Supporting information for: Organic Nanostructures on Hydrogen-Terminated Silicon Report on Electric Field Modulation of Dangling Bond Charge State

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1 Supporting Information

1.1 Self-consistent solution for band bending at the silicon surface in the presence of a biased STM tip, DBs, and adsorbed molecules

We assume an areal density of DBs on the surface is N_{DB}, and the energy of the DB^- and DB^+states with respect to the VBM are denoted by E_{DB-} and E_{DB+}. A CBMK intermediate has an energy level, E_{C*}, corresponding to the C* radical situated in the band gap of silicon . The presence of a lone electron in the C* level, in the immediate vicinity of the surface, implies the

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possibility of its escape via elastic tunneling to the bulk or via recombination with an itinerant hole from silicon. The latter is an inelastic capture event, characterized by an capture cross section σ_p^*. The rate of recombination, denoted by $R_{\rm rec}$, depends on the concentration of holes in the subsurface region

$$R_{\rm rec} = \sigma_p^* p v_p, \tag{1}$$

where p is the free electron concentration at the surface and v_p is their thermal velocity. In turn, p depends (self-consistently) on the total amount of band bending at the surface due to the biased STM probe and the charging of the surface states.

We formulated and solved a self-consistent boundary-value problem (BVP-1) for the electric potential U in the presence of the STM tip and surface states, consisting of the Poisson and Schroedinger equations written respectively as

$$\nabla^2 U(r) = -\frac{e}{\varepsilon_{Si}}[N_D^+ + p(r) - N_A^- - n(r) + \rho_0(r)] \tag{2}$$

and

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + U(r)\psi(r) = E\psi(r), \tag{3}$$

which can be compactly combined as

$$\nabla^2 U(r) = -\frac{e}{\varepsilon_{Si}}\rho_{total}\{U(r)\} \tag{4}$$

where { } denotes functional dependence. In the above, $N^+{}_D$ and $N^-{}_A$ are the concentrations of ionized donors and acceptors, ε_{Si} is the electric permittivity of silicon; ρ_0 is the charge on all surface states, while n and p are the concentrations of itinerant electron and holes in the crystal. Employing the semiclassical approximation, the latter quantities can be calculated with the help of the 1/2 Fermi-Dirac integral, $F_{1/2}$

$$n(r) = N_c F_{1/2}\{[E_F - E_{CBM}^{bulk} + eU(r)]/k_B T\} \tag{5}$$

$$p(r) = N_v F_{1/2}\{[E_{VBM}^{bulk} - eU(r) - E_F]/k_B T\} \tag{6}$$

where N_c and N_v are the effective density of states at the edges of the conduction (E_{CBM}) and valence (E_{VBM}) bands, respectively, E_F is the Fermi level and $k_B T$ is the temperature in energy units. The negative charge accumulated on the DBs is

$$\rho_0^- = N_{DB} f_{FD}(E_{DB}, E_F). \tag{7}$$

with a similar expression for the positive DB charge. We also include the possibility of charge on any molecular ad layer on silicon. Thus the net charge on the surface will be

$$\rho_0 = \rho_0^+ - \rho_0^-, \tag{8}$$

which is compensated by a subsurface space-charge layer in the bulk silicon. The BVP-1 also includes the appropriate set of boundary conditions (BC) denoted by BC-1, described below.

We solved the above BVP-1 by the finite element method (FEM). Even in the absence of an STM tip, surface states alone can accumulate charge and induce the crystal bands to bend at the surface. In the presence of the STM tip, the effects of tip-induced and surface state-induced band bending coexist and have to be solved self-consistently. However, we note that the tip-induced band bending has a finite spatial extent due to screening, while the surface state-induced band bending is more or less uniform along the surface (laterally). This means that far away from the tip, along the surface, the total band bending will be identical with that in the absence of the tip. Therefore, this lateral condition forms part of the set BC-1 for our BVP-1 problem. The other BCs in this set are the Dirichlet condition $U = U_{bias} + U_{cont}$ at the surface of the tip, and $U=0$ far inside the bulk of the crystal, where U_{bias} and U_{cont} are the values of the bias and the contact potential between tip and sample.

While the two latter BCs are easily imposed in an FEM calculation, the lateral BC presents

some technical difficulties. A straightforward but naive way to implement it would be to solve for U_0 (**r**) in the absence of the STM tip on a laterally large FEM domain and then impose a Dirichlet BC with the values of U_0 at the edges of the domain to solve BVP-1. However, when doing so, the results show unphysical behavior in the form of non-monotonic surface-parallel variations of U as a function of the lateral distance from the tip apex, which furthermore strongly depends on how fine the FEM mesh is at the lateral extremities of the domain. This approach is therefore deemed unreliable.

Another approach is therefore needed in order to impose the correct lateral BC on BVP-1. First we note that for the system in the presence of surface states only, the appropriate BVP-0 can be written as

$$\nabla^2 U_0(r) = -\frac{e}{\varepsilon_{Si}} \rho^0_{total}\{U_0(r)\}, \tag{9}$$

with the boundary condition set BC-0:

$$\nabla U_0(r) = 0, \text{ for z } > 0, \tag{10}$$

$$U_0(r) = 0, \text{ for z } < 0, \ |\text{z}| \to \infty. \tag{11}$$

Subtracting eq (9) from eq (4) we obtain a new differential equation

$$\nabla^2 U'(r) = -\frac{e}{\varepsilon_{Si}} [\rho_{total}\{(U' + U_0)(r)\} - \rho^0_{total}\{U_0(r)\}], \tag{12}$$

where $U'(r) \equiv U(r) - U_0(r)$ is the unknown function of a new BVP-2 to be solved (note that U_0 is previously and separately solved for). The advantage of this new BVP is that the lateral boundary condition simplifies to $U'(r) \to 0$ as $|r_{xy}| \to \infty$, due to the fact that U and U_0 have the same values asymptotically. To complete the set BC-2 for BVP-2, we must add the Dirichlet condition U'= U_{bias} + U_{cont} at the surface of the tip, and U'=*0* far inside the bulk of the crystal. This BVP-2 is actually the second problem (after BVP-0) that we solve by employing FEM, as it is easily amenable and well behaved on a finite element domain. Also, we further simplify the problem

by assuming both the tip and the whole domain to have axial symmetry. The above BVPs are self-consistently solved by iterations each consisting of an FEM calculation. Once U_0 and U' are computed, U is simply found by adding the two functions. Further details are given in an upcoming paper.

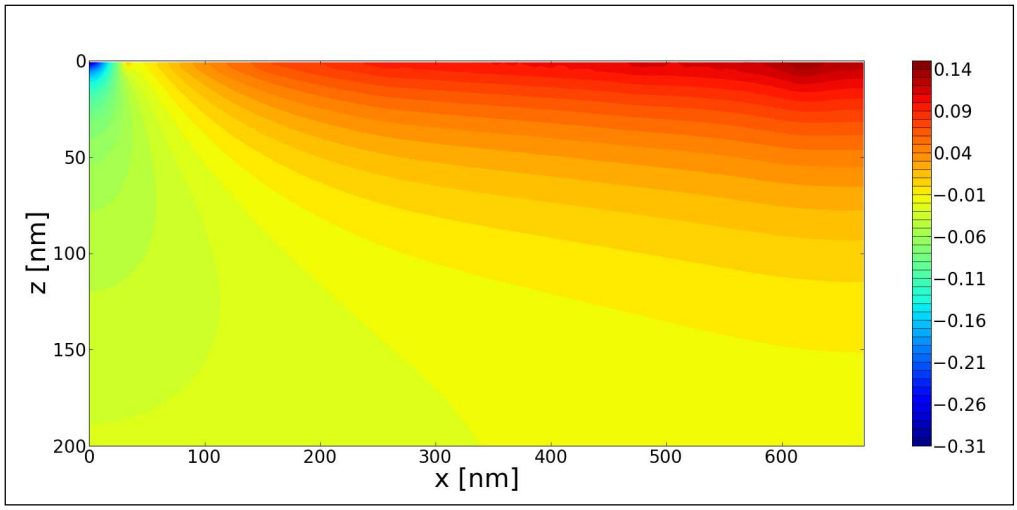

Figure S1: Images of a representative large cluster used for the *stage 1* (see manuscript) calculations. Shown are the transition state structure from H-abstraction by the CBMK addition intermediate.Views: a) end-on, b) top-down, c) side-on.

1.2 DFT models associated with the calculations described in the text

DFT calculations were performed with the Gaussian 03 package.[S1]

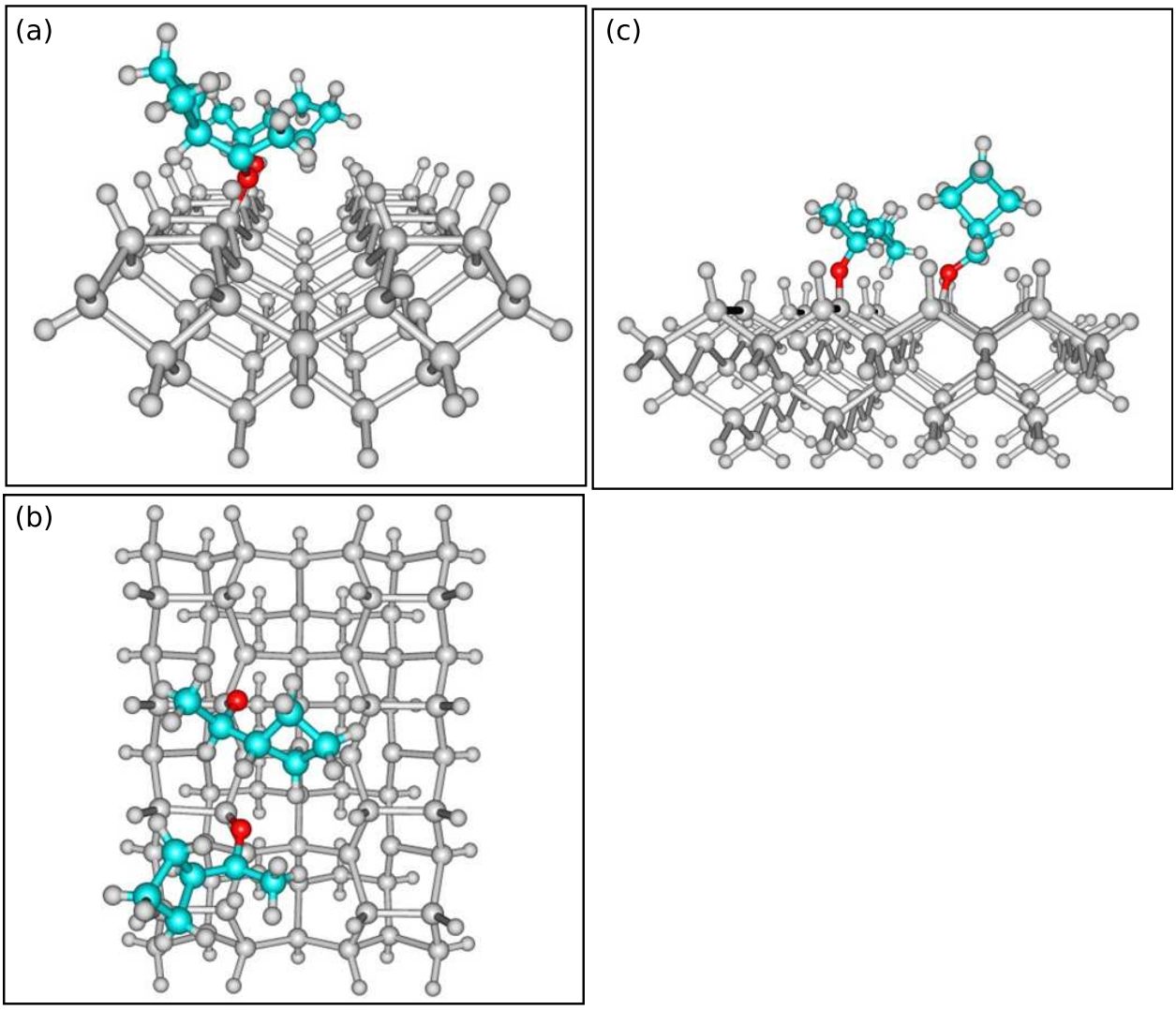

Figure S2: Images of a representative large cluster used for the *stage 1* (see manuscript) calculations. Shown are the transition state structure from H-abstraction by the CBMK addition intermediate.Views: a) end-on, b) top-down, c) side-on.

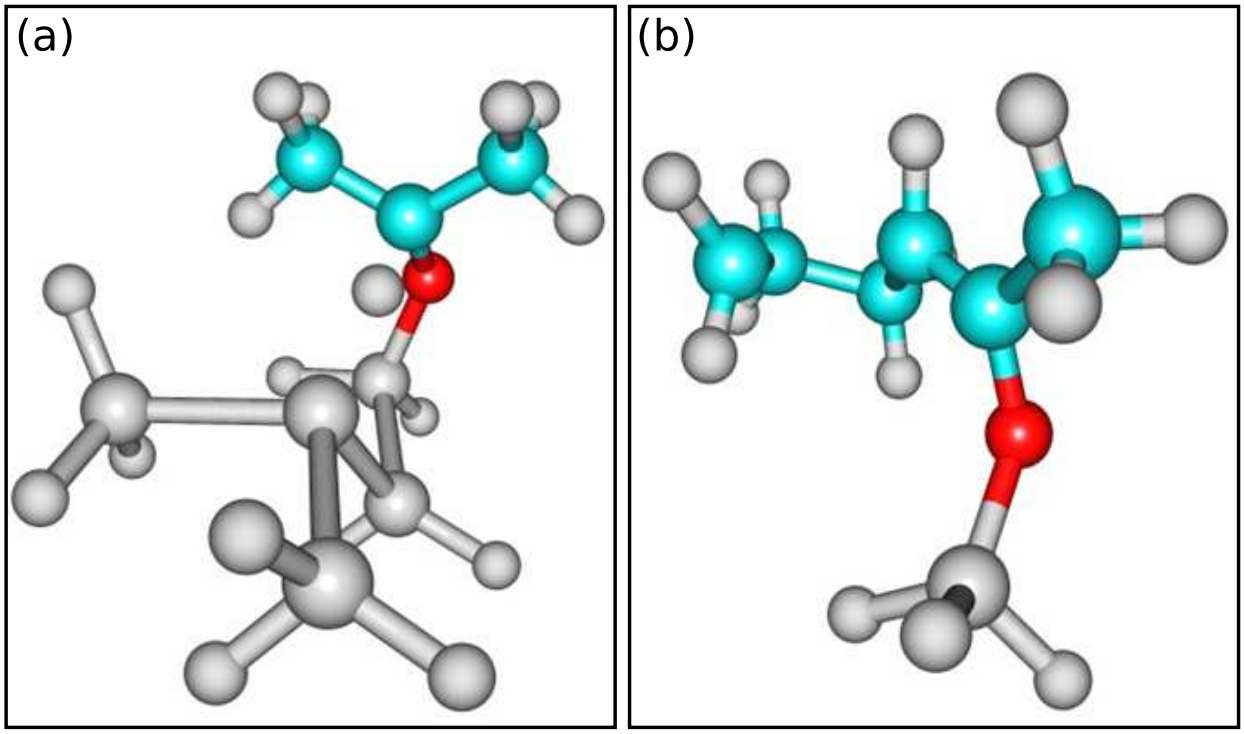

Figure S3: Images of representative small clusters used for the *stage 2* (see manuscript) calculations. Shown are the transition state structures for (a) H-abstraction and (b) ring opening.

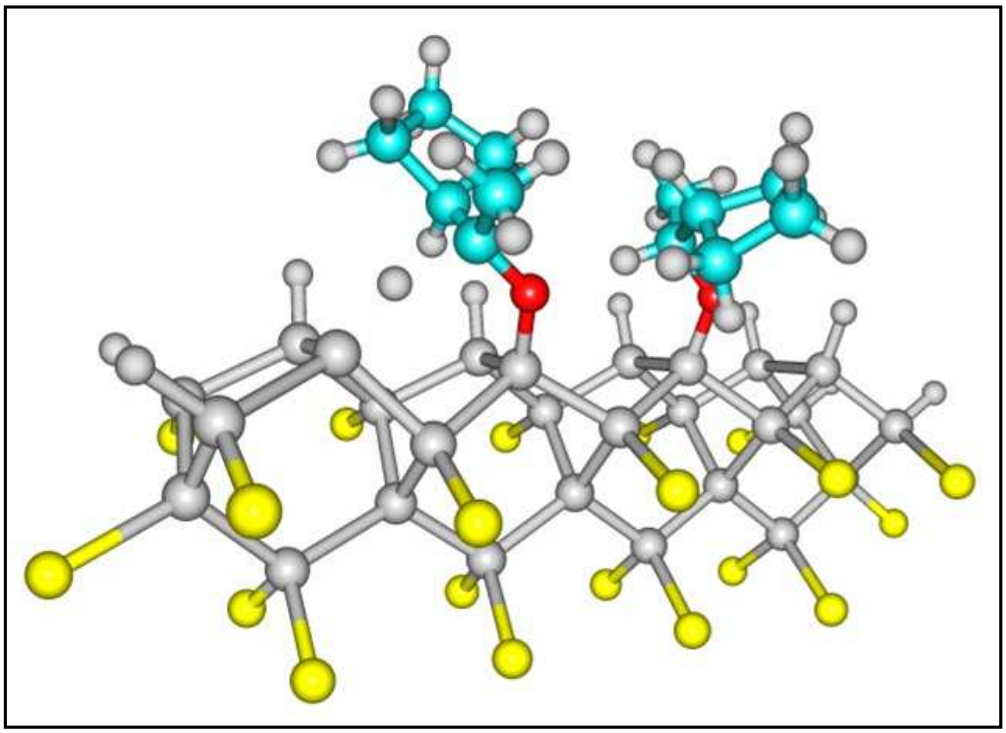

Figure S4: Image representative of a cluster used for the *stage 3* (see manuscript) calculations. Shown is the optimized structure for the transition state for H-abstraction.

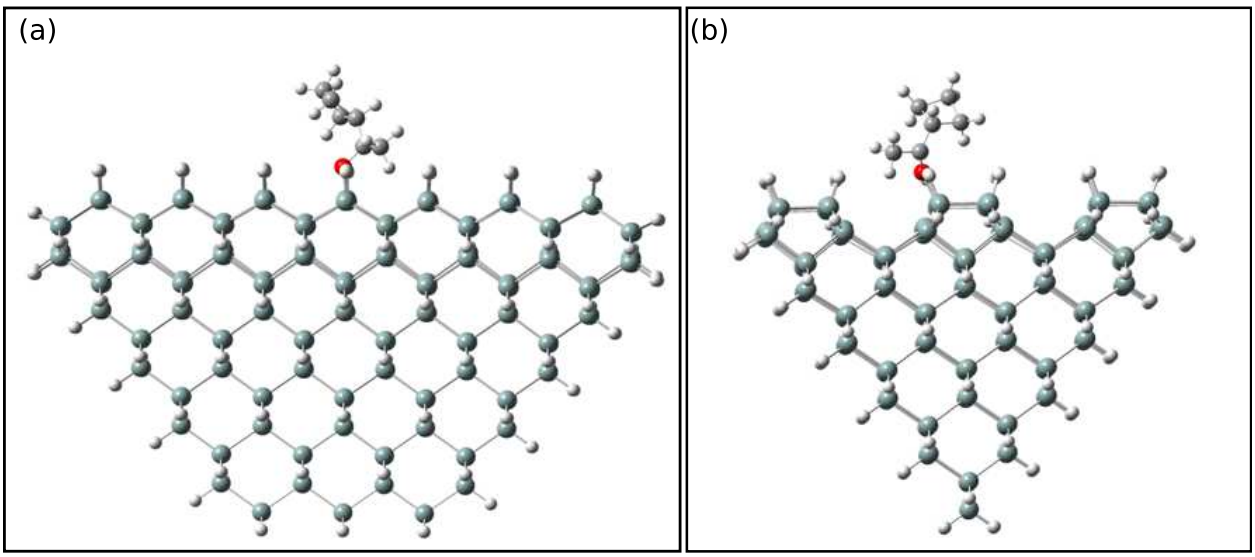

Figure S5: Side (a) and end view (b) of the cluster used to estimate the energy level of the SOMO of CBMK bound to a neutral DB on H-Si(100)-2x1. Key: Silicon - steel grey, carbon - grey, oxygen - red, hydrogen - white.

Table S1. Absolute B971-DCP electronic energies (Hartree) of systems related to the reaction of second CBMK on a cluster representing hydrogen-terminated silicon. See text for details of the calculation methods. Calculations utilized 6-31+G(d,p) basis sets for C, H, and O and 6-31G(d) basis sets for Si.

Number	Molecule/cluster system	Eel
1	CBMK	-309.655164
2	Passivated CBMK on H-Si with radical site	-20898.438157
3	Addition product of the reaction of 1 + 2	-21208.122311
4	Transition state structure associated with H abstraction from the next dimer in the row (from 3)	-21208.102693
5	Transition state structure associated with CBMK ring opening (from 3)	-21208.099687

Table S2. Absolute CBS-QB3 and B971-DCP electronic energies (Hartree) of systems related to the reaction of second CBMK on a cluster representing hydrogen-terminated silicon. See text for details of the calculation methods. Representative structures are shown in Figure S3. Structures were frozen in the geometries optimized from the large cluster optimizations.

Number	Molecule/cluster system	Eel (CBS)	Eel (B971)
1	Reduced model of addition species for ring opening	-600.861986	-600.853660
2	Reduced model of ring opening transition state (from 1)	-600.83 044	-600.830294
3	Reduced model of addition species for H-abstraction	-1646.421136	-1646.757590
4	Reduced model of H-abstraction transition state (from 3)	-1646.398331	-1646.736776

Table S3. Data used to compute the rate constants (at 300 K) for the ring-opening and H-abstraction reactions associated with CBMK on H-Si.

Quantity	Ring-opening	H-abstraction
ZPE (a.u.)	0.456437	0.45779
E_{therm}(a.u.)	0.555689	0.556033
Q	2.04E+72	1.4E+71
Eel (a.u.)	-21208.09969	-21208.1
RT (kcal/mol)	0.596	0.596
kT/h (s^{-1})	6.25093E+12	6.25E+12
E_0 (kcal/mol)	14.08	12.56
A (s^{-1})	1.98E+12	1.36E+11
E_a (kcal/mol)	13.35	12.45
k (s^{-1})	2.20E+02	96.79
k (s^{-1}) with tunneling	N/A	2.68E+02

Quantity terms are (in the order given in column one: zero-point energy, thermal energy correction term, partition coefficient, electronic energy, ideal gas constant time temperature (300K), Boltzmann constant times temperature (300 K) divided by Planck's constant, ZPE corrected energy barrier for the reaction, pre-exponential factor, Arrhenius activation barrier for the reaction, reaction rate constant.

Structures used for B971-DCP calculations (Cartesian corrdinates in Å) – see Table S1

Table S1, #1

C -3.37129263 0.64707912 0.01053606

C -1.95003135 0.03794019 0.04913263

C -2.20262623 1.46851897 -0.49423127

H -4.06152842 0.21902421 -0.71392074

H -3.82677898 0.93194639 0.95743905

H -1.71936920 -0.72254451 -0.69547979

H -1.86308549 2.31038417 0.10680192

H -2.07960834 1.60075392 -1.56742785

C -1.20951560 -0.19430949 1.34823558

O -0.37973594 -1.09243774 1.42780928

C -1.53532443 0.68290338 2.57376904

H -1.75294955 1.72540927 2.31156854

H -2.42285706 0.27250374 3.07676795

H -0.69294690 0.64047893 3.27049086

Table S2, #2

H 5.78120400 -5.77544000 3.25507000

H 1.88719000 -5.73156000 3.21960600

H -1.98737900 -5.70227900 3.16275600

H -5.87370400 -5.65416900 3.10041200

H 5.84693400 1.97089800 3.52189500

H 1.98068600 2.03598600 3.49090500

H -1.95020300 2.06639800 3.42740500

H -5.78755000 2.08929400 3.36704300

H 5.81303200 -2.20284800 3.38689800

H -0.53706400 -3.22187600 4.20587900

H -5.83703300 -2.08155000 3.23539700

H 5.88989200 5.54562000 3.62411100

H 1.99880400 5.57785400 3.58906600

H -1.87688400 5.61176600 3.53717300

H -5.76461100 5.66556300 3.46932000

Si 5.78687700 -5.16686500 1.89147900

Si 1.90835900 -5.14176500 1.84700000

Si -1.96153800 -5.09180900 1.79830100

Si -5.83271900 -5.04468400 1.73755700

Si 5.85546400 2.57857900 2.15726700

Si 1.98794700 2.62246900 2.11842200

Si -1.89229500 2.65808600 2.05903200

Si -5.75222400 2.69752200 2.00332000

Si 5.80647300 -2.71884400 1.98508900

Si 1.93304300 -2.69100500 1.92001600

Si -1.95304300 -2.62183300 1.89477900

Si -5.80592100 -2.59763800 1.83544300

Si 5.88524300 5.02701800 2.22372500

Si 2.01016600 5.07234000 2.18281100

Si -1.86241600 5.10848200 2.13011300

Si -5.73473600 5.14592600 2.06964500

Si 7.70596500 -5.66670900 0.58094800

Si 3.85780700 -5.66871900 0.59183900

Si -0.01928700 -5.63318200 0.54430400

Si -3.88091400 -5.58692700 0.48840900

Si -7.72890000 -5.50768600 0.37887100

Si 7.77425500 2.01811600 0.86230000

Si 3.92730500 2.02906600 0.86511700

Si 0.06159200 2.06478100 0.82531400

Si -3.80732300 2.10768800 0.75592600

Si -7.64755000 2.17651600 0.65923200

Si 7.73448900 -2.11539800 0.72625000

Si 3.89124000 -2.04122700 0.73566700

Si 0.01780800 -2.00143200 0.68713300

Si -3.85215600 -1.95973300 0.62795800

Si -7.68775800 -1.95659700 0.52440700

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Si 3.96694100 5.64592600 0.95885800

Si 0.09679200 5.68705000 0.91038500

Si -3.77245100 5.72518600 0.85511200

Si -7.61929500 5.73040500 0.74482100

Si 7.72203700 -3.84015300 -0.86774500

Si 3.88250100 -3.81086800 -0.85881700

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Si -3.83416100 -3.72858400 -0.96182000

Si -7.67084000 -3.68116700 -1.07020100

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Si -3.76147800 3.96771700 -0.71602500

Si -7.59515400 4.00132600 -0.81912800

Si 7.78454800 -0.00997600 -0.39526900

Si 3.92155400 0.03282100 -0.46137200

Si 0.06119300 0.07138800 -0.50758500

Si -3.80771100 0.11211300 -0.56842900

Si -7.66685800 0.14887600 -0.59931800

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Si -5.72803800 -3.67077600 -2.34451900

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Si -1.80986600 4.00503200 -2.01414300

Si -5.65379800 4.03788300 -2.09416500

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Si 2.00871600 0.09871000 -1.91748300

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Si -1.81308900 2.08732900 -3.36421000

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Si -1.85065900 -1.71787000 -3.48871200

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H 8.96714700 -3.83901000 -1.65708500

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H 7.08087200 -1.78005300 -4.23902200

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Table S3, #3

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Si -1.92540200 -2.72131500 1.47420100

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Si 1.77704900 5.06320500 2.35911100

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Si -5.96285000 4.84594500 2.49359200

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Si 3.94262300 -5.40210400 -0.31425600

Si 0.07883000 -5.50533600 -0.24707600

Si -3.78271200 -5.60865000 -0.17200400

Si -7.63476400 -5.66655200 -0.15724200

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Si 3.75194200 2.22728600 0.70866300

Si -0.11171900 2.12470900 0.77513700

Si -3.97586000 2.01915600 0.83965100

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Si 7.70303200 -1.73032700 0.03555400

Si 3.86270400 -1.81027200 0.17390800

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Si -7.71408200 -2.14666400 0.32987800

Si 7.51869500 5.89866100 1.00251000

Si 3.67063700 5.82361900 1.13882600

Si -0.19817400 5.71999600 1.21104800

Si -4.06503700 5.61333800 1.28067100

Si -7.91148700 5.48072800 1.28950600

Si 7.69531600 -3.29421000 -1.71309900

Si 3.85908500 -3.41394700 -1.58056900

Si -0.00171300 -3.51449800 -1.50156000

Si -3.85363000 -3.62246000 -1.44085600

Si -7.69220600 -3.70968600 -1.42338900

Si 7.50743400 4.32766400 -0.71984500

Si 3.67178900 4.21823900 -0.58870100

Si -0.18699800 4.11669200 -0.51637200

Si -4.04656900 4.01122300 -0.44974700

Si -7.88040300 3.91038800 -0.43330900

Si 7.63663600 0.47476900 -0.87395400

Si 3.77792900 0.37106900 -0.81167400

Si -0.08532000 0.26630500 -0.73840000

Si -3.94838000 0.16238500 -0.67594200

Si -7.80622500 0.05545600 -0.58665800

Si 5.74032300 -3.19025100 -2.96568900

Si 1.89847700 -3.30425200 -2.86627700

Si -1.95415000 -3.40858500 -2.79795100

Si -5.79555700 -3.50301400 -2.75099500

Si 5.55251200 4.45656700 -1.96984000

Si 1.71193300 4.35675200 -1.87094100

Si -2.14442600 4.25277600 -1.80009200

Si -5.98575700 4.14432000 -1.75769300

Si 5.67706200 0.61144600 -2.26414000

Si 1.81395400 0.50594900 -2.19390900

Si -2.04578200 0.40320900 -2.12505900

Si -5.91128100 0.29639700 -2.05153700

Si 5.60414400 2.67593800 -3.47699600

Si 1.73529700 2.57861900 -3.40103300

Si -2.12422100 2.47507200 -3.33005800

Si -5.99340600 2.36106600 -3.26214700

Si 5.69620600 -1.08096100 -3.96429400

Si 1.82805900 -1.19483900 -3.89072900

Si -2.03112000 -1.29871700 -3.81974000

Si -5.90045500 -1.39622700 -3.74959400

H 8.72323000 4.47782000 -1.54069900

H 8.79967600 0.62500800 -1.81114700

H 8.91166500 -3.16800500 -2.53477300

H 6.77317300 2.82421900 -4.35612400

H 6.86609900 -0.94629100 -4.84634900

H -7.20045400 2.44606100 -4.09635900

H -7.10752900 -1.32445100 -4.58658300

H -9.13115200 3.99463700 -1.20879200

H -9.00917000 0.14306000 -1.48008700

H -8.94271800 -3.65118600 -2.20286700

H -7.96044800 6.87603500 0.72560700

H -4.10243600 6.98046300 0.65391900

H -0.24467300 7.08488400 0.58223700

H 3.61308800 7.18926200 0.51049000

H 7.47110200 7.29364900 0.43874100

H -6.04982100 5.47584100 -2.38929600

H -2.19180800 5.58027000 -2.46098400

H 1.66659400 5.68468700 -2.53271000

H 5.52460700 5.78907100 -2.60446100

H -5.80074900 -4.63045400 -3.70327100

H -1.94273200 -4.52607600 -3.77496600

H 1.91567000 -4.42165800 -3.84669300

H 5.77368200 -4.31722300 -3.91843500

H -7.62164600 -6.87104100 -1.06172500

H -3.76363200 -6.76666300 -1.13341900

H 0.09413200 -6.66229000 -1.20510800

H 3.95189300 -6.55786100 -1.27684800

H 7.80990500 -6.45342700 -1.34859200

H -3.34244100 2.55044100 -4.16805500

H -4.80204000 2.51095500 -4.14095800

H 0.51662200 2.65483600 -4.23962500

H -0.94389300 2.61531200 -4.21247500

H 4.37475900 2.75930200 -4.31155100

H 2.91516200 2.71978600 -4.28438100

H -3.24951600 -1.22002300 -4.65827200

H -4.70911500 -1.25952800 -4.63117800

H 0.60954600 -1.11559300 -4.72983900

H -0.85097000 -1.15511700 -4.70268800

H 4.46768400 -1.01118300 -4.80177200

H 3.00808600 -1.05067800 -4.77459900

H 8.75793000 5.48707400 1.72955800

H 8.82357700 2.67221400 1.36900200

H 8.94275100 -2.16327900 0.74031300

H 9.01581100 -4.97657600 0.36912200

H -9.09889000 5.00382800 2.06151000

H -9.02559700 2.18917400 1.70081200

H -8.90642400 -2.64631900 1.07212300

H -8.84100800 -5.45982200 0.70107400

C -1.53309400 -2.85252000 4.25411600

O -2.05664600 -2.20431000 3.06768500

C -1.19388300 -1.77586200 5.31074800

C -0.25264700 -0.56346200 4.96441600

C -2.29902900 -0.73843400 5.74820900

H -0.80499100 -2.30258900 6.19693300

C -1.16082500 0.33944500 5.87675900

H -0.33329300 -0.29085000 3.90505300

H 0.80533700 -0.66233800 5.23021800

H -2.97179700 -0.51306300 4.91024200

H -2.89298800 -0.96773700 6.64202900

H -1.38403400 1.35486700 5.52804500

H -0.77311200 0.39602600 6.90283600

C -2.58565100 -3.85163700 4.79706600

H -2.20352100 -4.35974700 5.69299300

H -3.50705600 -3.31744300 5.06289800

H -2.83168700 -4.61652800 4.05164900

C 2.92784500 -2.06758400 3.89713600

O 1.88476300 -2.09914400 2.98224200

C 3.40818100 -3.39981300 4.40536000

C 4.41946900 -3.47586800 5.61059300

C 2.41009300 -4.30779600 5.24843700

H 3.80039600 -4.01788600 3.57279800

C 3.62960200 -4.72502400 6.14898800

H 4.30829600 -2.61533400 6.28352400

H 5.48100600 -3.60401200 5.36560800

H 1.68574000 -3.68877200 5.79418600

H 1.87726800 -5.10016100 4.70906400

H 3.45980500 -4.78070500 7.23073000

H 4.07968800 -5.66757800 5.81194200

C 3.60786200 -0.73240400 4.06995700

H 4.38778200 -0.78236200 4.83822200

H 4.08628600 -0.38825500 3.13396000

H 2.88587100 0.04787700 4.35446600

Table S4, #4

H 5.99904100 -5.60951400 2.17194000

H 2.13178300 -5.76806100 2.30485200

H -1.72601900 -5.96225500 2.40408300

H -5.62436100 -6.07513100 2.52499900

H 5.73528400 2.06506400 3.22980700

H 1.86462700 1.94881800 3.37510300

H -2.06689800 1.80086700 3.46861100

H -5.89574100 1.60182100 3.56551400

H 5.01896000 -2.16112000 2.68632100

H -0.25699500 -3.35946600 3.65860900

H -5.74799700 -2.53644800 3.01721600

H 5.61248100 5.60729600 3.68951200

H 1.72633300 5.44717800 3.81620400

H -2.14815300 5.29076700 3.92524900

H -6.03245500 5.14591200 4.02411600

Si 5.91794000 -4.84782500 0.88788600

Si 2.06977700 -5.03649500 1.00218200

Si -1.79698800 -5.20176800 1.11920200

Si -5.67263300 -5.33332800 1.22958100

Si 5.64886900 2.80272500 1.93243500

Si 1.78338300 2.65509900 2.06191300

Si -2.09549700 2.50890100 2.15941000

Si -5.94901700 2.34172500 2.26889600

Si 5.76685900 -2.43000700 1.26521300

Si 2.09857800 -2.59214500 1.31027900

Si -1.90180300 -2.76614900 1.50658000

Si -5.75227600 -2.91008900 1.57244100

Si 5.56676700 5.23115900 2.24496500

Si 1.69774100 5.08400200 2.36684300

Si -2.17301900 4.93300900 2.47446800

Si -6.04141200 4.76910700 2.57912300

Si 7.80733700 -5.13585800 -0.53240400

Si 3.97179400 -5.33967600 -0.38043700

Si 0.11001900 -5.49709900 -0.25667600

Si -3.75566500 -5.64963300 -0.14631800

Si -7.60537600 -5.75574400 -0.09118600

Si 7.53173200 2.47356000 0.51191300

Si 3.68983000 2.27352800 0.67721400

Si -0.17120000 2.13027600 0.80138900

Si -4.03709700 1.97756200 0.89156100

Si -7.87517800 1.85656900 0.95655000

Si 7.65707300 -1.61725200 0.00964900

Si 3.87694600 -1.76720600 -0.00834800

Si 0.01004300 -1.89596100 0.33829100

Si -3.87622500 -2.06010200 0.36717300

Si -7.72266000 -2.23983700 0.40969900

Si 7.41007700 5.99827200 0.95477400

Si 3.56645100 5.87254600 1.12824000

Si -0.29893200 5.72155300 1.24269600

Si -4.16684300 5.56520100 1.34897700

Si -8.01010500 5.38214900 1.39728700

Si 7.67560100 -3.16973400 -1.77642900

Si 3.84533200 -3.38391900 -1.69062200

Si 0.00251900 -3.48439500 -1.47300400

Si -3.85834000 -3.65471600 -1.39887500

Si -7.69987000 -3.79556200 -1.35022200

Si 7.40122600 4.43442200 -0.77302600

Si 3.56958400 4.27310700 -0.60510500

Si -0.28658000 4.12329300 -0.48887000

Si -4.14580600 3.97138000 -0.38884200

Si -7.97643500 3.81799600 -0.33111500

Si 7.57825300 0.57902800 -0.93676000

Si 3.72132800 0.44062700 -0.87419000

Si -0.12959000 0.26784900 -0.70788000

Si -3.99506600 0.11958400 -0.62115700

Si -7.85397500 -0.03569500 -0.49852300

Si 5.72370600 -3.09894300 -3.03779100

Si 1.85900900 -3.26260700 -2.89963600

Si -1.96951500 -3.41554600 -2.76993900

Si -5.81658700 -3.55988700 -2.69360100

Si 5.43281000 4.54165500 -2.00359000

Si 1.59396700 4.39210100 -1.86471200

Si -2.25844300 4.23786800 -1.75475800

Si -6.09949800 4.08084300 -1.67488300

Si 5.61042500 0.70577000 -2.32040200

Si 1.73467200 0.54807700 -2.20698100

Si -2.10739300 0.38443500 -2.08456000

Si -5.97482000 0.23253100 -1.97944400

Si 5.49256400 2.76911400 -3.51865500

Si 1.62259800 2.62136700 -3.40257900

Si -2.23064800 2.46230700 -3.28879100

Si -6.09825900 2.30136200 -3.18390700

Si 5.62707800 -0.98566200 -4.01957900

Si 1.75904200 -1.14864100 -3.90671900

Si -2.09459500 -1.30655100 -3.79276400

Si -5.96244700 -1.45223200 -3.68567000

H 8.60648100 4.60190400 -1.60528200

H 8.72935200 0.75132400 -1.89003400

H 8.88236900 -3.03747300 -2.62808900

H 6.64904100 2.93300700 -4.40652200

H 6.78509400 -0.83432300 -4.91091700

H -7.31523600 2.37507700 -4.00597700

H -7.17918400 -1.39225500 -4.51037100

H -9.23595300 3.88902300 -1.09349700

H -9.06757700 0.04026400 -1.37955500

H -8.96006700 -3.75035200 -2.11630600

H -8.08243900 6.77861100 0.83901000

H -4.22700900 6.93267300 0.72845400

H -0.37182800 7.08672400 0.61790600

H 3.48335200 7.24073300 0.50729400

H 7.33878400 7.39475300 0.39667600

H -6.18600700 5.41354700 -2.30006700

H -2.33057600 5.56761000 -2.41062300

H 1.52524400 5.72166500 -2.52122100

H 5.38067600 5.87568300 -2.63184000

H -5.82134000 -4.68422500 -3.65202100

H -1.96590400 -4.53021300 -3.76258500

H 1.88991600 -4.37615700 -3.87318400

H 5.74534600 -4.22208800 -3.98379400

H -7.58639900 -6.95687200 -0.99998400

H -3.73096600 -6.80286000 -1.11054600

H 0.12421700 -6.64885700 -1.22110100

H 3.97939600 -6.49479700 -1.33170700

H 7.83482600 -6.34072900 -1.44231900

H -3.45980400 2.52909100 -4.11654200

H -4.91842600 2.47082700 -4.07474000

H 0.39667900 2.68313200 -4.22699100

H -1.06285800 2.62481900 -4.18512600

H 4.25223200 2.83723400 -4.33778600

H 2.79361200 2.77894000 -4.29591100

H -3.32375200 -1.23819300 -4.62092800

H -4.78237500 -1.29647600 -4.57912900

H 0.53272900 -1.08411700 -4.73137400

H -0.92680900 -1.14243100 -4.68950900

H 4.38828300 -0.93007100 -4.84217600

H 2.92966200 -0.98834400 -4.80029800

H 8.66169500 5.60044500 1.66798000

H 8.75959400 2.78789300 1.29688400

H 8.93407600 -2.04352200 0.65002300

H 9.03925800 -4.85438100 0.26822200

H -9.18317600 4.88747000 2.17983400

H -9.07763600 2.07522200 1.80851900

H -8.90315500 -2.75619300 1.16165800

H -8.80561100 -5.56735600 0.78007600

C -1.12162200 -2.87982000 4.15278900

O -2.02437200 -2.36395500 3.13809700

C -0.58685500 -1.71935500 5.02318100

C -0.05157700 -0.39497300 4.36526300

C -1.58616600 -0.83948900 5.86893900

H 0.18466800 -2.14109600 5.68700300

C -0.65136900 0.39292300 5.58622400

H -0.60563400 -0.17355900 3.44377300

H 1.02129600 -0.32228700 4.16872100

H -2.54943100 -0.73502000 5.35173900

H -1.76247500 -1.12435200 6.91387000

H -1.13162500 1.35810800 5.38695600

H 0.09235200 0.52668100 6.38380500

C -1.87257900 -3.93203500 5.00356800

H -1.21094200 -4.33405900 5.78345500

H -2.74337900 -3.47129500 5.48704700

H -2.22089300 -4.76552900 4.38287500

C 3.61707400 -2.21339900 3.64652000

O 2.43779700 -2.06783500 2.90673200

C 3.80679700 -3.61190200 4.21483300

C 5.04230600 -3.96397700 5.12548000

C 2.85419300 -4.12076900 5.38182800

H 3.75523700 -4.33674400 3.38973100

C 4.09255900 -4.87525100 5.98914800

H 5.39714700 -3.09828200 5.69872700

H 5.89869400 -4.43914800 4.63229600

H 2.52183800 -3.29404300 6.02365300

H 1.98319600 -4.71645900 5.08196400

H 4.21777500 -4.83698200 7.07767400

H 4.12851600 -5.92261500 5.66387200

C 3.88307100 -0.97684000 4.49483600

H 4.88152400 -1.01380800 4.94514600

H 3.81549100 -0.07675700 3.87134800

H 3.14063200 -0.87966300 5.30512500

Table S5, #5

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H -5.72165100 -5.95705100 2.46423100

H 5.79111000 1.96758700 3.29689900

H 1.86789900 1.93889100 3.37868900

H -1.99305600 1.82599500 3.40901000

H -5.85728700 1.72310800 3.45542000

H 5.91743100 -2.20041000 2.75946700

H -0.64730300 -3.35396700 4.01114500

H -5.77523100 -2.41244800 2.92634500

H 5.72655100 5.50985000 3.72648400

H 1.83022400 5.42633000 3.79417400

H -2.03944900 5.33521100 3.84826700

H -5.92899700 5.27245600 3.89049600

Si 5.87788900 -5.00360000 0.99849800

Si 2.00126800 -5.10405200 1.04942100

Si -1.85945300 -5.16100100 1.11821700

Si -5.73708000 -5.22547200 1.16189100

Si 5.73252500 2.69359700 1.99219900

Si 1.85097000 2.62869200 2.05594900

Si -2.01277400 2.53632400 2.09939600

Si -5.87517100 2.45573400 2.15358400

Si 5.84224700 -2.58128700 1.32078000

Si 1.95512300 -2.66676800 1.39518100

Si -1.93872900 -2.71054700 1.46561800

Si -5.77493400 -2.79841400 1.48438500

Si 5.69401500 5.12379200 2.28428900

Si 1.81656000 5.05675100 2.34634000

Si -2.05266300 4.96674700 2.40003700

Si -5.92433700 4.88673300 2.44787200

Si 7.77278400 -5.31310600 -0.40257400

Si 3.92662400 -5.43923300 -0.29159500

Si 0.05578200 -5.51326800 -0.24172400

Si -3.80535600 -5.58957300 -0.18092400

Si -7.65807000 -5.62033200 -0.18374700

Si 7.62702000 2.31062500 0.59840100

Si 3.77895000 2.19675900 0.71468300

Si -0.08518900 2.12264800 0.76134600

Si -3.95032400 2.04232700 0.80848700

Si -7.79146000 2.00235900 0.81532700

Si 7.70502000 -1.79351400 0.06907300

Si 3.86340800 -1.85113400 0.20344200

Si -0.01413600 -1.91920000 0.27694900

Si -3.87632000 -1.99663400 0.28667700

Si -7.71492700 -2.09871600 0.29389700

Si 7.57112800 5.84110900 1.01511800

Si 3.72242700 5.79419100 1.13358500

Si -0.14917200 5.71798900 1.18807400

Si -4.01617800 5.63782900 1.24104400

Si -7.86295000 5.53236100 1.23341300

Si 7.69584400 -3.36074900 -1.67538800

Si 3.85690700 -3.45180200 -1.55728100

Si -0.00175300 -3.52144500 -1.49320700

Si -3.85655600 -3.60688900 -1.45656000

Si -7.69600000 -3.66643700 -1.45516900

Si 7.55664000 4.26522100 -0.70291100

Si 3.71979700 4.18390200 -0.58975100

Si -0.14058900 4.11058200 -0.53578000

Si -4.00091600 4.03150200 -0.48565500

Si -7.83515400 3.95734500 -0.48518800

Si 7.65984700 0.40955700 -0.84618100

Si 3.79786500 0.33004200 -0.79658000

Si -0.06103200 0.25298100 -0.73870300

Si -3.92831100 0.18108300 -0.70142400

Si -7.78722600 0.10165700 -0.62858200

Si 5.74681800 -3.24511700 -2.93625700

Si 1.90405800 -3.33200900 -2.85422100

Si -1.94788600 -3.40821400 -2.80312400

Si -5.79197800 -3.47650000 -2.77484500

Si 5.60870100 4.40488300 -1.96258500

Si 1.76671800 4.33251400 -1.88102200

Si -2.09111400 4.25580100 -1.82780500

Si -5.93326700 4.17464800 -1.80191600

Si 5.70603300 0.55636800 -2.24362700

Si 1.84308600 0.47862900 -2.19101800

Si -2.01477000 0.40269100 -2.13894200

Si -5.88406600 0.32557300 -2.08589200

Si 5.65376900 2.61902600 -3.46398000

Si 1.78430300 2.54940900 -3.40538000

Si -2.07565100 2.47284200 -3.35163400

Si -5.94635400 2.38766600 -3.30167400

Si 5.72182700 -1.13887200 -3.94170400

Si 1.85280800 -1.22520600 -3.88535800

Si -2.00717600 -1.30147600 -3.83174800

Si -5.87756200 -1.37159400 -3.77920000

H 8.77698300 4.40531000 -1.51874800

H 8.82753300 0.55137400 -1.77907500

H 8.91609300 -3.24417700 -2.49256400

H 6.82807700 2.75822700 -4.33878800

H 6.89667900 -1.01408900 -4.81902100

H -7.14889700 2.47892800 -4.14145200

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H -9.08167600 4.04844100 -1.26661000

H -8.98557800 0.19541800 -1.52758000

H -8.94256500 -3.60104500 -2.24042600

H -7.89947400 6.92650100 0.66576500

H -4.04053800 7.00363400 0.61131400

H -0.18185100 7.08076300 0.55686700

H 3.67683400 7.15784800 0.50235600

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H -2.12575700 5.58205700 -2.49132900

H 1.73356900 5.65917700 -2.54581700

H 5.59250600 5.73626700 -2.60033100

H -5.80081900 -4.60621500 -3.72407300

H -1.94187800 -4.52913100 -3.77853200

H 1.91744700 -4.45200900 -3.83302000

H 5.77638400 -4.37486800 -3.88752600

H -7.64935600 -6.82716200 -1.08514100

H -3.79041900 -6.75007800 -1.13959800

H 0.06826900 -6.67299700 -1.19405200

H 3.92695400 -6.59586000 -1.24855600

H 7.78589000 -6.51872000 -1.30306300

H -3.28996000 2.55601400 -4.19591200

H -4.74990800 2.52685400 -4.17533600

H 0.57002600 2.63310800 -4.25024000

H -0.89083800 2.60391700 -4.22961600

H 4.42908800 2.71027800 -4.30493000

H 2.96914100 2.68108800 -4.28428100

H -3.22135900 -1.21625700 -4.67613800

H -4.68130700 -1.24543600 -4.65556600

H 0.63862700 -1.13912800 -4.73046400

H -0.82223900 -1.16831900 -4.70983800

H 4.49768900 -1.06201300 -4.78516000

H 3.03774100 -1.09118200 -4.76450800

H 8.80400900 5.42269000 1.74906200

H 8.85147200 2.60652100 1.39594800

H 8.93945200 -2.23128800 0.78007100

H 8.99438700 -5.04597200 0.41635200

H -9.05708800 5.06577600 2.00123500

H -9.00197600 2.24975800 1.64801300

H -8.91399800 -2.58805100 1.03213600

H -8.86670800 -5.40288800 0.66852400

C -1.57878200 -2.81382500 4.25492100

O -2.08461300 -2.18117000 3.05401500

C -1.24668500 -1.72179700 5.29802100

C -0.27450000 -0.53420200 4.94980400

C -2.33992100 -0.65439900 5.69096700

H -0.89171900 -2.23639900 6.20518700

C -1.18092800 0.39943200 5.83228000

H -0.33337000 -0.27805100 3.88472000

H 0.77702700 -0.64499800 5.23566900

H -2.98563700 -0.42746600 4.83239600

H -2.96072800 -0.85738200 6.57266400

H -1.37295500 1.41616300 5.46977200

H -0.81284100 0.45654200 6.86549700

C -2.64157600 -3.80152700 4.79864300

H -2.27626100 -4.29208900 5.71121100

H -3.56731700 -3.26196300 5.03709100

H -2.87419800 -4.58073500 4.06359800

C 3.04583300 -2.04909400 3.82863100

O 1.90569900 -2.23161800 3.04600500

C 3.60513800 -0.64205000 3.80982100

H 4.52436800 -0.57731300 4.40319500

H 3.83315000 -0.31056300 2.78594600

H 2.87320000 0.07000500 4.22066900

C 3.41415300 -3.00457200 4.78753500

C 2.91409900 -4.46625200 4.85523000

C 2.69643800 -4.54436600 6.39715000

C 2.39934900 -3.05213700 6.62315900

H 4.39845500 -2.83256600 5.22938800

H 1.95299900 -4.55005200 4.33444300

H 3.62561100 -4.83346600 6.90717800

H 1.90517300 -5.23728400 6.71941900

H 2.89728900 -2.50055800 7.42237800

H 1.39040000 -2.70926500 6.39122900

H 3.60626900 -5.20391700 4.42173400

Structures used for CBS-QB3 calculations (Cartesian corrdinates in Å) – see Table S2

Table S2, #1

Si 1.83875395 -2.65946610 1.62525328

C 3.00871354 -2.05242544 3.98791675

O 1.81796533 -2.21848529 3.27719308

C 3.55011587 -0.63889812 4.01393324

H 4.54635062 -0.61317888 4.47267224

H 3.62620200 -0.21705157 3.00172884

H 2.89261738 0.03530412 4.59116384

C 3.25451747 -2.97041478 5.15647078

C 2.72232180 -4.45197013 5.17380238

C 2.45342915 -4.30717005 6.71540835

C 2.47920987 -2.74713255 6.54246805

H 4.33458618 -2.95864065 5.37073946

H 1.78161046 -4.53545549 4.61745711

H 3.30233434 -4.66307192 7.31346622

H 1.53207269 -4.75443991 7.10820192

H 2.98870008 -2.14828521 7.30744563

H 1.47598385 -2.34123847 6.36867116

H 3.41039734 -5.23806705 4.83805577

H 0.62281539 -2.20009323 0.93868939

H 1.86419222 -4.11560371 1.42546299

H 3.01245094 -2.16264876 0.89278626

Table S2, #2

Si 1.95946779 -2.63059937 1.40380093

C 2.76687294 -1.98463613 4.02667809

O 1.81535151 -2.18451920 3.04044635

C 3.52465710 -0.67574240 3.95239882

H 4.32633873 -0.64788132 4.69939623

H 3.97682725 -0.51579630 2.96212102

H 2.84746021 0.17170500 4.13480253

C 2.96386786 -2.95586825 5.01909184

C 4.15755720 -4.63653424 4.62912829

C 3.06538820 -5.25092281 5.52076041

C 1.99954415 -4.12973912 5.32249670

H 3.54285369 -2.60477810 5.87644171

H 4.06901935 -4.81495100 3.55773752

H 3.39837247 -5.29376497 6.56690388

H 2.73583830 -6.25932618 5.23008846

H 1.32723387 -3.94213551 6.17408603

H 1.38283457 -4.33903216 4.44038327

H 5.18393294 -4.54233256 4.98777911

H 1.99968433 -4.08606666 1.20156935

H 0.74571103 -2.18244313 0.70605419

H 3.13680647 -2.12878010 0.68064739

Table S2, #3

H 5.80643418 -5.73905442 2.53998754

H 5.81718766 -2.20772069 2.99524224

Si 5.75498217 -5.00726074 1.23867473

Si 5.72225554 -2.58502736 1.55685188

Si 1.83875395 -2.65946610 1.62525328

Si 7.58758178 -1.80243950 0.30385810

Si 3.74777117 -1.85139310 0.43389625

H 8.82129926 -2.23919292 1.01685179

C 3.00871354 -2.05242544 3.98791675

O 1.81796533 -2.21848529 3.27719308

C 3.55011587 -0.63889812 4.01393324

H 4.54635062 -0.61317888 4.47267224

H 3.62620200 -0.21705157 3.00172884

H 2.89261738 0.03530412 4.59116384

C 3.25451747 -2.97041478 5.15647078

H 4.33458618 -2.95864065 5.37073946

H 2.89281019 -3.97735524 5.16825022

H 2.73723596 -2.82144195 6.08120152

H 6.92753728 -5.20195714 0.37374246

H 4.54970961 -5.27553954 0.44102534

H 3.74296948 -2.84316110 -0.65112595

H 7.58153417 -2.78687222 -0.78781752

H 7.56251615 -0.44625459 -0.26274072

H 3.70967281 -0.51691676 -0.18142596

H 1.86419222 -4.11560371 1.42546299

H 0.62281539 -2.20009323 0.93868939

Table S2, #4

H 6.01452461 -5.68995502 2.19958201

H 5.07349818 -2.22754052 2.69225039

Si 5.95624696 -4.93181029 0.91219609

Si 5.83230801 -2.51094882 1.27977392

Si 2.16198263 -2.62607263 1.28791444

Si 7.74544580 -1.72681491 0.04084049

Si 3.96408732 -1.82854941 -0.01526167

H 9.01030711 -2.16710346 0.69566464

C 3.66136350 -2.25853858 3.63824974

O 2.49163275 -2.10052895 2.88596583

C 3.82737456 -3.65734405 4.21320114

H 3.77493138 -4.38436401 3.39007399

C 3.93453075 -1.02250280 4.48504917

H 4.92779662 -1.07063409 4.94565779

H 3.88482629 -0.12382731 3.85786087

H 3.18519424 -0.91300572 5.28737823

H 7.12913544 -5.12758556 0.04795963

H 7.75588948 -2.69510762 -1.06514330

H 4.75565804 -5.22365799 0.11575955

H 7.72022048 -0.37909573 -0.54560363

H 3.94191205 -2.85042602 -1.07175420

H 3.89078000 -0.46373410 -0.55637646

H 0.89788345 -2.18665103 0.67975169

H 2.12799780 -4.08473203 1.10886755

H 3.17404997 -3.98880075 4.99307513

H 4.65742054 -3.90509931 4.84132612

Example of optimized structure used to obtain vibration data: Addition product of CBMK on silicon. The P atoms in the cluster represent the quantum capping potentials.

H -2.972359174424 2.569208975455 -1.026722467290

C -0.364584919529 4.097515784161 -1.826702806641

Si 1.339144426199 2.228520393016 -0.831717389449

Si -2.506485600648 1.241668995360 -0.530285581467

Si 1.690220436461 0.542503655128 -2.554385153173

Si -2.164359498919 -0.390557248868 -2.291830055108

Si 3.376909914876 2.284569657425 0.413745118393

Si -0.375992309996 1.272648053555 0.546296838326

Si -4.068863101393 0.222408068396 0.974828646197

Si 3.876576375386 -0.338726920163 -2.143127881170

Si 0.091274856676 -1.123208761581 -1.958262301582

Si -3.586551239090 -2.229344183125 -1.716726998170

Si 4.064401151693 -0.001842857343 0.215955561876

Si 0.236606235790 -1.052670015623 0.438783744495

Si -3.586632832098 -2.098303312036 0.672155682916

Si 2.444880624017 -1.419065112931 1.269822466379

Si -1.362377389018 -2.497405840886 1.470400962929

P -0.433463045109 2.166961177141 2.747631042047

P 3.029147157828 2.970625958727 2.655488695282

P -3.736219399056 0.953048020307 3.205444876785

P -6.304235968123 0.715211458417 0.354628044770

P -1.269146671756 -2.185001762158 3.820553068493

P -5.123407774770 -3.563989716713 1.713666435614

P 2.423131533323 -1.057475977765 3.615103689508

P 3.026556106371 -3.690727248567 0.911594814254

P -0.720654626680 -4.739366480039 1.030053232464

P -2.740047099795 -4.283334577136 -2.543091029501

P 0.521648803135 -3.248287002555 -2.933579020075

P 4.036474665248 -2.621140640729 -2.768744723041

P -5.777284121420 -1.924018782106 -2.570534350598

P 4.945927650069 3.740606630473 -0.602998548612

P 5.527543703649 0.884226220423 -3.325607973556

P 6.219506439849 -0.418337515645 1.098498977840

H 1.510376015274 1.072787035805 -3.940222142150

H -2.409214852619 0.152742560371 -3.662672645061

O 0.929707683430 3.769733913399 -1.429592584498

C -0.947409249879 5.301095159139 -1.141782939383

C -0.848826696769 5.439173955418 0.430764910908

C -0.194096823457 6.710366069268 -1.242315174840

H -1.990381403793 5.420914386570 -1.468473656591

C -0.580316597569 6.977900920798 0.256005330444

H 0.037460478365 4.918544744526 0.813185852468

H -1.727816590944 5.129703964269 1.010204217604

H 0.885641755423 6.559194410884 -1.365033420782

H -0.555816844180 7.414040788438 -2.002620343555

H 0.186358542195 7.428764480798 0.898005066155

H -1.503218574317 7.566885522028 0.340324888049

C -0.743934014705 3.708663170386 -3.240978266966

H -1.802404598551 3.927584826661 -3.428609268657

H -0.142272713057 4.260386442767 -3.987268178738

H -0.577398743594 2.638094986459 -3.427888453542

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