

Supporting Information for

**Functional Role of Pyridinium During Aqueous
Electrochemical Reduction of CO₂ on Pt(111)**

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S1 Plane-wave-based DFT calculations

Density functional theory (DFT) calculations were carried out at the gradient-corrected PBE level of theory¹ within the plane-wave pseudopotential scheme as implemented in the Quantum ESPRESSO² software package. Ultra-soft pseudopotentials were employed for Pt, C, H, N and O atoms with plane wave kinetic energy cut off values of 40 Ry and 480 Ry for the wavefunctions and the charge densities, respectively. The Pt(111) surface was modeled by a periodically repeating 4×4 supercell ($11.32 \text{ \AA} \times 11.32 \text{ \AA}$) in a four-layer slab where the two bottom layers were fixed at the optimized bulk lattice constants. The Monkhorst-Pack type of k -point sampling with a $2 \times 2 \times 1$ was chosen for the slab calculations. The constrained optimizations mentioned were performed by fixing the distance between a hydrogen atom on Pt(111) surface and the carbon atom of carbon dioxide to investigate the proton-coupled-hydride-transfer (PCHT) step. Energies obtained via fully relaxed and constrained optimizations are listed in Tables ST1 and ST2, respectively, along with images of select structures in Figure SF1.

Table ST1: Electronic energies of optimized structures obtained via plane-wave-based DFT at the PBE level of theory.

	E (Ry)	E (kcal/mol)
H_2	-2.331168	-731.42
$[\text{Pt}_{64}]^0$	-5542.614031	-1739021.39
$[\text{Pt}_{64}]^-$	-5542.553692	-1739002.46
$[\text{Pt}_{64}\text{H}]^0$	-5543.808505	-1739396.17
$[\text{Pt}_{64}\text{PyrH}]^+$	-5626.538188	-1765353.00
$[\text{Pt}_{64}\text{PyrH}]^0$	-5626.538188	-1765353.00
$[\text{Pt}_{64}\text{H}_{16}]^0$	-5561.637584	-1744990.12

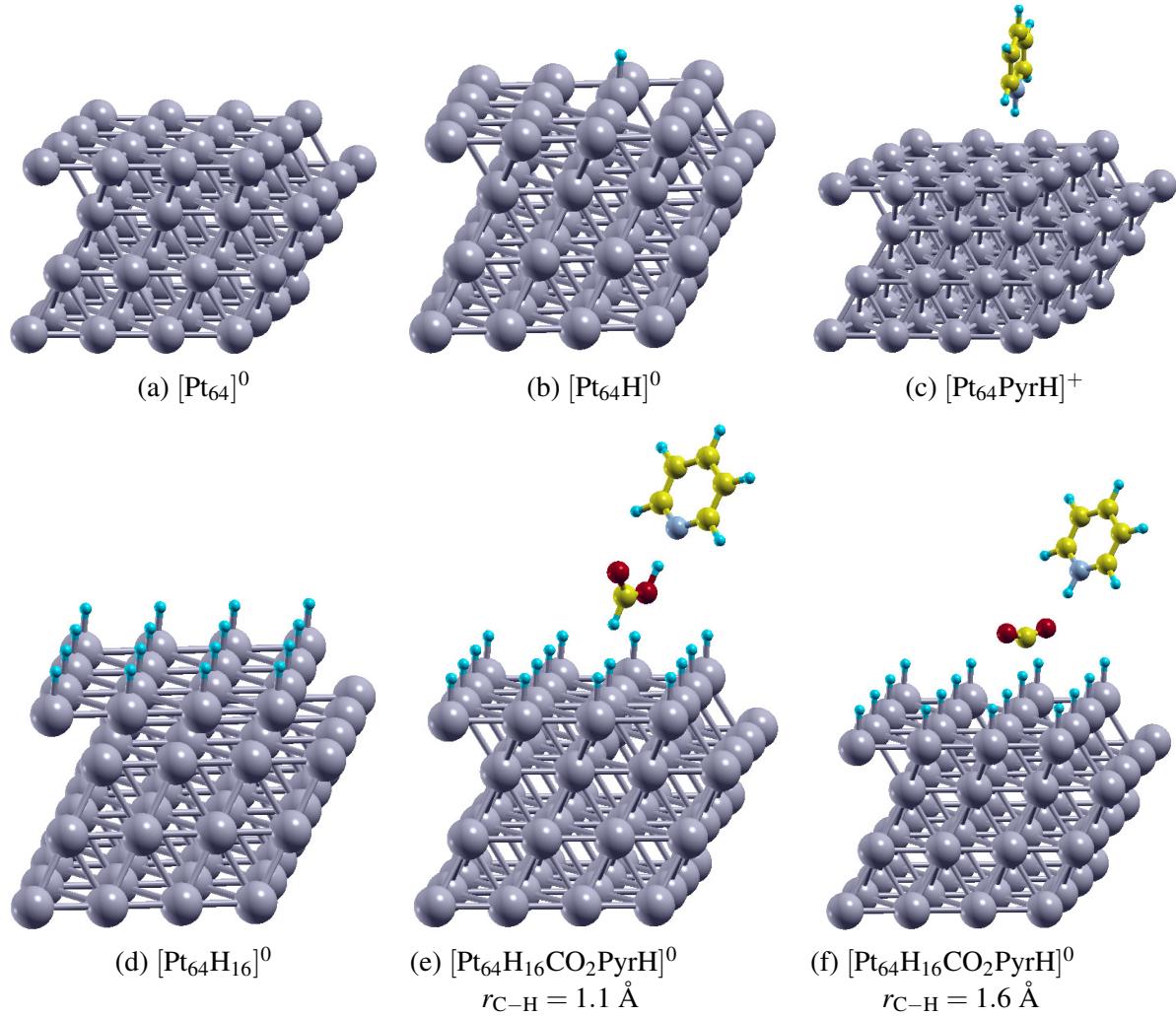


Figure SF1: Optimized structures of supercells employed in plane-wave-based density functional theory calculations.

Table ST2: Electronic energies of constrained optimizations of $[\text{Pt}_{64}\text{H}_{16}\text{CO}_2\text{PyrH}]^0$ with fixed (Pt)H-C(O₂) bond distance obtained using plane-wave-based DFT at the PBE level of theory.

$r_{\text{C}-\text{H}}$ (Å)	E (Ry)	E (kcal/mol)
1.1	-5720.673883	-1794888.52
1.2	-5720.668391	-1794886.79
1.3	-5720.654424	-1794882.41
1.4	-5720.636416	-1794876.76
1.5	-5720.631626	-1794875.26
1.6	-5720.631372	-1794875.18
1.7	-5720.632839	-1794875.64
1.9	-5720.644492	-1794879.29
2.1	-5720.652206	-1794881.71
2.5	-5720.654151	-1794882.32

S2 Cluster DFT calculations

Select geometries for the cluster calculations were fully optimized at the PBE level of density functional theory¹ using the Stuttgart ECP60MWB contracted pseudopotential basis set³ for Pt and the 6-31G(d) basis set⁴ for all other atoms. The `grid=ultrafine` option (in Gaussian 09)⁵ was chosen for integral evaluation and an automatically generated density-fitting basis set was used within the resolution-of-the-identity approximation for the evaluation of Coulomb integrals. The nature of all stationary points was verified by analytic computation of vibrational frequencies, which were also used for the computation of zero-point vibrational energies and molecular partition functions. Partition functions were further used in the computation of 298 K thermal contributions to free energy employing the usual ideal-gas, rigid-rotator, harmonic oscillator approximation (Table ST3).⁶ Solvation effects associated with water as solvent were accounted for by using the SMD aqueous continuum solvation model (Table ST4).⁷ Free energy contributions

were added to single-point PBE electronic energies computed with the SDD basis set for Pt and the 6-311+G(2df,p) basis set for all other atoms to arrive at final, composite free energies.

The aqueous solvation contribution to the plane-wave-based periodic DFT optimized structures were calculated via generating model clusters with 18 Pt atoms (Figure SF2) and performing single point calculations at the PBE level of density functional theory using SDD basis set for Pt and the 6-311+G(2df,p) basis set for all other atoms (Table ST5).

Table ST3: Electronic and free energies of species calculated at PBE level of theory with the SDD basis set for Pt and the 6-31G(d) basis set for C, H, N and O.

	<i>E</i> (kcal/mol)	<i>G</i> (kcal/mol)
H ₂	-730.44	-731.51
Pyr	-155600.99	-155563.86
[Pyr] ⁺	-155944.95	-155903.05
[PyrH] ⁺	-155833.39	-155787.50
[Pt] ⁺	-74843.56	-74855.17
[PtH] ⁺	-75252.51	-75262.57
[PtPyrH] ⁺	-230700.69	-230661.12

Table ST4: Single point calculations of select geometries listed in Table ST3 at the PBE level of theory with the 6-311+G(2df,p) basis set.

	<i>E</i> (kcal/mol)	ΔE_{solv} (kcal/mol)
Pyr	-155649.58	-4.44
[Pyr] ⁺	-155998.51	-3.79
[PyrH] ⁺	-155879.19	-59.21

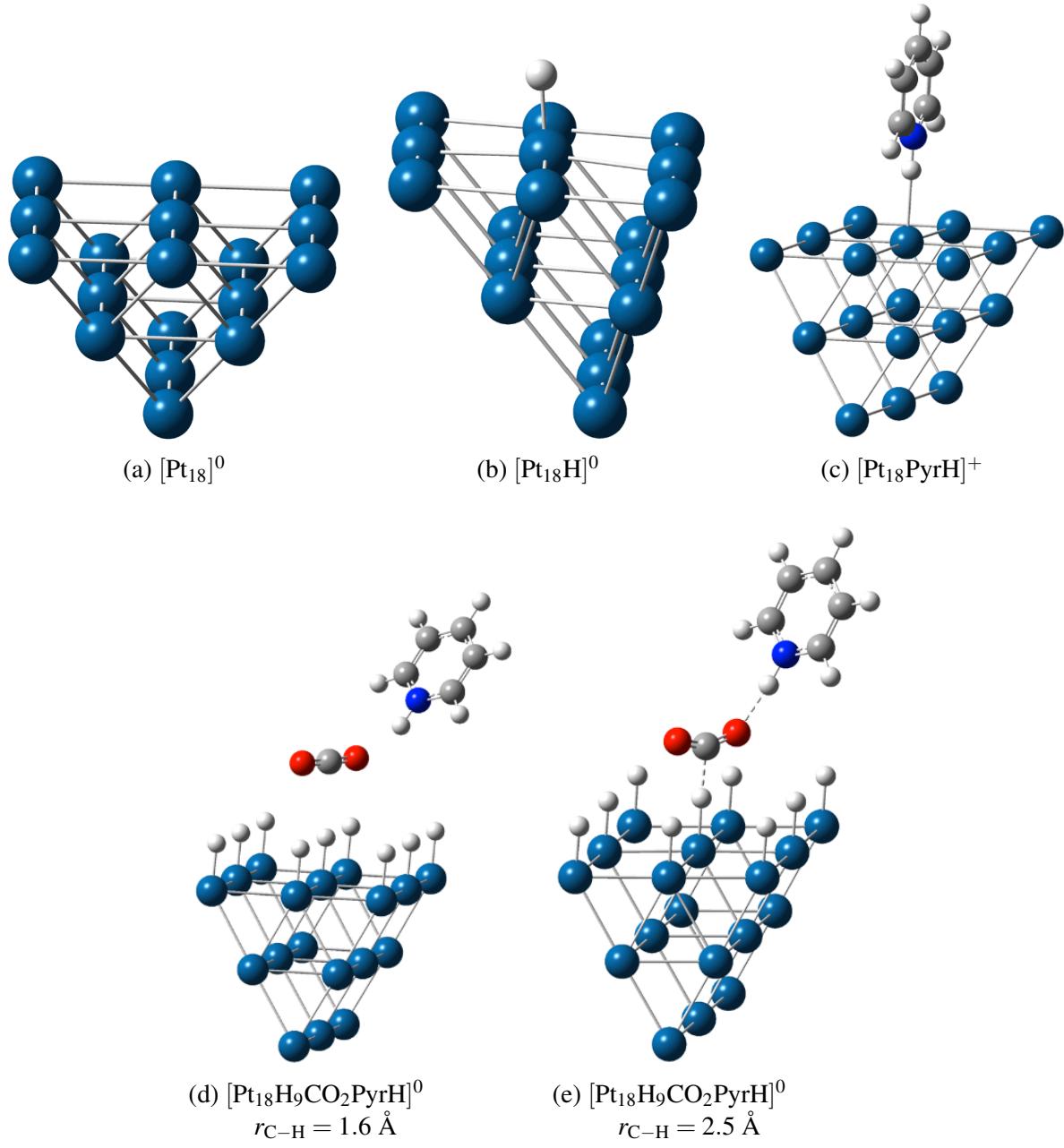


Figure SF2: Structures of model clusters.

Table ST5: Single point calculations at PBE level of theory with SDD basis set for Pt and 6-311+G(2df,p) basis set for C, H, N and O for model structures of select optimized geometries listed in Tables ST1 and ST2.

	E (Ry)	E (kcal/mol)
$[\text{Pt}_{18}]^0$	-2148.923527	-1348469.86
$[\text{Pt}_{18}]^-$	-2149.123428	-1348595.30
$[\text{Pt}_{18}\text{H}]^0$	-2149.567372	-1348873.88
$[\text{Pt}_{18}\text{PyrH}]^+$	-2397.362212	-1504367.49
$[\text{Pt}_{18}\text{H}_9\text{CO}_2\text{PyrH}]^0 \quad r_{\text{C}-\text{H}} = 1.6 \text{ \AA}$	-2591.806176	-1626382.92
$[\text{Pt}_{18}\text{H}_9\text{CO}_2\text{PyrH}]^0 \quad r_{\text{C}-\text{H}} = 2.5 \text{ \AA}$	-2591.811546	-1626386.29

S3 PyrH⁺ reduction calculations

In order to calculate the free energy change associated with the reduction of PyrH⁺ on the Pt(111) surface (i) to generate surface bound hydrogen atoms and Pyr(aq), we investigated three elementary reactions (i.1-3) which are the reduction of PyrH⁺ to H₂ and Pyr in aqueous solution (i.1), dissociative adsorption of H₂ to the Pt surface (i.2) and surface desorption of PyrH⁺ (i.3). The reduction potential of (i.1) was predicted to be -0.59 V (see Tables ST3 and ST4 for the detailed energetics). The free energy change associated with the dissociative adsorption of H₂ to the Pt surface (i.2) was calculated to be -6.9 kcal/mol, which was obtained by the sum of $\Delta E = -9.1$ kcal/mol (via plane-wave-based periodic DFT calculations; Table ST1), $-T\Delta S = 2.1$ kcal/mol and solvation contributions of +0.1 kcal/mol (via cluster calculations; Tables ST3 and ST4). The free energy change for the final step (i.3) was found to be $\Delta G_{\text{desorp}} = 9.9$ kcal/mol employing model clusters (Tables ST3 to ST5). In both steps (i.2) and (i.3) the zero-point energy and entropy contributions are calculated using single Pt models as tabulated in Table ST3. The free energy sum of (i.1) to (i.3) yields a calculated reduction potential of -0.72 V, in reasonable agreement with the estimated value of -0.58 V vs SCE reported by the partially reversible cyclic voltammogram wave.

S4 Geometries in cartesian coordinates

Table ST6: Optimized geometries obtained via plane-wave-based DFT at the PBE level of theory.

H₂

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
H	12.876085863	12.500000049	12.500000049
H	12.123914137	12.499999951	12.499999951

[Pt₆₄]⁰

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.322215785	6.546232370	5.598774710
Pt	5.663887907	6.545266843	5.597619693
Pt	8.492786507	1.645922945	5.598465121
Pt	2.834456865	1.645380956	5.599592586
Pt	14.150384042	6.545654239	5.599691681
Pt	12.736046827	8.995758147	5.599748239
Pt	15.564227395	8.995356438	5.598467312
Pt	8.491412095	6.544169936	5.598626747
Pt	11.321170545	1.646192303	5.599713269
Pt	5.663287598	1.645845571	5.599898312
Pt	7.077698128	8.994397915	5.598635876
Pt	9.906432920	4.096849725	5.598136399
Pt	4.248609829	4.095240345	5.599481474
Pt	9.906981361	8.995119617	5.599354429
Pt	12.735448700	4.096419264	5.599555483
Pt	7.078990691	4.095540681	5.597923970
Pt	8.499195680	4.926305299	7.915892355
Pt	2.842331464	4.930055232	7.913299717
Pt	5.670897164	0.026923096	7.913111999
Pt	0.013422346	0.027759967	7.912267599
Pt	11.326722100	4.927339229	7.911183890
Pt	5.672659688	4.927130705	7.908858584
Pt	8.500575495	0.027707751	7.912180813
Pt	9.911690474	7.375173043	7.908681107

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.258427092	7.377755791	7.911465876
Pt	7.085668279	2.477674272	7.910542410
Pt	12.743076894	7.377631208	7.913266203
Pt	7.084687600	7.375519629	7.913396740
Pt	9.913170722	2.479227954	7.910928587
Pt	2.839517025	0.026660520	7.911534327
Pt	1.427970267	2.479336984	7.912159043
Pt	4.255722073	2.477074115	7.912361541



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.322113152	6.546134893	5.598937120
Pt	5.663758525	6.545203798	5.597902098
Pt	8.492737757	1.645854558	5.598652047
Pt	2.834427120	1.645395941	5.599688558
Pt	14.150322137	6.545585170	5.599791316
Pt	12.735922000	8.995637419	5.599859853
Pt	15.564216208	8.995321865	5.598668778
Pt	8.491515691	6.544203657	5.598876801
Pt	11.321173207	1.646183320	5.599810254
Pt	5.663281299	1.645811818	5.599969112
Pt	7.077712672	8.994344267	5.598869201
Pt	9.906473850	4.096730509	5.598435361
Pt	4.248622670	4.095210152	5.599591129
Pt	9.906911746	8.995066983	5.599426263
Pt	12.735428042	4.096324425	5.599640878
Pt	7.078854545	4.095414831	5.598158205
Pt	8.499150080	4.926193043	7.915670192
Pt	2.842219968	4.929713057	7.913343751
Pt	5.670762254	0.026804930	7.913161762
Pt	0.013329040	0.027702811	7.912442391
Pt	11.326843558	4.927263966	7.911462445
Pt	5.672412807	4.926954762	7.909335363
Pt	8.500459742	0.027607598	7.912353616

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	9.911822094	7.375197520	7.909233529
Pt	4.258193491	7.377561031	7.911705869
Pt	7.085496021	2.477451597	7.910873307
Pt	12.742960570	7.377430482	7.913313477
Pt	7.084663989	7.375458539	7.913429506
Pt	9.913209151	2.478939211	7.911230695
Pt	2.839672293	0.026651054	7.911775317
Pt	1.427921732	2.479139499	7.912330042
Pt	4.255648837	2.476924337	7.912495236



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.323954207	6.547439714	5.596953390
Pt	5.661881696	6.545992093	5.596670161
Pt	8.492624808	1.645017971	5.597303858
Pt	2.834371568	1.645568435	5.596797415
Pt	14.150400723	6.544458218	5.598738821
Pt	12.734485983	8.996775442	5.598984470
Pt	15.565732409	8.996669540	5.598286977
Pt	8.492530588	6.530836327	5.619119514
Pt	11.319426592	1.649235963	5.592633410
Pt	5.665063757	1.648553771	5.592861042
Pt	7.079162603	8.991832744	5.591846073
Pt	9.895145734	4.104747916	5.618761114
Pt	4.251842078	4.095114349	5.592525148
Pt	9.905063555	8.992846141	5.591909843
Pt	12.732750494	4.096052706	5.592219014
Pt	7.090670243	4.102942274	5.618417625
Pt	8.498283132	4.924738622	8.037552360
Pt	2.841948175	4.931842819	7.916687043
Pt	5.672883405	0.025019918	7.916520600
Pt	0.010902199	0.026234972	7.916275412
Pt	11.342343088	4.921654917	7.899320884
Pt	5.656429203	4.920515383	7.898932004

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Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	8.500386465	0.027337614	7.911168264
Pt	9.914703410	7.390766270	7.897398703
Pt	4.257294037	7.377192465	7.910982029
Pt	7.071884031	2.466905958	7.900143628
Pt	12.742979101	7.377376393	7.911992151
Pt	7.082810264	7.390890142	7.899115000
Pt	9.926339987	2.468565261	7.899658818
Pt	2.840430449	0.031422070	7.909910852
Pt	1.432356385	2.476342624	7.910158991
Pt	4.250931473	2.473874897	7.910241452
H	8.499046829	4.928940885	9.596621047

 $[\text{Pt}_{64}\text{PyrH}]^0$

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350

Continued on Next Page...

Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.313594031	6.530599490	5.599589835
Pt	5.656721452	6.529043993	5.599385877
Pt	8.485211559	1.631197271	5.599989919
Pt	2.827932503	1.629919657	5.599193379
Pt	14.142697351	6.530481999	5.598562680
Pt	12.728091124	8.980527125	5.598998970
Pt	15.557566819	8.980464310	5.598763352
Pt	8.485011041	6.525930919	5.602368443
Pt	11.312517285	1.632035338	5.598472275
Pt	5.658110799	1.630713537	5.598543707
Pt	7.071063081	8.977195624	5.598741571
Pt	9.896651047	4.082016313	5.601365516
Pt	4.243765799	4.080433500	5.598776044
Pt	9.899471905	8.977117436	5.598883587
Pt	12.726675036	4.081715911	5.598490673
Pt	7.073278711	4.080632578	5.601693396
Pt	8.484069007	4.893781376	7.946583232
Pt	2.827534498	4.895245803	7.911017317
Pt	5.654610201	-0.006173925	7.912562996
Pt	-0.000334990	-0.004394579	7.911378542

Continued on Next Page...

Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	11.310925726	4.893695758	7.912892467
Pt	5.658386279	4.891420192	7.913271872
Pt	8.485137090	-0.003951798	7.911714532
Pt	9.896030587	7.342668714	7.916694897
Pt	4.242929290	7.344264487	7.910705927
Pt	7.069540628	2.444905048	7.916403393
Pt	12.727129123	7.344121240	7.911336353
Pt	7.071692276	7.341948857	7.914482000
Pt	9.899198157	2.446671997	7.914208163
Pt	2.827101042	-0.005754204	7.912107085
Pt	1.413507143	2.445461675	7.910813114
Pt	4.241901401	2.443836237	7.911786854
H	8.505265813	4.924589834	10.188482150
C	8.138869653	3.807108114	11.891756212
C	8.894220547	6.048672429	11.883506517
C	8.912345350	6.074606754	13.266939229
C	8.531517947	4.930510645	13.970975104
C	8.140585201	3.784851595	13.275742590
H	7.851912157	2.967491878	11.260554461
H	9.172659666	6.886604574	11.245790933
H	9.221341965	6.981012363	13.782895083
H	8.539580399	4.931991399	15.060795498
H	7.839234197	2.879672460	13.798303781
N	8.512031361	4.926889703	11.247866122



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000

Continued on Next Page...

Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.318507468	6.541724295	5.613516157
Pt	5.661340439	6.541691185	5.613411644
Pt	8.491352679	1.640610707	5.613601522
Pt	2.833114988	1.641239630	5.614929706
Pt	14.147834854	6.543696275	5.615237481
Pt	12.731159892	8.992623383	5.613969442
Pt	15.561675172	8.992653684	5.613590014

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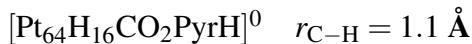
Table ST6 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	8.487721647	6.538575141	5.613431574
Pt	11.321366971	1.642539788	5.615683395
Pt	5.660581240	1.641907472	5.615860217
Pt	7.075419911	8.991090365	5.614454456
Pt	9.904461089	4.091264427	5.612328848
Pt	4.246682259	4.091995406	5.613474272
Pt	9.902200585	8.990251003	5.615735998
Pt	12.733751552	4.093004691	5.614272283
Pt	7.076401078	4.089466529	5.612741746
Pt	8.491294107	4.908848293	7.974147466
Pt	2.835262041	4.914058351	7.970821056
Pt	5.661432479	0.011942738	7.972503173
Pt	0.006530998	0.011226778	7.970643248
Pt	11.321503381	4.910510242	7.968914006
Pt	5.663986302	4.910922135	7.966771323
Pt	8.491366909	0.010368063	7.973089035
Pt	9.904855624	7.358610023	7.966304902
Pt	4.249654070	7.363328242	7.972216462
Pt	7.080597236	2.459784987	7.970724190
Pt	12.734008491	7.360639401	7.972965301
Pt	7.077043944	7.359216296	7.972601547
Pt	9.907491006	2.460609376	7.968256912
Pt	2.832943687	0.011149149	7.973055220
Pt	1.421600151	2.461673420	7.972867568
Pt	4.249410465	2.460975196	7.972290797
H	2.836950617	0.017487789	9.534981556
H	4.255192570	2.478756901	9.534208588
H	5.674617446	4.934563846	9.528458190
H	7.086435206	7.374566746	9.534532382
H	-0.007790068	0.017392803	9.532185449
H	1.423767928	2.482584959	9.534722160
H	2.836733716	4.931500832	9.532715118
H	4.260283756	7.389248461	9.534028733

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Table ST6 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	5.677604773	0.032372197	9.534289785
H	7.103222240	2.484651168	9.532271808
H	8.501427110	4.933725828	9.536085604
H	9.906970653	7.363580639	9.528049126
H	8.510225217	0.017958501	9.535055894
H	9.908593904	2.477835197	9.529932212
H	11.318101300	4.918301857	9.530769149
H	12.748339725	7.377493552	9.534953171

Table ST7: Geometries of constrained optimizations of $[\text{Pt}_{64}\text{H}_{16}\text{CO}_2\text{PyrH}]^0$ with fixed (Pt)H-C(O₂) bond distance obtained using plane-wave-based DFT at the PBE level of theory.

Atom	x (Å)	y (Å)	z (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.316472147	6.533743400	5.609219293
Pt	5.649654529	6.532434205	5.614579127
Pt	8.481885357	1.627417364	5.614615136
Pt	2.823919343	1.630494017	5.618420318
Pt	14.141029538	6.533170173	5.617355504
Pt	12.728466288	8.980233252	5.616922783
Pt	15.553403187	8.980293692	5.617532226
Pt	8.480577130	6.548332959	5.592823848
Pt	11.313992011	1.626834217	5.620827989
Pt	5.649445648	1.624999771	5.620805632
Pt	7.065397061	8.986236071	5.619897374
Pt	9.911208336	4.070891402	5.593419302
Pt	4.231611598	4.079517517	5.620196884
Pt	9.899535038	8.985296005	5.618984631
Pt	12.731110200	4.080606339	5.619228693
Pt	7.049332699	4.070429048	5.595424888
Pt	8.472830811	4.893192378	7.833314526
Pt	2.818816300	4.900285262	7.978098252

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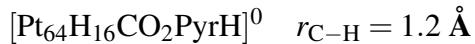
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.652941012	-0.009109594	7.978227129
Pt	-0.007968125	-0.003864212	7.979201126
Pt	11.298862890	4.896578250	7.963483333
Pt	5.651631293	4.894990107	7.972532793
Pt	8.479538874	-0.003322826	7.981430922
Pt	9.888909631	7.336159389	7.963571197
Pt	4.236311338	7.346504891	7.981652475
Pt	7.065654320	2.448816697	7.973638875
Pt	12.720914867	7.345395197	7.979030035
Pt	7.066810893	7.342614866	7.969903347
Pt	9.890918446	2.450420591	7.972219178
Pt	2.824840085	-0.005195602	7.976261997
Pt	1.407594213	2.448625007	7.976804077
Pt	4.234949847	2.444326211	7.977522386
H	2.828165241	-0.019446838	9.537929410
H	4.240363071	2.445100968	9.539166132
H	5.659837406	4.891000752	9.534284002
H	7.086594160	7.307621930	9.530912808
H	-0.015011410	-0.007191010	9.540969915
H	1.398581867	2.454596987	9.538531594
H	2.805341630	4.904118147	9.539874753
H	4.235141539	7.344375386	9.543048567
H	5.648841247	-0.023919883	9.539966152
H	7.074675659	2.465957087	9.535418945
H	8.020368334	4.763394259	10.502441708
H	9.844342046	7.197933012	9.518863909
H	8.475890073	-0.000863676	9.542777200
H	9.861293953	2.487157060	9.533279019
H	11.176584982	4.928500531	9.519930219
H	12.701723282	7.336005356	9.540230763
C	8.426023938	4.886675791	11.517624419
O	9.533319178	5.619909898	11.488894458
O	7.903416996	4.398070826	12.506957066

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	11.486152460	5.057431903	14.324296805
C	12.072518177	5.197903968	15.576608223
C	11.822549751	6.358516105	16.304143242
C	10.995617559	7.336596884	15.755222714
C	10.451351896	7.115764674	14.494663228
N	10.693433175	5.999096603	13.797260592
H	12.267319057	6.500811409	17.287505310
H	11.645689065	4.167450281	13.713592576
H	12.711358262	4.409243141	15.971694374
H	10.773167140	8.256034168	16.292969683
H	9.798396890	7.848106190	14.018100200
H	9.958287885	5.743058984	12.442611451



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.316441681	6.534261996	5.608501540
Pt	5.649007761	6.532667554	5.614522029
Pt	8.481336382	1.627502926	5.614441421
Pt	2.824776855	1.631470690	5.619697740
Pt	14.142709004	6.534317563	5.617006591
Pt	12.730114935	8.981518300	5.616311113
Pt	15.555418941	8.981857588	5.618622814
Pt	8.480337686	6.542708476	5.597078493
Pt	11.315491690	1.629407423	5.619321288
Pt	5.649282478	1.626684167	5.619717735
Pt	7.067759350	8.987003280	5.618246723
Pt	9.905421573	4.074594297	5.598006380
Pt	4.232523781	4.079019108	5.618999997
Pt	9.898832627	8.984718884	5.617445661
Pt	12.729807415	4.080918630	5.617891335
Pt	7.052641076	4.072780269	5.600659140
Pt	8.470489291	4.893906283	7.868457864
Pt	2.820487838	4.900217309	7.972484835
Pt	5.653089198	-0.007261719	7.972136096

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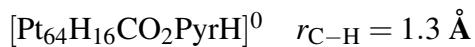
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	-0.005116615	-0.001677479	7.975936461
Pt	11.301900500	4.898143538	7.960036051
Pt	5.649479821	4.896399995	7.971766723
Pt	8.481073956	-0.002613440	7.983746424
Pt	9.891316730	7.338971215	7.960936951
Pt	4.237166008	7.348553527	7.984282872
Pt	7.065491811	2.447014038	7.973571489
Pt	12.722302302	7.346765369	7.974677954
Pt	7.066122684	7.344633296	7.964068604
Pt	9.891493309	2.449796842	7.965295124
Pt	2.825969640	-0.004449354	7.976819692
Pt	1.408279167	2.450218811	7.977923927
Pt	4.236665460	2.445731201	7.979772668
H	2.829501357	-0.014272755	9.538895238
H	4.241283104	2.446473738	9.541722035
H	5.662942039	4.889299856	9.533678068
H	7.082984530	7.320274348	9.525195776
H	-0.013309340	-0.005659917	9.537980815
H	1.402478725	2.454615190	9.540094655
H	2.812312457	4.904263080	9.534378775
H	4.236599156	7.345739412	9.546288784
H	5.650917826	-0.016862326	9.533941133
H	7.074747228	2.469437267	9.535617771
H	8.234076928	4.821618113	10.197435990
H	9.865593932	7.222474350	9.518142605
H	8.476806707	0.002063385	9.545649524
H	9.868631516	2.477352210	9.526451694
H	11.209048574	4.935954382	9.518044587
H	12.705389024	7.339410352	9.536126841
C	8.570249802	4.920710809	11.345297413
O	9.638913649	5.691321994	11.426316427
O	7.980546379	4.364557322	12.253164737
C	11.646557185	5.152552904	14.196935837

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	12.416162116	5.390613660	15.330666448
C	12.264567504	6.605410407	15.995299733
C	11.353491982	7.538248738	15.504218477
C	10.626005328	7.218297517	14.363236532
N	10.770721066	6.049756883	13.726786510
H	12.852191819	6.824613622	16.886263387
H	11.726111198	4.218526200	13.638338425
H	13.126353916	4.641111921	15.676751352
H	11.213758245	8.503062490	15.989242711
H	9.902574337	7.913555882	13.933436803
H	10.019681715	5.788052225	12.409733564



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.318505359	6.536062362	5.606344904
Pt	5.651858923	6.533800901	5.615424327
Pt	8.483443994	1.630163636	5.615298839
Pt	2.827798516	1.634329262	5.616649386
Pt	14.143838605	6.534061067	5.616324808
Pt	12.729448545	8.984036421	5.616065788
Pt	15.556546261	8.983109473	5.616665076
Pt	8.481185132	6.539117809	5.603607342
Pt	11.316193160	1.631750335	5.617399512
Pt	5.653893127	1.631766971	5.618298124
Pt	7.069504171	8.987027705	5.616706753
Pt	9.902556885	4.077748289	5.603897563
Pt	4.238686701	4.082390817	5.618007701
Pt	9.899411239	8.989464893	5.613811745
Pt	12.733504798	4.080842410	5.614196795
Pt	7.062113961	4.078706651	5.607082198
Pt	8.477924292	4.898873404	7.914593090
Pt	2.825382953	4.901542126	7.974446852
Pt	5.655797408	-0.001125625	7.974351093
Pt	-0.002326849	0.000955260	7.973400826

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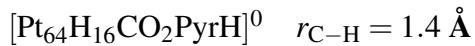
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Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
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Pt	5.651888496	4.900437017	7.972918381
Pt	8.483381253	0.000249455	7.979085079
Pt	9.899557519	7.350322185	7.948155117
Pt	4.239704728	7.350142165	7.979439874
Pt	7.068659105	2.448138690	7.973298709
Pt	12.727574460	7.350470074	7.974851827
Pt	7.066038183	7.350768838	7.967280381
Pt	9.896269148	2.448395843	7.967914798
Pt	2.827519181	-0.000319694	7.973905621
Pt	1.411603954	2.451997344	7.974414443
Pt	4.241211532	2.450219871	7.976350074
H	2.828022572	-0.005459114	9.536070392
H	4.248030636	2.454081849	9.538291443
H	5.686151943	4.884095371	9.534513137
H	7.070396433	7.336572541	9.528999193
H	-0.008434347	-0.001127045	9.535523433
H	1.407345801	2.455087104	9.536638531
H	2.820688690	4.904618058	9.536609945
H	4.240784647	7.352838772	9.541137277
H	5.655967538	-0.004246010	9.536483008
H	7.074530873	2.492341071	9.534791906
H	8.362919908	4.866845386	9.920538998
H	9.892356131	7.271372935	9.506329046
H	8.484747830	0.002808458	9.540777996
H	9.878776720	2.465392000	9.529583105
H	11.240552381	4.937621851	9.506664099
H	12.716788324	7.345553781	9.536573702
C	8.616082200	4.978951259	11.190906020
O	9.724568630	5.655692418	11.332389950
O	7.883899673	4.494328109	12.027289404
C	11.660366626	5.150711163	14.090751597
C	12.388093912	5.381199947	15.252290635

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	12.205018562	6.587589339	15.924404258
C	11.311163736	7.524207538	15.410428987
C	10.623206410	7.215156451	14.243079760
N	10.794013689	6.049589899	13.607036393
H	12.758033611	6.798005853	16.838876514
H	11.766302900	4.228165630	13.517997069
H	13.086490572	4.629911335	15.615383799
H	11.149821746	8.482601950	15.899952382
H	9.916182110	7.911133995	13.789255293
H	10.079814879	5.777890078	12.345330271



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.317790699	6.534561106	5.605865118
Pt	5.651869226	6.532826100	5.615383137
Pt	8.483233195	1.629332050	5.615629389
Pt	2.827200654	1.633051880	5.614488658
Pt	14.143559428	6.531596966	5.616830382
Pt	12.728072258	8.983549767	5.616650282
Pt	15.556841037	8.982368801	5.617420247
Pt	8.479613011	6.533254101	5.609160142
Pt	11.314820841	1.631303976	5.614469411
Pt	5.653892967	1.631833676	5.613440452
Pt	7.069493748	8.984898081	5.613336997
Pt	9.896902450	4.078173087	5.610386216
Pt	4.239524917	4.080940488	5.613112653
Pt	9.898682291	8.988140257	5.609512933
Pt	12.732292859	4.079284397	5.610618481
Pt	7.065907345	4.080050506	5.613085016
Pt	8.477188610	4.896919184	7.946909968
Pt	2.827806076	4.898911891	7.973083223
Pt	5.656002839	0.000313843	7.972878306
Pt	-0.001234453	0.000076239	7.970912572
Pt	11.318759378	4.901206675	7.941111923

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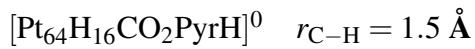
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
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Pt	8.484110658	-0.000290667	7.975438991
Pt	9.903740507	7.353670791	7.938871784
Pt	4.240725479	7.348940641	7.975437389
Pt	7.067523385	2.442622335	7.967301820
Pt	12.728640238	7.349614632	7.971167321
Pt	7.064843899	7.352922473	7.964823961
Pt	9.898558502	2.444270337	7.966781961
Pt	2.828339764	-0.001585565	7.968878185
Pt	1.411806000	2.451070192	7.969935352
Pt	4.242876496	2.450019148	7.970839902
H	2.832718158	-0.004207075	9.531285103
H	4.250063978	2.453470907	9.532917734
H	5.671323471	4.881163908	9.527720531
H	7.065730007	7.356010934	9.526899915
H	0.000401625	-0.000092210	9.533225841
H	1.413550464	2.453788272	9.532464126
H	2.835800350	4.897199411	9.535502589
H	4.247191992	7.347050904	9.537200936
H	5.656599693	0.005492967	9.535249898
H	7.063731069	2.472772039	9.528481586
H	8.428684978	4.892692382	9.717826714
H	9.891579970	7.288946222	9.497068360
H	8.485606275	0.006518551	9.537209544
H	9.896464989	2.445962827	9.528929457
H	11.258126481	4.927263208	9.499446416
H	12.723233799	7.347265877	9.533237148
C	8.601232264	4.992118969	11.103795665
O	9.656834491	5.631214887	11.328480664
O	7.720332743	4.453833741	11.736082031
C	11.688560324	5.143216428	14.002347517
C	12.362932620	5.369163306	15.189124544
C	12.152533062	6.570446290	15.869879225

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	11.273610960	7.516536500	15.337393732
C	10.626892189	7.235361231	14.147462803
N	10.840170369	6.067193672	13.514424078
H	12.670340814	6.768649005	16.806808320
H	11.802338308	4.238041614	13.407931108
H	13.043717652	4.613051726	15.573253095
H	11.089964014	8.463768815	15.839231180
H	9.932527534	7.919935818	13.662708250
H	10.271237343	5.847368624	12.568996250



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.320680057	6.540384168	5.612108451
Pt	5.658389599	6.539231136	5.615190232
Pt	8.488651378	1.637791995	5.615656015
Pt	2.830994999	1.639283219	5.614299956
Pt	14.147090890	6.537676641	5.616049071
Pt	12.732557330	8.989121845	5.615846300
Pt	15.561276284	8.988547587	5.615715411
Pt	8.487283536	6.538911197	5.618064294
Pt	11.318156962	1.638658505	5.613642393
Pt	5.657532584	1.637503900	5.610693826
Pt	7.074470460	8.990477045	5.612796740
Pt	9.901574771	4.087686704	5.618516572
Pt	4.242502687	4.086855167	5.610518429
Pt	9.903898413	8.992632823	5.610801842
Pt	12.734882232	4.086911784	5.611344118
Pt	7.071746937	4.087760752	5.615919624
Pt	8.489258039	4.912830593	7.968968431
Pt	2.836254217	4.910243600	7.972752746
Pt	5.663811125	0.014362548	7.971881839
Pt	0.005806571	0.012909961	7.969043791
Pt	11.329332107	4.913765641	7.953437674
Pt	5.654066309	4.912380546	7.961722129

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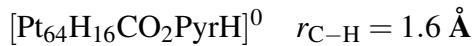
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Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	8.493087900	0.012721306	7.970848340
Pt	9.912499918	7.368962522	7.953843733
Pt	4.249141919	7.362118210	7.971017042
Pt	7.073888983	2.454898725	7.962409841
Pt	12.737394008	7.362739068	7.971596102
Pt	7.074390179	7.365316606	7.968575549
Pt	9.906670715	2.459165056	7.971078572
Pt	2.834990674	0.012125446	7.968538040
Pt	1.419497173	2.462620613	7.969360518
Pt	4.250292713	2.462495397	7.970793997
H	2.839928516	0.029367000	9.531270106
H	4.264127287	2.479341259	9.533274319
H	5.670416445	4.902804074	9.523077588
H	7.068338787	7.390010169	9.531293053
H	0.015420262	0.027816902	9.531674864
H	1.431032757	2.476650527	9.532240815
H	2.854605353	4.925965285	9.535378245
H	4.261065663	7.376063086	9.533420787
H	5.670643896	0.032627715	9.534522981
H	7.063715696	2.482324553	9.523691414
H	8.439839127	4.893709275	9.645946107
H	9.916075249	7.370113388	9.514563959
H	8.500660392	0.030182211	9.533269032
H	9.919112593	2.457138173	9.534002945
H	11.323136547	4.938164159	9.514039656
H	12.748543415	7.380456673	9.534443356
C	8.516666769	4.954265739	11.142970701
O	9.555737826	5.543905181	11.398980023
O	7.540000168	4.407666877	11.572308430
C	11.764260113	5.182170939	14.115559708
C	12.359369809	5.369094463	15.345288760
C	12.113756274	6.550855019	16.059056133
C	11.275948591	7.524831846	15.496003861

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	10.701669709	7.295736626	14.262994732
N	10.948052589	6.136741796	13.604527565
H	12.564030530	6.709818866	17.035760553
H	11.903080291	4.295360447	13.501826216
H	13.005590394	4.592501343	15.748753864
H	11.064622190	8.454295848	16.019236474
H	10.041480601	7.999286699	13.761714971
H	10.425867503	5.932192970	12.710594113



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.317635678	6.535321640	5.612361555
Pt	5.657007250	6.535195519	5.614655880
Pt	8.487262287	1.633366024	5.615097207
Pt	2.829269401	1.634835497	5.614580437
Pt	14.144873393	6.534119998	5.615419080
Pt	12.730453589	8.984426493	5.615361357
Pt	15.559167919	8.984322918	5.615970809
Pt	8.485534161	6.531012856	5.622095712
Pt	11.316258148	1.635231684	5.613506419
Pt	5.656758475	1.634126585	5.609691541
Pt	7.073041910	8.984639756	5.613090590
Pt	9.897677027	4.084915159	5.622455509
Pt	4.242500886	4.083342804	5.609451663
Pt	9.900786743	8.986385346	5.610523455
Pt	12.731740995	4.082875385	5.611011420
Pt	7.073888198	4.085100800	5.620177474
Pt	8.487005523	4.902988812	7.990799366
Pt	2.832091355	4.901238816	7.968391684
Pt	5.658945830	0.004819461	7.967857158
Pt	0.001915282	0.003149197	7.967645629
Pt	11.324224472	4.903226734	7.954293911
Pt	5.651971432	4.903225334	7.959210017
Pt	8.488407642	0.002407765	7.971652860

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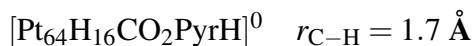
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	9.906742790	7.358613398	7.954180654
Pt	4.244313735	7.352962938	7.971366004
Pt	7.070571631	2.446495283	7.960380136
Pt	12.732604393	7.353131985	7.970756167
Pt	7.070652577	7.354664855	7.967084793
Pt	9.902515218	2.449571367	7.968136454
Pt	2.830535236	0.003495940	7.969876979
Pt	1.416414905	2.452559476	7.970712133
Pt	4.246290260	2.453620107	7.968993390
H	2.831895147	0.011960628	9.532236731
H	4.254608079	2.459600033	9.530992629
H	5.650893375	4.887392034	9.519731361
H	7.056536413	7.375345819	9.529315731
H	0.005819382	0.006298033	9.529724032
H	1.422588992	2.449789065	9.533092811
H	2.842746214	4.901411830	9.530488677
H	4.246083568	7.352760018	9.533455687
H	5.660932892	0.014664647	9.529914649
H	7.051733525	2.454848437	9.520883864
H	8.461255532	4.893624450	9.630215091
H	9.913464906	7.369217933	9.514548668
H	8.487471354	0.007558035	9.533686479
H	9.910492281	2.431599956	9.530353273
H	11.331686146	4.908900261	9.514679348
H	12.736644639	7.358475849	9.533214374
C	8.491621277	4.927359393	11.229802703
O	9.524899494	5.504081832	11.465723994
O	7.490781408	4.373905395	11.556097975
C	11.808610709	5.200429791	14.207926567
C	12.393821824	5.388289980	15.440398625
C	12.140739308	6.567911578	16.156943676
C	11.305988305	7.542170529	15.588979659
C	10.738843521	7.318387664	14.354216893

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
N	10.992291411	6.157913789	13.692291222
H	12.585648487	6.725092006	17.137389430
H	11.955387496	4.315615225	13.593831920
H	13.045850376	4.615406787	15.840457541
H	11.096573910	8.475135294	16.107403349
H	10.082619193	8.023731912	13.850718711
H	10.497264325	5.965034983	12.798519248



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.318119133	6.537482011	5.613952497
Pt	5.660102188	6.538137099	5.615263244
Pt	8.489230892	1.637663292	5.615448193
Pt	2.831084340	1.637571157	5.614043802
Pt	14.146578480	6.536845217	5.614395757
Pt	12.731469923	8.987745232	5.614388746
Pt	15.561007676	8.987594674	5.614407378
Pt	8.487787174	6.532749695	5.626177935
Pt	11.317247212	1.638725566	5.614256769
Pt	5.659441639	1.638344708	5.610382759
Pt	7.074995669	8.986826308	5.613890204
Pt	9.898001343	4.088910428	5.626585464
Pt	4.245376145	4.086527548	5.609884464
Pt	9.902142749	8.988320877	5.611787127
Pt	12.732198423	4.085673830	5.611465991
Pt	7.077834870	4.089983416	5.624321477
Pt	8.492087469	4.910489252	8.007162658
Pt	2.834538222	4.906845157	7.966952199
Pt	5.662248037	0.011098645	7.967411048
Pt	0.003891513	0.007924103	7.967768022
Pt	11.326392535	4.907282430	7.959507532
Pt	5.655801858	4.909036983	7.962138446
Pt	8.490987537	0.007584328	7.969590493
Pt	9.909063753	7.363797161	7.960340256

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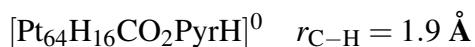
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.247378350	7.358440326	7.969525518
Pt	7.075279883	2.454430010	7.962930769
Pt	12.735193606	7.358629022	7.968796548
Pt	7.074295409	7.360111477	7.971471295
Pt	9.905465938	2.455021329	7.972275730
Pt	2.833113035	0.009299872	7.969591584
Pt	1.419679569	2.456940150	7.969844431
Pt	4.249440609	2.459140264	7.968042910
H	2.833065428	0.021716164	9.532168234
H	4.262595894	2.473942277	9.530328460
H	5.637666725	4.907633053	9.522817896
H	7.055453797	7.397500242	9.533792613
H	-0.002728434	0.010156897	9.530407336
H	1.429202070	2.459589946	9.532598400
H	2.845245027	4.916687823	9.529530356
H	4.252294526	7.372550750	9.532002144
H	5.672018546	0.033249451	9.529764269
H	7.064025936	2.458339950	9.523835595
H	8.480539383	4.913980546	9.621156592
H	9.926639121	7.393925517	9.520961995
H	8.498208099	0.009841159	9.532203162
H	9.920567076	2.428171872	9.535067869
H	11.354117609	4.912487143	9.520448814
H	12.747025403	7.371893164	9.531703963
C	8.479401213	4.928559089	11.321340080
O	9.511329718	5.500068428	11.526187363
O	7.465400968	4.370388564	11.558694334
C	11.820378356	5.207551784	14.335603529
C	12.384670859	5.385096048	15.577698755
C	12.126549892	6.560500277	16.301853171
C	11.301297890	7.541662332	15.728485467
C	10.752494811	7.332891404	14.484065209
N	11.013950310	6.175098419	13.812365272

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
H	12.558293755	6.708530781	17.288617029
H	11.976514928	4.326434630	13.719307145
H	13.026695301	4.606255345	15.982620916
H	11.085459933	8.469662795	16.252801964
H	10.107105513	8.046058425	13.979261270
H	10.547089782	6.000733912	12.909323634



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.313760015	6.529707283	5.612597597
Pt	5.651633863	6.534300404	5.611665400
Pt	8.485255496	1.624904230	5.611210736
Pt	2.822354743	1.628066426	5.616000914
Pt	14.140045485	6.529562370	5.616707377
Pt	12.726150820	8.978137613	5.617270931
Pt	15.556506771	8.979812872	5.616677677
Pt	8.481291909	6.525539539	5.620133627
Pt	11.312966362	1.629596565	5.615445338
Pt	5.647144202	1.625700844	5.607289920
Pt	7.070044179	8.980795544	5.615763506
Pt	9.892719277	4.079517818	5.619791766
Pt	4.232825059	4.076389554	5.607644809
Pt	9.895856071	8.979488662	5.614518212
Pt	12.724832923	4.077439681	5.614314458
Pt	7.064625931	4.078159772	5.609232224
Pt	8.463334910	4.882287120	7.975992508
Pt	2.820217145	4.891204793	7.971151142
Pt	5.650768869	-0.006265079	7.972081706
Pt	-0.005235714	-0.006864172	7.975237443
Pt	11.307762221	4.891594849	7.957504581
Pt	5.636025244	4.895630143	7.942591137
Pt	8.482211394	-0.011513698	7.974323452
Pt	9.895167772	7.343030049	7.955150093
Pt	4.233187948	7.346161147	7.974526924

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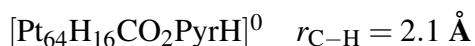
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Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
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Pt	12.721409341	7.340666751	7.973001748
Pt	7.063760945	7.345621966	7.965397931
Pt	9.895765427	2.438951753	7.966310656
Pt	2.823178749	-0.005830180	7.976216106
Pt	1.408039384	2.441087641	7.974891892
Pt	4.233483575	2.442307561	7.970497738
H	2.824413983	-0.000807957	9.539341459
H	4.241074178	2.447308625	9.533271455
H	5.569682450	4.888468119	9.501462804
H	7.042845872	7.367195108	9.528587048
H	-0.012852239	-0.020017643	9.538082795
H	1.411706524	2.424262243	9.537738222
H	2.814659196	4.876132026	9.534217952
H	4.219800504	7.335584122	9.537198162
H	5.652807665	-0.003132904	9.535558226
H	7.024979801	2.374767194	9.498759977
H	8.355741043	4.808433639	9.552152358
H	9.899265050	7.351216721	9.517790795
H	8.474563747	-0.021595010	9.537054133
H	9.902324145	2.400454852	9.529276041
H	11.316951895	4.874452701	9.520451963
H	12.716471366	7.328452128	9.536676834
C	8.158168123	4.758027614	11.440924591
O	9.125916837	5.409737879	11.626446360
O	7.184089760	4.109559047	11.506754537
C	11.922592860	6.012678097	13.937924772
C	12.613684112	6.552457028	14.996720764
C	12.335512342	7.862618933	15.417726589
C	11.349604992	8.598932516	14.740090367
C	10.676735486	8.031367807	13.683124958
N	10.972551853	6.755765571	13.301486887
H	12.875916282	8.301031029	16.253192503

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
H	12.083600331	5.007868628	13.554786709
H	13.372361812	5.950213624	15.492146393
H	11.106483878	9.617270467	15.031737276
H	9.907245367	8.538550455	13.107240619
H	10.438536375	6.331337252	12.536779835



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.243069860	5.716053740	3.309634350
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.313237781	6.532216566	5.614208884
Pt	5.654048710	6.534756805	5.612873794
Pt	8.485100528	1.629862959	5.612278938
Pt	2.824465624	1.631083476	5.616620316
Pt	14.141322089	6.532899317	5.615763085
Pt	12.727238033	8.981068259	5.616392052
Pt	15.556371302	8.981991242	5.615836074
Pt	8.482784835	6.531270990	5.617343079
Pt	11.313691419	1.631609693	5.615739442
Pt	5.650013380	1.628750116	5.609544677
Pt	7.070258273	8.982954285	5.615946136
Pt	9.896657357	4.081610323	5.616916979
Pt	4.235276163	4.080326298	5.610017678
Pt	9.898050377	8.981758994	5.615684227
Pt	12.726589298	4.081462419	5.615151393
Pt	7.064948508	4.080152862	5.609803623
Pt	8.470127096	4.890522049	7.961559700
Pt	2.822874867	4.897042368	7.971675715
Pt	5.652898818	-0.001927788	7.973394081
Pt	-0.004309360	-0.002784727	7.973978806
Pt	11.310247921	4.896832892	7.964388278
Pt	5.641667983	4.899371633	7.952783642
Pt	8.483183303	-0.005187471	7.973030829
Pt	9.896459590	7.347747975	7.964733975
Pt	4.236330882	7.349625664	7.973325581
Pt	7.062533274	2.437367667	7.950535359

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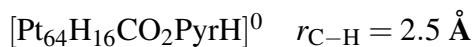
Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	12.723287174	7.345948608	7.972464781
Pt	7.065715651	7.349474201	7.969023397
Pt	9.897046896	2.444530048	7.967692544
Pt	2.824859019	-0.001902770	7.974990996
Pt	1.409795453	2.446716119	7.973720977
Pt	4.236790134	2.447623338	7.970261049
H	2.824782731	0.009619546	9.538219403
H	4.241519919	2.455013888	9.532998386
H	5.592011006	4.893123304	9.512909587
H	7.045958479	7.371348475	9.532436341
H	-0.007294843	-0.007441619	9.536804695
H	1.416713777	2.437055805	9.536659330
H	2.820241506	4.886501553	9.534704998
H	4.228221976	7.344281609	9.536114632
H	5.653610952	0.007371783	9.536715628
H	7.031762767	2.396943329	9.510320029
H	8.390581118	4.840286671	9.529627046
H	9.900024590	7.358028503	9.528396378
H	8.478607203	-0.007851330	9.535856131
H	9.906483399	2.413938563	9.531012032
H	11.321466248	4.885612534	9.527564449
H	12.721937218	7.339937833	9.536224204
C	8.164735865	4.699376980	11.612460241
O	9.160501690	5.309977039	11.762876322
O	7.169159835	4.086956114	11.602644185
C	11.998518801	6.080054709	13.984427551
C	12.618204844	6.577907316	15.106368362
C	12.317588035	7.875975394	15.552762296
C	11.384317154	8.643214349	14.835338489
C	10.781833503	8.118369819	13.715231042
N	11.096686153	6.853366041	13.310528932
H	12.799298485	8.279628481	16.440788474
H	12.179792382	5.088933035	13.577022734

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
H	13.335235810	5.954283049	15.635045680
H	11.126281664	9.651797209	15.148905749
H	10.056991497	8.651646206	13.105819854
H	10.615780982	6.457553458	12.500952745



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	5.657425640	0.000000000	1.000000000
Pt	2.828712820	4.899474320	1.000000000
Pt	8.486138460	4.899474320	1.000000000
Pt	0.000000000	0.000000000	1.000000000
Pt	2.828712820	-0.000000720	1.000000000
Pt	1.414355780	2.449737520	1.000000000
Pt	4.243069860	2.449737520	1.000000000
Pt	8.486138460	-0.000000720	1.000000000
Pt	7.071781420	2.449737520	1.000000000
Pt	9.900495500	2.449737520	1.000000000
Pt	5.657425640	4.899473600	1.000000000
Pt	4.243068600	7.349211850	1.000000000
Pt	7.071782680	7.349211850	1.000000000
Pt	11.314851280	4.899473600	1.000000000
Pt	9.900494240	7.349211850	1.000000000
Pt	12.729208320	7.349211850	1.000000000
Pt	14.143564100	8.165790540	3.309634350
Pt	8.486138460	8.165790540	3.309634350
Pt	11.314851280	3.266316220	3.309634350
Pt	5.657425640	3.266316220	3.309634350
Pt	9.900494240	0.816579420	3.309634350
Pt	4.243068600	0.816579420	3.309634350
Pt	7.071782680	0.816579420	3.309634350
Pt	5.657425640	8.165789820	3.309634350
Pt	2.828712820	3.266315490	3.309634350
Pt	4.243069860	5.716053740	3.309634350

Continued on Next Page...

Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	11.314851280	8.165789820	3.309634350
Pt	12.729207060	5.716053740	3.309634350
Pt	8.486138460	3.266315490	3.309634350
Pt	7.071781420	5.716053740	3.309634350
Pt	9.900495500	5.716053740	3.309634350
Pt	1.414357040	0.816579420	3.309634350
Pt	11.315427443	6.532485684	5.613519041
Pt	5.657150156	6.533629717	5.612473594
Pt	8.486616997	1.632368317	5.612779187
Pt	2.827615240	1.632600668	5.612676597
Pt	14.142760112	6.531701889	5.614692316
Pt	12.728086494	8.981657608	5.614526954
Pt	15.557516743	8.982519644	5.614542537
Pt	8.484753023	6.532160288	5.614895960
Pt	11.315144393	1.632936378	5.613453142
Pt	5.655020695	1.631306765	5.611564753
Pt	7.071617501	8.981710989	5.613937674
Pt	9.901009047	4.082466960	5.614971432
Pt	4.240335168	4.081414605	5.611355394
Pt	9.899876866	8.983263311	5.612043817
Pt	12.729959246	4.082135572	5.613863549
Pt	7.071881203	4.081604598	5.612213613
Pt	8.485120832	4.895598806	7.964248165
Pt	2.828072795	4.895526855	7.972855113
Pt	5.655401434	-0.003274518	7.970904215
Pt	0.000130804	-0.002608589	7.968283805
Pt	11.317037462	4.896444919	7.963835299
Pt	5.653990977	4.895928545	7.955144277
Pt	8.484938451	-0.002759046	7.966581956
Pt	9.900073884	7.348919400	7.958600823
Pt	4.241402301	7.346340447	7.966271506
Pt	7.068063602	2.443441784	7.959737054
Pt	12.729304749	7.346741135	7.969897866

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Table ST7 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	7.069151239	7.347344172	7.970532371
Pt	9.900095412	2.445260768	7.967222826
Pt	2.827763170	-0.001837566	7.966394034
Pt	1.414355675	2.446432712	7.968004998
Pt	4.241629115	2.446316207	7.968296012
H	2.831092533	0.007699588	9.528754195
H	4.241885848	2.440856775	9.530765789
H	5.639382992	4.880555404	9.516481785
H	7.060218188	7.354765435	9.533894574
H	0.018572034	0.003276588	9.530647772
H	1.418928686	2.431718064	9.530477998
H	2.834317151	4.884837826	9.535755098
H	4.234985457	7.327440685	9.528464469
H	5.648482035	-0.006618443	9.533661141
H	7.041114433	2.429031452	9.521284019
H	8.485019572	4.887550809	9.529465609
H	9.905978357	7.363234281	9.520913146
H	8.470843219	0.002381231	9.528859561
H	9.904587443	2.432271560	9.530339738
H	11.326979425	4.895758006	9.526594837
H	12.725446769	7.344402001	9.533069611
C	8.333942296	4.876393383	12.024704454
O	9.360953347	5.443628120	12.095990514
O	7.312240531	4.312613042	12.014943039
C	12.358203209	5.505163836	14.435596937
C	13.063004155	5.759638189	15.586849913
C	12.898492908	6.984312864	16.259363864
C	12.004281483	7.929866534	15.725200758
C	11.311803049	7.649004428	14.572492966
N	11.494536041	6.446461157	13.944477017
H	13.452052268	7.194675293	17.171592651
H	12.440983694	4.585284271	13.864139288
H	13.744406744	4.999801612	15.961867163

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Table ST7 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	11.845538130	8.890487944	16.209905421
H	10.610802267	8.333844024	14.104101714
H	10.948736506	6.230807907	13.109767914

Table ST8: Optimized geometries at PBE level of theory with SDD basis set for Pt and 6-31G(d) basis set for C, H, N and O.

H₂

Atom	x (Å)	y (Å)	z (Å)
H	0.000000	0.000000	0.376770
H	0.000000	0.000000	-0.376770

Pyr

Atom	x (Å)	y (Å)	z (Å)
C	-1.146523	0.724841	-0.000008
C	-1.204243	-0.677000	0.000024
C	0.000000	-1.393550	0.000031
C	1.204243	-0.677000	0.000006
C	1.146524	0.724841	-0.000025
H	-2.071822	1.316395	-0.000014
H	-2.171091	-1.190882	0.000043
H	0.000000	-2.488830	0.000056
H	2.171091	-1.190882	0.000010
H	2.071822	1.316395	-0.000045
N	0.000000	1.432145	-0.000032

[Pyr]⁺

Atom	x (Å)	y (Å)	z (Å)
C	0.658142	1.214438	-0.008832
C	-0.715452	1.217762	-0.007604
C	-1.457288	0.000000	0.008924

Continued on Next Page...

Table ST8 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	-0.715452	-1.217762	-0.007604
C	0.658141	-1.214438	-0.008832
H	1.269622	2.118776	-0.016522
H	-1.230735	2.183612	-0.020961
H	-2.548422	0.000000	-0.004087
H	-1.230736	-2.183612	-0.020961
H	1.269621	-2.118776	-0.016522
N	1.366800	0.000000	0.067547
H	2.334506	0.000000	-0.250086

 [PyrH]⁺

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	-0.670427	1.196037	0.000006
C	0.720421	1.216653	-0.000025
C	1.422892	0.000003	-0.000032
C	0.720427	-1.216649	-0.000007
C	-0.670421	-1.196040	0.000024
H	-1.295974	2.090987	0.000013
H	1.241858	2.176629	-0.000043
H	2.516820	0.000006	-0.000056
H	1.241868	-2.176624	-0.000011
H	-1.295965	-2.090993	0.000046
N	-1.315098	-0.000003	0.000029
H	-2.340272	-0.000005	0.000052

[Pt]

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	0.000000	0.000000	0.000000

 [PtH]⁺

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
H	0.000000	0.000000	-1.522345

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Table ST8 – Continued

Atom	x (Å)	y (Å)	z (Å)
Pt	0.000000	0.000000	0.019517



Atom	x (Å)	y (Å)	z (Å)
C	-2.304209	1.190671	-0.000097
C	-3.696695	1.215771	-0.000155
C	-4.400262	-0.000046	-0.000184
C	-3.696617	-1.215817	-0.000155
C	-2.304132	-1.190627	-0.000097
H	-1.677340	2.085734	-0.000071
H	-4.218042	2.176162	-0.000176
H	-5.494404	-0.000081	-0.000229
H	-4.217902	-2.176242	-0.000177
H	-1.677205	-2.085649	-0.000072
N	-1.656562	0.000043	-0.000070
H	-0.583109	0.000074	-0.000026
Pt	1.639429	0.000000	0.000069

Table ST9: Geometries of model clusters generated from optimized structures obtained via plane-wave-based DFT at the PBE level of theory.



Atom	x (Å)	y (Å)	z (Å)
Pt	-3.990614	-2.823212	-0.076082
Pt	-1.305169	-2.820071	-0.964894
Pt	1.380277	-2.816931	-1.853707
Pt	3.343971	-1.416203	-0.409374
Pt	-2.026568	-1.422301	1.368593
Pt	1.368440	-0.003400	-1.859264
Pt	-3.998924	-0.012477	-0.085611
Pt	0.657842	-1.416268	0.478321
Pt	-1.312218	-0.007116	-0.972400

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Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	0.658809	1.439226	0.501776
Pt	2.624260	0.000662	1.936972
Pt	-1.319611	2.821773	-0.967925
Pt	3.336601	1.418905	-0.404089
Pt	-2.031606	1.411772	1.373392
Pt	5.311190	0.001809	1.047802
Pt	1.365870	2.826656	-1.857136
Pt	-0.057233	-0.001931	2.826068
Pt	-4.005315	2.819106	-0.082441



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	-3.990614	-2.823212	-0.076082
Pt	-1.305169	-2.820071	-0.964894
Pt	1.380277	-2.816931	-1.853707
Pt	3.343971	-1.416203	-0.409374
Pt	-2.026568	-1.422301	1.368593
Pt	1.368440	-0.003400	-1.859264
Pt	-3.998924	-0.012477	-0.085611
Pt	0.657842	-1.416268	0.478321
Pt	-1.312218	-0.007116	-0.972400
Pt	0.658809	1.439226	0.501776
Pt	2.624260	0.000662	1.936972
Pt	-1.319611	2.821773	-0.967925
Pt	3.336601	1.418905	-0.404089
Pt	-2.031606	1.411772	1.373392
Pt	5.311190	0.001809	1.047802
Pt	1.365870	2.826656	-1.857136
Pt	-0.057233	-0.001931	2.826068
Pt	-4.005315	2.819106	-0.082441



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Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.015971	-2.806384	-0.077603
Pt	1.332315	-2.811452	-0.971792
Pt	-1.351344	-2.816519	-1.865981
Pt	-3.335889	-1.431199	-0.420412
Pt	2.036427	-1.420166	1.368595
Pt	-0.649987	-1.398559	0.474456
Pt	-1.356625	-0.000447	-1.850246
Pt	4.003930	-0.006290	-0.087684
Pt	1.305477	0.005397	-0.964865
Pt	-0.687189	1.504915	0.552063
Pt	-3.357666	1.388371	-0.424548
Pt	2.034095	1.399496	1.371072
Pt	-2.638767	-0.033931	1.937447
Pt	1.321954	2.813624	-0.977214
Pt	-5.320881	-0.022728	1.040432
Pt	0.047683	-0.028277	2.832592
Pt	-1.383458	2.807260	-1.877847
Pt	3.996460	2.821301	-0.076512
H	-0.975517	2.775666	1.407757

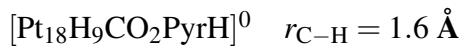


Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	-4.289541	-2.554602	0.509478
Pt	-1.645628	-2.986201	-0.398848
Pt	0.998288	-3.417800	-1.307174
Pt	3.126246	-1.943175	-0.211043
Pt	-2.161204	-1.079763	1.605900
Pt	1.237684	-0.676365	-1.893136
Pt	-4.047016	0.182965	-0.079843
Pt	0.481889	-1.508744	0.695564
Pt	-1.401582	-0.246177	-0.986666
Pt	0.738746	1.278296	0.129144

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Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	2.614484	-0.015666	1.802321
Pt	-1.156055	2.511853	-1.566045
Pt	3.372378	0.821076	-0.790914
Pt	-1.912859	1.683161	1.025734
Pt	5.259686	-0.449420	0.894036
Pt	1.488036	2.081866	-2.475122
Pt	-0.025437	0.416152	2.710755
Pt	-3.800295	2.943257	-0.661070
H	1.381438	3.268226	0.938237
C	0.822564	4.857581	2.140637
C	2.880292	4.696226	0.985236
C	3.285056	5.922486	1.482569
C	2.427459	6.626080	2.330588
C	1.183078	6.087721	2.662847
H	-0.122663	4.354850	2.339441
H	3.475012	4.072390	0.319295
H	4.260138	6.318187	1.207076
H	2.729017	7.593311	2.732213
H	0.495205	6.613720	3.321168
N	1.674457	4.208994	1.327392



Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.913981	-1.331386	-1.094550
Pt	2.578279	-2.553534	-0.068655
Pt	0.242575	-3.775684	0.957240
Pt	-2.306382	-2.806939	0.218059
Pt	2.366081	-0.359036	-1.835243
Pt	-0.646554	-1.265778	1.918268
Pt	4.029835	1.167899	-0.128734
Pt	0.027700	-1.573356	-0.807227
Pt	1.686218	-0.047382	0.894100
Pt	-0.895314	0.979473	0.141139

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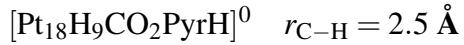
Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	-2.541534	-0.585650	-1.559300
Pt	0.785221	2.487486	1.855815
Pt	-3.218493	-0.276714	1.176474
Pt	1.461793	2.179062	-0.881898
Pt	-4.882508	-1.791098	-0.533349
Pt	-1.558217	1.269137	2.878654
Pt	-0.206403	0.652559	-2.586858
Pt	3.110594	3.712939	0.822614
H	2.278778	4.988217	0.473766
H	-0.026895	3.770704	1.496236
H	-2.386022	2.554001	2.554534
H	0.645246	3.467364	-1.212238
H	-1.738507	2.339530	-0.216221
H	-4.051355	0.997227	0.832496
H	-1.023414	1.932667	-2.953908
H	-3.371809	0.688824	-1.907507
H	-5.711665	-0.513010	-0.880210
C	-2.620132	3.628526	-0.565458
O	-3.705399	3.155351	-0.798337
O	-1.864524	4.540847	-0.459690
C	-6.304504	4.225029	-3.018170
C	-7.413029	4.884020	-3.501547
C	-8.367104	5.388547	-2.604781
C	-8.176549	5.192758	-1.228580
C	-7.055344	4.528813	-0.783108
N	-6.142039	4.065306	-1.677601
H	-9.241592	5.922504	-2.970957
H	-5.523211	3.807051	-3.647796
H	-7.531599	5.003431	-4.575893
H	-8.900245	5.557193	-0.502983
H	-6.838286	4.339445	0.265070
H	-5.261877	3.636200	-1.327937

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Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
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Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
Pt	4.940568	-1.234781	-1.162127
Pt	2.642094	-2.506007	-0.112074
Pt	0.343617	-3.777233	0.937979
Pt	-2.230313	-2.849116	0.238008
Pt	2.367485	-0.307081	-1.862381
Pt	-0.574963	-1.295484	1.928797
Pt	4.025228	1.245103	-0.171064
Pt	0.067576	-1.576621	-0.812532
Pt	1.724597	-0.027083	0.877789
Pt	-0.873127	0.941522	0.166783
Pt	-2.530042	-0.612115	-1.524548
Pt	0.787808	2.486767	1.860562
Pt	-3.171025	-0.335338	1.220443
Pt	1.430840	2.211058	-0.882576
Pt	-4.830936	-1.877389	-0.474094
Pt	-1.520534	1.227246	2.908186
Pt	-0.231031	0.663571	-2.574891
Pt	3.077873	3.767545	0.806639
H	2.229238	5.036227	0.472563
H	-0.045560	3.764688	1.527938
H	-2.372015	2.499087	2.589378
H	0.603998	3.495723	-1.207126
H	-1.721497	2.213153	-0.169661
H	-4.034753	0.926118	0.898324
H	-1.077975	1.931978	-2.917458
H	-3.387366	0.650525	-1.860780
H	-5.679420	-0.606512	-0.803445
C	-2.986671	4.322792	-0.614546
O	-3.966950	3.702637	-0.804412
O	-2.045111	4.989255	-0.438163

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Table ST9 – Continued

Atom	<i>x</i> (Å)	<i>y</i> (Å)	<i>z</i> (Å)
C	-7.032663	3.944636	-3.041350
C	-8.225369	4.440697	-3.508534
C	-9.231178	4.828838	-2.604730
C	-8.984700	4.694592	-1.226237
C	-7.782563	4.195931	-0.786523
N	-6.824961	3.829423	-1.693483
H	-10.178619	5.222834	-2.965235
H	-6.217165	3.621657	-3.681853
H	-8.372126	4.524964	-4.582620
H	-9.732934	4.980604	-0.490523
H	-7.528403	4.061824	0.260958
H	-5.921141	3.495138	-1.358065

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