

Supporting Information

Mechanistic insights into the C-H activation of methane mediated by the unsupported and silica-supported/ VO₂OH and CrOOH: A DFT Study

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1. The symmetry-adapted perturbation theory (SAPT) energy decomposition analyses

Table S1 The SAPT energy decomposition analyses of the complexes (**EC-i** ~ **EC-iv**) of methane molecule with unsupported/ silica-supported VO₂OH and CrOOH clusters in the reactions Rxn.i ~ Rxn.iv.

complexes	E_{tot} kcal/mol	E_{els} kcal/mol	E_{exc} kcal/mol	E_{ind} kcal/mol	E_{dis} kcal/mol
¹ EC-i	-9.78	-16.68	25.16	-18.26	-8.84
¹ EC-ii	-11.13	-18.16	27.57	-20.54	-10.01
⁴ EC-iii	-7.60	-4.44	4.25	-2.64	-4.76
⁴ EC-iv	-10.12	-8.11	11.65	-3.47	-10.18

2. Hirshfeld Spin Density and Charge Population Analyses

Table S2 Hirshfeld Spin Density and Charge Evolution along the Reaction Coordinates in the PCET and HAT Pathways of C-H Bond Activation of CH₄ on an Unsupported/ Silica-Supported VO₃H Cluster.

CH ₄ +VO ₂ OH		¹ EC-i	¹ TS _{HAT} -i	³ TS _{HAT} -i	¹ P _{HAT} -i	¹ TS _{PCET} -i	¹ P _{PCET} -i
spin density	V	0.00	0.85	1.04	1.07	0.00	0.00
	O _t	0.00	-0.25	0.56	0.02	0.00	0.00
	C	0.00	-0.39	0.30	0.77	0.00	0.00
	H _{tr}	0.00	-0.05	0.05	0.04	0.00	0.00
charge	V	0.58	0.63	0.58	0.60	0.59	0.59
	O _t	-0.32	-0.31	-0.25	-0.33	-0.29	-0.31
	C	-0.09	-0.08	-0.08	-0.08	-0.17	-0.21
	H _{tr}	0.07	0.08	0.05	0.14	0.10	0.18
CH ₄ +VO ₃ @Sili		¹ EC-ii	¹ TS _{HAT} -ii	³ TS _{HAT} -ii	¹ P _{HAT} -ii	¹ TS _{PCET} -ii	¹ P _{PCET} -ii
spin density	V	0.00	0.89	1.04	1.08	0.00	0.00
	O _t	0.00	-0.29	0.58	0.03	0.00	0.00
	C	0.00	-0.40	0.28	0.76	0.00	0.00
	H _{tr}	0.00	-0.05	0.05	0.04	0.00	0.00
charge	V	0.59	0.74	0.62	0.64	0.60	0.60
	O _t	-0.30	-0.27	-0.24	-0.33	-0.28	-0.30
	C	-0.09	-0.14	-0.08	-0.08	-0.16	-0.20
	H _{tr}	0.07	0.06	0.05	0.14	0.11	0.19

V, the metal center; C, the Methane carbon atom; O_t, the terminal oxygen atom abstracting hydrogen atom; H_{tr}, the transferring hydrogen.

Table S3 Hirshfeld Spin density and Charge Evolution along the Reaction Coordinates in the PCET and HAT Pathways of C-H Bond Activation of CH₄ on an Unsupported/ Silica-Supported CrOOH Cluster.

CH ₄ +CrOOH		⁴ EC-iii	⁴ TS _{HAT} -iii	⁶ TS _{HAT} -iii	⁴ P _{HAT} -iii	⁴ TS _{PCET} -iii	⁴ P _{PCET} -iii
spin density	Cr	3.18	3.82	3.98	3.94	2.99	3.01
	O _t	-0.21	-0.28	0.63	-0.03	-0.04	0.00
	C	0.01	-0.45	0.27	-0.76	-0.01	-0.05
	H _{tr}	0.00	-0.03	0.04	-0.02	0.02	0.01
charge	Cr	0.56	0.52	0.52	0.52	0.60	0.61
	O _t	-0.36	-0.36	-0.33	-0.41	-0.38	-0.37
	C	-0.15	-0.11	-0.11	-0.08	-0.19	-0.26
	H _{tr}	0.04	0.06	0.03	0.10	0.07	0.15
CH ₄ +CrO ₂ @Sili		⁴ EC-iv	⁴ TS _{HAT} -iv	⁶ TS _{HAT} -iv	⁴ P _{HAT} -iv	⁴ TS _{PCET} -iv	⁴ P _{PCET} -iv
spin density	Cr	3.21	3.82	3.94	3.90	3.01	3.00
	O _t	-0.25	-0.30	0.65	-0.01	0.03	0.00
	C	0.01	-0.45	0.25	-0.78	-0.02	-0.06
	H _{tr}	0.00	-0.03	0.05	-0.01	0.02	0.01
charge	Cr	0.62	0.59	0.59	0.60	0.65	0.65
	O _t	-0.32	-0.34	-0.31	-0.39	-0.36	-0.35
	C	-0.15	-0.10	-0.11	-0.10	-0.18	-0.24
	H _{tr}	0.04	0.07	0.03	0.13	0.07	0.16

Cr, the metal center; C, the Methane carbon atom; O_t, the terminal oxygen atom abstracting hydrogen atom; H_{tr}, the transferring hydrogen.

3. Schematic illustration of the mixed basis sets used in the $\text{Si}_{16}\text{O}_{30}\text{H}_3$ supported system

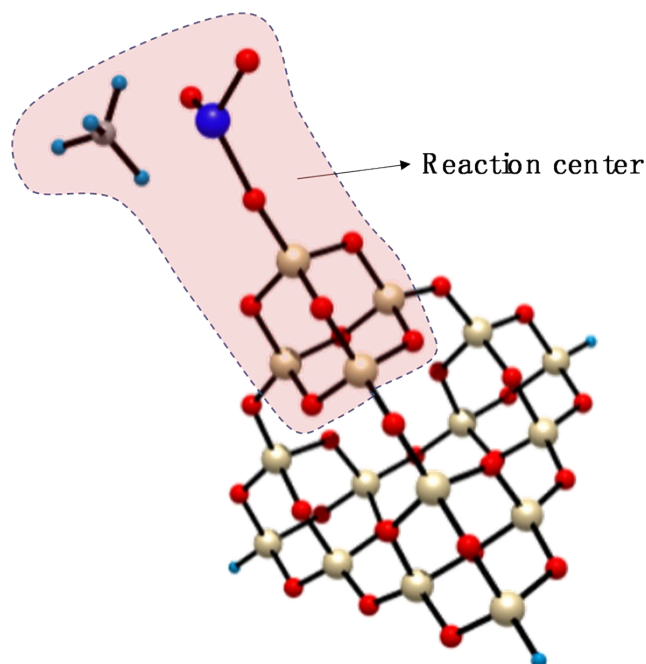


Figure S1. Schematic illustration of the mixed basis sets used in the $\text{Si}_{16}\text{O}_{30}\text{H}_3$ supported system in Rxn.v. The energy-consistent scalar-relativistic DF-adjusted 10-electron-core pseudopotential/ECP10MDF(8s7p6d1f/6s5p3d1f) basis set was used for V, and the def-TZVP basis set was applied for the C, H, O and Si atoms in the reaction center, while the smaller def-SV basis set was applied for all other atoms away from the reaction center (BSI), for the geometry optimization and frequency calculations. Then, the electronic energies were refined with the B3LYP-D3 functional and a larger mixed basis set (BSII), in which the DF-adjusted 10-electron-core pseudopotential/ECP10MDF(8s7p6d2f1g)/[6s5p3d2f1g] was used for V, and the ma-def2-TZVPP basis set was used for the other atoms in the reaction center, while the def-SV basis set was used for that away from the reaction center.

4. Cartesian Coordinates of All Optimized Structures

CH₄

5

C	2.139676000	-0.589399000	-0.689358000
H	3.103244000	-0.461090000	-0.196084000
H	2.283814000	-1.116609000	-1.632418000
H	1.697320000	0.387676000	-0.882622000
H	1.477306000	-1.169032000	-0.046561000

No imaginary frequency

G(298.15 K) = -40.51432 a.u.

VO₃H

5

V	0.498331000	-0.220772000	-0.021694000
O	-0.237378000	0.726300000	-1.342921000
O	-0.114978000	-1.649483000	0.291901000
O	0.845379000	0.585096000	1.300930000
H	-0.902442000	0.408341000	-1.965177000

No imaginary frequency

G(298.15 K) = -298.16322 a.u.

VO₃@Sili

17

Si	0.809971000	-3.370670000	-0.687890000
H	1.592118000	-4.600627000	-0.723471000
O	1.516420000	-2.086915000	0.217997000
O	-0.759861000	-3.515664000	-0.001567000
O	0.511579000	-2.644125000	-2.218112000
Si	0.715918000	-0.585851000	0.356470000
O	-0.834630000	-0.993768000	0.945871000
O	0.437069000	-0.123378000	-1.267140000
Si	-0.392715000	-1.186285000	-2.339828000
H	-0.571500000	-0.675350000	-3.693794000
O	-1.844219000	-1.544091000	-1.491058000
Si	-1.802395000	-2.152964000	0.116806000
H	-3.103789000	-2.412626000	0.720441000
V	1.653072000	2.061239000	2.183641000
O	1.503297000	0.543164000	1.245366000
O	0.484461000	3.121374000	2.085818000
O	2.182590000	1.951525000	3.670331000

No imaginary frequency

G(298.15 K) = -1909.62198 a.u.

VO₃@Sili2

53

Si	-2.35635200	0.04325200	1.42092000
O	-4.00229500	0.14410100	1.22469200
O	-1.88095700	-1.24048500	0.48303600
O	-1.74504600	1.40682800	0.69933200
Si	-4.52363500	0.30229300	-0.36324400
O	-3.89790300	-1.01204100	-1.20517900
O	-3.76047700	1.66201200	-0.98613400
Si	-2.10223600	1.64236800	-0.90332800
O	-1.64087900	0.26190800	-1.70024700
Si	-2.24685500	-1.17523300	-1.13372100
Si	-0.09911800	-0.22969800	3.33431600
O	0.45163800	-0.38853100	4.94001700
O	0.77095900	1.11761700	2.77428500
O	0.63167400	-1.55159100	2.55690500
Si	2.15272600	-0.50169000	5.25530700
O	2.81024700	0.89888400	4.46887600
O	2.67006100	-1.81667300	4.24768400
Si	2.31539300	-1.78381500	2.58261200
O	2.94623300	-0.28475100	2.08837000
Si	2.46890700	1.17160500	2.82350400
H	2.50714200	-0.63512000	6.66042000
O	-1.71016200	-0.11255800	2.92071200
O	-1.23198900	2.91233600	-1.47039100
O	3.03255200	2.48001500	1.95870300
O	2.75022700	-2.98311200	1.51035100
O	-1.50599800	-2.41751300	-1.90880300
Si	0.12543500	-2.75862100	-1.96592600
O	0.75887100	-2.95979700	-0.40283800
O	0.99755700	-1.44881600	-2.60602600
O	0.77884600	-4.08851800	-2.80947500
Si	2.43164900	-3.07192300	-0.12261100
O	3.07481900	-1.72591800	-0.93735400
O	2.89769200	-4.37476400	-1.11522000
Si	2.49339700	-4.34777000	-2.80255000
O	3.14048200	-2.83532300	-3.35574900
Si	2.69581900	-1.39655900	-2.56100100
Si	2.94930000	4.54530400	-2.07481500
O	1.21751500	4.46443700	-2.10771500
O	3.34133200	4.25962400	-0.40853700
O	3.44251400	3.08356800	-2.87020500
Si	0.42598200	3.08985700	-1.48236300
O	1.06491000	2.97335700	0.08688700

O	1.16430100	1.81667800	-2.33031300
Si	2.84870200	1.58822700	-2.31286000
O	3.24945500	1.61253000	-0.66116600
Si	2.73841500	2.86750600	0.36512700
O	3.23873700	0.11823000	-2.99398100
H	3.51622500	5.76376700	-2.63307200
H	2.93887700	-5.51093700	-3.55509400
V	-7.86871000	0.01048400	-0.21244000
O	-6.13198200	0.39329800	-0.48301500
O	-8.74841400	1.10728500	0.50917400
O	-8.22792900	-1.42860100	0.33116400

No imaginary frequency

G(298.15 K) = -7187.565240 a.u.

CrO₂H

4

Cr	-4.089916000	1.042072000	-0.212874000
O	-2.575625000	0.648514000	0.092937000
O	-5.786236000	0.635268000	0.103007000
H	-6.366214000	0.032432000	0.572680000

No imaginary frequency

G(298.15 K) = -238.1602220 a.u.

CrO₂@Sili

16

Si	-2.190710000	1.488863000	0.019504000
H	-2.912963000	2.757763000	0.035549000
O	-2.533373000	0.520382000	1.343822000
O	-0.526801000	1.680040000	0.018546000
O	-2.538320000	0.551645000	-1.325878000
Si	-1.747561000	-0.958848000	1.416632000
H	-2.098390000	-1.736909000	2.601235000
O	-0.113038000	-0.604514000	1.322540000
O	-2.123302000	-1.738646000	-0.018722000
Si	-1.752776000	-0.925275000	-1.436685000
H	-2.108005000	-1.675483000	-2.637843000
O	-0.117870000	-0.573345000	-1.340283000
Si	0.394684000	0.285880000	0.000464000
Cr	3.755371000	0.249718000	-0.000508000
O	4.862054000	-0.893593000	0.000975000
O	1.983090000	0.582118000	0.000805000

No imaginary frequency

G(298.15 K) = -1890.1501494 a.u.

¹EC-i

10

V	0.539939000	-0.225256000	-0.036921000
O	-0.227105000	0.731492000	-1.338960000
O	-0.141154000	-1.630796000	0.265575000
O	0.824160000	0.593994000	1.299946000
H	2.649132000	-0.214998000	-0.054742000
H	-0.906928000	0.380048000	-1.926601000
C	2.738816000	-0.790017000	-0.995625000
H	1.890618000	-1.428547000	-1.283624000
H	3.554462000	-1.482251000	-0.802173000
H	2.975143000	-0.105531000	-1.804745000

No imaginary frequency

G(298.15 K) = -338.68310 a.u.

¹TS_{HAT-i}

10

V	-0.677181000	-0.440517000	0.604143000
O	-1.402990000	0.536102000	-0.710357000
O	-1.547049000	-1.548281000	1.324563000
O	1.003377000	-0.717476000	0.623084000
H	1.989351000	-1.127839000	0.093213000
H	-2.304686000	0.519153000	-1.047962000
C	3.050005000	-1.603818000	-0.556100000
H	2.983111000	-2.673775000	-0.384170000
H	3.879752000	-1.111334000	-0.057773000
H	2.885033000	-1.293433000	-1.583272000

One and only one imaginary frequency: -2024.5411 cm⁻¹

G(298.15 K) = -338.62437 a.u.

³TS_{HAT-i}

10

V	-0.297922000	-0.106068000	0.611961000
O	-0.944065000	-1.198495000	-0.644819000
O	-1.250743000	0.794776000	1.490400000
O	1.451144000	0.045449000	0.953599000
H	2.152310000	-0.775905000	0.134383000
H	-1.832061000	-1.398633000	-0.956917000
C	2.567489000	-1.567988000	-0.679912000
H	3.225645000	-0.980391000	-1.315038000
H	1.697850000	-1.958942000	-1.201405000
H	3.089076000	-2.315021000	-0.086882000

One and only one imaginary frequency: -697.6984 cm⁻¹

G(298.15 K) = -338.61753 a.u.

¹TS_{PCET-i}

10

V	-0.677181000	-0.440517000	0.604143000
O	-1.402990000	0.536102000	-0.710357000
O	-1.547049000	-1.548281000	1.324563000
O	1.003377000	-0.717476000	0.623084000
H	1.989351000	-1.127839000	0.093213000
H	-2.304686000	0.519153000	-1.047962000
C	3.050005000	-1.603818000	-0.556100000
H	2.983111000	-2.673775000	-0.384170000
H	3.879752000	-1.111334000	-0.057773000
H	2.885033000	-1.293433000	-1.583272000

One and only one imaginary frequency: -2024.5541 cm⁻¹

G(298.15 K) = -338.65123 a.u.

¹P_{HAT-i}

10

V	-0.241835000	0.231601000	-0.350760000
O	-1.779891000	1.127221000	-0.262134000
O	-0.232995000	-1.343518000	-0.217870000
O	1.318401000	1.038701000	-0.610754000
H	2.175480000	0.586509000	-0.678964000
H	-2.689110000	0.835296000	-0.140759000
C	3.342531000	-1.391639000	-0.680897000
H	2.363918000	-1.819330000	-0.511198000
H	3.991341000	-1.179980000	0.156893000
H	3.731552000	-1.318205000	-1.686357000

No imaginary frequency

G(298.15 K) = -338.64456 a.u.

¹P_{PCET-i}

10

V	-0.068796000	-0.017361000	0.039003000
O	-1.047117000	-1.117979000	-0.944925000
O	-0.102657000	-0.439311000	1.547872000
O	-0.353106000	1.700086000	-0.219419000
H	-0.523928000	2.364548000	0.458035000
C	1.846765000	-0.340883000	-0.517668000
H	2.503239000	0.268088000	0.106943000
H	2.081874000	-1.397868000	-0.383217000
H	1.951526000	-0.054701000	-1.567357000
H	-1.338359000	-0.879148000	-1.834342000

No imaginary frequency
G(298.15 K) =-338.64456 a.u.

¹EC-ii

22

Si	0.728649000	-3.325677000	-0.731913000
H	1.466740000	-4.576315000	-0.879474000
O	1.467807000	-2.245674000	0.315245000
O	-0.824855000	-3.537741000	-0.142462000
O	0.550969000	-2.492645000	-2.177253000
Si	0.701027000	-0.785364000	0.557438000
O	-0.842170000	-1.157853000	1.062723000
O	0.530481000	-0.110224000	-0.975737000
Si	-0.281752000	-1.040539000	-2.112684000
H	-0.388988000	-0.381423000	-3.411680000
O	-1.766364000	-1.396989000	-1.427675000
Si	-1.748349000	-2.154760000	0.068323000
H	-3.083757000	-2.428586000	0.589337000
V	1.552437000	2.003931000	1.875822000
O	1.511330000	0.228913000	1.523098000
O	0.158377000	2.756120000	1.816027000
O	2.365803000	2.429815000	3.170746000
H	2.792689000	3.320140000	0.914976000
C	2.668636000	2.904698000	-0.106262000
H	1.881608000	2.159226000	-0.290030000
H	3.624235000	2.470510000	-0.386278000
H	2.413279000	3.764371000	-0.719709000

No imaginary frequency
G(298.15 K) =-1950.17649 a.u.

¹TS_{HAT}-ii

22

Si	4.438638000	-3.658580000	-1.213073000
H	5.837971000	-3.974175000	-0.937636000
O	4.002137000	-2.132514000	-0.670228000
O	3.367851000	-4.719208000	-0.482444000
O	4.064512000	-3.683773000	-2.844545000
Si	2.409205000	-1.665349000	-0.934066000
O	1.476056000	-2.857323000	-0.225973000
O	2.171851000	-1.823683000	-2.578448000
Si	2.479008000	-3.322221000	-3.257510000
H	2.237974000	-3.363314000	-4.696567000
O	1.534630000	-4.409030000	-2.398880000
Si	1.734631000	-4.431231000	-0.735659000

H	0.872885000	-5.400493000	-0.065209000
V	2.544918000	1.370523000	0.442138000
O	2.094227000	-0.191649000	-0.358802000
O	2.270660000	2.728899000	-0.310559000
O	3.972024000	1.362472000	1.378608000
H	4.995153000	0.714936000	1.417400000
C	6.048314000	-0.068411000	1.330574000
H	5.684418000	-0.861946000	0.684340000
H	6.231027000	-0.354802000	2.362146000
H	6.803105000	0.579137000	0.894752000

One and only one imaginary frequency: -1853.9755 cm⁻¹

G(298.15 K) = -1950.10137 a.u.

³TS_{HAT-ii}

22

Si	4.478294000	-4.140589000	-2.277830000
H	5.818624000	-4.657160000	-2.540699000
O	4.492740000	-2.590067000	-1.636846000
O	3.616140000	-5.069449000	-1.183006000
O	3.523683000	-4.051386000	-3.650506000
Si	2.999258000	-1.903905000	-1.298272000
O	2.240074000	-2.975602000	-0.268935000
O	2.147437000	-1.960099000	-2.731583000
Si	1.965785000	-3.463379000	-3.448926000
H	1.204126000	-3.418222000	-4.693141000
O	1.266061000	-4.438025000	-2.279234000
Si	2.065093000	-4.551696000	-0.810800000
H	1.386697000	-5.416169000	0.149939000
23	3.495057000	1.223795000	-0.025133000
O	3.150865000	-0.416980000	-0.688452000
O	2.340657000	2.246402000	0.290316000
O	5.130408000	1.834312000	0.326709000
H	6.064453000	0.851717000	0.003040000
C	6.748556000	-0.074885000	-0.319691000
H	6.104397000	-0.830576000	-0.761968000
H	7.214670000	-0.398244000	0.608046000
H	7.453771000	0.356242000	-1.026474000

One and only one imaginary frequency: -519.0928 cm⁻¹

G(298.15 K) = -1950.10137 a.u.

¹TS_{PCET-ii}

22

Si	2.726231000	-7.381969000	-1.359870000
H	4.057212000	-7.948396000	-1.163286000

O	2.430040000	-6.050368000	-0.384849000
O	1.491925000	-8.465992000	-1.025928000
O	2.455109000	-6.859992000	-2.928804000
Si	0.934622000	-5.328043000	-0.540794000
O	-0.181113000	-6.537790000	-0.251386000
O	0.778172000	-4.935282000	-2.154539000
Si	0.954189000	-6.187797000	-3.254007000
H	0.803525000	-5.759367000	-4.641155000
O	-0.165273000	-7.347753000	-2.795340000
Si	-0.075611000	-7.903814000	-1.217603000
H	-1.087743000	-8.907360000	-0.901616000
23	-0.219521000	-2.665059000	1.020157000
O	0.751067000	-4.049770000	0.442478000
O	-1.689410000	-2.585983000	0.462106000
O	0.498768000	-1.168409000	1.126041000
H	0.214598000	-1.588669000	2.313212000
C	-0.321275000	-2.604833000	3.197676000
H	-1.390760000	-2.684116000	3.380313000
H	0.188672000	-3.552601000	3.383364000
H	0.086750000	-1.879141000	3.908416000

One and only one imaginary frequency: -1501.9830 cm⁻¹

G(298.15 K) = -1950.14373 a.u.

¹P_{HAT-ii}

22

Si	1.264927000	-2.202770000	-1.001265000
H	2.621278000	-2.683759000	-1.248726000
O	1.233419000	-0.667909000	-0.322700000
O	0.401100000	-3.175526000	0.053187000
O	0.336334000	-2.099102000	-2.390567000
Si	-0.280642000	-0.020431000	0.002427000
O	-1.036406000	-1.133661000	0.989496000
O	-1.101373000	-0.059792000	-1.449724000
Si	-1.237338000	-1.548060000	-2.206545000
H	-1.974679000	-1.488104000	-3.464753000
O	-1.939392000	-2.565782000	-1.075362000
Si	-1.167607000	-2.698780000	0.405985000
H	-1.846774000	-3.600583000	1.331221000
23	0.178717000	3.085793000	1.325252000
O	-0.180376000	1.454604000	0.649885000
O	-0.988571000	4.087329000	1.654876000
O	1.824204000	3.673987000	1.619361000
H	2.647187000	3.183273000	1.449250000
C	3.869751000	1.411574000	0.804941000

H	3.053900000	0.795954000	0.451092000
H	4.248646000	1.277794000	1.808652000
H	4.426313000	2.021360000	0.106874000
No imaginary frequency			
G(298.15 K) = -1950.13664 a.u.			

¹P_{PCET-ii}

22

Si	2.130171000	-2.042228000	-0.696057000
H	3.473467000	-2.587898000	-0.526224000
O	1.871111000	-0.647986000	0.199324000
O	0.922019000	-3.106214000	-0.230036000
O	1.780412000	-1.628852000	-2.281651000
Si	0.361655000	0.050822000	0.069550000
O	-0.729327000	-1.139640000	0.492947000
O	0.127931000	0.335575000	-1.557071000
Si	0.259501000	-0.988118000	-2.577463000
H	0.039238000	-0.653670000	-3.981008000
O	-0.827029000	-2.119416000	-1.988149000
Si	-0.657997000	-2.567784000	-0.382804000
H	-1.645408000	-3.552538000	0.048527000
V	-0.800699000	2.684241000	1.630197000
O	0.222823000	1.385153000	0.987143000
O	-2.228215000	2.762235000	0.996964000
O	-0.079660000	4.293692000	1.703086000
H	0.861452000	4.410595000	1.890497000
C	-1.163391000	2.165460000	3.542633000
H	-1.804812000	2.914473000	4.008347000
H	-1.666481000	1.196032000	3.528376000
H	-0.205960000	2.093506000	4.064379000
No imaginary frequency			
G(298.15 K) = -1950.19956 a.u.			

⁴EC-iii

9

Cr	0.497534000	-1.246394000	1.480931000
O	0.917981000	-0.111496000	2.519751000
O	-0.873098000	-2.157206000	0.817083000
H	-1.822813000	-2.276177000	0.881826000
C	0.255318000	1.156545000	-1.137400000
H	1.215072000	0.686785000	-1.355625000
H	-0.539213000	0.411616000	-1.191389000
H	0.065605000	1.937427000	-1.873672000
H	0.283615000	1.598902000	-0.141504000

No imaginary frequency

G(298.15 K) = -278.6676501 a.u.

⁴TS_{HAT-iii}

9

Cr	-4.385191000	0.466139000	0.309775000
O	-4.043590000	2.174371000	0.132289000
O	-5.570927000	-0.864851000	0.581148000
H	-6.243081000	-1.046601000	1.242135000
C	-4.036080000	3.301436000	-2.164374000
H	-2.999213000	3.213450000	-2.471313000
H	-4.739791000	2.707829000	-2.738640000
H	-4.366276000	4.308854000	-1.931583000
H	-4.042725000	2.722046000	-0.845692000

One and only one imaginary frequency: -1529.8357 cm⁻¹

G(298.15 K) = -278.6195591 a.u.

⁶TS_{HAT-iii}

9

Cr	-4.260465000	0.590229000	0.452319000
O	-3.920519000	2.412563000	0.409092000
O	-5.508159000	-0.704049000	0.266504000
H	-6.202859000	-0.985257000	0.868545000
C	-4.112231000	3.138579000	-2.033449000
H	-3.182697000	2.841983000	-2.513289000
H	-4.972712000	2.598057000	-2.420395000
H	-4.261753000	4.216214000	-2.045263000
H	-4.005480000	2.874352000	-0.870319000

One and only one imaginary frequency: -649.51 cm⁻¹

G(298.15 K) = -278.5945501 a.u.

⁴TS_{PCET-iii}

9

Cr	-4.058238000	0.484923000	-0.543392000
O	-2.458232000	0.289444000	-0.053838000
O	-5.736747000	0.298882000	0.081867000
H	-6.288606000	0.751938000	0.723614000
C	-3.333114000	2.461171000	-1.250176000
H	-3.740051000	2.352550000	-2.258948000
H	-3.972526000	3.109748000	-0.651552000
H	-2.368210000	2.962951000	-1.365221000
H	-2.624800000	1.501369000	-0.622064000

One and only one imaginary frequency: -1357.6256 cm⁻¹

G(298.15 K) = -278.6264446 a.u.

⁴P_{HAT-iii}

9

Cr	-0.295558000	-1.857729000	0.766268000
O	1.101799000	-0.875158000	0.186810000
O	-1.641903000	-2.171324000	1.937057000
H	-1.614092000	-2.484197000	2.845432000
C	0.356338000	1.819802000	-1.346931000
H	0.953599000	2.412166000	-0.668984000
H	0.780633000	1.479175000	-2.280073000
H	-0.701440000	1.701831000	-1.164103000
H	1.060624000	-0.024566000	-0.275477000

No imaginary frequency

G(298.15 K) = -278.6269120 a.u.

⁶P_{HAT-iii}

9

Cr	-0.190824000	-1.956489000	0.939030000
O	1.022491000	-0.737074000	0.385954000
O	-1.626585000	-2.448409000	1.929632000
H	-1.697223000	-2.625170000	2.871756000
C	0.400984000	1.910849000	-1.468157000
H	1.130519000	2.430351000	-0.864237000
H	0.700311000	1.454821000	-2.400366000
H	-0.644018000	1.946774000	-1.197767000
H	0.904345000	0.024349000	-0.195845000

No imaginary frequency

G(298.15 K) = -278.6279404 a.u.

⁴P_{PCET-iii}

9

Cr	-0.030861000	-0.871645000	-0.035449000
O	1.535003000	-1.359838000	0.653886000
O	-1.699264000	-1.240389000	0.460322000
H	-2.232971000	-0.718104000	1.068605000
C	0.083617000	1.009159000	-0.764349000
H	-0.763607000	1.191624000	-1.431139000
H	0.062146000	1.738728000	0.048903000
H	1.016623000	1.123861000	-1.323041000
H	2.029313000	-0.873396000	1.322265000

No imaginary frequency

G(298.15 K) = -278.6865972 a.u.

⁴EC-iv

21

Si	0.088901000	-0.546394000	2.507689000
H	0.376105000	-0.311237000	3.919798000
O	0.882139000	-1.887356000	1.889148000
O	0.535781000	0.734050000	1.524895000
O	-1.538496000	-0.805474000	2.200614000
Si	0.618215000	-2.238102000	0.271691000
H	1.349311000	-3.415929000	-0.186879000
O	1.029958000	-0.844823000	-0.562646000
O	-1.042746000	-2.387937000	0.108190000
Si	-1.968275000	-1.080980000	0.603898000
H	-3.401591000	-1.293184000	0.424388000
O	-1.384267000	0.234593000	-0.251551000
Si	0.249243000	0.568103000	-0.112981000
Cr	0.840586000	2.869272000	-2.463728000
O	0.321431000	3.038841000	-3.958566000
O	0.718712000	1.845844000	-0.980436000
C	2.873091000	0.175895000	-3.523406000
H	3.517112000	1.003953000	-3.221404000
H	2.375821000	-0.243077000	-2.649444000
H	3.489236000	-0.590516000	-3.993711000
H	2.133617000	0.526312000	-4.244692000

No imaginary frequency

G(298.15 K) = -1890.1501494 a.u.

⁴TS_{HAT-iv}

21

Si	1.202429000	-2.863164000	1.636435000
H	1.340222000	-2.440507000	3.028012000
O	1.887609000	-4.364661000	1.340163000
O	1.924140000	-1.812018000	0.556036000
O	-0.396440000	-2.995012000	1.149521000
Si	1.782849000	-4.932320000	-0.234187000
H	2.406400000	-6.241887000	-0.408949000
O	2.465729000	-3.745682000	-1.192711000
O	0.147561000	-4.934564000	-0.603960000
Si	-0.653508000	-3.470568000	-0.438005000
H	-2.070467000	-3.555422000	-0.783143000
O	0.190975000	-2.380419000	-1.382136000
Si	1.831137000	-2.195861000	-1.072798000
Cr	3.141462000	-0.268447000	-3.528282000
O	3.337647000	-0.236599000	-5.260103000
O	2.556722000	-1.127529000	-2.021304000
C	5.477683000	-1.038734000	-6.387714000
H	6.233927000	-0.360366000	-6.006981000

H	5.561198000	-2.064862000	-6.044589000
H	5.241155000	-0.922229000	-7.440707000
H	4.265967000	-0.589357000	-5.811242000

One and only one imaginary frequency: -1643.2046 cm⁻¹

G(298.15 K) = -1890.0825898 a.u.

⁶TS_{HAT-iv}

21

Si	1.521107000	-2.659715000	1.194952000
H	1.631180000	-2.363225000	2.620892000
O	2.690633000	-3.737516000	0.660993000
O	1.680037000	-1.305724000	0.227651000
O	0.051866000	-3.350867000	0.780586000
Si	2.646746000	-4.139891000	-0.964857000
H	3.699335000	-5.077550000	-1.349840000
O	2.733638000	-2.688480000	-1.794382000
O	1.105949000	-4.734252000	-1.244358000
Si	-0.168355000	-3.720409000	-0.840042000
H	-1.474577000	-4.311743000	-1.117559000
O	0.104015000	-2.297421000	-1.671831000
Si	1.569559000	-1.522028000	-1.429436000
Cr	2.651737000	0.457677000	-3.760177000
O	3.093380000	-0.134952000	-5.441420000
O	1.762853000	-0.179436000	-2.284679000
C	4.544213000	-2.194597000	-4.873971000
H	4.379242000	-2.945746000	-5.644013000
H	5.581304000	-1.870175000	-4.825494000
H	4.153308000	-2.501984000	-3.906167000
H	3.917225000	-1.262173000	-5.243492000

One and only one imaginary frequency: -499.0279cm⁻¹

G(298.15 K) = -1890.1064411 a.u.

⁴TS_{PCET-iv}

21

Si	1.543398000	-2.523884000	1.328849000
H	1.877623000	-2.003016000	2.651765000
O	2.396614000	-3.915502000	0.941686000
O	1.862730000	-1.441514000	0.094943000
O	-0.074613000	-2.931155000	1.172953000
Si	2.083194000	-4.590785000	-0.560003000
H	2.867917000	-5.795611000	-0.819895000
O	2.370588000	-3.371721000	-1.671727000
O	0.430800000	-4.863276000	-0.599103000
Si	-0.553038000	-3.534363000	-0.316288000

H	-1.975921000	-3.858318000	-0.370373000
O	-0.093678000	-2.386098000	-1.440335000
Si	1.516390000	-1.930313000	-1.468139000
Cr	2.747702000	-0.704380000	-4.217229000
O	2.558891000	-0.965835000	-5.863251000
O	1.891986000	-0.846846000	-2.591108000
C	4.354411000	-2.188622000	-4.400207000
H	5.165270000	-1.579993000	-3.993709000
H	3.963528000	-2.872728000	-3.646237000
H	4.786369000	-2.788804000	-5.206558000
H	3.547452000	-1.731240000	-5.399047000

One and only one imaginary frequency: -1412.8782 cm-1

G(298.15 K) = -1890.1141454 a.u.

⁴P_{HAT-iv}

21

Si	-0.372232000	-0.535709000	2.811280000
H	-0.291410000	-0.216888000	4.234328000
O	0.826266000	-1.597039000	2.310860000
O	-0.225856000	0.804366000	1.825755000
O	-1.819588000	-1.263782000	2.385571000
Si	0.817884000	-2.024215000	0.691016000
H	1.896251000	-2.944368000	0.337585000
O	0.882046000	-0.583890000	-0.156421000
O	-0.706992000	-2.653988000	0.398176000
Si	-2.007839000	-1.661315000	0.767958000
H	-3.297053000	-2.284653000	0.480930000
O	-1.752122000	-0.246020000	-0.078974000
Si	-0.307022000	0.567627000	0.169123000
Cr	0.684912000	2.678760000	-2.154014000
O	1.189148000	2.383672000	-3.845830000
O	-0.128007000	1.895476000	-0.703967000
C	2.810509000	-0.527746000	-3.184916000
H	2.313275000	-0.914209000	-4.063346000
H	3.865461000	-0.297361000	-3.227992000
H	2.285787000	-0.498643000	-2.240524000
H	1.884344000	1.770366000	-4.114182000

No imaginary frequency

G(298.15 K) = -1890.1134974 a.u.

⁶P_{HAT-iv}

21

Si	-0.355302000	-0.538637000	2.797082000
H	-0.264931000	-0.227535000	4.221403000

O	0.845860000	-1.590706000	2.282570000
O	-0.223668000	0.810293000	1.819653000
O	-1.802883000	-1.271518000	2.377570000
Si	0.826359000	-2.008003000	0.659858000
H	1.906057000	-2.921005000	0.291796000
O	0.881454000	-0.561635000	-0.181301000
O	-0.696757000	-2.644362000	0.373210000
Si	-1.999655000	-1.659888000	0.758305000
H	-3.287826000	-2.287697000	0.475840000
O	-1.757376000	-0.238008000	-0.083725000
Si	-0.314249000	0.578973000	0.162652000
Cr	0.675707000	2.684375000	-2.153946000
O	1.206294000	2.317285000	-3.827873000
O	-0.152956000	1.916961000	-0.701471000
C	2.779625000	-0.524930000	-3.149562000
H	2.293397000	-0.915411000	-4.032097000
H	3.836792000	-0.303020000	-3.178010000
H	2.236018000	-0.467408000	-2.216791000
H	1.915801000	1.702317000	-4.052749000

No imaginary frequency

G(298.15 K) = -1890.1147676 a.u.

⁴P_{PCET-iv}

21

Si	-0.182582000	0.038725000	2.864410000
H	0.461232000	0.494917000	4.093450000
O	0.332401000	-1.483522000	2.383241000
O	0.101841000	1.045329000	1.559805000
O	-1.849416000	-0.073584000	2.999952000
Si	-0.349336000	-2.093037000	0.978723000
H	0.154147000	-3.419377000	0.629677000
O	-0.052242000	-0.946520000	-0.203350000
O	-2.005820000	-2.066747000	1.230974000
Si	-2.677388000	-0.583319000	1.634003000
H	-4.122718000	-0.647944000	1.832811000
O	-2.226267000	0.464676000	0.411632000
Si	-0.590871000	0.618693000	0.095984000
Cr	0.786301000	1.654824000	-2.591361000
O	0.434415000	1.162786000	-4.251087000
O	-0.243539000	1.634818000	-1.103567000
C	2.632062000	1.060308000	-2.069046000
H	2.927532000	1.618883000	-1.175766000
H	2.613223000	-0.006338000	-1.837293000
H	3.336208000	1.257329000	-2.880768000

H	0.520816000	0.269099000	-4.602425000
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No imaginary frequency

G(298.15 K) = -1890.1725488 a.u.

¹EC-v

58

Si	-0.17631400	2.14765100	1.15819000
O	-1.42842500	3.22911500	1.27703900
O	-0.76765600	0.71911500	1.76206600
O	0.05109000	1.91239900	-0.46903300
Si	-2.85136700	2.77099900	0.51171500
O	-3.27662100	1.27535200	1.15405200
O	-2.45034000	2.47974200	-1.09847400
Si	-1.24830700	1.36260900	-1.34109100
O	-1.77461400	-0.01972100	-0.58793500
Si	-2.11952000	0.09340300	1.03173500
Si	2.64373200	1.52869000	1.86389800
O	4.09475500	1.97932900	2.63824100
O	3.15719700	1.19642300	0.27877800
O	2.32855300	-0.00266100	2.52894200
Si	5.46454000	0.91913700	2.57679400
O	5.68698200	0.63149400	0.87962200
O	4.84435000	-0.58968100	3.16923400
Si	3.46135300	-1.26661700	2.44190900
O	3.88742300	-1.32789300	0.79744100
Si	4.37888000	0.06179600	-0.04922300
H	6.64674000	1.40539600	3.27237100
O	1.27007000	2.47248700	1.86288300
O	-0.75857200	0.99379000	-2.86439500
O	4.46035100	-0.24304000	-1.68587100
O	2.76443200	-2.70393600	2.91747500
O	-2.41003700	-1.40993600	1.62438900
Si	-1.39352500	-2.73083500	1.60081700
O	0.07608600	-2.38152400	2.37698000
O	-0.94357000	-3.12643300	0.01080900
O	-1.81107800	-4.24893800	2.25580700
Si	1.40229900	-3.44164700	2.30399200
O	1.58215300	-3.75991700	0.64395500
O	0.75819800	-4.90053100	2.90156300
Si	-0.67597800	-5.55718100	2.17805100
O	-0.27745700	-5.65756200	0.49166900
Si	0.27503900	-4.26462400	-0.31770400
Si	2.07872800	-1.54785600	-5.31384600
O	0.83878000	-0.39257600	-4.94772500

O	3.43417100	-1.00865200	-4.37391700
O	1.55556400	-2.98561700	-4.49403600
Si	0.42094900	-0.09195200	-3.32185600
O	1.91765500	0.29515900	-2.61888100
O	0.07214500	-1.64755100	-2.73475900
Si	1.20110300	-2.91485200	-2.82995900
O	2.61931400	-2.25239600	-2.16722400
Si	3.24457500	-0.76388300	-2.69915300
O	0.68361800	-4.22056500	-1.93281600
H	2.35304900	-1.72143400	-6.73248000
H	-1.13952800	-6.80472300	2.76677700
V	-4.96195400	5.39690500	0.73047900
O	-4.03535000	3.84897700	0.66198000
O	-4.34603100	6.61605600	-0.07673700
O	-5.42237300	5.86439100	2.17562300
H	-6.83524200	5.93876400	0.02559100
C	-7.06110300	4.95726500	-0.43180400
H	-7.18722700	5.13750400	-1.49522200
H	-6.32733500	4.13974000	-0.33030400
H	-7.97435000	4.61104700	0.04357700

No imaginary frequency

G(298.15 K) = -7228.29384 a.u.

¹TS_{HAT-V}

58

Si	1.88221100	-0.78168500	-0.38779900
O	0.65585500	0.33687400	-0.39354700
O	1.20522800	-2.17490800	0.20356600
O	2.23739200	-1.06150500	-1.98199000
Si	-0.72136300	-0.10514000	-1.27239700
O	-1.22936900	-1.57005100	-0.61879000
O	-0.18536500	-0.44443000	-2.82740900
Si	0.99674900	-1.60045700	-2.94577100
O	0.37367000	-2.94697200	-2.20229400
Si	-0.10085000	-2.78555800	-0.62121900
Si	4.61146100	-1.43193000	0.57823700
O	6.00291900	-0.98914000	1.45835300
O	5.24097600	-1.81547800	-0.95116600
O	4.20530700	-2.93562000	1.25537100
Si	7.34914200	-2.08031300	1.53501600
O	7.70059500	-2.41443100	-0.13089000
O	6.64652200	-3.55839800	2.11194400
Si	5.31205800	-4.22588600	1.29044300
O	5.86902900	-4.33683200	-0.31133400

Si	6.46090300	-2.98252500	-1.15071200
H	8.48087000	-1.60079300	2.31419900
O	3.26455900	-0.45714100	0.43811200
O	1.60322400	-2.02304800	-4.41065200
O	6.67296500	-3.33147600	-2.76582600
O	4.54161400	-5.63235700	1.74232600
O	-0.47593700	-4.26376300	-0.01368700
Si	0.50636000	-5.60775200	0.08198200
O	1.91356700	-5.26761100	0.97159000
O	1.07882800	-6.05414400	-1.45333800
O	0.00041300	-7.09775800	0.73941600
Si	3.21699300	-6.35648900	1.03590800
O	3.52760100	-6.72117700	-0.59454200
O	2.49244400	-7.78418700	1.61451800
Si	1.10833200	-8.43089200	0.78998000
O	1.64425600	-8.58326300	-0.85359100
Si	2.29441200	-7.22570200	-1.64992800
Si	4.57547500	-4.69086800	-6.54718900
O	3.33567200	-3.50151500	-6.31544800
O	5.85983400	-4.15167300	-5.51120400
O	3.95452400	-6.09335600	-5.73469400
Si	2.78962600	-3.14696300	-4.73968400
O	4.23110100	-2.76992900	-3.92276500
O	2.35971100	-4.67728900	-4.14066300
Si	3.46395000	-5.96897200	-4.10913300
O	4.83721600	-5.31673800	-3.34794500
Si	5.53620100	-3.85682000	-3.86583700
O	2.84112000	-7.23596500	-3.22378400
H	4.96371700	-4.91056600	-7.93238300
H	0.56877200	-9.65187000	1.36947100
V	-2.47218200	2.61553700	-0.56869200
O	-1.85557700	1.03173400	-1.21010400
O	-3.00631100	3.71298200	-1.56906200
O	-1.74567900	3.22660600	0.84205100
H	-0.70754700	3.10834400	1.46221700
C	0.45851400	2.90048500	2.03388600
H	0.88275300	2.11300800	1.41839800
H	0.18794000	2.60482000	3.04332000
H	0.94618900	3.86725900	1.95415400

One and only one imaginary frequency: -1908.4862 cm⁻¹
G(298.15 K) = -7228.23294 a.u.

³TS_{HAT-V}

Si	2.07978200	-0.81186600	-0.21039800
O	0.88858600	0.34441100	-0.15460500
O	1.36765900	-2.20201400	0.34651900
O	2.38812300	-1.04682700	-1.82265900
Si	-0.51675400	-0.02836500	-1.01529800
O	-1.06218500	-1.49225600	-0.39979400
O	-0.02883700	-0.32425600	-2.59423200
Si	1.11281800	-1.51486700	-2.77697400
O	0.46014500	-2.86368000	-2.06481600
Si	0.02631100	-2.74376200	-0.46839600
Si	4.80796800	-1.59226400	0.66389100
O	6.23251400	-1.22743100	1.52668600
O	5.39075500	-1.94233100	-0.89244400
O	4.36506200	-3.10432100	1.29742100
Si	7.54156600	-2.36565200	1.53588000
O	7.84492400	-2.65298900	-0.14836900
O	6.80085100	-3.83846200	2.07804200
Si	5.42736200	-4.43140500	1.26430800
O	5.94599200	-4.50498200	-0.35235300
Si	6.56495600	-3.14276600	-1.15868600
H	8.70593900	-1.95235800	2.30472200
O	3.49287200	-0.56844000	0.58832900
O	1.67126300	-1.90539200	-4.26896500
O	6.72777800	-3.44064600	-2.78978100
O	4.61776300	-5.82532300	1.68521200
O	-0.38619400	-4.22889000	0.09431700
Si	0.55022200	-5.60862400	0.12058300
O	1.98698500	-5.34525000	0.98801200
O	1.07345000	-6.01862200	-1.44264600
O	0.00852000	-7.10305400	0.73720000
Si	3.25364800	-6.47896300	0.98569900
O	3.51555400	-6.79612700	-0.66324000
O	2.49358200	-7.90099800	1.53149500
Si	1.07135600	-8.47325500	0.71707100
O	1.56596800	-8.58539100	-0.94261500
Si	2.24367500	-7.22291100	-1.70677800
Si	4.50163200	-4.59473600	-6.56598000
O	3.30825600	-3.37317400	-6.26488500
O	5.82551000	-4.13465200	-5.54185500
O	3.85163100	-6.00329700	-5.78752600
Si	2.80996300	-3.05728400	-4.66541700
O	4.28034500	-2.75624000	-3.86944200
O	2.34113800	-4.59218800	-4.10956500
Si	3.40145500	-5.92030700	-4.14778200

O	4.81188100	-5.34037800	-3.39648300
Si	5.54911000	-3.88749900	-3.88001000
O	2.75541000	-7.19592300	-3.29223900
H	4.85119700	-4.77823700	-7.96663100
H	0.50362700	-9.69526000	1.26662800
V	-2.60737300	2.63124200	-0.64441000
O	-1.59725900	1.15585000	-0.89025700
O	-3.92457800	2.87413100	-1.47297100
O	-2.21294100	3.95387000	0.47261500
H	-1.01328500	3.65589100	1.15207100
C	-0.00378400	3.27695900	1.65666800
H	0.38217400	2.45083200	1.06524400
H	-0.29312700	2.98186500	2.66246600
H	0.63763200	4.15517600	1.63641000

One and only one imaginary frequency: $-458.5206 \text{ cm}^{-1}$

G(298.15 K) = $-7228.2254463 \text{ a.u.}$

¹TS_{PCET-V}

58

Si	2.02540800	-0.80255100	-0.45338200
O	0.75854300	0.26319700	-0.32725600
O	1.45120300	-2.24010000	0.14496700
O	2.25181800	-1.02635600	-2.08187000
Si	-0.65624400	-0.21452200	-1.09441400
O	-1.06463700	-1.71293700	-0.45569700
O	-0.25640000	-0.48711300	-2.70573100
Si	0.95944300	-1.58926900	-2.95609900
O	0.44993300	-2.97998100	-2.20714000
Si	0.10712300	-2.88101000	-0.58649200
Si	4.85362100	-1.38870400	0.24539600
O	6.29966500	-0.92345700	1.01994300
O	5.36784200	-1.70744500	-1.34201600
O	4.55701900	-2.92645900	0.90391200
Si	7.68217400	-1.96723000	0.95165000
O	7.90493000	-2.24443100	-0.74709200
O	7.08031400	-3.48566000	1.53820100
Si	5.70494600	-4.17661200	0.80982800
O	6.12900000	-4.22508800	-0.83552100
Si	6.60278300	-2.82606300	-1.67683300
H	8.85938400	-1.46959700	1.64761800
O	3.46782700	-0.46175800	0.25088300
O	1.45171900	-1.94435600	-4.48084100
O	6.68560400	-3.12280200	-3.31473900
O	5.02694500	-5.62456000	1.28022800

O	-0.16353900	-4.38927200	0.00037500
Si	0.86882500	-5.69798600	-0.03045100
O	2.33492500	-5.33334000	0.74529700
O	1.32130700	-6.07931100	-1.62299800
O	0.47053800	-7.22342900	0.61819100
Si	3.67365000	-6.37745400	0.66548900
O	3.85497000	-6.68580700	-0.99620300
O	3.04798700	-7.84663600	1.25725600
Si	1.62108600	-8.51790500	0.53260000
O	2.01825200	-8.60487900	-1.15477600
Si	2.55272200	-7.20182300	-1.95860600
Si	4.31593900	-4.44139900	-6.94602100
O	3.06280400	-3.30231400	-6.57341100
O	5.66570200	-3.88982200	-6.00496700
O	3.81074600	-5.88830400	-6.13111300
Si	2.64364200	-3.01360800	-4.94616200
O	4.13604400	-2.61112700	-4.24253500
O	2.31382600	-4.57523000	-4.36406800
Si	3.45745900	-5.82900300	-4.46649800
O	4.86816100	-5.15208900	-3.80227700
Si	5.47529600	-3.65430100	-4.32911500
O	2.95769100	-7.14476200	-3.57407800
H	4.59061800	-4.60573500	-8.36564900
H	1.17374700	-9.77367600	1.11629100
V	-2.69603100	2.41192100	-1.18285400
O	-1.85733000	0.85160100	-0.93102500
O	-1.93832300	3.46109300	-2.08141200
O	-3.48356300	3.11626700	0.10003600
H	-4.35562100	2.73258600	-0.77860900
C	-4.66997000	2.10184100	-2.04409800
H	-4.61336200	2.66318100	-2.97414400
H	-4.57324000	1.02763200	-2.21812800
H	-5.66483600	2.26219600	-1.61630000

One and only one imaginary frequency: -1489.0131 cm⁻¹

G(298.15 K) = -7228.2586742 a.u.

¹P_{HAT-V}

58

Si	1.88511200	-0.85735300	-0.22960500
O	0.65544100	0.25950300	-0.19375000
O	1.21117800	-2.27126200	0.31256300
O	2.23250100	-1.07768600	-1.83524700
Si	-0.72318100	-0.15775000	-1.08120400
O	-1.22642500	-1.64136200	-0.47710200

O	-0.19300600	-0.43385500	-2.65029800
Si	0.99053000	-1.58526100	-2.81360900
O	0.37068500	-2.95702700	-2.11653000
Si	-0.09636200	-2.85536900	-0.52801400
Si	4.62240900	-1.53428100	0.69548800
O	6.01469500	-1.12033400	1.58739300
O	5.24891400	-1.85964700	-0.84880100
O	4.21977900	-3.06264800	1.31602900
Si	7.36266600	-2.21213100	1.62102900
O	7.71047400	-2.48595100	-0.05692500
O	6.66300900	-3.71063600	2.14648600
Si	5.32849000	-4.35170900	1.30515100
O	5.88221500	-4.40383600	-0.30082200
Si	6.46842200	-3.01905400	-1.09276600
H	8.49641800	-1.75813500	2.41243800
O	3.27220700	-0.55903300	0.59566300
O	1.59131500	-1.95249100	-4.29527800
O	6.67030900	-3.31101800	-2.72055000
O	4.56266300	-5.77419200	1.71196600
O	-0.46459200	-4.35445700	0.02737500
Si	0.52151600	-5.69855000	0.07216100
O	1.93081900	-5.38730200	0.96850900
O	1.09101300	-6.08512000	-1.48063400
O	0.02046100	-7.21176500	0.67607600
Si	3.23572700	-6.47663100	0.98816300
O	3.54193100	-6.78193800	-0.65543000
O	2.51516600	-7.92540800	1.51736100
Si	1.12959100	-8.54482200	0.67475300
O	1.65977500	-8.63568200	-0.97536300
Si	2.30536200	-7.24942000	-1.72396300
Si	4.55852500	-4.53702600	-6.53869000
O	3.31787200	-3.35795200	-6.26021800
O	5.84553500	-4.03344900	-5.48815300
O	3.94200900	-5.96874000	-5.77553100
Si	2.77738500	-3.06289200	-4.67088100
O	4.22029000	-2.71267300	-3.84524800
O	2.35072800	-4.61414500	-4.12655000
Si	3.45724900	-5.90442400	-4.14460700
O	4.83122000	-5.27673600	-3.36497900
Si	5.52795800	-3.79870400	-3.83200600
O	2.84271900	-7.20303700	-3.30052700
H	4.94128900	-4.70583100	-7.93252200
H	0.59468800	-9.78682100	1.21241700
V	-2.68113600	2.52409800	-0.53022500

O	-1.84924500	0.98552500	-0.98208500
O	-4.13016600	2.82257600	-1.06778700
O	-1.96111500	3.75987700	0.50028700
H	-1.08950800	3.78962400	0.93590100
C	0.90666400	3.25609000	1.60092900
H	0.91960200	2.30996100	1.07754800
H	0.63467400	3.28727100	2.64685900
H	1.35987500	4.12664600	1.14745400

No imaginary frequency

G(298.15 K) = -7228.2501506 a.u.

¹P_{PCET-V}

58

Si	-0.25335200	2.14026600	1.17809400
O	-1.52179400	3.20401400	1.30893900
O	-0.81983800	0.70596000	1.79195300
O	-0.04152500	1.90578300	-0.45051800
Si	-2.94081800	2.71833000	0.55478400
O	-3.34145500	1.22622700	1.21230100
O	-2.55570300	2.43725000	-1.05651500
Si	-1.34029900	1.33485700	-1.31023600
O	-1.84206000	-0.05052000	-0.54589100
Si	-2.16948000	0.05829500	1.07685800
Si	2.58147700	1.56400600	1.85722200
O	4.03318900	2.03703500	2.61623100
O	3.08250500	1.23438300	0.26803100
O	2.29219100	0.03091900	2.52977600
Si	5.41655700	0.99446200	2.54366600
O	5.62516300	0.70486900	0.84532500
O	4.82137400	-0.52017200	3.14679000
Si	3.44109100	-1.21842200	2.43507300
O	3.85102600	-1.27833000	0.78665900
Si	4.31600800	0.11479700	-0.06931600
H	6.59892500	1.49902900	3.22576400
O	1.19407300	2.48881400	1.86811900
O	-0.86004600	0.96879800	-2.83570700
O	4.38486800	-0.19422200	-1.70541400
O	2.76952900	-2.66369500	2.92277600
O	-2.43303100	-1.44534200	1.67820200
Si	-1.39885200	-2.75283300	1.64793500
O	0.07291300	-2.38056000	2.40927900
O	-0.95872600	-3.14436400	0.05465500
O	-1.78982100	-4.27384500	2.31104500
Si	1.41239800	-3.42354300	2.32521800

O	1.58053600	-3.74357700	0.66444300
O	0.79348100	-4.88914300	2.93298400
Si	-0.63826500	-5.56749700	2.22475600
O	-0.25502400	-5.66562700	0.53500200
Si	0.27102300	-4.26800900	-0.28370900
Si	1.98685800	-1.54272900	-5.30711300
O	0.73544800	-0.40258300	-4.93215700
O	3.34363700	-0.98260800	-4.38104600
O	1.49031700	-2.98408400	-4.47706000
Si	0.32915300	-0.10226300	-3.30395900
O	1.82672700	0.30717200	-2.61521000
O	0.00622800	-1.65990500	-2.70729900
Si	1.15070400	-2.91281900	-2.81022100
O	2.56586500	-2.22937400	-2.16245100
Si	3.16668300	-0.73480600	-2.70562800
O	0.66125500	-4.22239400	-1.90297800
H	2.24998800	-1.71743600	-6.72766100
H	-1.07888300	-6.81953400	2.82144200
V	-4.97096700	5.30849100	0.34702600
O	-4.14670500	3.78140200	0.72798000
O	-4.12440400	6.31247500	-0.50332900
O	-5.72767700	6.14681300	1.69749500
H	-6.15676100	5.68071300	2.42708900
C	-6.47900300	4.79294000	-0.88185500
H	-7.03629000	5.68326800	-1.17622900
H	-6.04210300	4.32093800	-1.76528500
H	-7.12830500	4.08792900	-0.35612800

No imaginary frequency

G(298.15 K) = -7228.3159731 a.u.
