316100
H	-2.94150500	-2.43926400	-3.39524200
H	-2.91724800	-3.54844800	-2.32756200
H	6.45049900	1.27482100	-1.63049600
O	5.55617900	1.00383200	-1.89857400
H	5.52803200	1.14947400	-2.85914200

P₅

O	3.36367900	-0.95888500	-1.33455000
O	3.73789400	1.21314700	0.14991200
O	3.01562800	-0.74947900	1.72032900
O	-1.43311500	-1.57990000	0.36854800
O	0.99542000	0.94681000	-0.11292200
Al	2.39199600	-0.13725000	0.05324100
O	-3.70756100	-0.74666400	1.65644500
O	-6.05167900	0.41969400	1.66859500
O	-4.18828900	0.79976200	-0.34390900
O	-3.51418000	-1.50108900	-1.38975900
Al	-2.77172000	-0.44953000	0.03461400
O	-1.57085800	0.87750000	-0.47109600
H	2.65952300	-1.51039300	2.20037200
H	3.81267600	-0.35984400	2.20897800

H	4.42027900	1.19631700	0.85252600
H	3.84534500	2.09899000	-0.37573200
H	4.18695000	-0.59885800	-1.69605700
H	3.19500300	-1.88726200	-1.69495200
H	1.17519400	1.88696500	0.00707700
H	-0.54885100	0.85081400	-0.34260200
H	-1.85129700	1.72369700	-0.88227500
H	-3.15738700	-2.35519600	-1.68118100
H	-4.31155700	-1.29787600	-1.90606900
H	-4.02769300	1.65804300	-0.82908300
H	-6.87112900	-0.09231200	1.56087400
H	-6.27563300	1.12230700	2.30180400
H	-4.62546700	-0.38267100	1.85920700
H	-3.38886000	-1.27133900	2.40593100
H	-1.59196100	-2.41292900	0.82658300
H	-5.02199100	0.85425300	0.18000500
H	1.40574700	-2.46364700	-0.54408600
O	1.19831900	-1.65443600	-0.03809700
H	0.20034100	-1.58823800	0.10441300
H	2.31224400	-3.61175400	-2.80150300
O	2.62191600	-3.37769500	-1.91182100
H	3.17350900	-4.12711600	-1.63311400
O	5.11095300	0.51971800	2.55979900
H	5.98365800	0.09385300	2.58765900
H	5.08971100	1.10695100	3.33309800
O	3.99604600	3.40497100	-1.09321800
H	4.44658200	3.50592600	-1.94410600
H	4.10206400	4.24956700	-0.63198500
H	-3.28808700	3.07495600	-2.50194400
O	-3.17851600	2.93083200	-1.54785400
H	-3.27775200	3.81065000	-1.14917600

R₆

O	-1.98897400	-1.64661000	-0.76151900
O	-3.66948500	-0.13075300	0.49748000
O	-2.03583600	0.93148400	-1.58531100
O	-1.87203100	1.88331700	0.82212300
O	0.18694300	0.05781700	-0.22472100
O	-1.34077500	-0.57740700	1.84260000
O	2.59611300	-2.04028100	0.11510100
O	2.82649300	0.27840900	-1.00723400

O	2.78629400	1.02699900	1.46289400
Al	-1.74735200	0.06251700	0.14306800
Al	1.84952900	-0.35552100	0.56722600
H	-1.28018000	-2.25153600	-1.01866900
H	-2.85769800	-2.14420700	-0.77557200
H	-4.23574700	0.51392600	0.94718000
H	-4.22118700	-0.91203700	0.22738200
H	-2.32060900	1.88357300	-1.67366100
H	-2.30081900	0.45218400	-2.38519500
H	-2.16589900	2.67438600	0.29792000
H	-1.71184100	2.13647800	1.74349000
H	2.71376200	1.17684500	2.41864400
H	3.47312400	1.64366000	1.06370000
H	3.28261600	-0.35338400	-1.61652000
H	3.38060100	1.09689200	-0.97053600
H	3.22808500	-2.22848900	-0.64455800
H	2.49570200	-2.82804600	0.67247700
H	0.32824000	0.47950300	-1.08466300
H	-1.96081400	-0.93294900	2.49369300
O	1.06627700	-0.95413200	2.05163900
H	-0.33125300	-0.80153500	2.08206200
H	1.46549400	-1.32890500	2.84552600
H	5.07706800	-2.03005100	-1.95841400
O	4.10909000	-1.96289600	-2.02734400
H	3.88709900	-2.43965300	-2.84494100
O	4.40085200	2.38054100	-0.09904600
H	5.36465700	2.26293600	-0.04102300
H	4.27898300	3.32657200	-0.28591900
H	-3.62701800	3.80541300	-1.22887300
O	-2.70458800	3.50175800	-1.17324700
H	-2.18314100	4.24272900	-1.52524000
H	-4.76776600	-3.22070700	0.06964800
O	-4.51259000	-2.48266700	-0.51033600
H	-5.12203000	-2.53917500	-1.26639900

TS₆

O	-2.28466600	-1.95997800	0.18895800
O	-2.17500700	-0.24209200	2.15626900
O	-3.25071000	0.26374100	-0.67609400
O	-1.54863200	1.79276200	0.47479400
O	-0.14454000	-0.43378800	-0.60949200

O	0.59890900	0.65946500	1.42105000
O	1.99679900	-1.69939600	1.04710700
O	3.37653000	0.64809500	0.76193300
O	2.44349500	-1.00078900	-1.38775400
O	1.78672500	1.58026400	-1.07273900
Al	-1.68940700	-0.08697400	0.31477000
Al	1.64197700	0.00138200	0.10483600
H	-1.78183100	-2.76463000	0.38304500
H	-3.15308500	-2.21924700	-0.24638300
H	-2.67240600	-0.97605300	2.55419100
H	-2.03059900	0.44020500	2.83265100
H	-3.90377100	-0.41705100	-0.98496200
H	-3.61511300	1.18546600	-0.79705300
H	-0.72277000	2.13578500	0.85970500
H	-2.20986000	2.47952900	0.19473600
H	1.15793200	1.86560100	-1.74875000
H	2.52932200	2.24364200	-1.01566500
H	2.75830600	-0.57829300	-2.20043400
H	2.92201500	-1.86702400	-1.27984900
H	3.81914700	1.48539300	0.46416700
H	3.92273700	0.23225900	1.44429600
H	2.57021600	-2.43832600	0.71297000
H	1.77229100	-1.85754400	1.97478900
H	-0.19327800	-0.99811500	-1.39223500
H	0.96541000	0.97112400	2.25536000
O	3.54194800	-3.29554700	-0.49366800
H	3.26293000	-4.16939000	-0.81457900
H	4.50100300	-3.37970500	-0.35771500
H	4.02268000	3.80246000	-0.01967000
O	4.02077700	2.95068200	-0.48798100
H	4.77130400	3.00433200	-1.10386200
H	-3.73458900	3.45241800	-1.40779800
O	-3.73831500	2.90075800	-0.60706400
H	-4.46186900	3.25895300	-0.06440300
O	-4.59345600	-2.04958600	-1.09899400
H	-5.43607200	-2.23827900	-0.65032000
H	-4.68232200	-2.45755400	-1.97772200

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O	1.84506600	1.71194200	0.99563600
O	2.48968100	-0.64228100	2.03048300

O	2.97640700	0.13277700	-0.72951300
O	1.64434800	-2.01174000	-0.08812400
O	0.11713800	0.31605800	-0.87118700
O	-0.20148100	-0.32354100	1.30770500
O	-1.86511000	1.85850400	0.72443700
O	-3.02688300	-0.55325200	1.09745600
O	-2.61907300	0.73405800	-1.47068400
O	-1.73454100	-1.74052700	-0.78561100
Al	1.44934100	-0.11641300	0.40840100
Al	-1.53369000	0.05798200	0.00086500
H	1.35322500	2.26297000	1.61832300
H	2.61517200	2.24047200	0.63437500
H	2.86277600	-0.02830000	2.68240900
H	2.82875400	-1.52702200	2.23752200
H	3.52399400	0.95646500	-0.75717400
H	3.44263200	-0.59923500	-1.20480700
H	1.12253500	-2.75857900	0.23491000
H	2.37825700	-2.34778900	-0.67879700
H	-1.24974800	-2.06339900	-1.55761700
H	-2.46192000	-2.38158500	-0.55615400
H	-2.96418200	0.20940800	-2.20770200
H	-3.02926700	1.64049900	-1.50523000
H	-3.49292300	-1.42677100	0.98568000
H	-3.55029900	-0.00072900	1.69626700
H	-2.42341500	2.54654500	0.26474100
H	-1.66792200	2.16523800	1.61991300
H	0.26353000	0.71541100	-1.73505800
H	-0.33913500	-0.68631600	2.18993800
O	-3.44011000	3.23790500	-0.95214500
H	-3.13643300	4.00511600	-1.46653300
H	-4.37086600	3.43075300	-0.74519600
H	-3.79106800	-3.76313000	0.87686500
O	-3.85938800	-2.97895700	0.30597300
H	-4.70193900	-3.09091900	-0.16709000
H	3.70151100	-2.53768200	-2.61963700
O	3.76480000	-2.29962000	-1.67928400
H	4.58681700	-2.71991800	-1.37356800
O	4.00485000	2.61539100	-0.26674400
H	4.85041900	2.73997900	0.19730700
H	3.98040200	3.32438000	-0.93134600