

Electronic Supplementary Information

Cooperative activating effects of metal ion and Brønsted acid on a metal oxo species

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Experimental details

Materials.

RuO_4 and $[\text{}^n\text{Pr}_4\text{N}][\text{RuO}_4]$ were prepared according to literature methods.^{1,2} Reagent grade acetonitrile and various alkanes were obtained from Sigma Aldrich and were purified according to standard methods.³ Boron trifluoride in acetonitrile ($\text{BF}_3 \cdot \text{CH}_3\text{CN}$) (Sigma, 15–18%) was stored at $-20\text{ }^\circ\text{C}$ and was used without further purification. Metal salts were purchased from Sigma Aldrich and were used as received.

Instrumentation.

Gas chromatographic analyses were performed on a HP 5890 gas chromatograph with a HP-5MS ($25\text{ m} \times 0.2\text{ mm} \times 0.33\text{ }\mu\text{m}$) or a HP-FFAP ($25\text{ m} \times 0.2\text{ mm} \times 0.33\text{ }\mu\text{m}$) column equipped with FID detector. GC-MS measurements were carried out on a HP 6890 gas chromatograph interfaced to a HP 5970 mass selective detector. UV-Vis spectroscopy was performed on an Agilent 8453 photodiode-array spectrophotometer. Electrospray ionization mass spectra were conducted on an AB Sciex API-3200 Qtrap mass spectrometer.

Stoichiometric oxidation of alkanes by RuO_4 /Lewis acid.

In a typical experiment, RuO_4 (0.04 mmol) in dichloromethane (270 μL) was added to a solution of CH_3CN containing Lewis acid (0.16 mmol), AcOH (0 - 250 equiv.), cyclohexane (433 μL) and chlorobenzene (5 μL) at $23\text{ }^\circ\text{C}$ (total volume = 4 mL). 100 μL of the mixture was sampled at various intervals and quenched by 50 μL isopropanol solution. The final solution was subjected to analysis by GC and GC-MS. The only product detected was cyclohexanone. This product was quantified by GC-FID. A calibration curve was constructed using pure cyclohexanone. Chlorobenzene was used as internal standard.

Stoichiometric oxidation of alkanes by $[\text{}^n\text{Pr}_4\text{N}][\text{RuO}_4]$ /Lewis acid.

In a typical experiment, $[\text{}^n\text{Pr}_4\text{N}][\text{RuO}_4]$ (0.04 mmol, 14 mg) was added to a solution of CH_3CN containing Lewis acid (0.16 mmol), AcOH (0 – 250 equiv.), cyclohexane (433 μL) and chlorobenzene (5 μL) at $23\text{ }^\circ\text{C}$ (total volume = 4 mL). The ruthenium complex dissolved within 5 s to give a clear brown solution. 100 μL of the mixture was sampled at various intervals and quenched by 50 μL isopropanol solution. The final solution was subjected to analysis by GC

and GC-MS. The only product detected was cyclohexanone. This product was quantified by GC-FID. A calibration curve was constructed using pure cyclohexanone. Chlorobenzene was used as internal standard.

DFT Calculations.

The structures and energies of all molecular species were calculated at the B3LYP⁴ level with the LanL2TZ(f) basis set⁵⁻⁷ for transition metal (Ru) and 6-311G(d,p) basis set for the nonmetal atoms. The polarizable continuum model (PCM)^{8,9} was used to account for the solvent effect in acetonitrile and the D3 version¹⁰ of Grimme's dispersion with Becke-Johnson damping were included. All calculations were performed with Gaussian 16 package of program.¹¹

Table S1. Oxidation of cyclohexane by RuO₄/Lewis acid in CH₃CN.^a

Entry	Lewis acid	Product Yield ^b		Time
		c-CyO	c-CyOH	
1	Nil	0.20	0	5 h
2	BF ₃	0.11	0	3 h
3	Ca(OTf) ₃	0.19	0	5 h

^aRuO₄ (0.01 M), Lewis acid (0.04 M), cyclohexane (1.0 M) and chlorobenzene (5 μL) in MeCN.^bYield = mole of product/mole of RuO₄.**Table S2.** Oxidation of cyclohexane by [nPr₄N][RuO₄]/Lewis acid in CH₃CN.^a

Entry	Lewis acid	Product Yield ^d		Time
		c-CyO	c-CyOH	
1	Nil	< 0.01	0	24 h
2	BF ₃	0.10	0	3 h
3	Mg(OTf) ₂	0.15	0	5 h
4	Ca(OTf) ₂	0.14	0	5 h
5 ^b	Ca(OTf) ₂	0.14	0	5 h
6 ^c	Ca(OTf) ₂	0.14	0	5 h
7	Sr(OTf) ₂	0.13	0	5 h
8	Ba(OTf) ₂	0.11	0	5 h
9	Sc(OTf) ₂	0.23	0	8 h

^a[nPr₄N][RuO₄] (0.01 M), Lewis acid (0.04 M), cyclohexane (1 M) and chlorobenzene (5 μL) at 23 °C in MeCN. ^bUnder argon. ^cIn the presence of 10 equiv. BrCCl₃, only a trace amount of bromocyclohexane was detected. ^dYield = mole of product / [nPr₄N][RuO₄].

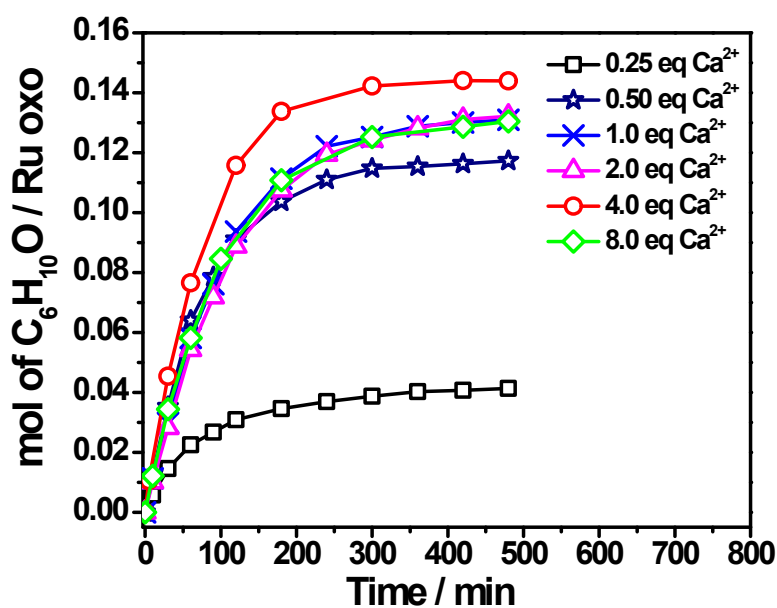


Figure S1. Time trace for cyclohexane oxidation by $[n\text{Pr}_4\text{N}][\text{RuO}_4]/\text{Ca}(\text{OTf})_2$ in CH_3CN . Conditions: $[n\text{Pr}_4\text{N}][\text{RuO}_4]$ (0.01 M), $\text{Ca}(\text{OTf})_2$ (0.024 – 0.08 M), cyclohexane (1.0 M) and chlorobenzene (5 μL) at 23 $^\circ\text{C}$.

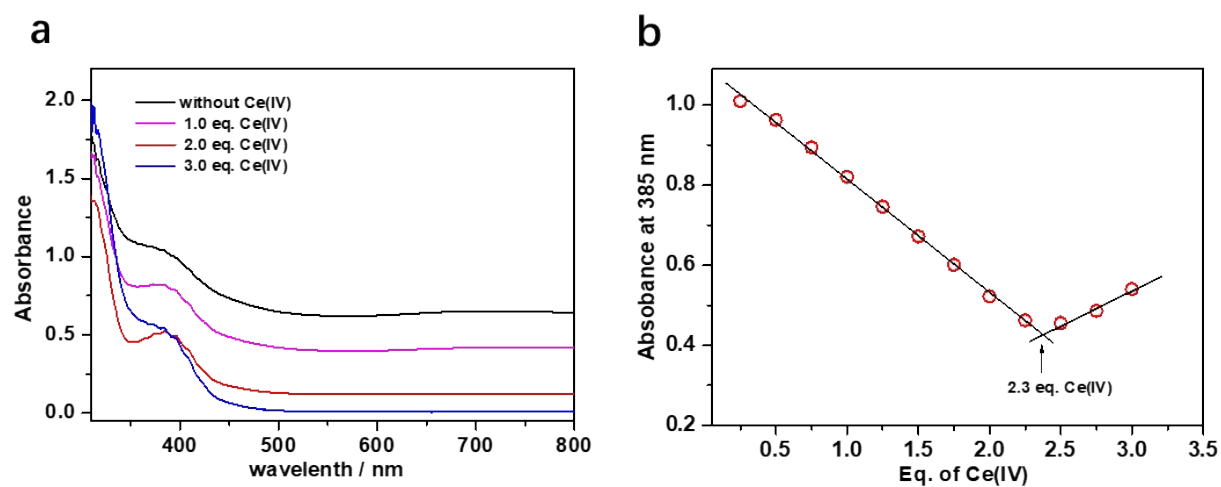


Figure S2. a) Spectrophotometric changes for the titration of the $\text{Ca}^{2+}/\text{RuO}_4^-$ + cyclohexane product in 0.1 M aqueous HNO_3 with $\text{Ce}(\text{IV})$ at 23 $^\circ\text{C}$. b) Plot of absorbance changes at 385 nm versus mol equiv. of $\text{Ce}(\text{IV})$.

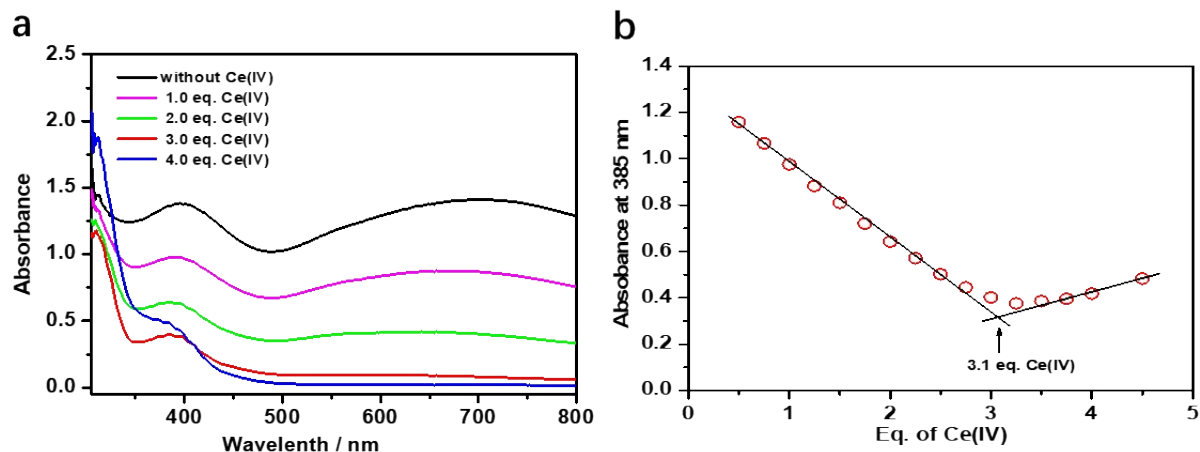


Figure S3. a) Spectrophotometric changes for the titration of the product solution of $\text{Ca}^{2+}/\text{AcOH}/\text{RuO}_4^-$ + cyclohexane with Ce(IV) in 0.1 M aqueous HNO_3 at 23 °C. b) Plot of absorbance changes at 385 nm versus mol equiv. of Ce(IV) .

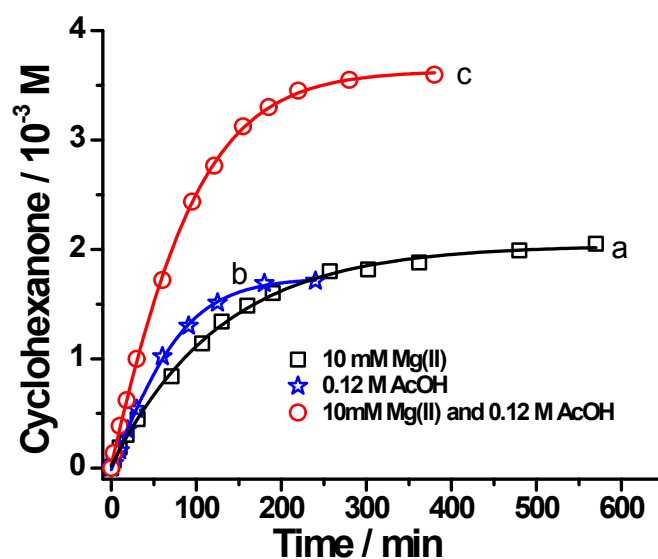


Figure S4 Time trace for cyclohexane oxidation by $[\text{Pr}_4\text{N}][\text{RuO}_4]$ (0.01 M) in CH_3CN at 23 °C in the presence of a) 1 equiv. Mg^{2+} , b) 12 mol equiv. of AcOH and c) 1 mol equiv. Mg^{2+} + 12 mol equiv. AcOH .

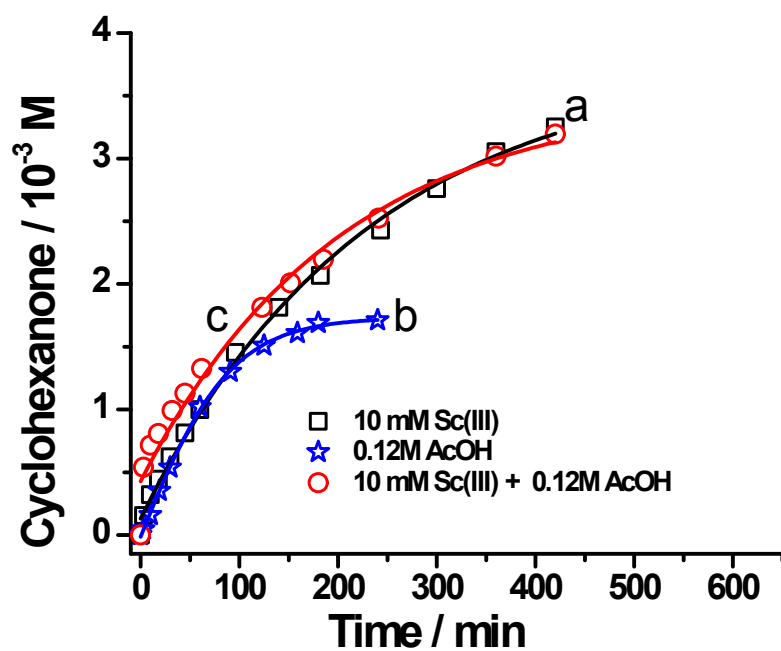


Figure S5. Time trace for cyclohexanone oxidation by $[\text{nPr}_4\text{N}][\text{RuO}_4]$ (0.01 M) in CH_3CN at 23 °C in the presence of a) 1 equiv. Sc^{3+} , b) 12 mol equiv. of AcOH and c) 1 mol equiv. Sc^{3+} + 12 mol equiv. AcOH.

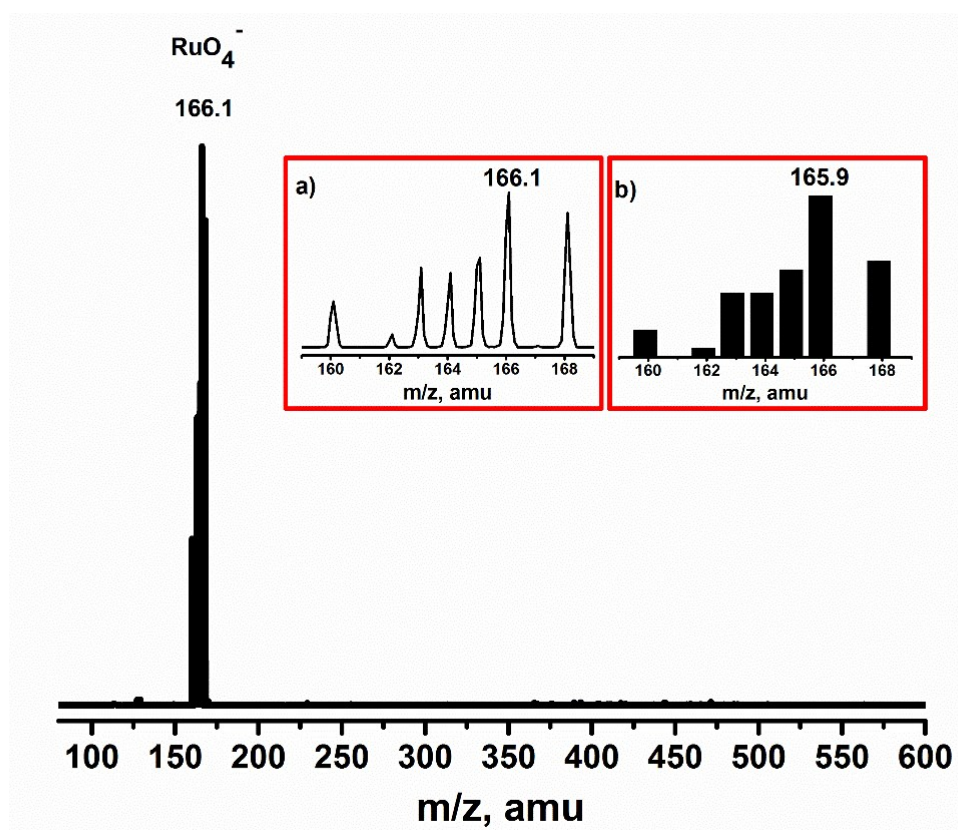


Figure 6. ESI-Mass spectrum of $[\text{nPr}_4\text{N}][\text{RuO}_4]$ in CH_3CN .

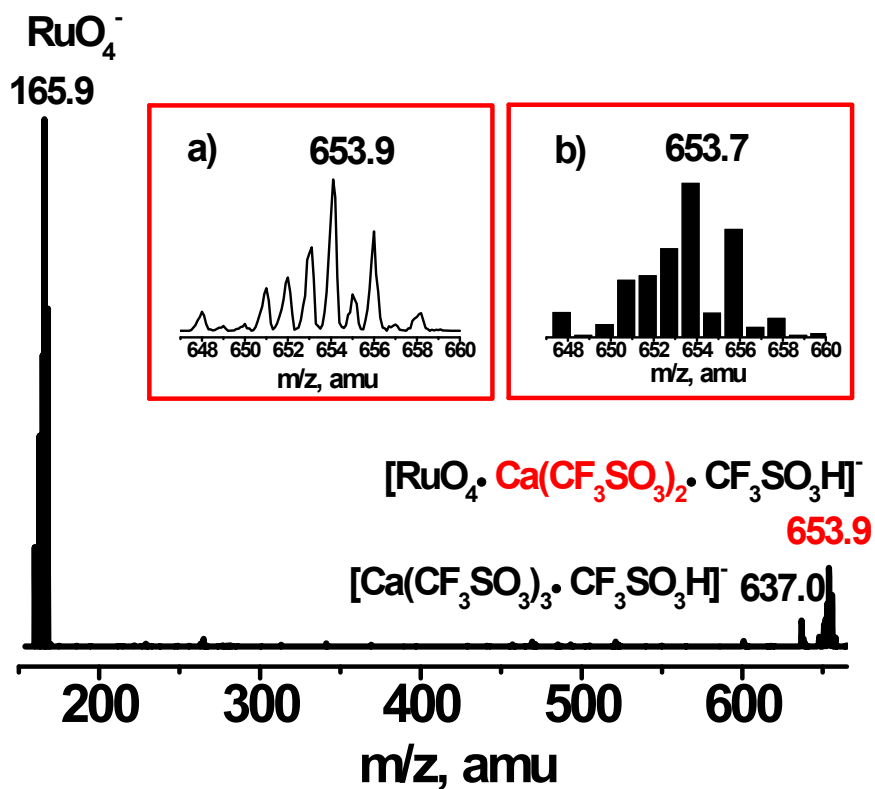


Figure S7. ESI/MS (negative mode) of a mixture of $[\text{nPr}_4\text{N}][\text{RuO}_4]$ (2 mM) and $\text{Ca}(\text{CF}_3\text{SO}_3)_2$ (0.5 mM) in CH_3CN . Insets show a) experimental and b) isotopic distributions of $[\text{RuO}_4 \cdot \text{Ca}(\text{CF}_3\text{SO}_3)_2 \cdot \text{CF}_3\text{SO}_3\text{H}]^-$. Note: If more $\text{Ca}(\text{OTf})_2$ is added, the MS will be overwhelmed by peaks due to $\text{Ca}(\text{OTf})_2$.

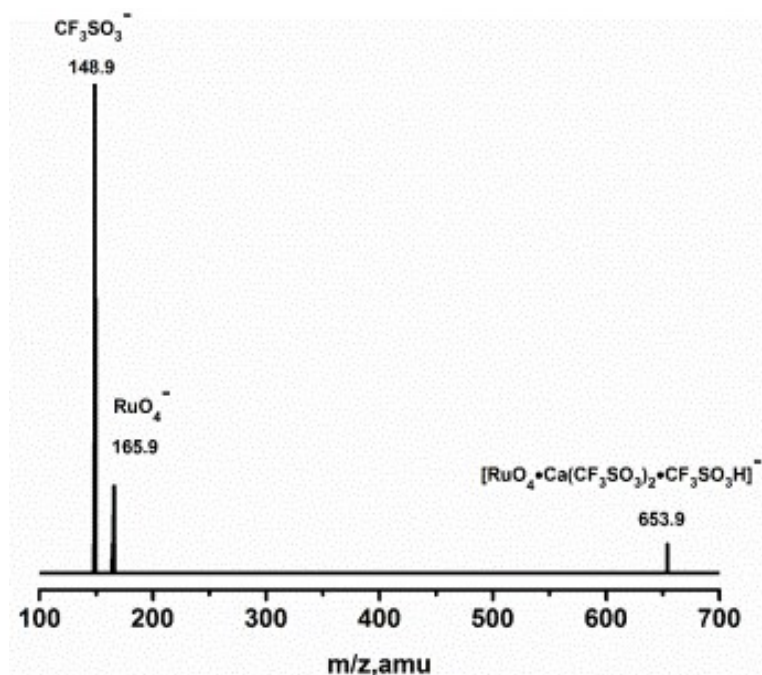


Figure S8. MS/MS of 653.9, CE = 5.

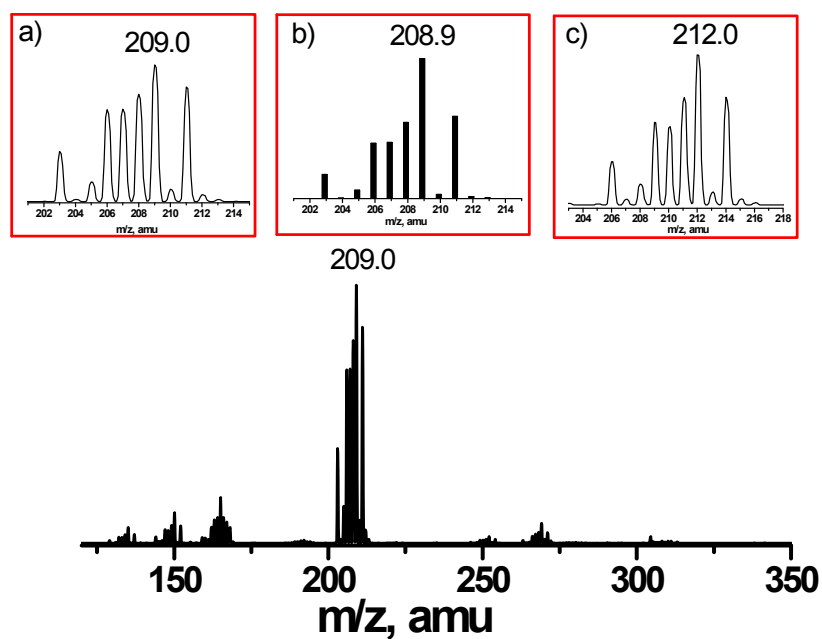


Figure S9. Mass spectrum of the reaction mixture of cyclohexane (1.0 M) with $[^{14}Pr_4N][RuO_4]$ (10 mM), 8 eq AcOH in CH_3CN . Reaction time = 6 h. Insets show isotopic distributions of $[RuO_3(CH_3CO_2)]^-$: a) experimental; b) simulation; c) $[RuO_3(CD_3CO_2)]^-$.

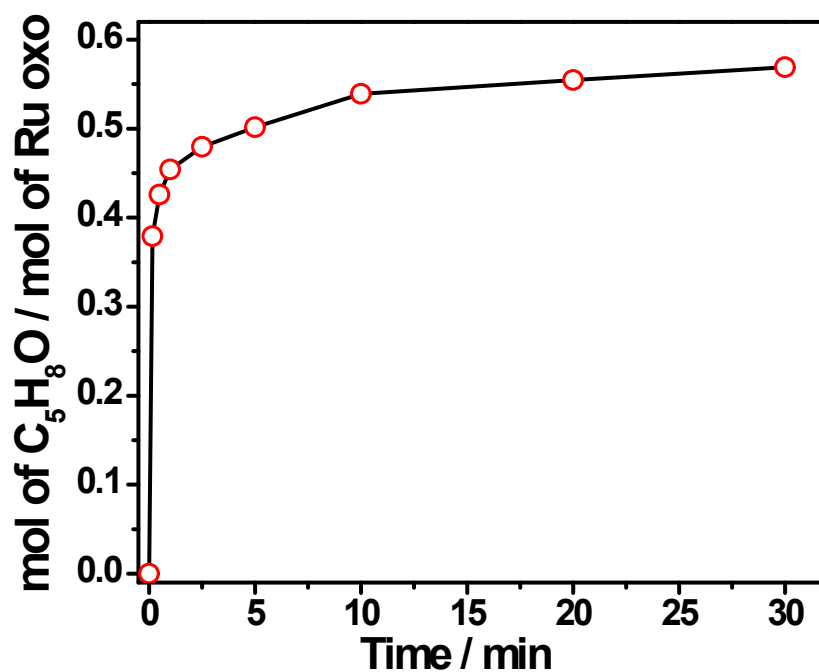


Figure S10. Competitive cyclohexane/cyclopentanol oxidation by $[^{14}Pr_4N][RuO_4]/Ca(OTf)_2$ in CH_3CN . Conditions: $[^{14}Pr_4N][RuO_4]$ (0.01 M); $Ca(OTf)_2$ (0.04 M); cyclohexane, 1.0 M; cyclopentanol (0.1 M) at 23 °C. No cyclohexanone was detected.

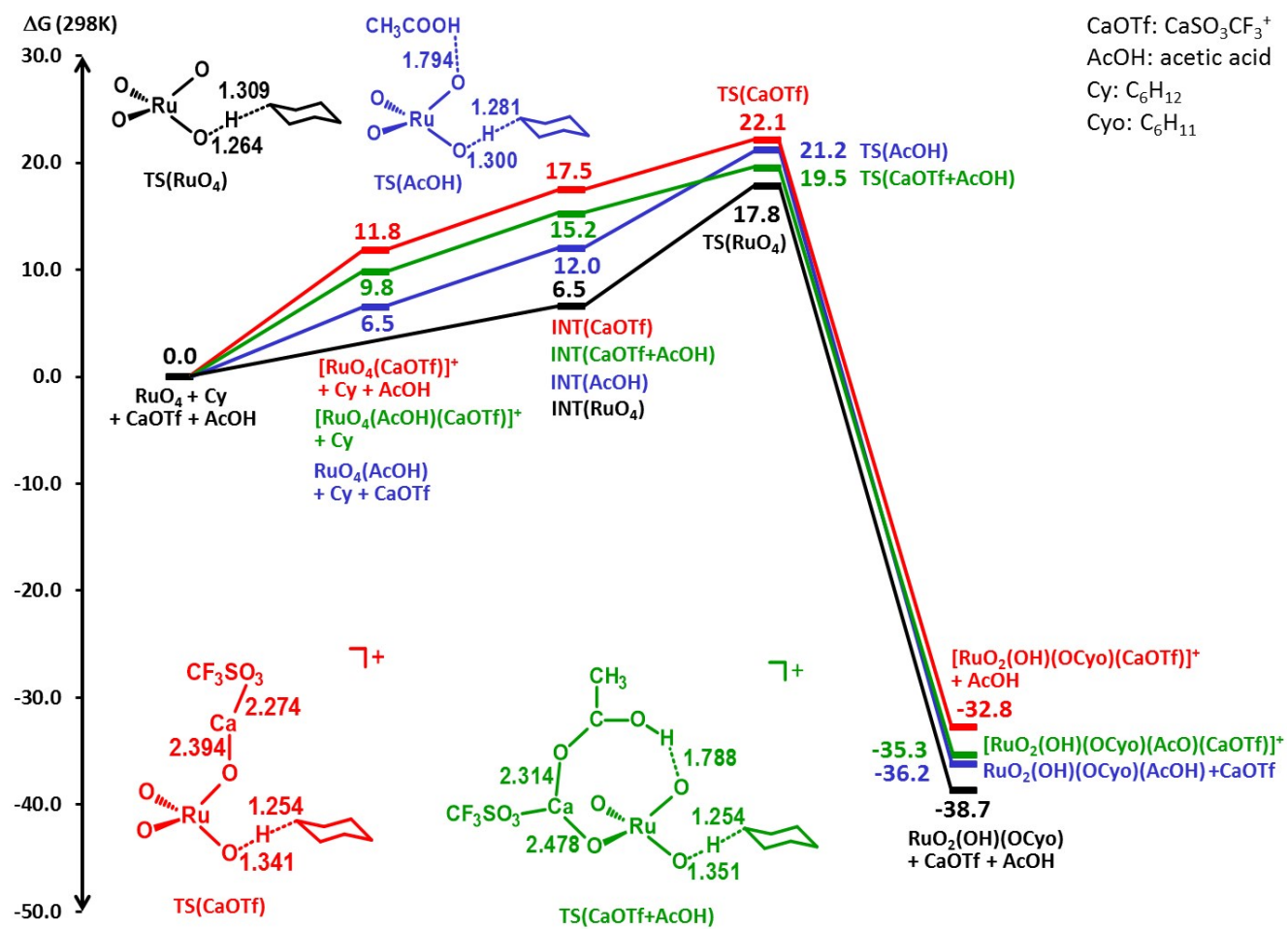


Figure S11. PES for the reaction of cyclohexane with Ru^{VIII}O₄ species.

Table S3. The structures of the intermediates (INT1) and transition states (TS1) in the oxidation of cyclohexane by $\text{RuO}_4^-/\text{RuO}_4$ in the presence and absence of Ca(II) and/or AcOH . at the B3LYP level using LanL2TZ(f) basis set (Ru) and 6-311++G(d,p) basis set (non-metals).

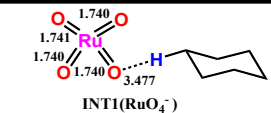
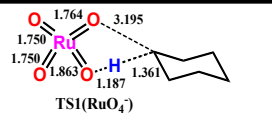
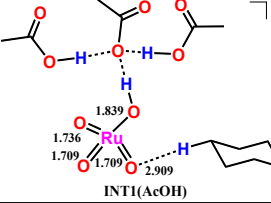
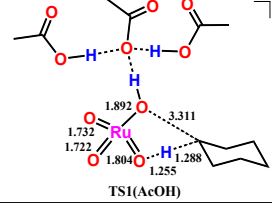
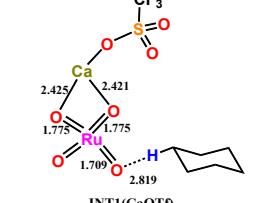
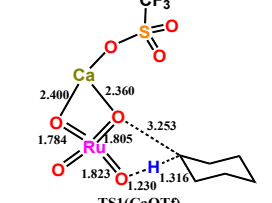
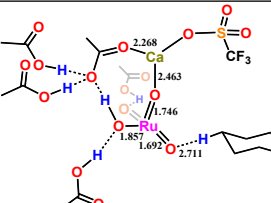
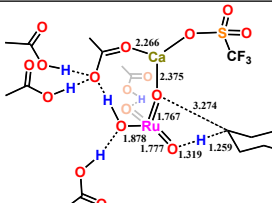
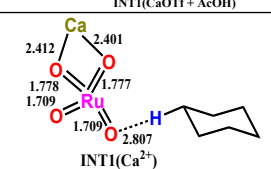
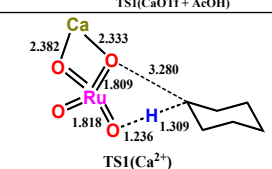
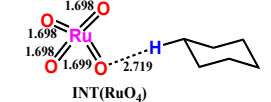
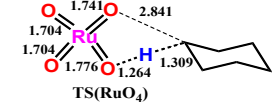
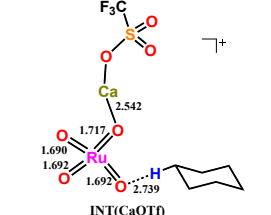
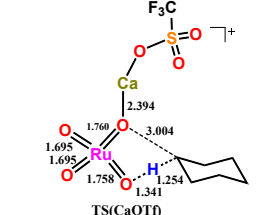
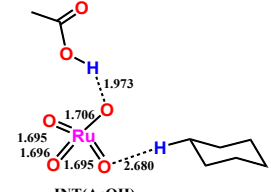
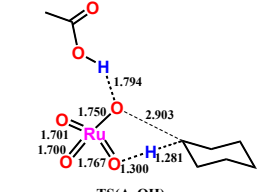
Entry		INT1	TS1	$\Delta G_{298}^\ddagger$ (TS1)
1	RuO_4^-	 INT1(RuO_4^-)	 TS1(RuO_4^-)	26.8
2	$\text{RuO}_4^-/\text{AcOH}$	 INT1(AcOH)	 TS1(AcOH)	15.2
3	$\text{RuO}_4^-/(\text{CaOTf})^+$	 INT1(CaOTf)	 TS1(CaOTf)	18.5
4	$\text{RuO}_4^-/(\text{CaOTf})^+/\text{AcOH}$	 INT1($\text{CaOTf} + \text{AcOH}$)	 TS1($\text{CaOTf} + \text{AcOH}$)	10.8
5	$\text{RuO}_4^-/\text{Ca}^{2+}$	 INT1(Ca^{2+})	 TS1(Ca^{2+})	22.5
6	RuO_4	 INT(RuO_4)	 TS(RuO_4)	17.8
7	$\text{RuO}_4/\text{Ca(OTf)}^+$	 INT(CaOTf)	 TS(CaOTf)	22.1
8	RuO_4/AcOH	 INT(AcOH)	 TS(AcOH)	21.2

Table S4. XYZ coordinates**RuO₄⁻**

INT1

O	1.32774200	-1.06190800	0.72530500
C	-3.13794500	1.20848000	-0.16667900
C	-2.72869300	-0.11540000	-0.82987000
C	-3.32313900	-1.32378700	-0.09074100
C	-4.84913000	-1.20837100	0.04394200
C	-5.25810000	0.11545100	0.70765200
C	-4.66386700	1.32419100	-0.03132600
H	-3.05802300	-2.25171200	-0.60867500
H	-3.08193000	-0.12069600	-1.86972500
H	-1.63747100	-0.19615000	-0.87025200
H	-2.68310200	1.26590000	0.83108700
H	-2.74340400	2.05544100	-0.73806600
H	-5.30363000	-1.26538800	-0.95417200
H	-5.24384500	-2.05550100	0.61513000
H	-6.34963100	0.19656300	0.74931100
H	-4.90439100	0.12039900	1.74726200
H	-5.10985300	1.38778400	-1.03285500
H	-4.92850200	2.25192500	0.48731400
H	-2.87758900	-1.38694700	0.91086000
Ru	2.52166400	0.00059200	0.03830800
O	3.72332200	-0.98537600	-0.74414800
O	3.19046000	0.96368600	1.32501400
O	1.85014800	1.07971700	-1.15000300

TS1

O	-0.50347500	0.00013300	-1.04782000
O	-1.18798900	-0.00016200	1.56591200
C	2.38814200	1.27060100	-0.24220000
C	1.70675700	0.00002600	0.21469000
C	2.38809100	-1.27057100	-0.24221500
C	3.86378400	-1.27046900	0.23091200
C	4.59474300	-0.00002800	-0.22399800
C	3.86383300	1.27043500	0.23093100

H	1.87039200	-2.15433200	0.14096800
H	1.44124000	0.00002500	1.27153300
H	0.49769400	0.00006200	-0.40943800
H	2.37264500	1.33241100	-1.33744800
H	1.87047700	2.15437900	0.14099400
H	3.88899300	-1.33502400	1.32541300
H	4.36866800	-2.16363800	-0.15176900
H	5.61969600	-0.00005100	0.16197000
H	4.67209200	-0.00002100	-1.31884400
H	3.88904200	1.33497200	1.32543300
H	4.36875300	2.16359000	-0.15173600
H	2.37259100	-1.33236600	-1.33746500
Ru	-2.03188700	-0.00000200	0.01713200
O	-2.94560200	-1.46345200	-0.27305600
O	-2.94560200	1.46349800	-0.27280600

INT2

O	-0.66832900	0.26382800	-1.09313100
O	-1.33521900	-0.33231900	1.52734600
C	2.69565400	1.30042000	-0.13096400
C	2.03495700	0.06001100	0.38301000
C	2.60105500	-1.24603600	-0.07806500
C	4.12863100	-1.29470000	0.20094400
C	4.83674500	-0.05967200	-0.37337300
C	4.22301900	1.24709600	0.14843800
H	2.09942100	-2.09087400	0.40059300
H	1.49372200	0.09800700	1.32368900
H	0.13995700	0.17268000	-0.54641600
H	2.56030100	1.37577800	-1.21999000
H	2.25911800	2.19963900	0.31110300
H	4.29238900	-1.33921500	1.28418100
H	4.54940300	-2.21193500	-0.22409600
H	5.90358700	-0.09416600	-0.12849700
H	4.76614300	-0.07965800	-1.46875800
H	4.39128700	1.32412300	1.22914300
H	4.70993000	2.11225400	-0.31359500
H	2.45789800	-1.35619600	-1.16311800

Ru	-2.22364000	-0.01359200	0.03940400
O	-3.03292500	-1.39257900	-0.68049100
O	-3.07644600	1.51668200	-0.01847000

TS2

O	-0.67213100	0.01809300	1.38018300
O	-0.72936900	-0.08889300	-1.27222600
C	2.29480000	-1.28788700	-0.05814000
C	1.76438600	-0.02337600	-0.65865100
C	2.24200400	1.25680500	-0.04600400
C	3.79762000	1.28861300	-0.09147700
C	4.39486100	0.02613500	0.54538700
C	3.85051200	-1.25397100	-0.10353800
H	1.82895900	2.12612200	-0.56303400
H	1.57874800	-0.02191200	-1.72468600
H	0.17372800	-0.01722100	0.89879900
H	1.99742200	-1.38178900	0.99442600
H	1.91874600	-2.16854000	-0.58407500
H	4.12408300	1.36387800	-1.13515000
H	4.15493400	2.18734700	0.42177600
H	5.48659100	0.04927500	0.46479400
H	4.16000800	0.01615000	1.61753600
H	4.17916900	-1.30498700	-1.14803200
H	4.24577400	-2.14195600	0.40047900
H	1.94243400	1.32856900	1.00758900
Ru	-2.00717000	-0.00072100	-0.02984000
O	-2.85322800	1.53369000	0.07328600
O	-2.93780100	-1.46803400	0.21089300

RuO₄-AcOH

INT1

O	-1.22146400	-3.81323300	-0.06230100
Ru	-0.34832700	-2.41857200	-0.52476400
O	-0.22076600	-1.30764600	0.93524500
O	1.19399600	-2.52308100	-1.25251400
O	-1.36538100	-1.46182200	-1.55699900

H	-1.97562500	3.22557000	3.18972300
C	-2.25594300	2.66844300	2.29682400
H	-2.20275100	3.30805100	1.41371500
H	-3.29133700	2.32993300	2.40003700
C	-1.36304600	1.45586600	2.12583500
O	-0.61406400	1.06981000	3.01825600
O	-1.46722600	0.84923300	0.95844900
H	-0.75852300	-0.38131300	0.91963600
C	4.20178300	0.89688500	-0.55462900
C	3.94991300	-0.20931400	0.48109300
C	5.23967200	-0.97469700	0.81348500
C	6.35981400	-0.02466200	1.26396200
C	6.61166300	1.08162900	0.22812400
C	5.32197200	1.84712900	-0.10479600
H	5.04560100	-1.72440000	1.58805000
H	3.55361800	0.24279000	1.39989000
H	3.18227500	-0.90004500	0.11671900
H	4.48337200	0.43653100	-1.51114100
H	3.28007000	1.45884000	-0.73860300
H	6.07753200	0.43583000	2.22009700
H	7.28167600	-0.58666900	1.44866700
H	7.37896500	1.77331500	0.59225900
H	7.00875400	0.62987000	-0.69071500
H	4.99050900	2.39704900	0.78606000
H	5.51663200	2.59670400	-0.87943200
H	5.57141100	-1.52444600	-0.07748100
C	-6.16839600	0.10772500	-0.31951400
H	-6.97107000	-0.25564900	0.31837200
H	-6.03184600	-0.57042600	-1.16518900
H	-6.43091900	1.08740300	-0.72534200
C	-4.88637900	0.20645000	0.46434800
O	-4.77051000	-0.09331800	1.63849800
O	-3.87380100	0.66641500	-0.27529700
H	-3.03141700	0.71222000	0.25600000
C	-0.03969100	3.73457100	-2.86118400
H	-0.39301900	4.72819600	-3.12755700
H	-0.21863100	3.04378000	-3.68852500

H	1.03759000	3.75831900	-2.68234700
C	-0.75207900	3.24481200	-1.62905200
O	-1.61217200	3.86548600	-1.03371500
O	-0.33274500	2.03149800	-1.25143200
H	-0.81912700	1.71994300	-0.44579900
TS1			
O	-0.27052000	-3.75675300	0.36700600
Ru	0.14592500	-2.27984600	-0.41329400
O	0.09525600	-0.94561500	0.92677700
O	1.85903300	-1.97784000	-0.89068300
O	-1.06481000	-1.74370900	-1.52989400
H	-3.04210700	2.21587000	3.63490500
C	-3.12827100	1.82460100	2.62208700
H	-3.68200700	2.53978300	2.00667500
H	-3.69784400	0.89239900	2.62974900
C	-1.75523800	1.59401400	2.01308200
O	-0.73083000	1.93648700	2.60706500
O	-1.74675900	1.02668100	0.83332900
H	-0.58854700	-0.23329600	0.78328700
C	3.40588900	0.89466600	-0.59010700
C	3.28678900	-0.28244400	0.34700900
C	4.57001600	-1.04549700	0.57379200
C	5.64837100	-0.06831000	1.11718700
C	5.81863600	1.14176800	0.19143100
C	4.48820800	1.86617500	-0.04382800
H	4.42182700	-1.86948300	1.27600300
H	2.73158900	-0.06589800	1.26104900
H	2.50671100	-1.12095900	-0.24214100
H	3.71375500	0.55386000	-1.58542700
H	2.45069600	1.41384900	-0.69541600
H	5.35413500	0.27011100	2.11723000
H	6.59217500	-0.61119800	1.22792500
H	6.54932300	1.83628400	0.61927900
H	6.22692200	0.80891600	-0.77092900
H	4.13459800	2.30412400	0.89654100
H	4.61271700	2.69006200	-0.75333700

H	4.92816100	-1.47117700	-0.37046300
C	-5.83487200	-0.81532400	-1.03402700
H	-6.45814500	-1.61325000	-0.63552100
H	-5.46839000	-1.09575300	-2.02491500
H	-6.42555500	0.09628000	-1.15022100
C	-4.66532400	-0.55950700	-0.11728200
O	-4.43296800	-1.20803300	0.88913300
O	-3.90846700	0.45473900	-0.52852500
H	-3.11465700	0.61169500	0.08081500
C	0.13689400	4.25468500	-2.32540400
H	-0.10336600	5.31312200	-2.39716500
H	-0.09610600	3.75888000	-3.27084700
H	1.20647500	4.12760500	-2.14476500
C	-0.65110400	3.61703500	-1.21055700
O	-1.46464000	4.20507500	-0.52098100
O	-0.36026300	2.32356400	-1.05949200
H	-0.89329200	1.91345600	-0.31754700

INT2

O	0.13692000	-3.26583200	-0.03777700
Ru	0.78988900	-1.88278100	-0.81580100
O	1.06413100	-0.16558900	0.29105500
O	2.65863300	-2.10521500	-1.32519100
O	0.01706200	-1.17628000	-2.21609200
H	-2.57872900	2.42017100	3.42119800
C	-2.62290000	1.79069500	2.53347400
H	-3.17092200	2.29548700	1.73505900
H	-3.16146200	0.86911600	2.77355100
C	-1.22839800	1.43166100	2.06177100
O	-0.23046300	1.68189500	2.73584000
O	-1.16972400	0.82929600	0.89293700
H	0.15499300	0.27238500	0.56000400
C	2.76483000	1.32896000	-0.71402600
C	2.18461700	0.73851700	0.56800300
C	3.23065300	0.05749000	1.44519800
C	4.37774400	1.03171200	1.76416400
C	4.98698600	1.62419000	0.48579900

C	3.91532800	2.29612600	-0.38386400
H	2.75657000	-0.29947900	2.36334600
H	1.71722000	1.53535400	1.15414800
H	3.25514300	-1.58289200	-0.77590700
H	3.13526800	0.52606100	-1.36076100
H	1.97488400	1.84472100	-1.26718500
H	3.99501100	1.84393400	2.39427200
H	5.14254300	0.51508500	2.35110400
H	5.76890200	2.34551200	0.74271000
H	5.47238900	0.82502000	-0.08877300
H	3.51398100	3.16890000	0.14600500
H	4.35471100	2.67007700	-1.31318800
H	3.64235500	-0.82541700	0.94097100
C	-4.47539300	-2.78432600	0.38277100
H	-4.80340200	-3.49576300	1.13741600
H	-4.01826700	-3.31760400	-0.45414000
H	-5.33474900	-2.23578800	-0.00951900
C	-3.47988000	-1.82124400	0.97371100
O	-3.08659200	-1.85524100	2.12544300
O	-3.06770800	-0.91101100	0.08770300
H	-2.39220700	-0.29454800	0.48830200
C	-2.71426700	3.67204400	-2.89901800
H	-3.63647600	4.24180600	-2.98821900
H	-2.64989000	2.94152300	-3.70874600
H	-1.85473800	4.33984000	-2.99208300
C	-2.66884800	2.96456400	-1.57110600
O	-3.54314100	3.02034200	-0.72713900
O	-1.54510000	2.25576100	-1.41409900
H	-1.53323200	1.79153300	-0.53701100

RuO₄⁻/(CaOTf)⁺

INT1

C	2.45393400	3.38700200	1.19421700
C	1.72312000	2.55454200	0.12992400
C	2.08472000	3.01362200	-1.29085600
C	3.60423900	3.00672100	-1.51622200

C	4.33604100	3.83820900	-0.45163700
C	3.97370600	3.38089400	0.96963000
H	1.59005500	2.37638800	-2.03168900
H	2.00138400	1.49910600	0.24683000
H	0.63986600	2.61070600	0.27998100
H	2.08888400	4.42206000	1.15505600
H	2.21842100	3.01126000	2.19581800
H	3.96831800	1.97152200	-1.47676800
H	3.84061400	3.38247300	-2.51760100
H	5.41911500	3.77836300	-0.60353700
H	4.06170000	4.89500400	-0.56991800
H	4.35610800	2.36376600	1.12815100
H	4.46868800	4.01891800	1.70972300
H	1.70220400	4.03093800	-1.44867800
Ru	-3.14281800	1.02915600	0.13593500
O	-3.29453200	-0.03544700	-1.27605900
O	-4.68862600	1.30667800	0.81601400
O	-2.11637600	2.34177600	-0.24578500
O	-2.25504300	-0.15140400	1.12097700
Ca	-2.12998900	-1.99335500	-0.44493200
C	2.24009900	-2.36090900	0.96499600
S	1.48581600	-2.73622900	-0.71925700
F	1.95548000	-3.33619400	1.83880500
F	1.76409100	-1.20617500	1.45001200
F	3.57194200	-2.26044000	0.86082700
O	0.02490000	-2.78868900	-0.39350500
O	1.86540400	-1.59230100	-1.55746900
O	2.04384900	-4.04208600	-1.08778100
TS1			
C	-2.00904200	2.60302800	0.91608500
C	-1.34405100	2.05991900	-0.32546800
C	-1.42341200	2.96584000	-1.53192200
C	-0.79732600	4.34094000	-1.17280800
C	-1.45073100	4.94182800	0.07776300
C	-1.38538000	3.97937800	1.26991000
H	-0.90487000	2.53000400	-2.38961700

H	-0.34953900	1.64838800	-0.14700100
H	-2.02640100	0.98991100	-0.67396800
H	-3.08189000	2.74174000	0.73782500
H	-1.89894600	1.91173500	1.75456700
H	0.27734700	4.21093900	-1.00082600
H	-0.90451000	5.01409600	-2.02916500
H	-0.96087400	5.88683700	0.33510700
H	-2.49947500	5.18024400	-0.13935700
H	-0.34089000	3.83368900	1.56903200
H	-1.90988900	4.39602900	2.13549700
H	-2.46956600	3.12228900	-1.81955800
Ru	-2.56930700	-1.42966000	0.04461700
O	-1.87551000	-2.83861300	-0.80074500
O	-3.82305000	-1.77500400	1.17157900
O	-2.73310000	0.04337900	-1.01597600
O	-1.03303100	-0.95192100	0.86397900
Ca	0.37402600	-2.64570300	0.01432800
C	3.53617400	0.40306400	0.85799600
S	3.30027200	-0.54245200	-0.75451800
F	4.14018100	-0.36555900	1.77456900
F	2.35430000	0.79876800	1.35140100
F	4.29306000	1.48878100	0.65031000
O	2.45014100	-1.69527700	-0.31635900
O	2.60656700	0.40487200	-1.63630600
O	4.65659200	-0.94112300	-1.14689800

INT2

C	1.27333200	1.86776400	-1.25240800
C	0.88498300	1.23508000	0.08546400
C	1.46907700	2.01304000	1.26793600
C	1.05094700	3.49280700	1.21360000
C	1.44196600	4.13756000	-0.12310100
C	0.86771100	3.35020300	-1.30872800
H	1.13006000	1.56052700	2.20617500
H	-0.21003700	1.26138100	0.17365600
H	2.62195600	-0.19911000	2.25638300
H	2.35749200	1.77442400	-1.38413300

H	0.79977200	1.30959000	-2.06643200
H	-0.03522800	3.56786700	1.34929800
H	1.50749800	4.03367500	2.04791800
H	1.09535200	5.17537300	-0.15592900
H	2.53604900	4.16800500	-0.20359900
H	-0.22668000	3.42910900	-1.29864600
H	1.20215000	3.78644900	-2.25497000
H	2.56360900	1.95212600	1.24254100
Ru	3.02023800	-0.98346300	-0.01287600
O	2.18793600	-2.52114400	-0.40899100
O	4.03718000	-0.14604300	-1.11186200
O	3.30814000	-0.76640600	1.87639700
O	1.18236500	-0.17359200	0.12732100
Ca	-0.09207400	-2.04185300	-0.46409900
C	-3.92821500	0.72363700	-0.13249900
S	-3.60765400	-1.08968400	0.26259400
F	-4.00274000	0.91480600	-1.45668900
F	-2.94438800	1.49595800	0.35099400
F	-5.08408300	1.11929900	0.41788200
O	-2.31315000	-1.33258200	-0.44700500
O	-3.50028700	-1.13184200	1.72712500
O	-4.74548900	-1.79916200	-0.33504600

TS2

C	1.02495600	1.96432700	-1.11008900
C	0.51490600	1.50691400	0.26581900
C	1.03710400	2.43807200	1.36850500
C	0.67650600	3.90588200	1.09066300
C	1.18105800	4.35979500	-0.28657400
C	0.67408400	3.43149100	-1.39903400
H	0.63124700	2.11845100	2.33425500
H	-0.58466900	1.58561200	0.25787000
H	1.94602200	-0.12995600	1.36090500
H	2.11460200	1.82824700	-1.13007200
H	0.60978300	1.31259900	-1.88693400
H	-0.41382600	4.02563900	1.13275400
H	1.08930200	4.54617800	1.87690700

H	0.86883600	5.39083900	-0.48289800
H	2.27885100	4.35832700	-0.28737700
H	-0.41545700	3.53352800	-1.48532800
H	1.09088800	3.73167100	-2.36600900
H	2.12814000	2.33395400	1.42763200
Ru	3.46988400	-0.96915100	-0.07275100
O	2.34168400	-2.03244700	-0.87928200
O	5.14129900	-1.01919100	-0.32239800
O	2.88315400	-0.58343000	1.65552200
O	0.86094500	0.14992700	0.51559100
Ca	-0.01194200	-1.70382300	-0.42791300
C	-4.29075500	0.29115600	-0.37145100
S	-3.53512300	-1.21981600	0.46082700
F	-4.62720300	0.01658100	-1.63937400
F	-3.42470800	1.31422400	-0.37641800
F	-5.39435000	0.67559200	0.28465000
O	-2.34150200	-1.48236300	-0.40407700
O	-3.19985400	-0.76160400	1.81585700
O	-4.57429900	-2.25118500	0.35224000

RuO₄⁻/(CaOTf)⁺/AcOH

INT1

C	3.66165400	3.76141400	1.10864000
C	3.08429000	3.11884200	-0.16163700
C	3.04754300	4.11444100	-1.33076700
C	4.43099100	4.73024900	-1.59019700
C	5.00991100	5.37230500	-0.32010500
C	5.04527400	4.37730900	0.85002400
H	2.67744800	3.62137200	-2.23609100
H	3.70406400	2.25732800	-0.44253300
H	2.07849100	2.73173700	0.03518200
H	2.97797900	4.54697000	1.45713800
H	3.72196900	3.02111000	1.91378000
H	5.11402400	3.94465100	-1.93956300
H	4.37043200	5.47120300	-2.39466000
H	6.01510600	5.76036700	-0.51704500

H	4.39114700	6.23507200	-0.03946000
H	5.75820200	3.57498800	0.61806600
H	5.41496100	4.87103800	1.75524000
H	2.33475300	4.91670000	-1.09768100
Ru	-0.86006400	1.06584600	1.32037700
O	-2.40612800	0.75575300	0.34052800
O	-1.02232000	0.29914400	2.83340500
O	-0.39711500	2.68314500	1.13936900
O	0.24298700	0.11789500	0.35500700
Ca	0.87890600	-2.05642500	-0.61081600
C	-2.07608300	-1.17935500	-4.04530200
H	-1.88597100	-0.22417600	-4.54588100
H	-1.43982400	-1.93772600	-4.49815700
H	-3.13008000	-1.42196800	-4.18062300
C	-1.74688000	-1.01345200	-2.58143800
O	-0.62436400	-1.35699300	-2.15798500
O	-2.65565400	-0.49832200	-1.82742000
H	-2.35109300	0.19249700	-0.53284200
C	5.55030800	-1.46231800	-0.46707600
S	4.33229000	-1.87716900	-1.84229600
F	5.79569800	-2.54012000	0.28983800
F	6.70879500	-1.03969100	-0.99111000
F	5.06346100	-0.49377100	0.32087200
O	4.15236600	-0.61526000	-2.57078600
O	4.96584400	-2.98006000	-2.57394400
O	3.12658200	-2.29958500	-1.05808800
C	-6.78383600	1.38266600	-3.87809300
H	-7.52806000	0.86660100	-4.48059600
H	-6.36394800	2.21885900	-4.44208600
H	-7.25375000	1.79581400	-2.98237400
C	-5.68684900	0.43124700	-3.48318000
O	-4.73652900	1.02744400	-2.75205800
H	-4.02955100	0.38050400	-2.49778000
O	-5.64835700	-0.74697900	-3.78350900
C	-4.69381700	-4.17941900	0.99294400
H	-4.15415600	-4.90213800	1.60056700
H	-5.31517900	-4.69876800	0.25985600

H	-5.35956700	-3.58687000	1.62482600
C	-3.72463300	-3.27186700	0.28773900
O	-4.34859500	-2.37310200	-0.49062800
H	-3.68997200	-1.79402800	-0.93302200
O	-2.51528400	-3.32419600	0.39343900
C	-6.00055300	3.53114200	2.36963700
H	-5.90828500	4.05872900	3.31618000
H	-6.83829100	2.83147300	2.41297300
H	-6.20957100	4.24301900	1.56747000
C	-4.72952400	2.78713600	2.06699400
O	-4.80502700	2.10019600	0.91599500
H	-3.95357100	1.63515500	0.75580400
O	-3.73387200	2.79075800	2.76355500
C	0.88535400	-3.83026100	5.12075800
H	1.68590300	-4.46140200	4.74219400
H	-0.00647200	-4.43225800	5.30959700
H	1.18432900	-3.38007300	6.07022300
C	0.56852500	-2.74974700	4.12579900
O	-0.42428500	-1.94709800	4.54908600
H	-0.58981100	-1.25741600	3.87659200
O	1.12534900	-2.59175900	3.05857500

TS1

C	2.89300400	3.77265000	-0.65648400
C	2.12215200	2.59965500	-1.21529500
C	1.87842500	2.65327300	-2.70461800
C	3.25096400	2.74703200	-3.43096100
C	4.07718500	3.92632900	-2.90759200
C	4.26328400	3.85810200	-1.38824400
H	1.33244000	1.77238300	-3.04972800
H	2.49080000	1.63309800	-0.86836200
H	0.97966700	2.67992700	-0.69151500
H	2.34478300	4.70518200	-0.82853600
H	3.05058100	3.66913400	0.41964700
H	3.80043200	1.81170800	-3.27864500
H	3.06913600	2.84151600	-4.50583800
H	5.05577000	3.93846500	-3.39947100

H	3.57987500	4.86733300	-3.17263000
H	4.86412000	2.98027600	-1.12664000
H	4.80021000	4.73713500	-1.01882300
H	1.28527700	3.53814600	-2.96015800
Ru	-0.88567900	1.51895700	0.74328000
O	-2.41559300	0.77270600	-0.04929600
O	-0.89486900	1.63471700	2.45021800
O	-0.22103300	2.88124300	-0.18502600
O	0.29053800	0.30321100	0.23113700
Ca	1.05043800	-1.94343200	0.35148600
C	-1.99797700	-3.14993000	-2.92846400
H	-1.94567000	-2.51483900	-3.81879200
H	-1.28330800	-3.96344800	-3.04104700
H	-3.01549400	-3.53524400	-2.85614800
C	-1.66128300	-2.30421100	-1.72165100
O	-0.50709200	-2.35988200	-1.24099200
O	-2.58418600	-1.54607400	-1.25034600
H	-2.32361700	-0.13839400	-0.47558500
C	5.61804000	-1.04323700	-0.23456100
S	4.42134600	-2.22319200	-1.08420000
F	5.99687100	-1.52688400	0.95586500
F	6.71147600	-0.87215000	-0.98977200
F	5.04551700	0.15377700	-0.04193600
O	4.08107300	-1.55642300	-2.34766500
O	5.15926200	-3.48775900	-1.18073900
O	3.29237800	-2.26695100	-0.10049000
C	-6.93855800	-1.28323100	-3.58329800
H	-7.66114700	-2.07942300	-3.74769300
H	-6.63292400	-0.85708400	-4.54184100
H	-7.39575600	-0.48077700	-2.99995700
C	-5.73297100	-1.81854700	-2.85817200
O	-4.82132000	-0.86971000	-2.61962300
H	-4.03448100	-1.24070100	-2.13546700
O	-5.58650100	-2.97928500	-2.52283400
C	-4.27068900	-3.02774900	3.26377000
H	-3.68804700	-3.22534500	4.16056100
H	-4.83946100	-3.91734800	2.98436700

H	-4.98915800	-2.22781300	3.45798700
C	-3.36185400	-2.62669200	2.13479700
O	-4.03605200	-2.41034800	0.99591200
H	-3.41959100	-2.14340100	0.27591000
O	-2.15547700	-2.50481500	2.22152800
C	-6.00029600	4.09819900	0.30380700
H	-5.92112200	5.01390800	0.88538800
H	-6.83175600	3.49272600	0.67123800
H	-6.20929500	4.34166200	-0.74085900
C	-4.71848600	3.31647500	0.39143900
O	-4.78748900	2.14949900	-0.26396400
H	-3.92666300	1.67324800	-0.17907000
O	-3.71815300	3.68154000	0.98016100
C	1.83059800	-0.36467600	6.19721000
H	2.58999500	-1.14066700	6.13548400
H	1.03467600	-0.67738000	6.87703200
H	2.26626300	0.55128800	6.60255800
C	1.25624900	-0.09549000	4.83431300
O	0.32352400	0.86979000	4.86002300
H	-0.02665200	1.02008900	3.95548000
O	1.57951300	-0.66897600	3.81336100

INT2

C	-2.47756400	-2.90412700	-1.07456700
C	-1.99203600	-1.50565100	-1.45267800
C	-1.48206400	-1.40992200	-2.88912200
C	-2.56386700	-1.89423900	-3.87065700
C	-3.05961200	-3.30309200	-3.51658300
C	-3.55661300	-3.37366100	-2.06604500
H	-1.20172100	-0.37517800	-3.10587800
H	-2.84704400	-0.82877000	-1.34279000
H	0.26957400	-3.56488000	-1.32556000
H	-1.64625800	-3.61873700	-1.09121000
H	-2.86576100	-2.89273000	-0.05256900
H	-3.40952400	-1.19613200	-3.85231100
H	-2.16380000	-1.87326400	-4.88833700
H	-3.86026100	-3.60130900	-4.20017600

H	-2.24240800	-4.02201700	-3.65578400
H	-4.44650800	-2.74264600	-1.95405200
H	-3.86183500	-4.39267300	-1.81261800
H	-0.58121100	-2.02140000	-3.00015800
Ru	0.70550800	-1.58886400	0.02849400
O	2.28417700	-0.81230800	-0.69044700
O	0.81367100	-2.38037200	1.52409100
O	1.03818500	-2.98265700	-1.24785100
O	-1.03154600	-0.97477500	-0.48680100
Ca	-1.37302000	1.30420900	0.55782900
C	1.72528900	3.74298000	-1.72761700
H	1.75448300	3.39829700	-2.76667800
H	0.88307500	4.42520600	-1.61990700
H	2.66568600	4.25245500	-1.51734200
C	1.55549700	2.53346100	-0.83632700
O	0.39524300	2.18423000	-0.50093300
O	2.60089600	1.89052100	-0.48172100
H	2.38664000	0.13935700	-0.42989500
C	-5.90516300	1.00715700	0.05701000
S	-4.70302300	2.31009500	-0.57961700
F	-6.19446500	1.21734000	1.34782700
F	-7.04444500	1.04945100	-0.64584300
F	-5.37870000	-0.22050100	-0.06326400
O	-4.46708200	1.93792400	-1.98025100
O	-5.38206300	3.58684500	-0.33577500
O	-3.51643500	2.09086600	0.30974100
C	6.90508700	2.94508700	-2.66709500
H	7.50320500	3.84977400	-2.58373500
H	6.64570800	2.77118600	-3.71448900
H	7.48161400	2.08256800	-2.32593700
C	5.64552800	3.07792000	-1.85299000
O	4.91482600	1.95887500	-1.86396100
H	4.08222200	2.06334500	-1.32611300
O	5.31333900	4.08325100	-1.25241900
C	4.06811100	1.96370500	4.29279500
H	3.47262000	1.80117100	5.18823300
H	4.53701100	2.94955900	4.33132100

H	4.86918000	1.22248200	4.24081300
C	3.20105100	1.85942300	3.06808800
O	3.89049800	2.07059900	1.94010600
H	3.30236600	1.99244600	1.15020400
O	2.00990600	1.61183500	3.07912200
C	6.46731100	-3.38430300	-1.07955200
H	6.69580200	-4.33697500	-0.60563800
H	7.21660500	-2.64983000	-0.76913000
H	6.51983400	-3.47435900	-2.16474300
C	5.11141200	-2.90061300	-0.63845900
O	4.59782900	-1.98993800	-1.47352700
H	3.72794600	-1.65311800	-1.13650400
O	4.54539300	-3.26915900	0.37330200
C	-1.46389700	-1.59913100	5.99003800
H	-2.14839800	-0.79132400	6.23820800
H	-0.59857700	-1.57271100	6.65622300
H	-1.95883800	-2.56236300	6.13513400
C	-1.01258000	-1.47097900	4.56204700
O	-0.14183900	-2.43573600	4.21865800
H	0.12950900	-2.31550900	3.28573000
O	-1.37517000	-0.60979200	3.78629700

TS2

C	2.57587100	3.20668100	0.33621300
C	2.69349200	2.06882500	-0.67177700
C	3.39034900	2.51926000	-1.95790700
C	4.77894800	3.10512400	-1.65544300
C	4.69288200	4.23970600	-0.62671300
C	3.97082800	3.78047200	0.64752800
H	3.46449300	1.67863000	-2.65221100
H	3.24464900	1.24290200	-0.21612100
H	0.71183600	2.19414900	-1.63418100
H	1.93821800	3.99667300	-0.07780000
H	2.10258900	2.84834700	1.25452700
H	5.43486700	2.31275000	-1.27549200
H	5.22708800	3.46295100	-2.58719100
H	5.69620100	4.60066600	-0.38084400

H	4.15070800	5.08698200	-1.06512400
H	4.57329100	3.01462400	1.15160400
H	3.86923900	4.61080300	1.35174600
H	2.76805900	3.28352600	-2.43935700
Ru	-0.57984000	1.57657500	-0.03281800
O	-2.37275400	1.02683000	-0.35902500
O	-0.49004700	2.39985700	1.43273700
O	-0.59010100	2.56466200	-1.57586900
O	1.38655400	1.50379400	-1.06692800
Ca	1.44953100	-1.01296600	-1.75437900
C	-1.90677100	-3.69309600	-1.50351200
H	-1.63735300	-3.73104900	-2.56300500
H	-1.22898200	-4.36592000	-0.97161600
H	-2.93602700	-4.02394400	-1.38012600
C	-1.71030100	-2.27996100	-0.99826500
O	-0.56454600	-1.76429100	-1.09709500
O	-2.70325900	-1.65629000	-0.49983500
H	-2.47143400	0.04020500	-0.25875300
C	5.44446700	-1.84041800	0.60839300
S	4.76356600	-2.45848100	-1.03603000
F	4.86295600	-2.47631800	1.63384700
F	6.76533400	-2.05748400	0.66865200
F	5.22519100	-0.52461200	0.74666400
O	5.48598000	-1.67747100	-2.04887300
O	5.01059700	-3.90446600	-1.01397900
O	3.31266900	-2.10009800	-0.92152600
C	-6.80467200	-1.54315200	-3.42776700
H	-7.43599400	-2.36336500	-3.76171600
H	-6.38067800	-1.02731900	-4.29270800
H	-7.40104800	-0.81534500	-2.87329800
C	-5.69458600	-2.06609800	-2.55736700
O	-4.91189500	-1.08165500	-2.09154100
H	-4.18457600	-1.44846300	-1.53477300
O	-5.50640300	-3.23789300	-2.29685500
C	-4.93332800	-3.55064000	3.51050400
H	-4.47157200	-3.79658400	4.46409100
H	-5.41488700	-4.44025200	3.09630300

H	-5.70898500	-2.79532900	3.65270400
C	-3.89311400	-3.05016800	2.54485200
O	-4.43041500	-2.64119800	1.38858100
H	-3.72550900	-2.33568000	0.76403000
O	-2.69764400	-3.02035400	2.76607700
C	-5.88049200	4.39313900	-0.90157800
H	-6.20183500	5.11961600	-0.15853500
H	-6.72639100	3.76769900	-1.19660000
H	-5.52732900	4.90914700	-1.79718900
C	-4.78131900	3.52924900	-0.34166100
O	-4.33700900	2.63555600	-1.23090900
H	-3.61283000	2.07273100	-0.84416800
O	-4.33971200	3.62200300	0.78844500
C	-0.37847400	0.18077300	5.97781700
H	0.12250400	-0.75832700	6.20122200
H	-1.43913600	0.10675800	6.22797400
H	0.04695300	0.98219500	6.58640300
C	-0.21953900	0.51348000	4.52115000
O	-0.84760100	1.65644700	4.19009800
H	-0.71229100	1.83151600	3.23667400
O	0.39866800	-0.14904800	3.71304000

RuO₄⁻/Ca²⁺

INT1

C	3.28971400	-0.74158700	-0.92858700
C	2.61628600	0.48464400	-0.29403900
C	3.30742100	0.89022500	1.01672500
C	4.81410100	1.11405800	0.81705700
C	5.48730200	-0.10951600	0.17683000
C	4.79516400	-0.51404900	-1.13373500
H	2.84237600	1.79307300	1.42723700
H	2.66322800	1.32298600	-1.00202900
H	1.55468100	0.28375200	-0.11514700
H	3.14300800	-1.61200300	-0.27537400
H	2.81053700	-0.98402500	-1.88341200
H	4.96549200	1.98761000	0.16914800

H	5.29121100	1.34961800	1.77444100
H	6.54850100	0.09359200	-0.00255200
H	5.44502400	-0.95216300	0.87981400
H	4.94014700	0.28111100	-1.87734700
H	5.26184400	-1.41505600	-1.54573400
H	3.15807700	0.09632200	1.76050100
Ru	-1.77848900	-0.77069300	0.16273900
O	-3.10749000	0.17778300	0.86667300
O	-2.38951500	-2.11504800	-0.69810200
O	-0.51912400	-0.97077100	1.30023700
O	-1.30059400	0.49903700	-0.98501900
Ca	-2.88483800	2.20975200	-0.41329500

TS1

C	2.96159900	-1.19083600	-0.27466900
C	2.07622900	0.02504200	-0.13122100
C	2.62629200	1.10176700	0.77285400
C	4.01863400	1.54235000	0.24415400
C	4.96160500	0.34308500	0.08880700
C	4.35209000	-0.74631300	-0.80182800
H	1.95411400	1.96214800	0.81993900
H	1.68483900	0.40030400	-1.07778300
H	0.99154100	-0.42899400	0.44485700
H	3.09504500	-1.67702000	0.69857500
H	2.51908700	-1.92403600	-0.95362700
H	3.89213500	2.03910300	-0.72480400
H	4.44106000	2.28312600	0.93010700
H	5.91745500	0.67417300	-0.33051300
H	5.18113700	-0.07721600	1.07812700
H	4.24371000	-0.36860200	-1.82512200
H	5.00869000	-1.62046500	-0.85193300
H	2.74471300	0.71594300	1.79198000
Ru	-1.56380100	-0.77357500	0.13855000
O	-2.80930000	0.22690300	0.93324500
O	-2.15574000	-2.13308100	-0.73112400
O	0.02476100	-0.95927500	1.00300400
O	-1.04666900	0.54019700	-0.99291700

Ca	-2.54746900	2.21051600	-0.35911300
INT2			
C	2.99703700	-1.16435600	-0.34224200
C	2.23684100	0.11798900	-0.24631500
C	2.78902800	1.16135300	0.66728200
C	4.25947800	1.47068700	0.25284700
C	5.09565200	0.18680300	0.17970600
C	4.46667300	-0.85318400	-0.75603700
H	2.18983900	2.07430800	0.64768500
H	1.64294600	0.43590900	-1.09796800
H	0.68457200	-0.56527400	0.65396500
H	3.02684800	-1.66586100	0.63407600
H	2.53965700	-1.85322500	-1.05573400
H	4.25726400	1.96593500	-0.72467800
H	4.69110500	2.17601100	0.96954500
H	6.10950200	0.42410500	-0.15870400
H	5.19226500	-0.24113200	1.18541100
H	4.47606800	-0.47831100	-1.78563000
H	5.04281700	-1.78348200	-0.74737600
H	2.80549600	0.79414200	1.70201400
Ru	-1.68632600	-0.76997200	0.13201400
O	-2.87256400	0.31765700	0.90830300
O	-2.31695900	-2.10009000	-0.75295200
O	-0.07908000	-1.02025900	1.10494000
O	-1.00963500	0.51353500	-0.94930400
Ca	-2.46511900	2.26965700	-0.35252900
TS2			
C	2.89393800	-1.33420600	-0.06172300
C	2.10364100	-0.10746300	-0.36970800
C	2.51253100	1.14896000	0.31391500
C	4.01249800	1.42997800	-0.01927800
C	4.88973500	0.21318400	0.29710100
C	4.38938000	-1.04957400	-0.41331500
H	1.89346600	1.99397800	0.00849900
H	1.60264900	-0.03611900	-1.32738200

H	0.54911600	-0.88257700	0.67883400
H	2.85080600	-1.57230600	1.00845600
H	2.53342400	-2.20205800	-0.61712300
H	4.09822100	1.68153100	-1.08201800
H	4.33993700	2.30692800	0.54686700
H	5.92419500	0.41726800	0.00253300
H	4.89906600	0.04161100	1.38050700
H	4.48518900	-0.93046100	-1.49788900
H	4.98533500	-1.92221600	-0.13015800
H	2.42813700	1.04075100	1.40276500
Ru	-1.76111300	-0.73402300	0.08039700
O	-2.76435400	0.51853300	0.87639700
O	-2.52485500	-1.87387100	-0.95520300
O	-0.25155200	-1.30821000	1.07393200
O	-0.75336700	0.46037900	-0.85106300
Ca	-1.87789400	2.40903800	-0.17729100

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