- Supporting Information -

Structure and Chemistry of the Heteronuclear Oxo-Cluster $[VPO_4]^{\bullet+}$: A Model System for the Gas-phase Oxidation of Small Hydrocarbons

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Complete ref 75.

Figure S1. Time-of-flight (TOF) mass spectra of helium-tagged $[VPO_4]^{\bullet+}$ (**13**) ions recorded after irradiation by an IR laser pulse. When the laser wavenumber is tuned off resonance (1475 cm^{-1}) with a vibrational transition, the spectrum (black trace) reflects the distribution of ion-He atom complexes **13**·He_n (n = 0 – 3) formed inside the ion trap. The red trace corresponds to the ion yield when the laser wavenumber is tuned on resonance with a vibrational transition around 1445 cm^{-1}. The laser pulse is triggered shortly after (~1 μs) the high voltages pulses have been applied to the TOF extraction plates. As a consequence, the photofragment ions arising from dissociation of the complexes n = 1 – 3 can be discriminated and detected background-free (red labels). For example, complex n = 2 loses two helium atoms leading to the formation of the helium complex **13''·He** (10.85 μs) and the bare ion **13''** (10.72 μs).

Table S1. Cartesian coordinates for all optimized structures.

Complete ref 75.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, **2009**.

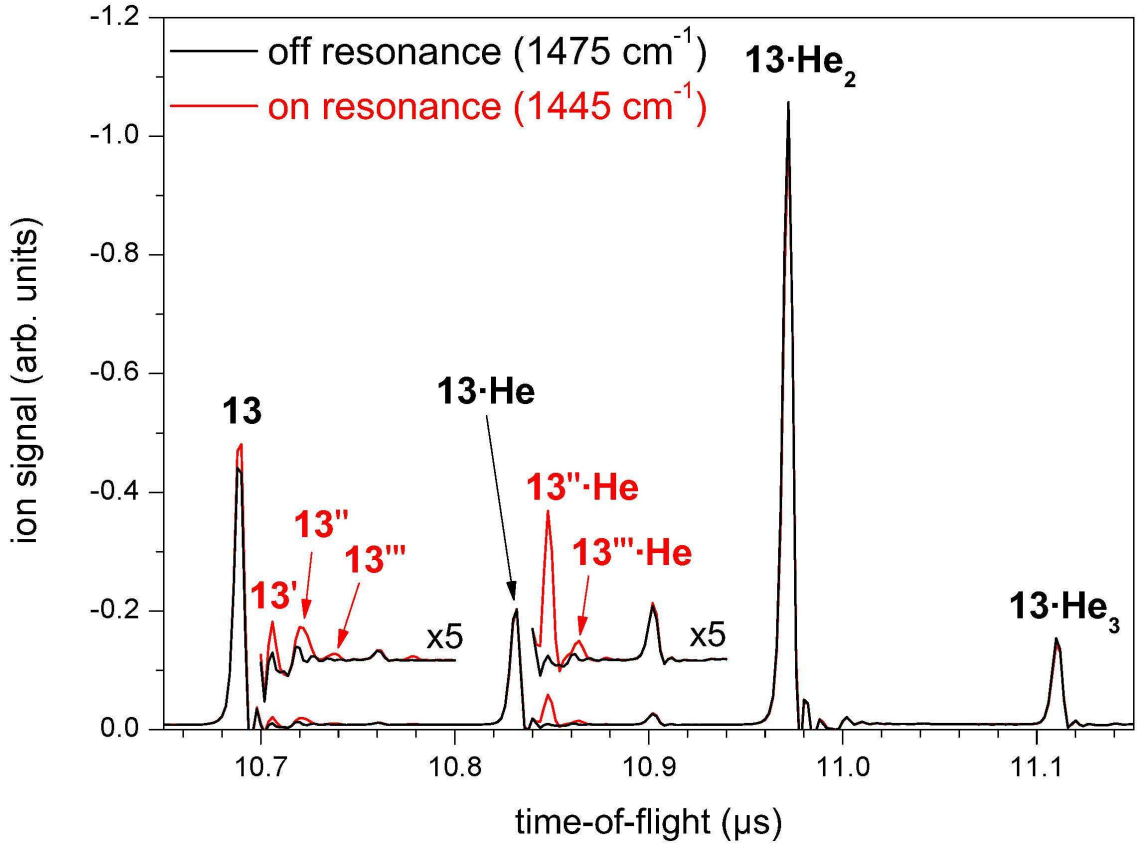

Figure S1. Time-of-flight (TOF) mass spectra of helium-tagged $[VPO_4]^{\bullet+}$ (**13**) ions recorded after irradiation by an IR laser pulse. When the laser wavenumber is tuned off resonance (1475 cm^{-1}) with a vibrational transition, the spectrum (black trace) reflects the distribution of ion-He atom complexes **13**·He_n (n = 0 – 3) formed inside the ion trap. The red trace corresponds to the ion yield when the laser wavenumber is tuned on resonance with a vibrational transition around 1445 cm^{-1}. The laser pulse is triggered shortly after (~1 μs) the high voltages pulses have been applied to the TOF extraction plates. As a consequence, the photofragment ions arising from dissociation of the complexes n = 1 – 3 can be discriminated and detected background-free (red labels). For example, complex n = 2 loses two helium atoms leading to the formation of the helium complex **13''**·He (10.85 μs) and the bare ion **13''** (10.72 μs).

Table S1. Cartesian coordinates for all optimized structures. All structures are singly positive charged and exhibit a spin multiplicity of 2; for each transition state the imaginary frequency ω_i is given.

Structure **13**:

V	-1.23980300	0.00002000	-0.33861100
O	0.30240700	-1.17512500	-0.13682700
O	0.30244200	1.17520300	-0.13671200
P	1.27842500	0.00002700	0.03882400
O	-2.13240100	-0.00009100	0.90771100
O	2.69493800	-0.00009400	0.26654000

Structure **16**:

V	1.68768100	-0.19042200	-0.09505400
O	0.12280500	-0.22964200	-1.17759000
O	0.28696300	-0.62037500	1.12492500
P	-0.82211100	-0.59410800	0.01926200
O	2.25997300	1.23205600	0.10429000
O	-1.93362200	-1.51528100	-0.05295600
C	-2.31507800	1.43861300	-0.49217400
H	-1.86660900	2.01305300	-1.29507500
H	-3.23903500	0.91483700	-0.71070400
C	-1.71496300	1.33175500	0.72455900
H	-0.84676700	1.93526200	0.96326300
H	-2.24129600	0.87190200	1.55615600

Transition state **TS16-17**: ω_i = -610.83

V	1.67676900	-0.10660300	-0.12488300
O	0.08648500	-0.01080700	-1.14444300
O	0.37139600	-0.78293300	1.05091100
P	-0.80693000	-0.63611900	0.00750200
O	2.24278400	1.28335600	0.27761100
O	-1.74387400	-1.71901500	-0.24448800
C	-2.35389400	1.76285900	-0.25003800
H	-1.17900500	1.69612800	0.81128600
H	-1.81758900	1.99510700	-1.16769700
C	-1.88708900	0.76842800	0.59855600
H	-3.20419900	2.38758300	0.01471000
H	-2.46937600	0.56230200	1.49365600

Structure **17**:

V	1.86041600	-0.06210000	-0.20589000
O	0.21019200	0.55510000	-0.96459400
O	0.50982300	-1.03170900	0.74656400
P	-0.65162000	-0.31684200	-0.00412800
O	2.60757600	0.99091800	0.63793600

O	-1.86370600	-1.10655300	-0.52458200
C	-3.12222700	1.13295100	0.09190600
H	-3.20092500	1.90035500	0.86790100
H	-2.75505100	1.59333900	-0.82314900
C	-2.23028100	0.05988500	0.60152900
H	-4.12203900	0.72843500	-0.07565900
H	-2.53328500	-0.46025000	1.50509000

Transition state **TS17-18**: ω_i = -390.46

V	1.85266600	-0.08243900	0.36168000
O	0.29286200	-1.09200700	0.00854000
O	0.60717400	1.25620900	-0.13861100
P	-0.53739300	0.19243800	-0.44811300
O	3.04021200	-0.30225000	-0.60682700
O	-1.66761400	0.35821900	0.82089400
C	-3.68067300	-0.63636700	-0.12149000
H	-4.12542600	-0.72945800	-1.11383700
H	-3.35248900	-1.59058800	0.28381900
C	-2.64568900	0.38439400	-0.10017600
H	-4.48182100	-0.23753900	0.52941600
H	-2.81359400	1.31758900	-0.63830600

Structure **18**:

V	-1.73004100	-0.58041900	-0.00010400
O	-0.59244400	0.35935200	1.18305100
O	-0.59259100	0.35986800	-1.18300200
P	0.20067200	1.07770000	0.00014100
O	-3.22245800	-0.16800000	0.00012600
O	1.74224500	-0.23871200	-0.00015200
C	4.06072100	-0.76388100	-0.00005200
H	4.68656700	-0.53691900	0.87136700
H	3.76002900	-1.80809200	-0.00028900
C	2.91567200	0.15257700	0.00006900
H	4.68656100	-0.53659800	-0.87140500
H	3.11133200	1.23350200	0.00031500

Structure **19**:

V	0.85431200	-0.00009000	-0.36449900
O	-0.63801700	1.17798300	-0.04346600
O	-0.63834800	-1.17796100	-0.04331400
P	-1.64137900	0.00009100	0.19794900
O	1.89780500	0.00006700	0.76355900

Structure **20**:

V	1.28775100	-0.00000400	-0.40015900

O	-0.09621000	1.22429100	-0.01707300
O	-0.09620800	-1.22429100	-0.01706100
O	2.46296200	0.00000700	0.60544900
O	-2.43608900	-0.00000400	-0.58002600
V	-1.23017000	0.00000300	0.40318900

Structure **21**:

V	1.86939900	-0.14843900	0.00006200
O	0.46492700	-0.30296200	-1.23117000
O	0.46491400	-0.30294300	1.23123100
O	2.62535000	1.20866000	-0.00015900
O	-1.61471000	-1.63772200	-0.00010600
C	-3.08122000	0.75623800	0.00002800
H	-1.67349600	2.05538000	-0.92787700
H	-3.53248700	0.40665400	-0.92194800
C	-2.03929900	1.62116800	0.00000300
H	-3.53249600	0.40672300	0.92202600
H	-1.67354500	2.05551700	0.92784200
V	-0.75586500	-0.32586400	-0.00000100

Transition state **TS21-22**: ω_i = -631.24

V	-1.84586900	0.05544700	0.09801100
O	-0.35807600	0.00316800	1.22695600
O	-0.65576700	-0.67463700	-1.13114000
O	-2.39694800	1.47540500	-0.23410700
O	1.40743100	-1.94507400	0.27941600
C	2.93401300	1.67853700	0.25749800
H	1.81331000	1.89881100	-0.57448100
H	2.52094200	1.95972200	1.22373600
C	2.29814600	0.75559800	-0.54876200
H	3.84753500	2.18653000	-0.04893000
H	2.78935000	0.58365500	-1.50716600
V	0.70077300	-0.58172700	-0.03168800

Structure **22**:

V	-1.90417500	0.03877700	0.10766900
O	-0.39919400	0.07773600	1.22199300
O	-0.68975900	-0.69433900	-1.11068900
O	-2.50512200	1.42296500	-0.27302100
O	1.49003300	-1.80847900	0.30499700
C	3.12675700	1.50958000	0.20102300
H	2.61990500	2.41966400	-0.25075400
H	2.92106400	1.54778400	1.26864500
C	2.36046900	0.60915200	-0.58869700
H	4.17855900	1.63551600	-0.06587500
H	2.73806200	0.46564400	-1.60699600
V	0.66293100	-0.50678000	-0.02789600

Transition state **TS22-23**: ω_i = -65.38

V	-1.96115100	-0.01431600	0.12935600
O	-0.43573600	0.25144500	1.19371100
O	-0.71146000	-0.78003700	-1.04074200
O	-2.66261900	1.27590700	-0.37939600
O	1.64723300	-1.53941700	0.39626400
C	3.31728700	1.28369900	0.12343800
H	3.20296000	2.23972200	-0.44864300
H	3.04940900	1.48818800	1.15763000
C	2.40841300	0.46337900	-0.62494500
H	4.37372300	1.02907000	-0.00812200
H	2.78804700	0.11752100	-1.59207300
V	0.63646900	-0.37786500	-0.01885300

Structure **23**:

V	-2.26806000	-0.07942200	-0.17947300
O	-0.76841700	-1.14702100	-0.48096800
O	-1.01868900	1.29855500	-0.06956700
O	-3.12008700	-0.37939900	1.09254800
O	2.27902300	0.32779300	0.06125500
C	3.49596000	0.42180500	0.24916500
V	0.33296700	0.18603100	-0.18906700
H	3.89685600	1.41729700	0.47513700
C	4.42773000	-0.71260400	0.18846400
H	5.20307100	-0.49149200	-0.55473800
H	4.95867100	-0.78008900	1.14568500
H	3.93176200	-1.65234400	-0.04158900

Structure **24**:

V	-1.04813200	0.00001100	-0.34075800
O	0.36231400	-1.23377000	-0.14356000
O	0.36176600	1.23381000	-0.14342700
O	-2.11413100	-0.00022000	0.78529500
V	1.53162700	0.00005200	0.16743400

Structure **25**:

V	-2.13079800	-0.19650000	-0.00797800
O	-0.80985900	0.58074000	-1.14674200
O	-0.77315200	0.40430700	1.19484100
P	0.13370300	0.94863700	0.04399000
O	-2.23039600	-1.73376800	-0.12223200
O	1.00631700	2.09791900	0.11679600
C	2.82329300	-0.84645400	1.26901200
H	3.20640100	0.16166600	1.42573500

H	3.67421000	-1.53490400	1.31196500
H	2.14629400	-1.11558900	2.07881000
C	2.19389900	-1.00409600	-0.08543400
H	1.68461100	-1.95954000	-0.22735100
H	1.17829400	-0.30054400	-0.06990100
C	2.97707600	-0.54747100	-1.28266500
H	3.84838200	-1.20595300	-1.36806500
H	2.41193500	-0.63253700	-2.20987400
H	3.34379400	0.47188700	-1.16446100

Transition state **TS25-26**: ω_i = -86.54

V	2.33364700	-0.00312700	-0.00005500
O	0.89976700	0.31845400	1.17562500
O	0.89959200	0.31661600	-1.17602900
P	-0.14323800	0.53564600	-0.00030000
O	2.91934300	-1.44312900	0.00104400
O	-1.04947800	1.68004400	-0.00114400
C	-3.26234500	-0.38848300	-1.27726700
H	-3.24552600	0.70002900	-1.25964900
H	-4.31427500	-0.70296300	-1.44615900
H	-2.70193000	-0.81033900	-2.11073000
C	-2.94032100	-0.99205700	0.00066400
H	-2.63610700	-2.03812700	0.00134500
H	-0.92810100	-0.67651600	0.00064800
C	-3.26247100	-0.38679800	1.27776100
H	-4.31458600	-0.70063800	1.44669000
H	-2.70244200	-0.80775800	2.11192900
H	-3.24532000	0.70168200	1.25876700

Structure **26**:

V	2.24877300	0.35308000	-0.20189300
O	0.63350600	0.75849900	0.72440900
O	1.02004900	-0.95202300	-0.84965200
P	-0.12481600	-0.46043400	0.09363400
O	3.39837500	-0.19433300	0.67532600
O	-1.38049300	-0.11576600	-0.69357200
C	-3.13312600	1.45221900	-0.02080500
H	-2.66852300	1.72423900	0.92846800
H	-4.21094100	1.59226400	0.07891900
H	-2.77790000	2.12332400	-0.80155900
C	-2.86609800	0.01002900	-0.37528200
H	-3.29215900	-0.24218100	-1.34360900
C	-3.27468600	-0.99976500	0.67042400
H	-4.36156700	-0.97036700	0.76281200
H	-3.00025800	-2.01601300	0.38584100
H	-2.86112600	-0.76591800	1.65376300
H	-0.40509000	-1.40560200	1.07628000

Transition state **TS26-27**: ω_i = -195.85

V	2.45734500	0.15384300	-0.47887600
O	1.02718900	1.09412200	0.29328600
O	1.23643600	-1.21869700	-0.10424900
P	0.20004100	-0.23265700	0.59500700
O	3.82132700	0.14918100	0.27132000
O	-1.20373800	-0.27059000	0.12175000
H	-2.84794500	-1.18763900	0.22712900
H	0.29099600	-0.46516500	1.96852400
C	-3.95669700	-1.18866000	-0.07862600
H	-4.55368200	-1.28734700	0.82364900
H	-4.04056600	-2.00406300	-0.79370300
C	-3.81216400	0.10845900	-0.61525600
H	-3.38081800	0.19192400	-1.61036300
C	-4.12072400	1.34647000	0.06971800
H	-3.31714500	2.07678100	-0.05611600
H	-4.97237800	1.77445800	-0.49201400
H	-4.41021100	1.22277700	1.11006900

Structure **27**:

V	2.56864800	-0.45965600	-0.12999400
O	1.09245800	0.24187000	-1.11296200
O	1.22192800	-0.19792900	1.19621100
P	0.21899400	0.41899100	0.17122800
O	3.79265300	0.47727400	-0.01920600
O	-1.11113600	-0.33737100	0.12931900
C	-4.68426000	-1.07444500	-0.29422100
H	-4.53250600	-1.04332300	-1.37295600
H	-5.75691500	-1.16130000	-0.09905400
H	-4.22762700	-1.98307600	0.10672000
C	-4.15309100	0.14145800	0.38621100
H	-4.24930500	0.16285900	1.46943300
H	-0.01649900	1.76739600	0.43112400
C	-3.60588500	1.20081300	-0.22340500
H	-3.32601200	2.08634500	0.33598200
H	-2.01817200	0.12030600	0.09713700
H	-3.54459100	1.26030400	-1.30536100

Structure **28**:

V	-1.20352800	-0.00972600	-0.40582700
O	0.25041500	-1.17260800	0.06020500
O	0.24157700	1.18325900	0.00291600
P	1.19145800	0.01524100	0.39651100
O	-2.35742300	0.00995600	0.61667000
O	2.48069500	-0.05788300	-0.46017600

H	3.34054500	0.22496700	-0.11372700
H	1.54660700	0.06833000	1.74316100

Structure **29**:

V	2.15917000	0.15503500	-0.00006100
O	0.86026800	-0.38472600	-1.23108800
O	0.86023900	-0.38413800	1.23112300
O	2.51039700	1.66912600	-0.00032700
O	-0.70162900	-2.27061000	0.00044300
C	-3.76195900	0.15117400	-0.00060200
H	-4.26026100	0.55124300	-0.88390300
H	-4.26080800	0.55073400	0.88262100
H	-3.86786300	-0.93253200	-0.00096400
C	-2.29604400	0.58528100	0.00000400
H	-1.84922500	0.15431500	0.93784000
H	-1.84863300	0.15479800	-0.93780700
C	-2.05596400	2.09306000	0.00045200
H	-2.51546300	2.53726800	0.88363800
H	-0.99769100	2.35717900	0.00082600
H	-2.51494500	2.53772400	-0.88278100
V	-0.30853900	-0.76047100	0.00007000

Transition state **TS29-30**: ω_i = -137.34

V	2.55617700	0.00009500	-0.03322300
O	1.17890000	1.23816100	-0.21780100
O	1.17914600	-1.23814200	-0.21841600
O	3.36407400	-0.00016000	1.30207800
O	-1.04993800	0.00013900	-1.49085100
C	-3.80667900	1.28102100	0.60637200
H	-3.87449500	1.27033500	1.69111400
H	-4.80802200	1.53869900	0.19690400
H	-3.16069000	2.07272400	0.22353000
C	-3.53352400	-0.00004900	-0.00198800
H	-3.24549600	-0.00018700	-1.05066100
H	-1.08845800	-0.00045500	1.04877800
C	-3.80698300	-1.28092300	0.60664800
H	-4.80841200	-1.53841200	0.19727000
H	-3.16121500	-2.07287700	0.22395500
H	-3.87476300	-1.26999100	1.69138900
V	-0.05499400	-0.00010000	-0.24888700

Structure **30**:

V	-2.38700400	0.13538100	-0.49536100
O	-1.06778200	-1.20566100	-0.31496400
O	-1.01281800	1.17679800	0.28099700
O	-3.66684900	-0.04863300	0.35580400

O	1.63325600	-0.10560000	0.09400300
C	3.80547700	-1.13576900	-0.08706000
H	3.96310900	-1.13104400	0.99172300
H	4.77860700	-1.06821100	-0.57619900
H	3.34397400	-2.07808800	-0.38023600
C	2.96619800	0.05039100	-0.51801400
H	2.76857200	0.01409200	-1.59161600
H	-0.05608500	-0.55802900	2.07497000
C	3.51292900	1.40369500	-0.11280000
H	4.47503200	1.55346300	-0.60541200
H	2.84847200	2.21137600	-0.41918000
H	3.66994500	1.45518600	0.96501800
V	0.01371200	-0.17207100	0.51803300

Transition state **TS30-31**: ω_i = -179.57

V	-2.60968200	0.24619200	-0.39008600
O	-1.33690300	0.99965600	0.73672300
O	-1.24605000	-0.95925900	-0.76986700
O	-3.93552400	-0.29466200	0.23181400
O	1.30480200	0.15920300	-0.04740200
C	4.55778000	-1.08591400	0.22365000
H	4.71740000	-0.84797900	1.27208300
H	5.52264600	-1.39615700	-0.22514500
H	3.91099500	-1.95619900	0.08032500
C	4.13203700	0.03013700	-0.58941000
H	3.81641200	-0.19506500	-1.60691400
H	0.00400300	-1.25457800	1.70666700
C	4.02684600	1.37463700	-0.16205700
H	4.07887600	2.13054600	-0.94366900
H	2.90650300	1.26183500	0.04450100
H	4.51371600	1.63277000	0.77447600
V	-0.17558500	-0.26914200	0.42723600

Structure **31**:

V	2.62079000	0.52272300	0.15603100
O	1.29577500	0.31105900	-1.17929600
O	1.29511400	-0.35019500	1.18148500
O	3.93670600	-0.26176700	-0.06250800
O	-1.37399000	-0.24605300	-0.05623800
C	-5.04814900	-0.72118700	-0.11352500
H	-5.01818800	-0.67710000	-1.20188700
H	-6.09474500	-0.70265600	0.20428700
H	-4.64764300	-1.68248700	0.21885400
C	-4.31926200	0.41460400	0.51876800
H	-4.28619700	0.41565200	1.60593600
H	0.43257600	-2.12984100	-0.59233000
C	-3.73816300	1.43063300	-0.13493300

H	-3.29912900	2.26458500	0.39986300
H	-2.26498300	0.25032700	0.01193200
H	-3.78985900	1.50976200	-1.21575700
V	0.26498300	-0.59302200	-0.16126100

Structure **32**:

V	-1.40714100	-0.00180900	-0.40683500
O	0.01893200	1.22636800	-0.08719300
O	0.01482500	-1.21786700	-0.08698400
O	-2.52035500	-0.00265000	0.66152400
O	2.71599000	-0.03980600	-0.30786600
H	1.18526200	0.00373000	1.90196700
H	3.42288500	0.15611200	-0.93821500
V	1.12699800	0.00666900	0.30250400

Structure **33**:

V	-2.18836100	-0.29796300	-0.11863400
O	-0.72447800	0.26321000	-1.22336800
O	-1.05057500	0.70491900	1.05841200
P	-0.00385800	0.99588700	-0.05395800
O	-2.19527600	-1.81198700	0.17331600
O	0.88061100	2.12994200	-0.14772700
C	1.91261200	-0.65956200	1.02735500
H	1.63997100	-1.71466900	1.09664200
H	1.12102100	-0.30996300	0.23308200
C	3.27663600	-0.37752300	0.44943800
H	3.98661500	-0.74317200	1.20283900
H	3.43616700	0.70099300	0.38953700
C	3.54228300	-1.04895900	-0.89337500
H	4.56285500	-0.85591900	-1.22163600
H	3.40996200	-2.13099400	-0.83438400
H	2.87419000	-0.66559600	-1.66912500
H	1.68796700	-0.13824400	1.95541600

Transition state **TS33-34**: ω_i = -488.92

V	-2.39749100	-0.11557000	0.10754400
O	-0.81203600	-0.48640800	1.05487600
O	-1.08490400	-0.07735500	-1.24393600
P	0.10022800	-0.38126200	-0.23707200
O	-3.09029800	1.23714100	0.43144300
O	1.10904800	-1.39379400	-0.53342100
C	2.57265700	1.51483600	-0.26274300
H	2.41729600	2.06297400	0.66264500
H	0.77306000	0.89564800	-0.08728900
C	3.46491700	0.42751500	-0.30458000
H	4.17138800	1.36740200	-0.45868800

H	3.52053400	-0.09705000	-1.25579200
C	3.89063800	-0.34372900	0.91727900
H	4.91289500	-0.70250000	0.80728800
H	3.81624000	0.24958400	1.82845900
H	3.23761500	-1.21445400	0.99824400
H	2.24608300	1.98702900	-1.18373300

Structure **34**:

V	-2.29551500	0.07137700	-0.44004200
O	-0.93219200	-1.21423100	-0.08239800
O	-0.83355300	1.12232000	0.18250500
P	0.05847600	-0.13463600	0.46022800
O	-3.51884000	0.01510900	0.50320300
O	1.39706100	-0.14530000	-0.27147400
C	3.60359000	-1.15273000	-0.18985100
H	3.65584900	-1.18138100	-1.27832300
H	0.28174600	-0.28204100	1.82918500
C	2.80888500	0.03986400	0.27960200
H	4.61966000	-1.07051600	0.19984400
H	2.69829400	0.03446900	1.36580800
C	3.29919900	1.37942300	-0.21226400
H	4.30484700	1.54742700	0.17680100
H	3.34678700	1.40004600	-1.30116800
H	2.66476700	2.19544200	0.13365500
H	3.17789700	-2.08811300	0.17213900

Transition state **TS34-35**: ω_i = -181.78

V	2.47397700	0.24186700	-0.42050600
O	1.19829200	0.89219500	0.79326100
O	1.08028700	-1.00035000	-0.60356900
P	0.20032300	-0.32097100	0.53627100
O	3.83302000	-0.26213200	0.14679300
O	-1.20467300	0.01484800	0.20515200
C	-3.67842800	1.33931400	-0.50028700
H	-4.00681000	1.32337000	-1.53572500
H	0.27321000	-1.15431300	1.65394200
C	-3.94934300	0.19413000	0.27718200
H	-3.75283800	2.29901400	0.00628100
H	-3.80012200	0.27338300	1.35193800
C	-4.34348100	-1.10202700	-0.23523300
H	-5.38141000	-1.24004000	0.12253600
H	-4.33152900	-1.17728200	-1.31949400
H	-3.78089400	-1.90651800	0.24492200
H	-2.55382300	1.08902100	-0.47990500

Structure **35**:

V	-2.18881400	-0.67800700	-0.05000200
O	-1.09371800	0.26796700	1.19181900
O	-0.99710700	0.31612200	-1.15843900
P	-0.35226000	1.05853700	0.06092400
O	-3.66511000	-0.22408100	-0.10223300
O	1.17496200	1.06409700	0.12457900
C	2.79245400	-1.42691700	0.00947300
H	2.65269600	-1.61819400	-1.04978500
H	-0.68483500	2.40670000	0.07393200
C	3.76034400	-0.61161200	0.44677600
H	2.21122400	-2.02238000	0.70461200
H	3.89934300	-0.50715900	1.52039700
C	4.70180800	0.16019400	-0.41308200
H	5.72635900	-0.16854000	-0.21687300
H	4.49489400	0.02854200	-1.47487000
H	4.67314200	1.22576900	-0.17099000
H	1.77395200	0.24854000	0.14495900

Structure **36**:

V	-1.21624000	-0.00048400	-0.40708500
O	0.24596600	-1.17658600	-0.01276000
O	0.24547900	1.17671200	-0.01534700
P	1.18533800	0.00067700	0.39231800
O	-2.33312800	0.00043400	0.65608000
O	2.58813700	0.00010000	-0.25887700
H	1.49969900	0.00288000	1.74430200
H	2.72211800	-0.00718000	-1.21887000

Structure **37**:

V	2.05536600	0.21392500	0.08027000
O	0.81983300	-0.49894200	-1.19080500
O	0.70783300	-0.61164300	1.15173400
P	-0.12457800	-1.07613600	-0.08758700
O	2.06122900	1.75720900	0.15161000
O	-0.90677700	-2.28654800	-0.18260600
C	-2.04356900	2.11481500	-0.24195600
H	-1.84209000	2.41639900	0.78556000
H	-2.94768200	2.63978100	-0.56981500
H	-1.23080500	2.43847500	-0.89092700
C	-2.32525900	0.64051400	-0.35781200
H	-2.41657300	0.29433700	-1.38753400
H	-1.25412400	0.11874500	-0.04444000
C	-3.34483800	0.03497900	0.56492500
H	-4.32487100	0.41388100	0.25545700
H	-3.37688500	-1.05076300	0.48644700

H	-3.18667800	0.32847500	1.60243900

Transition state **TS37-27**: ω_i = -150.47

V	2.25028100	0.13545900	0.03988600
O	0.95712300	-0.56035800	-1.14340000
O	0.81251500	-0.28416100	1.18541400
P	-0.10314400	-0.80896900	0.00558600
O	2.55996900	1.64922200	-0.11944400
O	-0.84174600	-2.06459800	0.10669000
C	-2.79870900	2.00863900	0.18891500
H	-2.79362200	1.95964700	1.27700100
H	-3.77183200	2.45317200	-0.10032600
H	-2.03329500	2.67762200	-0.19974300
C	-2.82297300	0.69679400	-0.45364600
H	-2.55616200	0.65705300	-1.50809900
H	-1.08719100	0.25398300	-0.17806700
C	-3.51144700	-0.45925700	0.08830000
H	-4.33847300	-0.70384800	-0.59666000
H	-2.86212900	-1.35153900	0.02388500
H	-3.87071900	-0.32502300	1.10532700

Transition state **TS29-38**: ω_i = -96.12

V	2.58108700	0.04431700	0.07424600
O	1.31982700	-0.60912200	-1.12485700
O	1.12367600	0.14730300	1.22470300
O	3.31471700	1.37338400	-0.29081900
O	-0.92152100	-1.60622500	0.31952400
C	-3.88841100	1.75000700	0.16296200
H	-4.00984400	1.67804000	1.24271900
H	-4.88534900	2.03251800	-0.24704800
H	-3.21241600	2.54487000	-0.14712900
C	-3.64970600	0.48768700	-0.49426300
H	-3.24657700	0.51801800	-1.50387600
H	-1.14896700	0.78031400	-0.45918300
C	-4.01177500	-0.79724500	0.03411500
H	-4.46724000	-1.43092100	-0.73574800
H	-3.03885900	-1.30860800	0.21985800
H	-4.57902800	-0.76785800	0.96094700
V	-0.00743300	-0.35439400	-0.01232500

Structure **38**:

V	-2.60577000	0.31364000	-0.48291400
O	-1.25861700	-0.98235600	-0.74803300
O	-1.32228600	0.95209700	0.75816800
O	-3.93404600	-0.20239100	0.12022500
O	1.37496500	-0.14933100	0.26871200

C	4.98808300	-0.85396800	-0.06162500
H	5.07002000	-0.75887300	1.02079000
H	5.99688500	-0.91699200	-0.48000500
H	4.49970000	-1.80159900	-0.30338000
C	4.26822200	0.29703400	-0.67706100
H	4.12628700	0.25151700	-1.75452400
H	-0.47132800	-1.35120500	1.76248400
C	3.81964200	1.37761700	-0.02257400
H	3.37797100	2.21344700	-0.55210800
H	2.27613200	0.27963600	0.04806500
H	3.98394300	1.50114100	1.04272800
V	-0.27229200	-0.36952400	0.50860700