Supporting Information

Silica-Supported Nb(III)-CH_3 Species can Act as an Efficient Catalyst for Non-Oxidative Coupling of Methane

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1. **The absolute electronic energies (E+ZPE, Hartree), the thermal enthalpies (H, Hartree) and free energies (G, Hartree) with zero-point correction at 723 K and 49.3 atm/50.0 bar, as well as the imaginary frequencies (I.F., cm^{-1}), calculated at the B3LYP/BS-1 level of theory.**

Species	E+ZPE	H (723.15 K,49.3 atm)	G (723.15 K,49.3 atm)
Methane	-40.489162	-40.477852	-40.531064
Hydrogen	-1.169509	-1.161491	-1.195557
Ethane	-79.781879	-79.765009	-79.836628
CA0 (= CB3)	-1682.749274	-1682.668232	-1722.250790
CB0	-1682.749274	-1682.668232	-1682.921895
CA[0-1]≠(= CB[3-4]≠)	-1762.539946	-1762.441139	-1762.732019
CA1 (= CB4)	-1762.572230	-1762.474129	-1762.760269
CA[1-2]≠	-1762.533562	-1762.433219	-1762.728465
CA2	-1761.394264	-1761.297302	-1761.581702
CA[2-3]≠	-1761.330751	-1761.236801	-1761.515197
CA3	-1761.360476	-1761.265115	-1761.553779
CA[3-4]≠	-1801.827211	-1801.722359	-1802.024831
CA4	-1801.873658	-1801.766575	-1802.074069
CA[4-0]≠	-1801.829365	-1801.724730	-1802.026310
CA[2-5]≠	-1801.818198	-1801.710573	-1802.016601
CA5	-1801.879003	-1801.769976	-1802.081919
CA[5-4]≠	-1801.793474	-1801.686042	-1801.992049
CA[2-6]≠	-1761.333259	-1761.238678	1761.516803
CA6	-1720.836621	-1720.753825	-1721.004847
CA[6-7]≠	-1761.286543	-1761.191855	-1761.471173

CA7	-1761.385675	-1761.290577	-1761.571510
CA[7-3]≠	-1761.355825	-1761.262376	-1761.540794
CB[0-1]≠	-1723.237100	-1723.145430	-1723.421327
CB1	-1723.275968	-1723.183583	-1723.456690
CB[1-2]≠	-1723.226538	1723.134514	-1723.409465
CB2	-1722.086584	-1721.998044	-1722.262693
CB[2-3]≠	-1722.056879	-1721.969755	-1722.235593
CB[4-5]≠	-1762.490320	-1762.390859	-1762.678265
CB5	-1762.554479	-1762.455569	-1762.746045
CB[5-0]≠	-1762.530564	-1762.432491	-1762.725338
CB[2-4]≠	-1762.510912	-1762.411484	-1762.698738
CA[2-5]≠	-1762.464664	-1762.365523	-1762.653141

2. Details of the refined single-point-energy calculations

To inspect the functional and basis set effects on the free energies, the energies of critical points in the catalytic cycle A were refined with the B3LYP functional including empirical dispersion correction computed with Grimme's D3 formula (B3LYP-D3). And larger basis set def2-TZVPP was applied for all atoms expect the metal atoms, which were described by the energy-consistent scalar-relativistic DF-adjusted 10-electron-core pseudopotential/ ECP10MDF(8s7p6d2f1g)/[6s5p3d2f1g] for V, WB-adjusted 28-electron-core pseudo-potential/ECP28MDF(10s9p8d2f1g)/[5s5p4d2f1g] for Nb, and WB-adjusted 60-electron- core pseudopotential/ECP60MWB(10s9p8d2f1g)/[5s5p4d2f1g] for Ta, respectively. These combined basis sets are denoted as BS-2.

The absolute calculated electronic energies (E_{BS-2}, Hartree) calculated at B3LYP-D3/BS-2 level of theory, the thermal correction to Gibbs free energy (G_{corr}, Hartree) obtained at B3LYP/BS-1 level of theory, as well as the corrected free energies (G_{BS-2}, Hartree) at 723 K and 49.3 atm/50.0 bar are summarized as following.

Nb(III)	**E_{BS-2}**	**G_{corr} (723.15 K,49.3 atm)**	**G_{BS-2} (723.15 K,49.3 atm)**
Methane	-40.539266	0.002685	-40.536581
Hydrogen	-1.180003	-0.015986	-1.195989
Ethane	-79.868025	0.019631	-79.848394
CA0	-1722.271461	-0.040557	-1722.312018
CA[0-1]$^{\neq}$	-1762.797036	-0.005347	-1762.802383
CA1	-1762.835051	-0.001167	-1762.836218
CA[1-2]$^{\neq}$	-1762.788838	-0.013913	-1762.802751

CA2	-1761.631376	-0.020834	-1761.652210
CA[2-3]≠	-1761.569007	-0.015720	-1761.584727
CA3	-1761.597432	-0.023154	-1761.620586
CA[3-4]≠	-1802.123496	0.019868	-1802.103628
CA4	-1802.170421	0.015258	-1802.155163
CA[4-0]≠	-1802.125875	0.021051	-1802.104824
CA0 (V)	-1737.143750	-0.036347	-1737.180097
CA[3-4]≠(V)	-1816.990156	0.020626	-1816.969530
CA0 (Ta)	-0.044017	-1722.974579	-1723.018596
CA[3-4]≠(Ta)	0.015152	-1802.814904	-1802.799752

3. Schematic orbital diagrams

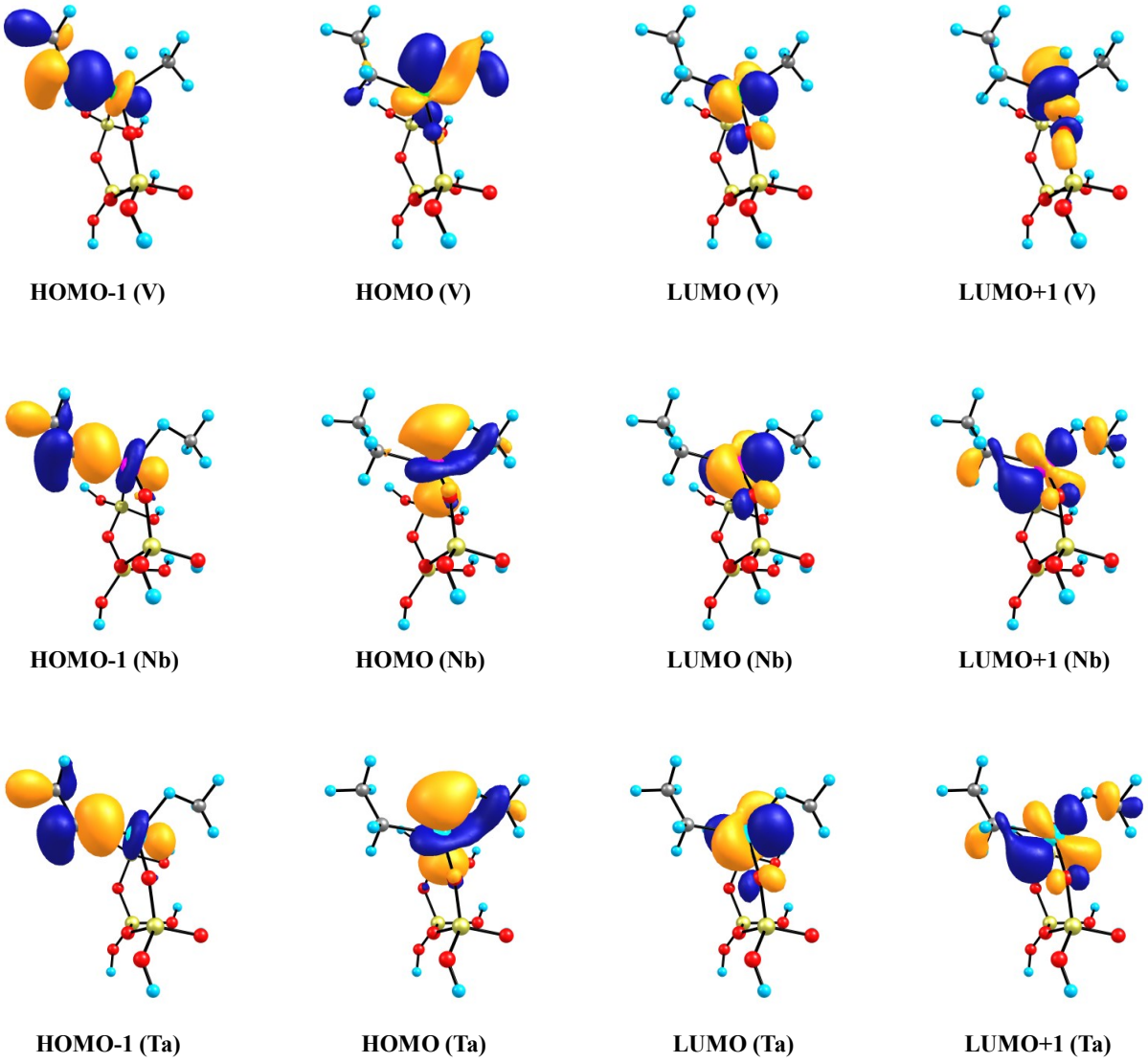

Figure S1. The diagram of frontier orbitals of the transition state **CA[3-4]$^{\neq}$** for the M(III)-CH_3 catalyzed systems.

4. Supplementary data for the $Si_9O_{24}H_{10}$ supported systems

To know whether the smaller model including 3 Si atoms is representative for a catalytic support of silica in this study. Some critical points, i.e., **CA0**, **CA3** and **CA[3-4]**$^{\neq}$ for the M(III)-catalyzed (where M = V, Nb, and Ta) non-oxidative coupling of methane were examined by using a larger $Si_9O_{24}H_{10}$ cluster model. As shown in Figure S2, the same the basis set was used for the reaction center as that by using the smaller $Si_3O_{10}H_6$ cluster model, that is, the 6-311G(d,p) was used for the C, H, O, and Si atoms, and SDD was used for V, Nb, and Ta atoms. While a smaller 6-31G(d) basis set was applied to the remaining atoms away from the reaction center, as illustrated in Figure S1. This combination of the mixed basis set applied for the $Si_9O_{24}H_{10}$ supported systems is denoted as BS-3. The optimized structures are schematically summarized in Figure S3.

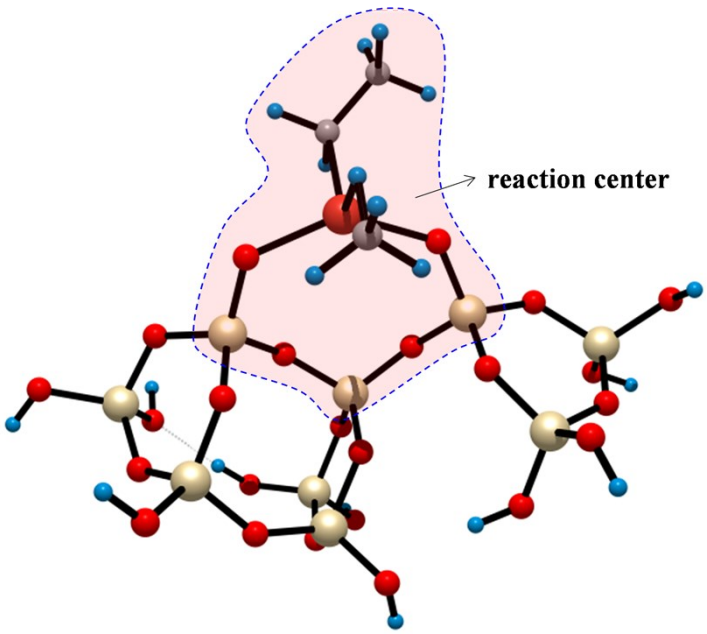

Figure S2. Schematic illustration of the mixed basis sets (BS-3) used for the calculations by using the larger $Si_9O_{24}H_{10}$ cluster.

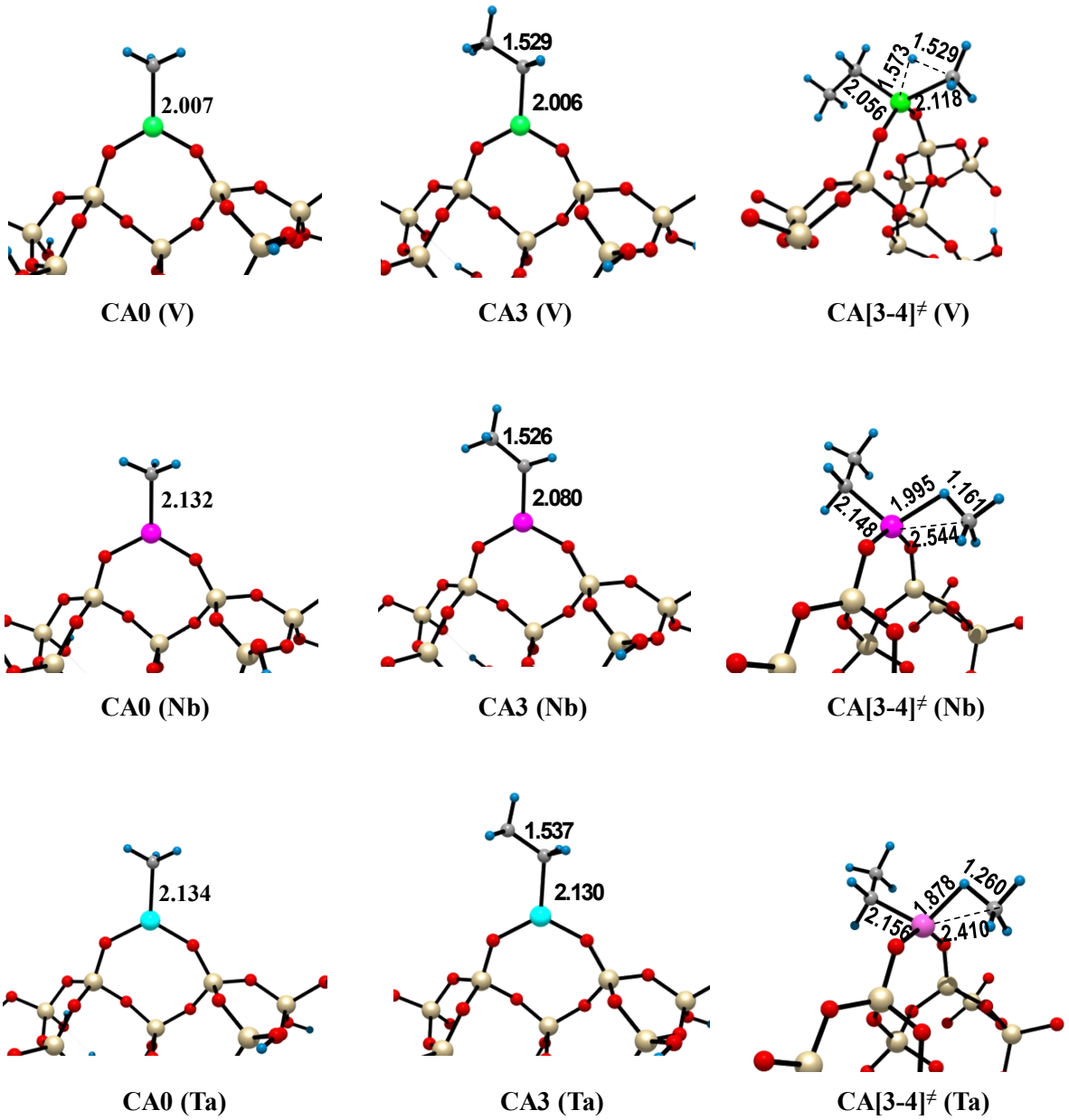

Figure S3. Schematically critical points with the key bond lengths/distances (Å) for M(III)-catalyzed (where M = V, Nb, and Ta) non-oxidative coupling of methane calculated by using the larger $Si_9O_{24}H_{10}$ cluster model.

5. The absolute electronic energies (E+ZPE, Hartree), the thermal enthalpies (H, Hartree) and free energies (G, Hartree) with zero-point correction at 723 K and 49.3 atm/50.0 bar, as well as the imaginary frequencies (I.F., cm^{-1}) for the $Si_9O_{24}H_{10}$ supported systems, calculated at the B3LYP/BS-3 level of theory.

Species	E+ZPE	H (723.15 K,49.3 atm)	G (723.15 K,49.3 atm)
CA0 (Nb)	-4515.528082	-4515.345246	-4515.839613
CA3 (Nb)	-4554.823557	-4554.634754	-4555.141557
CA[3-4]≠ (Nb)	-4595.290724	-4595.091499	-4595.616177
CA0 (V)	-4530.240701	-4530.058775	-4530.548569
CA3 (V)	-4569.533304	-4569.347134	-4569.843038
CA[3-4]≠ (V)	-4609.991986	-4609.792567	-4610.317676
CA0 (Ta)	-4515.586646	-4515.404131	-4515.898099
CA3 (Ta)	-4554.877525	-4554.688560	-4555.197378
CA[3-4]≠ (Ta)	-4595.335014	-4595.135214	-4595.663123

6. Cartesian coordinates of all the optimized structures obtained at the B3LYP/6-311G(d,p) level of theory.

Methane

C	0.00006000	0.00007400	-0.00002800
H	-0.21376600	-0.47016500	0.96070700
H	-0.26477600	-0.68496600	-0.80649100
H	1.06266900	0.23861100	-0.05962600
H	-0.58448500	0.91607600	-0.09442400

Hydrogen

H	0.00000000	0.00000000	0.37208700
H	0.00000000	0.00000000	-0.37208700

Ethane

C	0.00000000	0.00000000	0.76476700
H	0.00000000	1.01833500	1.16356900
H	0.88190400	-0.50916700	1.16356900
H	-0.88190400	-0.50916700	1.16356900
C	0.00000000	0.00000000	-0.76476700
H	0.00000000	-1.01833500	-1.16356900
H	-0.88190400	0.50916700	-1.16356900
H	0.88190400	0.50916700	-1.16356900

CA0 (= CB3)

Si	1.05484900	-2.19844700	-0.03067000
O	-0.54756300	-1.80679200	-0.11830500
Nb	-1.96929100	-0.55372100	-0.12781800
O	-1.61309100	1.33243800	-0.09574000
Si	-0.34538300	2.38826200	-0.03982500
O	-0.72348600	3.76592400	-0.83048700
O	0.08160100	2.76427600	1.50732600
O	0.97075500	1.63071800	-0.64829900
O	1.55819600	-2.44378800	1.51004600
O	1.25486600	-3.55418000	-0.91279400
O	1.90188700	-0.92390600	-0.66294400
H	2.05421200	-4.06497400	-0.77022000
H	1.81291100	-1.63594000	1.97561800
H	-1.16258400	3.70190900	-1.68172200
H	-0.50771700	3.31152800	2.03151900
Si	2.16676500	0.61695600	-0.17609900
O	2.15554700	0.52742400	1.48069500
O	3.54973300	1.19076700	-0.82443200
H	1.80959900	1.30047600	1.94464900
H	4.29383000	0.59030500	-0.90268800
C	-3.94242200	-1.25236800	0.31065200
H	-4.57072100	-0.51469000	0.81807600
H	-4.35743300	-1.43784700	-0.69744400
H	-3.95141900	-2.19186300	0.87063600

CB0

Si	2.48235400	0.22792300	-0.09232300
O	1.60131200	-1.18334100	0.00362000
Nb	0.02471600	-2.21989700	0.07172900
O	-1.71002000	-1.42862000	0.02042700
Si	-2.39264300	0.07234400	-0.15381500
O	-3.64990600	-0.00154000	-1.19168400
O	-2.93208200	0.67769800	1.27769900
O	-1.19622400	1.07754400	-0.62400600
O	3.50082000	0.30476100	1.18817600
O	3.37643800	0.27448600	-1.45552100
O	1.42919900	1.46649200	-0.15313200
H	0.17637800	-3.98746300	0.30077700
H	4.18581100	-0.24057200	-1.47542800
H	3.14190700	0.20578500	2.07299000
H	-3.54134400	-0.46654500	-2.02442000
H	-3.73903900	0.32590600	1.66045700
Si	-0.06995100	2.09595100	0.00880100
O	-0.34539400	2.25615900	1.62039100
O	-0.17736800	3.48577800	-0.84241400
H	-1.25288400	2.10350300	1.91002300
H	0.56496900	4.09279700	-0.81100300

CA[0-1]$^{\neq}$ (= CB[3-4]$^{\neq}$)

Si	-0.64975800	2.40600400	0.06455400
O	0.80063900	1.63482700	0.14501300
Nb	1.83785000	0.02224500	0.11285400
O	1.09529400	-1.77458200	0.20429500
Si	-0.41042200	-2.41900500	0.07485700
O	-0.36237100	-3.86249300	-0.69039000
O	-1.14715100	-2.63634900	1.53823700
O	-1.35323600	-1.30816000	-0.67841800
O	-1.27752100	2.74581600	1.54347000

O	-0.41949500	3.78751800	-0.77211600
O	-1.69834600	1.38558400	-0.71817300
C	4.18958600	0.36754800	0.74028800
H	-1.09103700	4.46835700	-0.69518700
H	-1.79670600	2.02551400	1.92500400
H	0.25153100	-3.96881200	-1.42069500
H	-0.88626600	-3.38744000	2.07622500
Si	-2.35998200	-0.06187600	-0.33625300
O	-2.56759900	0.00239400	1.30935200
O	-3.72815700	-0.30954500	-1.19097100
H	-2.48185200	-0.83982900	1.77527200
H	-4.30573100	0.44137600	-1.34266400
H	3.10299800	0.19726500	1.40765800
C	2.85801500	0.02547500	-1.83402100
H	3.89010900	-0.34563900	-1.87677100
H	2.26847800	-0.48653600	-2.60416600
H	2.88858000	1.08809200	-2.11817200
H	4.60514700	-0.50216600	0.23137400
H	4.33471400	1.25889500	0.12795400
H	4.72837300	0.50893800	1.68296900

CA1 (= CB4)

C	-0.16596600	3.70824200	-0.86092400
Nb	-0.09427100	1.73767700	-0.00614300
O	-1.95679500	1.10441900	-0.02532400
Si	-2.42689500	-0.47492500	-0.09553200
O	-1.25508200	-1.38324200	0.61333100
Si	0.13053500	-2.17691100	0.24019100
O	0.10876100	-3.56573800	1.10148900
O	1.78100100	1.26917300	0.02013900
Si	2.48591800	-0.22374900	-0.10637900
O	1.47357400	-1.31696600	0.62874300
O	2.72009200	-0.71831800	-1.65429800
O	3.91949100	-0.11845100	0.66963000
O	-3.89368100	-0.65529000	0.60934600
O	-2.53196700	-1.08462000	-1.62788900
O	0.20314100	-2.40471900	-1.40100000
C	-0.13900600	1.61837800	2.15654600
H	4.58938900	-0.76604100	0.44121500
H	2.00640900	-1.27144100	-2.00171600
H	-4.08987200	-0.12106800	1.38216400
H	-3.32114600	-0.89527700	-2.14042900
H	-0.63094900	-2.27160200	-1.87097600
H	0.94752900	-4.00103100	1.26651400
H	-0.03363400	0.39072100	-1.10536000
H	-1.03124100	2.14750900	2.50866200
H	-0.17332300	0.58070800	2.49795100
H	0.76202600	2.09887500	2.54881900
H	-0.13889000	3.62917900	-1.95552600
H	-1.08872800	4.22240700	-0.56920000
H	0.69528700	4.30079300	-0.53326100

CA[1-2]$^{\neq}$

Si	0.17383700	2.37378200	-0.18850600
O	-0.94823400	1.20857400	-0.31295700
Nb	-2.09109800	-0.36158900	-0.02238900
O	-0.68287500	-1.67268900	-0.07620000
Si	0.85086800	-2.23798700	-0.03998600
O	1.37687100	-2.63313800	1.46555500
O	0.89322500	-3.56141200	-0.99992600
O	1.83201100	-1.03946100	-0.62873300
O	0.10410700	3.50146600	-1.38353300
O	-0.04225400	3.17348300	1.22988300
O	1.66162700	1.66151500	-0.24332100
C	-2.99512200	0.70012000	1.66706000
H	-3.03609300	-1.69905200	0.91148700
C	-3.50998000	-0.78240700	-1.35673400
H	0.20517600	4.10072700	1.23926800
H	0.50408700	3.28107500	-2.22746700
H	1.87178400	-1.93028800	1.90925100
H	1.55517400	-4.22298000	-0.78894300
Si	2.54255200	0.31231800	-0.05101600
O	3.96251400	0.59732000	-0.81603200
O	2.72815000	-0.03343300	1.56785000
H	4.50640400	-0.16644600	-1.02056900
H	2.98688000	0.67803700	2.15880800
H	-3.54035100	-1.58175700	-0.02082600
H	-4.44016800	-0.20745300	-1.34564900
H	-3.47575400	-1.53416600	-2.14389400
H	-3.95939800	0.28868500	1.97639600
H	-2.31905100	0.67213500	2.52832800
H	-3.11580100	1.74900300	1.37221000

CA2

Si	0.99922400	-2.26412100	-0.04495300
O	-0.56808800	-1.76277200	-0.12197500
Nb	-1.89452900	-0.38469700	-0.12538700
O	-1.42330800	1.49833000	-0.13505500

Si	-0.07288700	2.43558600	-0.06305500
O	-0.31430600	3.85919400	-0.82592000
O	0.38926900	2.74925500	1.49173800
O	1.17054600	1.56495400	-0.68030900
O	1.49440300	-2.54396400	1.49476500
O	1.11333300	-3.63102800	-0.92543300
O	1.92990700	-1.04753000	-0.68074100
H	1.85316200	-4.21526500	-0.74777900
H	1.81819800	-1.75904600	1.95604700
H	-0.80634100	3.86165700	-1.65010700
H	-0.08754000	3.41838800	1.98838300
Si	2.29086800	0.47303700	-0.19484800
O	2.24480900	0.38723100	1.46287100
O	3.71903000	0.95155700	-0.82150900
H	1.96992100	1.19245900	1.92051200
H	4.41678700	0.29826000	-0.90422500
C	-3.29274800	-0.75886500	-1.39764800
H	-3.46479000	-1.74272000	-1.83659100
C	-2.98157100	-0.64823000	1.74925500
H	-3.96147700	0.02384300	-1.76275000
H	-3.36205400	-1.66955100	1.83927400
H	-2.30292400	-0.44836400	2.58878300
H	-3.83696800	0.03063900	1.81222400

CA[2-3]$^{\neq}$

Si	0.60145800	-2.40268100	-0.02145100
O	-0.83910400	-1.61031800	-0.08412800
Nb	-1.86789300	-0.00254900	-0.14507300
O	-1.03451100	1.74268100	-0.04369300
Si	0.46766500	2.41096800	-0.02730300
O	0.47248400	3.83821300	-0.82490000
O	1.02486600	2.67351100	1.50513200
O	1.51712500	1.31852900	-0.65077700
O	1.05148500	-2.77719300	1.51295200
O	0.44295900	-3.76743900	-0.90159700
O	1.75049800	-1.39391200	-0.66313100
H	1.10466800	-4.45091500	-0.77774000
H	1.51553200	-2.06280600	1.96943000
H	-0.00330300	3.89308800	-1.65690600
H	0.66950200	3.41284900	2.00351100
Si	2.40821600	0.02694500	-0.18614000
O	2.38398800	-0.05146500	1.47276700
O	3.89147300	0.21642900	-0.84138200
H	2.27858000	0.79134500	1.93247200
H	4.44137400	-0.56398100	-0.93578900
C	-3.70953700	-0.12660600	-0.89026600
H	-4.15692200	-1.07046700	-1.19969400
C	-3.99890400	-0.19323300	1.07110600
H	-4.32336200	0.73112000	-1.16227400
H	-5.04969300	-0.28928000	0.79710000
H	-3.72266400	-1.07566200	1.64847300
H	-3.89229000	0.70269500	1.68294200

CA3

Si	-0.21567400	2.42574800	-0.14210300
O	1.09920700	1.43455600	-0.19051500
Nb	1.79480300	-0.33425000	-0.27108200
O	0.64409700	-1.86093200	-0.22230300
Si	-0.90480000	-2.40360900	-0.02519300
O	-1.21458900	-3.57030400	-1.13177400
O	-1.16409900	-3.02409200	1.46717700
O	-1.90862400	-1.12526000	-0.16523200
O	-0.52396500	3.01777800	1.35567800
O	0.07506700	3.65409200	-1.17601900
O	-1.51659800	1.51818200	-0.62213200
C	3.81297700	-0.67148400	0.18945600
H	-0.39621900	4.47592000	-1.02521100
H	-1.11560400	2.46842800	1.88742200
H	-0.93097700	-3.42055600	-2.03655700
H	-0.76033900	-3.86961400	1.67469000
Si	-2.48093100	0.37866700	0.04379400
O	-2.47545900	0.77734600	1.65687700
O	-3.96699000	0.40101600	-0.63677000
H	-2.80936800	0.13145900	2.28525400
H	-4.34555000	1.25922700	-0.83949300
H	3.93791000	-1.68543200	0.58764100
H	3.94976100	-0.76545000	-0.93441400
C	4.80806000	0.32973300	0.77274200
H	4.67961800	0.40071400	1.85478200
H	5.84593700	0.03781600	0.57651900
H	4.66695000	1.33191000	0.35964500

CA[3-4]$^{\neq}$

Si	1.79937200	-1.83070000	-0.06590900
O	0.17741600	-2.11046600	-0.00613000
Nb	-1.35259600	-0.93736800	0.17212100
O	-1.72882100	0.99067700	0.43653300
Si	-0.76813200	2.28982600	0.17399700

O	-1.61566700	3.53979000	-0.45908900
O	-0.04181500	2.83665500	1.56191500
O	0.49895100	1.83460800	-0.77186400
O	2.43589700	-1.62253700	1.43897100
O	2.47929600	-3.11300300	-0.81399600
O	2.06252200	-0.42626500	-0.91553300
C	-1.53254900	-1.24710900	2.68398300
H	3.41667400	-3.26042100	-0.67370400
H	2.59780000	-0.69518900	1.66902800
H	-2.33495500	3.33698300	-1.06126900
H	-0.53124300	3.45116100	2.11359700
Si	1.98604700	1.17626200	-0.57604300
O	2.37979100	1.26771300	1.03793500
O	2.99116100	1.99600900	-1.56870800
H	1.93049800	1.96714600	1.53331100
H	3.79704800	1.55653400	-1.84756800
H	-2.17617300	-1.68034500	1.81364200
C	-2.55583100	-1.32176200	-1.56570600
H	-1.97255500	-0.74140400	-2.31732000
C	-4.04491300	-0.99004600	-1.67889600
H	-2.36379000	-2.37929400	-1.79246000
H	-1.67731900	-0.17994300	2.84895600
H	-2.00330700	-1.80233900	3.49763800
H	-0.47333500	-1.51478000	2.66336600
H	-4.42590800	-1.13568900	-2.69794200
H	-4.63218100	-1.62589800	-1.01166800
H	-4.24693100	0.04818000	-1.39975300

CA4

Si	1.29110100	-2.12644100	-0.05111300
O	-0.31739600	-1.81820500	-0.23719000
Nb	-1.75660700	-0.57070000	-0.37289200
O	-1.53388400	1.34363800	-0.14355400
Si	-0.28948800	2.41296100	-0.02560900
O	-0.66693900	3.82140800	-0.76093600
O	0.12082800	2.73784800	1.54132400
O	1.04354000	1.68393700	-0.64146200
O	1.71151300	-2.31048900	1.52562700
O	1.62257700	-3.48610300	-0.88611000
O	2.10592700	-0.81662600	-0.65759900
C	-2.83740700	-0.98314300	1.49987300
H	2.40126200	-3.98518300	-0.63114200
H	1.96988000	-1.48886300	1.96522400
H	-1.17838500	3.79249400	-1.57283200
H	-0.42354500	3.34926300	2.04302200
Si	2.29274100	0.73520100	-0.16868500
O	2.27714800	0.64383500	1.48877800
O	3.64627800	1.38027500	-0.80999900
H	1.88877400	1.39906700	1.94979800
H	4.42102900	0.82031200	-0.89164000
H	-3.31780300	-1.23339500	-0.69056900
C	-2.16590500	-0.57682900	-2.52576700
H	-3.04490900	0.00870100	-2.80663800
H	-1.27074300	-0.13700300	-2.99317100
H	-2.30345300	-1.59001200	-2.91237200
H	-3.76296200	-0.39935700	1.53761100
H	-3.13592100	-2.03532100	1.53201300
C	-1.90248800	-0.63791100	2.67233400
H	-0.98253700	-1.23137900	2.65075700
H	-1.61780500	0.41919700	2.67842500
H	-2.38487900	-0.84279100	3.63610600

CA[4-0]≠

Si	-0.30763300	2.48140600	0.00088800
O	1.05861200	1.68521500	-0.46179700
Nb	1.50734100	-0.18930300	-0.62396600
O	0.76462500	-1.96548200	-0.18116700
Si	-0.79805600	-2.35731700	0.11686900
O	-1.16902800	-3.82619800	-0.50285800
O	-1.15723800	-2.39882400	1.73594100
O	-1.75321200	-1.15186200	-0.46503300
O	-0.40592100	2.63908300	1.63651100
O	-0.27404900	3.94591500	-0.72046600
O	-1.62613300	1.59599300	-0.49445700
C	2.99825600	-0.22056600	1.41487900
H	-0.83457100	4.63171700	-0.35223900
H	-0.98730300	1.98784900	2.05669800
H	-0.75389300	-4.08337700	-1.32928800
H	-0.98226000	-3.21212100	2.21506300
Si	-2.39877400	0.26053400	0.06164000
O	-2.20816600	0.32987400	1.71166000
O	-3.95204900	0.27638700	-0.44306200
H	-2.10516500	-0.52633000	2.15094100
H	-4.38075400	1.12951100	-0.53662200
H	3.23139500	-0.24129900	0.26230300
C	1.78029800	-0.43939800	-2.76185700
H	2.29245800	-1.35827900	-3.05655300
H	0.76255200	-0.45112700	-3.19470300

H	2.31872700	0.41331900	-3.18488000
H	2.37704700	0.62261800	1.73410500
H	2.54503200	-1.15726500	1.74714100
C	4.42384500	-0.06439800	1.96594300
H	4.40770200	-0.04759800	3.05782600
H	5.06078200	-0.89255100	1.64682300
H	4.87582200	0.86701100	1.61846100

CA[2-5]≠

Si	0.66271000	-2.27284800	0.15868300
O	-0.63148900	-1.30103800	0.25333900
Nb	-1.98449300	0.11954200	0.01378900
O	-0.91063100	1.73056100	-0.00857700
Si	0.61840500	2.33687800	-0.01220200
O	0.63120300	3.82211000	-0.69891400
O	1.23352400	2.48742400	1.51440600
O	1.60751100	1.27097600	-0.75393100
O	1.30495500	-2.66498800	1.62262300
O	0.24251900	-3.65312700	-0.61968400
O	1.83160100	-1.44820500	-0.70023500
H	0.83672500	-4.40060600	-0.52406500
H	1.88463800	-1.97997000	1.98022200
H	0.15514500	3.95551400	-1.52132300
H	0.93405800	3.21527300	2.06391400
Si	2.55143500	-0.01855900	-0.37046600
O	2.78408700	-0.01957400	1.27191800
O	3.92024300	0.14153100	-1.24881600
H	2.62318900	0.82220600	1.71855300
H	4.45875900	-0.64285100	-1.37249300
C	-3.81404600	0.66683800	-0.58405300
H	-3.04511500	-0.14757400	-1.50131900
H	-4.79809900	0.43535500	-0.97802000
C	-2.34908100	-1.31303000	-1.91723500
H	-3.10995000	-1.32765900	-2.70453500
H	-1.37004100	-1.19627100	-2.38354300
H	-2.38457900	-2.26024600	-1.37948200
C	-2.62721400	-0.27700000	2.05644000
H	-3.66613400	1.74496400	-0.40353200
H	-3.28272400	0.48716300	2.47514900
H	-3.16685000	-1.23106800	2.04611800
H	-1.72666900	-0.39827300	2.66688000

CA5

Si	0.79570900	-2.30009300	0.05882600
O	-0.58689800	-1.42830600	0.11064200
Nb	-1.90571500	-0.01287400	-0.02243100
O	-0.96794800	1.67027800	0.01077700
Si	0.51996800	2.37818600	0.02539900
O	0.45140000	3.85342400	-0.67260000
O	1.10305800	2.56696100	1.55881200
O	1.57276700	1.35680800	-0.69311200
O	1.36950500	-2.66589000	1.55409000
O	0.51096300	-3.67056000	-0.78222100
O	1.92600600	-1.35054600	-0.70776400
H	1.16929500	-4.36685500	-0.73331800
H	1.89493000	-1.95786600	1.94982500
H	-0.03171800	3.95954000	-1.49499000
H	0.77528200	3.29543800	2.09133300
Si	2.55883800	0.10314400	-0.30372600
O	2.69951200	0.05041700	1.34911000
O	3.96014100	0.35610200	-1.10212300
H	2.54130900	0.88223300	1.81414400
H	4.54417700	-0.39456100	-1.22837900
C	-4.03410600	0.57621200	-0.24506900
H	-4.13774900	1.18563600	-1.15141300
H	-4.73649300	-0.25760300	-0.31900800
C	-2.34269400	-0.83059800	-2.00730500
H	-2.92348300	-0.15256900	-2.63482900
H	-1.39285600	-1.06999800	-2.49524500
H	-2.90612700	-1.76161000	-1.88032400
C	-2.69487100	-0.72547100	1.88907900
H	-4.32531500	1.19121300	0.61525900
H	-3.30650400	0.02613600	2.39238300
H	-3.30586100	-1.61847700	1.71966900
H	-1.84580800	-1.00049600	2.52247500

CA[5-4]≠

C	-3.96815100	-0.91584300	0.00098900
Nb	-1.67254300	-0.30286200	0.07618600
O	-1.30099600	1.58615700	0.33039000
Si	0.00076900	2.50413200	-0.10789800
O	1.34147500	1.61416300	0.20903100
Si	2.46838900	0.46311800	0.03686400
O	3.70327000	1.10817700	-0.81990900
O	-0.50350500	-1.81598500	-0.03393100
Si	1.07324500	-2.24797200	-0.24662700
O	1.89876700	-0.88511000	-0.69672700
O	1.76797300	-2.83878300	1.11703900

O	1.09270800	-3.38546800	-1.41867000
O	-0.13166500	2.91568700	-1.69353900
O	0.13883900	3.86604800	0.78375700
O	2.91627100	-0.09430000	1.53659600
C	-2.89046900	-0.38564100	-1.53221700
H	1.84502900	-3.98072500	-1.43647400
H	2.22753500	-2.17470000	1.64878500
H	-0.42091900	2.20001800	-2.27068500
H	-0.47753600	4.57713700	0.59709400
H	3.11203100	0.55351600	2.21849800
H	4.33600200	0.49998000	-1.20840200
C	-1.91894200	-0.47049400	2.29957800
H	-3.45557900	0.45700800	-1.92127700
H	-1.26559200	0.11550700	-1.79970400
H	-2.93384500	-1.26258800	-2.17396200
H	-4.29889200	-0.16408200	0.71848900
H	-4.74945800	-1.04178300	-0.74991400
H	-3.80989800	-1.87950100	0.48862400
H	-2.23240700	-1.47532300	2.60851700
H	-0.96211300	-0.25303500	2.79142100
H	-2.65348200	0.24322200	2.69022700

CA[2-6]≠

Si	-1.18672400	-2.13183700	-0.03788000
O	0.38093300	-1.85248800	-0.42430300
Nb	1.82517200	-0.58567100	-0.09831200
O	1.23753100	1.15580900	-0.74795600
Si	0.36325200	2.40174800	-0.10578300
O	1.08190500	2.92403600	1.27639800
O	0.23668300	3.66684300	-1.13806400
O	-1.16021300	1.85315300	0.13158000
O	-2.12359200	-2.44580700	-1.35162800
O	-1.24378400	-3.40793600	0.98442500
O	-1.76806200	-0.75160200	0.67973400
C	2.13971800	-0.42140400	1.68427200
H	-2.08113300	-3.87190700	1.04879800
H	-2.53273600	-1.65829200	-1.73625100
H	1.52723200	2.23118500	1.77826300
H	0.94635800	4.31200900	-1.11612100
Si	-2.31149600	0.71421000	0.20205600
O	-2.90767000	0.41035600	-1.32206400
O	-3.44826400	1.27505800	1.23814200
H	-3.14278100	1.16297100	-1.87073500
H	-4.05536000	0.62829500	1.60418500
H	2.31688500	-0.43265400	2.75560000
C	4.06570600	-1.22296000	-0.45556100
H	3.42487100	-0.87668800	0.74914200
H	3.86554800	-2.17687300	-0.95409200
H	4.32631100	-0.46549700	-1.20122400
H	4.94600500	-1.37094300	0.17333900

CA6

Si	-2.30474100	-0.53458600	-0.03666200
O	-1.12479200	-1.56272800	-0.53305500
Nb	0.72004100	-2.07168800	-0.21594200
O	1.73069900	-0.51933900	-0.81211000
Si	2.20392000	0.89964400	-0.10467000
O	2.97037500	0.57596300	1.31127500
O	3.21689000	1.75315100	-1.06781200
O	0.86525900	1.82195100	0.07616800
O	-3.19409900	0.04824900	-1.28946800
O	-3.28419900	-1.34549600	0.99240900
O	-1.56739400	0.75049200	0.70710400
C	0.93585700	-2.10589600	1.56350300
H	-4.15557900	-0.97402800	1.14532200
H	-2.84123100	0.86407100	-1.67048600
H	2.65428500	-0.22623000	1.74683800
H	4.15414700	1.57649300	-0.96491300
Si	-0.72882200	2.07033800	0.22802100
O	-1.39376200	2.41307900	-1.25855600
O	-0.90651200	3.28827800	1.30754700
H	-0.94393200	3.05612600	-1.81242600
H	-1.77541000	3.39330000	1.70106200
H	0.88619900	-1.99949600	2.64556000

CA[6-7]≠

Si	0.69193900	-2.32255500	-0.17887400
O	-0.70605400	-1.54730600	-0.54670400
Nb	-1.95588400	-0.10273300	-0.23389200
O	-0.99358500	1.57637100	-0.56776100
Si	0.38850200	2.36540800	-0.18818000
O	0.43541200	3.83339200	-0.91127300
O	0.56941300	2.57930900	1.44410900
O	1.66974200	1.42703800	-0.59964300
O	0.85153800	-2.69081000	1.41574200
O	0.73048500	-3.69964600	-1.05905700
O	1.93387300	-1.30211200	-0.59487000
H	1.30892600	-4.39676500	-0.74311800

H	1.21389300	-1.96695600	1.94453800
H	0.22103100	3.88272500	-1.84541000
H	-0.09648200	3.09040300	1.90999600
Si	2.45014200	0.12636300	0.01852700
O	2.08312900	0.03310700	1.63679200
O	4.03747000	0.32981800	-0.31058900
H	1.78656400	0.86035100	2.04031600
H	4.58592500	-0.45691400	-0.33406500
C	-2.52071300	-0.14097100	1.51206700
H	-3.50221300	-0.27233200	-1.07895600
H	-2.86000200	-0.22270200	2.54146100
C	-4.51247900	-0.24124200	0.16753300
H	-5.03090100	-0.96828600	-0.45481000
H	-4.69803000	-0.49358300	1.20478200
H	-4.85784900	0.76706600	-0.04735200

CA7

Si	0.02479800	2.44595900	-0.04100800
O	1.20601600	1.30692600	-0.20594900
Nb	1.72991400	-0.52250200	-0.39527800
O	0.54843200	-2.03704000	-0.07068300
Si	-1.07944100	-2.24802100	0.02945300
O	-1.53518500	-3.63143900	-0.70956100
O	-1.61742900	-2.29198800	1.59099200
O	-1.78805600	-0.90602300	-0.59370000
O	-0.22256200	2.87470100	1.52347900
O	0.48152900	3.74235500	-0.91657300
O	-1.37741200	1.77644400	-0.62220400
H	0.05754500	4.58124500	-0.72478700
H	-0.85748900	2.31533400	1.99080700
H	-1.10368300	-3.87703700	-1.53111600
H	-1.48445100	-3.09427400	2.10125400
Si	-2.34164900	0.55794200	-0.10743400
O	-2.23842500	0.62846800	1.54797200
O	-3.84838000	0.72100400	-0.71093000
H	-2.32327500	-0.21620600	2.01002700
H	-4.21660200	1.60466300	-0.77476700
C	3.47186100	-0.85568600	0.35053900
H	3.54236300	-1.95017000	0.46859500
H	2.27097200	-0.72629700	-2.05883500
C	4.67385300	-0.08039700	0.80708900
H	5.56241300	-0.37042300	0.23350700
H	4.53614100	0.99627600	0.68528900
H	4.89519100	-0.27360200	1.86375700

CA[7-3]$^{\neq}$

Si	-0.16189100	2.44701800	-0.02355600
O	1.09185200	1.38050400	-0.08230700
Nb	1.76707000	-0.40289700	-0.17439700
O	0.63698400	-1.96740600	-0.03968200
Si	-0.97448500	-2.30424300	-0.00808500
O	-1.28335400	-3.70674700	-0.78734800
O	-1.56237000	-2.42009300	1.53000900
O	-1.77222000	-1.02076100	-0.64079900
O	-0.52749700	2.91577900	1.50612700
O	0.26786600	3.74393800	-0.91448400
O	-1.48857000	1.68183500	-0.66064000
H	-0.21815200	4.55874700	-0.77265200
H	-1.12367300	2.31461200	1.97162400
H	-0.84082100	-3.87239000	-1.62289200
H	-1.32385000	-3.18441900	2.05957900
Si	-2.40794500	0.41656700	-0.17854200
O	-2.37303000	0.49125000	1.47899800
O	-3.89735700	0.50951000	-0.83956300
H	-2.41868400	-0.35698000	1.93917900
H	-4.29189900	1.37881600	-0.93502400
C	3.68685200	-0.70871400	0.18155600
H	3.85245200	-1.79101200	0.28577400
H	3.22483200	-0.64256800	-1.26732800
C	4.94013600	0.11636800	0.31037000
H	5.72334100	-0.21271800	-0.38254000
H	4.75323200	1.17789900	0.13721500
H	5.33345100	0.00958600	1.32583000

CB[0-1]$^{\neq}$

Si	2.61947100	-0.11050300	0.17205200
O	1.53281300	1.10022300	0.01403200
Nb	-0.31528700	1.61595400	-0.25625800
O	-2.22169000	1.22297300	0.16089800
Si	-2.42504500	-0.39380000	0.21444600
O	-3.00633000	-0.96630800	1.62374600
O	-3.33479700	-1.02934900	-0.99935900
O	-0.80612000	-0.82046600	0.03241100
O	3.78291500	-0.12642400	-0.98663600
O	3.37520700	0.05096900	1.61353000
O	1.76692000	-1.52840200	0.09015400
H	-0.23909100	3.51540600	-0.68461600
H	4.24940000	-0.33617300	1.69377400

H	3.53785400	-0.43401800	-1.86242100
H	-3.75027700	-1.57108200	1.60162100
H	-3.35378700	-0.54080300	-1.82673700
Si	0.25582900	-2.08233100	-0.12540900
O	0.20639600	-2.70586700	-1.64524000
O	-0.19171000	-3.16855300	1.01889600
H	-0.63748600	-3.03735500	-1.96213800
H	0.40711900	-3.89228700	1.21598400
H	-0.40244700	1.80618600	-1.99947300
C	-0.22592300	4.15492900	0.28623700
H	-0.19566800	5.12486900	-0.22055500
H	-1.12859700	4.10729200	0.89289800
H	0.66285900	4.05677200	0.90613400

CB1

Si	2.45520100	-0.10878800	-0.05421700
O	1.38152500	-1.35467700	-0.22290200
Nb	-0.40916800	-1.97928200	-0.36122200
O	-1.94361900	-0.82419300	-0.19720400
Si	-2.29222400	0.78350500	-0.06286600
O	-3.67665400	1.13853500	-0.84948200
O	-2.44052000	1.25340500	1.51074200
O	-0.99297800	1.61440800	-0.61381000
O	2.87424400	0.14074100	1.51149300
O	3.76841600	-0.48614400	-0.93918700
O	1.69976400	1.25283800	-0.61956500
H	-0.55176700	-2.36823400	-2.05974400
H	-0.62264900	-3.64184600	-0.77773600
C	-0.64143900	-3.18504600	1.44957400
H	4.60112200	-0.06996900	-0.70765700
H	2.28513100	0.73606600	1.99360400
H	-3.84805300	0.72211200	-1.69732200
H	-3.24984600	1.04006600	1.98127200
Si	0.45507500	2.17979100	-0.09859700
O	0.51359500	2.03525300	1.55424600
O	0.59552300	3.70296700	-0.66297500
H	-0.32747200	2.11662300	2.02108800
H	1.47484600	4.07923700	-0.73861700
H	-1.59963900	-3.70741300	1.50295600
H	0.15152100	-3.92831900	1.56225200
H	-0.57576300	-2.46565200	2.28122600

CB[1-2]$^{\neq}$

Si	0.22857100	2.41957800	-0.06125800
O	-1.01452900	1.37921500	-0.23344500
Nb	-2.18253500	-0.12592600	0.19001600
O	-0.95599900	-1.60211900	0.05390500
Si	0.51912400	-2.29588700	-0.10165500
O	1.14466100	-2.85043400	1.31118700
O	0.35284300	-3.53661700	-1.15267900
O	1.54026200	-1.13437900	-0.69789400
O	0.26648200	3.58338000	-1.22072700
O	0.11425100	3.18499100	1.38309300
O	1.62001800	1.54104800	-0.15220600
H	-2.61418900	0.79473800	1.63019900
H	-3.14756800	-1.17898900	1.39207400
C	-3.87843600	-0.30484000	-0.82833400
H	0.38809400	4.10431200	1.40634500
H	0.62579900	3.35014300	-2.07933400
H	1.71006000	-2.21425900	1.77061200
H	0.98239300	-4.25627700	-1.07436900
Si	2.39931000	0.11959000	-0.09970700
O	3.77992400	0.33906800	-0.95331400
O	2.66732500	-0.33668700	1.47841100
H	4.25403000	-0.45040700	-1.22352100
H	3.00832700	0.31961700	2.09113700
H	-3.81329600	-0.96293800	0.60117900
H	-4.48258200	0.60650200	-0.73422400
H	-4.33649600	-1.06613100	-1.45471300

CB2

Si	-2.45659700	0.08792000	0.00543000
O	-1.39261600	1.34820000	0.07760500
Nb	0.39452500	2.01098800	0.15755300
O	1.95662900	0.87391200	0.06643400
Si	2.31064200	-0.73482400	-0.01423500
O	3.72405900	-0.97544900	-0.79400200
O	2.40672200	-1.43139500	1.47813600
O	1.03448600	-1.47827300	-0.72343100
O	-2.94064300	-0.41395000	1.48958300
O	-3.74032200	0.58990100	-0.86300300
O	-1.66415200	-1.16245300	-0.74170300
H	-4.57074900	0.12508900	-0.74217200
H	-2.34335900	-1.04563900	1.91125700
H	3.92452200	-0.43936700	-1.56453900
H	3.19410700	-1.28610500	2.00799200
Si	-0.41354300	-2.13168600	-0.32214300
O	-0.50683000	-2.21198800	1.33325600

O	-0.51149100	-3.56699200	-1.09048900
H	0.32982100	-2.32718700	1.80193900
H	-1.37982200	-3.95615600	-1.21339000
C	0.61440400	3.62779300	-0.86787800
H	1.59630600	3.99142800	-1.17877200
H	-0.22208100	4.23568700	-1.21652000
H	0.51552800	2.81315400	1.71596800

CB[2-3]$^{\neq}$

Si	2.29440100	-0.84980600	-0.03806200
O	0.94328400	-1.78677700	0.06214500
Nb	-0.96204900	-1.80125100	-0.06820400
O	-2.03203500	-0.20711700	-0.06700300
Si	-2.03366300	1.44374900	-0.01107400
O	-3.10780200	2.03092300	-1.09755500
O	-2.42690200	2.01642000	1.47140900
O	-0.50974500	1.95585100	-0.30099000
O	3.00079500	-0.56956000	1.41474500
O	3.34062800	-1.61587500	-1.02782000
O	1.81044600	0.60563100	-0.66965700
H	4.27393900	-1.42623000	-0.91281200
H	2.68972300	0.22842900	1.86337300
H	-3.12620400	1.64113100	-1.97446900
H	-3.33665300	1.92039800	1.76175900
Si	1.10530100	1.98066500	-0.13710500
O	1.52009500	2.01316200	1.47177700
O	1.62879400	3.27752700	-0.98222600
H	1.05734700	2.62627000	2.04935300
H	2.55844600	3.30593200	-1.21847400
C	-1.87249500	-3.50674900	0.33100500
H	-2.95462500	-3.63916100	0.36558700
H	-1.61658400	-3.12326700	-1.16002000
H	-1.33139600	-4.44773600	0.44478500

CB[4-5]$^{\neq}$

C	-3.19784300	-1.46950000	1.38391900
Nb	-1.53788000	-0.74547000	-0.13071200
O	-1.60947800	1.16751100	-0.43672800
Si	-0.65358400	2.47328200	-0.10834900
O	0.90207200	1.97508500	-0.08467300
Si	2.16259500	0.96740200	0.06996800
O	3.41791100	1.71581200	-0.66905500
O	-0.18814300	-2.09309100	-0.31769300
Si	1.45736400	-2.03085900	-0.16344400
O	1.89897100	-0.49872900	-0.61324400
O	2.00960100	-2.31624700	1.35319300
O	2.05700700	-3.16010900	-1.18087100
O	-0.91922000	3.62714400	-1.24679300
O	-0.96666500	3.16177100	1.34566100
O	2.46340100	0.61745700	1.66412800
C	-3.33718000	-1.52607000	-0.56592100
H	2.91501700	-3.52885900	-0.96155700
H	2.13057400	-1.51599800	1.88370700
H	-1.00695200	3.34243100	-2.15914300
H	-1.63169500	3.85348600	1.35545000
H	2.26550400	1.29831000	2.31240600
H	4.20567200	1.19217300	-0.83038300
H	-0.65427600	-0.25728200	1.39600400
H	-4.22720200	-0.93065200	-0.75156100
H	-2.29893900	-1.04549800	-1.87244000
H	-3.47846900	-2.58533700	-0.76773400
H	-3.27830900	-0.51938300	1.91441300
H	-4.19088900	-1.91883700	1.32792500
H	-2.53975400	-2.15723400	1.91826600

CB5

C	-3.86095600	-1.66848900	1.27261600
Nb	-1.44310700	-0.61820400	-0.34036800
O	-1.70450700	1.31155700	-0.28775200
Si	-0.59676900	2.51902900	-0.05463500
O	0.89630700	1.86187500	-0.17993500
Si	2.16353200	0.87815100	0.07746400
O	3.44536300	1.61521500	-0.62506900
O	-0.22551200	-2.11970300	-0.31307600
Si	1.41264300	-2.12457000	-0.09702500
O	1.96143600	-0.62258900	-0.54072600
O	1.87706500	-2.39048800	1.45560200
O	2.01324300	-3.29735200	-1.06226100
O	-0.84518800	3.71806500	-1.14513500
O	-0.68348200	3.18223700	1.44256600
O	2.37155400	0.59609100	1.70075000
C	-3.40945700	-1.46772400	-0.18164100
H	2.86572800	-3.66635900	-0.82285400
H	2.04407000	-1.58482900	1.96310200
H	-0.99724600	3.47001400	-2.05978100
H	-1.39068700	3.81058000	1.60416400
H	2.25943600	1.33626600	2.30319500
H	4.22377500	1.07722400	-0.78516900

H	-0.56031400	-0.24407300	1.11251100
H	-4.08482900	-0.79138500	-0.72375500
H	-0.79303600	-0.30844200	-1.92839600
H	-3.38222400	-2.41916100	-0.72980700
H	-3.89050500	-0.72408500	1.82425100
H	-4.86791200	-2.09744700	1.31740400
H	-3.19831700	-2.35045100	1.81341700

CB[5-0]$^{\neq}$

Si	0.74471300	-2.39944500	-0.09621900
O	-0.77150700	-1.76268600	-0.13548300
Nb	-1.71072100	-0.09997500	-0.32797300
O	-0.91686500	1.65205000	-0.24803300
Si	0.46574300	2.53019400	-0.04661200
O	0.56955000	3.67364300	-1.21482200
O	0.52947600	3.27523700	1.40969700
O	1.72154900	1.48554000	-0.07356800
O	1.20861100	-2.90771300	1.39330800
O	0.78087600	-3.65061900	-1.14299100
O	1.76582100	-1.17807000	-0.56825200
C	-4.13202600	-0.23654700	-0.08055600
H	1.42457700	-4.34213700	-0.97648000
H	1.68884500	-2.24756900	1.91151200
H	0.28599000	3.44010600	-2.10165100
H	0.01205500	4.07609600	1.51897800
Si	2.54131500	0.09717900	0.09729200
O	2.63375700	-0.32211600	1.70340600
O	3.99884500	0.33619800	-0.60305600
H	2.91627400	0.34597800	2.33355100
H	4.51114200	-0.44188500	-0.83354100
H	-3.06543400	-0.12208200	0.79331800
H	-2.41361900	-0.14365500	-1.92785900
H	-4.37064800	0.60996100	-0.72735100
H	-4.23828600	-1.14568100	-0.67652700
C	-5.08485600	-0.27579900	1.12991000
H	-6.12292900	-0.36490800	0.79637400
H	-4.86858900	-1.12690300	1.78228400
H	-5.00425300	0.63301100	1.73401500

CB[2-4]$^{\neq}$

Si	0.64051900	-2.28110900	0.20608400
O	-0.68007100	-1.34596800	0.31415500
Nb	-2.06913900	0.05012000	0.24147800
O	-1.05465700	1.68854300	0.12804200
Si	0.45148600	2.34365800	-0.01761000
O	0.36189300	3.79422600	-0.76806400
O	1.16381300	2.58080700	1.45224500
O	1.41584300	1.27511600	-0.78536900
O	1.33510700	-2.63528700	1.65466800
O	0.23993100	-3.68215400	-0.54355500
O	1.75694600	-1.43092700	-0.69607500
H	0.85144600	-4.41495100	-0.44402100
H	1.89469700	-1.92626800	1.99618600
H	-0.13951800	3.86923100	-1.58260700
H	0.86052800	3.30431300	2.00532300
Si	2.42900600	0.03179800	-0.42029200
O	2.72796100	0.06913900	1.21009900
O	3.75091700	0.23578800	-1.35952400
H	2.58686500	0.92023100	1.64500600
H	4.32337800	-0.52384700	-1.48558200
C	-3.99931800	0.52124100	0.05577400
H	-3.40136900	-0.28015700	-1.02261900
H	-5.04241800	0.25043800	-0.06635000
C	-2.71177400	-1.39551900	-1.57946500
H	-3.57738500	-1.42626900	-2.24908100
H	-1.81517800	-1.25636400	-2.18593000
H	-2.64402300	-2.34327700	-1.04463200
H	-2.38668100	-0.30657500	1.91331200
H	-3.84468500	1.60913500	0.15503600

CB[2-5]$^{\neq}$

Si	1.34659000	-2.09277300	-0.06224800
O	-0.21260000	-1.67415300	-0.35282000
Nb	-1.86537000	-0.69159400	-0.38883100
O	-1.45569000	1.22441500	-0.26525300
Si	-0.24553200	2.30767600	-0.07482500
O	-0.62077300	3.73266000	-0.78707600
O	0.07420100	2.61410800	1.52143200
O	1.15064600	1.66038700	-0.63868700
O	1.65983300	-2.31040800	1.53670600
O	1.66296200	-3.46488300	-0.88690300
O	2.27690700	-0.82783300	-0.59878400
H	2.42625300	-3.97638000	-0.61088900
H	1.91481400	-1.49614300	1.99215800
H	-0.96866800	3.72289400	-1.68134400
H	-0.51786300	3.19712200	2.00190200
Si	2.38146500	0.72651200	-0.09346000
O	2.25671400	0.62900600	1.56040700

O	3.76522800	1.40213400	-0.63628600
H	1.79783800	1.36645500	1.98553000
H	4.54304400	0.84275300	-0.68708300
C	-2.66346200	-1.41169000	1.34287800
H	-3.58792800	-1.12337700	-0.61742800
H	-3.62325200	-1.84061500	1.60315000
C	-4.16145100	0.08231900	0.35418300
H	-5.07878200	-0.49934300	0.35200200
H	-4.05123700	0.62913000	1.28590300
H	-4.14449000	0.78344700	-0.48266000
H	-2.48257100	-1.03616300	-1.99966000
H	-2.01224600	-1.30151100	2.22368200

7. Cartesian coordinates of the optimized structures by using the larger $Si_9O_{24}H_{10}$ cluster obtained at the B3LYP/BS-3 level of theory.

CA0 (Nb)

Si	-1.92950700	1.73910200	-0.08251500
O	-1.06863600	3.12158300	-0.06377400
Nb	0.79940600	3.55775100	-0.31813400
O	2.13975600	2.22584300	-0.58451300
Si	2.55796600	0.63701600	-0.54624300
O	4.00237300	0.34595100	-1.23836500
O	2.63483800	0.13681500	1.01291800
O	1.38005400	-0.22126000	-1.31521500
O	-2.16312700	1.14308100	1.43783100
O	-3.42936700	1.88793600	-0.74410300
O	-1.10855500	0.63556800	-0.97082200
Si	-0.12943500	-0.68044200	-0.93172800
O	-0.14487400	-1.25410500	0.61196200
O	-0.73408500	-1.83204200	-1.91076300
C	1.45339500	5.53644300	0.13590000
H	2.45988500	5.56898800	0.56225900
H	1.46926100	6.02202600	-0.85653100
H	0.75781800	6.07815800	0.78366400
Si	-3.17842200	-0.07172300	1.92345700
Si	-4.62437600	0.76077400	-0.59805200
O	-3.77193300	0.21832800	3.41622300
H	-3.88733700	1.14888500	3.65434200
O	-4.35987600	-0.12925000	0.75836000
O	-6.03824800	1.58544300	-0.58279700
H	-6.84340400	1.06118500	-0.46585500
O	-4.54813200	-0.34391300	-1.84367600
H	-4.56845300	0.04527400	-2.73208900
Si	3.50140400	-1.10634600	1.67557800
Si	5.18345700	-0.74553600	-0.83128400
O	4.76578900	-1.36640800	0.64191800
O	4.04391000	-0.56975300	3.13248000
H	4.13842000	-1.25309500	3.81009300
O	2.66073800	-2.50708200	1.80051800
H	1.71407600	-2.47770800	2.02502900
O	5.22346400	-1.85746600	-2.03031700
H	6.04099500	-2.37046100	-2.09270000
O	6.67274500	-0.05603700	-0.72152200
H	6.89329600	0.31976300	0.14261200
Si	-1.75484600	-3.11437300	-1.59417800
Si	-1.19664000	-2.33522000	1.26401800
O	-1.77416200	-3.28382400	0.05810400
O	-3.23122200	-2.84135400	-2.22864800
H	-3.69024600	-2.00162900	-2.02278900
O	-1.16383500	-4.51252400	-2.20258400
H	-1.41338700	-4.70638200	-3.11661500
O	-2.41960900	-1.51661800	1.98554400
O	-0.33926000	-3.19942100	2.37099100
H	-0.41129500	-4.16292100	2.31193800

CA3 (Nb)

Si	-1.82388600	1.64381400	0.03774800
O	-0.88775100	2.97373500	0.05962600
Nb	0.94191900	3.37171700	-0.42760200

O	2.24972800	1.99761700	-0.68153300
Si	2.64792700	0.41974000	-0.51367700
O	4.04141800	0.02620700	-1.26033800
O	2.80785900	0.06280100	1.08118500
O	1.43240900	-0.52211600	-1.10958400
O	-2.22609000	1.10664300	1.54127700
O	-3.23878300	1.86651000	-0.77134800
O	-0.99841200	0.44603200	-0.71332000
Si	-0.10308300	-0.91900000	-0.77744700
O	-0.17351200	-1.66221000	0.71156900
O	-0.75267000	-1.93363900	-1.87004200
Si	-3.32331200	-0.08037800	1.90103600
Si	-4.55708500	0.88331900	-0.67302000
O	-4.11890700	0.20731600	3.29578500
H	-3.72754900	-0.16480800	4.09837100
O	-4.41200500	-0.07177400	0.65774700
O	-5.87302600	1.85603800	-0.65502000
H	-6.71600000	1.43777700	-0.42823300
O	-4.58507100	-0.18645900	-1.95003200
H	-4.64486600	0.22924500	-2.82438800
Si	3.53459200	-1.28691200	1.72947400
Si	5.13029300	-1.15814500	-0.85509800
O	4.62901600	-1.77458100	0.59602600
O	4.39967100	-0.93988400	3.07883200
H	3.89144300	-0.94509000	3.90196000
O	2.36540800	-2.38693000	2.06206100
H	1.49357400	-2.16826200	1.68062400
O	5.10780100	-2.25637200	-2.06636700
H	5.90766100	-2.79363200	-2.15046800
O	6.66441100	-0.58565700	-0.70060200
H	6.91529200	-0.30986900	0.19271000
Si	-1.94128400	-3.09054200	-1.68642900
Si	-1.48643700	-2.53147400	1.26945700
O	-2.14532700	-3.24775600	-0.04851400
O	-3.31042700	-2.66603700	-2.45874700
H	-3.76070600	-1.83239900	-2.21063400
O	-1.43557500	-4.53511600	-2.26489500
H	-1.70401400	-4.73469100	-3.17228800
O	-2.55479700	-1.52247700	1.98741600
O	-1.02213700	-3.58314800	2.42716500
H	-0.50067500	-4.34877100	2.14745900
C	1.69878400	5.29266900	-0.17564300
H	2.78479200	5.24467300	-0.03526000
H	1.53863100	5.33287900	-1.30770000
C	1.04662700	6.49433800	0.50124600
H	1.23223200	6.46410500	1.57675500
H	1.44157700	7.44231000	0.11944600
H	-0.03655300	6.50822600	0.35436000

CA[3-4]$^{\neq}$ (Nb)

Si	-2.02591600	1.65709900	0.08963600
O	-1.16250400	3.01536100	0.28719000
Nb	0.79876100	3.20560300	0.05743200
O	2.39097800	2.11426200	-0.23428000
Si	2.58165000	0.49776800	-0.40357400
O	3.98586500	0.09155400	-1.12640500
O	2.57792200	-0.18905600	1.09268700
O	1.31180900	-0.11562600	-1.26339100
O	-2.25673400	0.88919400	1.53933500
O	-3.53640100	1.88014500	-0.53679000
O	-1.25808100	0.62476900	-0.93595200
Si	-0.20011800	-0.63072700	-0.97241700
O	-0.24432400	-1.34435500	0.51393200
O	-0.72972400	-1.71512600	-2.06923900
Si	-3.28425300	-0.35626900	1.90147900
Si	-4.72067200	0.73628800	-0.52346800
O	-3.87040100	-0.23915500	3.42152900
H	-4.23944300	0.61745700	3.67753400
O	-4.47747300	-0.27686500	0.75004800
O	-6.14470400	1.54208000	-0.45112200
H	-6.94682400	1.00055900	-0.44749700
O	-4.62004600	-0.24340700	-1.86925800
H	-4.60251100	0.23663300	-2.71225700
Si	3.36241800	-1.53190100	1.65494600
Si	5.08266900	-1.10577200	-0.80578300
O	4.66230300	-1.75201400	0.65694800
O	3.84649500	-1.14399400	3.18085300
H	4.00895600	-1.90048800	3.76126300
O	2.47698100	-2.90678000	1.60390700
H	1.53396100	-2.89364600	1.85220600
O	4.99686200	-2.16475400	-2.05037400
H	5.75618300	-2.75628500	-2.14466700
O	6.62916400	-0.55176700	-0.71650800
H	6.89397500	-0.19567800	0.14339300
Si	-1.77475200	-3.00324400	-1.90186100
Si	-1.28008700	-2.50839600	1.02772100
O	-1.82645700	-3.33929800	-0.27446000
O	-3.24010800	-2.65079900	-2.52438200

H	-3.71059600	-1.84844100	-2.21926000
O	-1.19397100	-4.34082000	-2.64252700
H	-1.45196600	-4.44725100	-3.56844100
O	-2.52813500	-1.80230000	1.82159000
O	-0.41469900	-3.47389500	2.04754300
H	-0.51341000	-4.42836500	1.91790800
C	1.18070200	3.21083100	2.57310600
H	1.28990200	4.06180900	1.79154800
C	0.92780300	4.56852300	-1.59753900
H	0.67152100	3.86170500	-2.42079900
C	2.21687900	5.32202700	-1.93298100
H	0.07326000	5.25089000	-1.50839100
H	1.88115500	2.38332800	2.45121600
H	1.46907300	3.78348400	3.45662200
H	0.15864700	2.85389900	2.70958300
H	2.14463100	5.84870700	-2.89305100
H	2.44057600	6.06349200	-1.16201500
H	3.07137900	4.64348100	-1.99563700

CA0 (V)

Si	-1.75956100	1.81409000	-0.04170700
O	-0.83396500	3.14835400	-0.11988000
V	0.84468700	3.58180400	-0.53510500
O	2.12117500	2.39117400	-0.78454000
Si	2.63215300	0.85119700	-0.56170600
O	4.07418700	0.54751900	-1.25487200
O	2.76219700	0.54805600	1.04700700
O	1.50753300	-0.18959100	-1.17205900
O	-2.04806200	1.33945700	1.51166300
O	-3.23420300	2.01232700	-0.74466100
O	-1.01021000	0.58182000	-0.81139300
Si	0.00446600	-0.70199800	-0.85252400
O	-0.03276700	-1.43324900	0.64256200
O	-0.55304300	-1.77029600	-1.94652700
C	1.36294800	5.52077000	-0.50860800
H	2.40043900	5.63635500	-0.18476800
H	1.25422900	5.87316500	-1.54301900
H	0.69043500	6.08083800	0.14704000
Si	-3.09721700	0.14703000	1.98861500
Si	-4.54228000	1.03718200	-0.51158900
O	-3.62000800	0.40139000	3.51294800
H	-3.74059500	1.32496100	3.77419400
O	-4.32457200	0.17881100	0.87188800
O	-5.85284800	2.01932200	-0.47818000
H	-6.70397800	1.59585300	-0.29621300
O	-4.65165700	-0.10600800	-1.71845800
H	-4.73321700	0.26287000	-2.61231600
Si	3.57698000	-0.71920600	1.75841700
Si	5.24564500	-0.52750600	-0.77953500
O	4.75270500	-1.13315800	0.67795700
O	4.35211500	-0.26298500	3.12951200
H	3.82383900	-0.33305100	3.93693400
O	2.50213100	-1.91264700	2.07851500
H	1.62826800	-1.79548300	1.65874900
O	5.34860700	-1.66216900	-1.95209600
H	6.19203100	-2.13318100	-1.99877500
O	6.72172500	0.17629200	-0.60558200
H	6.92292400	0.50371300	0.28279800
Si	-1.79726200	-2.85923900	-1.76600200
Si	-1.33904400	-2.31377800	1.20564500
O	-2.02288900	-2.98933100	-0.12345100
O	-3.18469500	-2.40459200	-2.49301200
H	-3.71770000	-1.69575200	-2.07888200
O	-1.30532900	-4.27563000	-2.42032300
H	-1.98750900	-4.75571900	-2.90954700
O	-2.38889600	-1.31736900	1.95782800
O	-0.85731700	-3.40007000	2.32228200
H	-0.34430500	-4.15892500	2.01124400

CA3 (V)

Si	-1.77086600	1.67722100	-0.01264700
O	-0.84028500	3.00589800	-0.06820900
V	0.84893100	3.44705400	-0.45885400
O	2.14718400	2.27321700	-0.71520400
Si	2.63910800	0.72468800	-0.52329600
O	4.07202500	0.41631000	-1.23521400
O	2.78311700	0.38746000	1.07797900
O	1.50035500	-0.29684100	-1.13992000
O	-2.07289900	1.18215400	1.53264400
O	-3.24139100	1.88952900	-0.72179300
O	-1.02863600	0.44620200	-0.79268700
Si	0.00000500	-0.82574100	-0.84027600
O	-0.04398700	-1.57757600	0.64498000
O	-0.53895700	-1.88545000	-1.95243600
Si	-3.12482600	-0.01765300	1.98269900
Si	-4.55080900	0.91105600	-0.51308300
O	-3.65450400	0.20797100	3.50952900
H	-3.78897000	1.12611900	3.78276700

O	-4.34894500	0.03660500	0.86308700
O	-5.86325400	1.89124900	-0.48208700
H	-6.71531200	1.46303500	-0.31624200
O	-4.64718500	-0.21869100	-1.73412500
H	-4.71181700	0.16052900	-2.62504800
Si	3.58324400	-0.90763900	1.75387700
Si	5.22438000	-0.69474500	-0.79961300
O	4.73937100	-1.32098500	0.65215200
O	4.38202100	-0.49271900	3.12494800
H	3.86229400	-0.57462000	3.93679100
O	2.49255100	-2.08915400	2.06574300
H	1.61532700	-1.95210000	1.65910800
O	5.28635700	-1.80626300	-1.99728500
H	6.11666000	-2.29806200	-2.06177300
O	6.71883400	-0.02874300	-0.63126700
H	6.93835700	0.27501700	0.26118300
Si	-1.78580100	-2.97516500	-1.79770100
Si	-1.35383700	-2.46793500	1.18371300
O	-2.01812300	-3.13643600	-0.15888500
O	-3.16932000	-2.50480400	-2.52262600
H	-3.70207900	-1.79987600	-2.10149800
O	-1.29488900	-4.38051200	-2.47634600
H	-1.97540600	-4.84663600	-2.98114200
O	-2.41786700	-1.48189100	1.92915200
O	-0.88144300	-3.56164100	2.29734200
H	-0.35609500	-4.31205700	1.98625300
C	1.39416300	5.37683300	-0.50098600
H	2.25701800	5.40479100	0.17863900
H	1.77759200	5.46927300	-1.52900600
C	0.34217200	6.43615900	-0.16866400
H	-0.02784600	6.32566900	0.85353700
H	0.75569200	7.44744100	-0.25959600
H	-0.51825400	6.37494500	-0.83964800

CA[3-4]$^{\neq}$ (V)

Si	-1.68794400	1.71426400	-0.06224100
O	-0.73158900	3.01519100	-0.21002300
V	0.93307300	3.25185600	-0.85511800
O	2.21339400	2.04477600	-1.10976100
Si	2.59380200	0.49573800	-0.75522600
O	4.03845100	0.03315800	-1.34721800
O	2.62735100	0.32163300	0.87867900
O	1.41649900	-0.51145600	-1.32566000
O	-1.92018300	1.26388300	1.50943000
O	-3.19197200	1.94816300	-0.69297800
O	-1.01267800	0.45042200	-0.85380500
Si	-0.10297800	-0.91184300	-0.92613700
O	-0.12866100	-1.62235900	0.57828400
O	-0.78851700	-1.94098000	-1.98375100
Si	-3.00204600	0.14508400	2.07357400
Si	-4.53972000	1.06383300	-0.35770300
O	-3.42633200	0.45691100	3.61939200
H	-3.55979300	1.38746800	3.84786200
O	-4.28356100	0.20885500	1.02331700
O	-5.77902500	2.13006600	-0.24690000
H	-6.64607800	1.76167100	-0.02478600
O	-4.81046500	-0.08332200	-1.53359000
H	-4.92886200	0.27838500	-2.42623800
Si	3.40550800	-0.83789600	1.78329000
Si	5.14716500	-1.02294800	-0.70950000
O	4.60267600	-1.40943500	0.80346400
O	4.14723100	-0.19056300	3.09490400
H	3.58914200	-0.10723100	3.88048500
O	2.31114500	-1.95757500	2.26060400
H	1.51012400	-2.01228200	1.70593400
O	5.21164500	-2.30354600	-1.72355600
H	6.01872800	-2.83400700	-1.67159600
O	6.65272000	-0.37210400	-0.59430300
H	6.85121200	0.06995100	0.24361400
Si	-2.08899800	-2.94447000	-1.72815200
Si	-1.45507400	-2.41625500	1.20651800
O	-2.29041700	-2.98833400	-0.07627000
O	-3.47712500	-2.42915000	-2.41478800
H	-3.97068000	-1.71861300	-1.95781600
O	-1.68292300	-4.39501000	-2.36247500
H	-2.42661700	-4.94919300	-2.63633200
O	-2.36693900	-1.35745400	2.07028200
O	-0.95790900	-3.61711900	2.19253100
H	-1.06392800	-3.47064500	3.14251600
C	1.72510600	4.41178400	0.64619900
H	1.18024000	4.63311100	-1.56679900
C	0.60388100	3.97288400	-2.81913900
H	1.45147500	3.54911900	-3.36271900
H	-0.29524900	3.37386900	-3.01614800
H	0.42004200	4.98385600	-3.18627900
H	2.72995600	4.71590100	0.33224600
H	1.12142200	5.32378800	0.71758200
C	1.75584500	3.65904900	1.98135600

H	0.74885400	3.38156500	2.30719500
H	2.34979500	2.74255700	1.92625400
H	2.19197100	4.28142000	2.77383800

CA0 (Ta)

Si	-1.86451000	1.55884300	0.12586400
O	-0.90760700	2.87588100	0.20919600
Ta	0.95384600	3.21473000	-0.16303500
O	2.23684100	1.84125900	-0.49882200
Si	2.61314300	0.24734100	-0.42710600
O	3.99449400	-0.11921100	-1.20621200
O	2.77561500	-0.20515200	1.14186200
O	1.37671500	-0.63201300	-1.07137400
O	-2.30683400	0.98414900	1.60226100
O	-3.25356500	1.82712000	-0.70970600
O	-1.02451700	0.38183200	-0.63895100
Si	-0.17007800	-1.00526900	-0.76320000
O	-0.26707500	-1.81220500	0.68976600
O	-0.84098400	-1.94972800	-1.90411500
C	1.68083300	5.21524900	-0.01505800
H	2.68794700	5.25031000	0.41501500
H	1.72379200	5.59892600	-1.04752400
H	1.01845700	5.86154200	0.57084400
Si	-3.41833300	-0.21001800	1.89307400
Si	-4.59109800	0.86424800	-0.66689400
O	-4.24763300	0.03426200	3.27572700
H	-3.87200100	-0.35281000	4.07879900
O	-4.47296700	-0.15018200	0.62213900
O	-5.88829200	1.85997000	-0.61841800
H	-6.74240700	1.45012100	-0.41965100
O	-4.62355200	-0.14841700	-1.98867900
H	-4.67216300	0.30398700	-2.84531100
Si	3.46912500	-1.61516800	1.69378600
Si	5.05948900	-1.35202200	-0.88530500
O	4.54832300	-2.04995900	0.52481600
O	4.34508800	-1.38350300	3.06009400
H	3.83911400	-1.42850400	3.88341000
O	2.27118200	-2.70421900	1.95142400
H	1.40299300	-2.43454500	1.59523400
O	5.00566500	-2.36733300	-2.16551200
H	5.79285700	-2.91496800	-2.29170200
O	6.60608200	-0.82444000	-0.70430700
H	6.86777700	-0.60369000	0.20109300
Si	-2.04138500	-3.10320200	-1.77743300
Si	-1.60810500	-2.66794300	1.20192800
O	-2.27005400	-3.31598800	-0.14932700
O	-3.39314000	-2.63740400	-2.55541300
H	-3.83071800	-1.80084500	-2.29475300
O	-1.54008300	-4.53363300	-2.39326900
H	-1.75982000	-4.68638800	-3.32263000
O	-2.65709400	-1.65707800	1.94553100
O	-1.18447300	-3.77509700	2.32238900
H	-0.70411900	-4.55654400	2.01427500

CA3 (Ta)

Si	-1.84711900	1.49698900	0.09723000
O	-0.85954300	2.78994700	0.16813200
Ta	1.02102400	3.05532200	-0.19030000
O	2.28648700	1.65801100	-0.51491800
Si	2.60789100	0.05366700	-0.43074300
O	3.97244000	-0.36764900	-1.21289500
O	2.76410700	-0.39319800	1.14112900
O	1.34098300	-0.79167400	-1.06184400
O	-2.30679400	0.94779100	1.57869500
O	-3.22951400	1.78608400	-0.74368700
O	-1.03388100	0.29129400	-0.65339200
Si	-0.21579100	-1.11904700	-0.75310500
O	-0.33758700	-1.90069900	0.71196500
O	-0.90698300	-2.06463200	-1.88102100
Si	-3.44982800	-0.21163800	1.88461000
Si	-4.58929200	0.85616100	-0.69218300
O	-4.27342900	0.07334300	3.26310200
H	-3.90987700	-0.31533700	4.07093600
O	-4.50231600	-0.14145200	0.61230900
O	-5.86268200	1.88320900	-0.66455200
H	-6.72663500	1.49700700	-0.46108400
O	-4.64108500	-0.17508000	-1.99912500
H	-4.67117400	0.26591800	-2.86252300
Si	3.40672300	-1.82470100	1.69839900
Si	4.99354000	-1.63550600	-0.88843500
O	4.46354000	-2.30729300	0.52771500
O	4.29698400	-1.61797600	3.05970400
H	3.79275600	-1.63745500	3.88509400
O	2.16986900	-2.86666600	1.96826800
H	1.31129500	-2.56517300	1.61395500
O	4.89954600	-2.65589100	-2.16243000
H	5.66372900	-3.23628100	-2.28359200
O	6.55890400	-1.16287400	-0.71525200

H	6.83035100	-0.94566200	0.18813200
Si	-2.13376200	-3.18819700	-1.74106000
Si	-1.69744500	-2.72049600	1.23287800
O	-2.36872400	-3.37505400	-0.11060400
O	-3.47402000	-2.70167500	-2.52637900
H	-3.89210600	-1.85165000	-2.27746000
O	-1.66538100	-4.63705300	-2.33965500
H	-1.89975400	-4.79994800	-3.26369000
O	-2.72803900	-1.67806100	1.95834100
O	-1.29935000	-3.81840900	2.37176100
H	-0.81614700	-4.60467800	2.08078900
C	1.86952600	5.00734100	-0.10769400
H	2.72275500	4.90058600	0.58225700
H	2.29991000	5.09963100	-1.12231200
C	1.00606700	6.22867200	0.24482900
H	0.59457800	6.14741100	1.25399400
H	1.58831100	7.15498100	0.20202900
H	0.16660400	6.34008100	-0.44661200

CA[3-4]$^{\neq}$ (Ta)

Si	-2.03503200	1.49998100	0.11888600
O	-1.13240600	2.83382500	0.32498300
Ta	0.83244700	2.92708100	0.09014900
O	2.40744300	1.81288900	-0.18655300
Si	2.54695900	0.18909300	-0.36144400
O	3.93691800	-0.24901000	-1.09148800
O	2.52277600	-0.51335700	1.12496500
O	1.25741300	-0.36891000	-1.23034000
O	-2.29812300	0.72936900	1.55923600
O	-3.53206800	1.77489600	-0.51601600
O	-1.28395600	0.46052300	-0.91309800
Si	-0.27331800	-0.83493200	-0.95199700
O	-0.35321200	-1.56078000	0.52597200
O	-0.83428000	-1.88748200	-2.06365500
Si	-3.36653800	-0.48535200	1.90803600
Si	-4.75640100	0.67299800	-0.51387200
O	-3.95375500	-0.35975900	3.42663500
H	-4.26903200	0.51357500	3.69762300
O	-4.55083700	-0.35825100	0.75156600
O	-6.15122100	1.52761000	-0.43809400
H	-6.97172400	1.01434200	-0.43409900
O	-4.68531300	-0.29807400	-1.86760700
H	-4.65524900	0.18790100	-2.70687700
Si	3.25409700	-1.89675500	1.66184100
Si	4.99256900	-1.48840700	-0.79013900
O	4.54367700	-2.14808200	0.65786100
O	3.75355000	-1.55949900	3.19415200
H	3.87889300	-2.33227500	3.76209800
O	2.31318000	-3.23313700	1.58237400
H	1.37258600	-3.18683800	1.83550900
O	4.87622400	-2.51936400	-2.05540800
H	5.61707200	-3.13203400	-2.16095400
O	6.55581900	-0.98739100	-0.68497400
H	6.82991800	-0.65823300	0.18272400
Si	-1.92301200	-3.14180800	-1.91719800
Si	-1.43129800	-2.69437400	1.02142900
O	-2.00117100	-3.48880600	-0.29334000
O	-3.37030900	-2.73600400	-2.54910200
H	-3.82148000	-1.92627900	-2.23457400
O	-1.37937900	-4.49082500	-2.66494300
H	-1.63374500	-4.58217100	-3.59347500
O	-2.65803000	-1.95461500	1.81789400
O	-0.60253000	-3.70036800	2.03183600
H	-0.73998100	-4.64951700	1.89872400
C	1.26808500	3.28333300	2.43328900
H	1.38834700	4.07998300	1.46458900
C	0.84036200	3.91854400	-1.82405700
H	0.50758600	3.07560100	-2.47061300
C	2.12165300	4.53776000	-2.39408100
H	0.01580000	4.64079700	-1.82934200
H	1.92772600	2.41026100	2.46840900
H	1.64312200	4.01660400	3.15034400
H	0.24420700	3.02341900	2.71755200
H	1.98467200	4.86738500	-3.43128600
H	2.42576200	5.40722800	-1.80635500
H	2.95071500	3.82607500	-2.38222200