Supporting Information

Infrared spectroscopic study of solvation and size effects on the reactions between water molecules with neutral rare-earth metals

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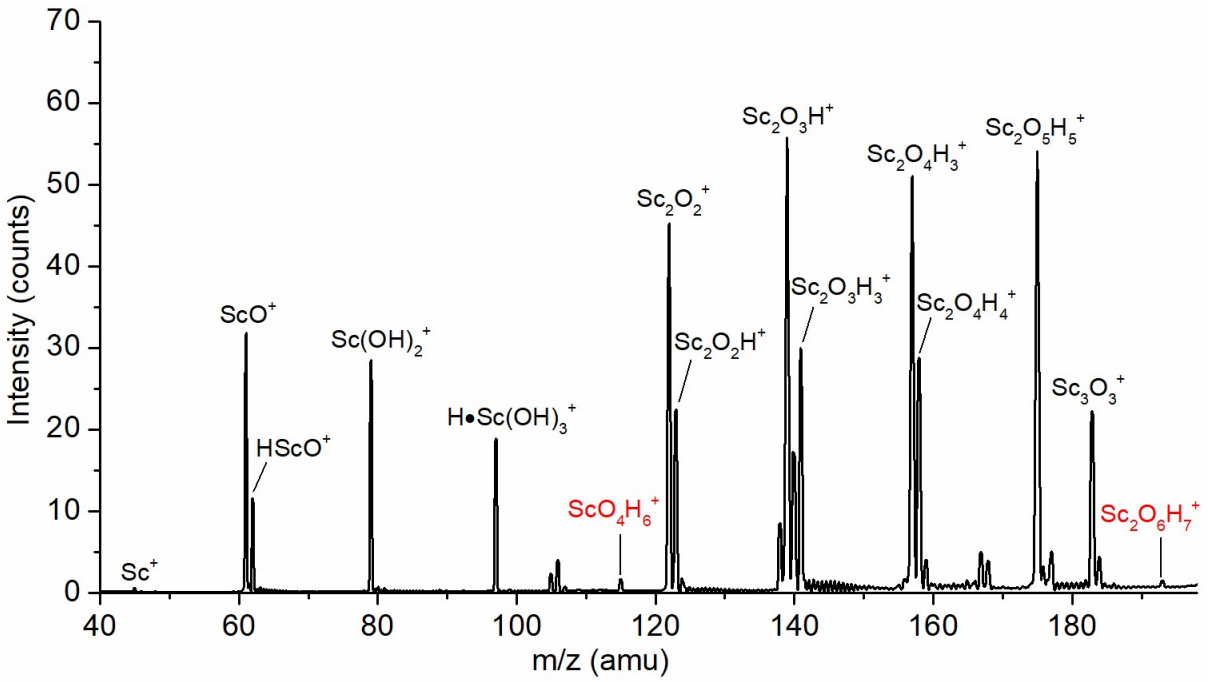


Fig. S1 Time-of-flight mass spectra of the species formed from the reactions between water molecules and scandium metals.

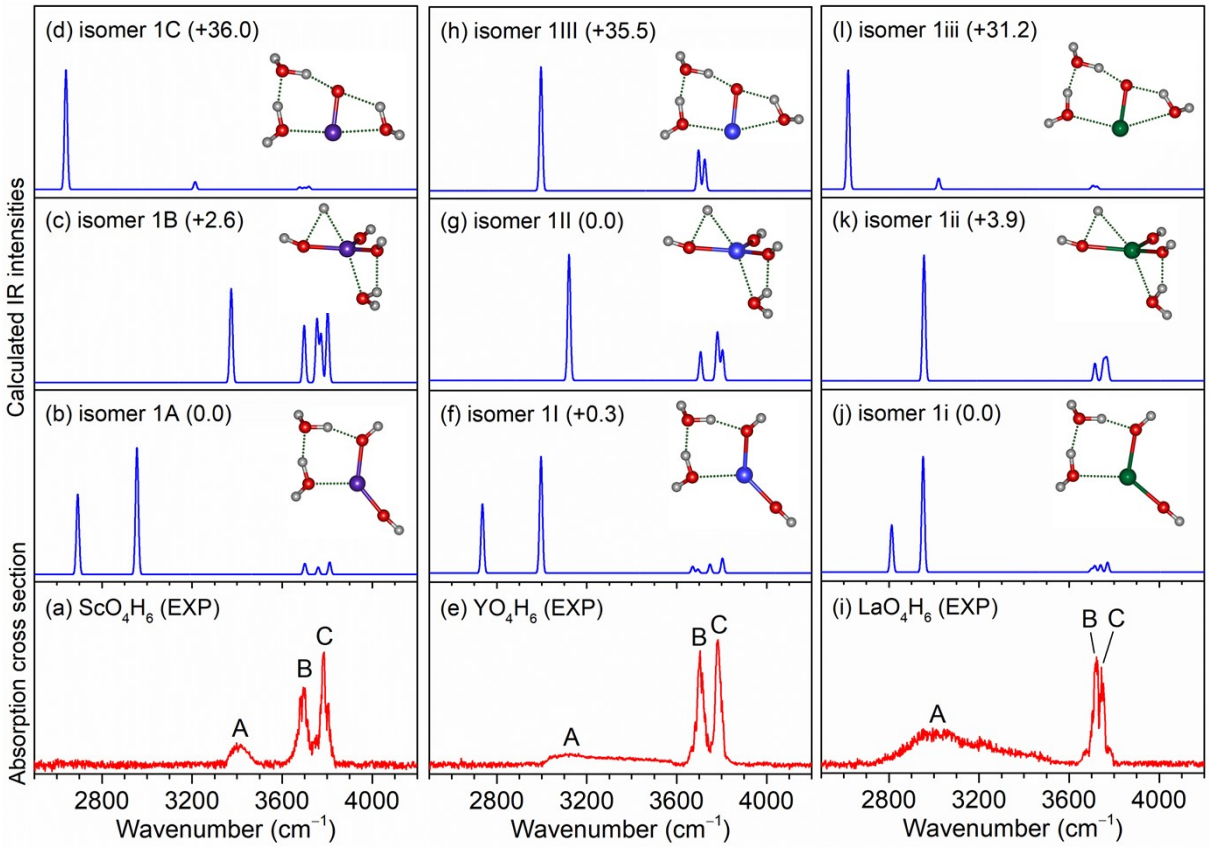


Fig. S2 Comparison of experimental IR spectra of neutral MO_4H_6 (M = Sc, Y, La) complexes and calculated IR spectra of the three types of isomers. Calculations were carried out at the TPSSh/def2-TZVP level of theory, with the harmonic vibrational frequencies scaled by a factor of 0.968. Relative energies (in parenthesis) are listed in kcal/mol. The structures are embedded in the inset (O, red; H, light gray; Sc, purple; Y, blue; La, olive).

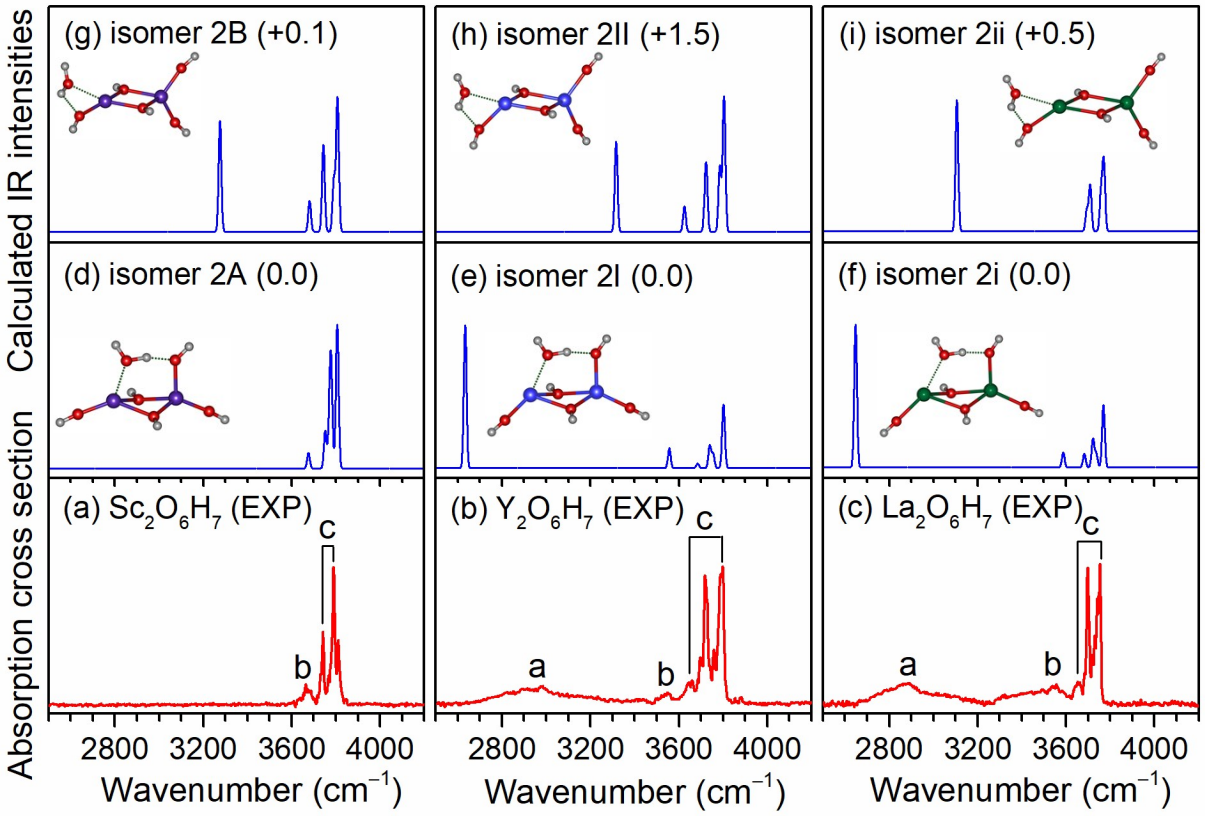
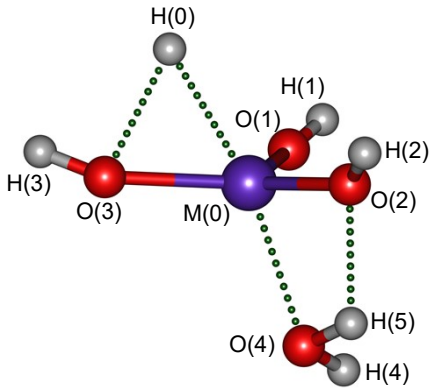


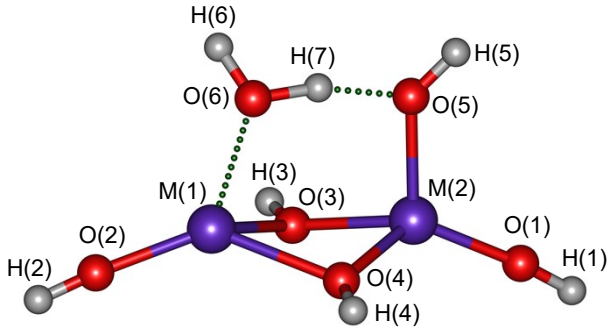
Fig. S3 Comparison of experimental IR spectra of neutral $M_2O_6H_7$ (M = Sc, Y, La) complexes and calculated IR spectra of the two types of isomers. Calculations were carried out at the TPSSh/def2-TZVP level of theory, with the harmonic vibrational frequencies scaled by a factor of 0.968. Relative energies (in parenthesis) are listed in kcal/mol. The structures are embedded in the inset (O, red; H, light gray; Sc, purple; Y, blue; La, olive).

Table S1. Comparison of the experimental band positions of MO_4H_6 (M = Sc, Y, La) with the calculated values of isomers 1B, 1II, and 1ii obtained at the THSSh/def2-TZVP level of theory (IR intensities are listed in parentheses in km/mol and the harmonic vibrational frequencies scaled by a factor of 0.968). The atoms are labeled for discussions.



Species	Label	Exptl	Calcd	Mode
ScO_4H_6	A	3398	3374 (162)	Symmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	B	3694	3698 (98)	Antisymmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	C	3786	3758 (109)	Stretching mode of the O(3)H(3) group
			3772 (83)	Stretching mode of the O(2)H(2) group
			3802 (125)	Stretching mode of the O(1)H(1) group
YO_4H_6	A	3104	3121 (397)	Symmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	B	3704	3706 (89)	Antisymmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	C	3784	3779 (106)	Stretching mode of the O(3)H(3) group
			3785 (67)	Stretching mode of the O(2)H(2) group
			3803 (94)	Stretching mode of the O(1)H(1) group
LaO_4H_6	A	2952	2956 (579)	Symmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	B	3722	3714 (80)	Antisymmetric stretching mode of the O(4)H(4) and O(4)H(5) groups
	C	3748	3751 (80)	Stretching mode of the O(3)H(3) group
			3762 (54)	Stretching mode of the O(2)H(2) group
			3769 (74)	Stretching mode of the O(1)H(1) group

Table S2. Comparison of the experimental band positions of $M_2O_6H_7$ (M = Sc, Y, La) with the calculated values of isomers 2A, 2I, and 2i obtained at the THSSh/def2-TZVP level of theory (IR intensities are listed in parentheses in km/mol and the harmonic vibrational frequencies scaled by a factor of 0.968). The atoms are labeled for discussions.



Species	Label	Exptl	Calcd	Mode
$Sc_2O_6H_7$			2474 (533)	stretching mode of the O(6)H(7) group
	b	3662	3675 (38)	stretching mode of the O(6)H(6) group
	c	3742	3751 (92)	stretching mode of the O(5)H(5) group
		3788	3770 (126)	stretching mode of the O(4)H(4) group
			3778 (210)	stretching mode of the O(3)H(3) group
		3810	3804 (209)	stretching mode of the O(2)H(2) group
			3806 (154)	stretching mode of the O(1)H(1) group
$Y_2O_6H_7$	a	2930	2631 (609)	stretching mode of the O(6)H(7) group
	b	3548	3555 (83)	stretching mode of the O(6)H(6) group
	c	3694	3684 (18)	stretching mode of the O(3)H(3) group
		3758	3738 (95)	stretching mode of the O(4)H(4) group
			3754 (59)	stretching mode of the O(5)H(5) group
		3798	3799 (140)	stretching mode of the O(2)H(2) group
			3802 (135)	stretching mode of the O(1)H(1) group
$La_2O_6H_7$	a	2880	2643 (528)	stretching mode of the O(6)H(7) group
	b	3556	3586 (54)	stretching mode of the O(6)H(6) group
	c	3656	3681 (48)	stretching mode of the O(3)H(3) group
		3698	3721 (104)	stretching mode of the O(4)H(4) group
		3754	3735 (49)	stretching mode of the O(5)H(5) group
			3767 (126)	stretching mode of the O(2)H(2) group
			3768 (102)	stretching mode of the O(1)H(1) group

Cartesian coordinates of the low-lying isomers, intermediates, and transition states for MO_4H_6 and $M_2O_6H_7$ shown in Figures 1-5, S2, and S3 calculated at the THSSh/def2-TZVP level of theory.

Isomer 1A

Sc	-0.74745000	-0.03500500	-0.03023800
H	-3.57406400	0.03125600	0.02488500
O	-2.62114400	0.09295600	-0.02194200
H	0.54727300	-2.47331800	0.20529400
O	0.54519500	-1.52381100	0.06506900
H	1.64149800	1.10240000	0.00843800
O	2.72317100	-0.05127700	0.03435100
H	0.76526900	2.34555400	0.56255100
O	0.73391000	1.56954600	-0.00889100
H	2.03759700	-0.78988300	0.06166400
H	3.22982200	-0.18020800	-0.77653900

Isomer 1B

O	-1.56476300	0.00341600	1.25012300
H	-1.99293900	0.84987600	1.43194400
O	1.67941900	-1.02189900	0.65781000
H	2.61112600	-0.99293400	0.89017000
O	-1.15472700	-0.88965700	-1.14512500
H	-1.27312400	-1.58466500	-1.79504800
H	1.89743100	-0.81039000	-1.21870400
H	-2.05130200	-0.42890300	0.51166300
O	0.46456000	1.87778500	-0.31999600
H	0.50590700	2.76173200	-0.68368900
Sc	0.23366600	0.02133900	-0.12756400

Isomer 1C

O	-0.11342100	-1.12591000	-0.10252900
Sc	-0.58141600	0.57198800	-0.08181300
O	1.45715700	1.29721500	0.00765400
H	1.88117400	2.00375300	0.50610200
H	2.02887800	0.43107900	0.06563000
O	-2.61435700	-0.40309500	0.03883100
H	-2.01592600	-1.19573600	0.08132000
H	-3.17678000	-0.40738700	0.82426000
O	2.42087600	-1.03657800	0.15524100
H	2.86486500	-1.40328800	-0.61856700
H	1.42549300	-1.29323400	0.06575500

Isomer 2A

H	-0.04079200	-0.73316800	-2.24122300
H	-0.01875600	-0.66354000	2.26153200
Sc	1.54297900	-0.19316100	-0.01269200
Sc	-1.62290900	-0.20300100	-0.01092100
O	1.37995500	1.78873100	-0.09027700
H	1.99956000	2.51582000	0.00895500

O	3.26587800	-0.94085800	0.05209800
H	4.09920500	-1.40944600	0.07465900
O	-1.15915200	1.93445200	0.09827600
H	-1.55127700	2.51081900	-0.56999600
O	-3.39949300	-0.82226700	0.02583200
H	-4.27076500	-1.21605400	0.03435800
O	0.06428400	-0.56907800	1.31137600
O	0.04771500	-0.73209200	-1.28647600
H	-0.13214800	2.04387000	0.04096000

Isomer 2B

H	-0.01845500	1.82936900	1.17906200
H	-0.29312200	-2.00160600	-1.20161700
Sc	-1.77523700	0.02302300	0.01181700
Sc	1.46814900	-0.18292200	-0.07553800
O	-2.76706200	0.70513900	-1.43087900
H	-3.48228000	1.01408100	-1.98560100
O	-2.76346600	-0.55389200	1.50092200
H	-3.47545600	-0.79354000	2.09281300
O	3.06717700	1.42517900	0.25240300
H	3.68362400	0.66187700	0.12245400
O	3.17874300	-1.12359200	-0.07464400
H	3.71630000	-1.90428400	0.06122300
O	-0.24248800	-1.24542900	-0.61019400
O	-0.08790900	1.10358600	0.55260700
H	3.23827400	2.06406800	-0.45190300

Isomer 1I

Y	-0.61662100	0.02283600	-0.20728400
H	-3.43049700	-0.01019700	0.72971800
O	-2.53164800	0.02990700	0.40510200
H	0.72490800	-2.47996500	0.39885100
O	0.72753000	-1.56516500	0.10568500
H	1.94901900	1.08000600	0.19956000
O	2.96848500	-0.15419000	0.18918800
H	1.19769600	2.46825300	-0.15820300
O	1.06711400	1.58911300	0.21921500
H	2.25482200	-0.86161000	0.16615800
H	3.50040300	-0.28441100	-0.60551200

Isomer 1II

Y	0.21490100	0.03685200	-0.10165700
O	-1.74242400	-0.20180000	1.30396000
H	-2.23686000	0.54280100	1.66696100
O	1.73774000	-1.26029300	0.53257500
H	2.55561600	-1.74450400	0.65795800
O	-1.46051100	-0.66323800	-1.18835400
H	-1.84795500	-1.09756500	-1.94888400
H	1.90284800	-0.96671400	-1.29056600
H	-2.15378900	-0.45676700	0.43064000
O	0.54540600	2.03975600	-0.07489200
H	0.75731000	2.97011900	-0.13781700

Isomer 1III

O	-0.06310600	1.28224800	0.01128600
O	-1.72552400	-1.13358600	0.04859700
H	-2.29959300	-1.87001400	-0.18466300
H	-2.25509900	-0.22321300	0.00889900
O	2.46217400	0.85984300	-0.08696400
H	1.69782300	1.50978800	-0.01133700
H	3.13267600	1.07979800	0.57075200
O	-2.57435900	1.21454800	-0.10230000
H	-2.96723900	1.61558500	0.68187300
H	-1.54971700	1.44428700	-0.07215300
Y	0.49865800	-0.54719600	0.00106900

Isomer 2I

H	0.05583500	-0.47055400	2.38963900
H	0.28056600	-0.83378000	-2.14260900
O	-1.58128700	1.94816700	-0.16581600
H	-2.12672300	2.72881800	-0.28740100
O	-3.44436000	-1.16003200	-0.11487800
H	-4.25593000	-1.66517400	-0.14685200
O	1.01634200	2.12308200	-0.21840000
H	1.33420600	2.71548900	0.48328500
O	3.40105900	-1.06176200	-0.52805400
H	4.18521400	-1.55485800	-0.76736500
O	0.09291400	-0.55540200	-1.24181200
O	-0.05418400	-0.55935200	1.43618700
H	-0.00518600	2.20119000	-0.24020100
Y	-1.67623400	-0.16643800	-0.00663200
Y	1.80669900	-0.06429900	0.19570100

Isomer 2II

H	-0.15069200	-1.48617500	1.62918400
H	0.27145700	1.47847500	-1.91323100
Y	1.88602400	-0.00611100	0.06683500
Y	-1.66229800	0.02097700	-0.32425600
O	3.10376700	-1.21262900	-1.02195000
H	3.75771800	-1.74676800	-1.47070900
O	2.78374400	1.23066900	1.40739700
H	3.34973700	1.75156700	1.97560100
O	-3.34158100	-1.26986600	0.89884900
H	-3.89774300	-0.46137700	0.78932600
O	-3.31317700	1.22524700	0.04126800
H	-3.77179000	2.05677800	0.16704500
O	0.21031700	0.93340100	-1.12210100
O	-0.00820600	-0.93120700	0.85587500
H	-3.76291100	-1.97721600	0.38750200

Isomer 1i

La	-0.50738300	0.06833500	-0.07675000
H	-3.60150600	-0.10464000	0.31639200
O	-2.66200900	-0.05603600	0.13252500
H	0.86403000	-2.65491400	0.42547000
O	0.85358000	-1.72448400	0.18496900

H	2.24143200	1.07049900	0.09276200
O	3.07444500	-0.32432400	-0.00664900
H	1.71031000	2.44949600	0.70890500
O	1.46332000	1.71465500	0.13677100
H	2.34605000	-1.01716300	0.08749300
H	3.52581700	-0.51687100	-0.83720800

Isomer 1ii

O	-2.04917300	-0.29000900	1.26324000
H	-2.63572400	0.32857400	1.71276400
O	1.77140200	-1.52968900	0.42509300
H	2.51769800	-2.13252500	0.47083400
O	-1.69670800	-0.43298500	-1.25405000
H	-2.17623500	-0.72653300	-2.03119100
H	1.85876000	-1.21397400	-1.37436100
H	-2.35703900	-0.39309100	0.30966400
O	0.77957000	2.13794900	0.06668800
H	1.08282900	3.04719400	0.05854200
La	0.19770100	0.03523200	-0.05533400

Isomer 1iii

O	-0.21102600	1.41075400	-0.05656700
O	-1.99375600	-1.05576900	0.10623700
H	-2.62410900	-1.74881400	-0.11538000
H	-2.46882500	-0.13710500	0.05535900
O	2.37618900	1.28803600	-0.01397300
H	1.51666100	1.80573000	0.00319600
H	2.97540100	1.66235500	0.64178400
O	-2.75481100	1.35811200	-0.09311600
H	-3.11316800	1.80255800	0.68401600
H	-1.74143900	1.57222200	-0.10568100
La	0.45829300	-0.50817600	-0.01235000

Isomer 2i

H	0.14177500	-0.71714500	2.40212800
H	0.22333100	-0.81891700	-2.26760100
O	-1.70334900	2.12765400	-0.11352800
H	-2.20531600	2.93955800	-0.22650300
O	-3.74373300	-1.22181900	-0.14232100
H	-4.56101200	-1.72004300	-0.19575100
O	0.90097400	2.31834900	-0.18578400
H	1.19046300	2.90328200	0.53200600
O	3.70122600	-1.17358900	-0.49197700
H	4.48055200	-1.67735900	-0.73298300
O	0.05697900	-0.50668000	-1.37266300
O	0.00451500	-0.69388300	1.44801000
H	-0.12089200	2.36785200	-0.20332400
La	-1.83517700	-0.15585300	0.01268600
La	1.96005800	-0.02094500	0.11991300

Isomer 2ii

H	0.04435900	1.44953000	1.83988900
H	-0.21705500	-1.55373900	-1.93528200

La	-2.06105900	0.01074200	0.04667100
La	1.82781100	-0.04035000	-0.19389400
O	-3.30827600	1.34625500	-1.16205400
H	-3.92571100	1.90416000	-1.63755100
O	-3.14902600	-1.31980400	1.40683600
H	-3.73417000	-1.85427600	1.94594600
O	3.85885700	1.27226000	0.88621700
H	4.29979900	0.42168500	0.60532000
O	3.80680700	-1.13585800	-0.09288800
H	4.37206700	-1.90100700	0.03307700
O	-0.16802100	-0.98037800	-1.16264800
O	-0.02560500	0.96972900	1.00734400
H	4.33796600	2.00370000	0.47787100

H_2

H	0.00000000	0.00000000	0.37118300
H	0.00000000	0.00000000	-0.37118300

ScO

O	0.00000000	0.00000000	-1.20379000
Sc	0.00000000	0.00000000	0.45858700

OH

O	0.00000000	0.00000000	0.10877400
H	0.00000000	0.00000000	-0.87019400

H_2O

O	0.00000000	0.00000000	0.11775500
H	0.00000000	0.76397200	-0.47102000
H	0.00000000	-0.76397200	-0.47102000

$HSc(OH)_3$

O	-1.75326900	-0.74390900	-0.20429600
H	-2.65691300	-0.41110400	-0.19216800
O	1.50898500	-1.14966200	-0.06184500
H	2.23698900	-1.75702200	-0.18770700
H	-1.36144400	-0.49417100	1.50010100
O	0.25553700	1.86359400	-0.06579100
H	0.65731700	2.72523200	-0.17822200
Sc	0.04924000	0.00842300	0.08159300

HSc_2O_2

Sc	1.34274400	0.00013000	0.06921200
Sc	-1.43266600	-0.00002700	-0.03793900
O	-0.05763600	-1.27707400	0.02729100
O	-0.05759600	1.27702400	0.02708400
H	2.81022500	-0.00175200	-1.09172700

HScO

Sc	0.05509400	-0.41674300	0.00000000
H	-1.59773100	-1.31101400	0.00000000
O	0.05509400	1.25782700	0.00000000

$Sc(OH)_2(H_2O)$

O	-1.60424900	-1.27653800	-0.10139200
H	-2.40197800	-0.81051200	-0.40252300
O	1.92887300	-0.62033400	-0.05187500
H	2.86876500	-0.77564800	-0.13610800
H	-1.79887600	-1.61215100	0.79632700
O	-0.55412500	1.79558300	-0.01849300
H	-0.61870000	2.74770600	-0.09014900
Sc	0.18032400	0.06004400	0.05745400

$Sc(OH)_2$

Sc	0.00000000	0.41742200	0.00000000
O	1.65995300	-0.41177800	0.00000000
H	2.33425600	-1.09183100	0.00000000
O	-1.66004100	-0.41099500	0.00000000
H	-2.33355300	-1.09184800	0.00000000

$ScO(H_2O)$

O	0.76586200	1.16918000	0.01248200
Sc	0.51478600	-0.50530100	0.00310800
O	-1.65203700	0.04874700	-0.08848100
H	-2.37465300	-0.10888900	0.53366800
H	-1.34644200	0.97679900	0.00905300

IM1

Sc	-0.83527600	-0.05954600	-0.28782800
Sc	1.91044500	0.04261400	0.16543000
O	0.59843800	-1.28370200	0.01614900
O	0.51434600	1.26822800	-0.11887800
H	-2.19640200	-0.12992400	-1.69291900
O	-2.85616400	-0.00460400	0.57039100
H	-3.02005000	-0.02758100	-0.44689400
H	-3.41505700	0.67369500	0.96887900

IM2

Sc	1.68397200	-0.41126600	-0.06035800
Sc	-0.86949600	0.72470700	0.02459800
O	0.94436600	1.31531000	-0.01429700
O	-0.10926500	-1.04712700	-0.03090000
H	3.17404300	-1.06642100	0.90095900
O	-2.69202300	-0.67609400	0.09067000
H	-2.00596100	-1.38071800	0.00150600
H	-3.41670800	-0.87184100	-0.51529000

IM3

H	-0.49807300	2.38516800	0.13181300
Sc	1.05292200	-0.00848200	-0.01999400
Sc	-1.83479200	-0.11225900	-0.10529200
O	2.94079900	-0.07324500	-0.07402000
H	3.85785000	-0.34831600	-0.06059900
O	-0.46210300	1.42378500	0.15029500
O	-0.38615300	-1.23504800	0.23362300
H	-3.68084200	-0.42523000	0.08059900

IM4

H	-0.52315800	3.78879600	-0.12397500
Sc	0.96165600	-0.07825200	-0.22796700
Sc	-1.80247300	-0.19165000	0.13242600
O	2.78710700	-0.05555400	0.29441900
H	3.64738700	-0.05547400	0.71331300
O	-0.49488700	1.14724300	0.03369800
O	-0.41049800	-1.41598500	-0.12531200
H	-0.52084900	4.52898500	-0.20541300

IM5

Sc	0.90798000	-0.00001100	0.14731300
Sc	-1.87154000	-0.00006200	-0.11794700
O	-0.51464600	-1.28412700	0.01419400
O	-0.51441500	1.28403500	0.01120000
H	1.44552500	0.00599600	2.50187500
O	2.67703600	-0.00087900	-0.55396500
H	2.12842200	0.00468500	2.18909200
H	3.47701000	-0.00138600	-1.07907000

IM6

Sc	0.94636200	0.00000800	-0.23094700
Sc	-1.81890600	-0.00000200	0.12559600
O	2.77350500	0.00008500	0.28982700
H	3.63386100	-0.00060400	0.70850300
O	-0.46865700	1.28453500	-0.05090900
O	-0.46865400	-1.28456100	-0.05093500

IM7

Sc	1.34873200	-0.05126300	-0.16728700
Sc	-1.36019600	0.66142000	-0.00206400
O	3.11439200	-0.62239100	0.28204500
H	3.97345500	-0.85239800	0.63432600
O	0.32467400	1.52023000	0.15189200
O	-0.34768800	-0.94948800	-0.31850100
O	-2.88414800	-1.06545800	0.13874800
H	-2.04370800	-1.57728200	-0.00588100
H	-3.34685900	-1.44675400	0.89445400

IM8

H	-0.00023500	2.42349600	-0.08662600
Sc	-1.45565600	-0.02309700	0.04047200
Sc	1.45571900	-0.02317500	0.03971900
O	-3.34616400	-0.16008500	0.07542800
H	-4.24595000	-0.48560400	0.04430300
O	3.34623600	-0.15996400	0.07598700
H	4.24594200	-0.48583100	0.04609300
O	-0.00015000	-1.20319700	-0.22167700
O	-0.00005600	1.46320300	-0.14071200

IM9

H	-0.15971300	-0.00249700	2.39932900

Sc	-1.62725400	0.04174900	-0.05097200
Sc	1.32759700	-0.18756300	-0.00894200
O	-3.49082800	-0.29516900	-0.09650200
H	-4.36904900	-0.60266500	-0.31972500
O	2.97718200	-1.11972800	-0.03349900
H	3.61264500	-1.78647800	-0.29607200
O	-0.11417600	-0.43064900	-1.16069400
O	-0.15118200	-0.10675000	1.44336900
O	1.40011800	2.03462500	-0.10083400
H	0.42259600	2.24009700	-0.13597100
H	1.81738900	2.55500300	-0.80407400

IM10

H	-0.15263500	-0.00359700	2.29233600
H	-0.15422200	0.00225900	-2.29204300
Sc	1.42645800	0.00014900	-0.00021500
Sc	-1.78736300	-0.00091600	0.00048000
O	2.41984800	-1.58798600	-0.00156900
H	3.13343200	-2.22509200	-0.00135800
O	2.41745500	1.58972300	0.00111400
H	3.12927400	2.22879000	0.00211100
O	-3.66625000	0.00118500	-0.00061400
H	-4.62247600	0.00263400	-0.00077500
O	-0.19547000	0.00056400	-1.33173300
O	-0.19487900	-0.00209900	1.33207000

IM11

Sc	-1.83485500	0.00000300	-0.29965500
Sc	0.95800200	-0.00000400	-0.01621000
O	-0.40560500	-1.35028500	0.54005300
O	-0.40560100	1.35028300	0.54004800
O	2.83187200	0.00000700	-0.23146100
H	-0.28525800	-0.00000400	-1.47783300
H	3.75708700	0.00001800	-0.47720300
H	-0.61160300	-2.21413000	0.89951000
H	-0.61165400	2.21408600	0.89957200

IM12

Sc	-1.70234300	-0.00165600	0.34720500
Sc	1.03192600	0.00202200	-0.11666800
O	-0.48163600	-1.36778400	-0.59818400
O	-0.48523600	1.36967300	-0.59501700
O	2.79997200	-0.00215900	0.48573200
H	-3.30624100	-0.00503800	1.28787600
H	3.69170200	-0.00241500	0.83199800
H	-0.48258700	-2.32780100	-0.65274800
H	-0.48891500	2.32972800	-0.64866500

IM13

H	0.07582200	2.29305600	0.11589900
Sc	-1.56183800	0.00027600	-0.04448200
Sc	1.61383500	0.00175400	0.35366300
O	-3.42428400	-0.00247000	-0.26071200

H	-4.37472300	-0.00323100	-0.36747500
O	0.03700200	1.33230300	0.14155200
O	0.03704900	-1.33025700	0.14950400
H	0.07821000	-2.29076700	0.11894200
H	2.28840500	0.01060000	2.06162200
O	2.99244500	-0.00524100	-0.89150800
H	3.70266400	-0.00696300	-1.53247600

IM14

H	-0.22030000	0.14182500	2.26823300
Sc	1.40236300	-0.06959000	0.00165600
Sc	-1.79394500	0.41614900	-0.00636500
O	2.64885300	1.31891900	-0.01423600
H	3.33774500	1.98186500	-0.03004000
O	-0.21638700	0.19978200	1.30837700
O	-0.22093200	0.14977900	-1.31217700
H	-0.22696100	0.01590500	-2.26445400
H	-2.42496400	2.14179900	-0.03692200
O	-3.19305000	-0.80862100	0.01332100
H	-3.91264600	-1.43849300	0.02346000
O	2.09236600	-1.81520100	0.01872300
H	2.78355300	-2.47789300	0.02656400

IM15

Sc	-1.65663700	-0.00905600	-0.00349100
Sc	1.59571100	0.04350300	0.03910400
O	-0.01084100	-0.20139300	-1.27153500
O	2.55081000	1.63047900	-0.16209900
H	3.50766200	-1.95894400	-0.07845300
O	2.61406800	-1.60665300	-0.09521900
H	0.02742800	-0.75352800	-2.05898100
O	-2.64438600	1.57858000	-0.14259000
H	-3.29822400	-2.28118900	0.17881200
O	-2.61366800	-1.61806400	0.09770500
H	-0.04696500	0.57745800	2.19648400
O	-0.05396900	0.20369900	1.31058000
H	2.65972900	-0.88955800	1.68479100
H	-3.32677600	2.23964500	-0.25209800
H	3.02048400	2.44956200	-0.31314800

TS1

O	0.37647700	1.28149700	0.00895400
Sc	0.57822400	-0.45673900	0.00609800
O	-1.50974800	-0.15641200	-0.09606300
H	-2.18950700	-0.24672900	0.58096600
H	-0.88701400	0.83757900	-0.01214800

TS2

O	-1.75709700	-0.85638700	-0.17440600
H	-2.61671500	-0.41844900	-0.23932600
O	1.58211700	-1.07806000	-0.07375400
H	2.40785800	-1.54544900	-0.19489400
H	-1.47979400	-0.72876500	1.14031100

O	0.12682400	1.88053500	-0.06337500
H	0.43898800	2.77887500	-0.17275000
Sc	0.07785300	0.01643300	0.09328300

TS3

Sc	1.65670300	-0.36626300	-0.05752700
Sc	-0.96686500	0.74897700	0.03030200
O	0.86457400	1.32222500	-0.03309000
O	-0.10434800	-1.11248400	-0.00735100
H	3.22240600	-0.89769200	0.84113600
O	-2.41495400	-0.78242100	0.05096100
H	-1.31765000	-1.31471800	-0.00083200
H	-3.15351300	-1.24314400	-0.35273300

TS4

Sc	-0.84401500	0.03506100	0.25697000
Sc	1.91043400	-0.02687000	-0.14732300
O	0.58017200	1.28089000	0.00958000
O	0.52193500	-1.27277700	0.08548500
H	-2.28927600	0.05568300	1.63992900
O	-2.82326700	0.03483000	-0.54458000
H	-2.88716600	0.02263200	0.57526800
H	-3.44909400	-0.59386300	-0.92165500

TS5

H	-1.38519500	1.73335600	0.39934000
Sc	1.01458100	0.00891600	-0.15543400
Sc	-1.82415300	-0.17531600	0.03290600
O	2.87474100	0.03785500	0.20863800
H	3.77821900	-0.05946500	0.50866300
O	-0.43789200	1.31677600	-0.14089400
O	-0.30880000	-1.32410300	0.03710900
H	-2.41641200	1.57628400	0.82625000

TS6

Sc	1.31888400	-0.05741500	0.15676100
Sc	-1.44023700	0.66078600	-0.00422800
O	0.27128400	1.49395700	-0.10875100
O	-0.34672300	-1.03431400	0.27652200
O	-2.64951700	-1.08935600	-0.14337000
H	-1.50322100	-1.42878100	0.05320900
H	-3.13392200	-1.62249100	-0.77894900
O	3.12174000	-0.49474000	-0.26054900
H	4.01129500	-0.62390300	-0.58826500

TS7

H	-0.10535900	-0.44147000	2.34761900
Sc	-1.61332800	0.09543300	0.00892100
Sc	1.35718300	-0.04500100	-0.08196600
O	-3.47482500	-0.23534400	-0.09869900
H	-4.32926900	-0.50212900	-0.43935300
O	2.63961500	-1.42487400	-0.12246400
H	3.34451100	-2.05436100	-0.26675000

O	-0.25832500	-0.14042600	-1.23855600
O	-0.19518500	-0.30602300	1.40041100
O	1.87084900	1.78809200	0.08826700
H	-0.30516600	1.78264000	-0.30646300
H	2.11730300	2.70485000	-0.03275900

TS8

Sc	-1.53210300	-0.00000600	0.49993400
Sc	0.90539300	0.00000600	-0.30209100
O	-0.56961400	1.44551600	-0.61656800
O	-0.56960400	-1.44551300	-0.61657600
O	2.62675300	-0.00000400	0.53886800
H	-0.39384700	0.00000400	2.00568900
H	3.05424500	-0.00001200	1.39880400
H	-0.69989300	2.31981100	-1.00247900
H	-0.69987700	-2.31980000	-1.00250600

TS9

H	-0.23922500	1.33527600	-1.54241400
H	-1.59371300	2.49310300	-0.89422400
H	0.12254700	-1.17654600	2.00686800
Sc	-1.56905600	-0.12176400	0.10345100
Sc	1.61228600	-0.02591900	-0.03554400
O	-2.20928800	1.79493900	-0.00292100
H	-3.08274100	2.20650300	0.04508600
O	-2.80071300	-1.51641800	-0.09288800
H	-3.35527400	-2.23633900	-0.39270300
O	2.61741400	1.48604500	0.40879800
H	3.26451200	2.16079400	0.61047600
O	2.50815900	-1.60765900	-0.50277700
H	3.19623700	-2.22190100	-0.75717200
O	0.05257900	-0.51988700	1.30634500
O	-0.07066900	0.43053800	-1.17930000

TS10

H	-0.08815000	-1.25466500	-1.97802700
H	0.11656600	-0.21957600	2.25603000
Sc	1.57886000	-0.14040700	-0.04472500
Sc	-1.64753400	-0.24664400	0.05575500
O	1.78340600	1.62505100	-0.74844100
H	2.41418300	2.28151500	-1.04942600
O	3.08358500	-1.17576600	0.38534700
H	3.87477300	-1.68479400	0.55550700
O	-1.40665500	2.00393500	0.23295200
H	-1.34442900	2.47348700	-0.61061200
O	-3.40224000	-0.88710300	-0.16728300
H	-4.28030800	-1.26519000	-0.14726200
O	0.12159200	0.13976900	1.36392500
O	-0.01973800	-0.99062100	-1.05591900
H	-0.53008000	2.07518600	0.65750700