

*Supplementary Information*

**Effect of hydrogen adsorption on Pt nanoparticle encapsulated in NaY zeolite: Combined study of WT XAFS and DFT calculation**

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**Table S1.** Optimized Crystallographic Information File for Pt55 in NaY zeolite

data\_Pt55-NaY

|                   |           |
|-------------------|-----------|
| _cell_length_a    | 18.010520 |
| _cell_length_b    | 18.090904 |
| _cell_length_c    | 17.998944 |
| _cell_angle_alpha | 59.795380 |
| _cell_angle_beta  | 59.303386 |
| _cell_angle_gamma | 59.353345 |

|                                |       |
|--------------------------------|-------|
| _symmetry_space_group_name_H-M | 'P 1' |
|--------------------------------|-------|

loop\_

|                            |            |
|----------------------------|------------|
| _symmetry_equiv_pos_as_xyz | '+x,+y,+z' |
|----------------------------|------------|

loop\_

|                        |  |
|------------------------|--|
| _atom_site_type_symbol |  |
| _atom_site_fract_x     |  |
| _atom_site_fract_y     |  |
| _atom_site_fract_z     |  |

|    |          |          |          |
|----|----------|----------|----------|
| Al | 0.727195 | 0.906689 | 0.091601 |
| Al | 0.962641 | 0.517937 | 0.165813 |
| Al | 0.335557 | 0.968758 | 0.158974 |
| Al | 0.901169 | 0.727439 | 0.267730 |
| Al | 0.085840 | 0.902628 | 0.267857 |
| Al | 0.148708 | 0.517023 | 0.343909 |
| Al | 0.517196 | 0.974096 | 0.336546 |
| Al | 0.967575 | 0.337385 | 0.523622 |
| Al | 0.155781 | 0.981837 | 0.514887 |
| Al | 0.085714 | 0.266887 | 0.731478 |
| Al | 0.904226 | 0.090668 | 0.726031 |
| Al | 0.271322 | 0.898921 | 0.730864 |
| Al | 0.094641 | 0.725861 | 0.903311 |
| Al | 0.511992 | 0.156738 | 0.978587 |
| Al | 0.149375 | 0.337911 | 0.979447 |
| Al | 0.333843 | 0.519481 | 0.978083 |
| Na | 0.079221 | 0.079442 | 0.079651 |
| Na | 0.067145 | 0.767997 | 0.083452 |
| Na | 0.760929 | 0.080238 | 0.072227 |
| Na | 0.481706 | 0.170711 | 0.166564 |
| Na | 0.169828 | 0.169562 | 0.169824 |
| Na | 0.167751 | 0.486534 | 0.175819 |
| Na | 0.890836 | 0.886607 | 0.313378 |
| Na | 0.333448 | 0.337943 | 0.341869 |
| Na | 0.177745 | 0.173780 | 0.472718 |

|    |          |          |          |
|----|----------|----------|----------|
| Na | 0.076204 | 0.068216 | 0.764892 |
| Na | 0.880646 | 0.335739 | 0.884497 |
| Na | 0.328939 | 0.885405 | 0.881602 |
| Na | 0.891751 | 0.891679 | 0.891737 |
| Na | 0.334714 | 0.342743 | 0.965306 |
| O  | 0.512604 | 0.303117 | 0.090421 |
| O  | 0.300414 | 0.086967 | 0.087418 |
| O  | 0.086205 | 0.496154 | 0.106392 |
| O  | 0.799605 | 0.303225 | 0.077299 |
| O  | 0.303569 | 0.803842 | 0.073362 |
| O  | 0.803319 | 0.803161 | 0.077855 |
| O  | 0.299283 | 0.517184 | 0.094164 |
| O  | 0.487088 | 0.093585 | 0.099474 |
| O  | 0.078695 | 0.295128 | 0.097842 |
| O  | 0.905783 | 0.627488 | 0.110448 |
| O  | 0.336772 | 0.905374 | 0.110933 |
| O  | 0.618670 | 0.336327 | 0.123434 |
| O  | 0.340258 | 0.619548 | 0.126439 |
| O  | 0.615137 | 0.922215 | 0.118482 |
| O  | 0.901480 | 0.336733 | 0.119477 |
| O  | 0.736604 | 0.163245 | 0.161564 |
| O  | 0.159211 | 0.930853 | 0.151613 |
| O  | 0.928968 | 0.732650 | 0.157570 |
| O  | 0.447785 | 0.946363 | 0.146899 |
| O  | 0.943039 | 0.436877 | 0.152009 |
| O  | 0.439211 | 0.441146 | 0.152474 |
| O  | 0.165972 | 0.733740 | 0.166161 |
| O  | 0.737806 | 0.938774 | 0.164055 |
| O  | 0.918007 | 0.163955 | 0.167688 |
| O  | 0.962719 | 0.258173 | 0.262856 |
| O  | 0.262429 | 0.487380 | 0.261932 |
| O  | 0.479585 | 0.975389 | 0.262771 |
| O  | 0.483161 | 0.262838 | 0.258407 |
| O  | 0.954699 | 0.491625 | 0.279384 |
| O  | 0.249615 | 0.980219 | 0.264260 |
| O  | 0.990647 | 0.758981 | 0.249223 |
| O  | 0.754479 | 0.991339 | 0.265689 |
| O  | 0.970286 | 0.988957 | 0.258447 |
| O  | 0.791183 | 0.089914 | 0.307618 |
| O  | 0.068752 | 0.802079 | 0.307379 |
| O  | 0.806009 | 0.817115 | 0.303388 |
| O  | 0.507859 | 0.095171 | 0.298539 |
| O  | 0.082284 | 0.094240 | 0.303089 |
| O  | 0.082069 | 0.500276 | 0.311452 |
| O  | 0.905618 | 0.621026 | 0.347803 |
| O  | 0.614382 | 0.130983 | 0.332745 |
| O  | 0.106971 | 0.918803 | 0.339977 |
| O  | 0.905282 | 0.115400 | 0.341582 |
| O  | 0.626986 | 0.914053 | 0.340137 |
| O  | 0.110851 | 0.626047 | 0.341665 |
| O  | 0.938559 | 0.452299 | 0.453792 |

|    |          |          |          |
|----|----------|----------|----------|
| O  | 0.139545 | 0.954885 | 0.442669 |
| O  | 0.433747 | 0.158927 | 0.436076 |
| O  | 0.159872 | 0.430208 | 0.446434 |
| O  | 0.946973 | 0.152043 | 0.442072 |
| O  | 0.443239 | 0.954729 | 0.450457 |
| O  | 0.967220 | 0.266739 | 0.483119 |
| O  | 0.258028 | 0.254431 | 0.487616 |
| O  | 0.266761 | 0.979681 | 0.487737 |
| O  | 0.302875 | 0.086164 | 0.516357 |
| O  | 0.094777 | 0.105377 | 0.487377 |
| O  | 0.088581 | 0.299645 | 0.512677 |
| O  | 0.920903 | 0.118379 | 0.612428 |
| O  | 0.126328 | 0.332105 | 0.619947 |
| O  | 0.344707 | 0.906595 | 0.620573 |
| O  | 0.897935 | 0.336355 | 0.634833 |
| O  | 0.111129 | 0.918773 | 0.625631 |
| O  | 0.332840 | 0.123496 | 0.622466 |
| O  | 0.159837 | 0.930491 | 0.737903 |
| O  | 0.158623 | 0.152405 | 0.745543 |
| O  | 0.926574 | 0.162857 | 0.746110 |
| O  | 0.970505 | 0.266515 | 0.766494 |
| O  | 0.983583 | 0.978997 | 0.766639 |
| O  | 0.270778 | 0.982381 | 0.758821 |
| O  | 0.303065 | 0.085934 | 0.799312 |
| O  | 0.796620 | 0.306881 | 0.810686 |
| O  | 0.089669 | 0.802098 | 0.795917 |
| O  | 0.795712 | 0.085484 | 0.802554 |
| O  | 0.307549 | 0.802409 | 0.816352 |
| O  | 0.065211 | 0.303838 | 0.815040 |
| O  | 0.331588 | 0.119793 | 0.909535 |
| O  | 0.619094 | 0.336062 | 0.913831 |
| O  | 0.126510 | 0.610486 | 0.922392 |
| O  | 0.623541 | 0.118665 | 0.913577 |
| O  | 0.106753 | 0.336517 | 0.913782 |
| O  | 0.340352 | 0.626176 | 0.906315 |
| O  | 0.733876 | 0.164141 | 0.930537 |
| O  | 0.156709 | 0.159376 | 0.930556 |
| O  | 0.163714 | 0.737783 | 0.938349 |
| O  | 0.433961 | 0.155700 | 0.946505 |
| O  | 0.445820 | 0.439497 | 0.955574 |
| O  | 0.151188 | 0.441676 | 0.960462 |
| O  | 0.257632 | 0.254579 | 0.983752 |
| O  | 0.479770 | 0.262852 | 0.991439 |
| O  | 0.254347 | 0.475446 | 0.999680 |
| O  | 0.979152 | 0.250750 | 0.992064 |
| O  | 0.266474 | 0.749495 | 0.990734 |
| O  | 0.762815 | 0.990998 | 0.980160 |
| O  | 0.750034 | 0.262134 | 0.987488 |
| O  | 0.979031 | 0.761868 | 0.980650 |
| O  | 0.262143 | 0.982999 | 0.975561 |
| Pt | 0.632342 | 0.213317 | 0.662662 |

|    |          |          |          |
|----|----------|----------|----------|
| Pt | 0.639493 | 0.204303 | 0.507402 |
| Pt | 0.476266 | 0.220033 | 0.660392 |
| Pt | 0.779955 | 0.203618 | 0.517185 |
| Pt | 0.789773 | 0.349066 | 0.507925 |
| Pt | 0.783890 | 0.343430 | 0.357298 |
| Pt | 0.638224 | 0.359956 | 0.505533 |
| Pt | 0.472055 | 0.242154 | 0.801837 |
| Pt | 0.525001 | 0.367440 | 0.778596 |
| Pt | 0.487195 | 0.369772 | 0.649751 |
| Pt | 0.317458 | 0.371922 | 0.778362 |
| Pt | 0.699929 | 0.294583 | 0.688300 |
| Pt | 0.648663 | 0.465849 | 0.664594 |
| Pt | 0.644978 | 0.507458 | 0.498161 |
| Pt | 0.491415 | 0.518547 | 0.641282 |
| Pt | 0.488618 | 0.211512 | 0.512159 |
| Pt | 0.492460 | 0.363159 | 0.503490 |
| Pt | 0.503294 | 0.351693 | 0.354215 |
| Pt | 0.343215 | 0.358863 | 0.508760 |
| Pt | 0.678790 | 0.298886 | 0.333220 |
| Pt | 0.646670 | 0.505256 | 0.349250 |
| Pt | 0.661338 | 0.461588 | 0.215039 |
| Pt | 0.498245 | 0.507317 | 0.351220 |
| Pt | 0.299289 | 0.306563 | 0.688149 |
| Pt | 0.343116 | 0.520279 | 0.642161 |
| Pt | 0.345539 | 0.512223 | 0.499557 |
| Pt | 0.206433 | 0.480682 | 0.666669 |
| Pt | 0.495744 | 0.512772 | 0.494944 |
| Pt | 0.497623 | 0.660627 | 0.490291 |
| Pt | 0.500425 | 0.656468 | 0.342423 |
| Pt | 0.346603 | 0.661246 | 0.493022 |
| Pt | 0.340800 | 0.516962 | 0.352276 |
| Pt | 0.341048 | 0.513689 | 0.794199 |
| Pt | 0.799357 | 0.505184 | 0.348368 |
| Pt | 0.481758 | 0.529587 | 0.790268 |
| Pt | 0.500397 | 0.504382 | 0.209782 |
| Pt | 0.197468 | 0.802749 | 0.494127 |
| Pt | 0.467917 | 0.664344 | 0.207761 |
| Pt | 0.475087 | 0.670768 | 0.647671 |
| Pt | 0.785820 | 0.499960 | 0.508668 |
| Pt | 0.194765 | 0.506207 | 0.511599 |
| Pt | 0.502974 | 0.796519 | 0.196383 |
| Pt | 0.197356 | 0.660297 | 0.486338 |
| Pt | 0.650093 | 0.657642 | 0.490482 |
| Pt | 0.297392 | 0.696349 | 0.312847 |
| Pt | 0.344538 | 0.799041 | 0.339188 |
| Pt | 0.790966 | 0.495346 | 0.209862 |
| Pt | 0.183828 | 0.530303 | 0.798962 |
| Pt | 0.500711 | 0.802266 | 0.490495 |
| Pt | 0.186864 | 0.662515 | 0.647290 |
| Pt | 0.658999 | 0.656690 | 0.197264 |
| Pt | 0.313176 | 0.685444 | 0.666401 |

|    |          |          |          |
|----|----------|----------|----------|
| Pt | 0.340952 | 0.808132 | 0.498533 |
| Pt | 0.667790 | 0.671365 | 0.329432 |
| Pt | 0.503413 | 0.808423 | 0.338289 |
| Si | 0.902493 | 0.728278 | 0.085086 |
| Si | 0.266007 | 0.903149 | 0.085588 |
| Si | 0.723430 | 0.268674 | 0.091384 |
| Si | 0.270352 | 0.723734 | 0.094236 |
| Si | 0.897435 | 0.266477 | 0.093229 |
| Si | 0.514080 | 0.339385 | 0.156740 |
| Si | 0.333204 | 0.519640 | 0.159534 |
| Si | 0.968975 | 0.334021 | 0.158860 |
| Si | 0.510261 | 0.980941 | 0.157116 |
| Si | 0.721724 | 0.095266 | 0.270804 |
| Si | 0.728279 | 0.908782 | 0.269363 |
| Si | 0.085783 | 0.726995 | 0.271652 |
| Si | 0.895734 | 0.089622 | 0.272918 |
| Si | 0.148366 | 0.979627 | 0.338366 |
| Si | 0.512202 | 0.157869 | 0.334152 |
| Si | 0.967836 | 0.519180 | 0.346214 |
| Si | 0.969737 | 0.156277 | 0.339949 |
| Si | 0.980814 | 0.161226 | 0.509533 |
| Si | 0.338002 | 0.973563 | 0.522255 |
| Si | 0.151810 | 0.332696 | 0.521130 |
| Si | 0.333751 | 0.154540 | 0.520262 |
| Si | 0.265185 | 0.088732 | 0.729985 |
| Si | 0.899720 | 0.267259 | 0.734483 |
| Si | 0.089538 | 0.904164 | 0.729655 |
| Si | 0.265386 | 0.090636 | 0.901435 |
| Si | 0.723460 | 0.267730 | 0.905277 |
| Si | 0.727434 | 0.089568 | 0.902928 |
| Si | 0.083520 | 0.267412 | 0.906932 |
| Si | 0.269615 | 0.726735 | 0.908205 |
| Si | 0.514135 | 0.336757 | 0.979325 |
| Si | 0.151334 | 0.510142 | 0.995456 |
| Si | 0.330812 | 0.153737 | 0.979935 |

**Table S2.** Optimized Crystallographic Information File for Pt13 in NaY zeolite

data\_Pt13-NaY-

|                   |           |
|-------------------|-----------|
| _cell_length_a    | 18.215432 |
| _cell_length_b    | 17.939984 |
| _cell_length_c    | 17.989095 |
| _cell_angle_alpha | 58.338140 |
| _cell_angle_beta  | 59.086279 |
| _cell_angle_gamma | 58.923725 |

\_symmetry\_space\_group\_name\_H-M      'P 1'

loop\_

\_symmetry\_equiv\_pos\_as\_xyz  
'+x,+y,+z'

loop\_

\_atom\_site\_type\_symbol  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z

|    |          |          |          |
|----|----------|----------|----------|
| Al | 0.901250 | 0.271440 | 0.092526 |
| Al | 0.720451 | 0.899816 | 0.102214 |
| Al | 0.520949 | 0.338383 | 0.149612 |
| Al | 0.983186 | 0.513629 | 0.154425 |
| Al | 0.340914 | 0.968085 | 0.161710 |
| Al | 0.726652 | 0.092125 | 0.269086 |
| Al | 0.905601 | 0.730433 | 0.267423 |
| Al | 0.093308 | 0.898554 | 0.279948 |
| Al | 0.973192 | 0.154892 | 0.343030 |
| Al | 0.516059 | 0.969917 | 0.347005 |
| Al | 0.340385 | 0.152956 | 0.520576 |
| Al | 0.904213 | 0.089698 | 0.732989 |
| Al | 0.087469 | 0.270761 | 0.726084 |
| Al | 0.721689 | 0.274509 | 0.898944 |
| Al | 0.515558 | 0.154349 | 0.973942 |
| Al | 0.157270 | 0.342829 | 0.970417 |
| Na | 0.075200 | 0.079476 | 0.083782 |
| Na | 0.068061 | 0.773299 | 0.080238 |
| Na | 0.755055 | 0.082170 | 0.078298 |
| Na | 0.180072 | 0.445896 | 0.183886 |
| Na | 0.166443 | 0.170752 | 0.174565 |
| Na | 0.479922 | 0.160538 | 0.176683 |
| Na | 0.882604 | 0.902937 | 0.321570 |
| Na | 0.371445 | 0.895961 | 0.359099 |
| Na | 0.375522 | 0.342760 | 0.367235 |

|    |          |          |          |
|----|----------|----------|----------|
| Na | 0.902978 | 0.362310 | 0.362204 |
| Na | 0.174655 | 0.170837 | 0.481672 |
| Na | 0.079153 | 0.075318 | 0.760229 |
| Na | 0.866184 | 0.894998 | 0.899130 |
| Na | 0.885760 | 0.324397 | 0.889869 |
| Na | 0.338651 | 0.883689 | 0.883692 |
| Na | 0.362275 | 0.358162 | 0.898873 |
| O  | 0.300090 | 0.086023 | 0.085173 |
| O  | 0.507507 | 0.304035 | 0.082157 |
| O  | 0.105106 | 0.499541 | 0.087567 |
| O  | 0.803209 | 0.306980 | 0.070036 |
| O  | 0.299471 | 0.803572 | 0.077482 |
| O  | 0.811925 | 0.803509 | 0.073148 |
| O  | 0.509680 | 0.080764 | 0.093926 |
| O  | 0.085888 | 0.311713 | 0.090014 |
| O  | 0.303223 | 0.509676 | 0.087536 |
| O  | 0.340187 | 0.892343 | 0.127426 |
| O  | 0.626796 | 0.343880 | 0.110550 |
| O  | 0.918476 | 0.627524 | 0.114277 |
| O  | 0.906253 | 0.344883 | 0.122927 |
| O  | 0.324687 | 0.623350 | 0.125857 |
| O  | 0.614316 | 0.893458 | 0.145643 |
| O  | 0.738025 | 0.164847 | 0.151447 |
| O  | 0.934331 | 0.745692 | 0.151999 |
| O  | 0.163763 | 0.930296 | 0.160063 |
| O  | 0.942609 | 0.441362 | 0.164050 |
| O  | 0.434790 | 0.447082 | 0.158711 |
| O  | 0.442466 | 0.937812 | 0.172125 |
| O  | 0.933662 | 0.155648 | 0.168817 |
| O  | 0.155128 | 0.746149 | 0.155950 |
| O  | 0.737639 | 0.926224 | 0.172315 |
| O  | 0.975549 | 0.265901 | 0.261772 |
| O  | 0.259676 | 0.484196 | 0.258259 |
| O  | 0.479604 | 0.975254 | 0.270191 |
| O  | 0.985757 | 0.479523 | 0.266304 |
| O  | 0.483940 | 0.262642 | 0.262963 |
| O  | 0.263286 | 0.969915 | 0.274623 |
| O  | 0.982608 | 0.770054 | 0.259542 |
| O  | 0.759862 | 0.973750 | 0.270656 |
| O  | 0.981300 | 0.977609 | 0.274748 |
| O  | 0.807494 | 0.074097 | 0.307132 |
| O  | 0.090750 | 0.788382 | 0.309701 |
| O  | 0.794246 | 0.793632 | 0.319331 |
| O  | 0.093312 | 0.081841 | 0.316266 |
| O  | 0.502075 | 0.090605 | 0.313912 |
| O  | 0.095581 | 0.490590 | 0.312036 |
| O  | 0.615186 | 0.124079 | 0.339768 |
| O  | 0.926014 | 0.613986 | 0.337159 |
| O  | 0.130958 | 0.897250 | 0.351897 |
| O  | 0.902175 | 0.114687 | 0.348243 |
| O  | 0.120675 | 0.620244 | 0.324598 |



|   |          |          |          |
|---|----------|----------|----------|
| ○ | 0.624520 | 0.901780 | 0.351165 |
| ○ | 0.441464 | 0.167687 | 0.439203 |
| ○ | 0.943428 | 0.438864 | 0.442261 |
| ○ | 0.164594 | 0.938498 | 0.451483 |
| ○ | 0.946574 | 0.172267 | 0.443085 |
| ○ | 0.167026 | 0.444305 | 0.434614 |
| ○ | 0.434486 | 0.937608 | 0.455738 |
| ○ | 0.258617 | 0.265768 | 0.483705 |
| ○ | 0.261823 | 0.971291 | 0.495879 |
| ○ | 0.987799 | 0.258198 | 0.491107 |
| ○ | 0.299136 | 0.082269 | 0.520142 |
| ○ | 0.094311 | 0.087991 | 0.506693 |
| ○ | 0.091618 | 0.315280 | 0.498541 |
| ○ | 0.333919 | 0.903100 | 0.630400 |
| ○ | 0.917508 | 0.118608 | 0.620462 |
| ○ | 0.121378 | 0.343731 | 0.612395 |
| ○ | 0.337866 | 0.115013 | 0.632944 |
| ○ | 0.916548 | 0.339089 | 0.617735 |
| ○ | 0.126794 | 0.908110 | 0.627863 |
| ○ | 0.159375 | 0.151851 | 0.737924 |
| ○ | 0.937814 | 0.163360 | 0.737823 |
| ○ | 0.163136 | 0.929957 | 0.743144 |
| ○ | 0.991044 | 0.974358 | 0.767238 |
| ○ | 0.971508 | 0.273849 | 0.759467 |
| ○ | 0.266538 | 0.973931 | 0.765481 |
| ○ | 0.294919 | 0.074336 | 0.811500 |
| ○ | 0.797790 | 0.314753 | 0.782982 |
| ○ | 0.102311 | 0.795040 | 0.799821 |
| ○ | 0.803647 | 0.072867 | 0.811777 |
| ○ | 0.086010 | 0.299655 | 0.803198 |
| ○ | 0.302861 | 0.799507 | 0.807524 |
| ○ | 0.611287 | 0.344124 | 0.897797 |
| ○ | 0.336461 | 0.123153 | 0.902306 |
| ○ | 0.131737 | 0.622656 | 0.909775 |
| ○ | 0.625842 | 0.131595 | 0.897726 |
| ○ | 0.123125 | 0.340588 | 0.898039 |
| ○ | 0.335997 | 0.623365 | 0.909728 |
| ○ | 0.738690 | 0.158965 | 0.929984 |
| ○ | 0.160980 | 0.158564 | 0.934758 |
| ○ | 0.160128 | 0.737749 | 0.938223 |
| ○ | 0.438077 | 0.155401 | 0.942909 |
| ○ | 0.442019 | 0.446962 | 0.942609 |
| ○ | 0.175775 | 0.446752 | 0.934706 |
| ○ | 0.266794 | 0.260123 | 0.969715 |
| ○ | 0.475722 | 0.271733 | 0.971867 |
| ○ | 0.270596 | 0.487697 | 0.971286 |
| ○ | 0.987640 | 0.262035 | 0.979800 |
| ○ | 0.262803 | 0.758376 | 0.982363 |
| ○ | 0.744771 | 0.987040 | 0.989277 |
| ○ | 0.758244 | 0.274512 | 0.971786 |
| ○ | 0.987759 | 0.762971 | 0.975416 |

|    |          |          |          |
|----|----------|----------|----------|
| O  | 0.270310 | 0.979060 | 0.983272 |
| Pt | 0.561514 | 0.507058 | 0.533136 |
| Pt | 0.556279 | 0.640196 | 0.367142 |
| Pt | 0.403423 | 0.514234 | 0.689820 |
| Pt | 0.427132 | 0.669238 | 0.524155 |
| Pt | 0.705451 | 0.537491 | 0.415971 |
| Pt | 0.564772 | 0.425491 | 0.698753 |
| Pt | 0.754167 | 0.532346 | 0.531737 |
| Pt | 0.563731 | 0.718806 | 0.450660 |
| Pt | 0.734577 | 0.678130 | 0.383089 |
| Pt | 0.588197 | 0.582014 | 0.627039 |
| Pt | 0.417138 | 0.658608 | 0.678287 |
| Pt | 0.699524 | 0.433933 | 0.703752 |
| Pt | 0.525955 | 0.757788 | 0.586563 |
| Si | 0.268610 | 0.902103 | 0.094781 |
| Si | 0.906816 | 0.731269 | 0.087908 |
| Si | 0.729610 | 0.273537 | 0.080780 |
| Si | 0.261909 | 0.731175 | 0.091566 |
| Si | 0.974197 | 0.341592 | 0.157338 |
| Si | 0.336698 | 0.514981 | 0.155001 |
| Si | 0.513962 | 0.969379 | 0.167623 |
| Si | 0.903031 | 0.085725 | 0.276465 |
| Si | 0.085669 | 0.733165 | 0.267789 |
| Si | 0.724118 | 0.902466 | 0.278394 |
| Si | 0.515211 | 0.157516 | 0.339062 |
| Si | 0.981421 | 0.510692 | 0.337605 |
| Si | 0.160946 | 0.970804 | 0.345970 |
| Si | 0.157436 | 0.513768 | 0.333586 |
| Si | 0.980014 | 0.156376 | 0.517401 |
| Si | 0.159382 | 0.341400 | 0.512024 |
| Si | 0.336108 | 0.973147 | 0.522645 |
| Si | 0.981158 | 0.337736 | 0.515729 |
| Si | 0.160203 | 0.974321 | 0.519344 |
| Si | 0.268385 | 0.902577 | 0.732696 |
| Si | 0.264200 | 0.088230 | 0.732122 |
| Si | 0.905133 | 0.270750 | 0.726773 |
| Si | 0.093887 | 0.903056 | 0.732616 |
| Si | 0.266371 | 0.090396 | 0.906945 |
| Si | 0.094147 | 0.726710 | 0.907010 |
| Si | 0.723724 | 0.091558 | 0.906645 |
| Si | 0.088857 | 0.271831 | 0.902748 |
| Si | 0.266254 | 0.726180 | 0.908987 |
| Si | 0.337822 | 0.155171 | 0.975053 |
| Si | 0.513273 | 0.336758 | 0.972269 |
| Si | 0.166008 | 0.512400 | 0.975749 |
| Si | 0.341206 | 0.514843 | 0.974721 |

**Table S3.** Optimized Crystallographic Information File for Pt13-H12 in NaY zeolite

data\_Pt13-H12-NaY-

|                   |           |
|-------------------|-----------|
| _cell_length_a    | 18.145901 |
| _cell_length_b    | 17.916829 |
| _cell_length_c    | 17.955316 |
| _cell_angle_alpha | 59.134984 |
| _cell_angle_beta  | 59.605031 |
| _cell_angle_gamma | 59.666138 |

|                                |       |
|--------------------------------|-------|
| _symmetry_space_group_name_H-M | "P 1" |
|--------------------------------|-------|

loop\_

|                            |            |
|----------------------------|------------|
| _symmetry_equiv_pos_as_xyz | '+x,+y,+z' |
|----------------------------|------------|

loop\_

|                        |  |  |  |
|------------------------|--|--|--|
| _atom_site_type_symbol |  |  |  |
| _atom_site_fract_x     |  |  |  |
| _atom_site_fract_y     |  |  |  |
| _atom_site_fract_z     |  |  |  |

|    |          |          |          |
|----|----------|----------|----------|
| Al | 0.902635 | 0.268504 | 0.094618 |
| Al | 0.724234 | 0.903167 | 0.095974 |
| Al | 0.519826 | 0.341947 | 0.154800 |
| Al | 0.980834 | 0.517346 | 0.155107 |
| Al | 0.341137 | 0.972142 | 0.157711 |
| Al | 0.723799 | 0.094743 | 0.270290 |
| Al | 0.903471 | 0.724940 | 0.269365 |
| Al | 0.092054 | 0.902431 | 0.274019 |
| Al | 0.975441 | 0.156161 | 0.340810 |
| Al | 0.518131 | 0.971291 | 0.344429 |
| Al | 0.339937 | 0.154665 | 0.519947 |
| Al | 0.903692 | 0.092717 | 0.728427 |
| Al | 0.090626 | 0.273398 | 0.724587 |
| Al | 0.721785 | 0.274780 | 0.899877 |
| Al | 0.518431 | 0.154657 | 0.973052 |
| Al | 0.157780 | 0.343591 | 0.974031 |
| H  | 0.567073 | 0.545351 | 0.740478 |
| H  | 0.528502 | 0.751888 | 0.584417 |
| H  | 0.317580 | 0.464282 | 0.776264 |
| H  | 0.359443 | 0.714287 | 0.694966 |
| H  | 0.406530 | 0.580265 | 0.368192 |
| H  | 0.540515 | 0.796203 | 0.300912 |
| H  | 0.718500 | 0.680086 | 0.350939 |
| H  | 0.787994 | 0.403650 | 0.528795 |
| H  | 0.585722 | 0.278828 | 0.712429 |

|    |          |          |          |
|----|----------|----------|----------|
| H  | 0.672235 | 0.535611 | 0.297909 |
| H  | 0.258225 | 0.711715 | 0.597544 |
| H  | 0.531534 | 0.329664 | 0.525745 |
| Na | 0.074636 | 0.083572 | 0.083418 |
| Na | 0.071946 | 0.772160 | 0.081614 |
| Na | 0.755904 | 0.079341 | 0.079543 |
| Na | 0.169665 | 0.474262 | 0.180988 |
| Na | 0.167508 | 0.172648 | 0.172656 |
| Na | 0.490440 | 0.161925 | 0.168139 |
| Na | 0.884747 | 0.890527 | 0.316569 |
| Na | 0.355485 | 0.919351 | 0.354836 |
| Na | 0.367084 | 0.344548 | 0.358521 |
| Na | 0.911915 | 0.363193 | 0.355107 |
| Na | 0.177198 | 0.172550 | 0.471789 |
| Na | 0.070235 | 0.091272 | 0.765416 |
| Na | 0.880761 | 0.892584 | 0.891327 |
| Na | 0.885632 | 0.313536 | 0.897204 |
| Na | 0.327964 | 0.894313 | 0.884049 |
| Na | 0.371422 | 0.351165 | 0.912494 |
| O  | 0.301728 | 0.090371 | 0.084179 |
| O  | 0.502807 | 0.312052 | 0.086441 |
| O  | 0.098538 | 0.515494 | 0.084566 |
| O  | 0.802969 | 0.302816 | 0.076377 |
| O  | 0.295144 | 0.809935 | 0.073361 |
| O  | 0.815332 | 0.803913 | 0.072750 |
| O  | 0.507594 | 0.082112 | 0.091355 |
| O  | 0.086298 | 0.311890 | 0.091040 |
| O  | 0.304726 | 0.515872 | 0.087433 |
| O  | 0.337394 | 0.897900 | 0.123445 |
| O  | 0.626233 | 0.346150 | 0.114154 |
| O  | 0.910698 | 0.626973 | 0.115672 |
| O  | 0.907491 | 0.340471 | 0.128024 |
| O  | 0.334293 | 0.627143 | 0.121695 |
| O  | 0.616579 | 0.900908 | 0.135135 |
| O  | 0.733255 | 0.166776 | 0.154730 |
| O  | 0.941911 | 0.731755 | 0.154395 |
| O  | 0.161903 | 0.936688 | 0.154997 |
| O  | 0.946164 | 0.439886 | 0.164818 |
| O  | 0.431641 | 0.449456 | 0.168756 |
| O  | 0.444103 | 0.939576 | 0.165865 |
| O  | 0.936354 | 0.153440 | 0.167574 |
| O  | 0.160666 | 0.735266 | 0.159900 |
| O  | 0.732252 | 0.934303 | 0.168782 |
| O  | 0.978821 | 0.266397 | 0.262191 |
| O  | 0.255320 | 0.493381 | 0.256982 |
| O  | 0.483330 | 0.975347 | 0.265539 |
| O  | 0.986210 | 0.481764 | 0.266992 |
| O  | 0.485434 | 0.264073 | 0.264984 |
| O  | 0.262161 | 0.974557 | 0.269834 |
| O  | 0.990290 | 0.755249 | 0.260080 |
| O  | 0.754528 | 0.978866 | 0.270630 |

|   |          |          |          |
|---|----------|----------|----------|
| ○ | 0.979325 | 0.975988 | 0.271638 |
| ○ | 0.806890 | 0.079249 | 0.303822 |
| ○ | 0.093973 | 0.791357 | 0.303234 |
| ○ | 0.802157 | 0.803895 | 0.304160 |
| ○ | 0.093965 | 0.084180 | 0.310219 |
| ○ | 0.507122 | 0.090329 | 0.313319 |
| ○ | 0.088136 | 0.507560 | 0.311679 |
| ○ | 0.613963 | 0.131199 | 0.341416 |
| ○ | 0.907281 | 0.612788 | 0.344749 |
| ○ | 0.131318 | 0.901649 | 0.344680 |
| ○ | 0.907883 | 0.112374 | 0.344632 |
| ○ | 0.124891 | 0.620441 | 0.336828 |
| ○ | 0.626162 | 0.898619 | 0.346831 |
| ○ | 0.440087 | 0.169295 | 0.438739 |
| ○ | 0.949451 | 0.435931 | 0.443423 |
| ○ | 0.163491 | 0.945837 | 0.445742 |
| ○ | 0.947034 | 0.172007 | 0.442628 |
| ○ | 0.167785 | 0.442387 | 0.434746 |
| ○ | 0.430403 | 0.941026 | 0.450332 |
| ○ | 0.258360 | 0.265597 | 0.483788 |
| ○ | 0.258187 | 0.975372 | 0.494311 |
| ○ | 0.987963 | 0.260011 | 0.489352 |
| ○ | 0.298835 | 0.081987 | 0.521145 |
| ○ | 0.090579 | 0.088682 | 0.512301 |
| ○ | 0.092446 | 0.310414 | 0.504864 |
| ○ | 0.333007 | 0.901699 | 0.628503 |
| ○ | 0.908815 | 0.125647 | 0.617907 |
| ○ | 0.127568 | 0.344910 | 0.611831 |
| ○ | 0.339680 | 0.116245 | 0.631024 |
| ○ | 0.911062 | 0.340550 | 0.618284 |
| ○ | 0.124417 | 0.906939 | 0.625947 |
| ○ | 0.163994 | 0.156543 | 0.733188 |
| ○ | 0.940847 | 0.164932 | 0.730242 |
| ○ | 0.158463 | 0.936963 | 0.740207 |
| ○ | 0.988658 | 0.976430 | 0.761534 |
| ○ | 0.978815 | 0.269452 | 0.755554 |
| ○ | 0.266629 | 0.977263 | 0.760358 |
| ○ | 0.295021 | 0.075620 | 0.810857 |
| ○ | 0.804726 | 0.306018 | 0.792233 |
| ○ | 0.095212 | 0.800681 | 0.800761 |
| ○ | 0.803438 | 0.079296 | 0.808138 |
| ○ | 0.089046 | 0.300551 | 0.803510 |
| ○ | 0.297499 | 0.804002 | 0.806842 |
| ○ | 0.611373 | 0.349034 | 0.902013 |
| ○ | 0.332113 | 0.129551 | 0.903304 |
| ○ | 0.133127 | 0.625202 | 0.902605 |
| ○ | 0.627511 | 0.122406 | 0.900654 |
| ○ | 0.123495 | 0.339496 | 0.902629 |
| ○ | 0.337379 | 0.626562 | 0.906541 |
| ○ | 0.731837 | 0.160615 | 0.933474 |
| ○ | 0.160637 | 0.159194 | 0.935202 |

|    |          |          |          |
|----|----------|----------|----------|
| O  | 0.158870 | 0.737661 | 0.939251 |
| O  | 0.436282 | 0.163145 | 0.941747 |
| O  | 0.437963 | 0.446697 | 0.944784 |
| O  | 0.171452 | 0.448336 | 0.942035 |
| O  | 0.267262 | 0.264356 | 0.974706 |
| O  | 0.485260 | 0.268559 | 0.975197 |
| O  | 0.266107 | 0.493441 | 0.975741 |
| O  | 0.988391 | 0.261193 | 0.979900 |
| O  | 0.260189 | 0.757832 | 0.983624 |
| O  | 0.753823 | 0.985695 | 0.982223 |
| O  | 0.754705 | 0.271472 | 0.978723 |
| O  | 0.989043 | 0.758775 | 0.975721 |
| O  | 0.268207 | 0.982281 | 0.980006 |
| Pt | 0.485123 | 0.429242 | 0.528428 |
| Pt | 0.464610 | 0.599299 | 0.394303 |
| Pt | 0.378864 | 0.501721 | 0.675224 |
| Pt | 0.348965 | 0.659631 | 0.538717 |
| Pt | 0.633271 | 0.476804 | 0.400372 |
| Pt | 0.544755 | 0.383865 | 0.660791 |
| Pt | 0.688845 | 0.430539 | 0.536818 |
| Pt | 0.508092 | 0.724411 | 0.397158 |
| Pt | 0.672685 | 0.604955 | 0.402353 |
| Pt | 0.522089 | 0.557113 | 0.529618 |
| Pt | 0.424294 | 0.629228 | 0.662095 |
| Pt | 0.589516 | 0.518099 | 0.659720 |
| Pt | 0.563274 | 0.686922 | 0.531010 |
| Si | 0.265963 | 0.907084 | 0.090925 |
| Si | 0.908408 | 0.727706 | 0.087666 |
| Si | 0.726810 | 0.273218 | 0.085304 |
| Si | 0.264228 | 0.730776 | 0.090883 |
| Si | 0.976355 | 0.340606 | 0.158826 |
| Si | 0.337120 | 0.520287 | 0.157314 |
| Si | 0.515401 | 0.971746 | 0.162177 |
| Si | 0.904746 | 0.084267 | 0.274095 |
| Si | 0.089470 | 0.728193 | 0.269656 |
| Si | 0.725520 | 0.903772 | 0.274382 |
| Si | 0.515826 | 0.159957 | 0.339907 |
| Si | 0.976934 | 0.513811 | 0.341619 |
| Si | 0.160081 | 0.975001 | 0.340961 |
| Si | 0.155855 | 0.518650 | 0.337642 |
| Si | 0.977259 | 0.159163 | 0.518237 |
| Si | 0.160529 | 0.340326 | 0.513749 |
| Si | 0.335009 | 0.974512 | 0.521297 |
| Si | 0.982095 | 0.336401 | 0.518534 |
| Si | 0.156554 | 0.976857 | 0.519413 |
| Si | 0.265322 | 0.905950 | 0.729422 |
| Si | 0.266359 | 0.089902 | 0.729099 |
| Si | 0.905207 | 0.270452 | 0.726849 |
| Si | 0.091543 | 0.906375 | 0.729420 |
| Si | 0.265541 | 0.092752 | 0.906038 |
| Si | 0.093985 | 0.727604 | 0.904426 |

|    |          |          |          |
|----|----------|----------|----------|
| Si | 0.725689 | 0.091191 | 0.905093 |
| Si | 0.090265 | 0.271194 | 0.904051 |
| Si | 0.264683 | 0.728000 | 0.907747 |
| Si | 0.336592 | 0.160540 | 0.975658 |
| Si | 0.515191 | 0.340149 | 0.976078 |
| Si | 0.162688 | 0.518811 | 0.976309 |
| Si | 0.340334 | 0.519113 | 0.975821 |