

Theoretical study of ether group substitution effects on electrochemical properties of Ti-modified vanadium-oxide clusters

Kexin Wang,[†] Shuang Wu,[†] Sihan Wei, Likai Yan*

Key Laboratory of Polyoxometalate Science of Ministry of Education, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China

*E-mail: yanlk924@nenu.edu.cn

[†] These authors contributed equally to this work.

Table S1 Redox potentials (V) of $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$ calculated by thermodynamic cycling using different functionals.

	PBE	TPSSh	B3LYP	PBE0	Exp
$[\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^+ - e^- \rightleftharpoons [\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^{2+}$	-0.10	0.28	0.62	0.68	0.70
$[\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}] - e^- \rightleftharpoons [\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^+$	-0.88	-0.19	0.19	0.23	0.22
$[\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}] + e^- \rightleftharpoons [\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^-$	-2.01	-1.80	-1.48	-1.62	-1.53
$[\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^- + e^- \rightleftharpoons [\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}]^{2-}$	-2.53	-2.37	-2.02	-2.01	-2.10

Note: The experimental values are taken from reference.²⁶

Table S2 Redox potentials (V) of Ti_2V_4 , $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$ and $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$ calculated by PBE0 functional.

	E_{red}^2	E_{red}^1	E_{ox}^1	E_{ox}^2
Ti_2V_4	-2.05 (-2.10)	-1.67 (-1.58)	0.11 (0.15)	0.57 (0.64)
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$	-2.01 (-2.11)	-1.62 (-1.53)	0.23 (0.22)	0.68 (0.70)
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$	-1.94 (-2.02)	-1.67 (-1.50)	0.23 (0.25)	0.67 (0.73)

Note: Data in parentheses are experimental values, quoted from reference.²⁴

Table S3 Redox potentials (V) of Ti_3V_3^+ , $\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{B}+}$ and $\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{C}+}$ calculated by PBE0 functional.

	E_{red}^2	E_{red}^1	E_{ox}^1	E_{ox}^2
Ti_3V_3^+	-1.71	-1.29	0.46	0.98
$\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{B}+}$	-1.68	-1.13	0.88	1.28
$\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{C}+}$	-1.69	-1.15	0.86	1.28

Table S4 Recombination energies λ_{total} (kcal mol⁻¹) for **Ti₂V₄**, **Ti₂V₄TRIOI^B** and **Ti₂V₄TRIOI^C**.

	R ₂	R ₁	O ₁	O ₂	Total
Ti₂V₄	40.9	37.5	26.1	30.2	134.7
Ti₂V₄TRIOI^B	36.2	35.8	26.7	32.5	131.1
Ti₂V₄TRIOI^C	35.0	31.3	26.7	32.6	125.6

Table S5 Recombination energies λ_{total} (kcal mol⁻¹) for **Ti₃V₃⁺**, **Ti₃V₃TRIOI^{B+}** and **Ti₃V₃TRIOI^{C+}**.

	R ₂	R ₁	O ₁	O ₂	Total
Ti₃V₃⁺	33.2	34.4	29.0	34.2	130.8
Ti₃V₃TRIOI^{B+}	32.8	33.2	28.0	35.6	129.7
Ti₃V₃TRIOI^{C+}	32.3	33.3	30.1	35.8	131.5

Table S6 Diffusion coefficients of studied systems.

System	D^{cal} (10 ⁻⁶ cm ² s ⁻¹)	System	D^{cal} (10 ⁻⁶ cm ² s ⁻¹)
Ti₂V₄	7.5	Ti₃V₃⁺	5.8
Ti₂V₄TRIOI^B	7.3	Ti₃V₃TRIOI^{B+}	7.8
Ti₂V₄TRIOI^C	5.5	Ti₃V₃TRIOI^{C+}	9.2

Table S7 Interaction energy between Ti_2V_4 , $\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{B}}$ and $\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{C}}$ with CH_3CN and $[\text{NBu}_4][\text{PF}_6]$ (kJ mol^{-1}).

	POVs- CH_3CN	POVs- $[\text{NBu}_4][\text{PF}_6]$
Ti_2V_4	-196.2	-69.9
$\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{B}}$	-172.0	-71.6
$\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{C}}$	-187.1	-75.3

Table S8 Interaction energy between Ti_3V_3^+ , $\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{B}+}$ and $\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{C}+}$ with CH_3CN and $[\text{NBu}_4][\text{PF}_6]$ (kJ mol^{-1}).

	POVs- CH_3CN	POVs- $[\text{NBu}_4][\text{PF}_6]$
Ti_3V_3^+	-239.9	-183.1
$\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{B}+}$	-240.0	-180.9
$\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{C}+}$	-258.8	-174.3

Table S9 Dipole moments of the studied systems (in Debye).

	Dipole Moment (Debye)
Ti_2V_4	14.76
$\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{B}}$	13.19
$\text{Ti}_2\text{V}_4\text{TRIOL}^{\text{C}}$	12.85
Ti_3V_3^+	16.82
$\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{B}+}$	16.72
$\text{Ti}_3\text{V}_3\text{TRIOL}^{\text{C}+}$	19.52

Table S10 Solubility and solvation energies of Ti_2V_4 , $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$ and $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$.

System	Solubility (M)	ΔG_{solv} (kcal mol ⁻¹)
Ti_2V_4	0.19	-12.4
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$	0.32	-14.2
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$	0.66	-15.3

Note: Solubility data are quoted from references.^{24,26}

Table S11 Solvation energies of Ti_3V_3^+ , $\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{B}+}$ and $\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{C}+}$.

	ΔG_{solv} (kcal mol ⁻¹)
Ti_3V_3^+	-37.6
$\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{B}+}$	-37.9
$\text{Ti}_3\text{V}_3\text{TRIOI}^{\text{C}+}$	-39.4

Table S12 Maximum and minimum values of electrostatic potential (kcal mol⁻¹) for Ti_2V_4 , $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$ and $\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$.

System	Minimum	Maximum
Ti_2V_4	-47.65	34.55
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{B}}$	-51.02	34.37
$\text{Ti}_2\text{V}_4\text{TRIOI}^{\text{C}}$	-50.43	34.55

Table S13 Maximum and minimum values of electrostatic potential (kcal mol⁻¹) for **Ti₃V₃⁺**, **Ti₃V₃TRIOL^{B+}** and **Ti₃V₃TRIOL^{C+}**.

System	Minimum	Maximum
Ti₃V₃⁺	5.80	90.55
Ti₃V₃TRIOL^{B+}	0.19	89.69
Ti₃V₃TRIOL^{C+}	-5.95	90.04

Optimize the Cartesian coordinates of the structure

Ti₂V₄

V 1.81299700 -1.66502500 0.27335700
V -1.49481000 -1.96618400 0.33734100
V 0.00140600 -0.55528900 -2.26965000
V 0.01869400 0.18716200 2.35393000
Ti -1.67331000 1.22595100 -0.18179000
Ti 1.45229700 1.50729400 -0.23287600
O 3.04321100 -2.65120600 0.38569000
O -2.50801600 -3.16397700 0.53261400
O -0.03540000 -0.74352700 -3.84150800
O 0.03418300 0.40082100 3.92418200
O -3.00431400 2.35690600 -0.33455300
O 2.58516700 2.82560700 -0.44551800
O 0.26598200 -2.86988700 0.49829600
O 1.50929900 -1.69279100 -1.69552200
O 2.75692600 0.09337300 -0.00666900
O 1.51417400 -1.09241800 2.15240600
O -1.26947000 -1.93691500 -1.64006500
O 1.27512400 1.00025600 -2.13135400
O 1.25044400 1.65012000 1.72123400

O	-1.24982400	-1.32495900	2.19631600
O	-1.49771000	0.79327700	-2.06660000
O	-0.20465500	2.58641500	-0.43282300
O	-1.46870800	1.39832400	1.75102600
O	-2.73534800	-0.40722200	0.07657500
O	-0.00176300	0.00053400	0.01084400
C	-3.98739500	3.34915900	-0.29370900
H	-4.29100200	3.61435900	-1.31220700
H	-3.59802500	4.24206700	0.20730200
H	-4.86100200	2.98266700	0.25582300
C	3.46481800	3.90008800	-0.59866800
H	4.47098600	3.60170500	-0.28553000
H	3.13367800	4.74385200	0.01616700
H	3.49315900	4.21210500	-1.64824500
C	0.36805200	-3.80929000	1.56139200
H	-0.46044600	-4.52185800	1.48567200
H	0.32676200	-3.30584000	2.53185100
H	1.31880100	-4.34632100	1.47131000
C	1.80722900	-2.91565000	-2.34611800
H	2.89220800	-3.07289200	-2.32986400
H	1.46609600	-2.87524600	-3.38587700
H	1.32656900	-3.76182200	-1.84399300
C	4.15481800	0.29370200	0.12519600
H	4.64420700	-0.67140300	0.28002100
H	4.37122800	0.94770200	0.97702900
C	2.65396200	-0.81276900	2.94927400
H	2.37544300	-0.89280300	4.00640700
H	3.02904800	0.19951600	2.76291100
H	3.44401300	-1.53776100	2.72692700
C	-1.44809800	-3.17067300	-2.31179000
H	-1.14956600	-3.06888900	-3.36035600

H	-2.50703200	-3.45322600	-2.26709700
H	-0.85804800	-3.96878700	-1.84856100
C	2.42153200	0.94533300	-2.96385400
H	3.03422400	1.83972800	-2.80981700
H	2.10088900	0.90044600	-4.00999700
H	3.01317200	0.05306000	-2.73108800
C	1.18010500	2.92216600	2.34329600
H	2.09060300	3.48695500	2.11689800
H	1.09565200	2.79074200	3.42656400
H	0.31298000	3.48250600	1.97607200
C	-2.43536200	-1.25194400	2.97231700
H	-2.18860200	-0.89774200	3.97899400
H	-2.87924300	-2.25189800	3.03796700
H	-3.16419500	-0.57202200	2.51774200
C	-2.27830600	1.19821600	-3.17351600
H	-3.04599700	1.90493300	-2.84379700
H	-2.76367200	0.33035500	-3.63263900
H	-1.64221700	1.68106800	-3.92321400
C	-0.29018300	3.60742000	-1.41147300
H	0.46922200	4.36893900	-1.20689000
H	-1.28241900	4.06703700	-1.37544700
H	-0.11951100	3.18651100	-2.40860800
C	-2.26044400	2.20763200	2.60171300
H	-3.31586800	1.92414000	2.52190800
H	-2.15652800	3.26285700	2.32477400
H	-1.93324800	2.07730300	3.63689000
C	-3.88279700	-0.66253100	-0.71893800
H	-4.45628900	0.26167000	-0.84358300
H	-4.50300000	-1.41144000	-0.21539800
H	-3.58475700	-1.04260200	-1.70147200
H	4.55138800	0.75668800	-0.78466800

Ti₂V₄TRIOI^B

V	1.35461600	0.03502500	2.21509000
V	-1.03049100	-1.82886200	0.87640900
V	-0.74471000	-0.12602200	-1.95235600
V	-1.31874700	1.46512500	0.90011600
Ti	1.85373400	-1.49543800	-0.58929600
Ti	1.55142600	1.63242000	-0.57015700
O	3.06456900	-2.62290200	-1.16662200
O	2.56113100	2.96149100	-1.10966100
O	2.09088200	0.02453800	3.61871200
O	-1.89274900	-3.07405300	1.33561900
O	-1.40465300	-0.15774300	-3.39259200
O	-2.39850600	2.47854100	1.45714400
O	2.78460600	0.15458000	-1.17528900
O	2.56243800	-1.23728000	1.21322300
O	0.58765600	-2.77241100	0.16806000
O	0.74718400	-1.43983000	-2.20683600
O	2.30621300	1.50566300	1.22228800
O	0.02913200	-1.40781600	2.48428300
O	-1.69043100	-1.57559300	-0.99142600
O	0.57019900	1.37399200	-2.23393400
O	0.04013400	2.69610600	0.10539300
O	-0.13114600	1.30205600	2.48621300
O	-2.16053100	-0.27648800	1.35004600
O	-1.92812200	1.13277900	-0.97323900
O	0.47219500	-0.01080600	0.04865400
O	-5.99318300	0.52111600	-0.15300000
C	4.08196300	-3.41250700	-1.70990300
H	5.05401800	-3.08522100	-1.32566600
H	4.08010900	-3.32418800	-2.80170000
H	3.92316200	-4.46064700	-1.43517300

C	3.49066800	3.96150600	-1.40786600
H	4.50313700	3.61158000	-1.17925100
H	3.27747200	4.85523300	-0.81178900
H	3.43261600	4.21852700	-2.47105600
C	3.46277800	0.20265300	-2.41912900
H	2.77151300	-0.04006600	-3.23401500
H	4.28288100	-0.52191900	-2.41337100
H	3.86903000	1.20633400	-2.57533800
C	3.96165100	-1.16968600	1.43432500
H	4.15126200	-1.06930400	2.50714600
H	4.39220600	-0.31065700	0.90707600
H	4.43143900	-2.08712900	1.06475500
C	1.06303500	-3.87213500	0.93409300
H	0.25136500	-4.59647700	1.05135000
H	1.39160300	-3.52660900	1.91945100
H	1.90306100	-4.34086900	0.41236800
C	0.45395400	-2.62290300	-2.93544700
H	0.06212500	-2.34603000	-3.91918900
H	-0.29472200	-3.21559500	-2.39959400
H	1.36705000	-3.21352300	-3.05669100
C	3.31923500	2.33595200	1.76232200
H	4.24520000	2.22289100	1.18735000
H	3.50808200	2.05105900	2.80089200
H	3.00877100	3.38604900	1.72961900
C	-0.67583400	-1.38751100	3.71814300
H	-1.35587100	-0.53175400	3.76375400
H	0.04725200	-1.32008300	4.53812200
H	-1.25129800	-2.31472300	3.81424600
C	0.61825500	2.10527900	-3.44385500
H	-0.35337400	2.56854300	-3.64518300
H	0.86744500	1.43697300	-4.27506000

H	1.37988100	2.88737500	-3.36995500
C	-0.46474100	3.80867800	-0.61813000
H	-1.01422900	4.45812500	0.07139400
H	-1.14074500	3.46864700	-1.40924600
H	0.36635800	4.36683100	-1.06051800
C	0.15941300	2.52133600	3.15159600
H	0.63263600	3.23887500	2.47240900
H	0.82942500	2.32479100	3.99553400
H	-0.77618200	2.95325800	3.52432200
C	-3.10166200	-1.59863500	-1.14414100
H	-3.47443900	-2.53049000	-0.69692900
H	-3.32605400	-1.61595300	-2.21987000
C	-3.53868700	-0.38996600	1.01619500
H	-4.06979900	0.45317800	1.47187900
H	-3.91803300	-1.32219800	1.45754000
C	-3.32277800	0.90654400	-1.13226100
H	-3.54306200	0.88522100	-2.20896600
H	-3.86103900	1.74903500	-0.68368900
C	-3.80108400	-0.40083000	-0.49274200
C	-5.30107800	-0.55620100	-0.73669900
H	-5.49853400	-0.59519200	-1.82211400
H	-5.65010700	-1.51221400	-0.30911100
C	-7.38341700	0.42574300	-0.35263200
H	-7.84391500	1.29245100	0.12604700
H	-7.79390800	-0.49074300	0.09629800
H	-7.63882300	0.43044200	-1.42256700

Ti₂V₄TRIOI^C

V	-1.74523300	0.08932400	2.25507200
V	0.65688800	1.79958900	0.75214600
V	0.17674800	0.01428400	-1.99843800
V	0.80606800	-1.50177200	0.88301600

Ti	-2.29986000	1.54224100	-0.57952400
Ti	-2.12983600	-1.59318300	-0.45937900
O	-3.48426100	2.70177400	-1.14782000
O	-3.21724200	-2.89532000	-0.90520200
O	-2.41828100	0.17921200	3.68714800
O	1.59071400	3.01995700	1.13106300
O	0.77498100	-0.03279200	-3.46501600
O	1.86430400	-2.54221900	1.43148000
O	-3.32417100	-0.08448200	-1.06570100
O	-2.94076200	1.37779400	1.25891300
O	-0.94875100	2.78805900	0.07678700
O	-1.26773100	1.38252200	-2.23873500
O	-2.80052300	-1.37111900	1.35726100
O	-0.35028200	1.48214700	2.41616100
O	1.22406500	1.45336900	-1.13110700
O	-1.21176000	-1.43529600	-2.17088100
O	-0.63734800	-2.69810300	0.19150300
O	-0.30279800	-1.23034000	2.51030500
O	1.73940900	0.21597300	1.23356300
O	1.34735300	-1.26108400	-1.02519100
O	-0.95517900	0.02162800	0.05354200
O	5.46114800	-0.80587500	-0.39837800
C	-4.48315400	3.52112000	-1.68135100
H	-5.44755200	3.28214700	-1.22043700
H	-4.55493500	3.36583300	-2.76326800
H	-4.24347200	4.57159700	-1.48553200
C	-4.19593900	-3.87013600	-1.11738700
H	-5.18597800	-3.46332400	-0.88481800
H	-4.00352500	-4.73470200	-0.47315800
H	-4.17875800	-4.19314900	-2.16385900
C	-4.05695800	-0.14563700	-2.27757800

H	-3.39129300	0.03486200	-3.12913900
H	-4.84243500	0.61627400	-2.26508700
H	-4.51443500	-1.13426200	-2.37834300
C	-4.33071700	1.37854400	1.54049000
H	-4.47773400	1.32711600	2.62341400
H	-4.81861600	0.51942500	1.06606600
H	-4.77796700	2.30052500	1.15465700
C	-1.34490400	3.93270600	0.82194700
H	-0.50002400	4.62563400	0.87878700
H	-1.64441700	3.63535300	1.83198900
H	-2.18695200	4.41849800	0.31944700
C	-0.95734000	2.52728000	-3.01962000
H	-0.60085200	2.20131400	-4.00170000
H	-0.17679100	3.11561300	-2.52611100
H	-1.85481600	3.14159900	-3.14008300
C	-3.82010300	-2.14074600	1.96995300
H	-4.76436900	-2.01394900	1.42863300
H	-3.95484900	-1.80981500	3.00328300
H	-3.55022900	-3.20251300	1.96603500
C	0.40277000	1.47651900	3.62131800
H	1.03803800	0.58776100	3.67936500
H	-0.28884500	1.48367800	4.47073700
H	1.02950600	2.37433700	3.65344700
C	-1.34516900	-2.20248900	-3.35186600
H	-0.41005400	-2.72944600	-3.56906200
H	-1.58424600	-1.54847400	-4.19722400
H	-2.14796100	-2.93495900	-3.22493000
C	-0.21336300	-3.85736300	-0.51033400
H	0.34044600	-4.50397900	0.17833400
H	0.43830500	-3.57665600	-1.34400300
H	-1.08678000	-4.39491100	-0.89256500

C	-0.61365200	-2.41074100	3.23395200
H	-1.14788200	-3.13067700	2.60434500
H	-1.23504500	-2.15455600	4.09883200
H	0.31899000	-2.86997300	3.58050700
C	2.62656000	1.40888500	-1.34433600
H	3.05844800	2.33814500	-0.94777900
H	2.80393500	1.37903300	-2.42853000
C	3.10516400	0.25727500	0.83856000
H	3.61906300	-0.59219900	1.30213800
H	3.54258300	1.18664500	1.22949100
C	2.74197300	-1.10209900	-1.25107300
H	2.91564400	-1.12708000	-2.33619800
H	3.26358400	-1.95131700	-0.79576800
C	3.30217500	0.20436200	-0.67977000
C	4.79530900	0.28860100	-0.99221000
H	4.94743000	0.27400700	-2.08435900
H	5.19060300	1.24626500	-0.61909000
C	6.83568700	-0.88036300	-0.70822300
H	7.14293900	-1.91700700	-0.53821100
H	7.01365200	-0.64485400	-1.76796800
C	7.67679100	0.03478200	0.16940800
H	7.39253100	1.09019000	0.02660700
H	7.50371800	-0.21165000	1.22977800
O	9.02140200	-0.16789700	-0.18677900
C	9.89841000	0.63027600	0.56963900
H	9.82543600	0.40695600	1.64447300
H	10.91463500	0.41430600	0.23198200
H	9.69625500	1.70238000	0.42696800
Ti₃V₃⁺			
V	-0.17575600	2.36606500	0.71889700
V	-1.56736900	0.66768300	-1.79300400

V	-2.07181200	-0.26947500	1.35488100
Ti	-0.16092400	-2.02223900	-0.61834300
Ti	1.18329000	-0.41071900	1.78522000
O	-0.16051500	3.85433700	1.23746300
O	-2.48706400	1.03402800	-3.01906200
O	-3.31052700	-0.61226800	2.26549700
O	3.05222100	0.81226800	-2.20918200
O	-0.12717400	-3.68492600	-1.12625600
O	2.22019300	-0.82559900	3.11917400
O	-1.31177400	2.42136700	-0.89901300
O	-1.72001600	1.63756600	1.70399900
O	1.05068500	1.50765900	2.06609600
O	1.41569700	2.28559500	-0.51723100
O	-2.88016900	0.18867200	-0.38795800
O	-0.55307300	-0.60547700	2.63393500
O	2.59725600	-0.05362800	0.43585700
O	0.27375800	0.86178100	-2.58301800
O	-1.68121600	-2.09239500	0.56794300
O	0.99875000	-2.22299600	1.01195500
O	1.44514600	-1.43300500	-1.62057800
O	-1.29462200	-1.30747500	-2.04057600
O	-0.00335300	0.00519400	0.00812200
C	0.08669900	-4.98539900	-1.60443100
H	-0.62961700	-5.66743600	-1.13652600
H	1.10477900	-5.30429800	-1.36070200
H	-0.05062800	-5.00217200	-2.68991200
C	3.10067000	-1.25435200	4.12183200
H	3.67161300	-0.39975000	4.49713000
H	3.78987300	-1.99999700	3.71329200
H	2.52976600	-1.69873100	4.94284700
C	-1.10911600	3.51225500	-1.79250400

H	-2.00477600	3.63053400	-2.41137800
H	-0.24869100	3.33141300	-2.44536000
H	-0.94355000	4.42848400	-1.21695200
C	-2.77730500	2.55679800	1.94915000
H	-2.43185000	3.30255700	2.67329900
H	-3.63926800	2.02437700	2.36199600
H	-3.07412800	3.07058000	1.02975300
C	2.19824800	2.23869300	2.48706000
H	1.91249400	3.27956100	2.66050200
H	2.97971700	2.19356200	1.72121200
C	2.21283700	3.41224000	-0.87099300
H	2.14351900	3.59815200	-1.94731200
H	3.25771800	3.22397000	-0.60499400
H	1.85526000	4.29027400	-0.32840800
C	-4.14529900	0.83153300	-0.48046800
H	-4.73602600	0.61206800	0.41401500
H	-4.67168600	0.44902300	-1.36210000
H	-4.03388500	1.91549400	-0.58263200
C	-0.73797700	-0.13569200	3.96792600
H	0.09276600	-0.47864700	4.59090200
H	-1.67865500	-0.53830600	4.35372000
H	-0.77521400	0.95792500	3.97206300
C	3.79150900	-0.82520400	0.42254000
H	4.32174200	-0.68147600	1.36835600
H	4.42932700	-0.49603200	-0.40197000
H	3.55182900	-1.88675100	0.29786200
C	0.41836800	0.43336500	-3.93333300
H	1.45914800	0.55510300	-4.24679100
H	-0.22841400	1.04706400	-4.56722200
H	0.12676000	-0.61744700	-4.02904700
C	-2.61442100	-3.14814600	0.75982400

H	-2.27587300	-4.03843100	0.22323000
H	-3.59821300	-2.85068700	0.38486300
H	-2.69319800	-3.37396600	1.82748000
C	0.85708000	-3.34973700	1.86973300
H	1.72270000	-3.40709300	2.53522300
H	0.80166300	-4.25973600	1.26656200
H	-0.05595900	-3.24975000	2.46646600
C	2.22339900	-2.25961000	-2.47488300
H	1.59431900	-2.67144000	-3.27002500
H	2.66121300	-3.08035600	-1.89837400
H	3.02609300	-1.66918400	-2.92310200
C	-2.42898100	-2.02235000	-2.52052400
H	-2.20281600	-3.09200900	-2.55301200
H	-2.66673800	-1.66782000	-3.52791400
H	-3.28703200	-1.84882200	-1.86378000
H	2.57861600	1.80320300	3.41579700
Ti	1.64372600	0.51197000	-1.23609900
C	4.20615900	1.16461000	-2.92316500
H	3.93882100	1.85725200	-3.72686400
H	4.92006300	1.64691500	-2.24855800
H	4.66111000	0.26667600	-3.35242000

Ti₃V₃TRIOI^{B+}

V	1.01069500	1.96342100	-0.52309800
V	1.01204500	-1.17235300	-1.60145800
V	1.31421100	-0.52765300	1.64838500
Ti	-1.74529900	0.58553000	-1.63303300
Ti	-1.42367400	-1.81334200	0.44258900
O	-2.90627200	1.00451900	-2.85826200
O	-2.36299600	-3.22809600	0.81652000
O	1.80414900	3.27386900	-0.89763200
O	1.79785800	-2.01993000	-2.67314100

O	2.33056200	-0.87539000	2.80325400
O	-2.58883100	-1.10087500	-1.03467800
O	-2.61638700	1.50448100	-0.09921600
O	-0.55837200	2.12342800	-1.76171100
O	-0.47527000	-0.41236200	-2.71015200
O	-2.34570800	-0.57893200	1.69065400
O	-0.21789700	2.57828900	0.92968500
O	1.83766800	0.61992300	-1.72479500
O	-0.28225700	-2.55890700	-0.92450300
O	0.02293200	-2.05139100	1.73859200
O	-0.04977100	0.53356900	2.67095100
O	2.08165400	1.15200300	0.92466400
O	2.08156500	-1.42242500	0.04628300
O	-0.45374100	0.01205900	0.00096800
O	6.04172900	-0.16579900	0.57928000
C	-3.91676400	1.24876000	-3.79884500
H	-4.89592300	1.16391400	-3.31752400
H	-3.84464000	0.51674400	-4.60902000
H	-3.79847800	2.25661300	-4.20793800
C	-3.24570500	-4.24974500	1.19500500
H	-4.27769200	-3.90119400	1.09064700
H	-3.05726700	-4.52681200	2.23660700
H	-3.08955500	-5.12176000	0.55274400
C	-3.20479500	-1.96755000	-1.98104100
H	-2.46980600	-2.28717600	-2.72771200
H	-4.02123900	-1.43634100	-2.47773500
H	-3.60415900	-2.84411700	-1.46449300
C	-4.02916900	1.66123200	-0.04499800
H	-4.30466800	2.16776900	0.88320800
H	-4.51643200	0.68105800	-0.08417500
H	-4.35604300	2.26404900	-0.89679100

C	-1.09684700	3.43211500	-1.93613000
H	-0.29269600	4.10296400	-2.25011600
H	-1.52682900	3.78943300	-0.99477000
H	-1.87400600	3.40311100	-2.70494900
C	-0.12423100	0.04436500	-4.01597900
H	0.36844100	-0.77243700	-4.55047500
H	0.55583200	0.89779900	-3.93772600
H	-1.03033500	0.34244400	-4.55024700
C	-3.47430200	-0.91479900	2.48721100
H	-4.31618000	-1.18786700	1.84337700
H	-3.75659700	-0.05733300	3.10223200
H	-3.22775300	-1.75805200	3.13911500
C	0.33011500	3.48942600	1.88146800
H	1.11775200	2.99112400	2.45436500
H	-0.46047500	3.82713000	2.55650500
H	0.74778300	4.34563700	1.34480600
C	-0.19857700	-3.90038600	-1.39085100
H	0.78475500	-4.31617500	-1.15223300
H	-0.34154000	-3.92027500	-2.47520300
H	-0.97349300	-4.50291000	-0.90984600
C	0.59380400	-3.33336500	1.98581000
H	1.05952900	-3.32318200	2.97580000
H	1.35291600	-3.55547800	1.22947200
H	-0.18965700	-4.09582300	1.95704100
C	-0.35308300	0.05608900	3.97845000
H	-0.73375100	-0.96915100	3.92613000
H	-1.10524000	0.70365000	4.43797500
H	0.56142200	0.07271100	4.57798600
C	3.26235500	0.63545100	-1.75593700
H	3.58049900	1.65999800	-1.98942100
H	3.58616500	-0.02302700	-2.57282600

C	3.49027000	1.12115600	0.69994200
H	3.97457100	0.80392800	1.62936600
H	3.81615300	2.14365100	0.46655800
C	3.48967000	-1.26057000	-0.11979400
H	3.81019600	-1.92141400	-0.93643000
H	3.98079100	-1.58511200	0.80363000
C	3.89743500	0.18105400	-0.43839000
C	5.41509400	0.24022400	-0.61253100
H	5.71859100	-0.41292800	-1.44873000
H	5.71870600	1.26794300	-0.87625300
C	7.44615100	-0.13346700	0.47627100
H	7.85217600	-0.46049100	1.43555100
H	7.81093000	0.88126700	0.26024000
H	7.80772300	-0.80723400	-0.31412200
Ti	-1.45149300	1.18521900	1.48029000
O	-2.39108300	2.07754500	2.63927800
C	-3.14838500	2.88086000	3.50428000
H	-3.33362100	3.84988400	3.03118100
H	-4.10381500	2.39254900	3.71993400
H	-2.59711800	3.02973000	4.43761600

Ti₃V₃TRIOLO⁺

V	0.67680800	-1.61214700	1.05961600
V	0.34931900	1.68213600	1.24878800
V	0.85217200	0.22405700	-1.69937800
Ti	-2.23802600	-0.26696600	1.70603300
Ti	-2.04020700	1.50823500	-0.93598200
O	-3.40940900	-0.45645400	2.97709600
O	-3.08657500	2.67146900	-1.69495300
O	1.56858700	-2.68888900	1.78938100
O	1.00786000	2.85904400	2.06452100
O	1.88374700	0.34798500	-2.88601600

O	-3.20116800	1.10569800	0.65705100
O	-2.95307500	-1.64392500	0.46149000
O	-0.92418500	-1.58982200	2.26682800
O	-1.11120800	1.10311000	2.49421500
O	-2.79205500	-0.09873600	-1.82040700
O	-0.42623200	-2.71315800	-0.19381100
O	1.32661100	0.07851300	1.86783500
O	-1.03256900	2.70263200	0.19831100
O	-0.56482300	1.53389400	-2.22172700
O	-0.36413000	-1.20193500	-2.42034600
O	1.73356700	-1.11788600	-0.53455900
O	1.46475100	1.58451200	-0.38464100
O	-0.93142600	-0.02708800	0.00004200
O	5.53351800	0.62655900	-0.49228600
C	-4.43834200	-0.54514100	3.92524900
H	-5.39353000	-0.70917300	3.41701700
H	-4.48625500	0.38547500	4.49890400
H	-4.23844400	-1.38026400	4.60326600
C	-4.04346700	3.45692500	-2.35341400
H	-5.04153900	3.04379600	-2.17850200
H	-3.83355400	3.46263800	-3.42723400
H	-4.00072700	4.48050600	-1.96904200
C	-3.93692500	2.12836500	1.31943600
H	-3.26825000	2.71347100	1.96005000
H	-4.71871400	1.67050600	1.93142300
H	-4.39670700	2.78460700	0.57606500
C	-4.34127000	-1.95263600	0.42861300
H	-4.52861600	-2.71012500	-0.33617700
H	-4.92004500	-1.05156900	0.19922100
H	-4.64554900	-2.34157600	1.40434900
C	-1.34848900	-2.85188500	2.77714700

H	-0.50249700	-3.32881600	3.27927300
H	-1.69663200	-3.48976300	1.95830500
H	-2.16196800	-2.69749400	3.49150500
C	-0.77889400	1.05193000	3.88138600
H	-0.38838700	2.02774200	4.18275000
H	-0.02010100	0.28210500	4.05041800
H	-1.67652400	0.81835500	4.46013300
C	-3.91056900	-0.10096300	-2.69783700
H	-4.80384200	0.23525500	-2.16223300
H	-4.07761600	-1.11241900	-3.07505000
H	-3.71942800	0.56936900	-3.54098000
C	0.24301900	-3.78480900	-0.85722100
H	1.00159300	-3.38047000	-1.53385000
H	-0.48509400	-4.36931700	-1.42562700
H	0.71829800	-4.41931200	-0.10418500
C	-1.09149600	4.12136200	0.28650700
H	-0.13852600	4.55336200	-0.03272800
H	-1.28854100	4.41577500	1.32149500
H	-1.89236500	4.49398200	-0.35732000
C	-0.10054200	2.75429000	-2.79238900
H	0.40766200	2.52803700	-3.73449100
H	0.60141000	3.24214200	-2.10899100
H	-0.94954600	3.41650200	-2.98394000
C	-0.64982900	-1.12669400	-3.81391400
H	-1.12695600	-0.16981800	-4.04972000
H	-1.31604100	-1.94748400	-4.09421300
H	0.28881400	-1.20984800	-4.36893000
C	2.74388000	0.21159300	1.92882500
H	3.14169700	-0.67632400	2.43754400
H	2.97119600	1.09374600	2.54194300
C	3.12200300	-0.89023200	-0.29978200

H	3.61736000	-0.78775900	-1.27103000
H	3.52679900	-1.77585600	0.20820200
C	2.87305500	1.61258700	-0.15529200
H	3.09623900	2.49596600	0.45806600
H	3.37364200	1.72477700	-1.12267900
C	3.39319600	0.35583200	0.54894100
C	4.90119000	0.49154300	0.76171300
H	5.11017800	1.37413000	1.38848300
H	5.27112800	-0.39178000	1.30473000
C	6.91750700	0.89476000	-0.41819100
H	7.20501200	1.32826300	-1.38088600
H	7.13211000	1.63657700	0.36516100
Ti	-1.75352000	-1.64553200	-1.12418500
O	-2.55819300	-2.90225600	-2.01664100
C	-3.21091300	-3.97335200	-2.64410900
H	-3.33979700	-4.79047400	-1.92794900
H	-4.19162500	-3.64763900	-3.00461700
H	-2.60967800	-4.32061300	-3.48973000
C	7.74036500	-0.36189800	-0.17580700
H	7.48365400	-0.82203800	0.79232000
H	7.52122000	-1.10259300	-0.96213500
O	9.09357800	0.01886200	-0.19854800
C	9.95561600	-1.07138400	0.02402500
H	10.97974400	-0.69280900	-0.01218200
H	9.78029800	-1.53196900	1.00766800
H	9.83480500	-1.84719500	-0.74654900